UNIVERSITA' DEGLI STUDI DI URBINO CARLO BO

Department of

Pure and Applied Sciences

Ph.D. PROGRAMME IN

Research Methods in Science and Technology

CYCLE 37

THESIS TITLE

Development of Ultrasound Assisted Synthesis of Natural Acidic Deep Eutectic Solvents (NADESs) for Extraction of Bioactive Compounds from Agrifood Wastes Valorization: Antioxidant and Antiradical Scavenging Elucidation

ACADEMIC DISCIPLINES: CHEM-01/A; CHEM-07/B

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ACADEMIC YEAR
2023/2024

APPROVAL

Development of Ultrasound Assisted Synthesis of Natural Acidic Deep Eutectic Solvents (NADESs) for Extraction of Bioactive Compounds from Agrifood Wastes Valorization: Antioxidant and Antiradical Scavenging Elucidation.

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This dissertation is approved as a credible and independent investigation by a candidate for the Doctor of Philosophy degree in Research Methods in Science and Technology and is acceptable for meeting the dissertation requirements for the degree. Acceptance of this dissertation does not imply that the conclusions reached by the candidate are necessarily the conclusions of the major department.

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DEDICATION

I dedicate this dissertation to my late parents,

Ichie Ohoezie Robert Okeke (1878-1982), and Ezinne Nnalunwa Felicia Okeke (1938-2013).

ACKNOWLEDGEMENT

I expressed my deepest gratitude to my Supervisor, Professor Achille Cappiello, for giving me the opportunity to work in the Liquid Chromatography & Mass Spectrometry laboratory, and for the guidance, support, and invaluable advice on my research without which I would never have been able to accomplish this work. I am very grateful to my Co-supervisor, Dr. Matteo Micucci, for admitting me to the Food Chemistry laboratory, and for the tutelage on nutraceuticals, bioactive compounds, and the circular economy.

I am thankful to Professor Dasha Mihaylova for accepting me into the Biotechnology Laboratory, the University of Food Technology, Plovdiv, Bulgaria, for my first research experience abroad, and for providing all the resources required to execute the synthesis and extraction studies. Your support, insight, and encouragement cannot be fully expressed by words. I am also indebted to Professor Dimitrios Rafailidis of the Electrical and Computer Engineering Department, University of Thessaly, Volos, Greece, my second foreign supervisor, and gave me great insight on Scikit-learn, deep learning, and data modeling.

To the academic Lecturers: Prof. Pierangela Palma, Prof. Giorgio Famiglini, Prof. Andrea Duranti, Prof. Fabio Mantellini, Prof. Simone Lucarini, Prof. Janusz Pawliszyn, Prof. Valeria Freschi, Prof. Antonella Penna, Prof. Matteo Montani, Prof. Raffaella Servadei, Prof. Gino Tarozzi, Prof. Pierluigi Graziani, Prof. Vincenzo Fano, Prof. Michele Mattioli, and Prof. Cuno Lorenz Klopfenstein, I will forever be grateful to all of you for providing the springboard on which my research and this dissertation gathered momentum. I count myself privileged to have studied under your feet and gained immense knowledge from your excellent academic backgrounds.

The members of the LCMS lab, specifically Adriana Arigo, and Elizabeta Perini, immensely assisted me in one way or another, and I am very grateful to you. My fellow (cycle 37) PhD candidates in the LCMS lab, namely Genny Grassely, and Malvika Dutt, deserve my appreciation for their wonderful cooperation during these years. To other PhD candidates and Master's students in the lab, I thank you all for your understanding and friendliness.

It was a great experience associating with wonderful comrades in the cycle 37 PhD in Research Methods in Science and Technology program. Space will not allow me to mention everyone's

names, however, the PhD rep., Christel Chiroci did excellent work in her representation. I say a big thank you to all the wonderful comrades, see you all at alumni events.

I am indebted to all support and assistance given to me during these years by the former coordinator of ReMeST PhD program, Prof. Alessandro Bogliolo, and the program manager, Dott. Alessandra Petronio. I will not forget to thank the Doctorate Office, specifically Dott. Pieri Eugenio for the great work they offer. Eugenio has helped me in ways that I lack words to express. I will be forever grateful for your kindness. Without their dedication and kindliness this dissertation wouldn't have been possible at this time.

I am most especially thankful to the Rector, University of Urbino Carlo Bo, Prof. Giorgio Calcagnini, and the University Management for offering me a generous PhD scholarship without which the journey would have been impossible. Thank you very much.

Finaly to my dearest family, my beloved wife, Comfort, my lovely daughter, Oluebube, and my impeccable son, Ugochieze, I cannot appreciate you enough for your sacrifices in these long years of my absence. Thank you, my dear family, for you are my absolute treasure, every sacrifice is greatly appreciated. From the bottom of my heart, I agree to owe you all unrepayable debts.

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LIST OF PAPERS/PRESENTATIONS FROM THE RESEARCH

Udodinma Jude Okeke, Matteo Micucci, Dasha Mihaylova, Achile Cappiello (2024) Optimization of NADESs-UAE extraction of phytochemicals from African nutmeg (*Monodora myristica* (Gaertn.) Dunal*)* Peels: antioxidant and antiradical scavenging activity by Rotatable Center Composite Design-Response Surface Methodology (RCCD-RSM)(preprints) https://doi.org/10.21203/rs.3.rs-4256212/v1

Udodinma Jude Okeke, Matteo Micucci, Dasha Mihaylova, Achile Cappiello (2024) The effects of experimental conditions on extraction of polyphenols from African Nutmeg (*Monodora myristica* (Gaertn.) Dunal*)* peels using NADESs-UAE: A Multifactorial Modelling Technique. *Research Square* (preprints). https://doi.org/10.21203/rs.3.rs-3931581/v1

Udodinma Jude Okeke, Matteo Micucci, Dasha Mihaylova, Achile Cappiello (2024) Synthesis and Application of Novel Natural Deep Eutectic Solvents (NADESs) for Extraction of Polyphenols from African Nutmeg Peels: Antioxidant and Antiradical Scavenging Characterization. Oral Presentation at World Food Congress of International Union of Food Science and Technology (IUFoST), Rimini Italy, September 8-12, 2024.

LIST OF ABBREVIATIONS

Deep eutectic solvents..... DESs
Natural Acidic deep eutectic solvents ..... NADESs
Total phenolic content..... TPC
Total flavonoid content ..... TFC
Antiradical activity ..... ARA
Fractional factorial experiment ..... FFE
Rotatable central composite design response surface methodology ..... RCCDRSM
Cupric ion reducing antioxidant capacity. ..... CUPRAC
Ferric reducing antioxidant power ..... FRAP
2,2- diphenil-1-picrylhydrazyl ..... DPPH

Fourier transform infrared spectroscopy ..... FTIR
Hydrogen bond donor ..... HBD
Hydrogen bond acceptor ..... HBA
Ultrsound temperature ..... UT
Extraction time ..... ET
Solvent volume ..... SV
Solvent concentration ..... SC
Micro molar trolox equivalent ..... µMTE
Microgram quercetin equivanlent ..... µgQE
Microgram garlic acid equivalent ..... µgGAE
Many factors at a time ..... MFAT
Mililitre ..... ml
Gram ..... g
Hour(s) ..... h
Second(s) ..... s
Kilo hertz ..... kHz
Ultrasound assisted extraction ..... UAE
Citric acid/sucrose ..... CaSu
Citric acid/fructose ..... CaFr
Citric acid/xylitol ..... CaXy
Citric acid/glycerol ..... CaGr
Citric acid/glycine ..... CaGc
Citric acid/glucose ..... CaGl
Quartenary ammonium salts ..... QASs
Choline chlorideitric ..... ChCl

ABSTRACTS

Natural acidic deep eutectic solvents (NADESs)-ultrasound-assisted technique was developed and used to valorize agrifood waste. The extraction capacity of the synthesized NADESs was comprehensively evaluated using the peels of African nutmeg. The antioxidant and antiradical scavenging properties of the extracts were investigated using various in vitro methods.

The extraction process was studied using many factors at a time (MFAT) experimental design and further optimized through a rotatable central composite design response surface methodology (RCCDRSM). The effects of different operating conditions were evaluated comprehensively to determine the parameters necessary for antioxidant recovery in terms of TPC and TFC, and antiradical scavenging activity based on CUPRAC and FRAP methods. The conditions that gave the highest values of 908.17 µgGAE/g DW, 1431.51 µgQE/g DW, 11.5568 µMTE/g DW, and 14.7903 µMTE/g DW for TPC, TFC, CUPRAC, and FRAP were found in CaFr12, CaGc11,

CaFr11, CaXy11 as solvents respectively. These results underscore the potential of using specific NADES formulations to tailor the extraction process for desired antioxidant and antiradical scavenging properties. The findings give insights into the capacity of NADESs as powerful solvents for extraction applications, and further optimized.

Four independent factors of temperature, time, volume, and concentration, determined from the MFAT studies which significantly affected bioactive molecule extraction were optimized to elucidate the best conditions that produce the maximum TPC extracts, maximum TFC extracts, and maximum antiradical scavenging activity through CUPRAC, FRAP, and DPPH inhibition. The optimized conditions with maximum desirability for TPC, TFC, CUPRAC, FRAP, and DPPH were temperature, time, volume, and concentration of 45ºc, 5 min, 25 ml, & 90%; 30ºc, 5min, 25 ml, & 90%; 30ºc, 5 min, 25 ml, % 90%; 45ºc, 25 min, 25 ml, & 50%; and 50ºc, 15 min, 15 ml, & 70%, respectively. CaFr11 was observed to be the best performing solvents among the NADESs studied as it outperforms others by extracting the highest TPC, and TFC as well as highest CUPRAC antiradical scavenging activity at the optimized conditions. CaSu11 had the highest FRAP power, while CaXy12 gave the highest DPPH inhibition at optimized conditions. Besides, all the studied NADESs outperformed water, the greenest solvent, in TPC, and TFC extraction, as well as in DPPH inhibition. However, water extracts performed better than CaGC21, CaGl11, and CaGl21 in FRAP tests. The results are like findings obtained by other researchers who performed optimization of UAE-Choline chloride NADESs extraction using other plant materials.

This study demonstrated the feasibility and effectiveness of using ultrasound-assisted synthesis of natural acidic deep eutectic solvents (NADESs) for the extraction of bioactive compounds from agrifood wastes. The combination of NADESs and UAE not only provided higher yields of antioxidants but also offered a sustainable, green alternative to conventional solvents. The antioxidant and antiradical scavenging assays confirmed the potential of these extracts for applications in the food, pharmaceutical, and cosmetic industries. The findings highlight the role of NADESs in enhancing extraction processes and valorizing agrifood wastes, paving the way for further research on the scalability and commercial viability of this approach.

CHAPTER ONE

INTRODUCTION

1.1 Background

The world is currently facing tremendous challenges arising, particularly from the impact of climate change and the inefficient management of natural resources. In addition to the above, the exponential growth of the world population, which is estimated to reach 9.8 billion in 2050 according to the United Nations (UN) requires optimized utilization of natural resources, including the use of value-derived products from wastes as well as a significant reduction in food loss/waste. Moreover, the recent pandemic situation, COVID-19, has contributed indisputably to the present worsening economic situation. Along the agrifood supply chain, several amounts of waste or by-products are generated, and in most cases, these biomasses cause serious environmental impacts and high costs to enterprises. The valorizations of the agrifood loss/food industry wastes are a useful strategy to produce certain value-added compounds with several potential applications, namely in the food, health, pharmaceutical, cosmetic, and environmental fields.

Green processing technologies to extract different compounds such as polyphenols and phenolic compounds from agrifood materials such as fruits and vegetables have been studied in recent times[1] [2]. Green techniques such as ultrasound[3], microwave[4], pulsed electric field[5], pressurized liquids[6], and supercritical fluid processing[7], have gained special attention due to their exceptional practices focused on economic, environmental, and safety concerns. However, outstanding green extraction chemistry has been linked to the principles of ultrasonication because it showcases advantages such as shorter operating times, energy savings, high extraction yields, preferential selection of extracts, and reduction in the generation of effluents due to reduced volume of solvents including water[8].

Green extraction procedures capture some principles of the green chemistry techniques, namely, use of renewable and sustainable bio-resources, use of green solvents or water, use of lower energy consuming apparatus, co-products production from waste, minimal number of unit operations, resulting non-denatured and biodegradable extract, and sustainability of production and processes.

1.2 Problem Statement

The search for greener solvents capable of replacing conventional toxic VOCs in daily applications continues both at the laboratory and industrial levels[9] [10]. The challenge rages when it becomes difficult to design a more sustainable green alternative to toxic chemicals with desired chemical and physical properties. In most cases, ensuring the availability of greener solvents tunable to replace nongreen solvents is problematic for most scientists[11]. Despite the numerous publications about NADES since its first inception in 2011, most research works concentrated mainly on the use of choline chloride as HBA which limits the utilization of other capable candidates. The availability of greener solvents in all the four solvent categories (high basicity-low polarity, low basicity-low polarity, high basicity-high polarity, and low basicity-high polarity) is pivotal to ensuring sustainability, therefore expansion of candidate HBAs should be a priority.

To date, the ratio of choline chloride based natural deep eutectic solvents to other viable candidates is not encouraging. A Web of Science search of the phrase "choline chloride based natural deep eutectic solvents" shows 22 publications at which 12 indicated it being an HBA, while the same search with “citric acid based natural deep eutectic solvents” shows only 2 publications of which 1 is as an HBA.

Regarding the environmental impacts of agrifood wastes evaluated as contributing more than 20% of total global production of greenhouse gases, including methane (CH_4), nitrous oxide (N_2O), and carbon dioxide (emission of 3.3 billion tons of CO_2 per year), which contribute significantly to climate changes[12] [13]. Concerning the hunger crisis, about 805 million people are already suffering from hunger worldwide[14], while approximately 1.3 billion tons of agrifood wastes are produced annually worldwide throughout the supply chain (30%–40% of food production)[15]. In Europe alone, over 58 million tons of food waste (131 kg/person) are produced yearly representing a market value worth €132 billion[16].

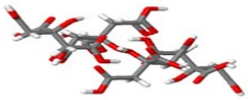
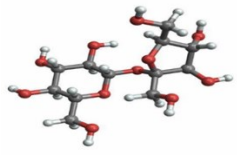
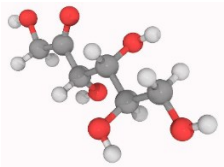
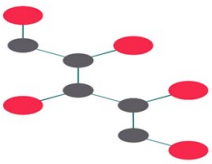
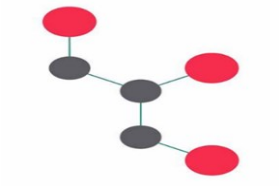
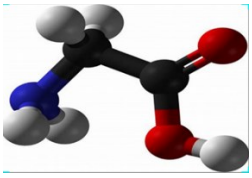
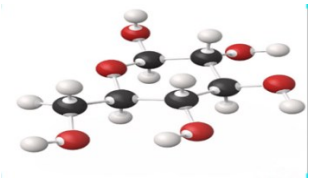
1.3 Aim and objectives of the study

The main aim of this research is to develop ultrasound assisted techniques to synthesize cost effective neoteric deep eutectic solvents (NADESs) and apply them for extraction of bioactive compounds from agrifood materials. The objectives therefore include:

1. Develop and characterize the physicochemical properties of the synthesized NADESs,
2. Apply the NADESs coupled to ultrasonication to extract bioactive compounds from African nutmeg peels,
3. Develop extraction modelling using the synthesized NADESs coupled with ultrasonication
4. Optimize the extraction conditions to maximize extraction efficiency,
5. Investigate the antioxidants and antiradical scavenging potentials of the NADESs extracts in vitro,
6. Compare the antioxidant and antiradical scavenging power of the NADESs extracts with those of water extracts at the optimized conditions.

1.4 Justification of the study

Since the introduction of natural deep eutectic solvents (NADESs) by Choi et al[17] in 2011, choline chloride, quaternary ammonium salts (QAS) continues to be the major HBA in NADESs synthesis. Active research to substitute choline chloride as HBA in NADESs preparation has been ongoing to investigate how NADESs could be synthesized with other hydrogen donating species than choline chloride, and fields that suit the application of these new solvents. The concept of DES in analytical extraction is still in its infancy compared to ionic liquids, nonetheless, the increasing number of research publications make the field very promising. This study employs citric acid as HBA and plant secondary metabolites (sucrose, glucose, fructose, xylitol, glycerol, and glycine) as HBDs at different molar ratios to synthesize NADESs see scheme 1.1. The solvents are easy to prepare, starting materials are biodegradable, and the solvents have good physicochemical properties with excellent extraction capabilities.

Citric Acid		$C_6H_8O_7$
Sucrose		$C_{12}H_{22}O_{11}$
Fructose		$C_6H_{12}O_6$
Xylitol		$C_5H_{12}O_5$
Glycerol		$C_3H_8O_3$
Glycine		$C_2H_5NO_2$
Glucose		$C_6H_{12}O_6$

Scheme 1.1 Compounds used in the synthesis of NADESs, their structures and chemical formulae

CHAPTER TWO

REVIEW OF THE LITERATURE

2.1. Ultrasound Technology

Ultrasound is the sound waves having frequency higher than a human ear can detect. It is basically mechanical waves with frequencies ranging from 16 kHz to 100 MHz[18 19]. The commencement and speeding up of chemical reactions in the field of ultrasonication is related to the appearance of cavitation. Cavitation is the formation of cavities inside the liquid and their collapse followed by intensive hydraulic shocks. When high intensity ultrasound wave is generated inside the liquid, interruption in the continuity of liquid occurs followed by the formation of cavities at the negative pressure (rarefaction). At the site of negative pressure these cavities are not formed promptly but require some time, the duration of the low-pressure phase, during which cavitation bubbles grow, and decrease with increasing ultrasonic frequency. Power ultrasound can be used for extraction of organic compounds as it can possibly improve the kinetics of solvent extraction of component from the plants and seeds[20]. Compared to conventional extraction methods, ultrasonication is a non- thermal technology which has attracted prominent interest in the food industry. Ultrasonication is a sound wave of high intensity which by means of mechanical vibration can make changes in food either by disrupting its structure or by stimulating chemical reactions. The use of this technology improves the quality and productivity of product, reduction of physical and chemical hazards, enhancement of extract yield as well as environmental friendliness[21]. The mechanical vibrations generated through liquid, gases, and solid media with a frequency which exceeds the human hearing limit and depending on the frequency range, can be divided into low and high intensity applications. The frequency above 100 kHz and energy below 1 W/cm^2 are classified under low intensity applications and are used for analytical purposes with no remarkable effect of the ultrasonic wave on the material being tested. The low intensity ultrasound is used in food industry as an analytical technique to control a process or to acquire information regarding different physicochemical properties of food[22 23]. In the case of high intensity ultrasound, the frequency used is between 20-24 kHz, sometimes above 100 kHz, and the applied energy ranges from 10-1000 (W/cm^2)[24 25], and these conditions generate intense cavitation which physically

ruptures the materials. The occurrence of cavitation during high intensity ultrasound involves emergence, expansion and collapse of bubbles in liquid. The waves of acoustic energy promote cycles of compression and rarefaction of the molecules in the solution through pressure changes leading to the formation and collapse of microbubbles in the medium that result in micro-jetting. The microjets generate effects such as surface peeling, erosion and particle breakdown[26 27].

Thornycroft and Barnaby (1895) were the first to report the formation of cavitation when they postulated that the cause for the faulty performance of a new torpedo was the ineffectiveness and the loss of power caused in the water due to formation of cavities[28]. The physical and chemical changes in liquid medium are improved by power ultrasound through the generation and destruction of cavitation bubbles. When subjected to high intensity ultrasound, the liquid expands and compresses forming cavities or small bubbles. The collapse of cavitation bubble creates a transitory hot spot generating extreme temperature (up to 5000 K) and pressure (up to 1000 Atm.), which can accelerate dramatically chemical reactivity into the medium[29]. The extent of cavitation can be determined by energy and intensity along with the medium viscosity, surface tension, vapour pressure, presence of solid particle, temperature and pressure of treatment[30]. Power ultrasound promotes different applications such as the extraction of different compounds[31], microbial and enzymatic inactivation[32], emulsion formation[33 34], and physical modifications[35]. Among these applications, ultrasound has been increasingly studied for the extraction of high value ingredients from plant materials.

The use of high intensity ultrasound in food processing is an encouraging area with a broad range of current and future applications. It has been seen as an alternative efficient method to improve the extraction processes of high value compounds in food materials. It can improve the mass transfer by accelerating the eddy and internal diffusion and thus allows better penetration of solvent into the sample matrix[25 36]. The frequency of ultrasound has an appreciable influence on the extraction yield and kinetics, and depending on the plant material, differences exist between the extraction yield and kinetics.

Ultrasound assisted extraction can be utilized to increase the extraction process by enhancing the mass transfer between solvent and plant material. This extraction permits better penetration of solvent into the plant material and breaks down the cell walls[37]. Ultrasound assisted extraction has been carried out to extract essential oil from aromatic compounds such as peppermint leaves,

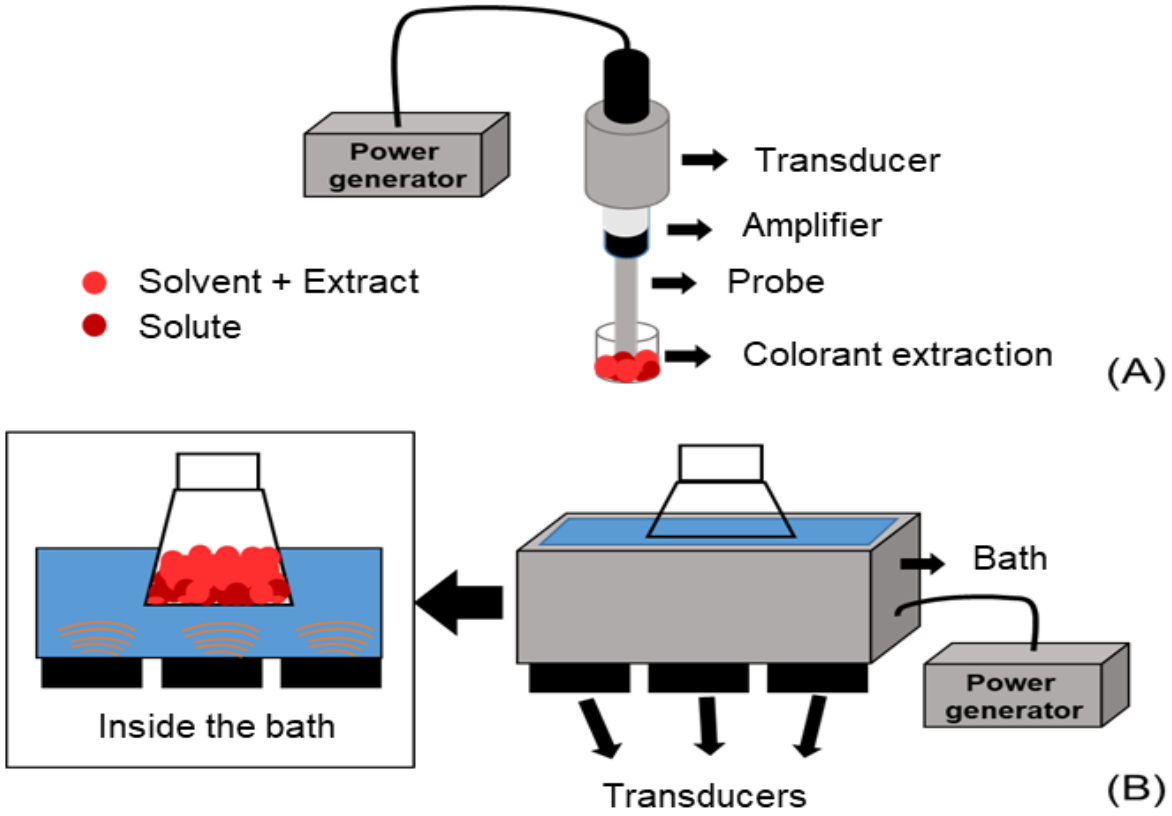
Artemisia, and citrus flowers, and has been found to increase the yield[38]. Ultrasound extraction permits changes in the processing conditions like decreasing the temperature and pressure as compared to those without ultrasound extraction. Therefore, it is desirable to use ultrasound assisted extraction for thermolabile compounds. Key parameters of interest in UAE include the ultrasound system utilized; the matrix or compound to be extracted; the solvent; the ratio of solvent to sample; and the specific energy applied to the system.

2.1.1 Ultrasonic Systems

The UAE systems used for high value ingredients processing include probe and bath systems and are shown in **scheme 2.1 A** and **B** respectively. The probe system contains a power generator which produces high-frequency electrical energy of 20 kHz, a transducer that converts the electrical energy to mechanical energy, an amplifier that amplifies the mechanical energy and a probe that dissipates the acoustic energy directly into the sample in form of waves[26]. In the bath system, the power generator produces energy of about 20-40 kHz, which is dissipated into the bath in form of waves by the transducer(s)[24]. Extraction of high value materials has been performed with either the probe or bath system with great efficiency. The frequencies employed in the bath system are normally more than 24 kHz[39 40], but lower frequencies seems to produce better physical effects[41]. For example, in a study to extract anthocyanins, a bath ultrasonic system with operating frequency of 37 kHz was used and the authors reported longer extraction time and lower yield of anthocyanin content than the control[42]. Tandem UAE with other techniques have also been employed such as ultrasound-microwave-assisted extraction of natural bioactive compounds from sorghum husk using a conventional shaking method with a frequency of 25 kHz, and obtained a yield of 3.6 times those of the control[43]. A combined treatment to obtain anthocyanins from blueberry using a probe system and a cell grinder was investigated by Liu *et al*., and observed that the cell grinder destroyed the cell walls and released the water-soluble anthocyanins into the concentrated ethanol used as solvent[44].

2.1.2 Matrix contents and compounds

Agrifood matrices such as fruits and vegetables are typical resources for various extraction applications because they contain vast diversity of bioactive molecules[45]. Some of these bioactive molecules are highly sensitive in variable conditions and therefore care must be taken to avoid denaturing their potency during extraction. For instance, anthocyanins are sensitive to temperature, pH, light, oxygen and metals[46], curcumin degrades in the presence of sunlight and visible light[47], and therefore must be considered during the separation processes to avoid loss.



Scheme 2.1 Ultrasound systems (A. probe; B. bath)[48].

2.1.3 Solvent and Feed

The effectiveness of the cavitation process is strongly influenced by the physical properties of the mixture of solvent and feed (S/F). Hence, proper manipulation of solvent and feed to enhance acoustic energy transformation is very important because solvent characteristics affect the

cavitation phenomenon. Example, viscosity and surface tension govern cavitation transient threshold while the bubble collapse intensity is ruled by steam pressure[41]. The solvent therefore should be well compatible with the compound of interest[49]. For instance, the best organic solvent for anthocyanins extraction should be acidified ethanol because they are stable under acidic conditions[36]. Carotenoids on the other hand possess non-polar characteristics, hence, a good option is to utilize vegetable oils as solvent[50].

The effects of the choice of solvent employed on the extraction and activities of extracts have been demonstrated using residues of European blackberry, European blueberry and Brazilian cherry and obtained different yields of anthocyanins when water and ethanol were employed as solvents[40]. There was higher extraction yield by using water as solvent, but in relation to the antioxidant activity, the water extract had lower antioxidant power. In vitro analysis gave better antioxidant activity to the alcohol extracts than the water extracts. The observation may be linked to extractive non active water-soluble compounds into the water sample.

Another important factor to consider in solvent selection for food and pharmaceutical application is the GRAS (generally regarded as safe) status of the solvent[51], which is also required to minimize environmental impact of solvents. Most research employ green solvents such as water and ethanol while some still use non-green solvents such as methanol and acetone to perform ultrasound-assisted extractions[26 52]. Apart from GRAS status, the amount of solvent used is also a key factor, excess solvents should be avoided to minimize environmental impacts. The relationship between S/F is extremely important, however, it has been noted that a ratio of 5:1 gave the best results for anthocyanins extraction from fig[53].

2.1.4 Temperature

The thermal effects in addition to the cavitation and mechanical effects significantly influence the UAE technique[54], making temperature another important variable in the extraction process. Studies of high-intensity ultrasound as an economically feasible technology for the extraction of thermolabile compounds indicate that fast rise in temperature of the reaction system happens during prolonged extraction time and thermally degrades the extracts[55 56]. However, increase in temperature was observed to be favorable in some UAE processes, such as a 10°C (40 to 50°C)

increase in temperature, increased the yield of carotenoid by 8%[57], but with further temperature increase, the yield was reduced, which was attributed to the degradation of thermolabile carotenoids. Recovery of chlorophyll on the other hand, was noted to favor a positive increase in temperature up to 20°c (from 40°c to 60°C)[58]. Most researchers employed controlled temperatures between 25°c to 80°C, while some do not consider temperature as a factor to be controlled in UAE processes. However, the importance of temperature control cannot be overemphasized particularly when working with thermolabile compounds.

2.1.5 Specific Energy

The energy applied by ultrasound in extraction has been standardized following Equation 2.1 which shows that the energy applied is a function of the nominal power, the sample volume and the extraction time. But the volume is a function of the pressure and temperature therefore, the energy factor can be expressed as a function of mass, which does not depend on other variables hence, the relation can be expressed in specific energy following Equation 2.2[59 26].

$$ED\left(\frac{j}{ml}\right) = \frac{Nominal\ Power\ (w) x\ Extraction\ time\ (s)}{Sample\ volume\ (ml)} \tag{2.1}$$

$$E\left(\frac{j}{g}\right) = \frac{\text{Nominal Power (w) x Extraction time (s)}}{\text{Sample mass (g)}} \tag{2.2}$$

2.1.5.1 Nominal Power

The power provided by the ultrasound device is called the nominal power; however, not all the nominal power is converted into the cavitation phenomenon because of energy dissipated by the equipment during conversion to cavitation from mechanical energy[60], therefore, energy efficiency studies recorded only about 9%[61] conversion from electrical to cavitation, and 5.6%[62] with calorimetric method. As a result, most authors prefer using the highest nominal power of the equipment to do the extractions[50]. A high nominal power produces greater shearing in plant materials and leads to achieving better solvent penetration. The critical pressure and temperature

from oscillation and collapse of cavitation bubbles within the solvent is also enhanced resulting in high extraction yields[55]. Majority of studies in literature selected higher nominal powers as the best condition for the extraction process because with more intense ultrasonic treatments, better results for obtaining extracts are assured[57].

2.1.5.2 Extraction Time

The extraction time is one of the most important variables to consider during ultrasonication, because as shown in Equation 2.2, the extraction time is directly related to the nominal power and the sample mass (solvent and feed). Too short or long exposure of samples to time that is inappropriate leads to incomplete extraction or degraded/contaminated extracts[63], therefore, the extraction time to be employed must factor the values of nominal power and sample mass. For example, to extract anthocyanin from mulberry, the maximum time should not exceed 10 min to avoid anthocyanins degradation and obtain a quantitative extracts, however, the extraction time can be reduced when using a higher nominal power greater than 200 W[64].

2.2. Solvents

Solvents are substances mostly liquids which dissolve other materials to form solutions. Solvents serve in several applications as an integral part of the process. Many processes cannot proceed without solvents. For instance, extractions, chemical synthesis, pharmaceutical formulations, food product development, agrochemical formulations, paints, inks, and coatings productions, as well as industrial cleaning and washing may be practically impossible without solvents. The pharmaceutical industry is acclaimed to use the highest volume of solvents. According to data from GlaxoSmithKline (GSK)[65], solvents constitute more than 1/2 the mass of material required to produce an active pharmaceutical ingredient (API), and when water is included reaches 4/5.

Until about three decades ago, most industrial applications employed the use of organic solvents, for example, during the first four decades of the 20th century, benzene was used as a hand-cleanser and also as an aftershave until its carcinogenic properties were established [66]. The lack of precaution on the exposure to benzene and the resultant impact of its increased harm was in part

due to inadequate data on benzene toxicity as well as its cheaper price compared to alternatives[65]. Organic solvents, known as carbon bonded solvents, are typically volatile (organic) compounds which often vaporize even at room temperature[67]. These volatile organic compounds (VOCs) have been implicated with numerous environmental and health concerns[68]. However, these concerns notwithstanding, the global Solvents market held a market value of USD 26 billion in 2021, selling around 27.4 million metric tons (MMT) in the same year. Solvents is projected to reach USD 49.6 billion sales by 2030. The market is anticipated to grow at a cumulative annual growth rate (CAGR) of 7.5% from 2022 to 2030 (source: https://www.researchandmarkets.com ; assessed on 12/04/2024).

Solvents constitute pivotal materials for chemical reactions and chemical processing not only in pharmaceutical and fine chemistry operations, but also in almost all industrial systems, and can be as game changing as catalysts[66]. Solvents are integral constituents of the Green Chemistry principles[67], which changed the ways organic chemical processes are practiced in the last 30 years. Under the banner of circularity, solvents have also gained importance for chemical process engineers, food scientists, pharmaceuticals drugs developments, and others making their designs fit into the framework of recovery, recycling, repurpose, remanufacture, refurbish, repair, reuse, reduce, rethink, refuse (10R framework of circular economy)[69]. Solvents do much more than simple carriers for reactants and reaction spaces for interactions as they determine solubility, as well as productivity and economic benefits. Solvents can support the stability of excited states, guiding the potential-energy curves of activation, and govern the stability and activity of the catalysts, including labile catalysts such as biocatalysts/enzymes or sophisticated transition metal catalysts[70]. Process media usually constituted 70–80% solvents[66], and therefore are crucial in process wastes reduction.

2.2.1 Solvent selection guidelines

Solvents have received much attention as seen on the large volumes of solvents typically used in reactions or in formulation[71]. However, solvents are not directly responsible for the composition of reaction products, nor are they an active component of the formulation, yet, toxic, flammable, and environmentally damaging solvents are still being used in laboratory and industrial operations.

This practice would seem unnecessary because these characteristics have no impact on the function or progress of the system in which the solvent is applied. Nonetheless, these unfortunate consequences of solvents' use are often linked to the assumed beneficial attributes of the solvent needed for the application. For instance, the volatility of solvents permits recovery and purification of the solvent by distillation, but also creates unwanted air emissions and the risk of exposure of harm to workers. Broadly speaking, amide solvents in one end, have high polarity required to dissolve a wide range of substrates and accelerate reactions but often produce toxic by-products, while on the other end, hydrocarbon solvents provide the ability to dissolve oils in extractions and perform separations, but are still highly combustible with low water solubility (high $\log^{P}$) which is linked to bioaccumulation and aquatic toxicity[72]. Sustainable and green solvents selection can solve the problems related to the environmental and human health cost, and also contribute to the optimization of the overall process[73].

To eliminate undesirable solvents, replacement strategies often seek structurally related compounds not yet covered by legislative and regulatory measures. For example, as benzene became recognized as a carcinogen, toluene became it's replacement[71]. The Montreal protocol restricted the use of carbon tetrachloride since 1989 because it was linked to ozone layer depletion[71], and as such has been replaced with the halogenated solvents chloroform and dichloromethane (DCM). However, these measures have proven to be ineffective with respect to strict chemical controls worldwide because alternative chemicals are not harmless. For instance, toluene is suspected of unborn child and organ damage when exposed to humans for a long time, and chloroform and DCM have also been declared carcinogenic to humans by World Health Organization IARC evaluations[71]. Furthermore, DCM has also been implicated for ozone depletion even at short exposure duration[71].

The European regulation concerning the 'Registration, Evaluation, Authorization and Restriction of Chemicals' (REACH) also introduced specific restricting conditions on toluene, chloroform and DCM[71].REACH affects the importation and usage of a wide range of chemicals in Europe by ensuring that any product found not to comply with the established conditions are removed from the market through the 'rapid alert system for dangerous non-food products' (RAPEX) information scheme[71]. Future European bans on solvents, candidate chemicals are placed on a list of 'substances of very high concern' (SVHC) prior to imposition of REACH restrictions. A non-

exhaustive list has been drawn since 2015 as SVHC for REACH scrutiny notable among which are the amides such as *NN*-dimethylformamide (DMF), *NN*-dimethylacetamide (DMAc), and *N*-methyl pyrrolidinone (NMP), certain hydroxy ethers, and chlorinated solvents.

Structurally similar solvents can easily be sourced as alternative replacements for the restricted ones, however, the likelihood of presenting many of the same environmental, health, and safety (EHS) problems is high. Therefore, solvent selection guidelines have been produced to give more information than the 'black and white's conclusions of regulatory assessments as an attempt to categorize solvents with respect to their EHS profiles by prominent pharmaceutical and chemical companies, notably GlaxoSmithKline (GSK), Pfizer, and AstraZeneca among others.

The GSK solvent selection guide provides useful guidance on selection and replacement of solvents primarily for Chemists and Engineers working in chemical process development. The guide is also useful for medicinal chemistry and other scientists working in analytical laboratories. The most updated version of the guideline consists of 110 solvents provided at different levels of detail depending on specific user requirements[65]. The guide could be used to reconcile the competing environmental, health and safety demands in the application of solvents providing alternatives. However, the alternatives may present many of the same health, environmental, and safety concerns of the primary solvent (i.e., the solvent to be substituted)[71]. In terms of the above reference, DCM may be regarded as a greener (safer) solvent when compared to chloroform or carbon tetrachloride and could be selected for their replacement in a process, even though DCM is an occupational health threat and has high vapor pressure[73]. Indeed, solvent replacement should be done without compromising the compatibility and process functionality of the primary solvent as much as occupational health and the environment is not compromised.

Pfizer, AstraZeneca, and others also published solvent selection guidelines which follow closely to the GSK guidelines and will not be discussed further.

2.2.2. Green solvents

The concept of green chemistry emerged during the early works by Trost and Sheldon about economical use of mass and environmental factors, respectively. The field of green chemistry revamped after the 12 principles by Warner and Anastas were stipulated in 1987[74]. Since then, a

few industries and pharmaceutical companies like Pfizer have laid down a restrictive guideline to help in the selection of solvents and reagents. According to the Pfizer solvent selection guide for medicinal chemistry, if one is to choose any solvent, water is preferred rather than cyclohexane and pentane. Nevertheless, in chemical synthesis and processing, cyclohexane is usable compared to pentane. Due to the environmental, health, and safety implications of organic solvents, the impetus in organic solvent replacement with green solvents such as ionic liquids (ILs) and deep eutectic solvents (DESs) are growing globally.

A green solvent therefore should encompass the environmental and health safety (EHS), life cycle analysis (LCA), energy demand, and toxicity of the solvent in question. A detailed assessment of solvents for these parameters is invaluable in the call for environmental sustainability. The concept of green chemistry and green solvents is actively under research in the quest to design and develop new solvents to replace conventional organic solvents. Ionic liquids and deep eutectic solvents are among the new generation of solvents under study due to their tunability and lower volatility issues into a single methodology for selection[65]. This growth in green solvents is driven by strict US Environmental Protection Agency (EPA) regulations to shift solvents toward a more eco-friendly and biodegradable alternatives with reduced emissions and toxicity. Due to the increasing regulatory measures and continued amendments of the EPA regulations, especially concerning VOCs, the exponential rise in market demand for green solvents in this decade is not shocking. As a result, an 8.7% increase in sales of green solvents is estimated by CAGR for 2022 to 2030. (source: https://www.grandviewresearch.com/industry-analysis/solvent-market) (assessed 12/04/2024).

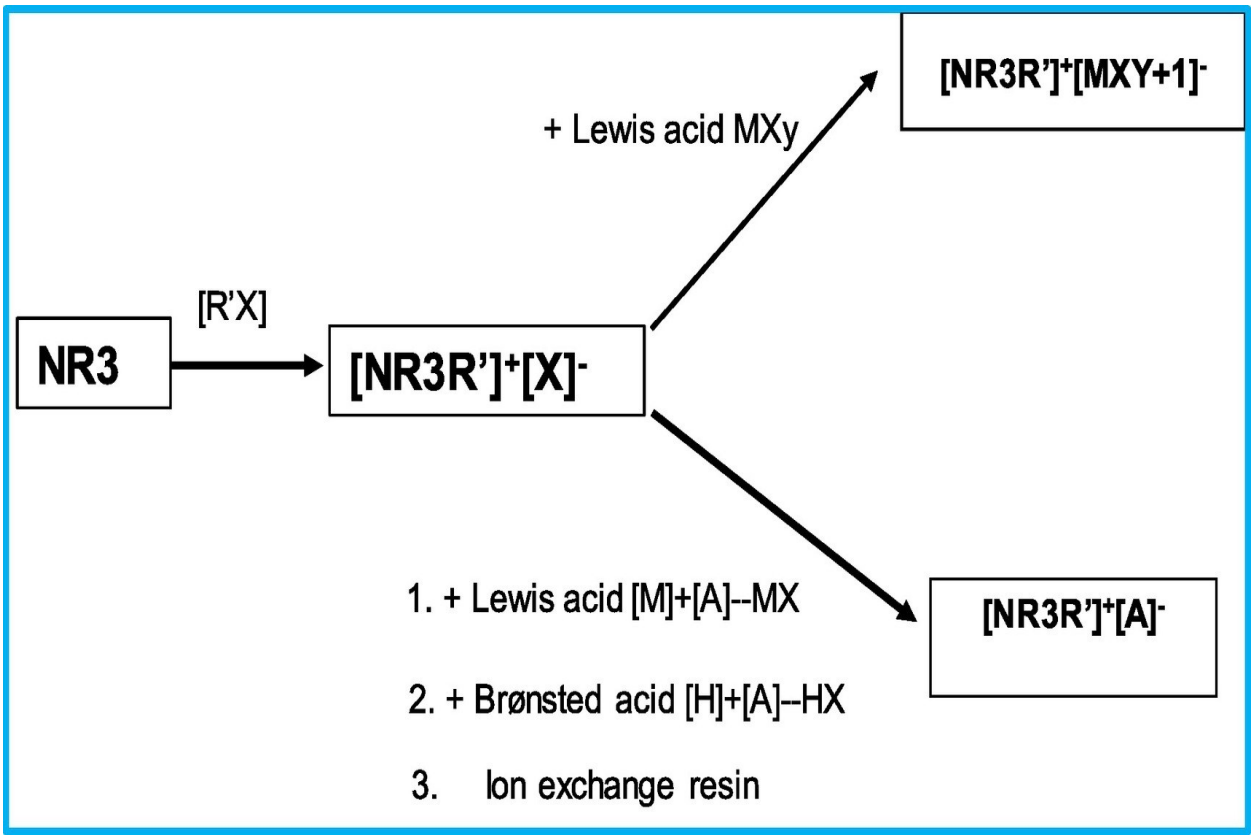
2.2.2.1 Ionic liquids

Ionic liquids (ILs) are salts with melting temperature lower than the boiling point of water (< 100 °C)[75]. ILs are completely ionic consisting of organic cations and organic or inorganic polyatomic anions[76].The first report of ionic liquids could be traced to 1914 during the preparation of ethyl ammonium nitrate from a concentrated nitric acid and ethylamine followed by water removal by distillation[77], and the resulting pure salt remained liquid at room temperature. Most importantly, the formation of the desired cation and the anion exchange processes are key steps to ILs

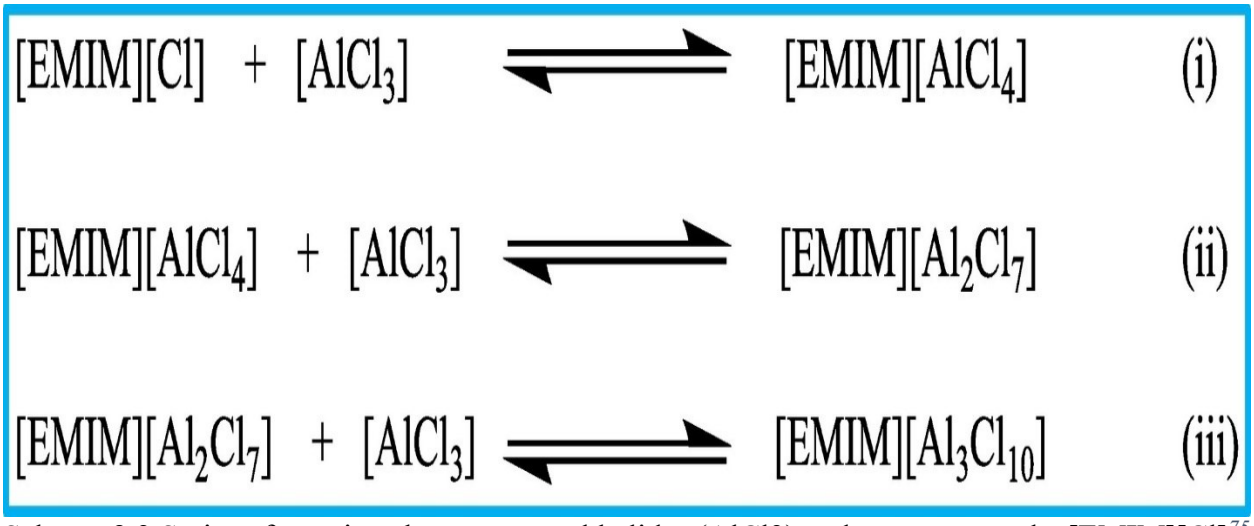
formation. In 1948, Hurley and Weir found that an anion exchange reaction between a Lewis acid ($AlCl_3$, 67% by mole) dissolved infused ethyl pyridinium bromide forms a very low melting eutectic with a melting point at -40 °C[78]. The addition of Lewis acid to a halide salt is by far one of the simplest methods of synthesizing ionic liquids[75].

2.2.2.1.1 Synthesis of ILs

The first room temperature ILs started in 1914 with the synthesis of ethyl ammonium nitrate (m. p. 12 °C)[79]. The ethyl ammonium nitrate IL was synthesized by the addition of concentrated nitric acid with ethylamine. The additional aqueous layer was removed by distillation to generate a pure salt, which was a liquid at room temperature. Generally, there are two basic methods that are employed for the synthesis of ILs and is summarized in Scheme 2.2. Normally in most of cases, a single step is sufficient for the ILs synthesis, for example with 1-butyl-3-methylimidazolium chloride, ethyl-ammonium nitrate, and so on, although, many counter cations are generated as zwitterions and further react with desired anions to form highly viscous products[75]. The counter cation parts of ILs are also common in commercial availability in a halide form and require only the anion exchange reactions. The anions exchange reaction occurs between halides and metal halides to form Lewis acidic ILs[80]. Brønsted acidic and ion exchange resin based ILs also are synthesized *via* anion exchange reactions. The $AlCl_3$ based salts acting as Lewis acidic ILs are broadly studied for various applications because it is a very simple addition reaction in which Lewis acid or metal halides are added into the halide salts and results in the formation of respective acidic ILs with one extra halide species[81]. The ratio of Lewis acid or metal halides (MXn) and quaternary salts (Q^+X^-) is a very simple reactions between $AlCl_3$ and [EMIM][Cl] and is shown in Scheme 2.3. Similarly, few of the examples of metal halides could also be used to prepare $FeCl_3$, BCl_3, $AlEtCl_2$, CuCl, and $InCl_3$ acidic ILs with one more halide species[82].



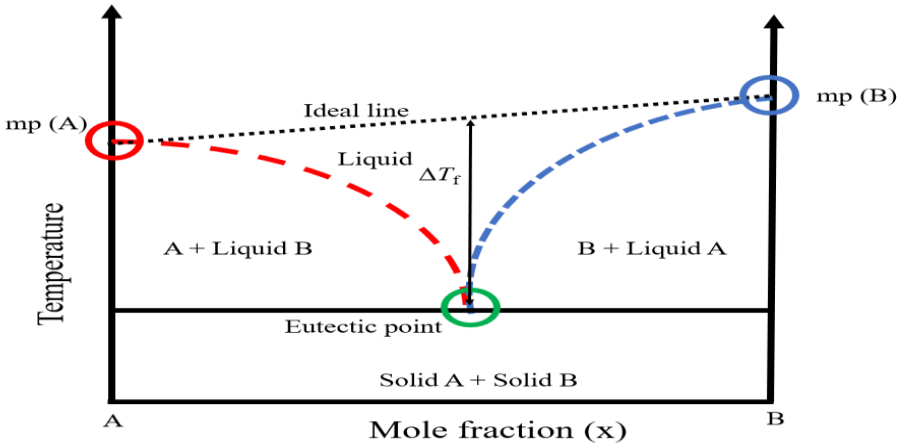
Scheme 2.2 Typical procedure for synthesis of ILs[75]



Scheme 2.3 Series of reactions between metal halides (AlCl3) and quaternary salts [EMIM][Cl][75]

2.2.2.2 Deep eutectic solvents (DESs)/Natural deep eutectic solvents (NADESs)

DESs are a mixture of two or more components which are individually solid at room temperature but converts to liquid after synthesis due to the development of intermolecular hydrogen bond that keeps them in liquid form[83]. Abbott *et al* synthesized the first Deep Eutectic Solvent in 2003 by mixing choline chloride (ChCl) and urea (Ur) in a molar ratio of 1:2 (called reline) with a melting point (MP) of 12 °C, which is lower than the MP of ChCl (302 °C) and Ur (133 °C)[84] Scheme 2.4. It is suggested that high MP depression of eutectic mixture may be due to charge delocalization, for instance, halide anion (HBA) to HBD via hydrogen bond formation[85]. Deep Eutectic Solvents (DESs) are mainly categorized into four groups as: organic salts + metal salts (type 1), organic salts + metal hydrates (type 2), organic salts + hydrogen bond donor (HBD) (type 3) and metal chlorides + HBD (type 4)[86]. The term 'Natural Deep Eutectic Solvents' (NADESs) comprising of quaternary ammonium salts and natural substances such as amino acids, polyols, sugars, organic acids, amides, amines and diols were coined later by Choi *et al* [87]. In type 3, the HBD is mainly natural compounds or primary metabolites which are used by plants for its own survival such as organic acids, sugars, etc.[88 89]. It is considered that these solvents are present in all living cells as third class of liquids other than water and lipids which help them to fight against odd conditions such as drought[90]. NADESs shows better extraction properties than DESs, as the former solubilizes polar as well as non-polar compounds and also acts as a stable media for oxidation sensitive compounds, than the later[91]



Scheme 2.4 Eutectic points of two-phased component diagram[92]

2.2.2.2.1 Synthesis of DESs and NADESs

There are various methods for the preparation of DESs and NADESs such as heating and stirring (known as thermal mixing), microwave, ultrasonication, grinding, freeze drying and vacuum evaporation[93]. The first and one of the widely used methods of synthesis is heating and stirring which involves mixing the individual components with or without known amount of water, followed by heating in water bath or on a hot plate (50–100 °C) until a clear homogenous liquid is formed. This method is among the simplest, cheap and safe but requires more time (10-48 h) for preparation[83 94]. Microwave assisted synthesis of DESs is the fastest method where individual components are mixed in glass bottles and exposed to microwaves for a few seconds (less than 30 s at 180 W) that makes it ultra-fast[95]. Similarly, in ultrasound (US) assisted preparation, individual components along with known amount of distilled water is added in a glass vial consisting of screw cap or in a beaker and treated with US waves (20-47 kHz, 30-300 W) using a bath or probe system at controlled or uncontrolled temperature till a clear homogenous liquid is formed[96]. Under grinding method, components are mixed and ground in pestle-mortar at room temperature till clear solution is formed[97]. In freeze-drying method, aqueous solution of DESs or of the individual components are freeze-dried in order to sublimate the water to get solvent in its pure form[98]. Lastly, vacuum evaporation method in which HBA and HBD are mixed in water and evaporated at 50 °C with the help of rotator evaporator, keeping the obtained solution in charged desiccator until it reaches a constant weight[99]. Irrespective of different preparation methods, high temperature results in degradation of DESs based on ChCl and carboxylic acids due to esterification reaction[100]. However, no change in physicochemical properties of NADESs was found when prepared using three different methods of heating and stirring, microwave and ultrasonication[95 101].

2.2.2.3 Application of DESs and NADESs

DESs and NADESs prepared using various methods can be applied in various materials such as fruits, vegetables, cereals, pulses, spices, herbs, plantation crops, oil seed crops, medicinal and aromatic plants, seaweeds, eggs, animal products, and milk for different purposes including

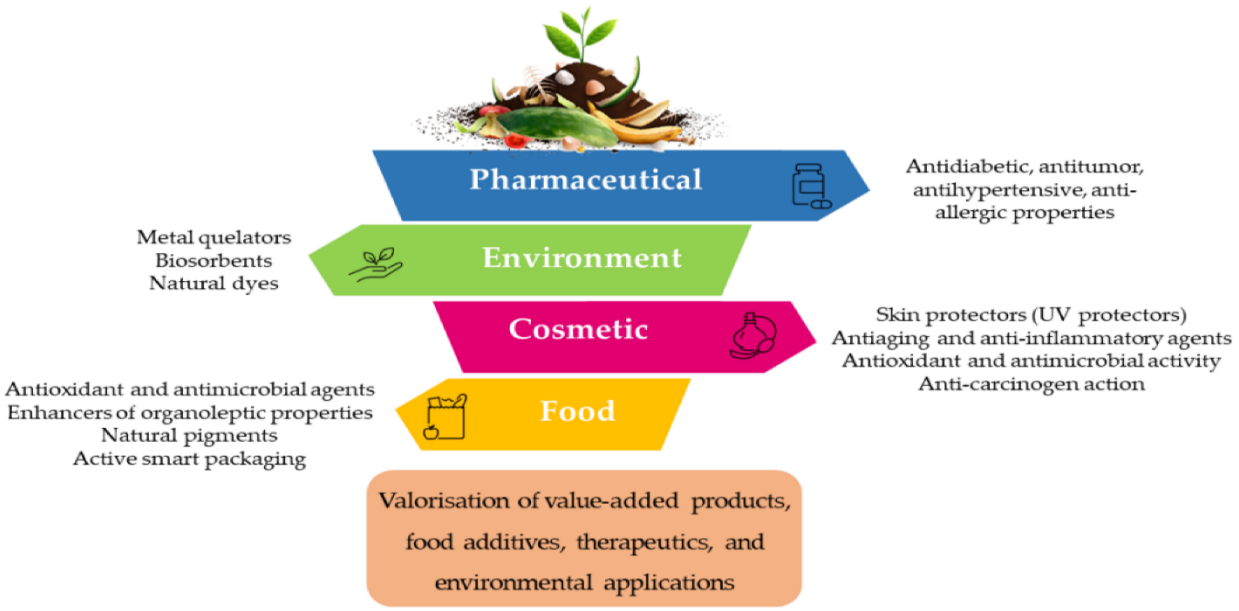
extraction of bioactive compounds, removal of heavy metal, etc. Scheme 2.5 presents a map of DES and NADES synthesis and application in agrifood systems.

Scheme 2.5 DES/NADES preparation and application in the agrifood sector [102]

2.3. Agrifood loss/waste valorization.

Valorization of agrifood wastes moved from a fancy ecological trend to an urgent human survival strategy because the destructive effects of unstable and extreme climate variations on agriculture, soil exhaustion, and water scarcity, among others has dealt negatively on agrifood production[103]. However, the continuous exponential growth of the human population requires more food but currently, around 700 million people are estimated to be suffering from hunger[103]. In contrast, nutrient loss due to agrifood waste is estimated to provide balanced diets to more than 2 billion people. Added to this, agrifood waste disposal in landfills is responsible for greenhouse gas (GHG) emissions, air pollution, and groundwater contamination. In summary, the impact of agrifood wastes on the world economy is very high, affecting different aspects of sustainability, such as water and land management, energy production, transport, and storage. The European Commission has already proposed many efforts to address these enormous challenges which included the mitigation of food waste as a priority area of the Action Plan for the European Circular Economy Strategy[104]. To make such a strategy economically viable, the valorization of agri-food wastes can be achieved by the extraction of valuable compounds for different industrial sectors, like the nutraceutical, cosmetic and pharmaceutical industries[105 106]. Diverse phytochemicals are present

in different agrifood wastes, mostly from those of plant origin like peels, leaves, seeds, pomaces, as well as from meat derivatives, egg products, and food industry rejects, thereby constituting promising raw materials for other industries as presented in scheme 2.6.



Scheme 2.6 Main sectors bioactive compounds recovered from agrifood wastes valorization can be applied [103]

CHAPTER THREE

MATERIALS AND METHODS

3.1. Materials

3.1.1. Chemicals

All the chemicals and solvents used were of analytical and standard grades. Citric acid monohydrate (≤ 100% purity), sucrose (99.8% purity), glucose monohydrate (99.0% purity), fructose (98.5-101.2% purity), xylitol (99% purity), glycerol (99-101% purity), sodium carbonate (99% purity), sodium acetate (99% purity), potassium acetate (99% purity), iron (iii) chloride hexahydrate (99% purity), Glycine (99% purity), and potassium persulfate (≥ 99% purity) were supplied by (Fluka Analytica, Germany), methanol (HPLC grade) (≥ 99.9% purity) was supplied by (Sigma–Aldrich, France), ethanol (96% purity) was purchased from (Fillab, Bulgaria), ammonium acetate (≥ 98% purity) was supplied by (Sigma–Aldrich, Netherlands), 2,4,6-tris(2-pyridyl)-s-triazine (TPTZ) (≥ 99% purity), and Folin-Ciocalteu's phenol reagent were supplied by (Sigma–Aldrich Switzerland), copper (ii) chloride (99% purity) was bought from (Sigma–Aldrich United Kingdom), aluminum (iii) nitrate nonahydrate (98.5% purity) was purchased from (Chem-Lab NV Belgium), Neocuprine (99.9% purity) was supplied by (Sigma–Aldrich Austria), (±)-6-hydroxy-2,5,7,8-tetramethylchromane-2-carboxylic acid (Trolox) (≥ 99% purity), 3,4,5-trihydroxybenzoic acid (Gallic acid) (99% purity) were purchased from (Sigma–Aldrich Milan, Italy). Water was purified using a Milli-Q Plus 185 system from Millipore (Milford, MA, USA).

3.1.2. Samples

Dried seeds of African Nutmeg (*Monodora myristica* (Gaertn. Dunal) fruits from the 2022 harvest were purchased from the Zuba Fruit Market, Abuja, Nigeria. The seeds were cleaned, packed under vacuum following WTO guidelines on sanitary and phytosanitary measures adopted in Nigeria as provided by the Standards Organisation of Nigeria through (**https://epingalert.org/**), and brought

to the Biotechnology Laboratory at the University of Food Technologies, Plovdiv, Bulgaria. In the laboratory, the seeds were peeled, and the peels were collected and ground with an electric coffee grinder. The ground peels were vacuum sealed and stored in a desiccator for further use.

3.2 Methods

3.2.1 Synthesis of Natural Deep Eutectic Solvents (NADESs)

The ultrasound-assisted synthesis of NADESs was first screened with a general factorial experimental design with three factors at three levels to obtain a total of 27 experimental runs as shown in Table 3.1 for coded and uncoded display. The NADESs were synthesized by weighing into synthesis bottles the designated mole ratios of the HBA and HBD (1:1, 1:2, 2:1), then 5 ml of water was added to moisten the two materials. The bottle was vigorously shaken to mix them into a homogenous mixture before sonicating in an ultrasonic bath operated at a frequency of 35kHz with maximum input power of 240 w (USTS 5.7150 Siel, Gabrovo, Bulgaria) at three designed temperatures (50, 70, 90 °c) and three designated times (60, 90, 120 min) with intermittent vigorous stirring to achieve uniformity (Figure 3.1). Three sonication temperatures (50ºc, 70ºc, and 90ºc), and three sonication times (60 min, 90 min, and 120 min) were selected for the synthesis based on information found in the literature for the synthesis of NADESs using heating and stirring (3-6 h)[107 108 109 110]; rotary evaporation (1-3 h)[111 112]; freeze-drying (24-48 h) [111]; and microwave radiation (0.25-0.75 h)[113 114]. At the end of each synthesis time using the corresponding temperature, the solvent was observed for proper and complete solvation. Those that did not completely solvate were further sonicated for a quarter of the experimental time at that temperature. After the extra sonication, those that failed to form clear solvents were discarded. The synthesis was taken to be successful when clear solutions were obtained after sonication, cooling and storing in a desiccator to minimize moisture absorption for 24 h. The temperature and time values that were appropriate from the screening study were then applied to different HBA:HBD ratios following the same steps. Using an infrared drier, the water contents in the solvents were between 0.5–2% depending on the molar ratio and the type of HBD used. The fourteen well formed NADESs, the molar ratios, the synthesis temperature, and synthesis time used for the synthesis is presented in Table 4. 1.

Table 3.1 Screening experiment for ultrasound-assisted synthesis of NADESs

Run	A	B	C	Temperature (°c)	Time (h)	HBA:HBD ratio
1	2	3	1	70	2.0	1:1
2	2	1	2	70	1.0	1:2
3	2	2	3	70	1.5	2:1
4	2	3	2	70	2.0	1:2
5	1	1	1	50	1.0	1:1
6	3	2	2	90	1.5	1:2
7	1	1	2	50	1.0	1:2
8	3	3	3	90	2.0	2:1
9	1	2	3	50	1.5	2:1
10	1	3	2	50	2.0	1:2
11	2	2	2	70	1.5	1:2
12	3	1	2	90	1.0	1:2
13	1	1	3	50	1.0	2:1
14	2	3	3	70	2.0	2:1
15	3	3	1	90	2.0	1:1
16	1	3	3	50	2.0	2:1
17	1	3	1	50	2.0	1:1
18	3	1	1	90	1.0	1:1
19	3	1	3	90	1.0	2:1
20	3	3	2	90	2.0	1:2
21	2	2	1	70	1.5	1:1
22	1	2	1	50	1.5	1:1
23	2	1	1	70	1.0	1:1
24	3	2	1	90	1.5	1:1
25	2	1	3	70	1.0	2.1
26	1	2	2	50	1.5	1:2
27	3	2	3	90	1.5	2:1

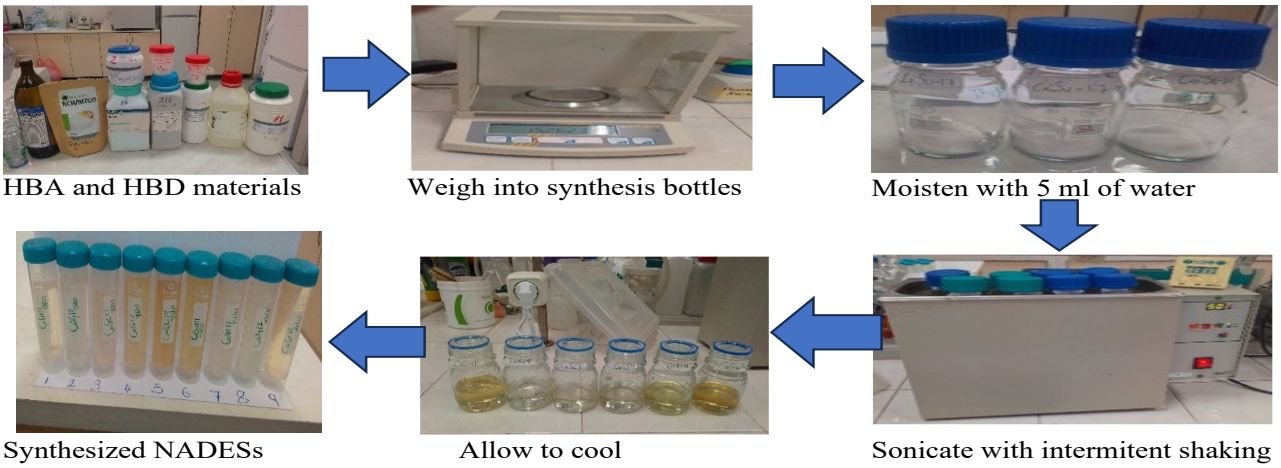


Figure 3.1 Pictorial flowchart for the synthesis of natural deep eutectic solvents (NADESs.)

3.2.2 Physical Properties and characteristics of NADESs.

3.2.2.1 Density

The density of the samples at 25ºC was determined in triplicate using a glass pycnometer following equation (**3.1**):

$$\boldsymbol{\rho s = d\ x\ \rho w}\ \ \mathbf{[kg/m3]} \qquad (\mathbf{3.1})$$

where:

ρs = density of sample.

mp = weight of pycnometer.

mpw =weight of pycnometer + water.

mw = weight of water = mpw-mp [kg].

mps = weight of pycnometer + sample.

ms = weight of sample = mps-mp [kg].

d = relative density of the sample to water = ms/mw.

ρw = 0.997 at 25ºC taken from appropriate table.

3.2.2.2 Water activity

A digital water activity meter AMTAST WA-60A (China) was used to measure the water activity of the samples in triplicate at 25ºC.

3.2.2.3 Viscosity

The viscosity of the samples at 25ºC was measured in triplicate using a glass pycnometer and calculated using equation (**3.2**):

$$\eta s = \eta w \left(\frac{\rho sts}{\rho wtw}\right) \ [pa.s] \qquad (3.2)$$

where:

ηs = viscosity of sample in [pa. s].

ρs = density of sample as measured [kg/m^3].

ts = average time for which the sample flows out (s).

ηw = viscosity of distilled water obtained from table [mpa. s] (0.89 at 25ºC).

ρw = density of distilled water obtained from table [kg/m^3] (0.997 at 25ºC).

tw = average time for which the water flows out (s).

3.2.2.4 PH

An Orion 2 digital pH meter Thermos scientific (Germany) was used to measure the pH of the synthesized NADESs in triplicates at 25ºC.

3.2.3 Effects of ultrasonication on the formation of NADESs

The effects of ultrasonication factors on the synthesis of NADESs were studied to elucidate the appropriate condition for synthesis of NADESs with ultrasound.

3.3. Storage Stability of NADESs

The effects of storage time on the physical properties of the synthesized NADESs were investigated to evaluate the shelf stability of the solvents. The physical properties of the synthesized NADESs were measured on the day of preparation, after 45 days of storage, and after ninety days of storage to investigate the effects of storage on the physicochemical properties of the solvent. All measurements were carried out in triplicates.

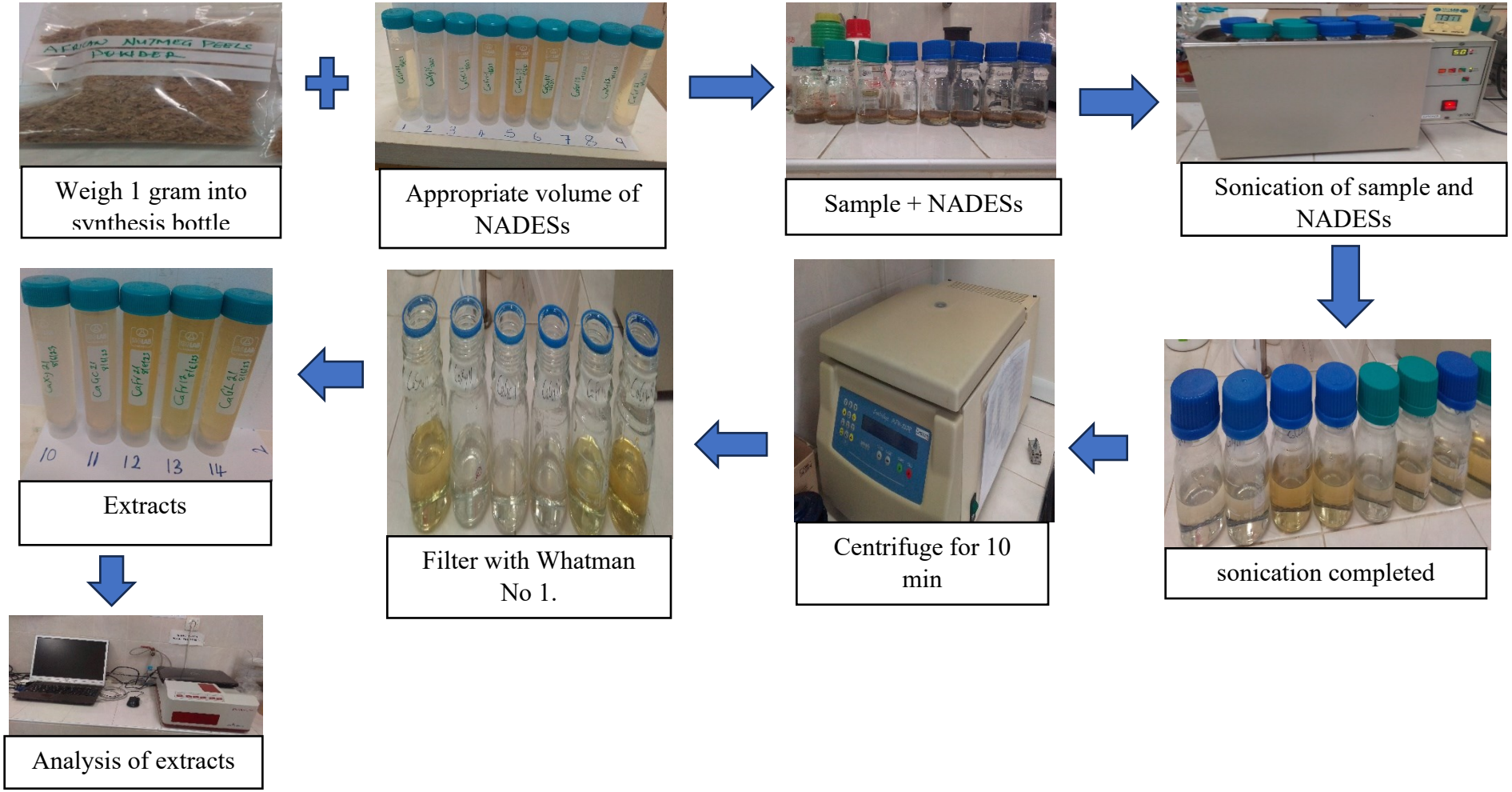


Figure 3.2 Pictorial flowchart for extraction and analysis of bioactive compounds from African Nutmeg peels

3.4 Application of NADESs for extraction of bioactive compounds

3.4.1 Extraction of Total Phenolic Contents (TPC)

The TPC assay was performed spectrophotometrically modifying the method of Ianni et al.,[115]. The Folin–Ciocalteu's (F-C) reagent method determined the TPC by measuring the absorbance at 765 nm. In a reaction tube, 0.1 mL of extract samples were mixed with 0.5 ml of F-C reagent. After approximately 1 min, 0.4 mL of 7.5% Na2CO3 was added, the mixture was incubated at 50°C for 5 min, and the absorbance was measured in a microplate reader (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany) against the appropriate blank sample. In this study, the TPC was evaluated using a gallic acid standard curve and reported in mgGAE/g dry weight of sample using **Equation 3.3**

TPC = ((Y-0.04)/0.0204*D*C)/B*1000) mgGAE/g, DW) ……. (3.3)

Where:

Y = Area of standard curve measured at 765 nm

B = Weight of sample used in the extraction

C = Volume of solvent used in the extraction

D = Dilution factor (where applicable)

DW= Dry weight of sample

3.4.2 Extraction of Total Flavonoid Contents (TFC)

The TFC was evaluated according to the method described in Kivrak et al., with minor adjustments[116]. In Eppendorf tubes (2 mL), aliquots of 0.25 mL of the extracts were added to 0.025 mL of 10% Al-$(NO_2)^3$, 0.025 mL of 1 M CH_3COOK, and 0.95 mL of ethanol. The mixture was incubated at room temperature (RT) for 40 min, after which the absorbance was read at 415 nm in a microplate reader (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany) against the designated blank control. The TFC calibration curve was determined by relying on the quercetin equivalence (QE) and was used as a standard to calibrate and standardize

the spectrophotometric measurements. **Equation 3.4** was used to determine and express the TFC in microgram equivalent of quercetin per gram of dry sample (µgQE/g, DW).

TFC = (((Y-0.0075)/0.0128) *D*C)/B) µgQE/g…… (3.4)

Where:

Y = Area of the standard curve measured at 415 nm

B = Weight of sample used in the extraction

C = Volume of solvent used in the extraction

D = Dilution factor (where applicable)

3.5 Antiradical scavenging activity of extracts

3.5.1 2,2-diphenil-1-picrylhydrazyl (DPPH) Radical Scavenging Assay

The antioxidant assay of the African nutmeg peels extracts was performed by using the radical 2,2-diphenyl-2-picrylhydrazyl (DPPH) based on the method of Brands-Williams et al. [117] with adjustments for specificity to our samples. To prepare the DPPH stock solution we dissolved 24 mg of DPPH in 100 mL of methanol. This solution was then diluted to achieve the absorbance of 1± 0.02 using the spectrophotometer (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany). For the assay, we combined forty microliters of extract with 3 mL of the prepared DPPH working solution and kept in the dark for 30 min at room temperature. Subsequently, we measured the absorbance at 515 nm using a spectrophotometer (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany), to assess the reduction in DPPH concentration, indicative of the antiradical activity utilizing the formula:

$$ARA\ (\%) = \left(\frac{AC - AS}{AC}\right) X100 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{3.5})$$

Where:

ARA (%) = Antiradical activity

AC = absorbance of control

AS = absorbance of sample

3.5.2 Ferric-Reducing Antioxidant Power (FRAP) Assay

The FRAP assay was carried out according to the procedure of Benzie and Strain, as slightly modified in subsequent studies [118 119]. The FRAP reagent was prepared fresh each day and warmed up to 37°C before use. The FRAP reagent consists of (1) 300 mM acetate buffer (pH 3.6), (2) TPTZ (10 mM in 40 mM HCl), and (3) ($FeCl_3.6H_2O$, 20 mM). Solutions (1), (2), and (3) were mixed at a ratio of 10:1:1 to form the FRAP reagent. In a 15 mL tube, 2.85 mL of freshly prepared and warmed FRAP reagent was blended with 0.15 mL of sample and incubated at 37°C for 4 min, after which the absorbance was measured at 593 nm in a microplate reader (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany) against the appropriate blank. The result is expressed as µMTE/g dry sample derived from **Equation 3.6**.

FRAP = (((Y+0.0017)/0.0013) *D*C)/B) µMTE/g, DW……. (3.6)

Where:

Y = Area of standard curve measurement at 593 nm

B = Weight of sample used in the extraction

C = Volume of solvent used in the extraction

D = Dilution factor where applicable

3.5.3 Cupric Ion-Reducing Antioxidant Capacity (CUPRAC) Assay

The CUPRAC assay was performed according to the procedure of Apak *et al*., as described in Akyuz *et al*. [120 121] with slight modifications. Briefly, 0.25 mL of 1.0×10^{-2} M copper (II) chloride solution, 7.5×10^{-3} M Neocuprine (Nc), 1 M CH_2COONH_4 buffer (pH 7.0) solution, and distilled water were mixed in a 2 mL Eppendorf tube, after which 0.025 mL sample was added and mixed. The resultant mixtures were allowed to stand at RT for 30 min to incubate. At the end of the incubation period, the absorbance was measured at 450 nm against the blank using a microplate reader (SPECTROstar Nano Microplate Reader, BMG LABTECH, Ortenberg, Germany). Trolox was used to prepare a standard curve, and the total antioxidant capacities of the samples were calculated following **Equations 3.7** and are expressed as µMTE/g dry weight (DW).

CUPRAC = (((Y+0.0372)/0.4128) *C*D)/B) µMTE/g, DW…… (3.7)

Where:

Y = Area of the standard curve measured at 450 nm

B = Weight of sample used in the extraction

C = Volume of solvent used in the extraction

D = Dilution factor where applicable

3.6 Experimental designs

3.6.1 Fractional experiments

A 2^4 fractional factorial experiment (FFE) with eight (8) corners and two (2) central points was performed three times, for a total of thirty experimental runs. The following factors were selected for the study: ultrasound temperature (UT), extraction time (ET), solvent volume (SV), and solvent concentration (SC). Many factors at a time (MFAT) experiments were chosen because they have many advantages over one factor at a time (OFAT) experiments. Some of the advantages of this approach include simultaneous investigation of independent factors and their interaction effects on the dependent factor (response), a reduction in the number of experiments to be executed to fully grasp the behavior of the process, guiding the choice of an optimization method that best fits a process, and saving time and resources during the process. The selected factors were set at two levels, low and high, for the corner points, with a central point set at the mean value of the sum of the corner points. The central point is necessary to elucidate changes in the process direction (if a curvature could be detected). The experiment was randomized and the design showing the coded and the actual factor values is presented in **Table 3.2.**

3.6.2 Response surface methodology

To investigate the effect of independent variables related to temperature (UT), time (ET), volume (SV), and concentration (SC) on total phenolic content, total flavonoid content, and antiradical

scavenging activity by CUPRAC, FRAP, and DPPH, a rotatable central composite response surface methodology design with five levels in and four factors was used.

Table 3.2 Fractional factorial experimental design for screening of extraction, antioxidant, and antiradical scavenging power studies.

Run	Blk	A	B	C	D	UT (ºc)	ET (min)	SV (ml)	SC (%)
1	1	0	0	0	0	50	15	15	70
2	1	+	+	-	-	60	20	10	60
3	1	+	-	-	+	60	10	10	80
4	1	+	+	+	+	60	20	20	80
5	1	-	-	-	-	40	10	10	60
6	1	-	-	-	-	40	10	10	60
7	1	-	-	+	+	40	10	20	80
8	1	0	0	0	0	50	15	15	70
9	1	-	+	-	+	40	20	10	80
10	1	-	-	-	-	40	10	10	60
11	1	+	+	+	+	60	20	20	80
12	1	-	+	+	-	40	20	20	60
13	1	-	+	+	-	40	20	20	60
14	1	+	+	-	-	60	20	10	60
15	1	-	+	-	+	40	20	10	80
16	1	0	0	0	0	50	15	15	70
17	1	0	0	0	0	50	15	15	70
18	1	-	+	-	+	40	20	10	80
19	1	+	+	-	-	60	20	10	60
20	1	-	-	+	+	40	10	20	80
21	1	+	-	-	+	60	10	10	80
22	1	-	+	+	-	40	20	20	60
23	1	+	+	+	+	60	20	20	80
24	1	-	-	+	+	40	10	20	80
25	1	0	0	0	0	50	15	15	70
26	1	+	-	+	-	60	10	20	60
27	1	0	0	0	0	50	15	15	70
28	1	+	-	+	-	60	10	20	60
29	1	+	-	+	-	60	10	20	60
30	1	+	-	-	+	60	10	10	80

The coded and uncoded levels of independent variables that were used in the design are presented in **Table 3.3**. Actual values of independent variables were calculated by following **Equation 3.8**. Central points used for temperature (ºC), time (min), volume (ml), and concentration (%) were 50, 15, 15, and 70, respectively. The step change for temperature and concentration was 10, while that for time and volume was 5, respectively. The full design matrix is shown in **Table 3.4**.

$$X = \frac{X0 - XC}{\Delta X} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{3.8})$$

Where:

X = coded values of independent variables

X0 = actual values of independent variables

ΔX = change in step, and

XC = the values at central points.

The analysis of variance technique was used to calculate the RCCRSD statistical parameters. For building the model, calculating the predicted values and optimal desirability for each of the solvents, plotting three-dimensional surface graphs to show the effects of independent variables on the response factors, calculating regression equations for the best-fitted model having non-significant lack of fit with effect to pure error, the response optimizer, and every other data analysis, Minitab statistical software 21.4.0 (Minitab LLC, Penn, USA) was used. The Fisher least significant difference (LSD) test value (F-value), coefficient of determination R^2, and lack of fit were used to determine the quality and adequacy of the model at ($p > 0.05$).

Table 3.3 Coded and actual levels of independent variables used in response surface methodology

	Coded levels				
	-α	**-1**	**0**	**+1**	**+α**
Variables	**Experimental Actual Values**				
Ultrasound temperature (UT) (ºc)	30	40	50	60	70
Extraction time (ET) (min)	5	10	15	20	25
Solvent volume (SV) (ml)	5	10	15	20	25
Solvent concentration (SC) (%)	50	60	70	80	90

Table 3.4 Randomized Design Table of Rotatable Central Composite Response Surface Experiment for the study of potential of NADESs-UAE extracts from African nut peels.

		Coded Factors and levels				Uncoded (Actual) Factors and levels			
Run	**Blk**	**A**	**B**	**C**	**D**	**Ultrasound Temperature (UT) (ºc)**	**Extraction Time (ET) (min)**	**Solvent Volume (SV) (ml)**	**Solvent Concentration (SC) (%)**
1	1	1	1	1	1	60	20	20	80
2	1	1	1	-1	1	60	20	10	80
3	1	1	1	1	-1	60	20	20	60
4	1	-1	-1	-1	-1	40	10	10	60
5	1	1	-1	1	-1	60	10	20	60
6	1	0	0	0	0	50	15	15	70
7	1	1	-1	1	1	60	10	20	80
8	1	1	-1	1	-1	60	10	20	60
9	1	0	0	0	0	50	15	15	70
10	1	1	1	-1	1	60	20	10	80
11	1	1	-1	-1	-1	60	10	10	60
12	1	0	0	0	0	50	15	15	70
13	1	-1	1	1	1	40	20	20	80
14	1	1	1	1	-1	60	20	20	60
15	1	0	0	0	0	50	15	15	15
16	1	-1	-1	-1	-1	40	10	10	70
17	1	-1	1	1	-1	40	20	20	60
18	1	1	-1	-1	-1	60	10	10	60
19	1	1	1	1	1	60	20	20	80
20	1	-1	-1	1	1	40	10	20	80
21	1	1	-1	-1	1	60	10	10	80
22	1	1	-1	-1	-1	60	10	10	60
23	1	-1	1	-1	1	40	20	10	80
24	1	-1	-1	-1	1	40	10	10	80
25	1	-1	-1	1	-1	40	10	20	60
26	1	0	0	0	0	50	15	15	70
27	1	1	-1	1	1	60	10	20	80
28	1	-1	1	-1	-1	40	20	10	60
29	1	-1	1	1	-1	40	20	20	60
30	1	-1	1	1	1	40	20	20	80
31	1	0	0	0	0	50	15	15	70
32	1	-1	-1	-1	-1	40	10	10	60
33	1	1	1	-1	-1	60	20	10	60
34	1	0	0	0	0	50	15	15	70
35	1	1	1	1	1	60	20	20	80

Table3.4 contd.

36	1	-1	1	1	-1	40	20	20	60
37	1	0	0	0	0	50	15	15	70
38	1	1	-1	-1	1	60	10	10	80
39	1	-1	-1	1	-1	40	10	20	60
40	1	1	1	1	-1	60	20	20	60
41	1	-1	-1	-1	1	40	10	10	80
42	1	-1	1	-1	-1	40	20	10	60
43	1	0	0	0	0	50	15	15	70
44	1	-1	-1	1	1	40	10	20	80
45	1	-1	1	-1	-1	40	20	10	60
46	1	0	0	0	0	50	15	15	70
47	1	-1	-1	1	-1	40	10	20	60
48	1	1	1	-1	1	60	20	10	80
49	1	0	0	0	0	50	15	15	70
50	1	-1	1	1	1	40	20	20	80
51	1	0	0	0	0	50	15	15	70
52	1	1	1	-1	-1	60	20	10	60
53	1	-1	1	-1	1	40	20	10	80
54	1	-1	-1	-1	1	40	10	10	80
55	1	1	-1	1	-1	60	10	20	60
56	1	-1	1	-1	1	40	20	10	80
57	1	-1	-1	1	1	40	10	20	80
58	1	1	-1	-1	1	60	10	10	80
59	1	1	-1	1	1	60	10	20	80
60	1	1	1	-1	-1	60	20	10	60
61	1	0	-α	0	0	50	5	15	70
62	1	0	0	0	0	50	15	15	70
63	1	0	0	-α	0	50	15	5	70
64	1	0	0	α	0	50	15	25	70
65	1	0	0	0	0	50	15	15	70
66	1	0	0	0	0	50	15	15	70
67	1	0	-α	0	0	50	5	15	70
68	1	0	α	0	0	50	25	15	70
69	1	0	0	α	0	50	15	25	70
70	1	0	0	0	-α	50	15	15	50
71	1	-α	0	0	0	30	15	15	70
72	1	0	0	-α	0	50	15	5	70
73	1	0	0	0	-α	50	15	15	50
74	1	0	0	0	α	50	15	15	90
75	1	-α	0	0	0	30	15	15	70
76	1	0	0	0	0	50	15	15	70

Table 3.4 contd.

77	1	0	0	0	-a	50	15	15	50
78	1	0	a	0	0	50	25	15	70
79	1	0	0	0	a	50	15	15	90
80	1	0	0	0	0	50	15	15	70
81	1	0	0	0	a	50	15	15	90
82	1	a	0	0	0	70	15	15	70
83	1	a	0	0	0	70	15	15	70
84	1	0	0	a	0	50	15	25	70
85	1	0	0	-a	0	50	15	5	70
86	1	a	0	0	0	70	15	15	70
87	1	-a	0	0	0	30	15	15	70
88	1	0	-a	0	0	50	5	15	70
89	1	0	a	0	0	50	25	15	70
90	1	0	0	0	0	50	15	15	70

3.7 Instrumentation and Characterization

3.7.1 Fourier Transform Infrared Spectroscopy (FTIR) Analysis.

Chemical characterization of the prepared NADES was instrumentally confirmed by analyzing different bonds energies and peaks through infrared induced absorption at a frequency related to bond vibration using FT-IR spectrometer system (IRAffinity-1S, A221357, SHIMADZU, Japan).

3.8. Chemometric Analysis

3.8.1 Principal Component Analysis (PCA)

Chemometric methods are a combination of processing raw data and extracting information. Chemometric methods comprise experimental design, classification and clustering studies, multivariate calibration and multivariate analysis. Through PCA, complicated data sets can be simplified and displayed. Dimension reduction and classification of data tables are assembled with this method. PCA was used to evaluate the quantitative physical properties results and profiles of the synthesized NADESs in terms of the HBD components. NADESs prepared with different HBDs, and molar ratios were tested using PCA for the purpose of creating physical properties data correlations with the eutectic energies derived from the FTIR peaks. PCA analysis was executed with Minitab 21.3 Software.

CHAPTER FOUR

RESULTS

4.1 Synthesis of natural deep eutectic solvents (NADESs)

Natural deep eutectic solvents (NADESs) were synthesized with citric acid as HBA and sucrose, fructose, xylitol, glycerol, glycine, and glucose as HBDs. The HBA and HBDs were varied in three molar ratios: 1:1, 1:2, and 2:1 respectively based on some preliminary studies that eliminated other molar ratios from the study. In the preliminary investigation, three ultrasonic temperature ranges (50ºC, 70ºC, and 90ºC), three-time intervals (60 min, 45 min, and 30 min), and six molar ratios of HBA and HBD (1:1, 1:2, 1:3, 2:1, 2:3, 3:1), respectively were tested before selecting the molar ratios and operating temperature and time. **Table 4.1** shows the NADESs that were synthesized, the molar ratios, the synthesis conditions of temperature and time, as well as the physical characteristics of the synthesized NADESs.

Table 4.1 Natural deep eutectic solvents (NADESs), synthesis conditions, and physical characteristics.

S/No	Code	HBA	HBD	HBA: HBD ratio	Synthesis temperature (ºc)	Synthesis time (min)	Remarks
1	CaSu11	Citric acid	Sucrose	1:1	70	60	Orange yellow
2	CaFr11	Citric acid	Fructose	1:1	70	60	Faintly yellow
3	CaFr12	Citric acid	Fructose	1:2	70	60	Yellow
4	CaFr21	Citric acid	Fructose	2:1	70	60	Yellow
5	CaXy11	Citric acid	Xylitol	1:1	70	60	Colourless
6	CaXy12	Citric acid	Xylitol	1:2	70	60	Colourless
7	CaXy21	Citric acid	Xylitol	2:1	70	60	Colourless
8	CaGr11	Citric acid	Glycerol	1:1	70	60	Colourless
9	CaGr12	Citric acid	Glycerol	1:2	70	60	Colourless
10	CaG21	Citric acid	Glycerol	2:1	70	60	Colourless
11	CaGc11	Citric acid	Glycine	1:1	70	60	Colourless
12	CaGc21	Citric acid	Glycine	2:1	70	60	Colourless
13	CaGl11	Citric acid	Glucose	1:1	70	60	Yellow
14	CaGl21	Citric acid	Glucose	2:1	70	60	yellow

4.2. Physical Properties of NADESs

The physical properties (density, water activity, viscosity, & pH) of the synthesized NADESs were measured in triplicates and analyzed using a one-way analysis of variance and Fisher's least significant difference (LSD) to compare and separate the NADESs into groups to further investigate if similarity in the physical properties could lead to similarity in performance of the solvents during application. The physical properties of the synthesized NADESs are shown in **Table 4.2.**

4.2.1 Density

The mean density obtained among the NADESs ranged from 1.2344 in CaGr11 & CaGr12 to 1.377 in CaFr21. The mean and standard deviation of the density measurements is presented in **Table 4.2.** Analysis of variance and Fisher's LSD shows that the solvents could be separated into four groups: **A** (CaSu11, CaFr12, & CaFr21), **B** (CaFr11, CaXy21, CaGr21, CaGc11, CaGc21, & CaGl21), **C** (CaXy11, CaXy12, & CaGl11), **and** D (CaGr11 & CaGr12) respectively, **Figure 4.1.**

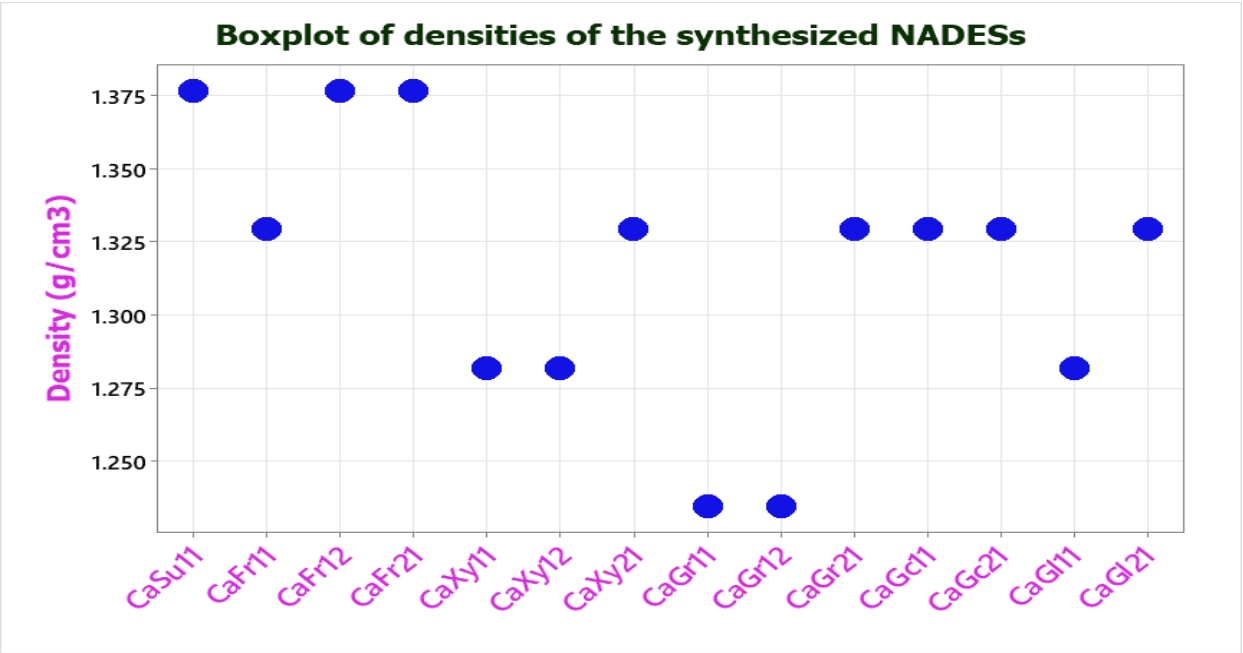


Figure 4.1 Box plots of the densities of the synthesized NADESs

Table 4.2 Physical Properties of the synthesized NADESs

NADESs	HBA	HBD	Ratio	pH	Water activity	Viscosity (pa. s)	Density (g/cm^3)
CaSu11	Citric acid	sucrose	1:1	1.92±0.00^{C}	0.73±0.010^{F}	0.3545±0.0003^{A}	1.3768±0.0002^{A}
CaFr11	Citric acid	fructose	1:1	1.75±0.01^{H}	0.77±0.006^{DE}	0.0805±0.0001^{F}	1.3293±0.0003^{B}
CaFr12	Citric acid	fructose	1:2	1.90±0.01^{C}	0.76±0.010^{E}	0.1797±0.0002^{B}	1.3768±0.0008^{A}
CaFr21	Citric acid	fructose	2:1	1.84±0.00^{EF}	0.72±0.010^{FG}	0.1221±0.0001^{D}	1.3770±0.0000^{A}
CaXy11	Citric acid	xylitol	1:1	1.85±0.05^{E}	0.78±0.010^{CD}	0.0269±0.0001^{J}	1.2818±0.0004^{C}
CaXy12	Citric acid	xylitol	1:2	1.90±0.03^{C}	0.76±0.010^{E}	0.0806±0.0002^{F}	1.2818±0.0008^{C}
CaXy21	Citric acid	xylitol	2:1	1.89±0.03^{CD}	0.72±0.006^{FG}	0.0871±0.0001^{E}	1.3293±0.0002^{B}
CaGr11	Citric acid	glycerol	1:1	1.68±0.02^{I}	0.79±0.000^{C}	0.0131±0.0001^{M}	1.2344±0.0004^{D}
CaGr12	Citric acid	glycerol	1:2	1.86±0.02^{DE}	0.77±0.010^{DE}	0.0191±0.0020^{L}	1.2344±0.0006^{D}
CaGr21	Citric acid	glycerol	2:1	1.78±0.01^{GH}	0.77±0.010^{DE}	0.0525±0.0005^{H}	1.3293±0.0003^{B}
CaGc11	Citric acid	glycine	1:1	2.61±0.04^{A}	0.83±0.010^{A}	0.0204±0.0000^{K}	1.3293±0.0004^{B}
CaGc21	Citric acid	glycine	2:1	2.39±0.01^{B}	0.81±0.000^{B}	0.0760±0.0020^{G}	1.3293±0.0004^{B}
CaGl11	Citric acid	glucose	1:1	1.81±0.01^{FG}	0.77±0.010^{DE}	0.0438±0.0001^{I}	1.2818±0.0004^{C}
CaGl21	Citric acid	glucose	2:1	1.71±0.01^{I}	0.71±0.010^{G}	0.1313±0.0002^{C}	1.3293±0.0003^{B}

Means that do not share a letter are significantly different.

4.2.2 Water activity

The water activity of the synthesized NADESs were measured with a digital water activity meter and the results presented in **Table 4.2.** The water activity values were between 0.71 and 0.83. The solvent with the highest water activity values was CaGc11, while CaGl21 has the lowest water activity value. Scatterplot of the water activity of the synthesized NADESs are shown in **Figure 4.2**

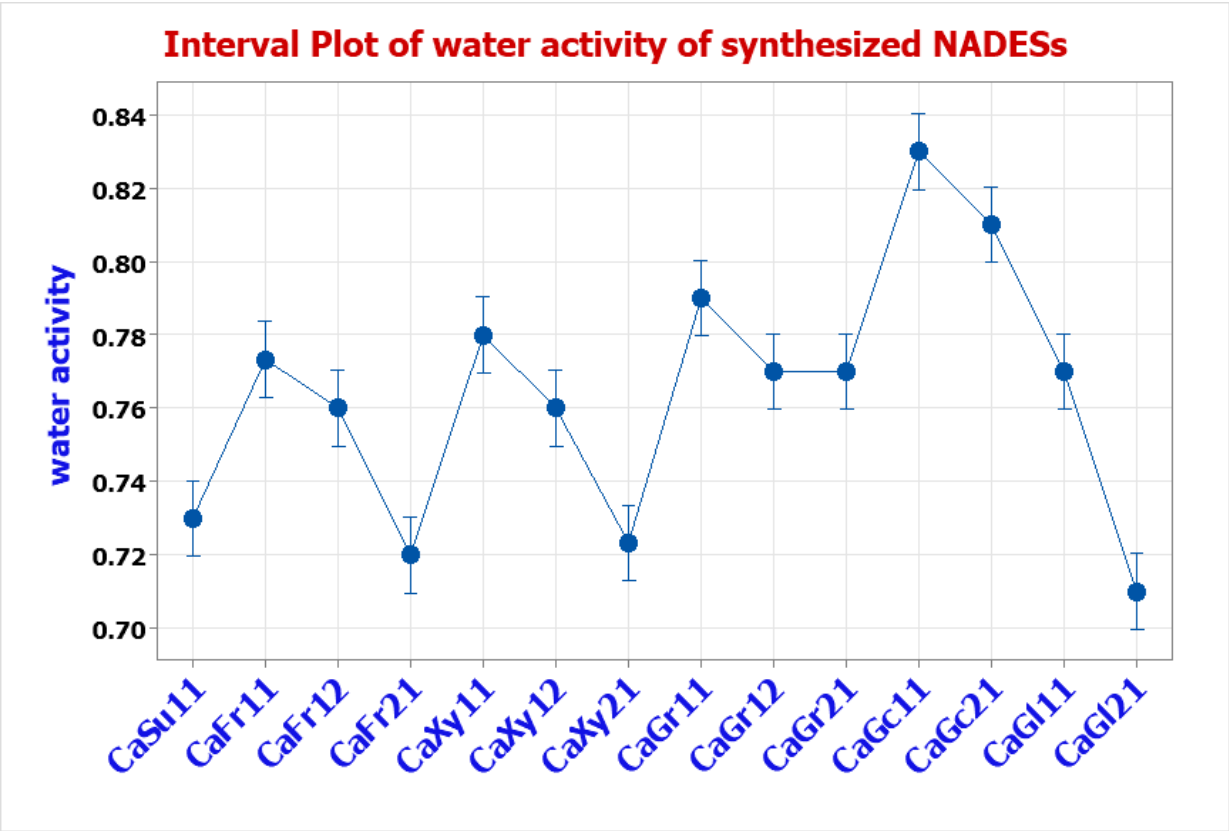


Figure 4.2 Water activity of synthesized NADESs at 25°c

4.2.3 Viscosity

Dynamic viscosity measures the resistance of fluid to flow and the molecular bond strength of the fluid. The viscosities of the synthesized NADESs for all functional groups of HBD at different molar ratios are shown in **Table 4.2.** The analysis of the relationships of the viscosity of the

NADESs are shown in **Figure 4.3,** and in comparison, CaSu11 is the most viscous among the solvents while CaGr11 is the least viscous. All the solvents seem to be more viscous than water.

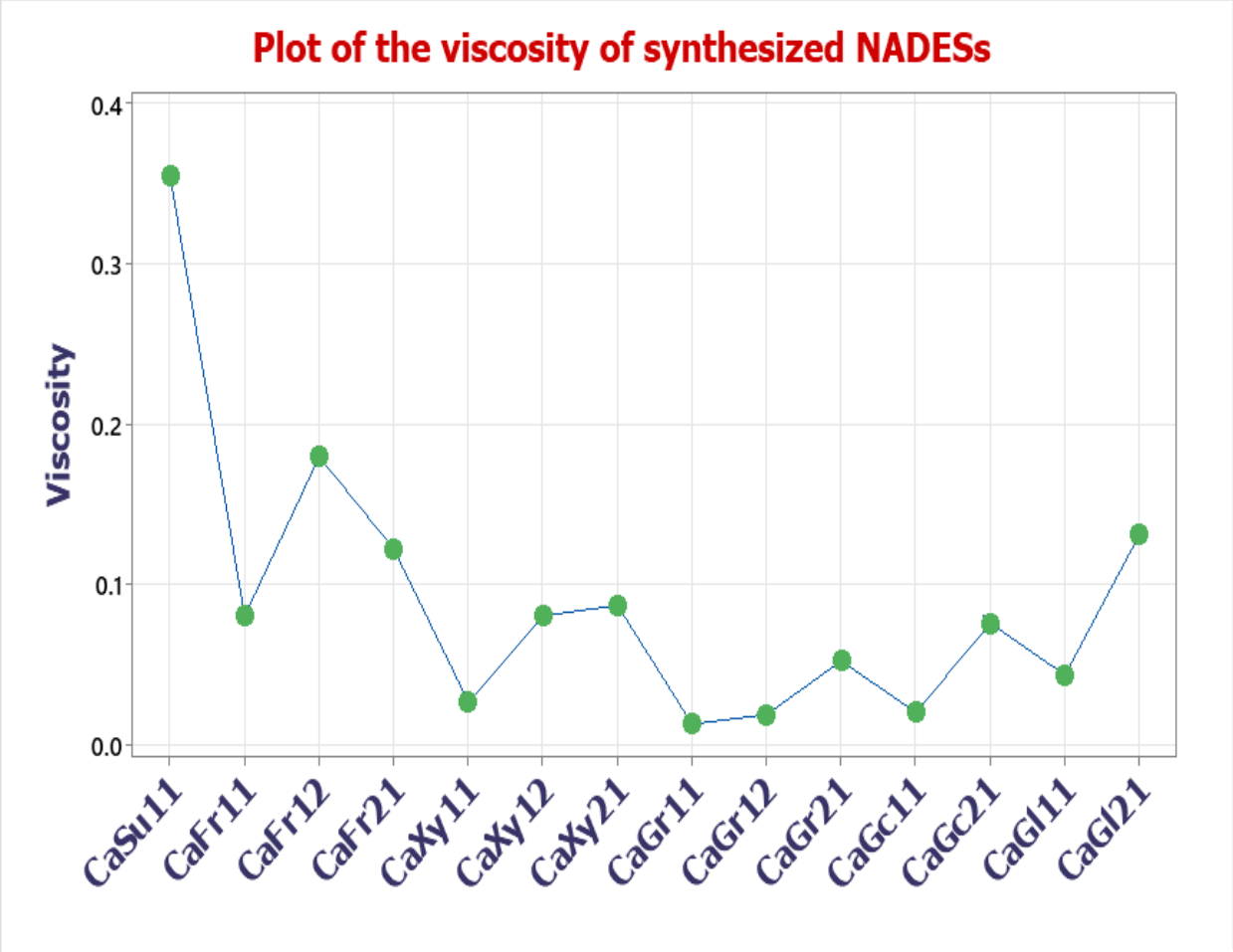


Figure 4.3 Viscosity of synthesized NADESs at 25°c

4.2.4 pH

The pH values at 25°c of the synthesized NADESs ranged from 1.68±0.02 to 2.61±0.04, and is shown in **Table 4.2.** All synthesized NADESs display acidic condition as the pH were below 2.0 except in CaGc11 and CaGc21 where the pH values were above 2.0 as can be seen in figure 4.4.

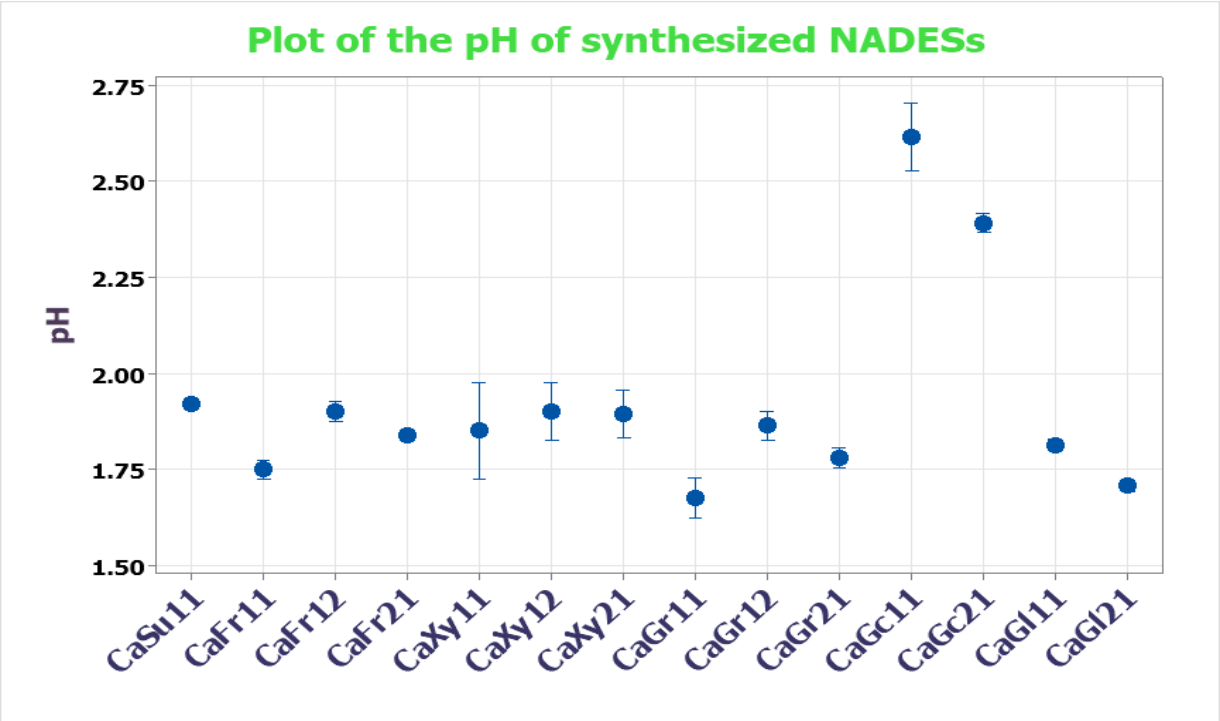


Figure 4.4 pH of synthesized NADESs at 25°c

4.3 Storage Stability of NADESs

The synthesized NADESs were stored in the desiccator at 25°c to avoid moisture loss or gain for ninety days and the physical properties measured first after 45 days and next after a second 45 days bring them to a storage period of 90 days to study the effect of time on the stability of the solvents. The mean and standard deviation of the solvents at the end of the storage period is presented in **Table 4.3.**

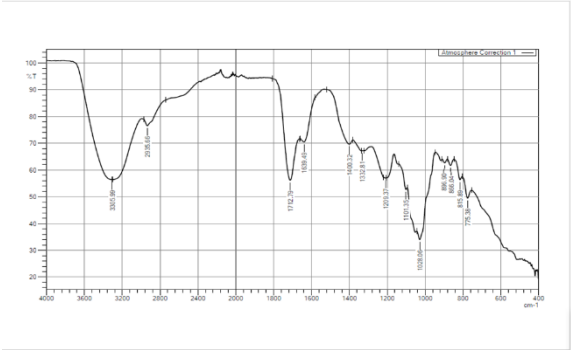
4.4 Instrumentation and Characterization NADESs

FT-IR spectroscopy was employed to identify the chemical structure of the NADES and validate the presence of bonds between hydrogen bond donor and acceptor in NADES molecules. FTIR analysis has been used to identify chemical structures and confirm the existence of intermolecular bonds among the individual components of mixtures. In this study, Citric acid was used as the hydrogen bond acceptor, while sucrose, fructose, xylitol, glycerol, glycine, and glucose were applied as hydrogen bond donors respectively. The synthesized NADESs FTIR spectra is shown in **Figure 4.5** while the peaks are presented in **Table 4.4**. The peaks show the presence of the following characteristic functional groups: OH (3400−3200 cm^{-1}); 3392 cm^{-1} in CaGc21 to 3286 cm^{-1} in CaGr12, CH (3000-2800 cm^{-1}); 3246 cm^{-1} in CaXy21 to 2935 cm^{-1} in CaSu11.

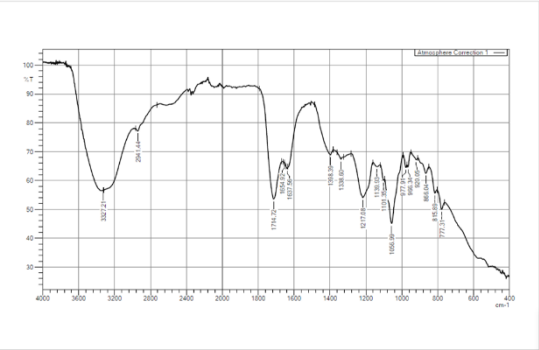
Table 4.3 Physical properties of NADESs over storage period

NADESs	Physical properties and storage period of synthesized NADESs											
	Density			Viscosity			Water activity			pH		
	Day 1	Day 45	Day 90	Day 1	Day 45	Day 90	Day 1	Day 45	Day 90	Day 1	Day 45	Day 90
CaSu11	1.377±0.00	1.363±0.00	1.360±0.00	0.355±0.00	0.338±0.00	0.313±0.00	0.73±0.01	0.70±0.01	0.70±0.01	1.92±0.00	2.21±0.01	2.02±0.02
CaFr11	1.329±0.00	1.320±0.00	1.314±0.00	0.081±0.00	0.089±0.00	0.098±0.00	0.77±0.01	0.78±0.01	0.76±0.01	1.75±0.01	1.90±0.01	1.86±0.00
CaFr12	1.377±0.00	1.337±0.00	1.314±0.00	0.180±0.00	0.181±0.00	0.182±0.00	0.76±0.01	0.70±0.02	0.71±0.00	1.9±0.01	1.89±0.01	1.95±0.02
CaFr21	1.377±0.00	1.361±0.00	1.360±0.00	0.122±0.00	0.134±0.00	0.140±0.00	0.72±0.01	0.69±0.00	0.70±0.01	1.84±0.00	1.73±0.01	1.76±0.01
CaXy11	1.282±0.00	1.271±0.00	1.269±0.00	0.027±0.00	0.027±0.00	0.029±0.00	0.78±0.01	0.77±0.01	0.78±0.00	1.85±0.05	1.88±0.01	1.91±0.01
CaXy12	1.282±0.00	1.297±0.00	1.318±0.00	0.081±0.00	0.096±0.00	0.105±0.00	0.76±0.01	0.73±0.00	0.73±0.00	1.9±0.03	1.91±0.01	1.95±0.01
CaXy21	1.329±0.00	1.320±0.00	1.318±0.00	0.087±0.00	0.084±0.00	0.083±0.00	0.72±0.01	0.71±0.00	0.72±0.00	1.89±0.03	1.73±0.03	1.79±0.01
CaGr11	1.234±0.00	1.221±0.00	1.227±0.00	0.013±0.00	0.014±0.00	0.014±0.00	0.79±0.00	0.79±0.01	0.78±0.00	1.68±0.02	1.82±0.02	1.88±0.01
CaGr12	1.234±0.00	1.280±0.00	1.318±0.00	0.019±0.00	0.044±0.00	0.074±0.00	0.77±0.01	0.75±0.00	0.74±0.00	1.86±0.02	1.88±0.01	1.92±0.00
CaGr21	1.329±0.00	1.302±0.00	1.273±0.00	0.053±0.00	0.048±0.00	0.045±0.00	0.77±0.01	0.73±0.00	0.72±0.00	1.78±0.01	1.60±0.02	1.77±0.00
CaGc11	1.329±0.00	1.305±0.00	1.273±0.00	0.020±0.00	0.032±0.00	0.042±0.00	0.83±0.01	0.83±0.00	0.83±0.00	2.61±0.04	2.67±0.01	2.61±0.01
CaGc21	1.329±0.00	1.321±0.00	1.318±0.00	0.076±0.00	0.074±0.00	0.073±0.00	0.81±0.00	0.76±0.01	0.76±0.00	2.39±0.01	2.36±0.01	2.43±0.03
CaGl11	1.282±0.00	1.281±0.00	1.273±0.00	0.044±0.00	0.047±0.00	0.050±0.00	0.77±0.01	0.76±0.02	0.76±0.00	1.81±0.01	1.87±0.01	1.86±0.02
CaGl21	1.329±0.00	1.320±0.00	1.318±0.00	0.131±0.00	0.106±0.00	0.096±0.00	0.71±0.01	0.69±0.01	0.71±0.00	1.71±0.01	1.70±0.01	1.71±0.01

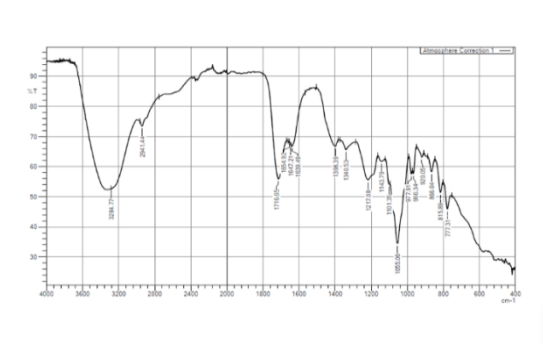
CaSu11



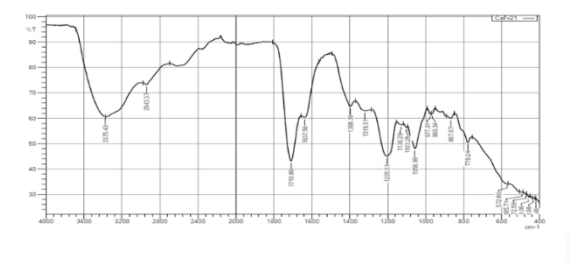
CaFr11



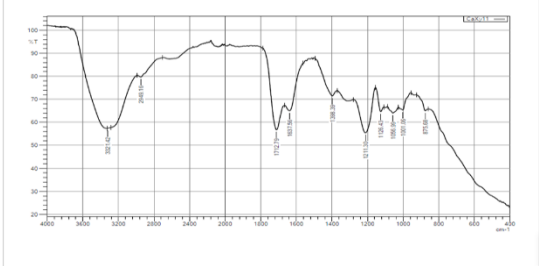
CaFr12



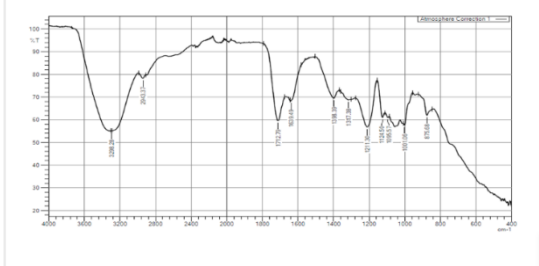
CaFr21



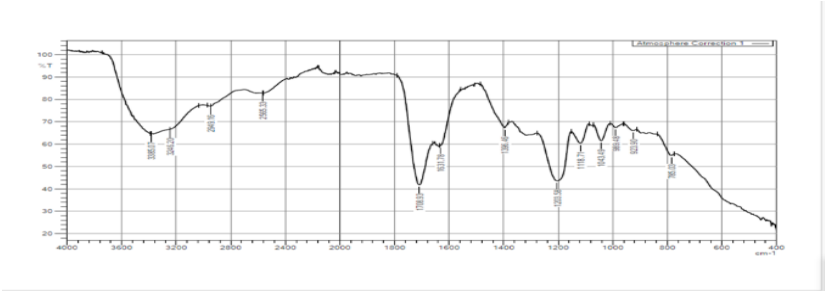
CaXy11



CaXy12



CaXy21



CaGr11

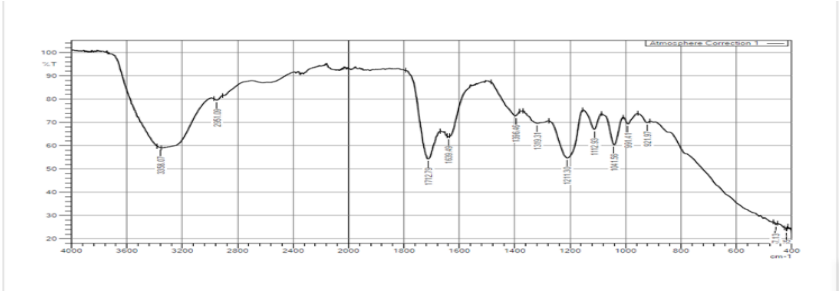
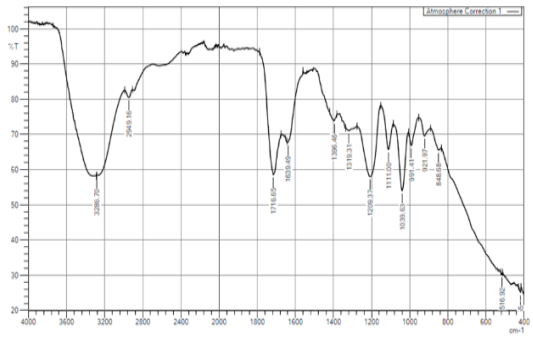
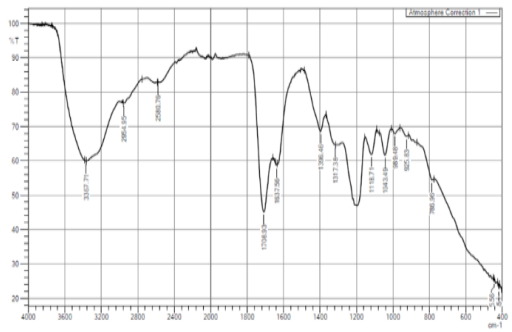


Figure 4.5 FTIR spectra of synthesized NADESs

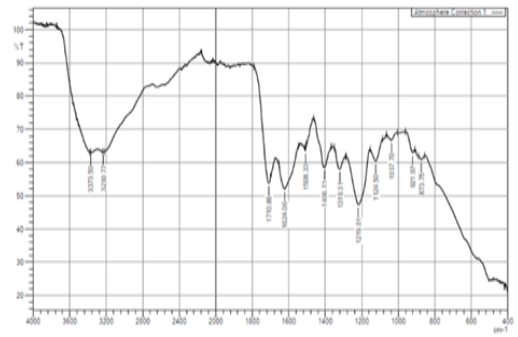
CaGr12



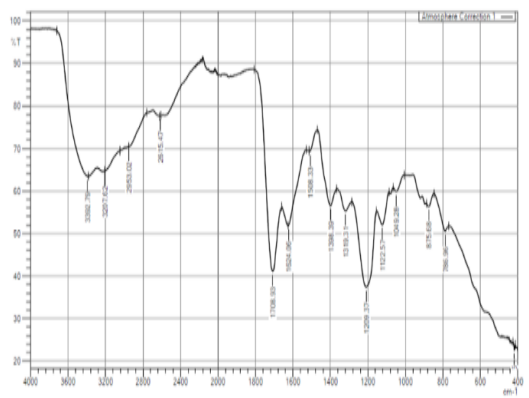
CaGr21



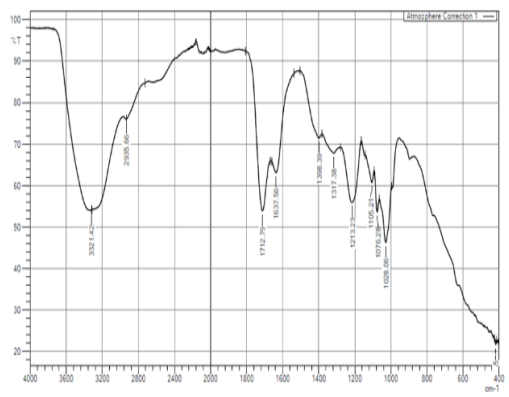
CaGc11



CaGc21



CaGl11



CaGl21

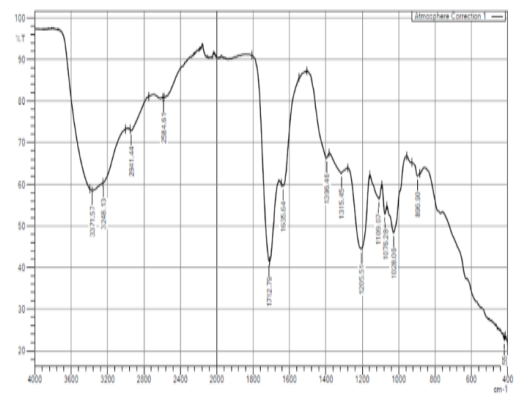


Figure 4.5 contd.

Table 4.4 FTIR peaks of the synthesized NADESs

Peaks	**NADESs**													
	CaSu11	**CaFr11**	**CaFr12**	**CaFr21**	**CaXy11**	**CaXy12**	**CaXy21**	**CaGr11**	**CaGr12**	**CaGr21**	**CaGc11**	**CaGc21**	**CaGl11**	**CaGl21**
1	3306	3327	3288	3375	3321	3298	3385	3358	3287	3368	3374	3393	3321	3372
2	2936	2941	2941	2943	2949	2943	3246	2951	2949	2955	3231	3208	2936	3218
3	1713	1715	1717	1711	1713	1713	2949	1713	1717	2581	1711	2953	1713	2941
4	1639	1655	1655	1638	1638	1639	2565	1639	1639	1709	1624	2615	1638	2585
5	1400	1638	1647	1398	1398	1398	1709	1396	1396	1638	1508	1709	1398	1713
6	1333	1398	1639	1319	1211	1317	1632	1319	1319	1396	1406	1624	1317	1636
7	1209	1339	1398	1206	1126	1211	1396	1211	1209	1317	1319	1508	1213	1396
8	1101	1217	1341	1130	1057	1125	1204	1113	1111	1119	1219	1398	1105	1315
9	1028	1140	1217	1103	1001	1096	1119	1042	1040	1043	1125	1319	1076	1206
10	897	1101	1144	1057	876	1001	1043	991	991	989	1038	1209	1028	1109
11	866	1057	1101	978		876	989	922	922	936	922	1123	419	1076
12	816	978	1055	966			924	457	849	787	874	1049		1028
13	775	966	978	868			785	419	517	446		876		897
14		920	966	779					419	419		787		419
15		866	920	573								419		
16		816	866	496										
17		777	816	473										
18			777	459										
19				434										
20				420										

4.5. Chemometric Analysis

Chemometric analysis of the principal components was performed by Minitab and shows the similarities and differences among the groups as well as the relationship between the variables (physical properties and FTIR peaks). The loading plot of the PCA is presented in **Figure 4.6** while the score plot is shown in **Figure 4.7**, respectively. The result of the loading plot illustrates a 98.99% variation in the data (73.18% PC2, 25.81% PC1). The score plot on the other hand shows a separation of the solvents into four main groups

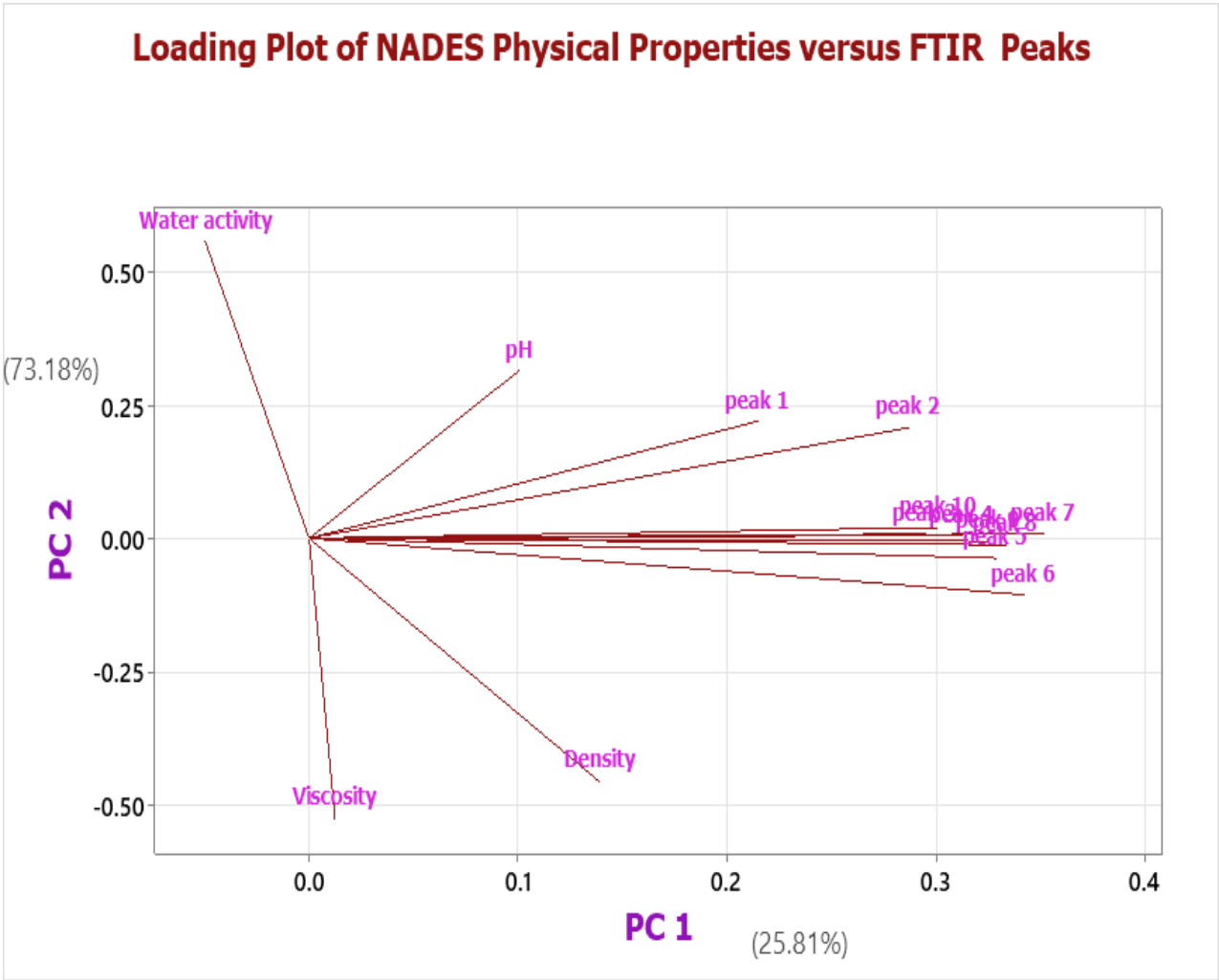


Figure 4.6 Loading plot of physical properties versus FTIR peaks of synthesized NADESs

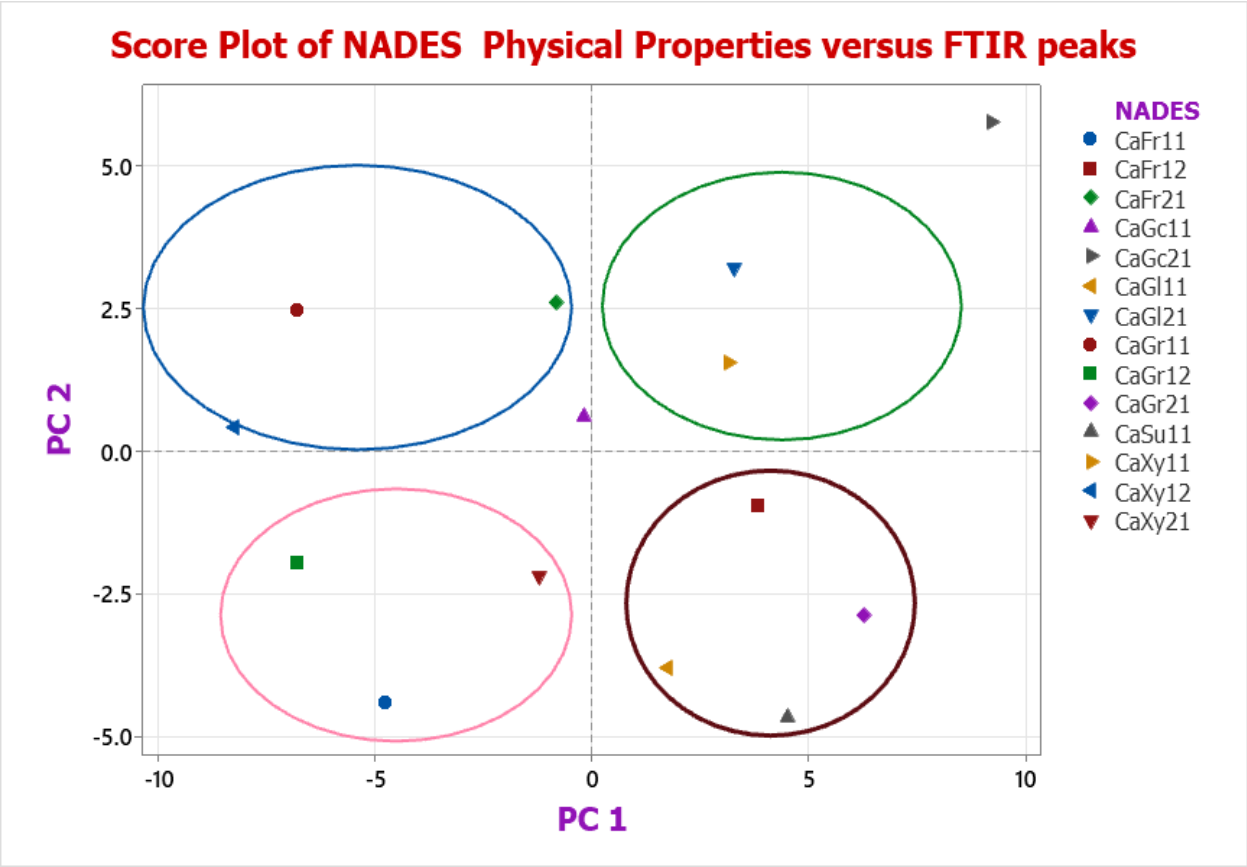


Figure 4.7 score plot of physical properties versus FTIR peaks of synthesized NADESs

4.6 Application of NADESs for extraction of bioactive compounds

4.6.1 Factorial experiments

The study applied a multifactorial (MFAT) experimental design to investigate the capacity of the synthesized NADESs in extraction of bioactive compounds from African nutmeg peels (plant food waste) and evaluate the antioxidant and antiradical scavenging activities of the extracts. The use of MFAT in conjunction with NADES highlights an innovative approach, bridging the gap between traditional extraction methods and modern, sustainable techniques. The behaviour of the solvents under different extraction conditions was elucidated. The effects of operational variables on the yield of polyphenols and flavonoids from the extracts were thorough studied. The findings could pave the way for more efficient and environmentally friendly extraction processes, contributing significantly to the field of green chemistry and sustainable agriculture. The antioxidant capacity

was measured in terms of total polyphenol content (TPC) and total flavonoid content (TFC) via spectrophotometric methods. The antiradical scavenging power of the extracts were analyzed via the cupric ion reducing antioxidant capacity (CUPRAC) assay and the ferric reducing antioxidant power (FRAP) assay.

4.6.1.1 Model performance on extraction of polyphenols and flavonoids from African Nutmeg peels

The experimental model used in the study was found to contribute significantly to TPC and TFC extraction from the sample. The model performance is presented in **Table 4.5** as a percentage of the contributions of individual components. As shown in **Table 4.5**, the model contributions presented as coefficient of determination (**R^2**) for the TPC extraction ranged from 85.26% for CaSu11 to 99.72% for CaGc21, while for the TFC, the **R^2** ranged from 99.93% for CaXy21 to 100% for CaFr11, CaGc11, and CaGl21, with nonsignificant differences with effect to pure error. The four-way interaction term (UT*ET*SV*SC) was found to be completely confounded with the center points, while the following two-way and three-way interaction terms (ET*SV, ET*SC, SV*SC) and (UT*ET*SC, UT*SV*SC, ET*SV*SC) were found to be completely confounded with the corner points. All confounding terms were removed from the model. The uncoded regression models for TPC extraction are given as equations **(4.1)** to **(4.14),** while for TFC extraction they are given as equations **(4.15)** to **(4.28)** and are presented in **Table 4.6** respectively**.**

4.6.1.2 Model performance on Antiradical scavenging activity of African Nutmeg peels measured by CUPRAC and FRAP methods

The antiradical scavenging activities were measured to investigate the effects of the experimental model on the scavenging power of the extracts. The model performance, presented as coefficient of determination (**R^2**) in **Table 4.7** indicates that CUPRAC ranged from 0.736 in CaGc11 to 0.998 in CaGl21, while in FRAP, the design was almost a perfect fit (0.9999- 1.0000) as can be seen in **Table 4.7**. The four-way interaction term (UT*ET*SV*SC) was found to be completely confounded with the center points (Ct Pt), while the following two-way and three-way interaction terms (ET*SV, ET*SC, and SV*SC) and (UT*ET*SV, UT*ET*SC, UT*SV*SC, and

ET*SV*SC) were found to be completely confounded with the corner points. All confounding terms were removed from the model. The uncoded regression models for CPRAC and FRAP antiradical scavenging activity are given as equations **(4.39-4.42)**, and **(4.43-4.57),** and are presented in **Table 4.8,** respectively

4.6.1.3 Effects of experimental factors on antioxidant and antiradical scavenging activity of African nutmeg peels extracts using NADESs.

The Effects of experimental factors and their interactions on antioxidant and antiradical scavenging activity of African nutmeg peels extracts was determined and results presented in **Figure 4.8** to **Figure 4.11** for TPC, TFC, CUPRAC, and FRAP respectively. The results show that the interaction between extraction temperature and solvent concentration was significant among all the synthesized NADESs in TPC extraction and CUPRAC capacity, while all main factors were significant across the solvents in TFC extraction and FRAP power respectively.

4.6.1.4 The behaviour of NADESs at different experimental conditions

The behaviour of the synthesized NADESs at different conditions were further elucidated using TPC extraction, and the results presented in **Figure 4.12.** At different TPC extraction conditions, the solvents showed nonlinear behaviour except CaFr11, which behaves linearly.

Table 4.5 Percentage contribution of model components to TPC and TFC extraction

NADESs	TPC							TFC						
	R^2 (%)	R^2(Adj) (%)	R^2(Pred) (%)	Linear (%)	Interaction (%)	Curvature (%)	Error (%)	R^2 (%)	R^2(Adj) (%)	R^2(Pred) (%)	Linear (%)	Interaction (%)	Curvature (%)	Error (%)
CaSu11	85.26	79.65	78.76	32.92	40.51	11.83	14.74	99.99	99.99	99.98	87.80	11.08	1.11	0.01
CaFr11	85.80	80.40	79.55	29.59	53.88	2.33	14.20	100.00	99.99	99.99	55.42	44.57	0.01	0.00
CaFr12	98.40	97.79	97.69	82.35	8.13	7.92	1.60	99.99	99.98	99.97	51.37	29.23	19.39	0.01
CaFr21	98.07	97.34	97.21	52.30	45.72	0.05	1.93	99.98	99.97	99.96	65.73	19.85	14.40	0.02
CaXy11	96.07	94.57	94.31	19.46	71.85	4.75	3.93	99.95	99.94	99.90	65.24	30.02	4.46	0.05
CaXy12	99.67	99.54	99.50	38.54	38.33	22.79	0.33	99.99	99.99	99.99	66.38	33.59	0.02	0.01
CaXy21	95.92	94.37	94.11	48.20	42.59	5.13	4.08	99.93	99.91	99.85	62.58	37.35	0.00	0.07
CaGr11	96.82	95.60	95.40	70.69	19.06	7.06	3.18	99.99	99.99	99.99	61.97	34.91	3.11	0.01
CaGr12	95.58	93.90	93.62	52.86	34.38	8.34	4.42	99.99	99.99	99.98	57.41	36.76	5.83	0.01
CaGr21	93.41	90.91	90.48	64.20	18.84	10.38	6.59	99.99	99.99	99.99	59.94	35.12	4.92	0.01
CaGc11	99.69	99.58	99.47	77.85	21.82	0.02	0.31	100.00	99.99	99.99	83.98	10.77	5.25	0.00
CaGc21	99.72	99.61	99.56	54.68	36.68	8.36	0.28	99.99	99.99	99.99	43.70	47.80	8.49	0.01
CaGl11	89.54	85.55	84.90	51.38	36.22	1.94	10.46	99.99	99.99	99.99	65.82	26.10	8.07	0.01
CaGl21	97.67	96.79	96.62	24.95	65.46	7.26	2.33	100.00	99.99	99.99	84.01	15.97	0.01	0.00

Table 4.6 Regression model equations for uncoded TPC and TFC factors

NADESs	Regression Model Equation	
CaSu11	TPC = 1882- 41.51 UT+ 28.3 ET+ 46.8 SV- 39.30 SC- 0.361 UT*ET - 0.690 UT*SV+ 0.816 UT*SC+ 109.2 Ct Pt	4.1
CaFr11	TPC = 1399- 25.0 UT+ 48.4 ET+134.9 SV- 49.31 SC- 0.810 UT*ET -2.340 UT*SV+ 0.948 UT*SC- 72.5 Ct Pt	4.2
CaFr12	TPC = -508+ 17.81 UT+ 51.82 ET+ 91.89 SV-15.51 SC-1.080 UT*ET -0.951UT*SV+ 0.1603 UT*SC-162.7 Ct Pt.....	4.3
CaFr21	TPC = 1848-39.98 UT- 5.83 ET+ 37.57 SV- 30.90 SC+ 0.1920 UT*ET - 0.4714 UT*SV+ 0.6315 UT*SC+ 5.11 Ct Pt	4.4
CaXy11	TPC = -321+5.86UT-29.05ET+77.63SV- 3.91SC+0.5053UT*ET -1.4816UT*SV+ 0.1395UT*SC-45.73Ct Pt	4.5
CaXy12	TPC = -72.5-0.458UT- 13.02ET+ 60.03SV- 6.80 SC+0.1442UT*ET - 1.0543 UT*SV+ 0.2016 UT*SC- 98.10CtPt	4.6
CaXy21	TPC = 563-12.38UT-18.32ET+44.84 SV-12.13 SC+0.2042UT*ET - 0.8587 UT*SV+0.3235 UT*SC- 42.48CtPt	4.7
CaGr11	TPC = 130- 6.38UT- 3.29ET+ 31.99SV- 7.17SC- 0.0776 UT*ET - 0.5498 UT*SV+ 0.2541 UT*SC - 51.23 Ct Pt	4.8
CaGr12	TPC = -179+ 1.56UT- 9.06ET+ 54.17SV- 6.85SC+ 0.0376UT*ET - 1.0408 UT*SV+ 0.2390 UT*SC- 63.1Ct Pt	4.9
CaGr21	TPC = 596- 18.07UT- 6.11ET+ 27.57SV- 13.74 SC+ 0.034 UT*ET - 0.427 UT*SV+ 0.4003 UT*SC- 75.4 Ct Pt	4.10
CaGc11	TPC = -48.8+3.346UT-12.606 ET+21.005SV-1.368SC+0.2394UT*ET - 0.3374UT*SV+ 0.02042UT*SC+1.39 Ct Pt.....	4.11
CaGc21	TPC = -499.9+10.821UT-9.306ET+39.257SV+2.373SC+0.2717UT*ET - 0.7986UT*SV+ 0.00592UT*SC-45.04Ct Pt.....	4.12
CaGl11	TPC = 536- 14.97UT-1.58ET+42.88SV-15.49 SC- 0.094UT*ET - 0.804 UT*SV+ 0.4287 UT*SC- 30.5 Ct Pt	4.13
CaGl21	TPC = -450+6.89UT-30.77ET+72.68SV-1.09SC+0.5400UT*ET -1.3832UT*SV+0.0960UT*SC-55.76 Ct Pt.....	4.14

Table 4.6 contd.

CaSu11	TFC	=	-180.9-16.751UT-53.138ET+81.615SV- 4.72SC +0.74023UT*ET-1.23633UT*SV+0.46777UT*SC- 60.84Ct Pt	**4.15**
CaFr11	TFC	=	-4804.9+ 84.753UT - 60.13ET+ 243.424SV+ 43.659SC +0.64583UT*ET- 4.48177UT*SV- 0.55469UT*SC+7.68Ct Pt	**4.16**
CaFr12	TFC	=	-1923.3+31.465UT-19.961ET+104.74SV+12.233SC +0.09505UT*ET-1.96875UT*SV-0.4167UT*SC+179.62Ct Pt.....	**4.17**
CaFr21	TFC	=	-1943.9+31.738UT-36.576ET+69.245SV+22.52SC +0.46549UT*ET-1.20768UT*SV-0.25944UT*SC+132.78Ct Pt....	**4.18**
CaXy11	TFC	=	-1043.1+17.012UT+11.445ET+68.411SV-2.819SC -0.4714UT*ET- 1.4245UT*SV+0.22852UT*SC- 69.34Ct Pt	**4.19**
CaXy12	TFC	=	-3507.9+57.91UT-74.049ET+169.219SV+35.788SC +0.86328UT*ET-3.14453UT*SV-0.38802UT*SC-10.03 Ct Pt.....	**4.20**
CaXy21	TFC	=	-1256.6+21.699UT+3.32ET+69.896SV+3.223SC -0.2826UT*ET-1.3789UT*SV+0.07682UT*SC+0.26Ct Pt	**4.21**
CaGr11	TFC	=	-1521.6+28.398UT+23.385ET+105.716SV-8.437SC -0.86914UT*ET-2.23763UT*SV+0.37467UT*SC-83.887Ct Pt	**4.22**
CaGr12	TFC	=	-1673.6+31.374UT+11.888ET+110.339SV-3.431SC- 0.6263UT*ET-2.30339UT*SV+0.26562UT*SC-108.854 Ct Pt	**4.23**
CaGr21	TFC	=	-591.4+10.013UT+39.974ET+72.721SV-18.477SC- 1.09375UT*ET-1.59635UT*SV+0.54818UT*SC-93.099 Ct Pt	**4.24**
CaGc11	TFC	=	-3938.9+69.746UT-40.56ET+142.396SV+45.163SC +0.72852UT*ET-1.57096UT*SV-0.78418UT*SC+ 182.32Ct Pt ...	**4.25**
CaGc21	TFC	=	-5575.8+100.143UT- 43.073ET+128.633SV+76.042SC +0.96029UT*ET-2.5332UT*SV-1.26009UT*SC+174.38 Ct Pt	**4.26**
CaGl11	TFC	=	-4455.2+101.042UT+ 44.766ET+56.133SV+37.096SC- 1.37956UT*ET-0.97331UT*SV- 0.75684UT*SC-140.983 Ct Pt ...	**4.27**
CaGl21	TFC	=	-1308.7+25.527UT-72.695ET+36.016SV+16.725SC +1.61263UT*ET-0.68034UT*SV-0.27311UT*SC-7.129Ct Pt.....	**4.28**

Table 4.7 Contribution of model components to the antiradical scavenging activities based on CUPRAC and FRAP methods

NADESs	CUPRAC							FRAP						
	R^2	R^2(Adj)	R^2(Pred)	Linear	Interaction	Curvature	Error	R^2	R^2(Adj)	R^2(Pred)	Linear	Interaction	Curvature	Error
CaSu11	0.865	0.801	0.7920	0.4965	0.3036	0.0560	0.144	1.000	1.000	0.9999	0.5765	0.3871	0.0363	0.0000
CaFr11	0.971	0.960	0.9585	0.5787	0.2955	0.0970	0.029	1.000	1.000	0.9999	0.4726	0.4797	0.0477	0.0000
CaFr12	0.918	0.887	0.8820	0.8042	0.0632	0.0505	0.082	1.000	1.000	1.0000	0.5383	0.4583	0.0034	0.0000
CaFr21	0.927	0.899	0.8950	0.4098	0.4172	0.0999	0.073	1.000	1.000	0.9999	0.5895	0.4050	0.0055	0.0000
CaXy11	0.983	0.976	0.9740	0.5616	0.2894	0.1315	0.174	1.000	1.000	1.0000	0.5931	0.4068	0.0001	0.0000
CaXy12	0.996	0.994	0.9937	0.4317	0.4569	0.1071	0.004	1.000	1.000	1.0000	0.5862	0.3787	0.0050	0.0000
CaXy21	0.964	0.951	0.9483	0.3773	0.4420	0.1450	0.036	1.000	1.000	0.9999	0.5980	0.3841	0.0179	0.0000
CaGr11	0.923	0.894	0.8883	0.3507	0.5537	0.0187	0.077	1.000	0.9999	0.9999	0.5115	0.4791	0.0094	0.0000
CaGr12	0.967	0.955	0.9520	0.3051	0.5158	0.1461	0.033	1.000	1.000	0.9999	0.6018	0.3460	0.0523	0.0000
CaGr21	0.977	0.969	0.9670	0.5940	0.3092	0.0741	0.023	1.000	1.000	0.9999	0.5785	0.3993	0.0222	0.0000
CaGc11	0.736	0.635	0.6188	0.3741	0.3575	0.0040	0.264	1.000	1.000	1.000	0.6548	0.2613	0.0839	0.0000
CaGc21	0.994	0.992	0.9905	0.6835	0.2692	0.0416	0.006	1.000	1.000	0.9999	0.6713	0.2346	0.0940	0.0000
CaGl11	0.996	0.995	0.9940	0.6057	0.2879	0.1027	0.004	0.9999	0.9999	0.9998	0.5685	0.3666	0.0648	0.0001
CaGl21	0.998	0.997	0.9960	0.4043	0.4519	0.1418	0.002	0.9999	0.9999	0.9998	0.5698	0.3517	0.0784	0.0001

Table 4.8 Regression model equations for antiradical scavenging activity

NADESs			Regression Model Equation	
CaSu11	CUPRAC	=	-0.21+0.0535UT-0.233ET+0.729SV- 0.0478SC+0.00202UT*ET - 0.01272UT*SV+0.001353UT*SC-0.632Ct Pt.....	**4.29**
CaFr11	CUPRAC	=	-27.38+0.5416UT-0.033ET+1.936SV+ 0.1508SC-0.00531UT*ET -0.03450UT*SV- 0.00108 UT*SC-2.240Ct Pt.....	**4.30**
CaFr12	CUPRAC	=	-7.10+0.082UT-0.384ET+0.734SV+0.0921SC+0.00527UT*ET -0.00850UT*SV- 0.00049UT*SC-1.004 Ct Pt.....	**4.31**
CaFr21	CUPRAC	=	-12.56+0.208UT-0.388ET+1.722SV-0.04SC+0.00422UT*ET -0.03111UT*SV+0.00282UT*SC-1.745 Ct Pt.....	**4.32**
CaXy11	CUPRAC	=	-12.76+0.1669UT-0.5229ET+1.3865SV+0.0591SC +0.00735UT*ET-0.02354UT*SV+0.00107UT*SC-1.865Ct Pt.....	**4.33**
CaXy12	CUPRAC	=	-31.02+0.6016UT-0.1244ET+1.4895SV+0.189SC -0.001292UT*ET-0.027818UT*SV-0.002099UT*SC-1.5241Ct Pt.	**4.34**
CaXy21	CUPRAC	=	-21.12+0.3727UT-0.725ET+1.647SV+0.1623SC +0.01157UT*ET-0.02941UT*SV-0.001423UT*SC-2.032Ct Pt....	**4.35**
CaGr11	CUPRAC	=	-38.28+0.76UT-0.646ET+1.811SV+0.3585SC+0.00874UT*ET -0.03418UT*SV-0.00538UT*SC-0.758Ct Pt.....	**4.36**
CaGr12	CUPRAC	=	-24.35+0.4449UT-0.659ET+1.815SV+0.1268SC +0.01062UT*ET-0.03492UT*SV-0.00038UT*SC-2.172Ct Pt.....	**4.37**
CaGr21	CUPRAC	=	-13.09+0.1573UT-0.3186ET+1.6522SV-0.068SC +0.00147UT*ET-0.03079UT*SV+0.004774UT*SC-1.765Ct Pt...	**4.38**
CaGc11	CUPRAC	=	-9.11+0.198UT-0.26ET+0.939SV+0.0204SC+0.00388UT*ET -0.01611UT*SV+0.00018UT*SC-0.196Ct Pt.....	**4.39**
CaGc21	CUPRAC	=	-5.80+0.0541UT-0.7485ET+0.8056SV+0.0965SC +0.013303UT*ET-0.011850UT*SV-0.000474UT*SC-0.7843CtPt.	**4.40**
CaGl11	CUPRAC	=	1.71-0.1712UT-0.5757ET+1.0607SV-0.1385SC +0.011244UT*ET-0.018593UT*SV+0.0054UT*SC-1.62CtPt.....	**4.41**
CaGl21	CUPRAC	=	1.853-0.1189UT-0.493ET+1.3559SV-0.1706SC +0.008055UT*ET-0.024770UT*SV+0.005602UT*SC-.7755Ct Pt.	**4.42**

Table 4.8 contd.

CaSu11	FRAP	=	55.022-1.22404UT+0.655ET+0.904SV-1.05763SC -0.006378UT*ET-0.010096UT*SV+0.020696UT*SC-.47596CtPt….	**4.43**
CaFr11	FRAP	=	88.728-1.99256UT-0.93974ET+1.06156SV-1.18013SC +0.022994UT*ET-0.011545UT*SV+0.025298UT*SC+2.0003CtPt……	**4.44**
CaFr12	FRAP	=	95.032-2.0782UT-0.28493ET+0.5888SV-1.32451SC +0.013998UT*ET-0.003434UT*SV+0.026653UT*SC+0.52811CtPt……	**4.45**
CaFr21	FRAP	=	90.904-2.05865UT-0.21167ET+0.71374SV-1.32301SC +0.012622UT*ET-0.003827UT*SV+0.027208UT*SC-0.7279Ct Pt……	**4.46**
CaXy11	FRAP	=	91.808-1.97115UT+0.89974ET+1.10926SV-1.65218SC -0.007154UT*ET-0.011526UT*SV+0.031551UT*SC-0.1038Ct Pt…….	**4.47**
CaXy12	FRAP	=	72.86-1.58929UT+0.19244ET+0.67964SV-1.1666SC +0.004282UT*ET-0.005603UT*SV+0.022776UT*SC-1.56731Ct Pt……	**4.48**
CaXy21	FRAP	=	64.701-1.47468UT+0.23141ET+0.66272SV-1.05917SC +0.003654UT*ET-0.006179UT*SV+0.02159UT*SC-1.05513 Ct Pt……	**4.49**
CaGr11	FRAP	=	79.854-1.78526UT+0.26769ET+0.56079SV-1.27385SC +0.001622UT*ET-0.003109UT*SV+0.025907UT*SC-0.8119 Ct Pt……	**4.50**
CaGr12	FRAP	=	48.964-1.15487UT-0.32282ET+1.42079SV-0.84833SC +0.012327UT*ET-0.019327UT*SV+0.017388UT*SC-1.8099 Ct Pt……	**4.51**
CaGr21	FRAP	=	57.344-1.34UT+0.83872ET+1.12438SV-1.18397SC-0.009404UT*ET -0.012929UT*SV+0.023779UT*SC-1.3221Ct Pt ……	**4.52**
CaGc11	FRAP	=	38.135-0.86019UT+0.76192ET+0.68528SV-0.79955SC - 0.009026UT*ET-0.005897UT*SV+0.015135UT*SC-2.03526 Ct Pt….	**4.53**
CaGc21	FRAP	=	26.7718-0.67064UT-0.1541ET+0.04849SV-0.36885SC +0.005718UT*ET+0.003769UT*SV+0.008269UT*SC-1.26667Ct Pt….	**4.54**
CaGl11	FRAP	=	36.097-0.85282UT+0.21205ET+0.70413SV-0.69551SC +0.000532UT*ET-0.008545UT*SV+0.014285UT*SC-1.4016 Ct Pt……	**4.55**
CaGl21	FRAP	=	42.676-0.96006UT+0.26551ET+0.64451SV-0.76494SC -0.000122UT*ET-0.006955UT*SV+0.015119UT*SC-1.6381Ct Pt……	**4.56**

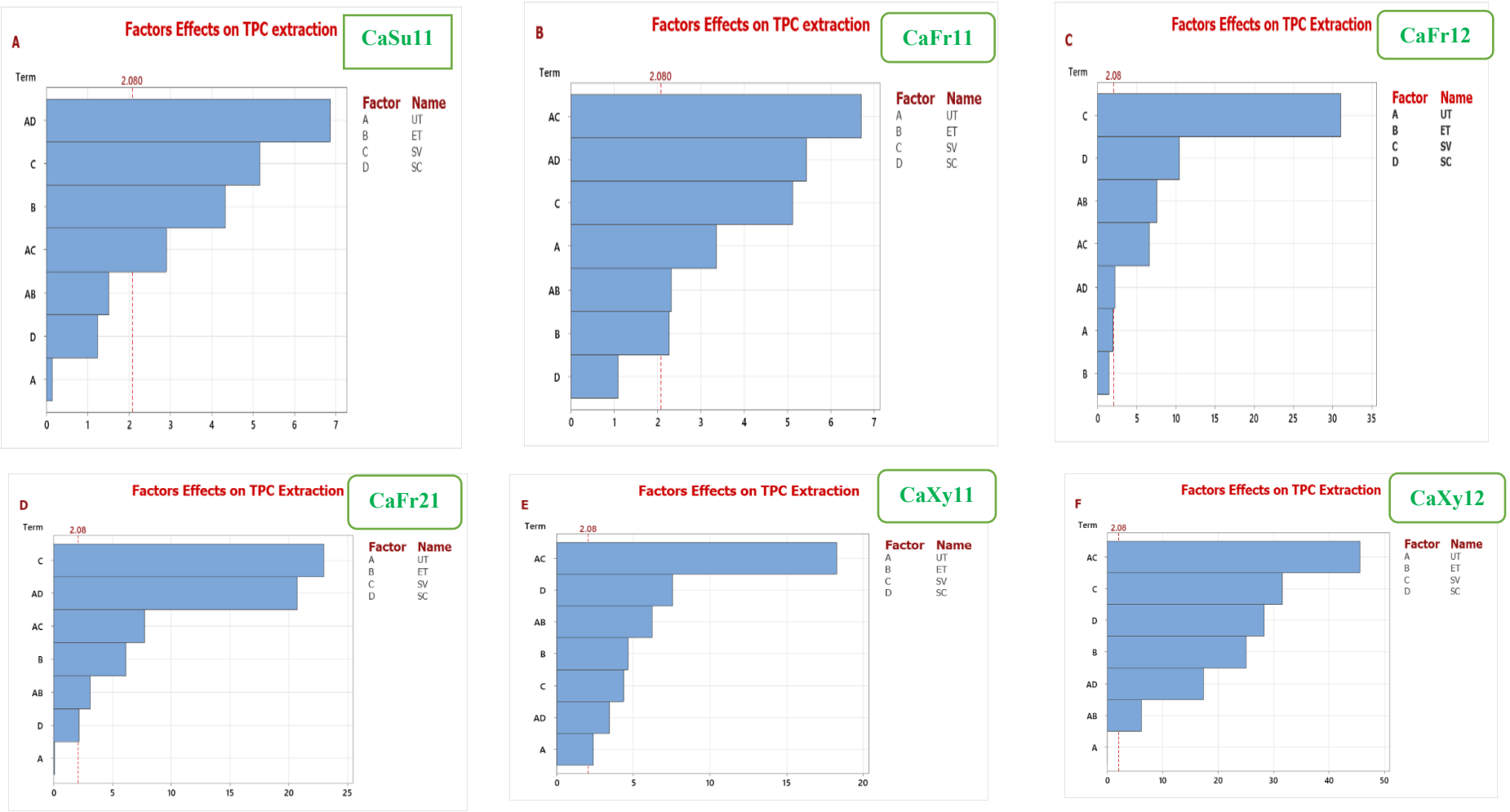


Figure 4.8 Effects of experimental factors on TPC extraction from African nutmeg peels using NADESs

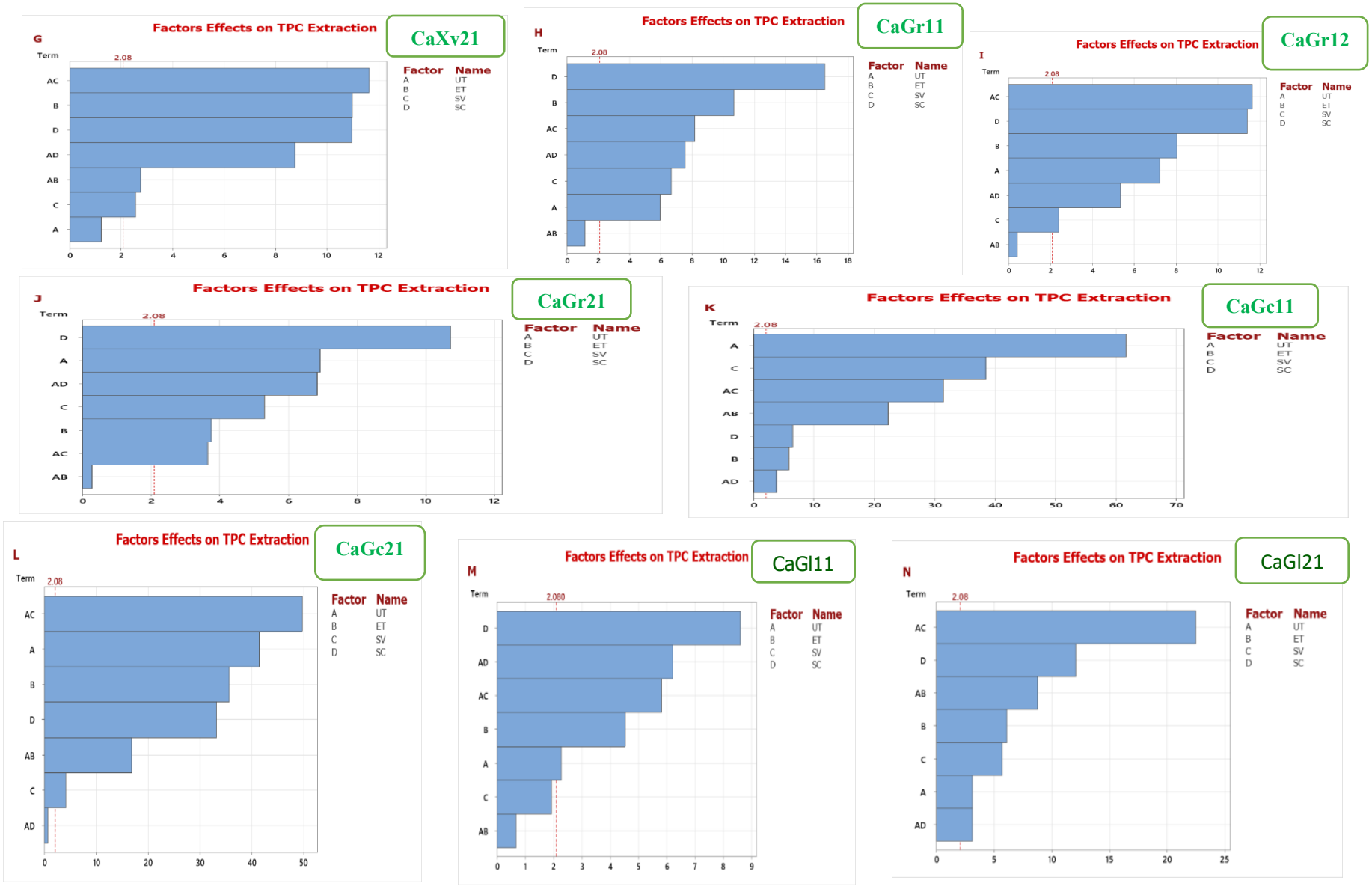


Figure 4.8 contd.

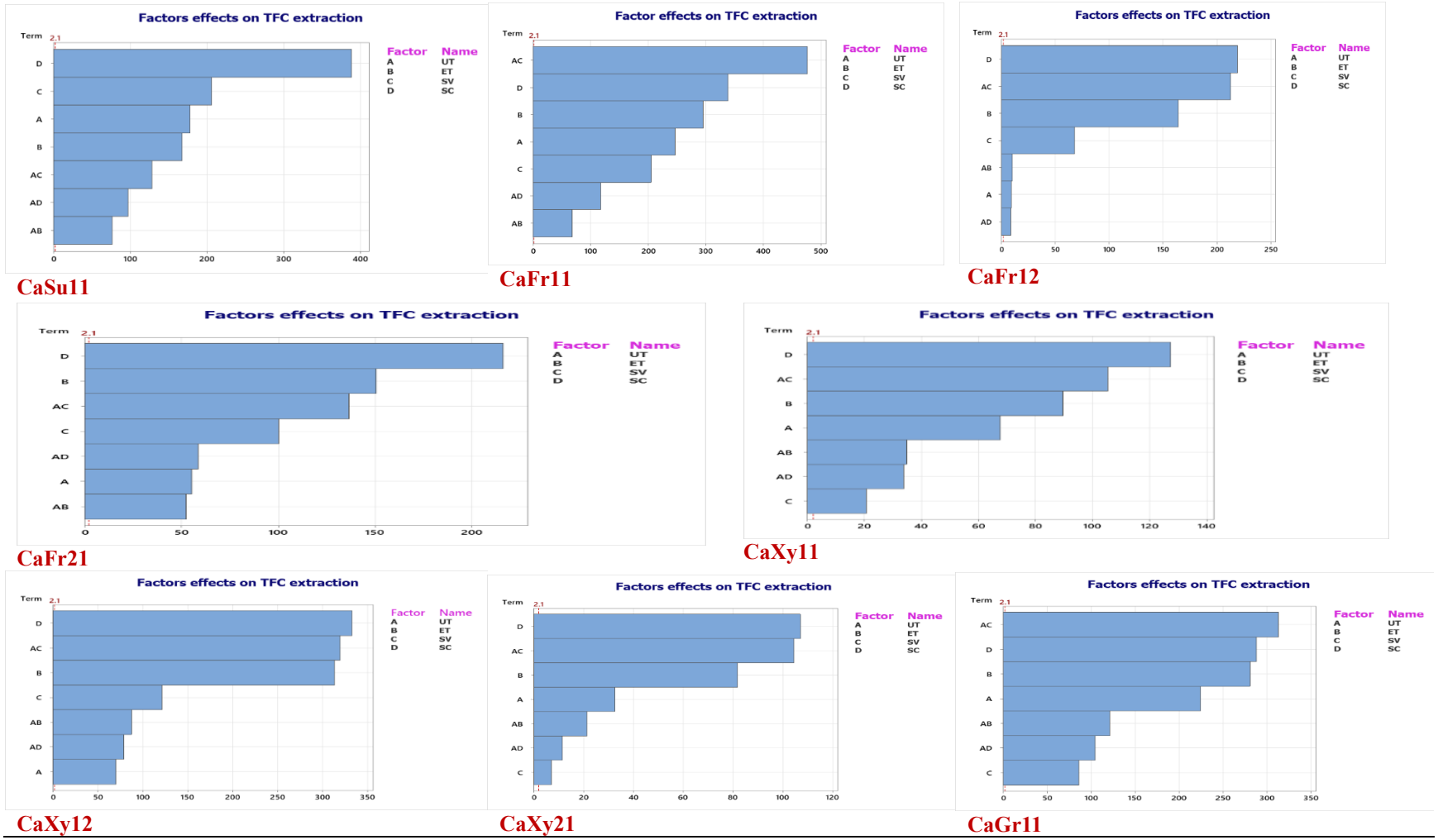
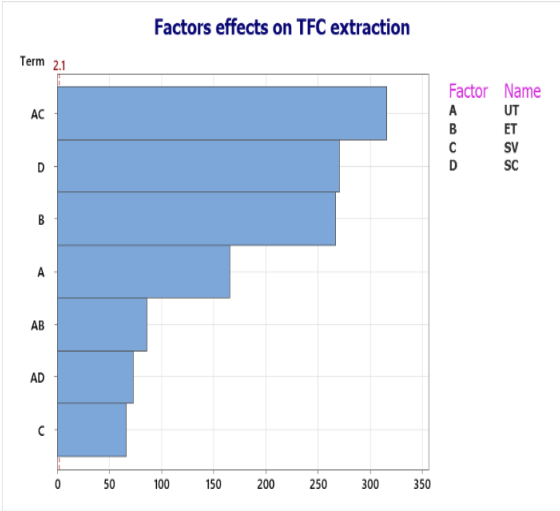
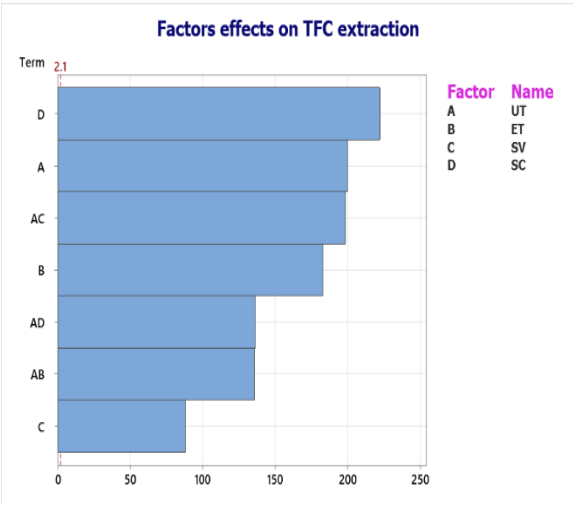


Figure 4.9 Effects of experimental factors on TFC extraction from African nutmeg peels using NADESs.



CaGr12



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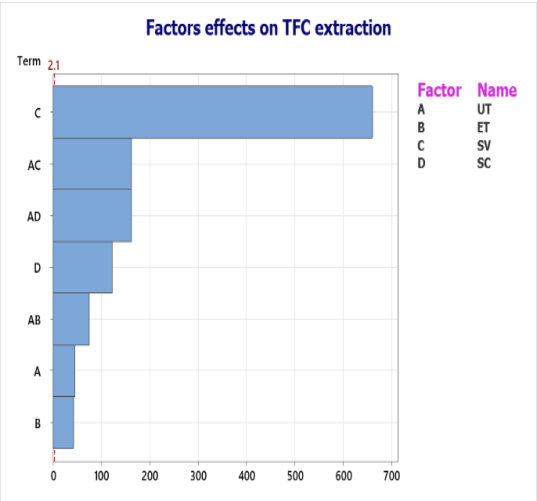

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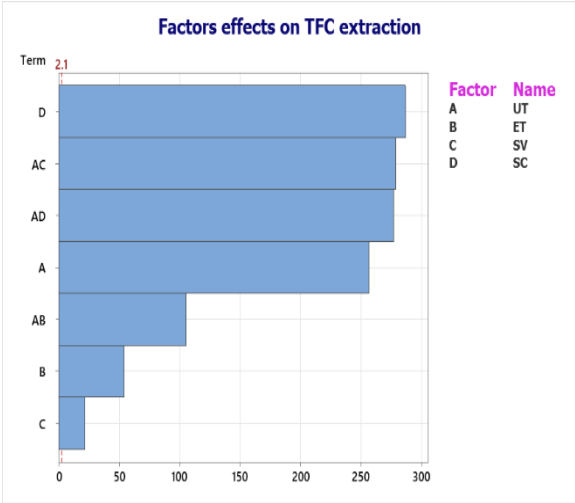

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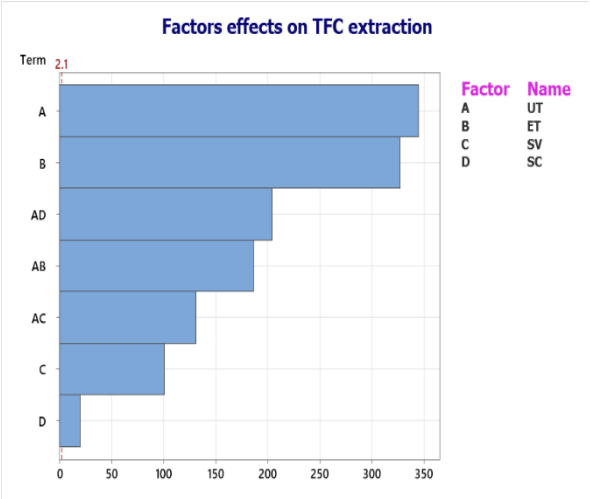

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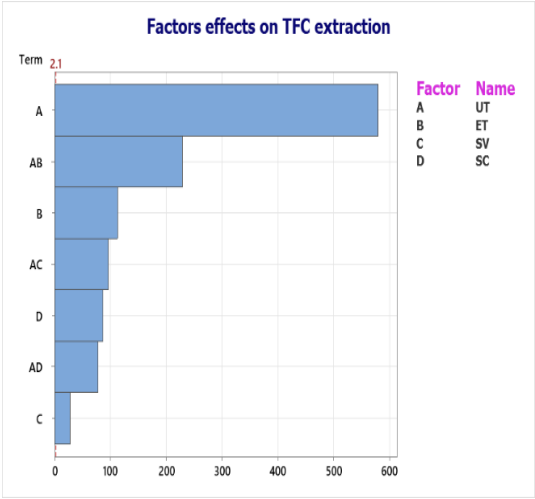

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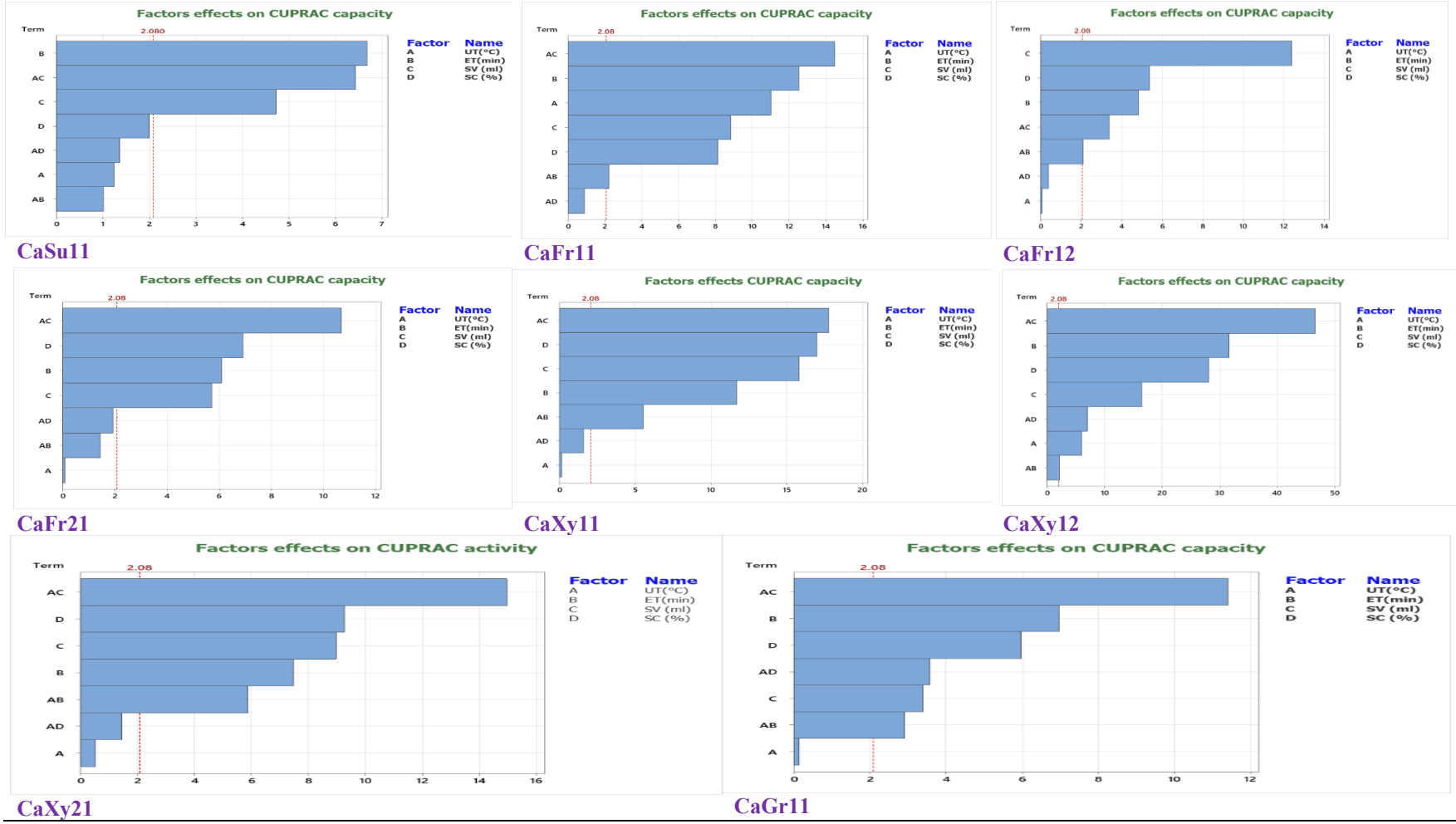
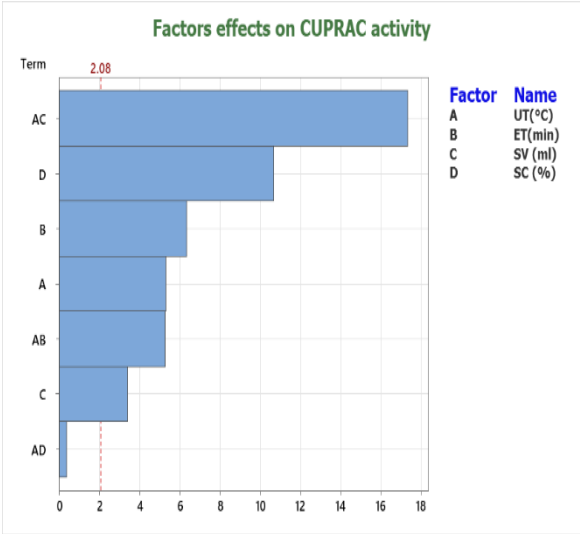
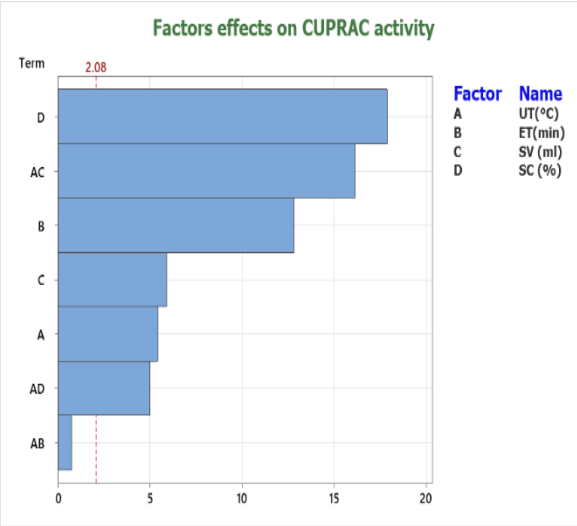


Figure 4.10 Effects of experimental factors on CUPRAC capacity of African nutmeg peels using NADESs



CaGr12



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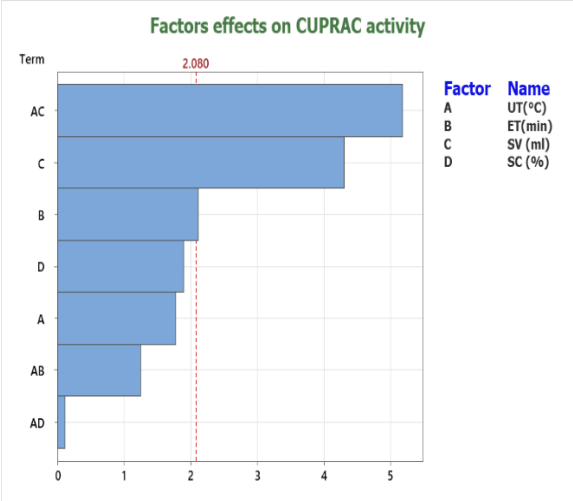

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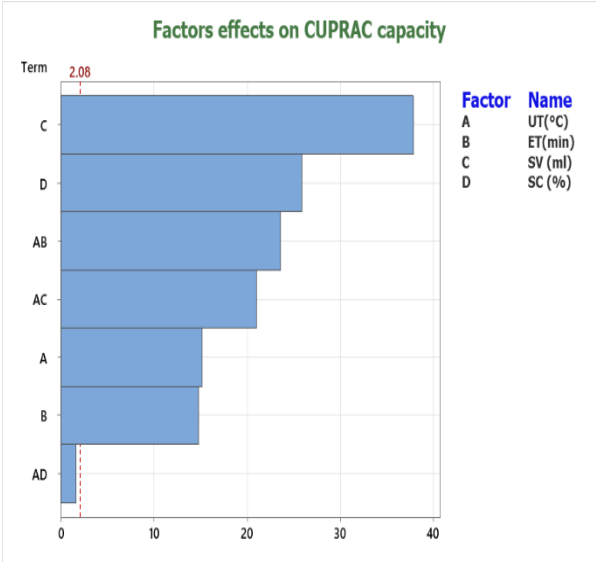

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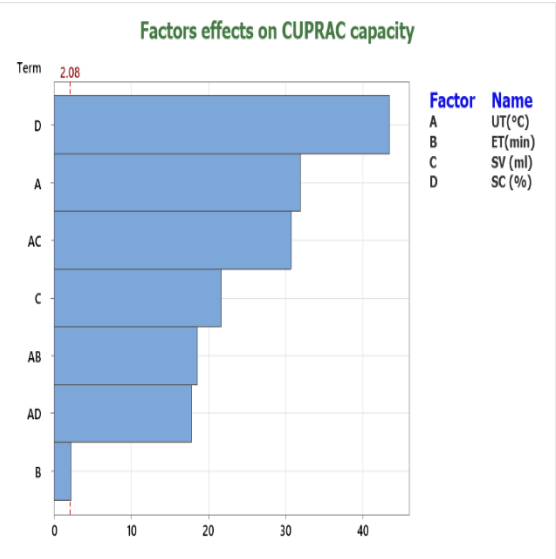

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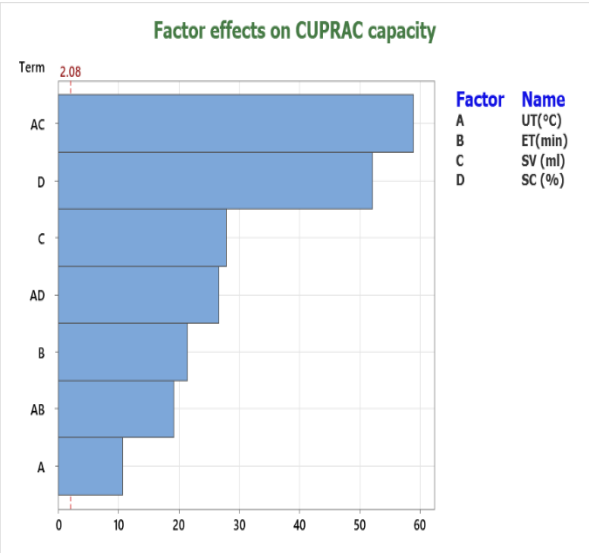

CaGl21

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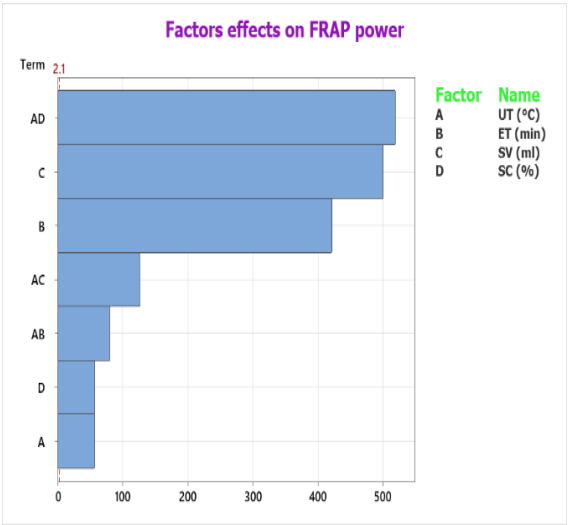
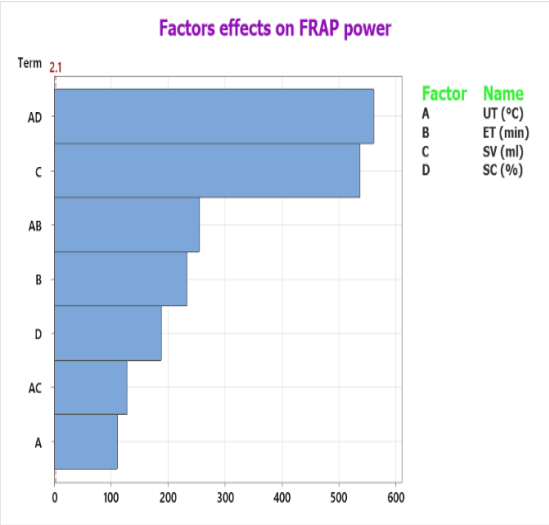
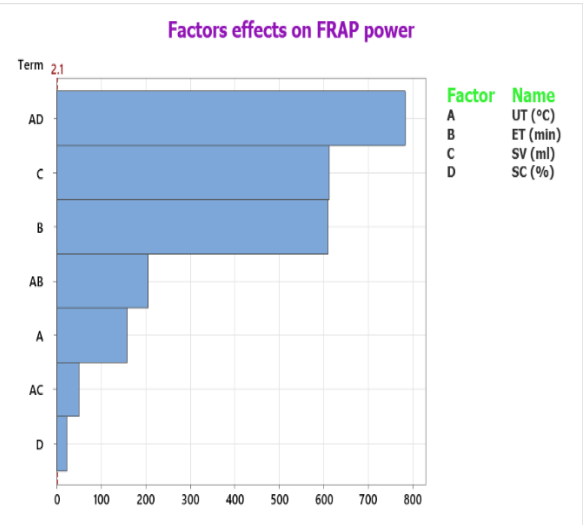


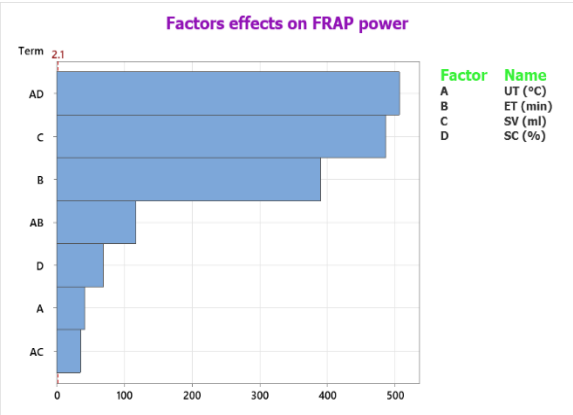
CaSu11



CaFr11



CaFr12



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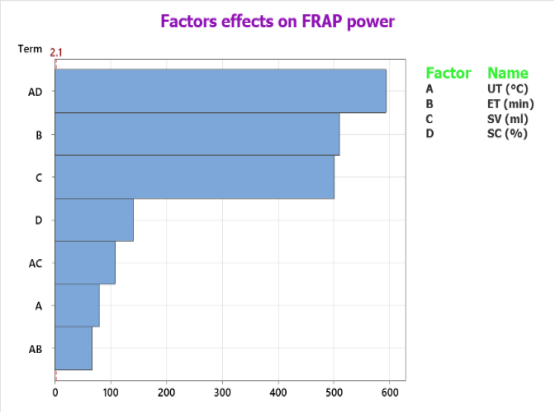
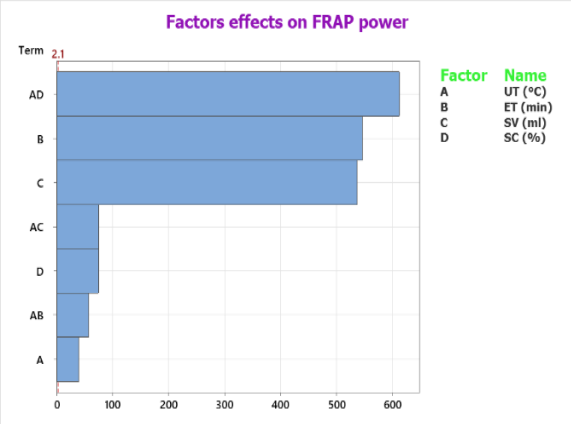
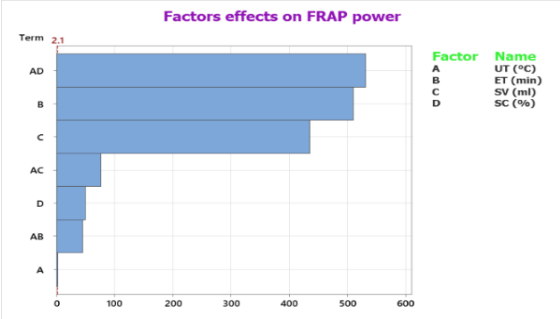


CaXy11

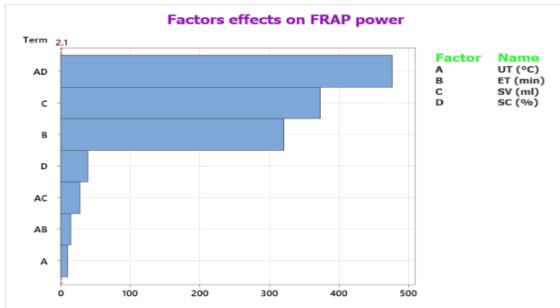


CaXy12

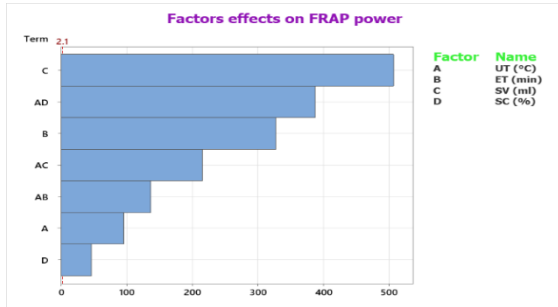
Figure 4.11 Effects of experimental factors on FRAP power of African nutmeg peels using NADESs



CaXy21



CaGr11



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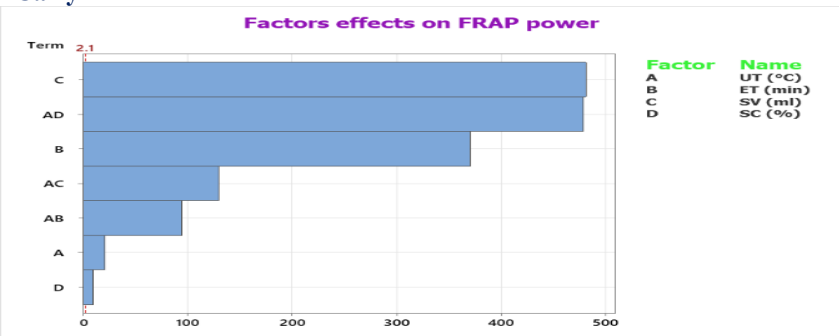

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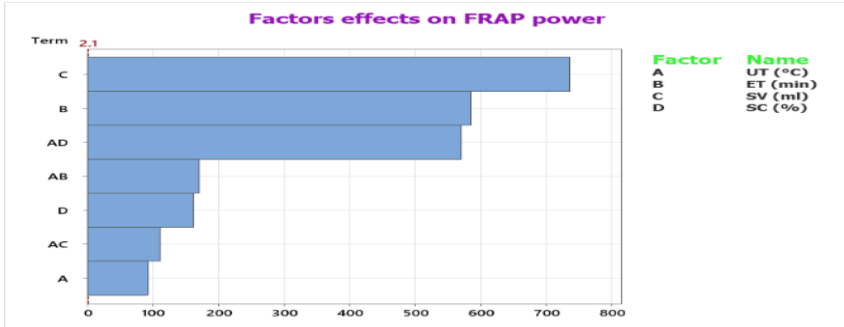
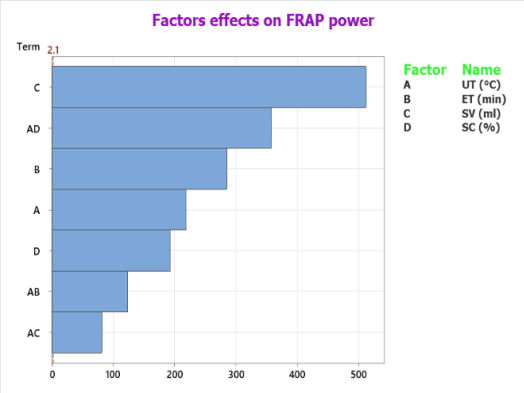
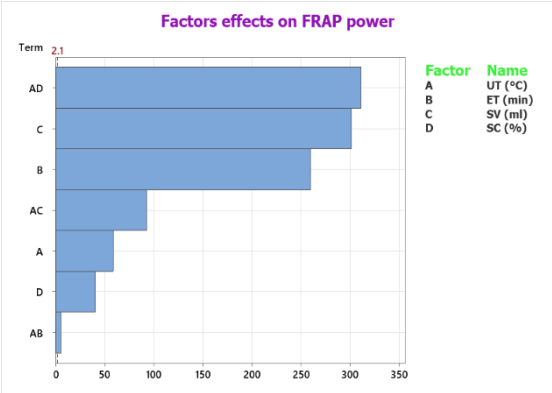


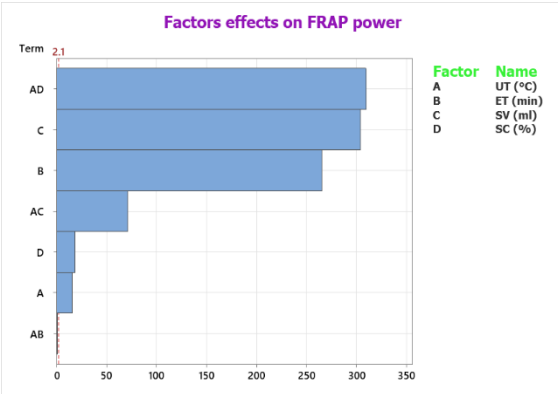
CaGc11



CaGc21



CaGl11



CaGl21

Figure 4.11 contd.

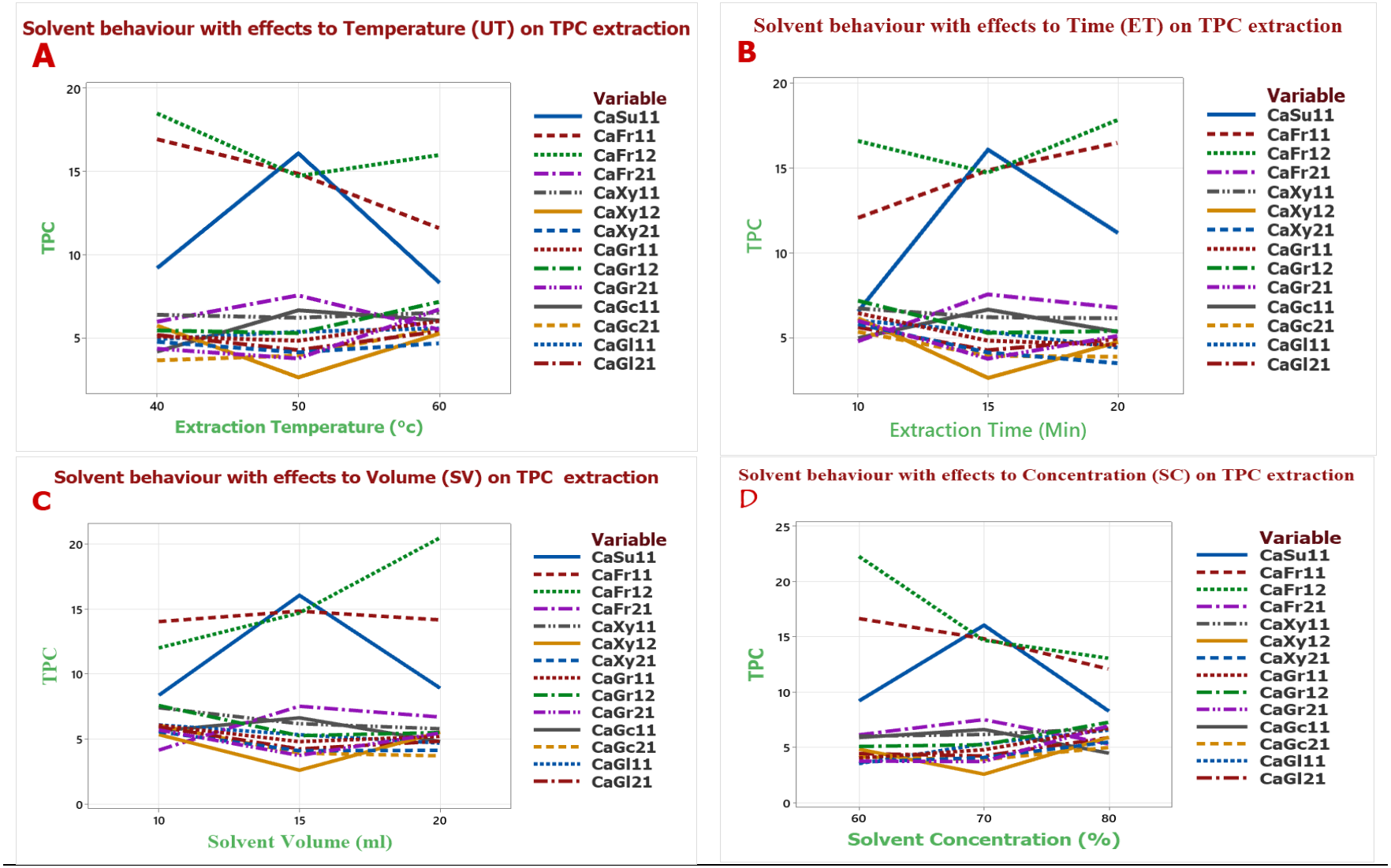


Figure 4.12 Solvents behaviour at different extraction conditions for TPC

4.6.2 Extraction of antioxidant and antiradical scavenging potential of African nutmeg peels

4.6.2.1 Total phenolic content (TPC) and total flavonoid content (TFC)

The TPC and TFC values extracted from African Nutmeg peels using the NADESs are presented in **Table 4.9**. The results show that the minimum TPC (123.0 mgGAE/g) was obtained from the CaGc21, while the maximum (458.0 mgGAE/g) was obtained from the CaFr12 extracts. On the other hand, the minimum TFC (172.1 µg QE/g) was extracted from CaXy12, while the maximum (897.3 µgQE/g) was obtained from CaGc11. The results are presented as the means from 30 experimental runs and were ranked using the Tukey group of significance. CaFr12 produced the highest TPC, followed by CaFr11, while CaGc21 produced the smallest TPC. In terms of TFC, CaGc11 produced the highest TFC, followed by CaGc21, while CaXy12 produced the smallest TFC.

Table 4.9 Antioxidant and antiradical scavenging power of African nutmeg peels extracted with NADESs

NADESs	**Runs**	**TPC (mgGAE/g)**	**TFC (µgQE/g)**	**FRAP (µMTE/g)**	**CUPRAC (µMTE/g)**
CaSu11	30	270.6^{B}	331.3^{BCD}	2.954^{BC}	3.147^{A}
CaFr11	30	389.2^{A}	421.4^{BC}	5.848^{A}	4.718^{A}
CaFr12	30	458.0^{A}	262.7^{CD}	4.278^{ABC}	4.341^{A}
CaFr21	30	163.7^{C}	271.3^{CD}	4.571^{AB}	4.359^{A}
CaXy11	30	174.3^{BC}	172.1^{D}	4.132^{ABC}	3.910^{A}
CaXy12	30	136.7^{C}	249.2^{CD}	3.225^{ABC}	3.274^{A}
CaXy21	30	125.3^{C}	175.0^{D}	3.696^{ABC}	3.934^{A}
CaGr11	30	147.8^{C}	208.7^{D}	3.246^{ABC}	4.241^{A}
CaGr12	30	167.6^{C}	199.0^{D}	3.552^{ABC}	4.101^{A}
CaGr21	30	143.4^{C}	188.7^{D}	3.123^{ABC}	4.393^{A}
CaGc11	30	146.93^{C}	897.3^{A}	2.236^{BC}	3.852^{A}
CaGc21	30	123.0^{C}	482.6^{B}	1.641^{C}	3.790^{A}
CaGl11	30	143.3^{C}	265.3^{CD}	2.222^{BC}	3.798^{A}
CaGl21	30	139.0^{C}	330.1^{BCD}	2.057^{BC}	3.626^{A}

(Means that do not share a letter are significantly different.)

*The effects of the factor combinations (UT, ET, SV, and SC) on the extraction of TPC and TFC are presented in **Figure 4.13** and **Figure 4.14,** respectively,* 4.6.2.1 Factor effects on the extraction of Total Phenolic Contents (TPC) and Total Flavanol content (TFC) from African nutmeg peels using NADESs

which indicates that different experimental conditions had different effects on the TPC and TFC extracted from African Nutmeg peels using different NADESs. The highest TPC extracts, as shown in **Table 4.9**, was produced from CaFr12 (TPC = 908.17 mgGAE/g) under the experimental conditions shown in **Figure 4. 13D** (UT = 40°C, ET = 20 min, SV = 20 ml, SC = 60%). However, the experimental conditions that produced comparable TPC extracts across the synthesized NADESs is given in **Figure 4. 13B** (UT = 40°C, ET =10 min, SV = 20 ml, SC = 80%). Furthermore **Figure 4.13F (**UT = 60°C, ET= 10 min, SV = 10 ml, SC = 80%) and **Figure 4.13I** (UT=60°C, ET = 20 min, SV = 20 ml, SC = 80%) should also be considered for good TPC extraction from African Nutmeg peels. On the other hand, the conditions that produced the least amount of TPC extracts is given in **Figure 4.13C** (UT = 40°C, ET =20 min, SV = 10 ml, SC = 80%), **Figure 4.13A** (UT = 40°C, ET =10 min, SV = 10 ml, SC = 60%), and **Figure 4.13H (**UT = 60°C, ET= 20 min, SV = 10 ml, SC = 60%). The best conditions for extracting TFC from African Nutmeg peels using the synthesized NADESs is shown in **Figure 4.14F** (UT = 60°C, ET = 10 min, SV = 10 ml, SC = 80%), in which all the NADES samples extracted more than 300 µgGAE/g of TFCs from the peels. However, in terms of the highest yield of flavonoids from a given NADES, **Figure 4.14B** (UT = 40°C, ET = 10 min, SV = 20 ml, SC = 80%) shows the highest TFC extract of 1431.51 µgGAE/g from CaGc11 and the lowest of 224.74 µgGAE/g from CaGr21. Other important experimental conditions that generated at least 500 µgGAE/g of TFC from African Nutmeg peels in one or more individual NADESs are as follows: **Figure 4.14C** (UT = 40°C, ET = 20 min, SV = 10 ml, SC = 80%) with a maximum TFC of 660.807 µgGAE/g from CaGc21; **Figure 4.14D** (UT = 40°C, ET = 20 min, SV = 20 ml, SC = 60%) with a maximum of 1041.41 µgGAE/g from CaGc11; **Figure 4.14E** (UT = 50°C, ET = 15 min, SV = 15 ml, SC = 70%) with 1043.55 µgGAE/g from CaGc11; **Figure 4.14G** (UT = 60°C, ET =10 min, SV = 20 ml, SC = 60%) gave 1126.82 µgGAE/g from CaGc11; **Figure 4.14H** (UT = 60°C, ET = 20 min, SV = 10 ml, SC = 60%) produced 676.953 µgGAE/g and 676.432 µgGAE/g from CaGc11 and CaGl21, Finally, as shown in **Figure 4.14I** (UT = 60°C, ET = 20 min, SV = 20 ml, SC = 80%), 1120.57 µgGAE/g of TFC extract was generated from CaGc11.

4.6.2.2 Effects of Factor Interaction on the TPC and TFC Extraction from African Nutmeg Peels

The effects of two factors (UT*ET; UT*SV; UT*SC; ET*SV; ET*SC; and SV*SC) interaction on the extraction of TPC and TFC from African Nutmeg peels was examined for each of the synthesized NADESs, and the results presented in **Figure 4.15 – Figure 4.28** for TPC, and **Figure 4.29- Figure 4.43** for TFC, respectively. From the figures, it was clearly shown that the conditions necessary to maximize the extraction of TPC and TFC from the sample using the NADESs were different.

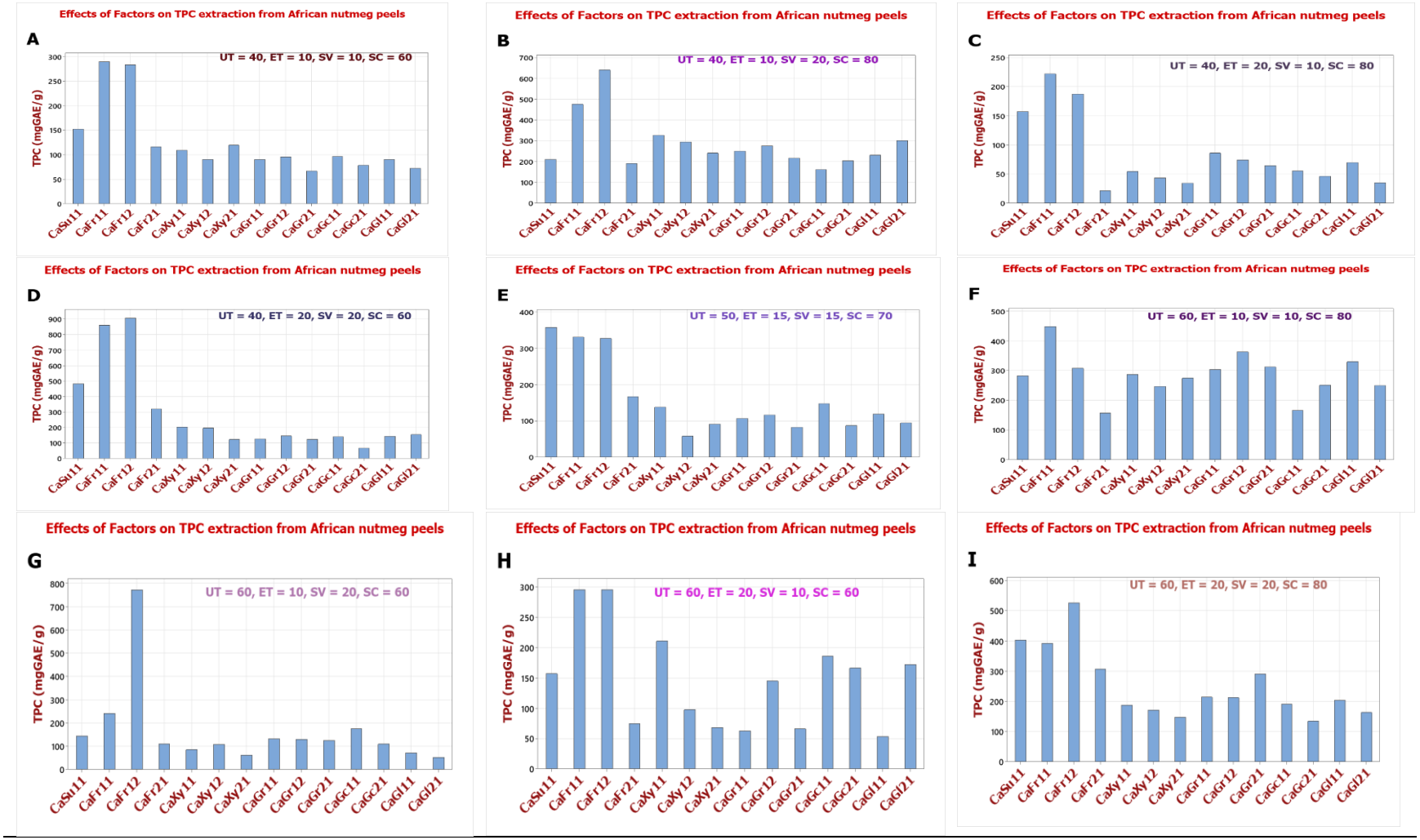


Figure 4.13 Effects of experimental conditions on TPC extraction from African nutmeg peels using NADESs

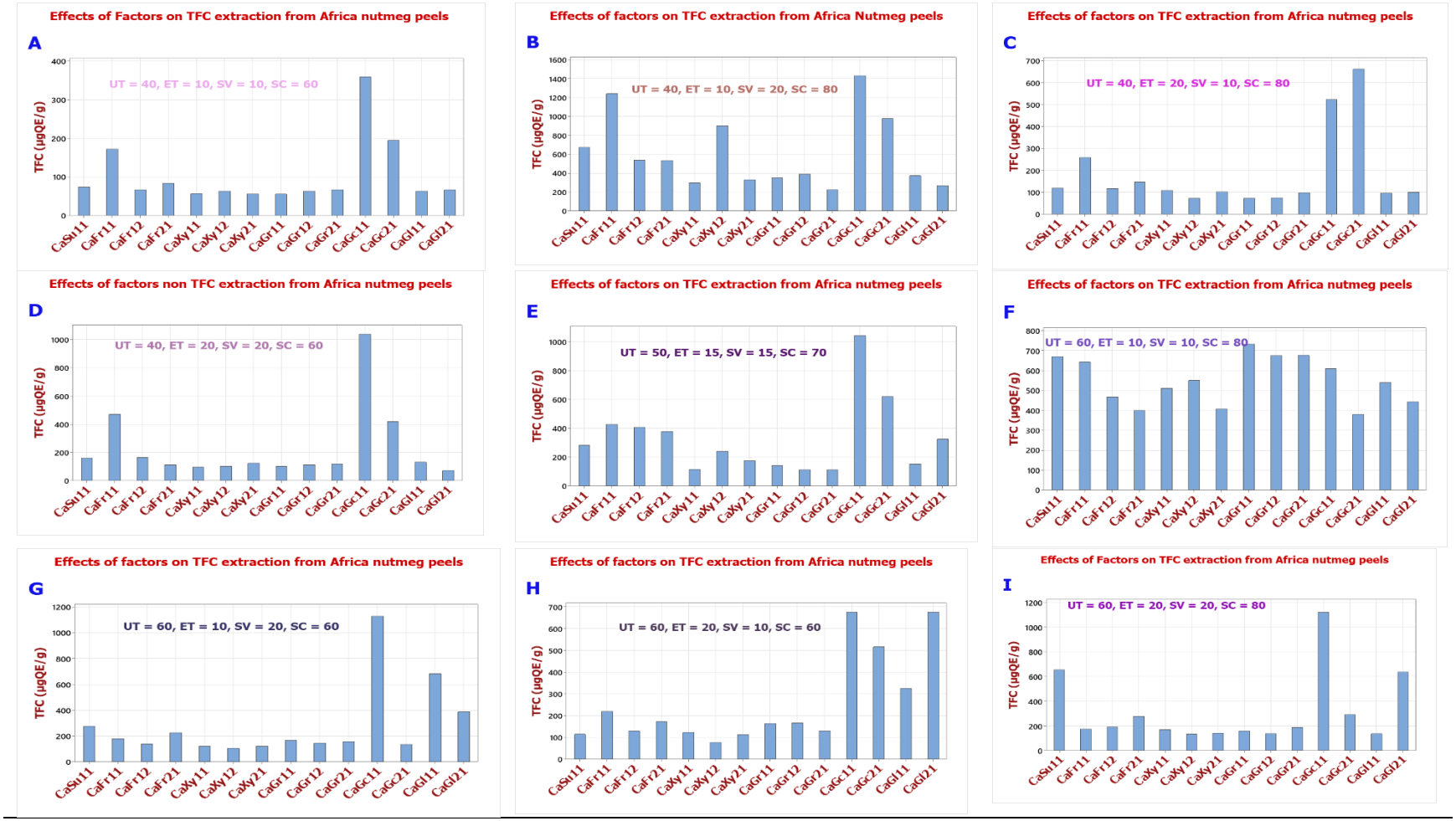


Figure 4.14 Effects of experimental conditions on TFC extraction from African nutmeg peels using NADESs

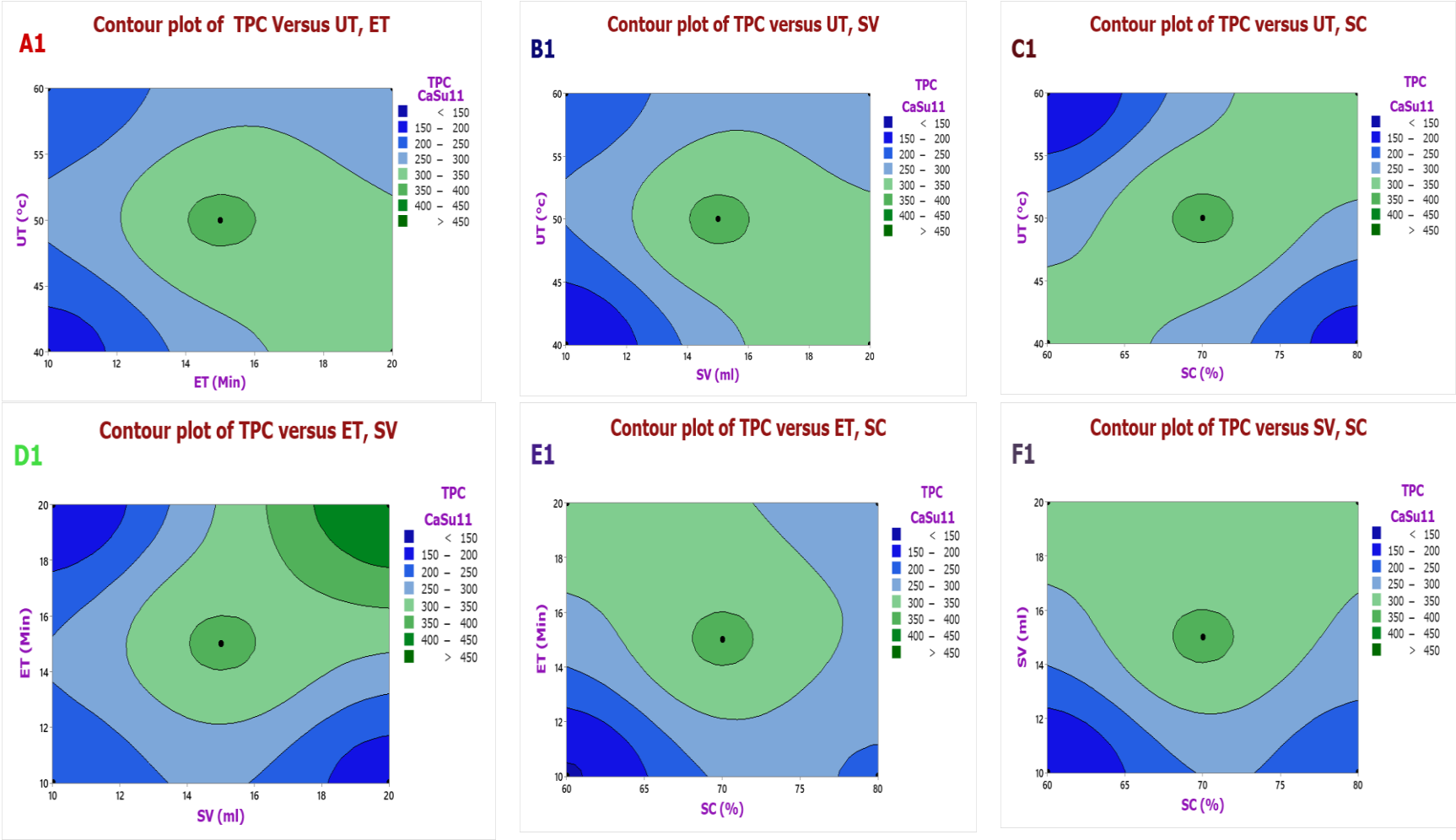


Figure 4.15 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaSu11

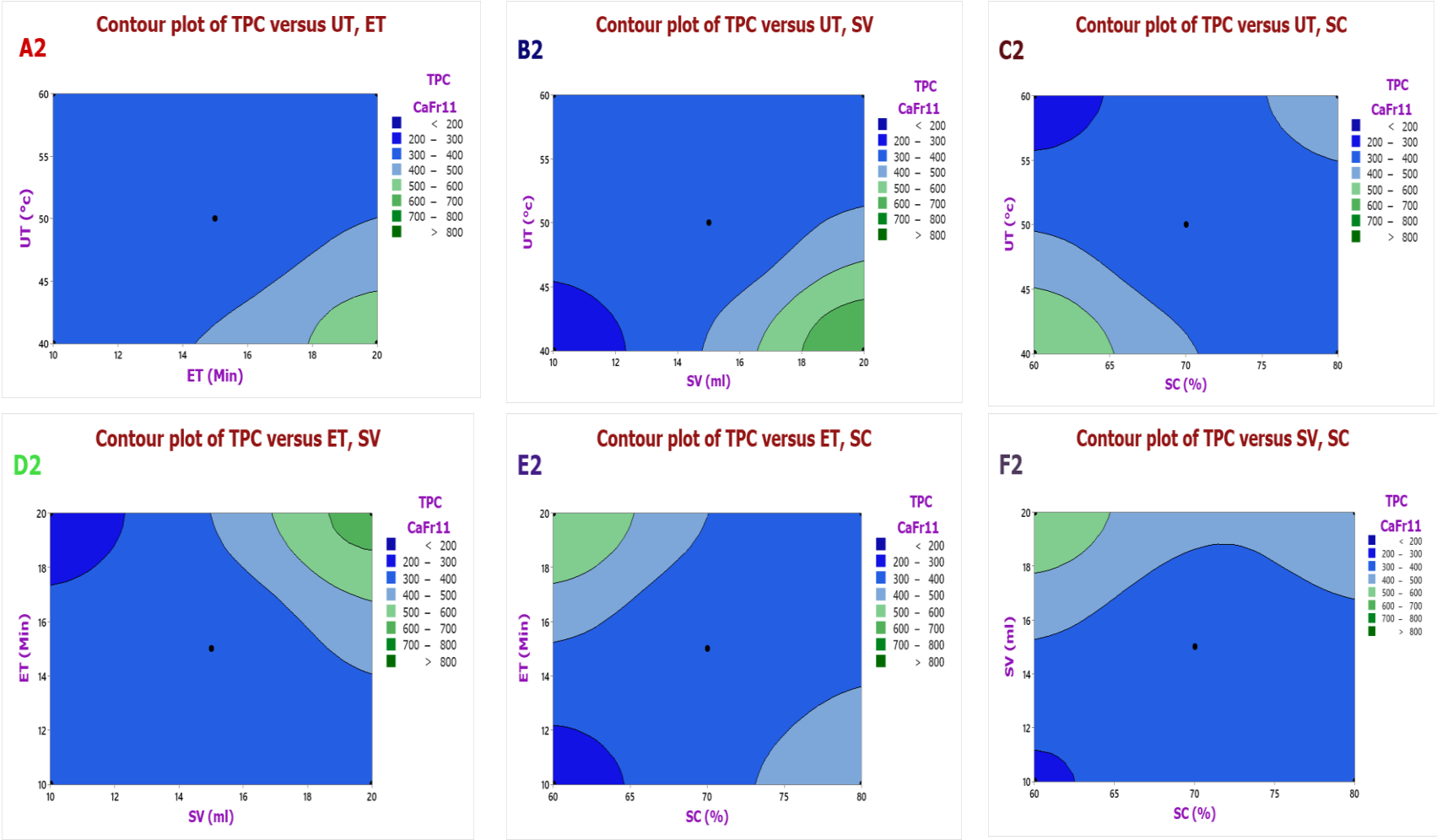


Figure 4.16 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaFr11

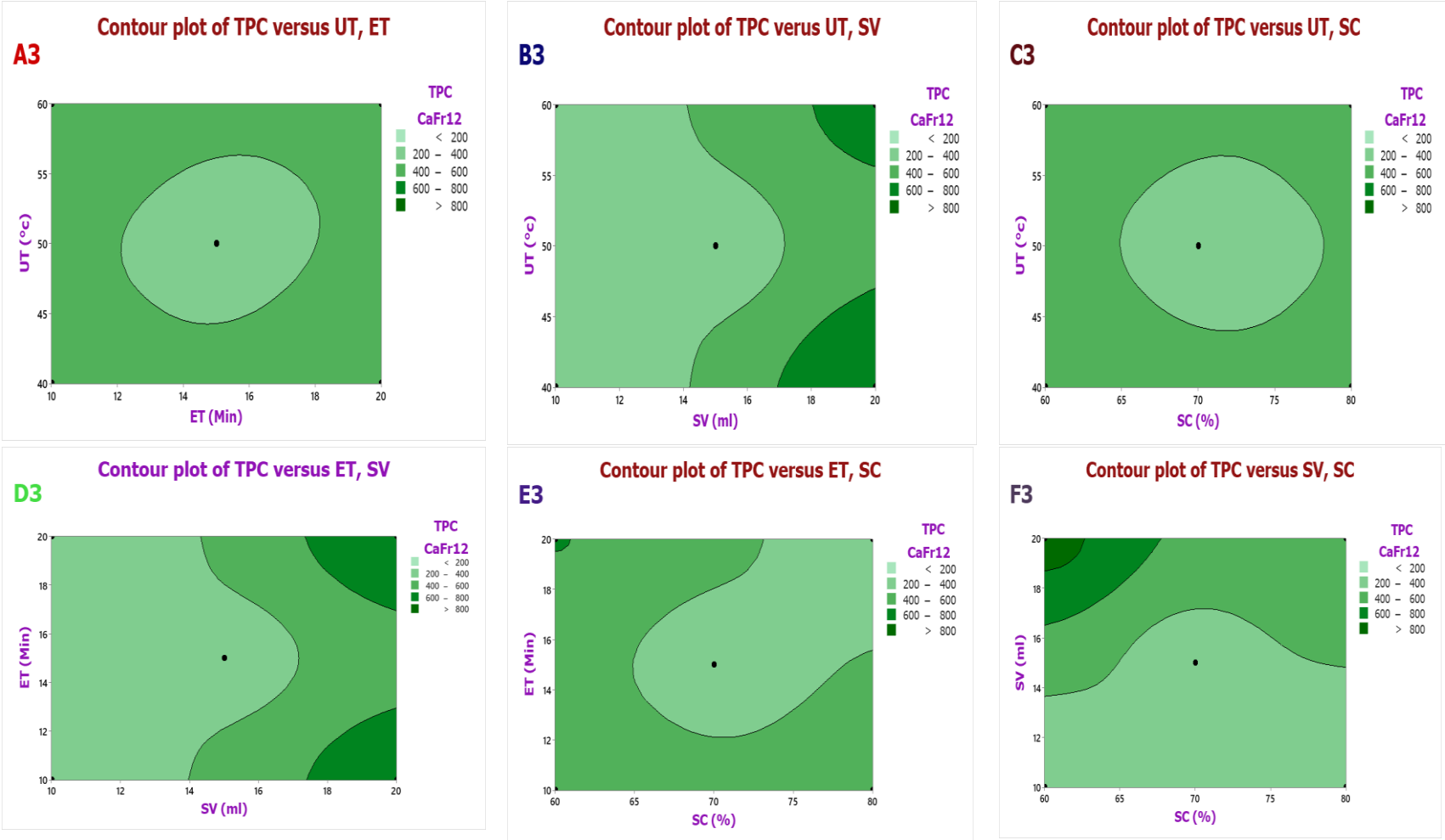


Figure 4.17 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaFr12

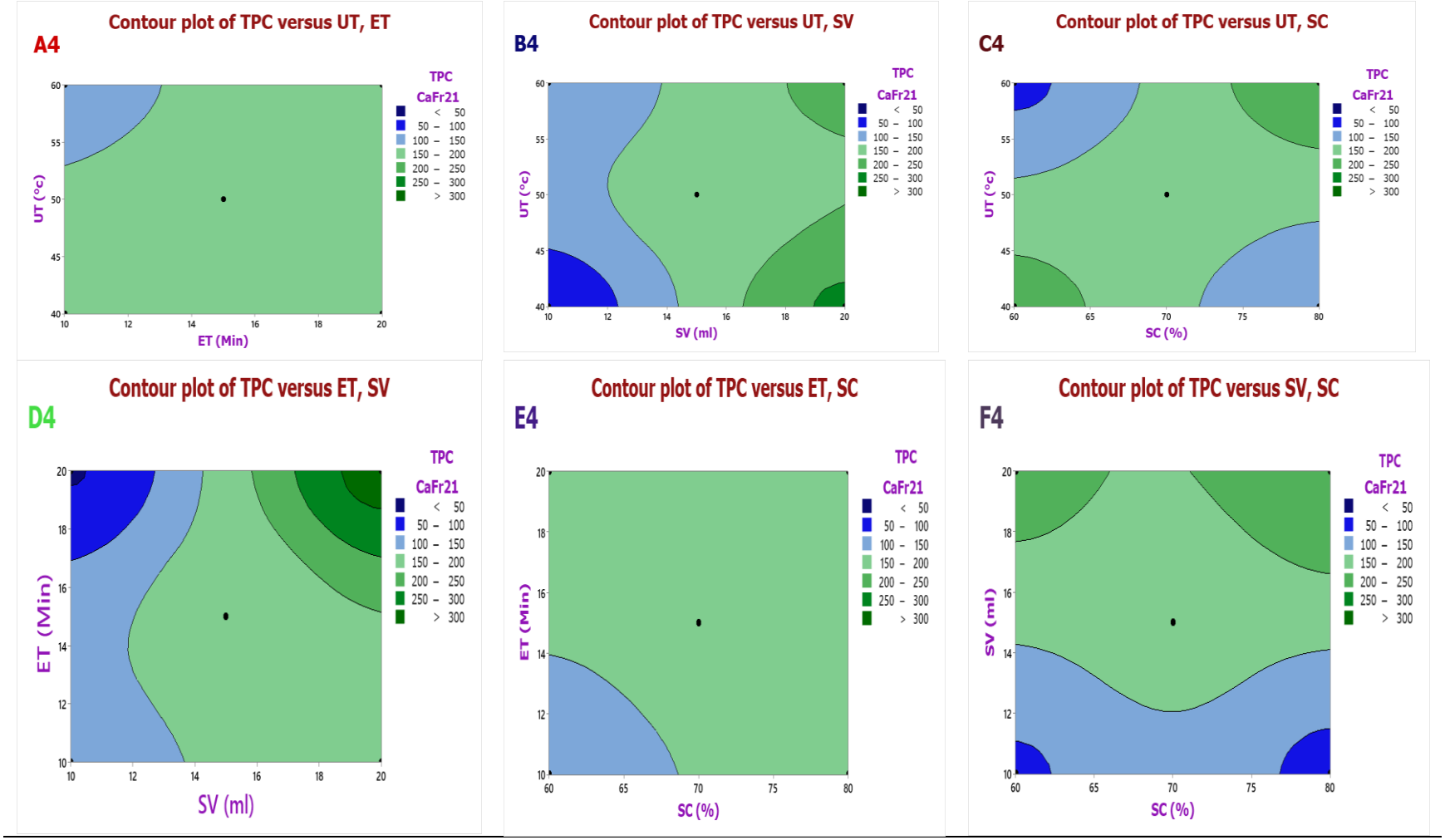


Figure 4.18 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaFr21

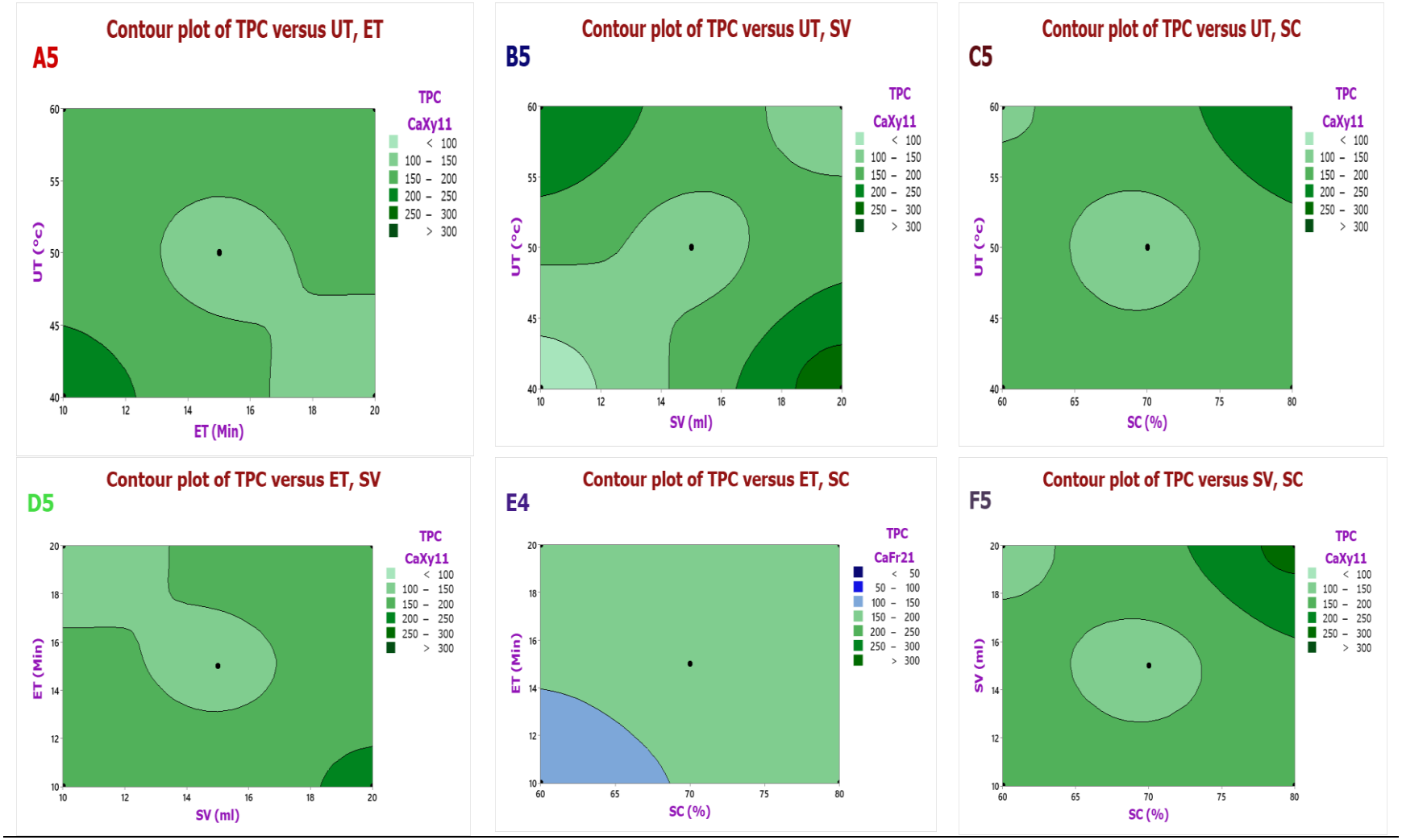


Figure 4.19 Contour plots of factor effects on TPC extraction from African nutmeg peels using CaXy11

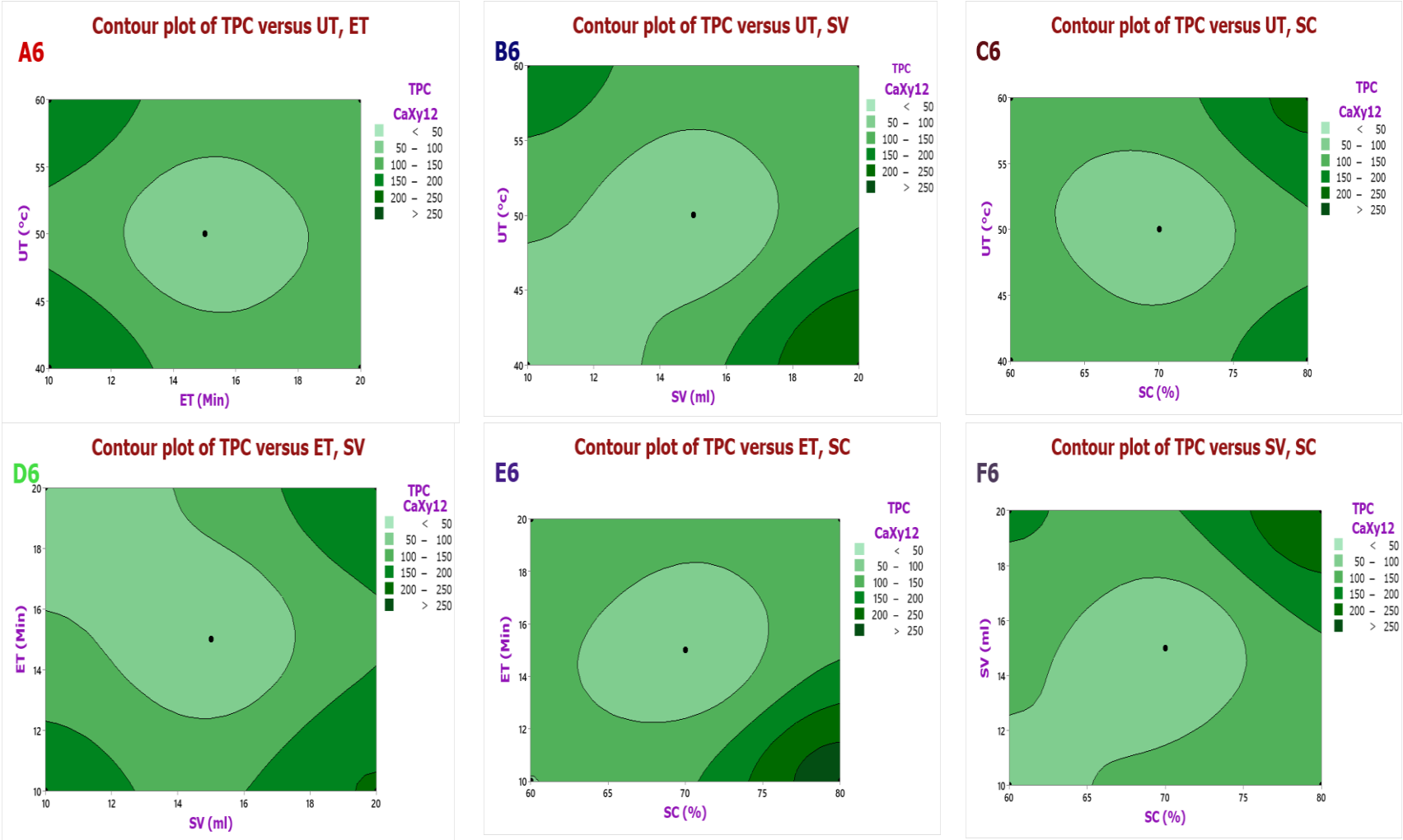


Figure 4.20 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaXy12

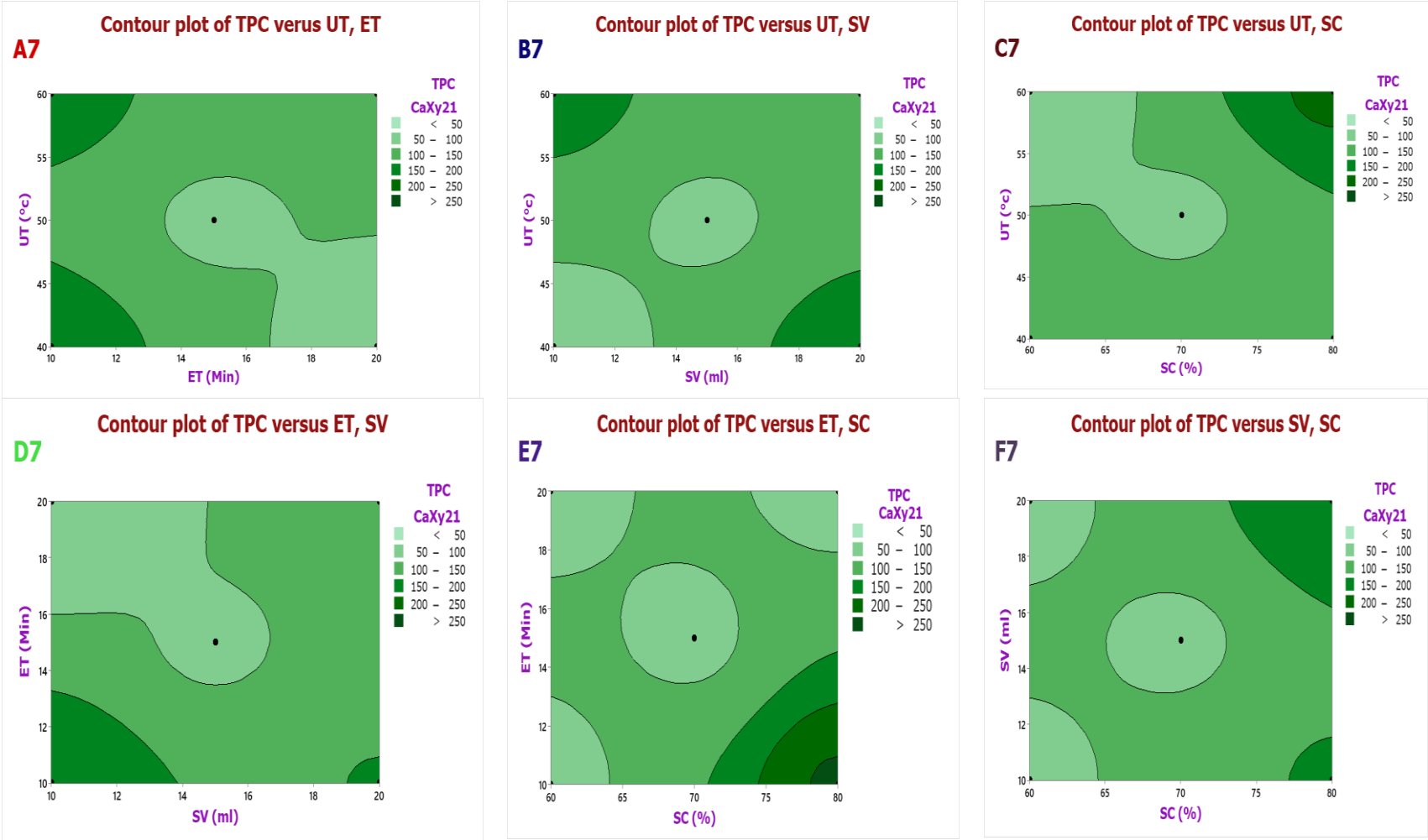


Figure 4.21 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaXy21

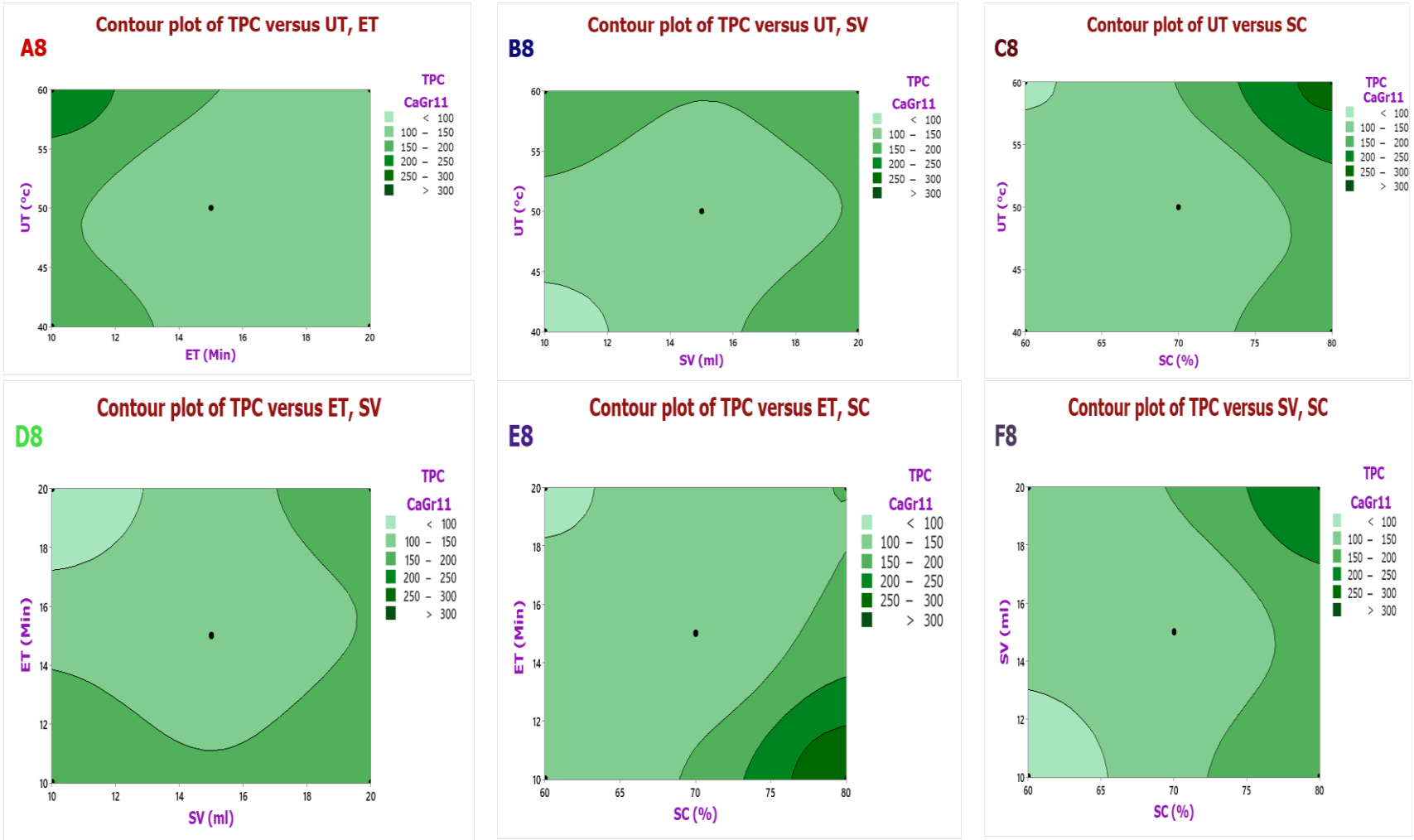


Figure 4.22 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGr11

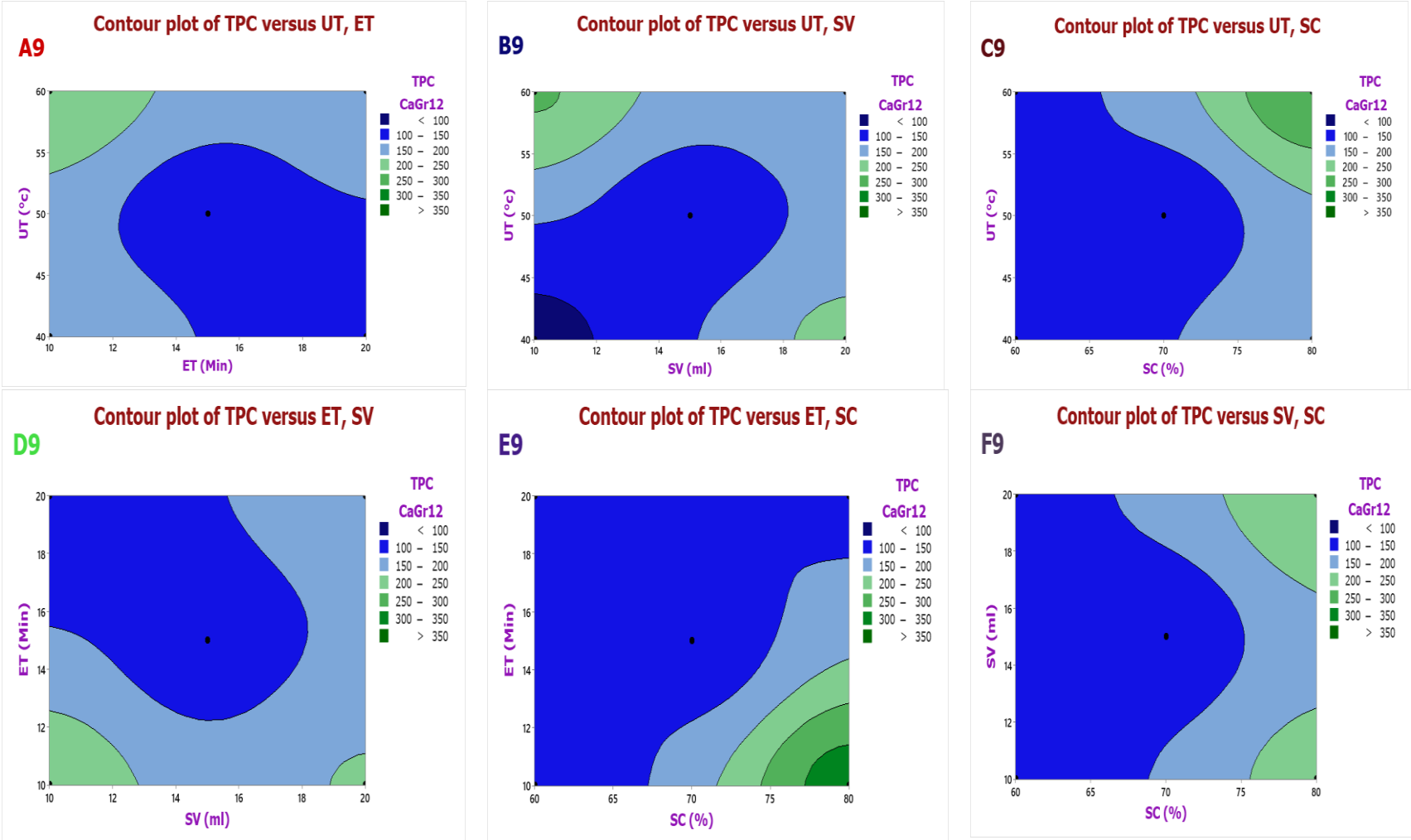


Figure 4.23 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGr12

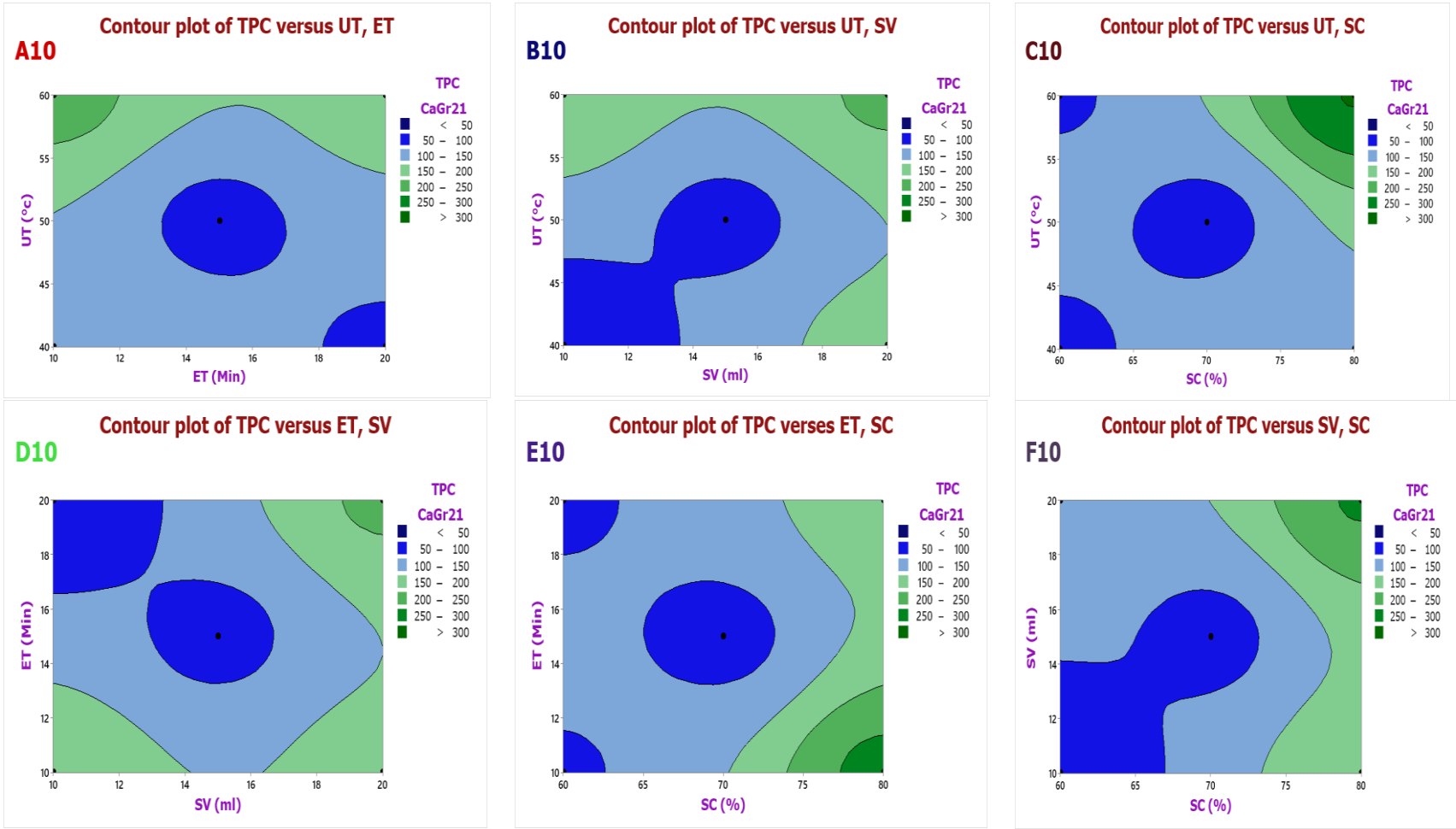


Figure 4.24 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGr21

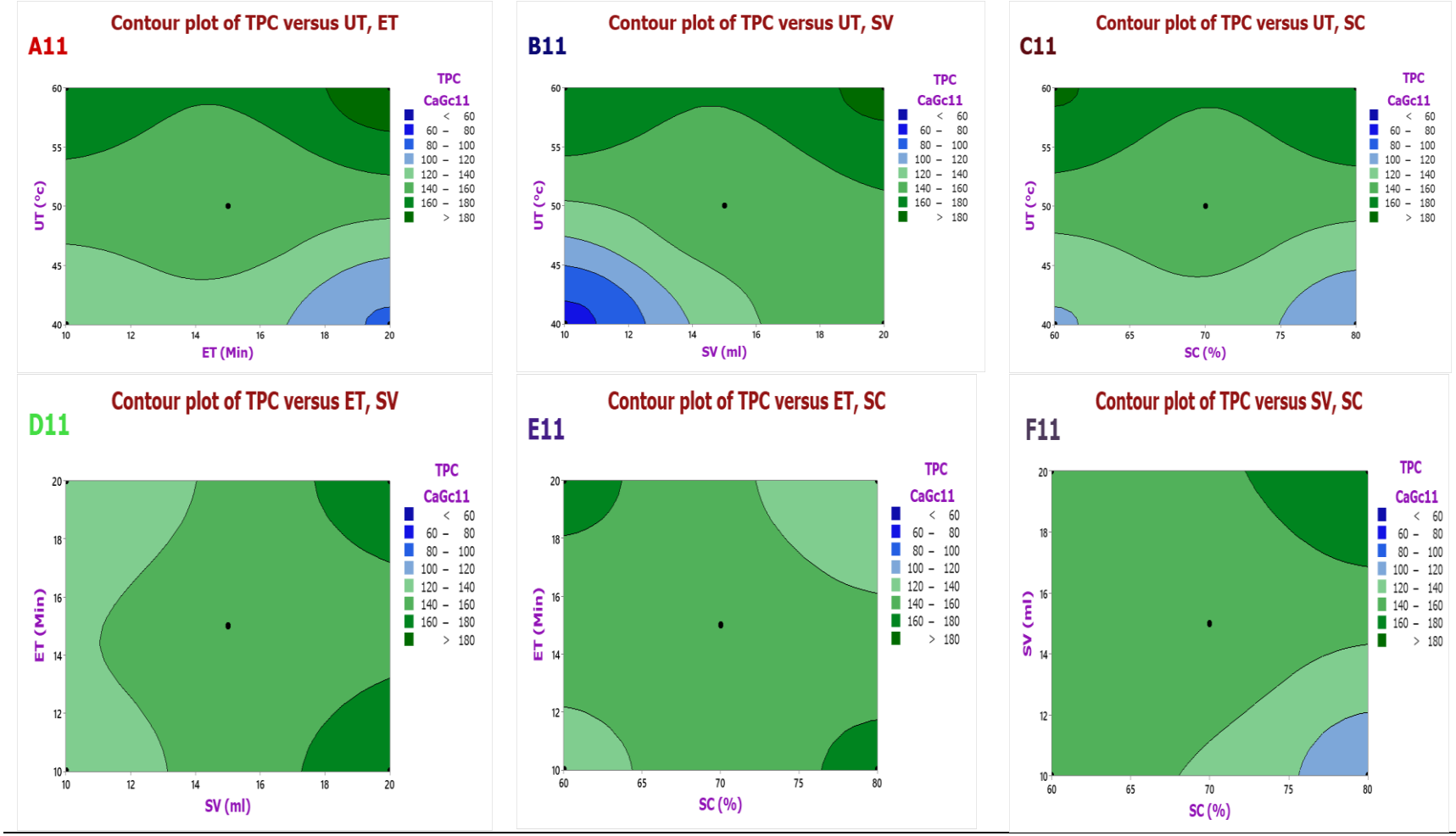


Figure 4.25 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGc11

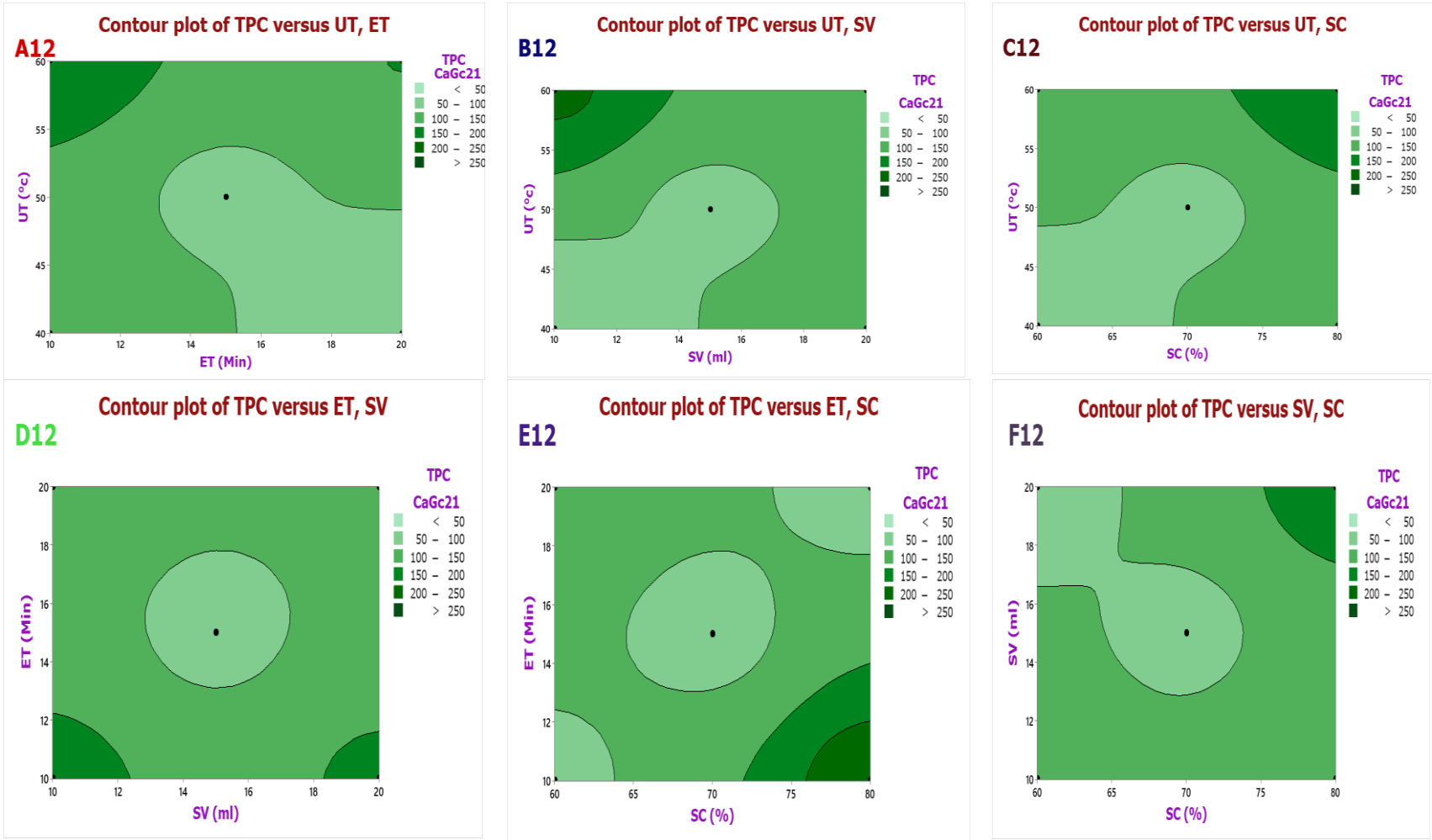


Figure 4.26 Contour plots of factor effects on TPC extraction from African nutmeg peels using CaGc21

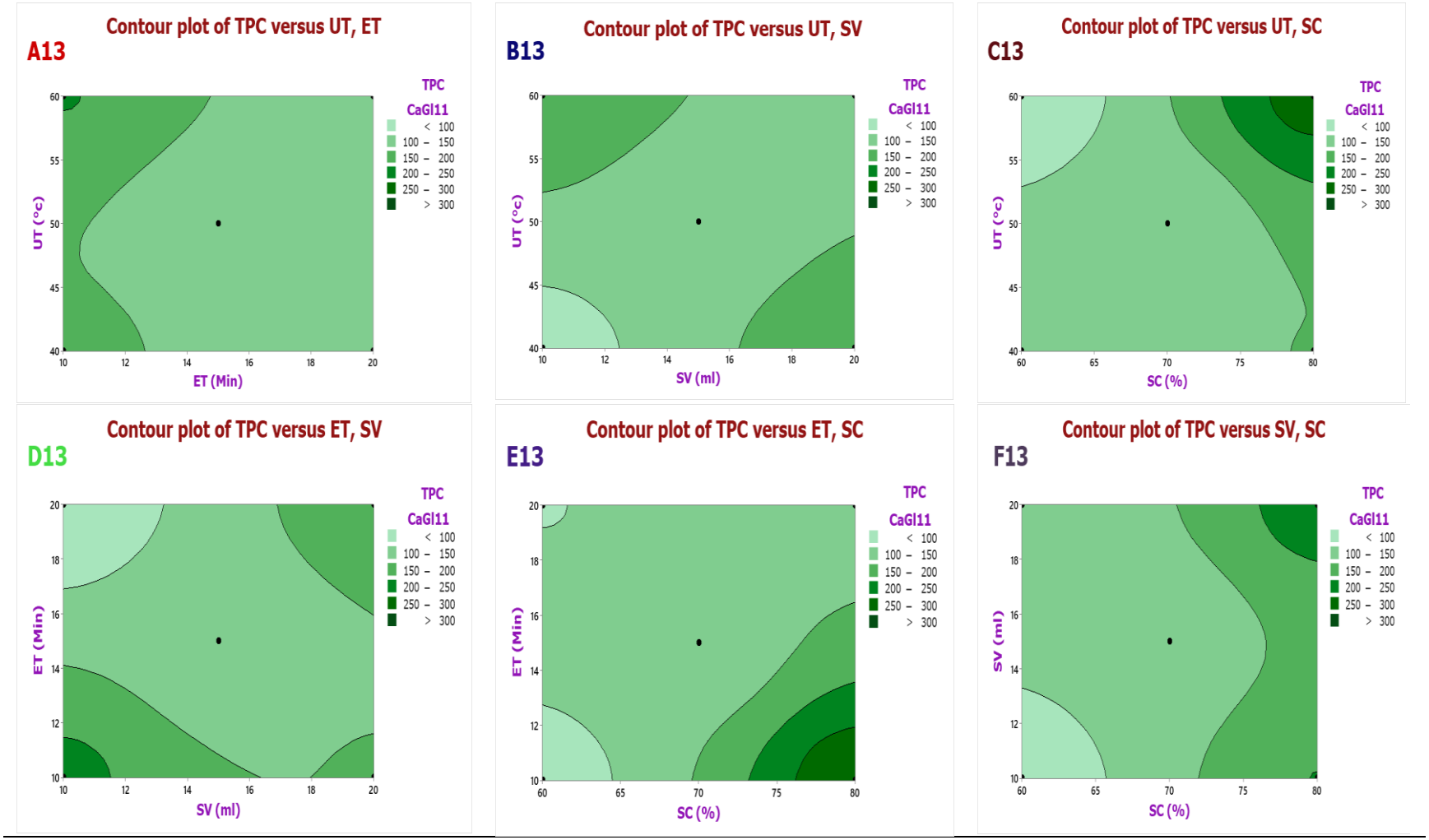


Figure 4.27 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGl11

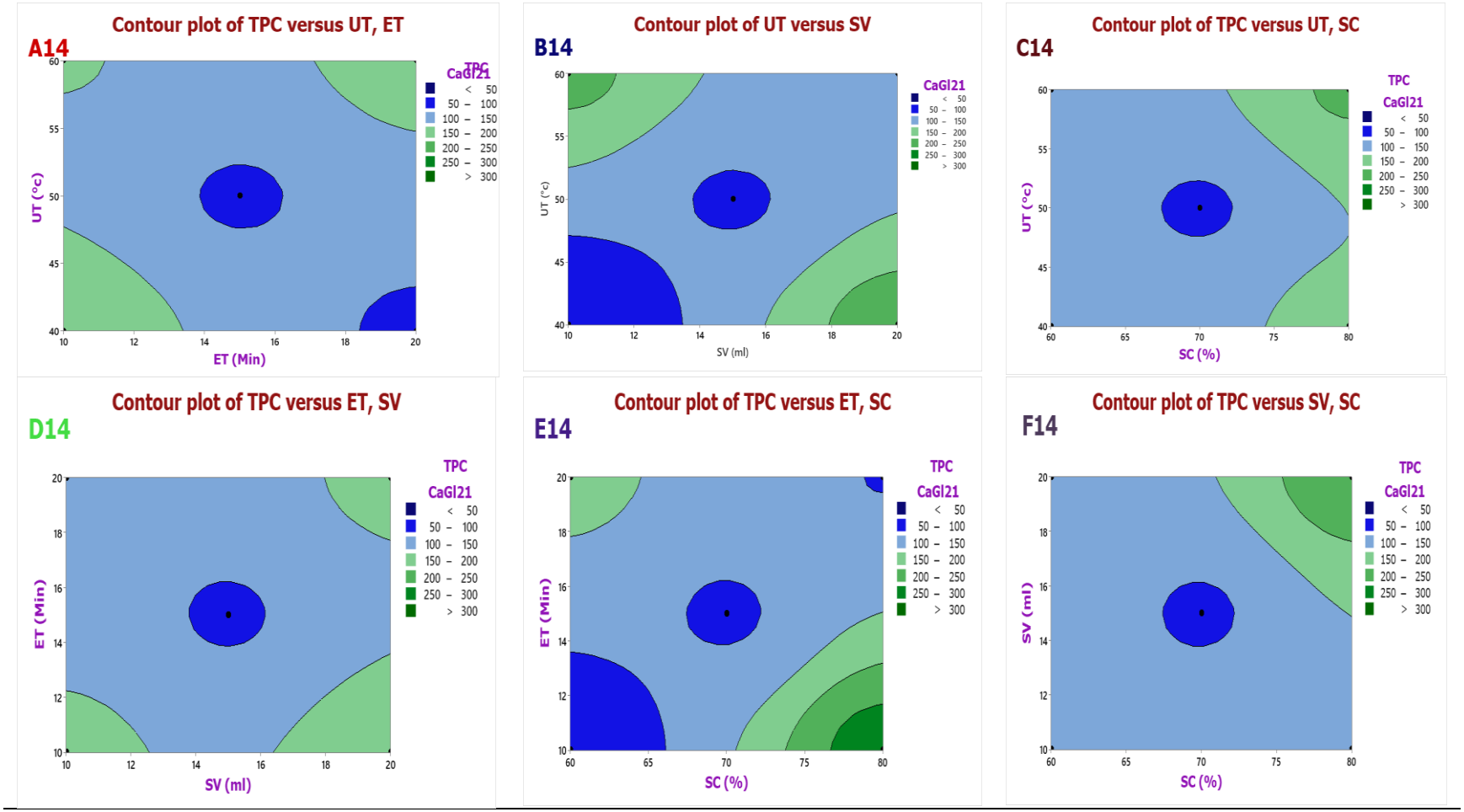


Figure 4.28 Contour plots of factors effects on TPC extraction from African nutmeg peels using CaGl21

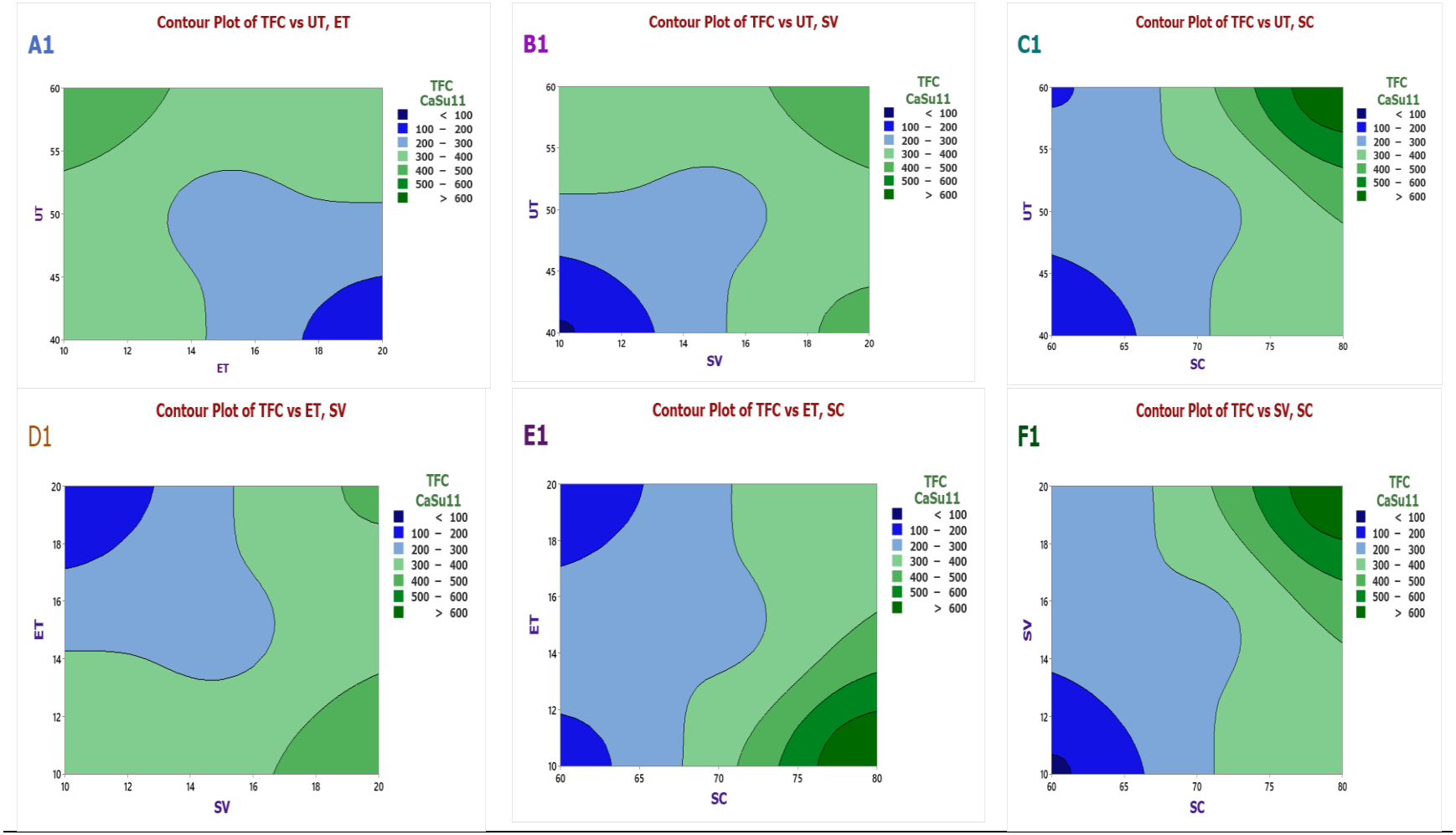


Figure 4.29 Contour plots of factors effects on TFC extraction from African nutmeg peels using CaSu11

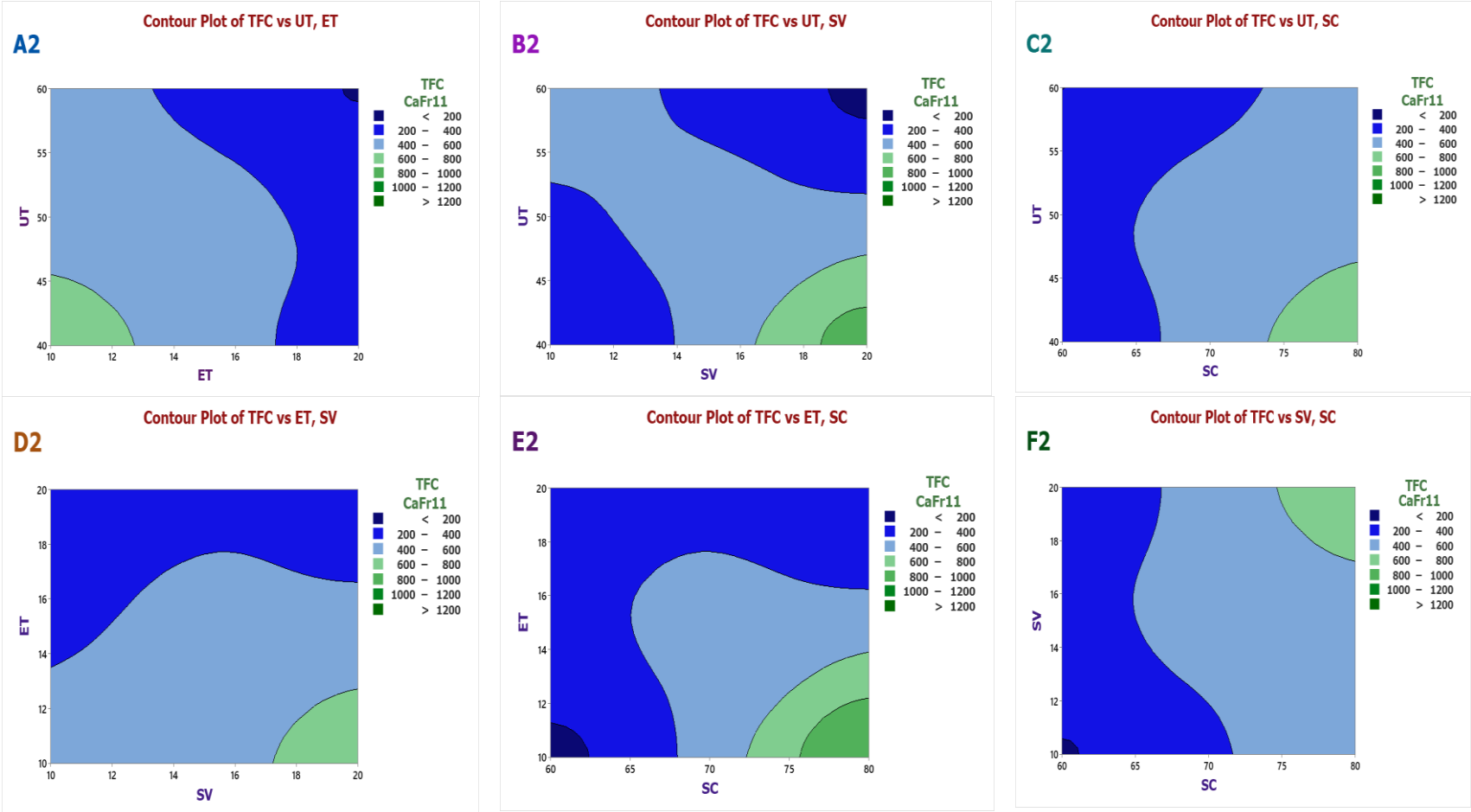


Figure 4.30 Contour plots of factors effects on TFC extraction from African nutmeg peels using CaFr11

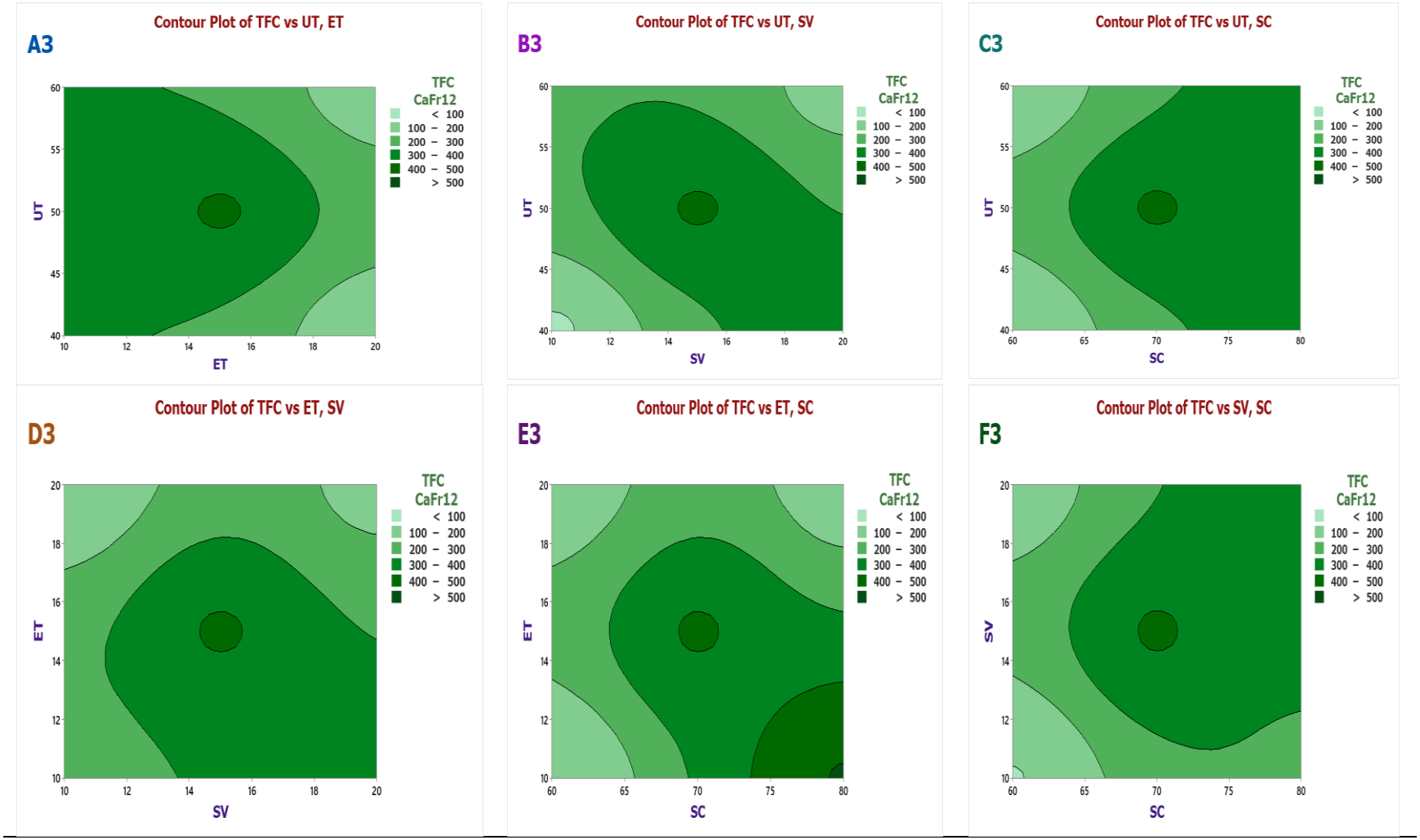


Figure 4.31Contour plots of factors effects on TFC extraction from African nutmeg peels using CaFr12

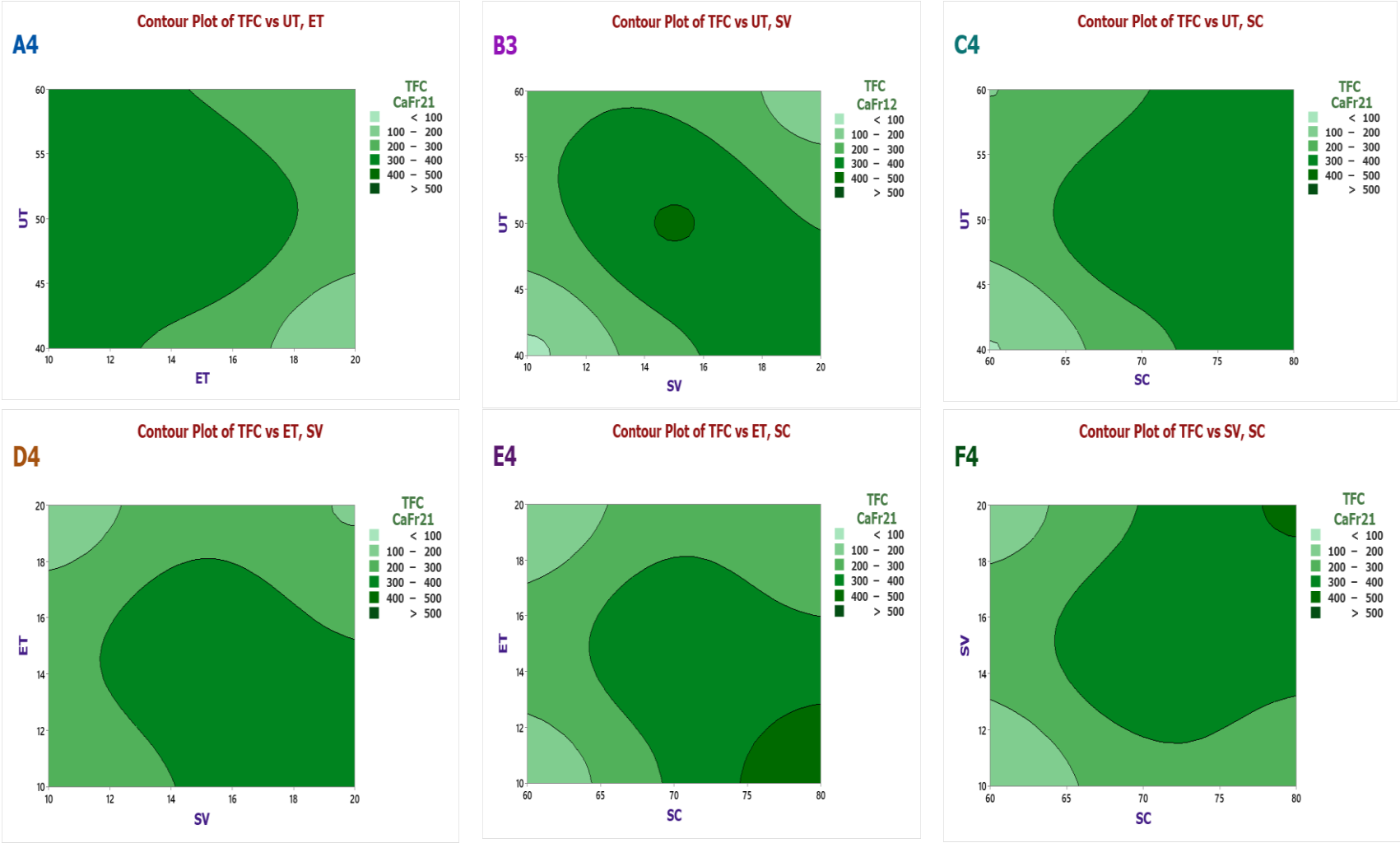


Figure 4.32 Contour plots of factors effects on TFC extraction from African nutmeg peels using CaFr21

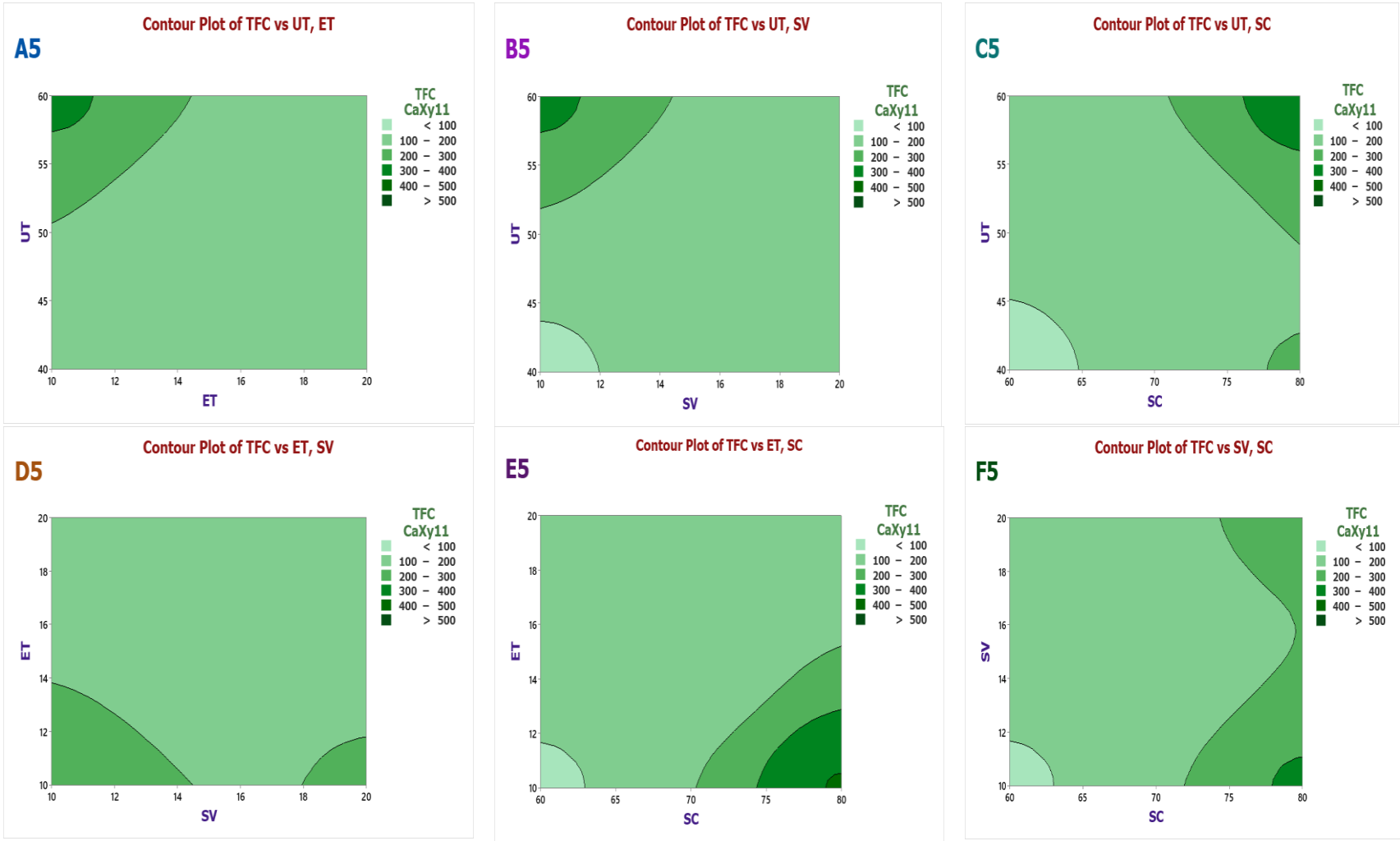


Figure 4.33 Contour plots of factors effects on TFC extraction from African nutmeg peels using CaXy11

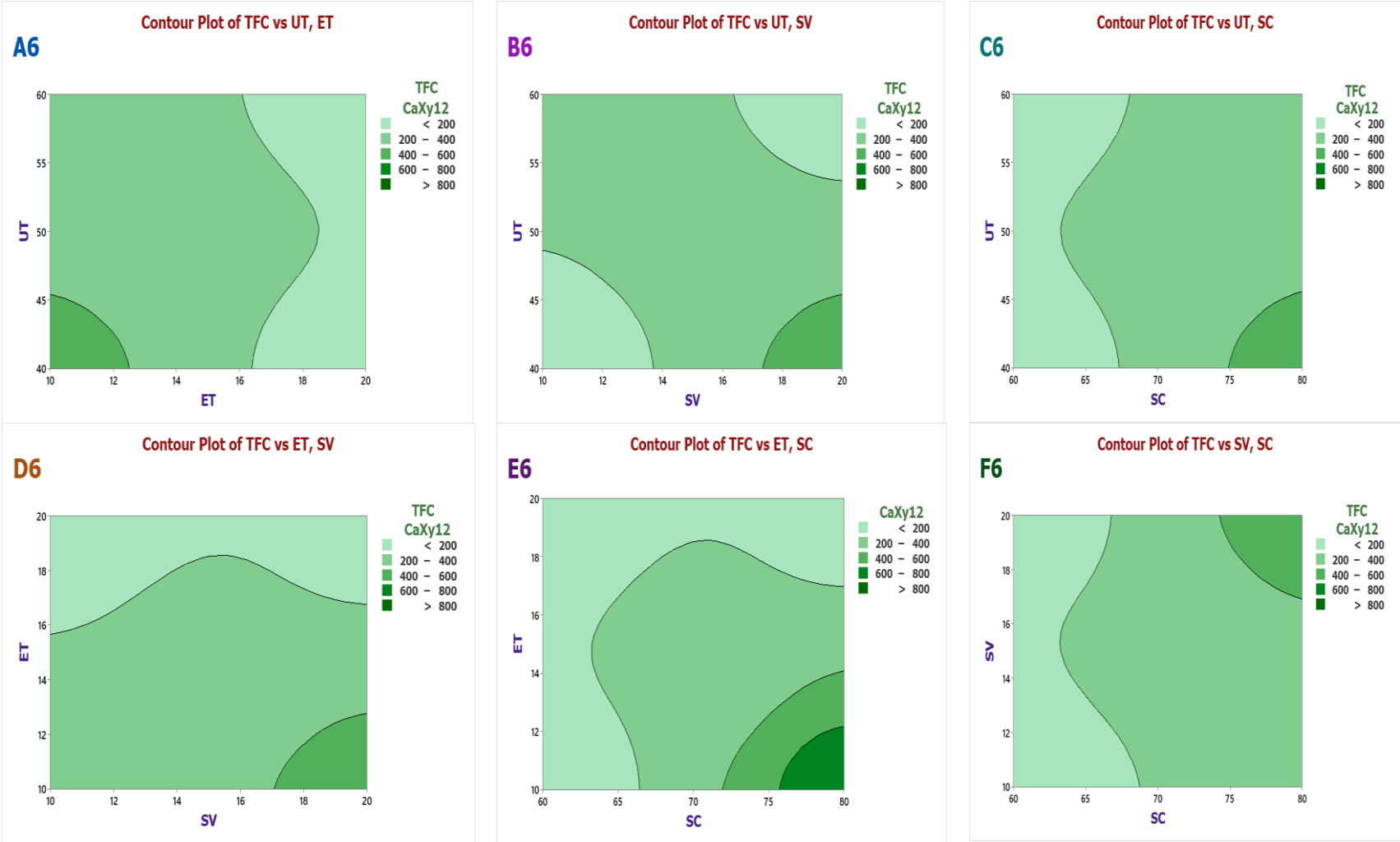


Figure 4.34 Contour plots of factors effects on TFC extraction from African nutmeg peels using CaXy12

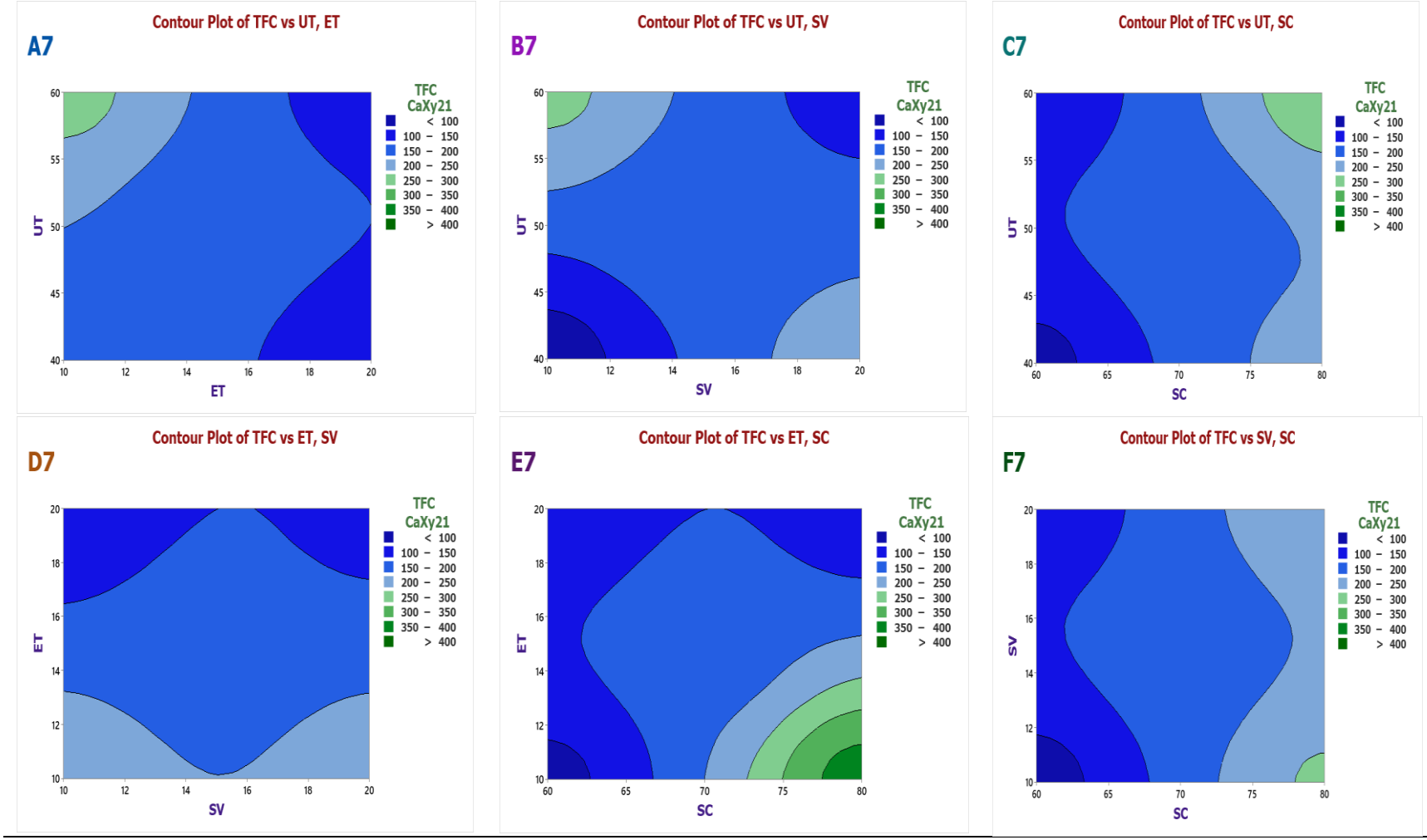


Figure 4.35 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaXy21

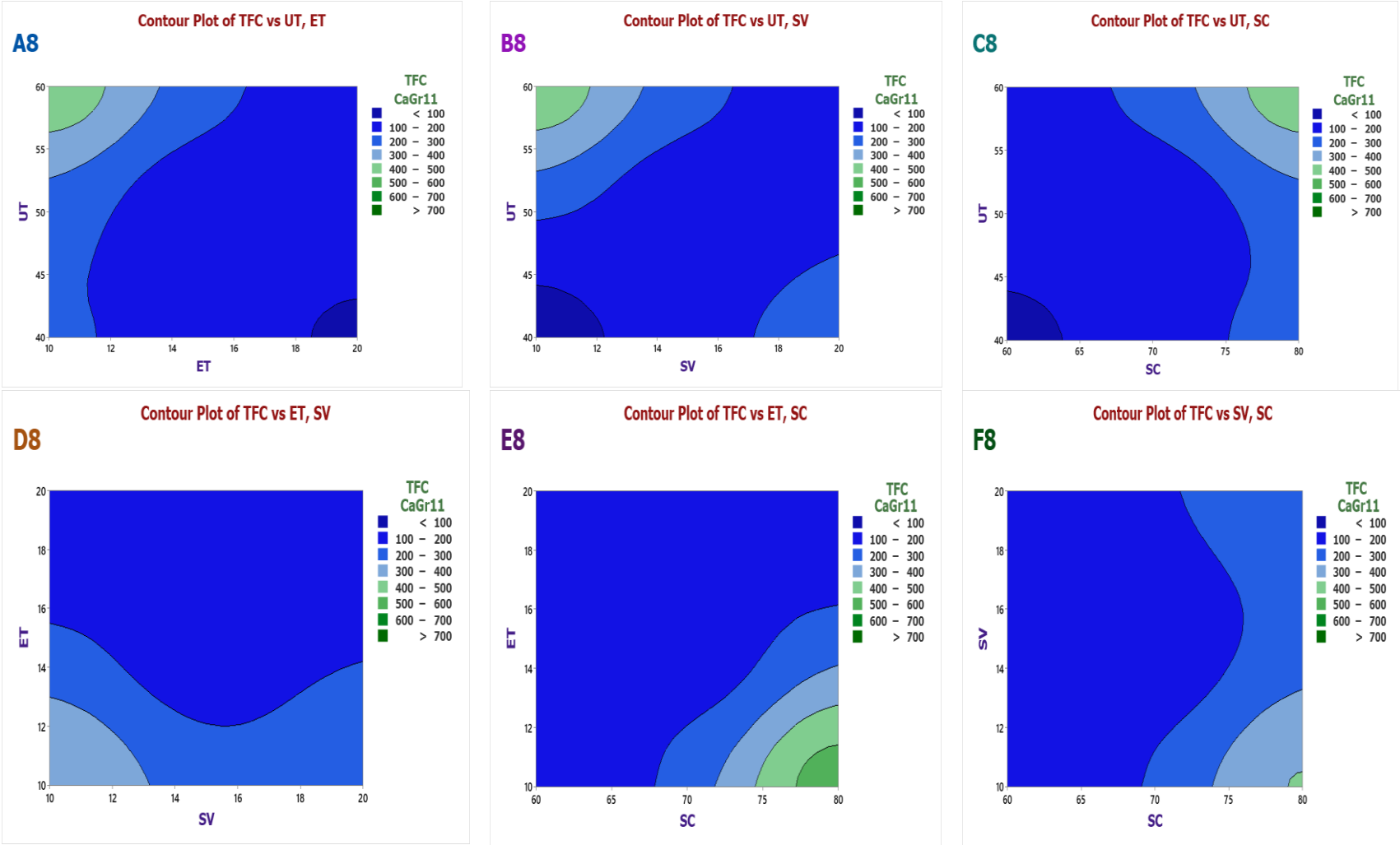


Figure 4.36 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGr11

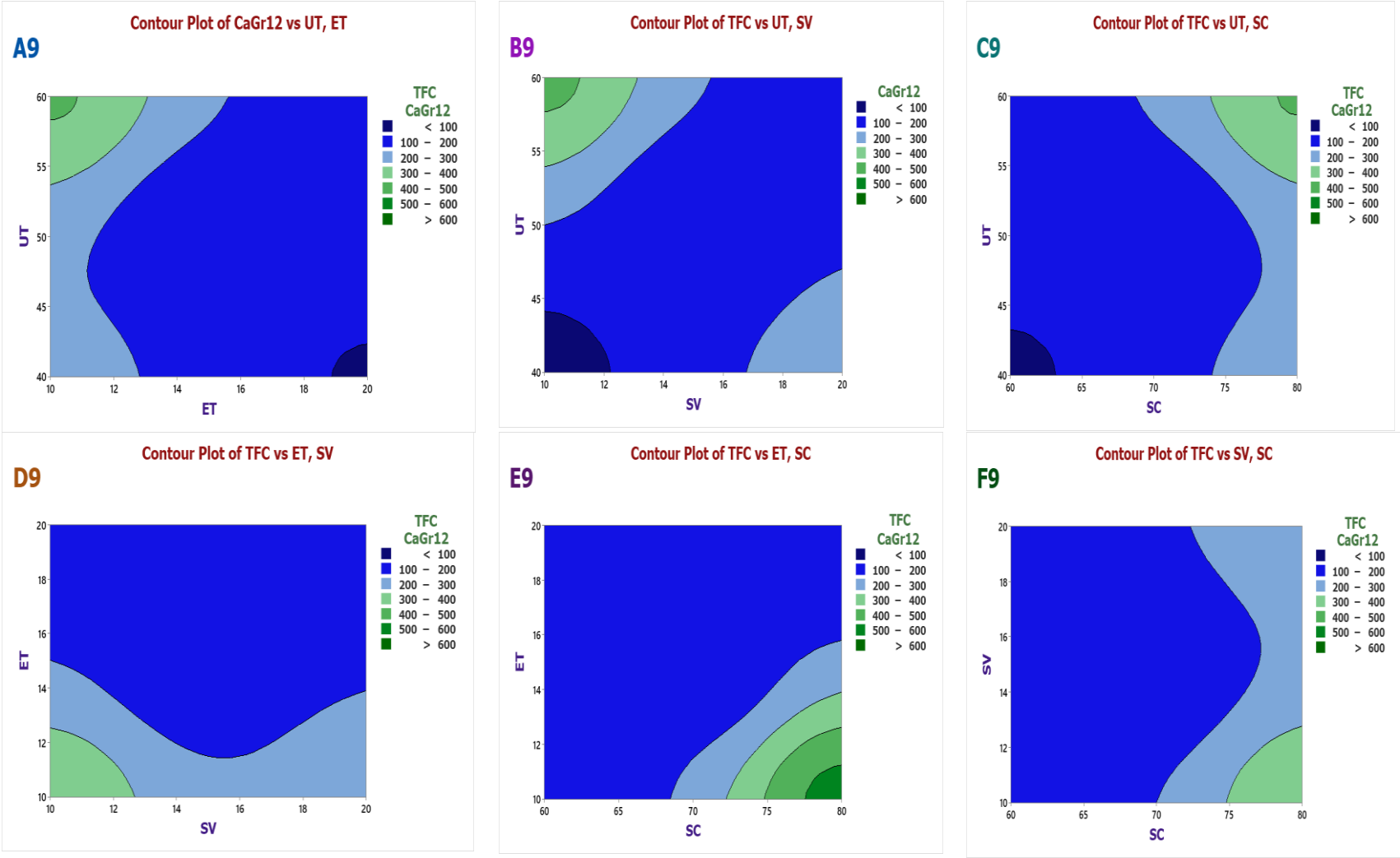


Figure 4.37 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGr12

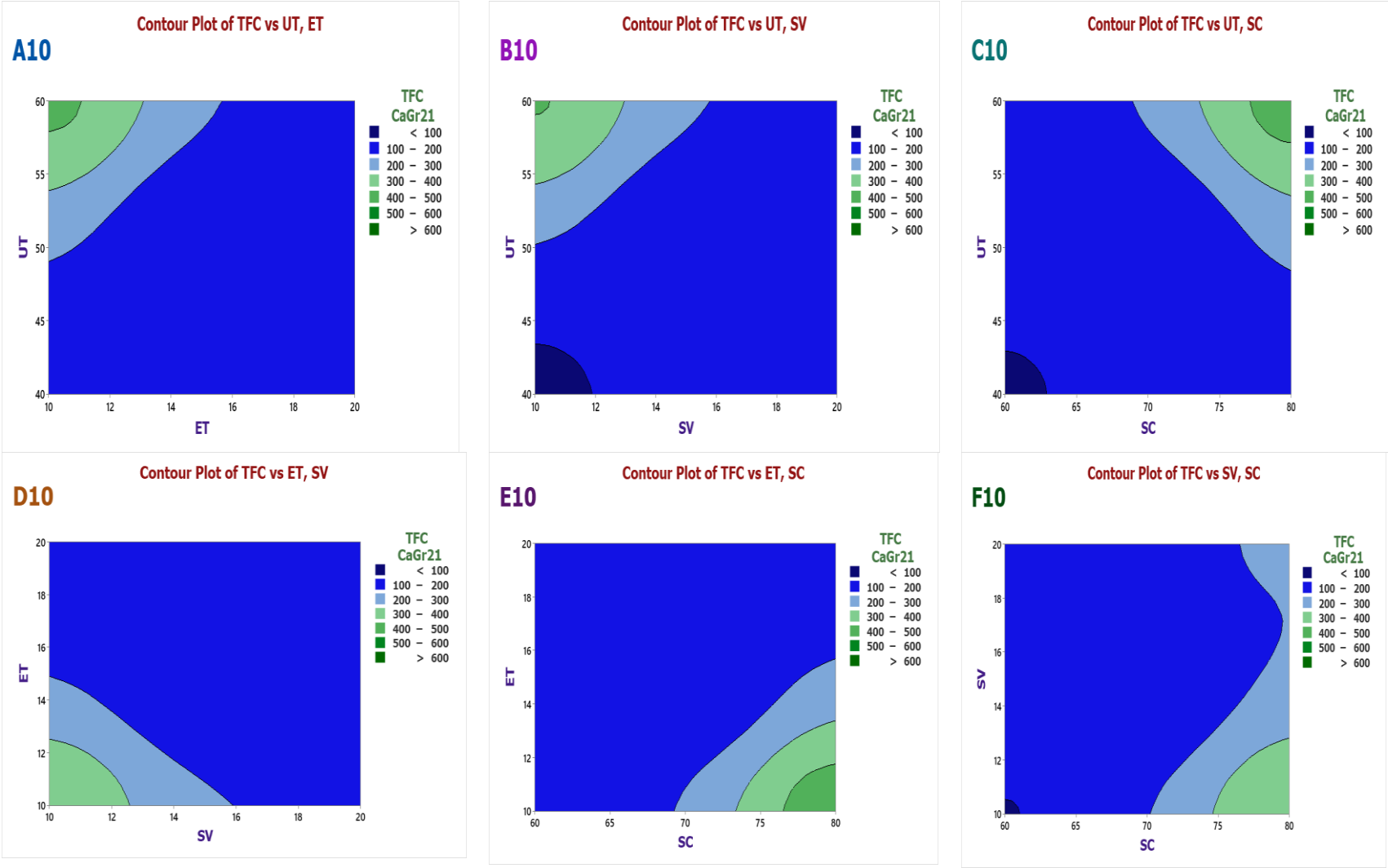


Figure 4.38 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGr21

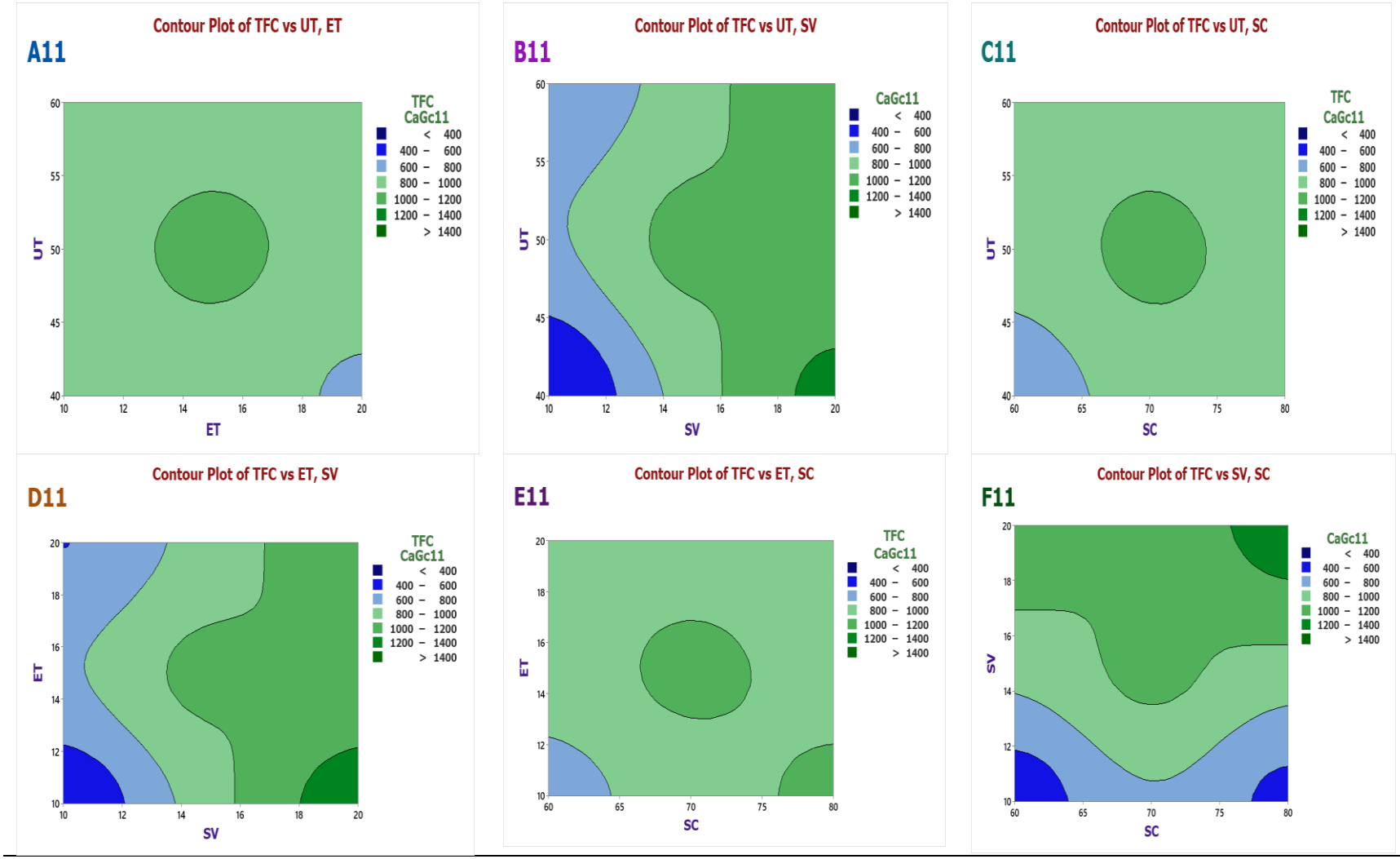


Figure 4.39 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGc11

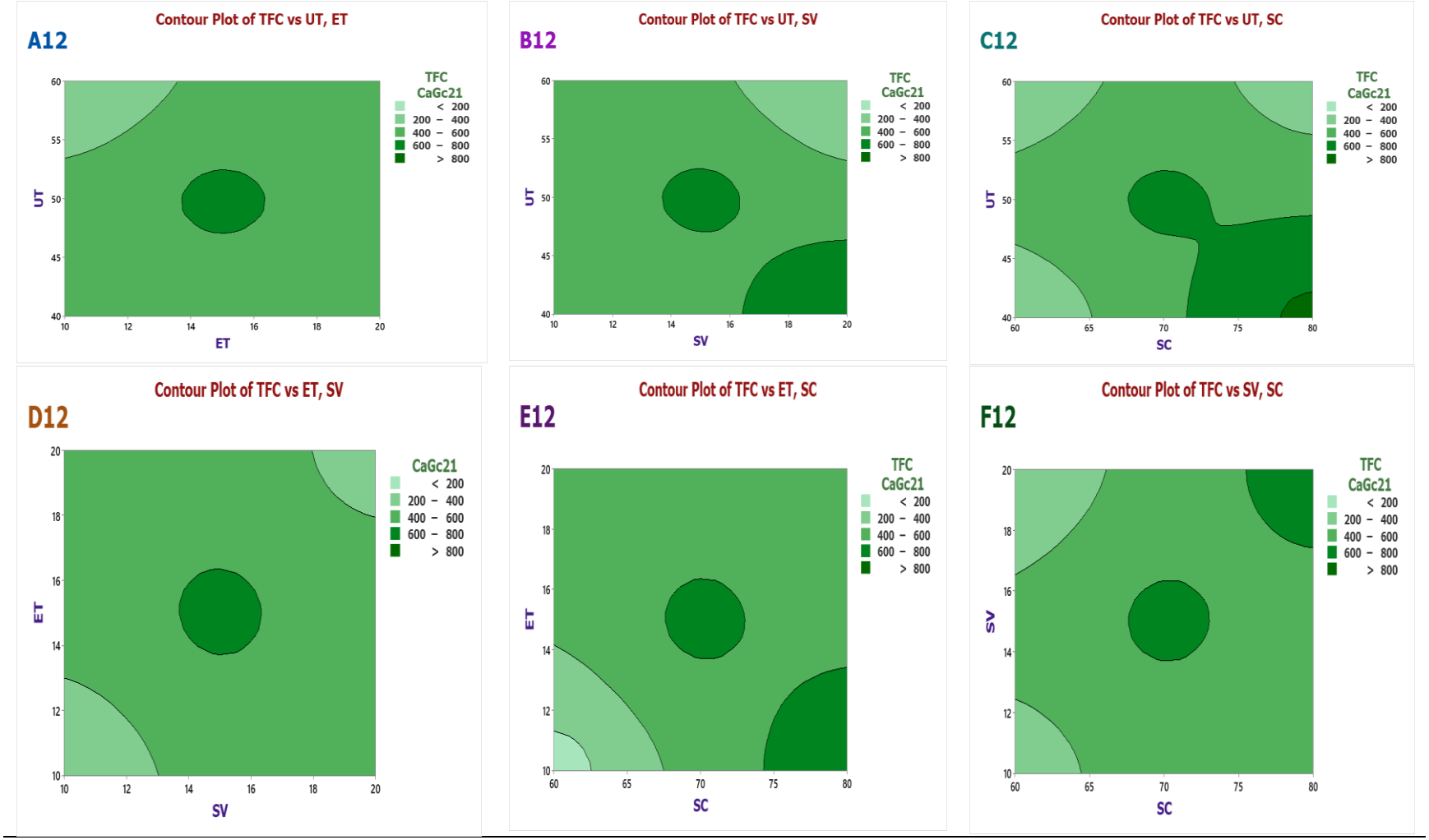


Figure 4.40 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGc21

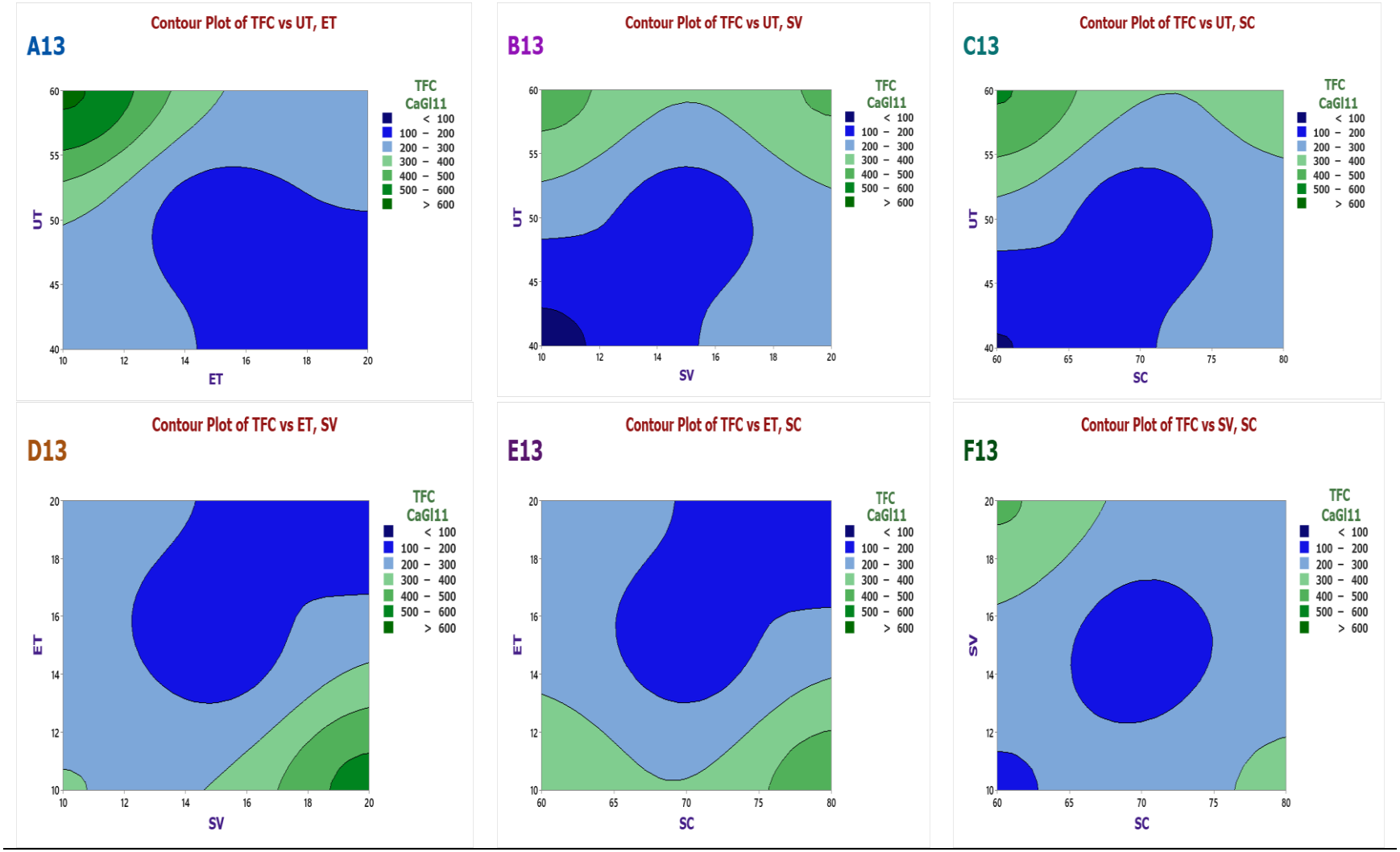


Figure 4.41Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGl11

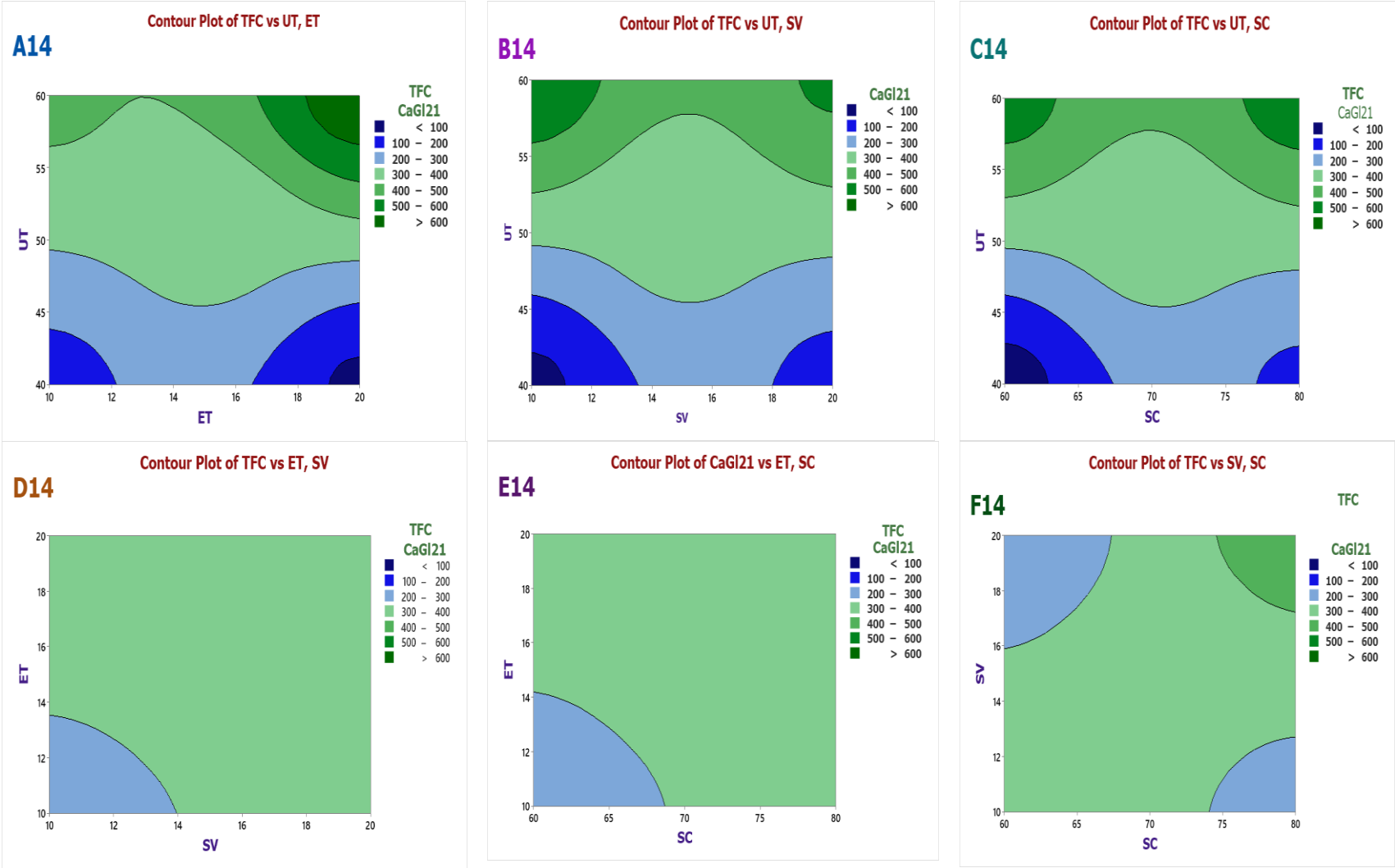


Figure 4.42 Contour plots of factors effects on TFC extracted from African nutmeg peels using CaGl21

4.6.2.3 Cupric Ion-Reducing Antioxidant Capacity (CUPRAC) and Ferric-Reducing Antioxidant Power (FRAP) Antiradical Scavenging Power

The antiradical scavenging potentials of African Nutmeg peel extracted using NADESs were measured in vitro by the CUPRAC and FRAP methods, and the results presented in **Table 4.9**. CaFr11 had the highest mean CUPRAC value (4.718 µMTE/g), while CaSu11 had the lowest mean value (3.147 µMTE/g). However, there was no significant difference among the mean CUPRAC values across the synthesized NADESs. On the other hand, the highest mean FRAP value of 5.848 µMTE/g was obtained from CaFr11, while the lowest mean FRAP value of 1.641 µMTE/g was obtained from CaGc21. The difference between the mean FRAP values of the highest and the lowest groups were statistically significant.

4.6.2.4 Effects of Experimental Conditions on the Antiradical Scavenging Power of CUPRAC and FRAP

The effects of the experimental conditions on CUPRAC and FRAP were evaluated, and the results presented in **Figure 4.43** and **Figure 4.44,** respectively. The conditions for obtaining the highest antiradical scavenging power from CUPRAC are shown in **Figure 4.43B** (UT = 40°C, ET = 10 min, SV = 20 ml, SC = 80%), followed by **Figure 4.43F** (UT = 60°C, ET = 10 min, SV = 10 ml, SC = 80%). On the other hand, the conditions that gave the least CUPRAC antiradical scavenging power are shown in **Figure 4.43C** (UT = 40°C, ET = 20 min, SV= 10 ml, SC = 80%), followed by **Figure 4.43A** (UT = 40°C, ET = 10 min, SV= 10 ml, SC = 60%). Furthermore, the conditions that gave rise to the highest FRAP antiradical scavenging power are shown in **Figure 4.44D** (UT = 40°C, ET = 20 min, SU = 20 ml, SC = 60%), followed by **Figure 4.44I** (UT = 60°C, ET = 20 min, SU = 20 ml, SC = 80%), whereas **Figure 4.44C** (UT = 40°C, ET = 20 min, SU = 10 ml, SC = 80%), followed by **Figure 4.44G** (UT = 60°C, ET = 10 min, SU = 20 ml, SC = 60%), produced the least FRAP antiradical scavenging power.

Figure 4.43 Effects of experimental conditions on CUPRAC capacity of African nutmeg peels extracted using NADESs

Figure 4.44 Effects of experimental conditions on FRAP power of African nutmeg peels extracted using NADESs

4.6.2.5 Effects of Factor Interaction on CUPRAC antiradical scavenging capacity of African nutmeg peels extracted using NADESs

A further analysis of the relationship between the responses and two factor interactions (UT*ET; UT*SV; UT*SC; ET*SV; ET*SC; and SV*SC) on CUPRAC capacity was studied with two-dimensional contour plots for each of the synthesized NADESs as shown in **Figure 4.45** to **Figure 4.58**. From the figures, important factor combinations for maximal CUPRAC capacity of African nutmeg peels were derived.

4.6.2.6 Effects of Factor Interaction on FRAP antiradical scavenging potentials of African nutmeg peels extracted using NADESs

The effects on two factor interaction on FRAP scavenging potential of the extracts were also elucidated with two-dimensional contour plots as shown in **Figure 4.59** to **Figure 4.72.,** and from which factors that were of great importance to FRAP potentials in African nutmeg peel extracts emerged.

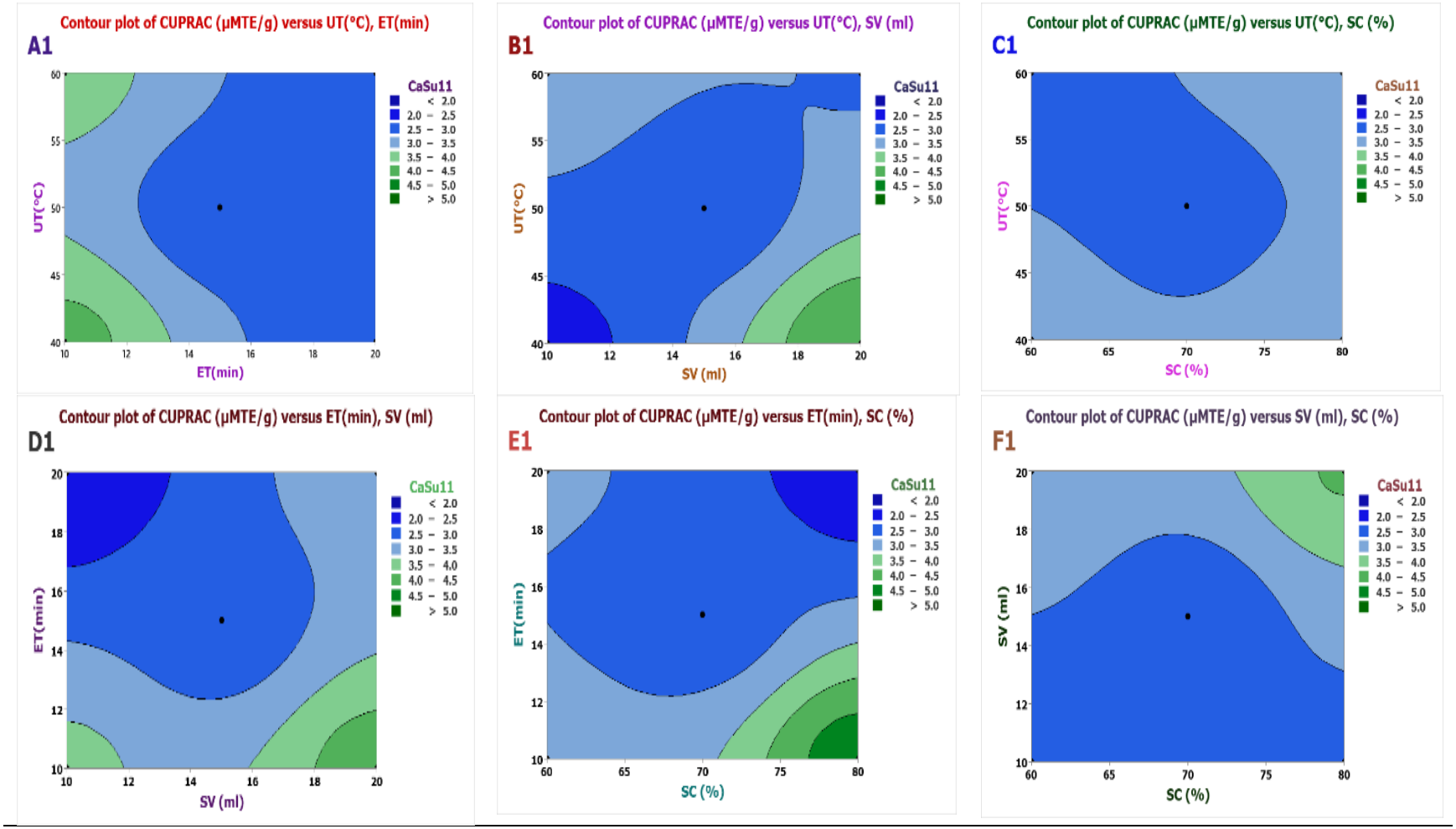


Figure 4.45 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaSu11

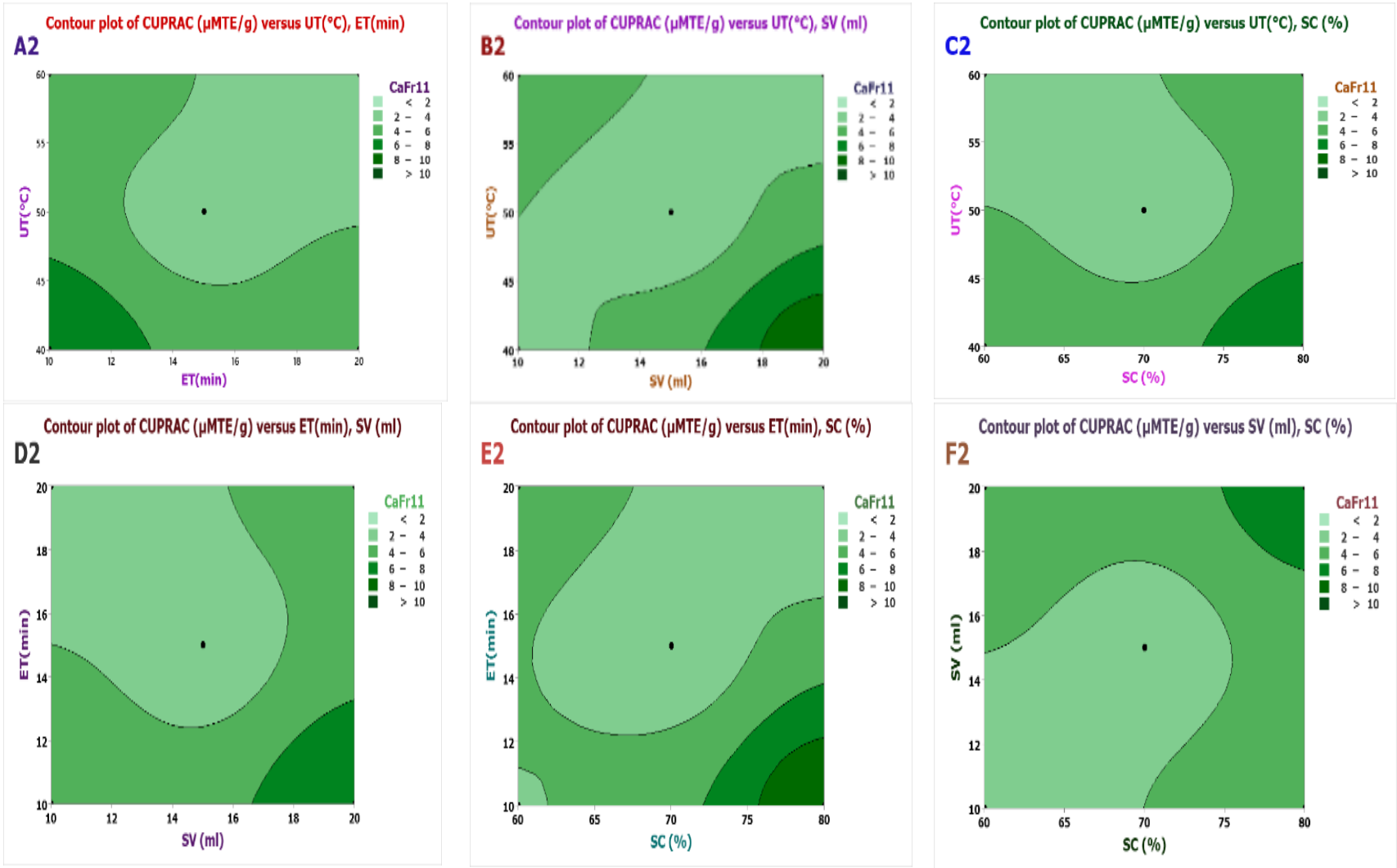


Figure 4.46 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaFr11

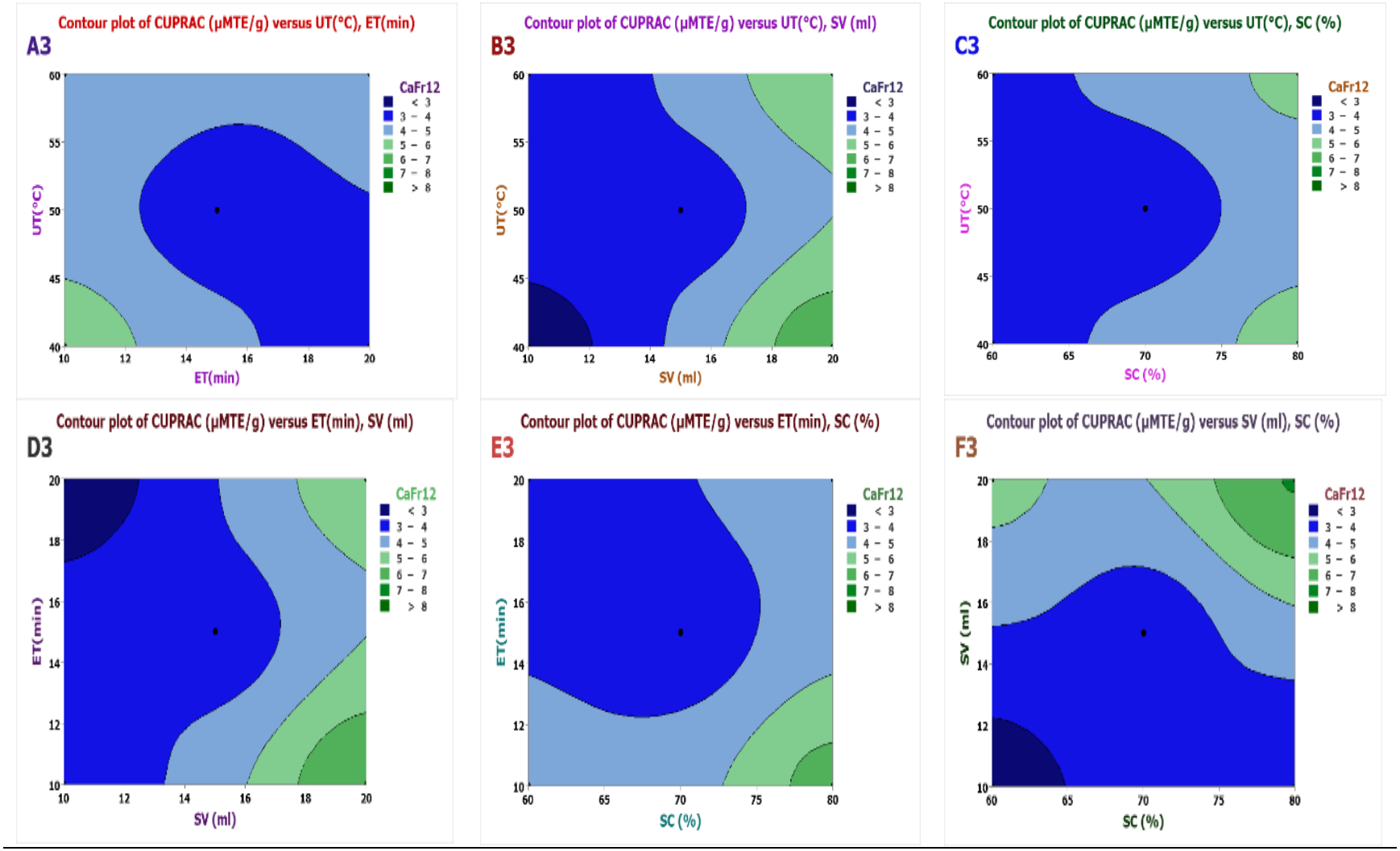


Figure 4.47 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaFr12

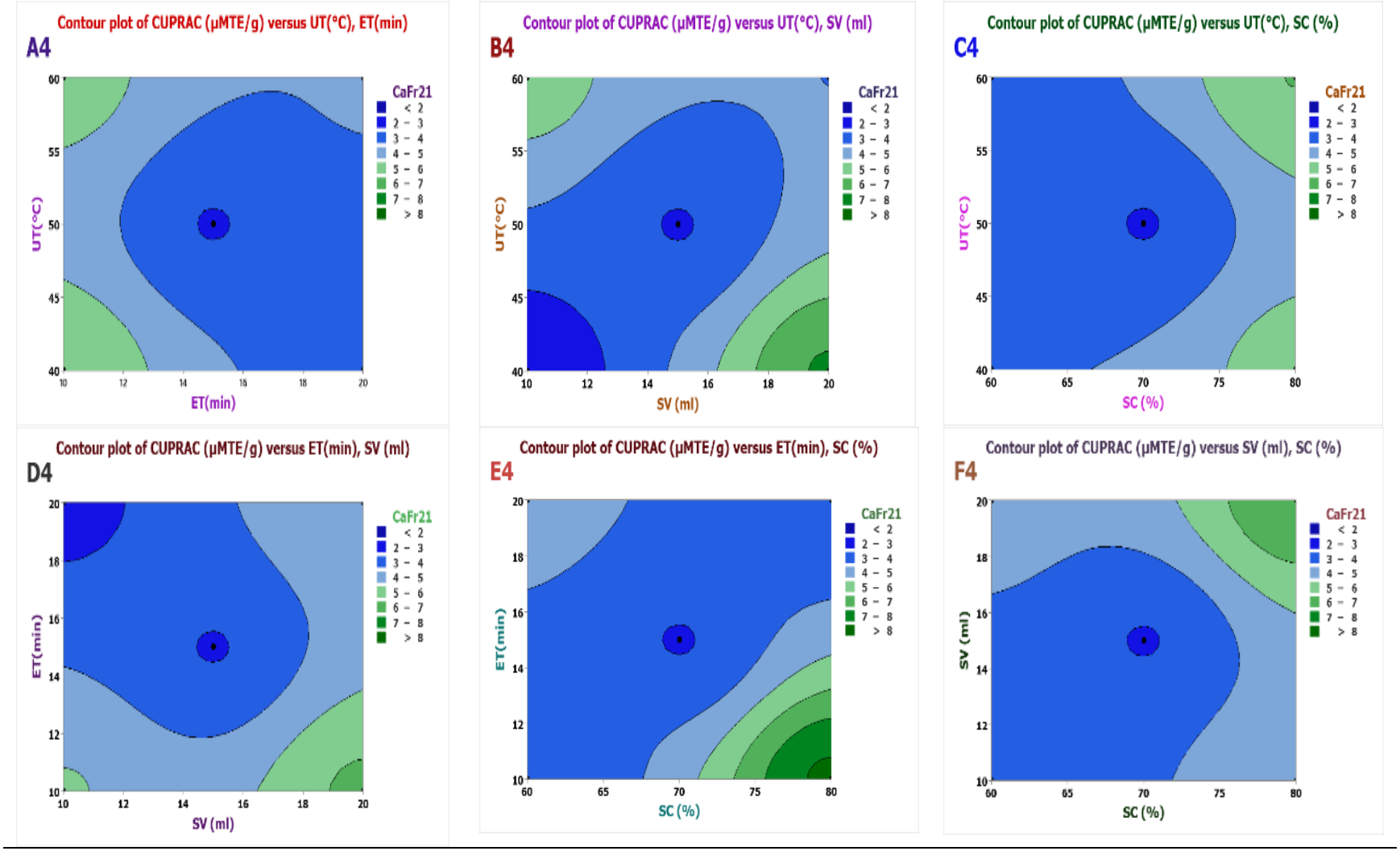


Figure 4.48 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaFr21

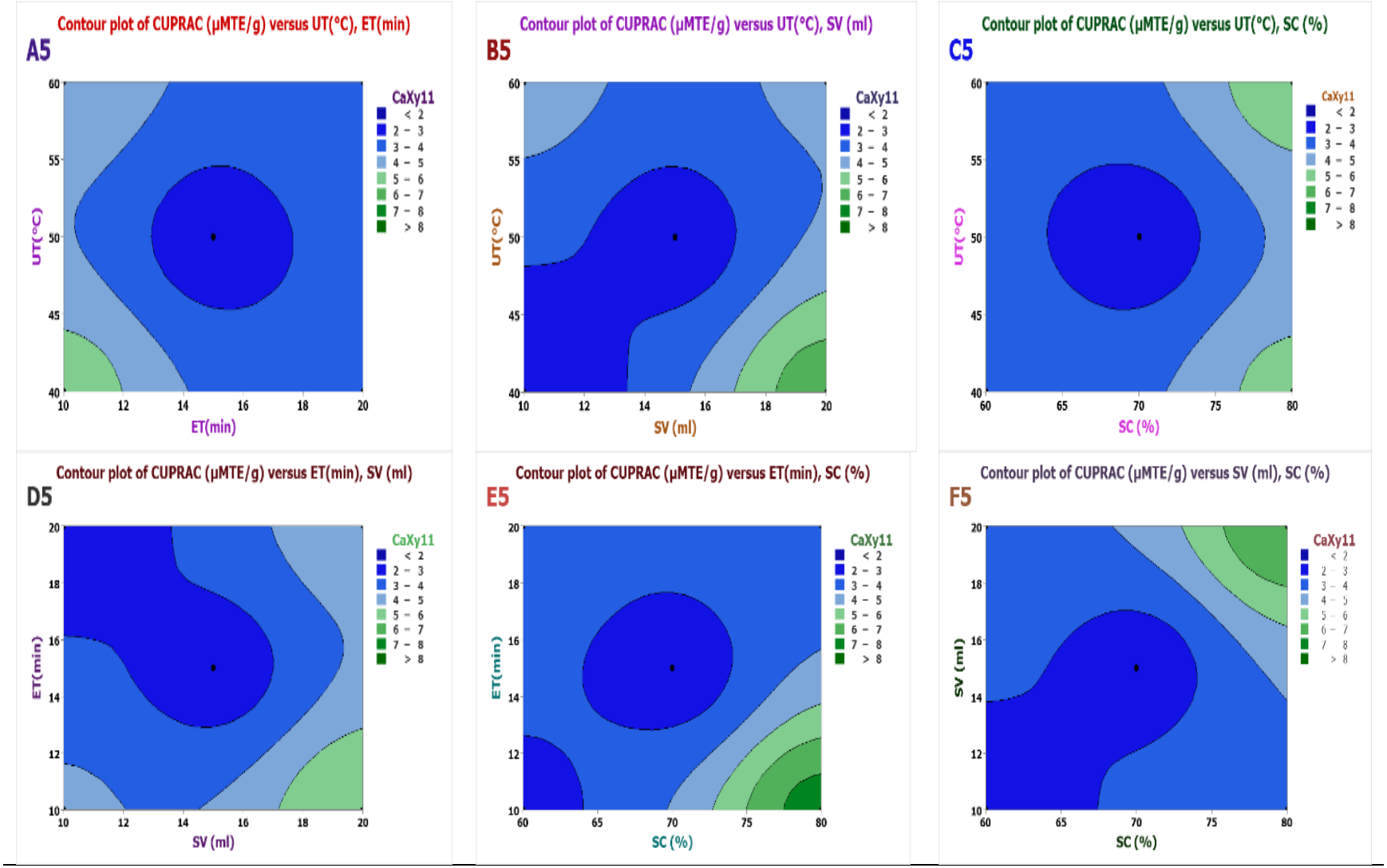


Figure 4.49 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaXy11

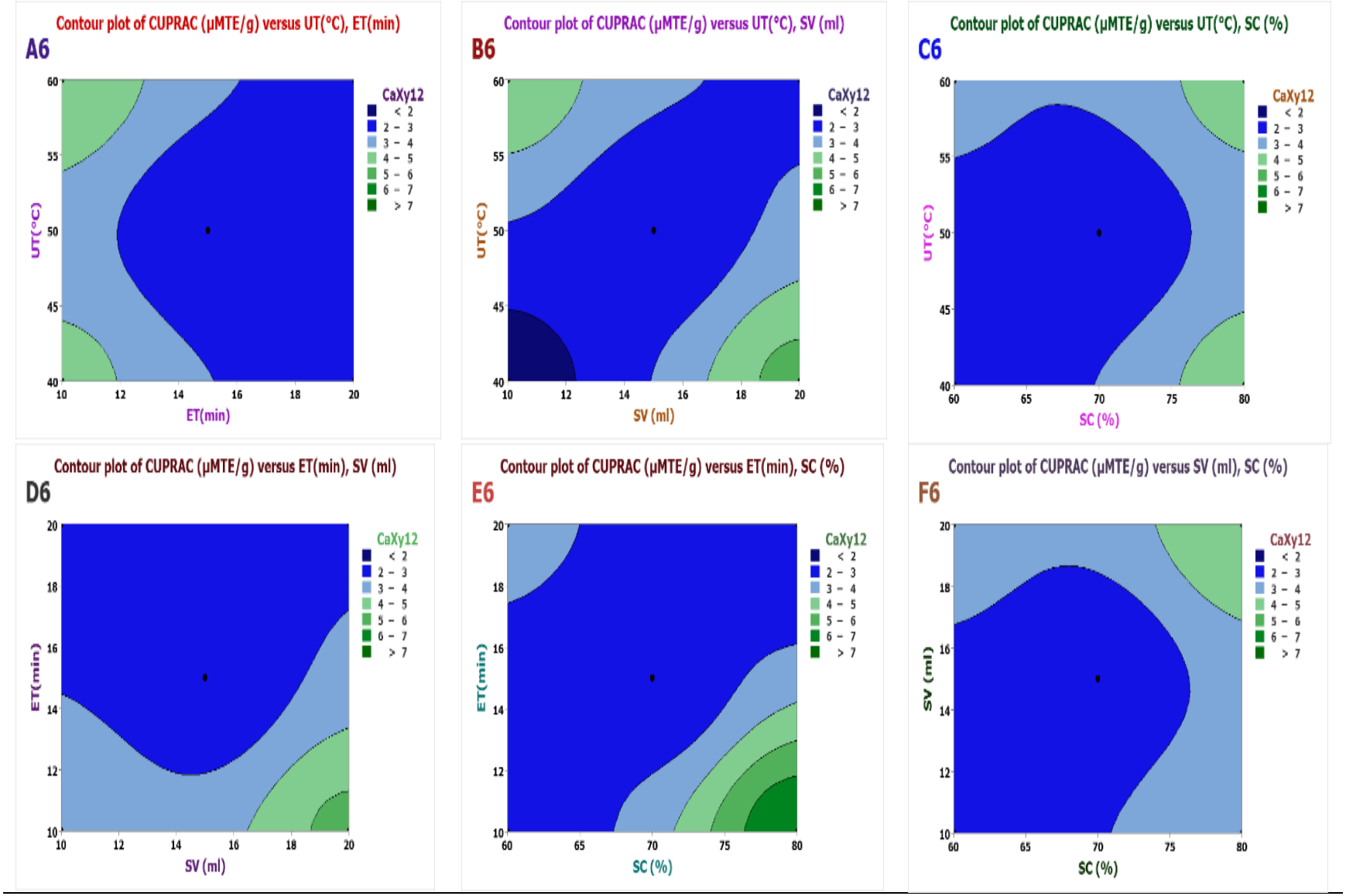


Figure 4.50 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaXy12

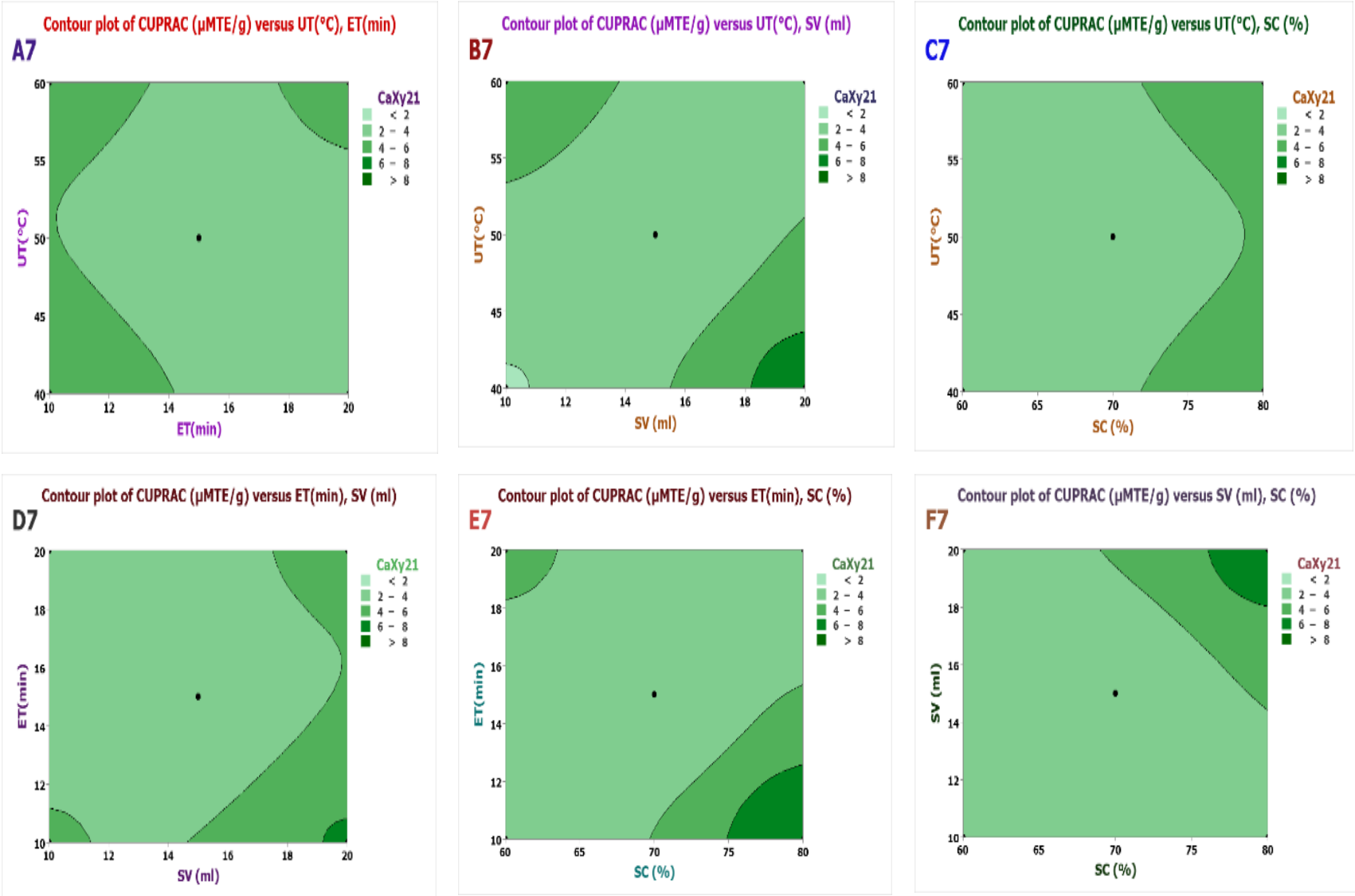


Figure 4.51 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaXy21

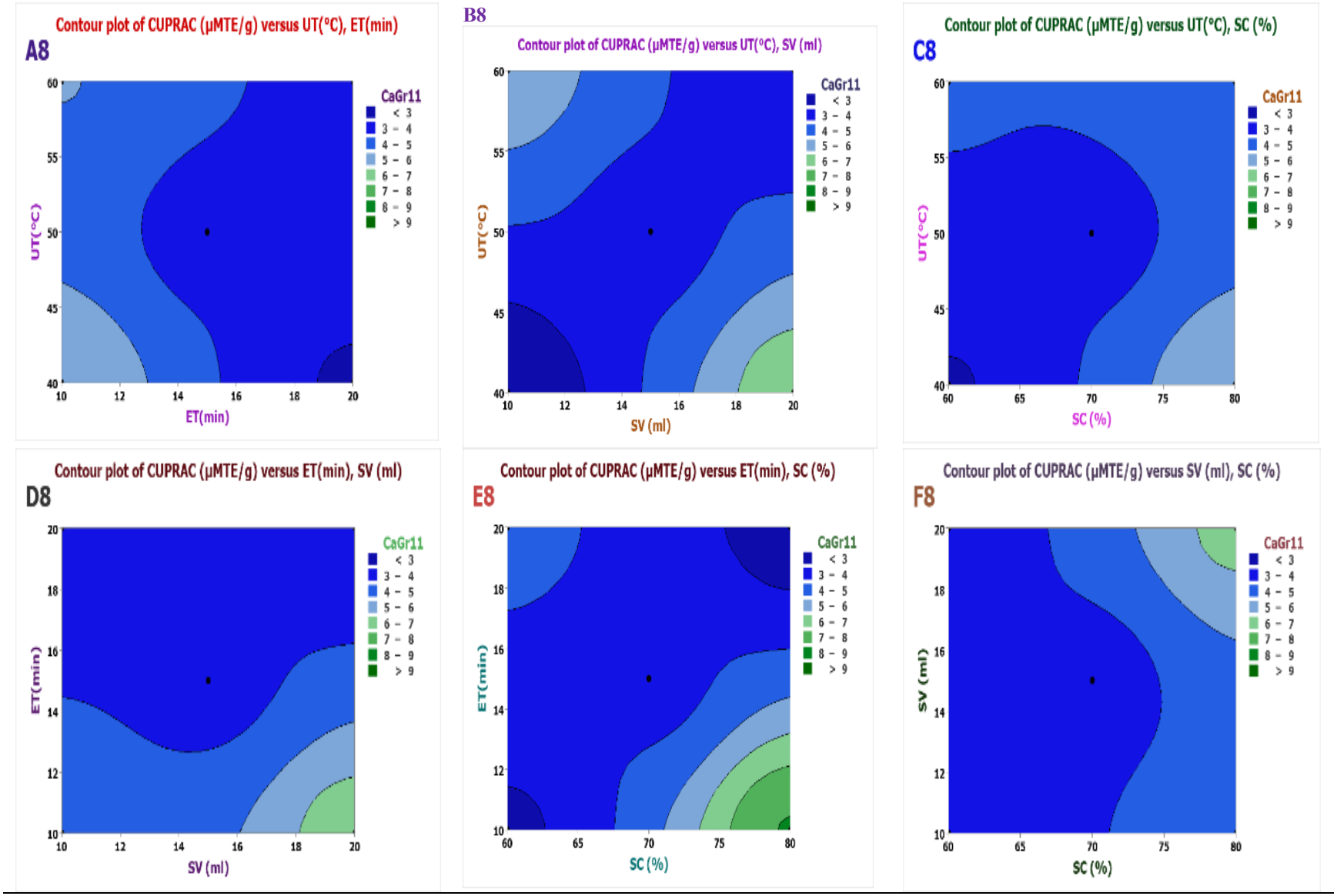


Figure 4.52 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGr11

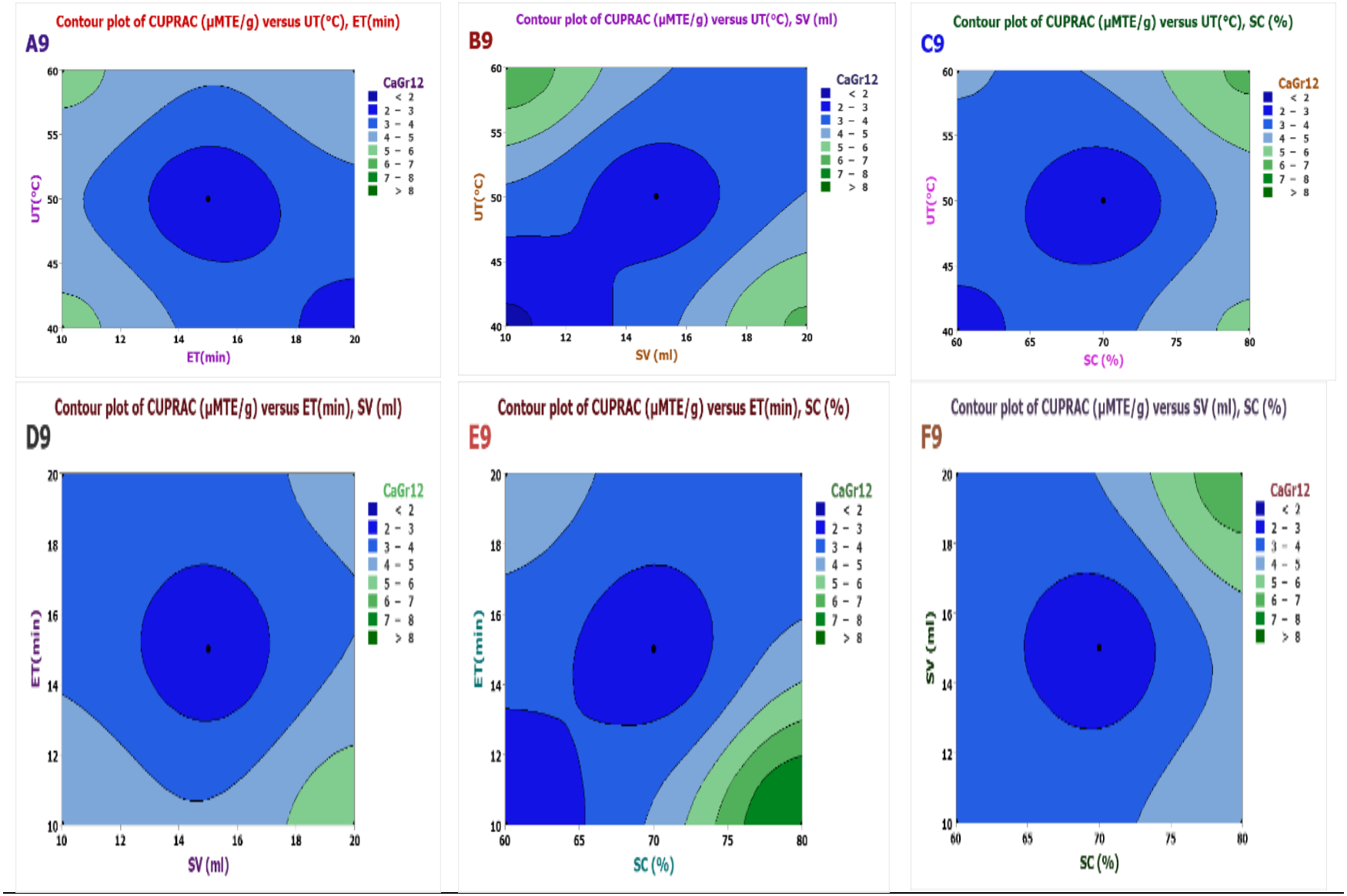


Figure 4.53 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGr12

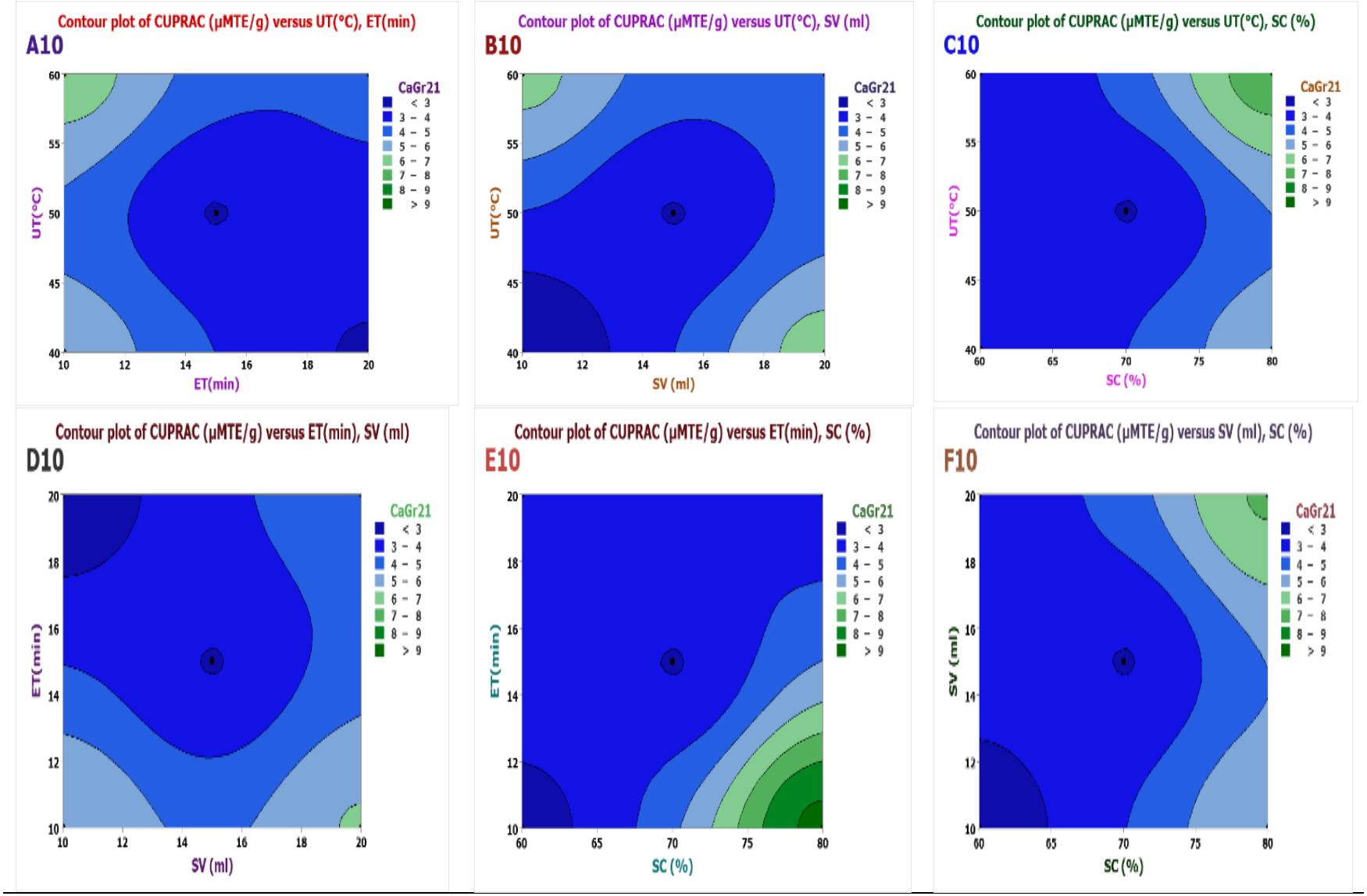


Figure 4.54 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGr21

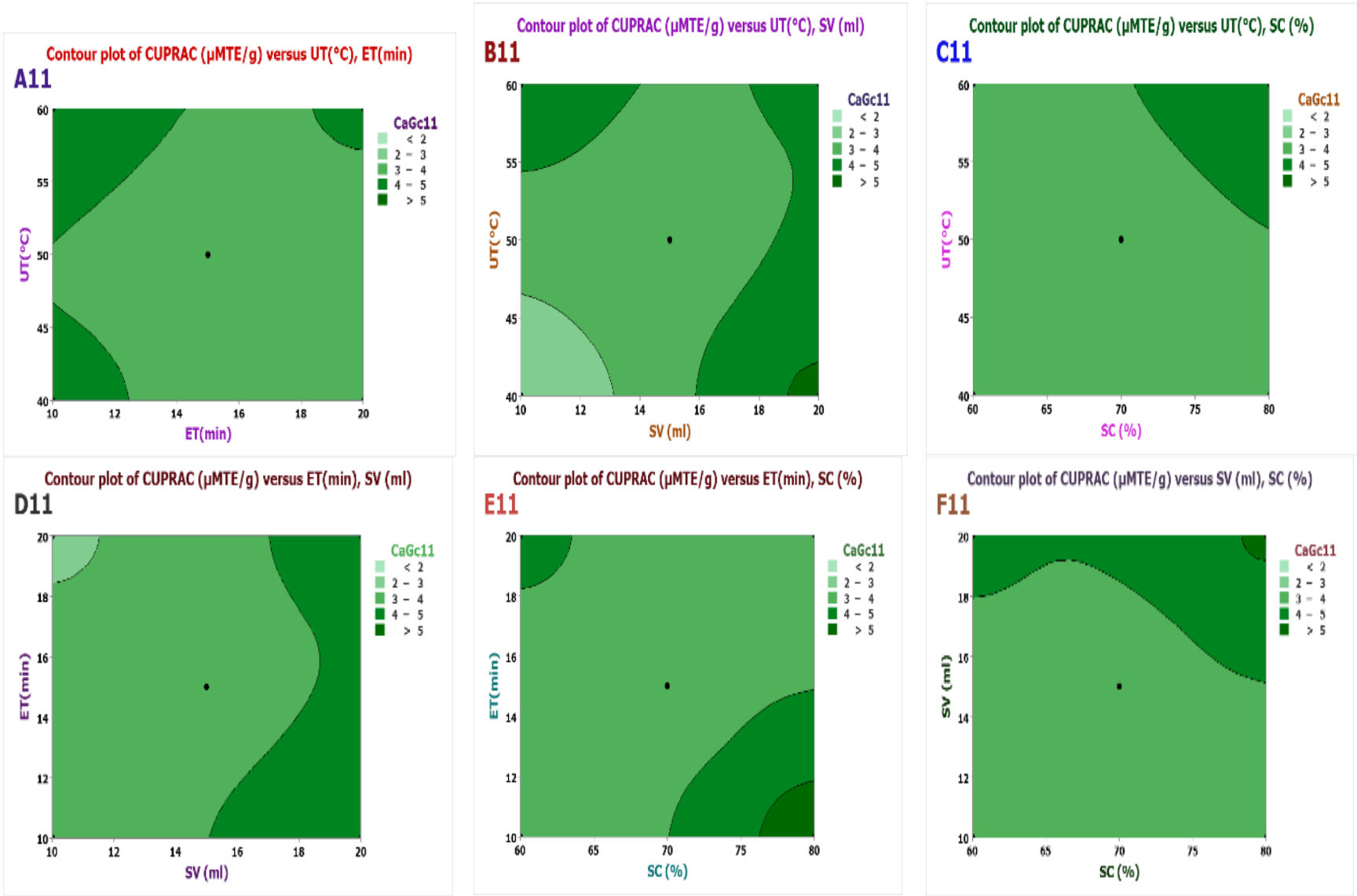


Figure 4.55 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGc11

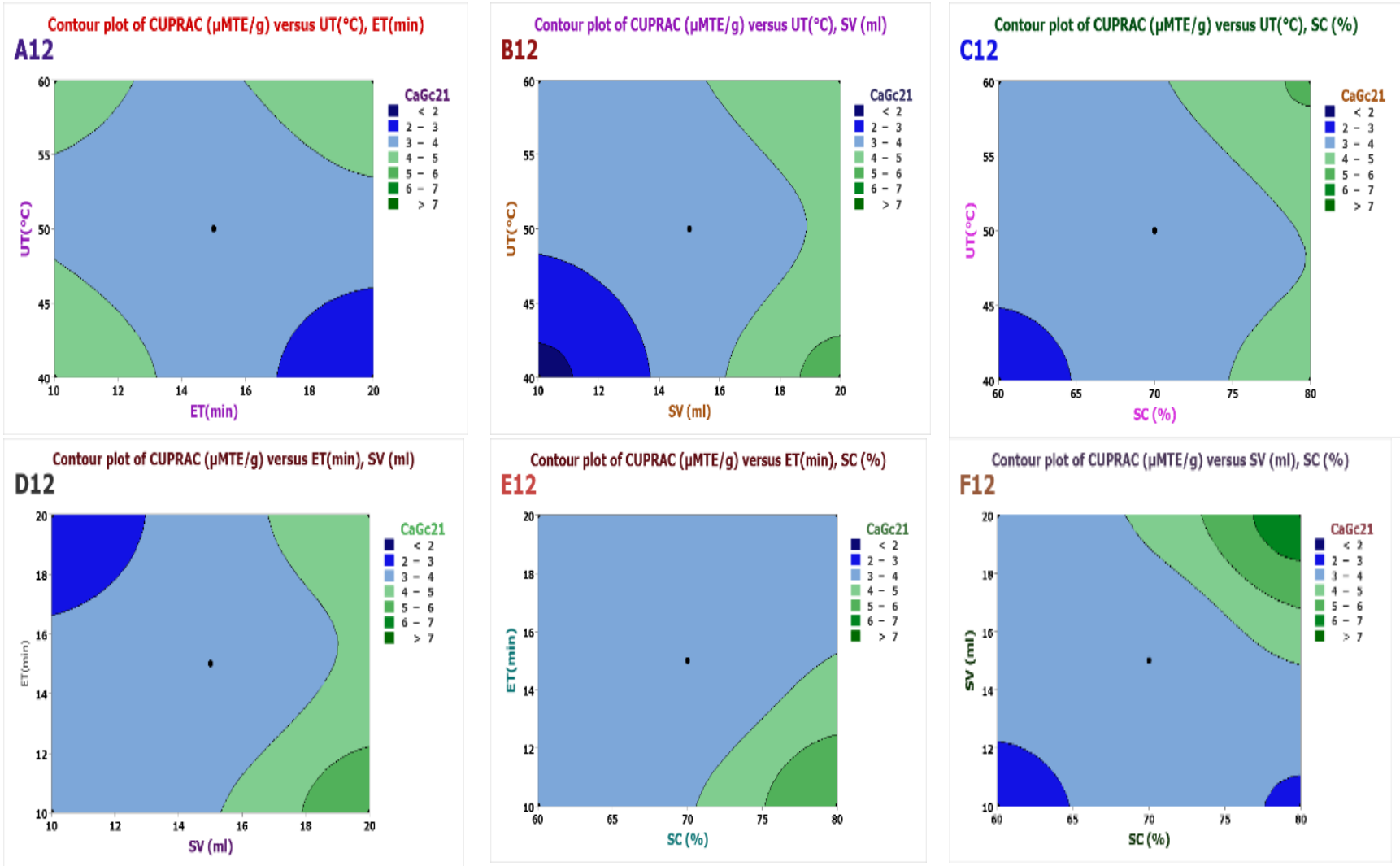


Figure 4.56 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGc21

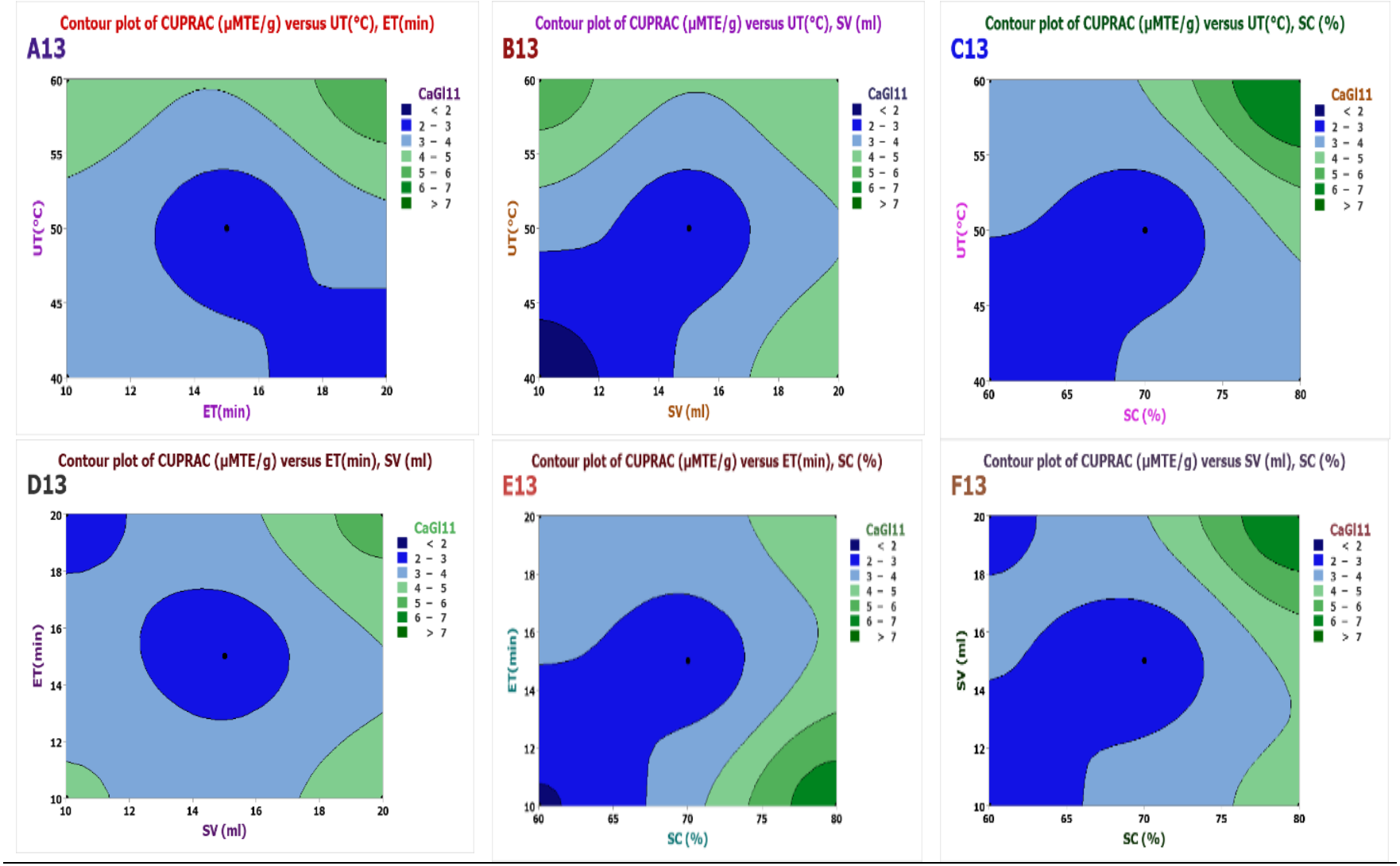


Figure 4.57 Contour plots of factors effects on CUPRAC capacity of African nutmeg peels extracted with CaGl11

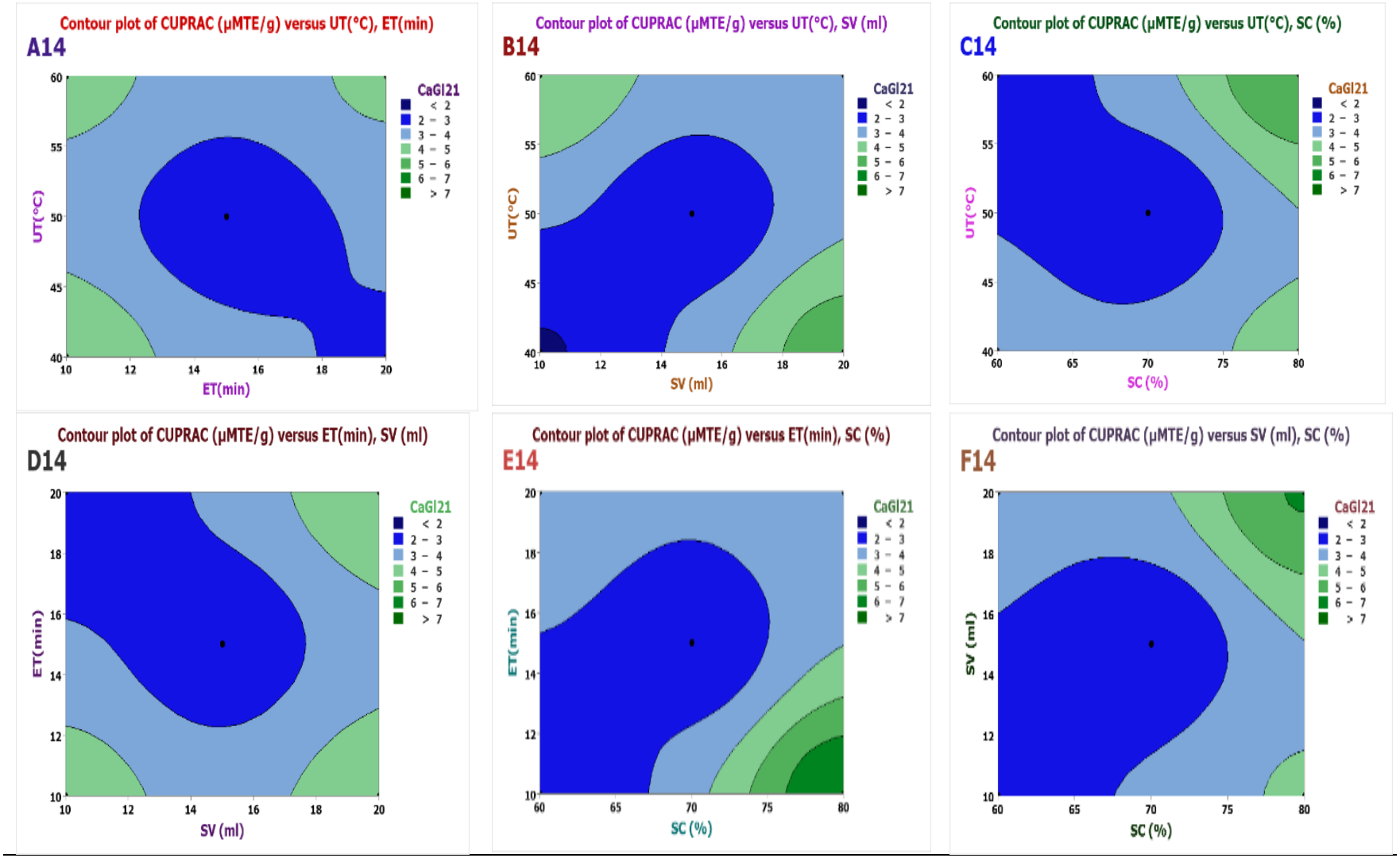


Figure 4.58 Contour plots of factor effects on CUPRAC capacity of African nutmeg peels extracted with CaGl2

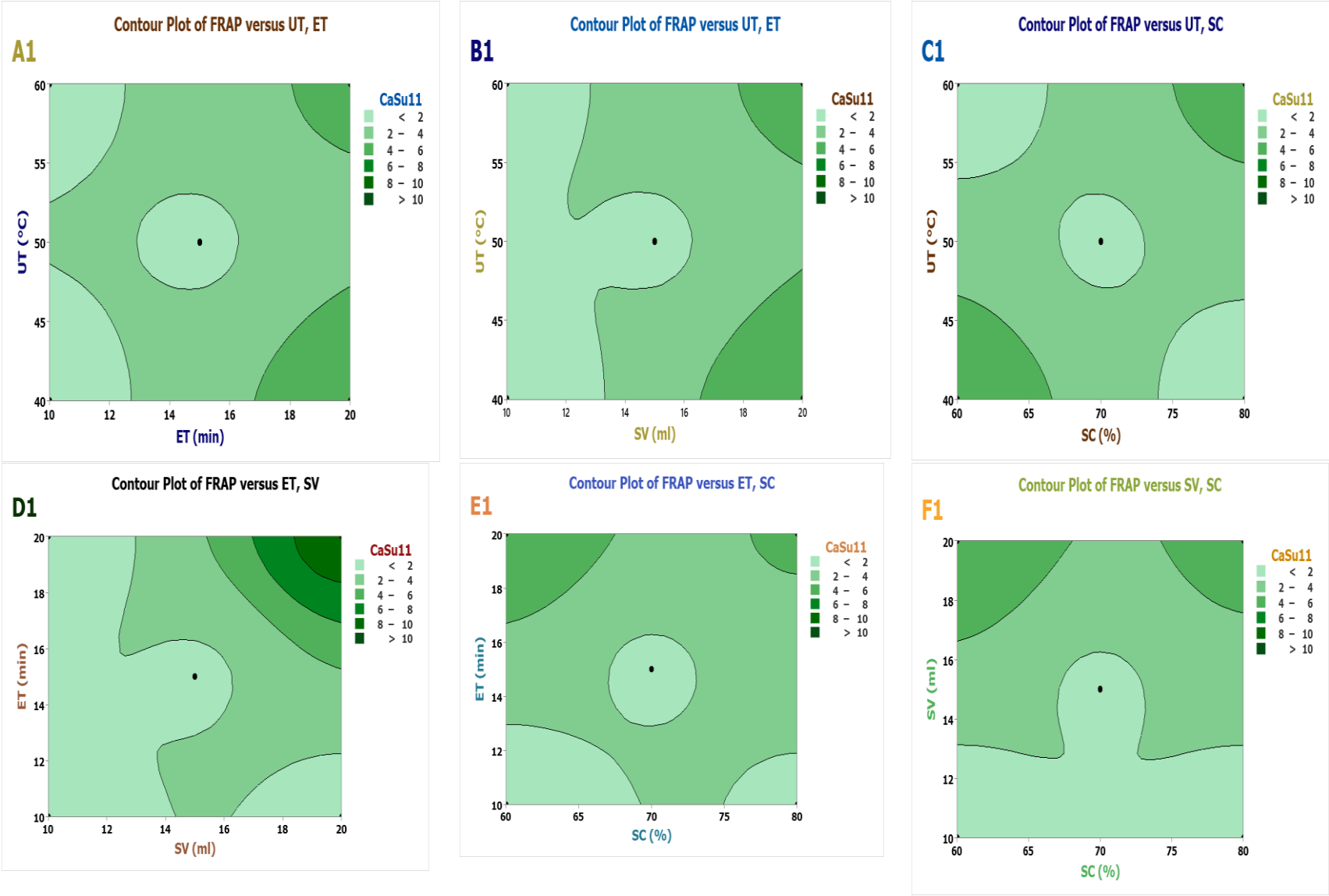


Figure 4.59 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaSu11

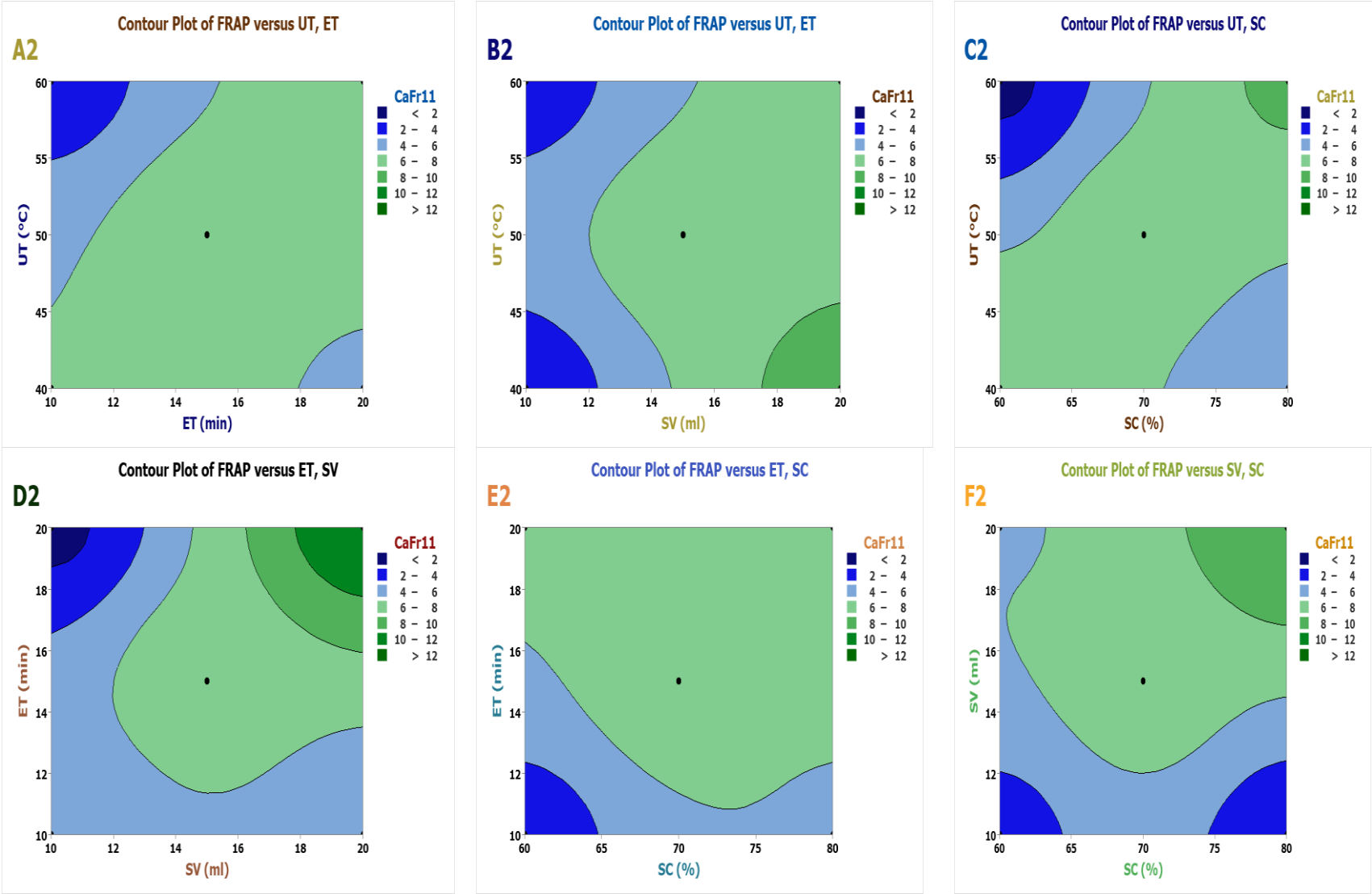


Figure 4.60 Contour plots of factors effects on FRAP potential of African nutmeg peels extracted using CaFr11

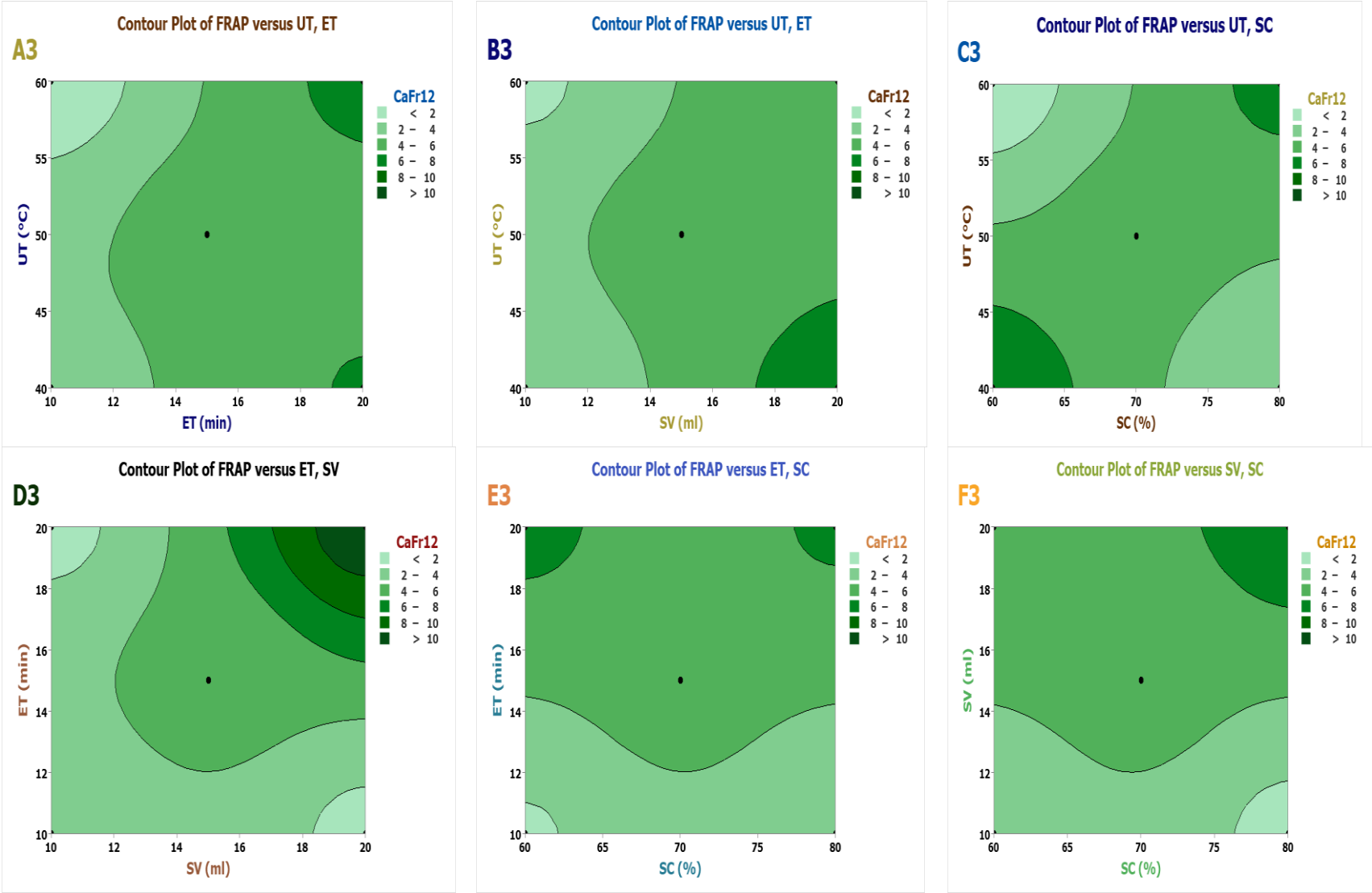


Figure 4.61 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaFr12

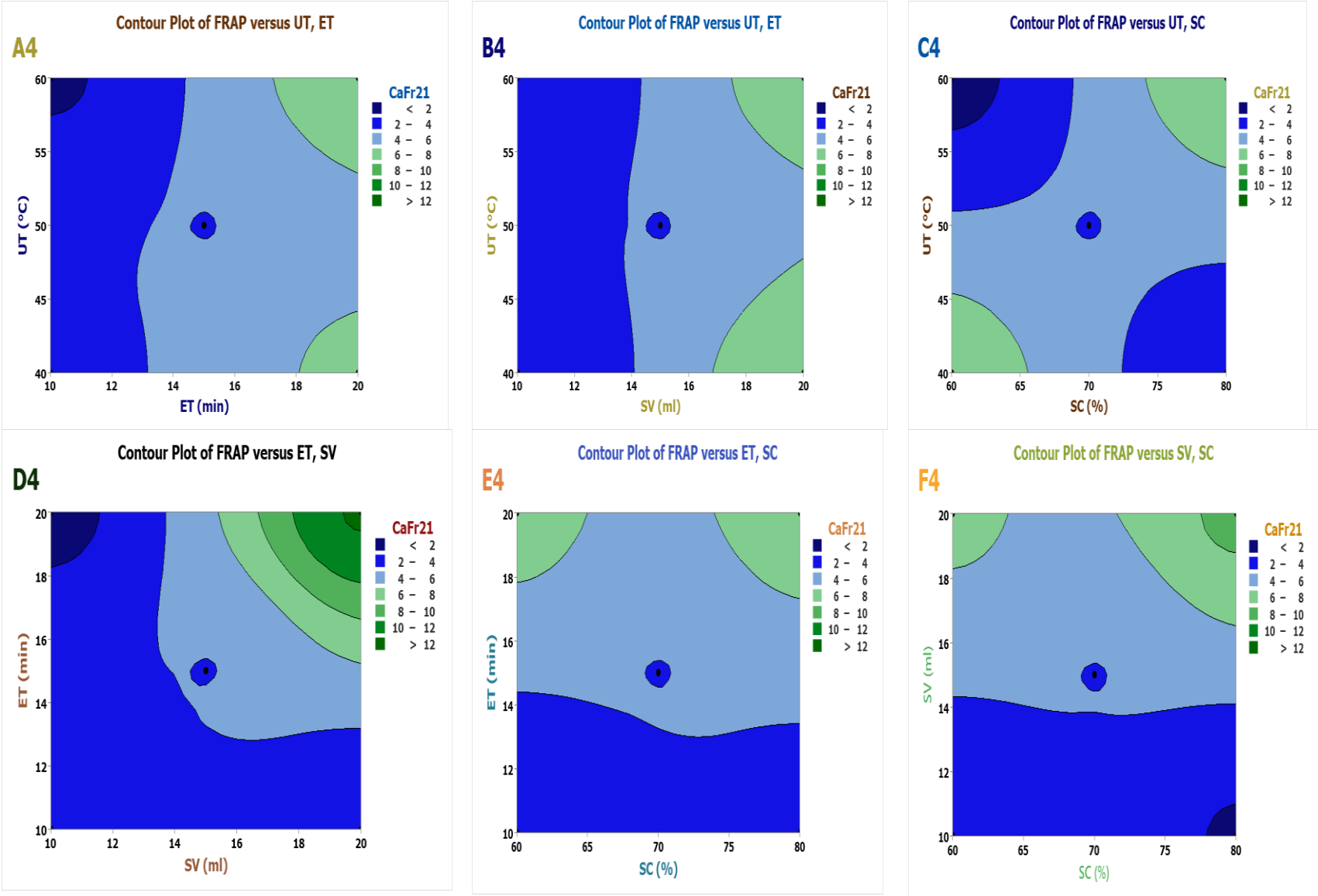


Figure 4.62 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaFr21

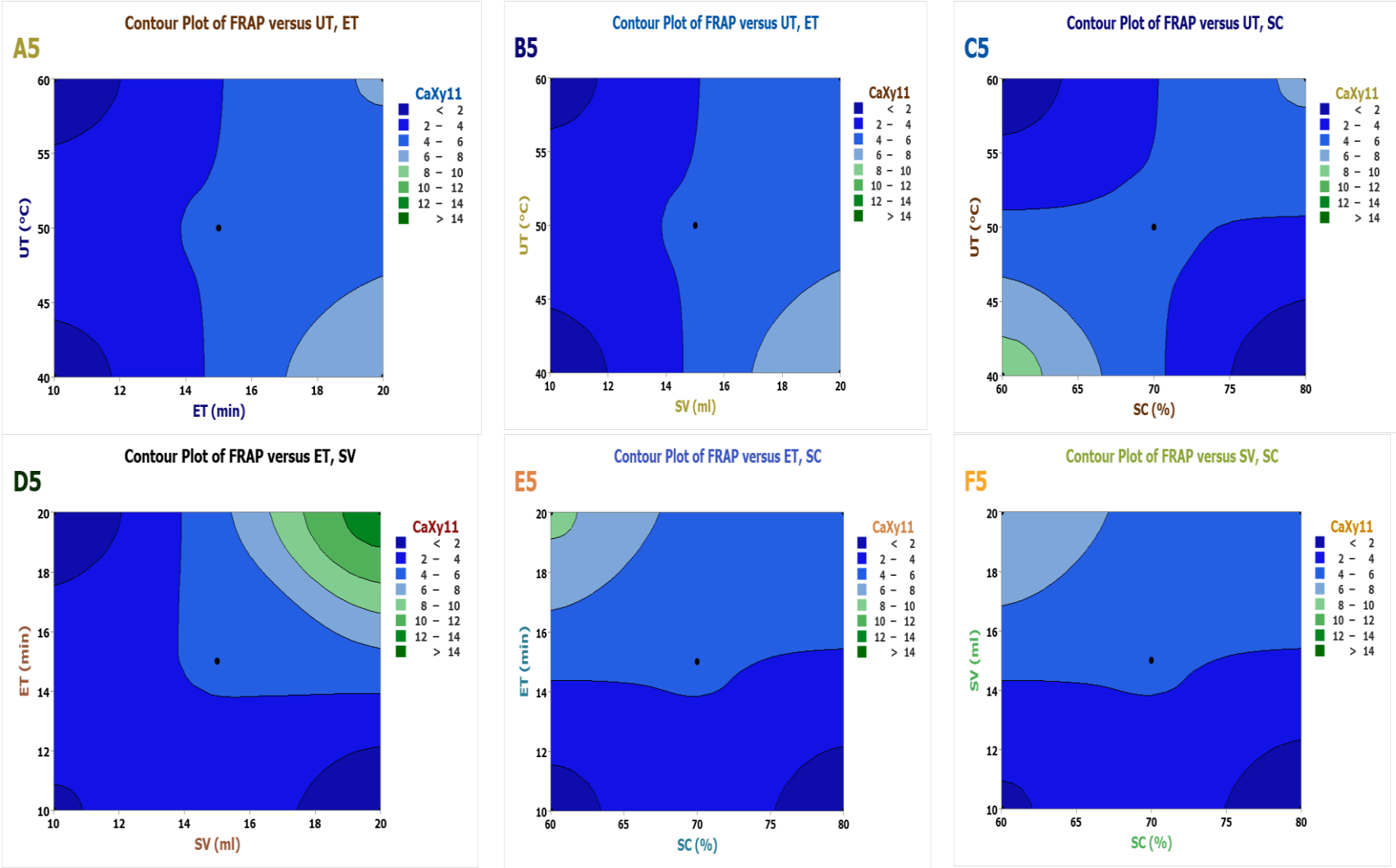


Figure 4.63 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaXy11

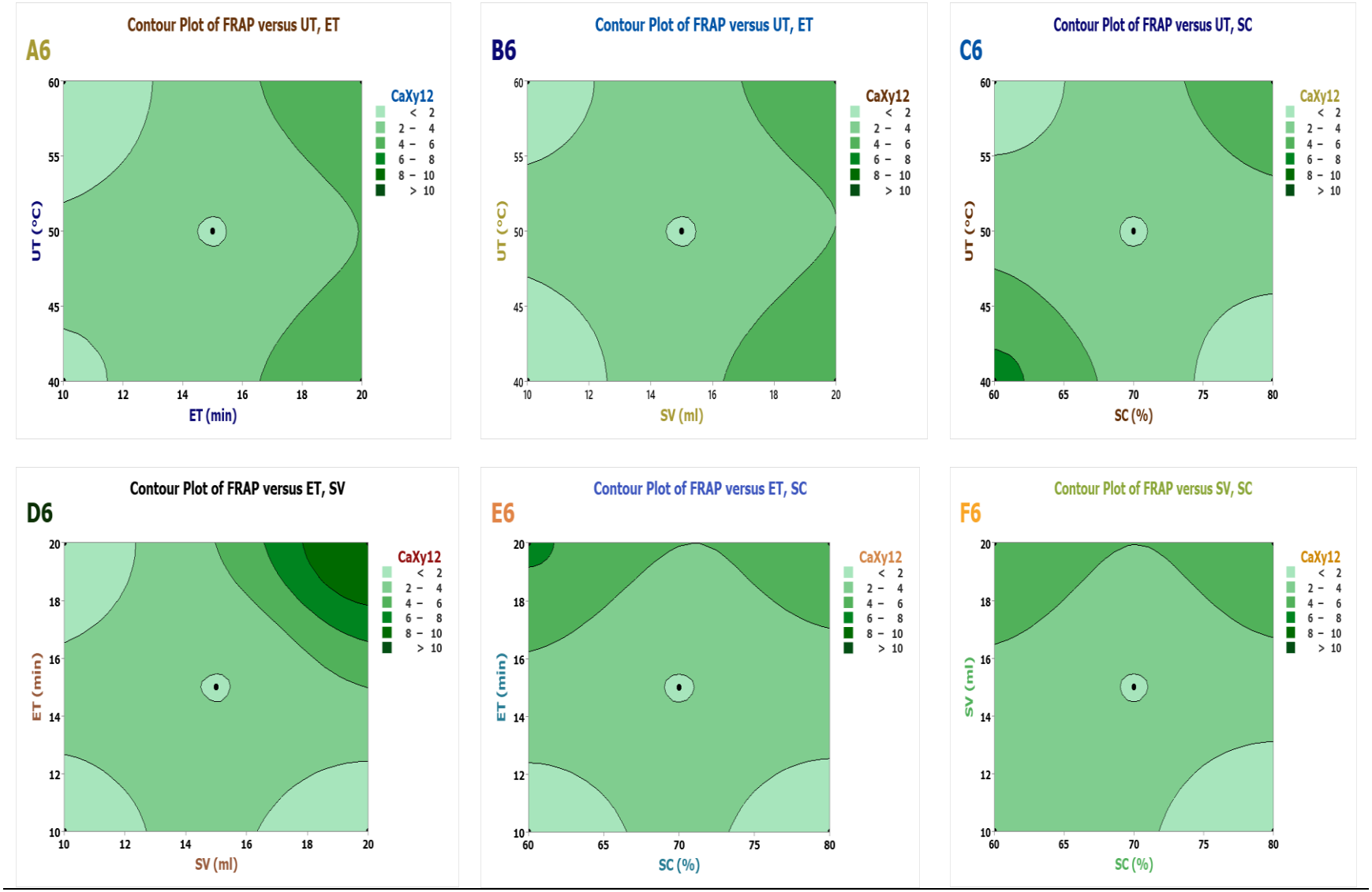


Figure 4.64 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaxY12

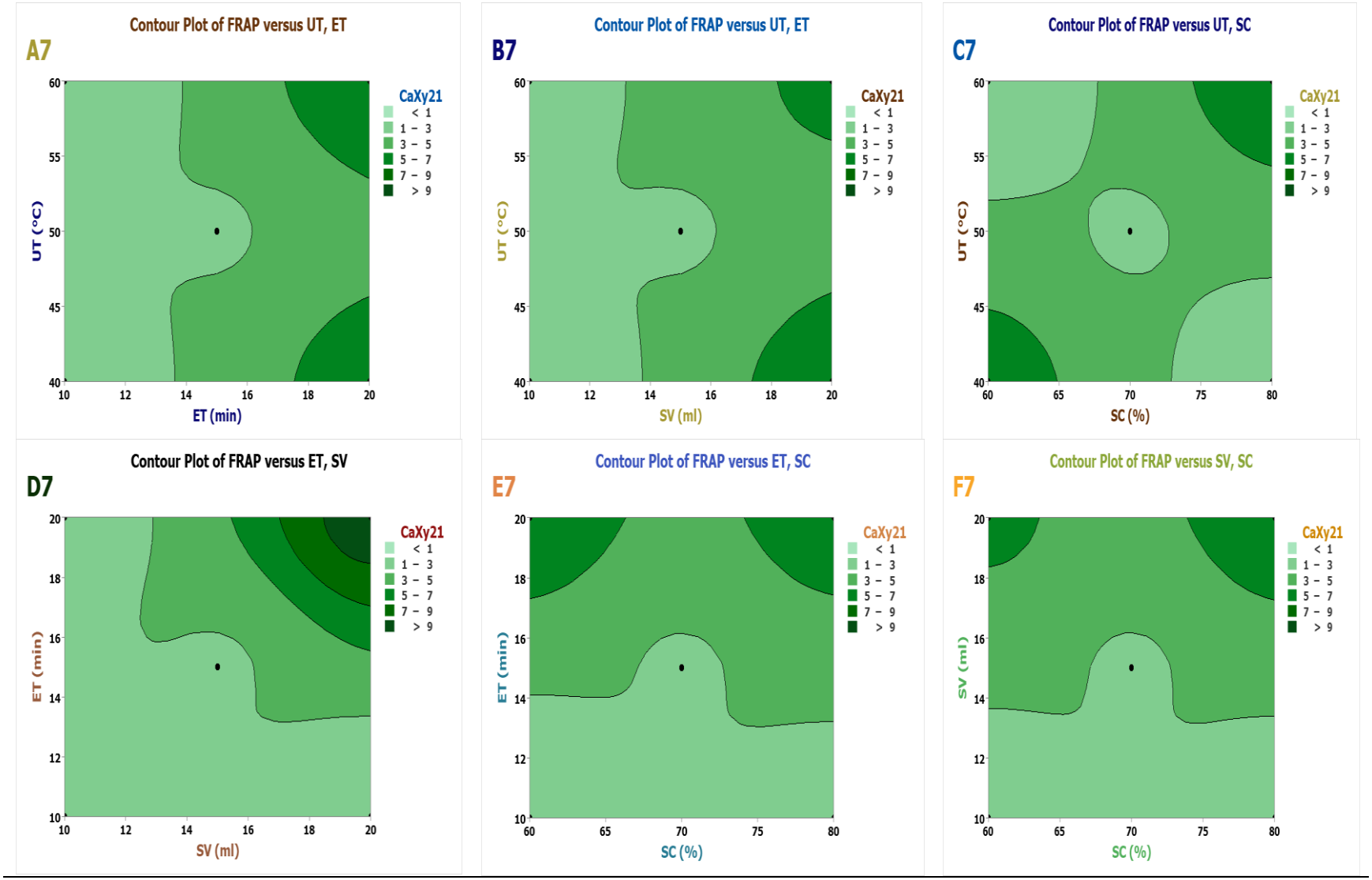


Figure 4.65 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaXy21

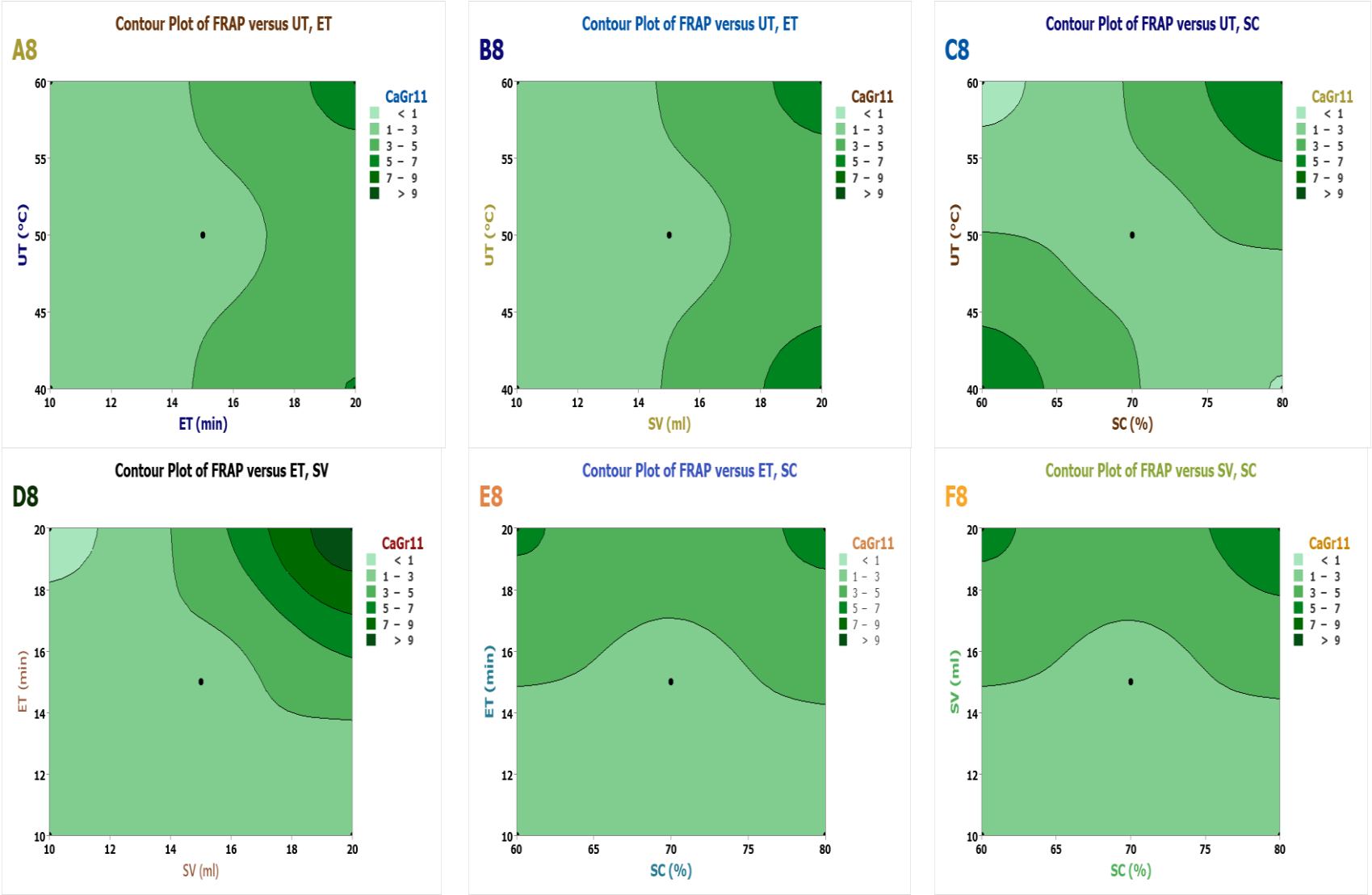


Figure 4.66 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGr11

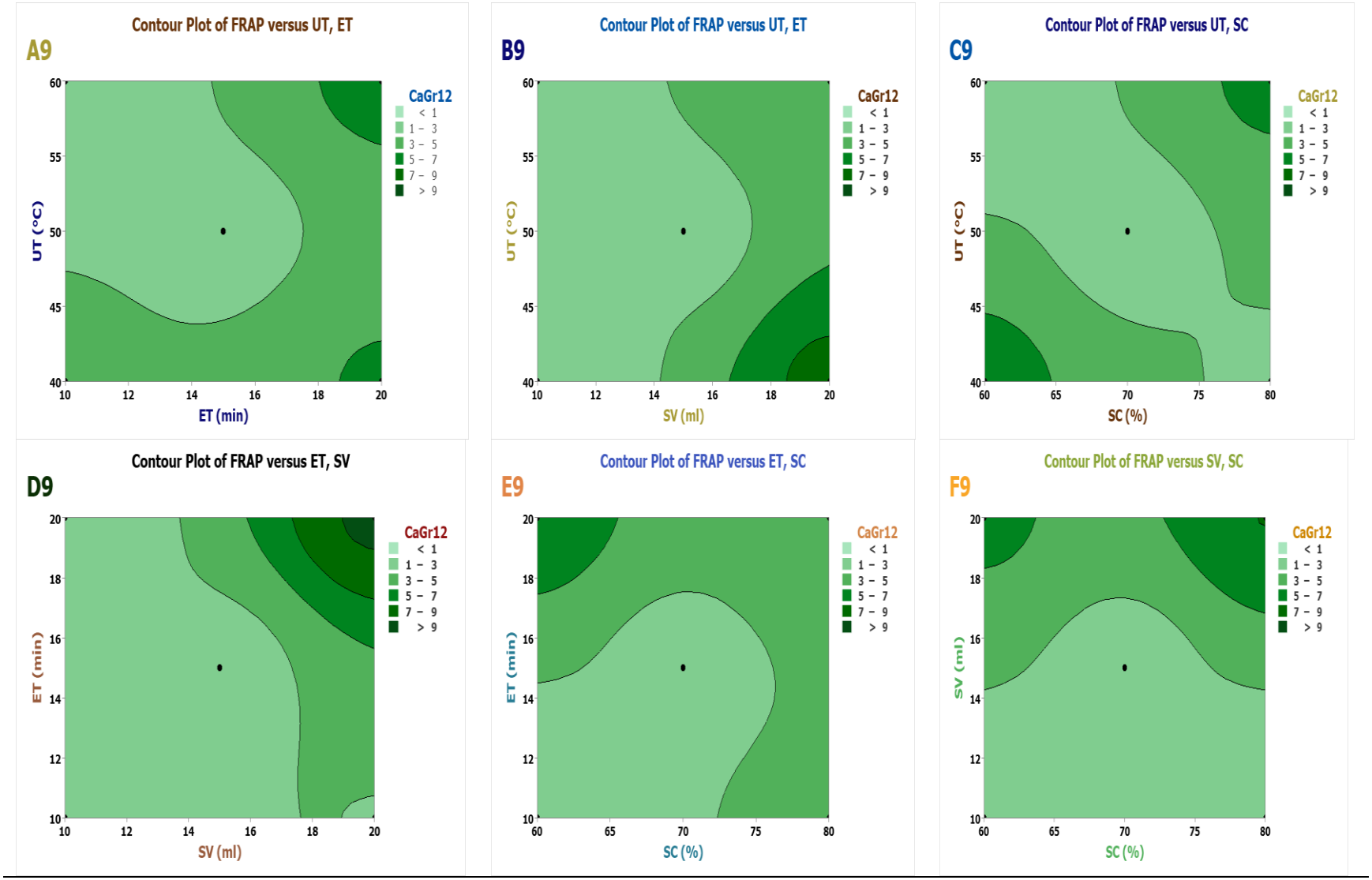


Figure 4.67 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGr12

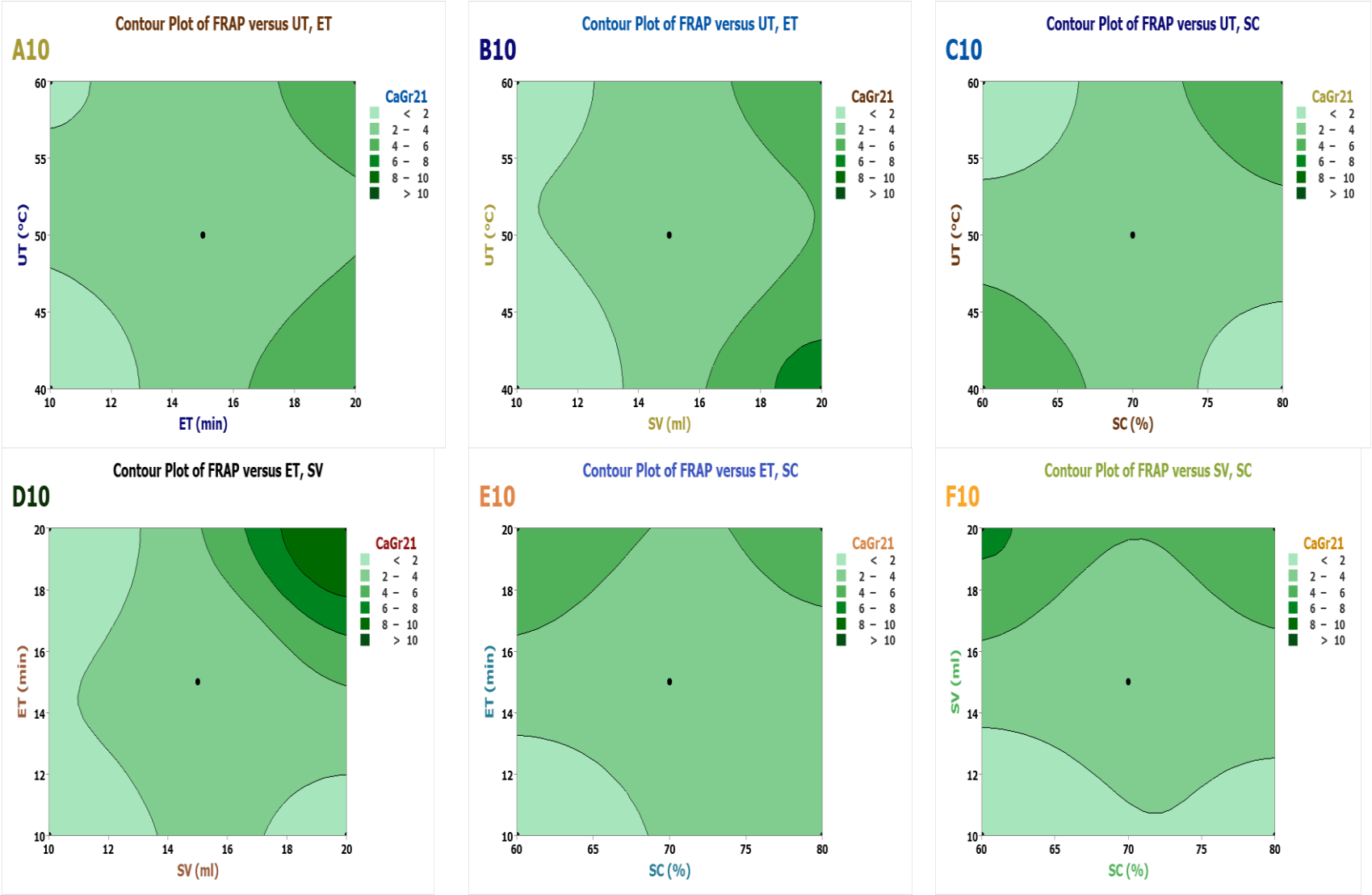


Figure 4.68 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGr21

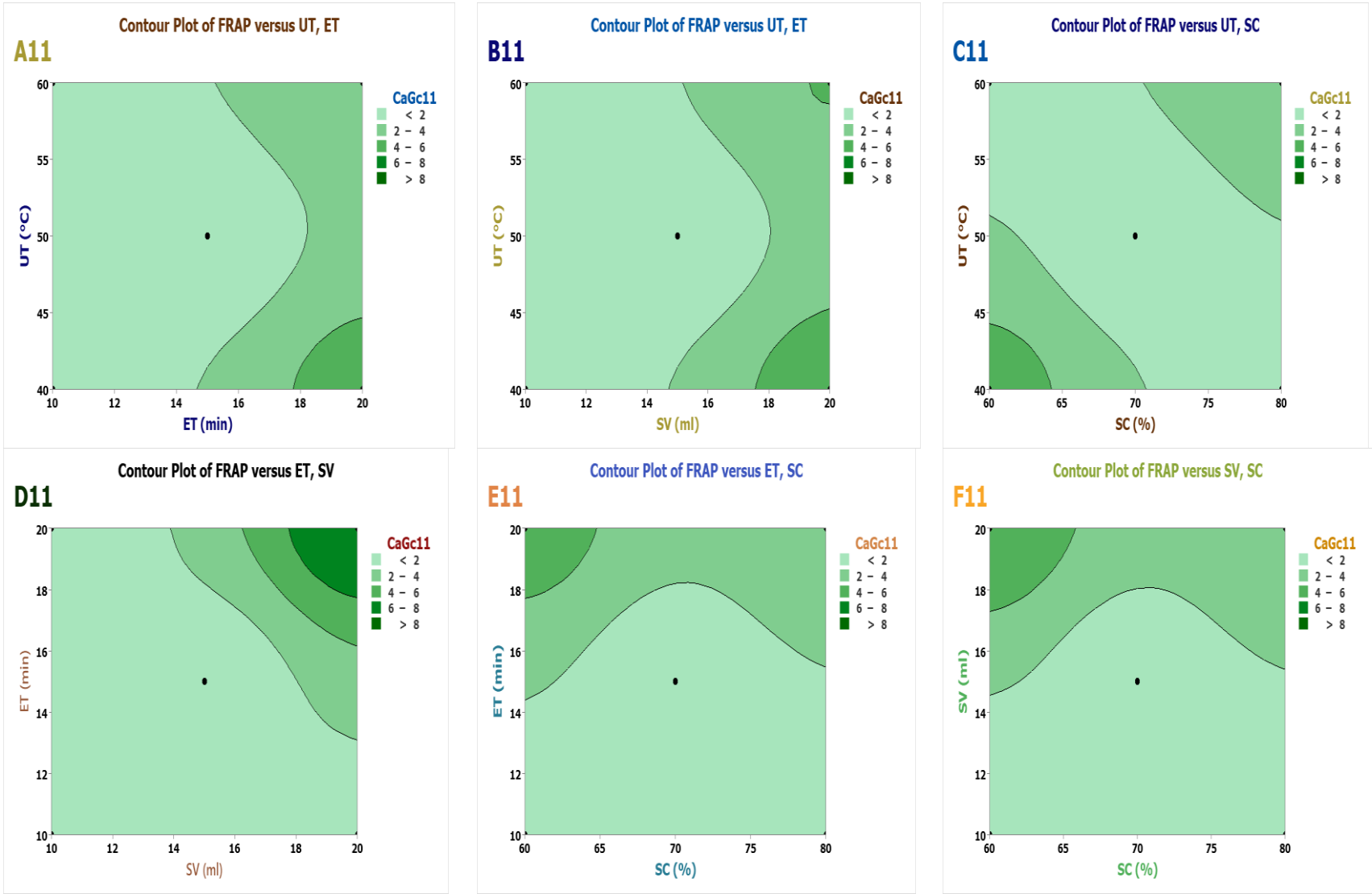


Figure 4.69 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGc11

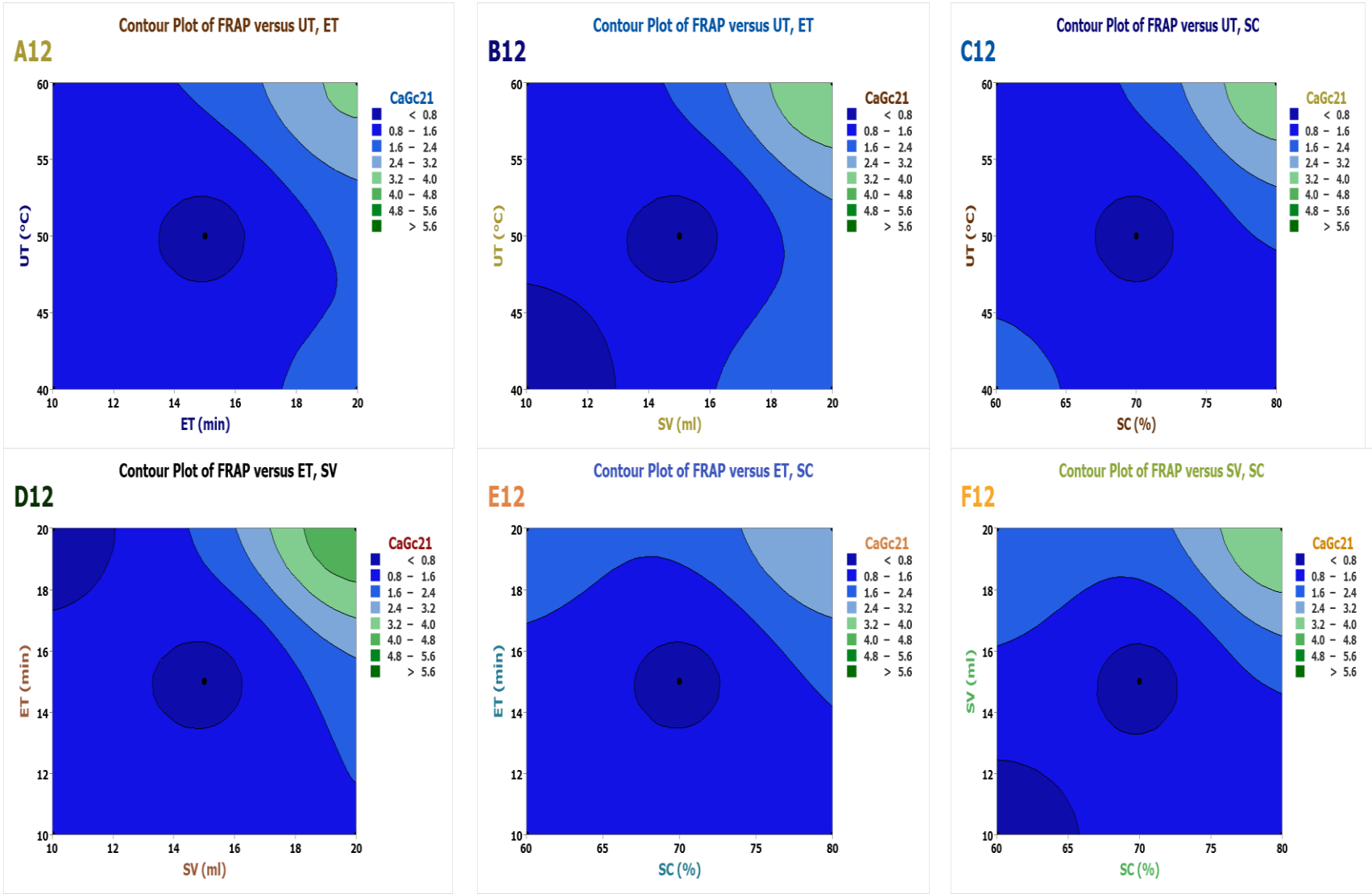


Figure 4.70 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGc21

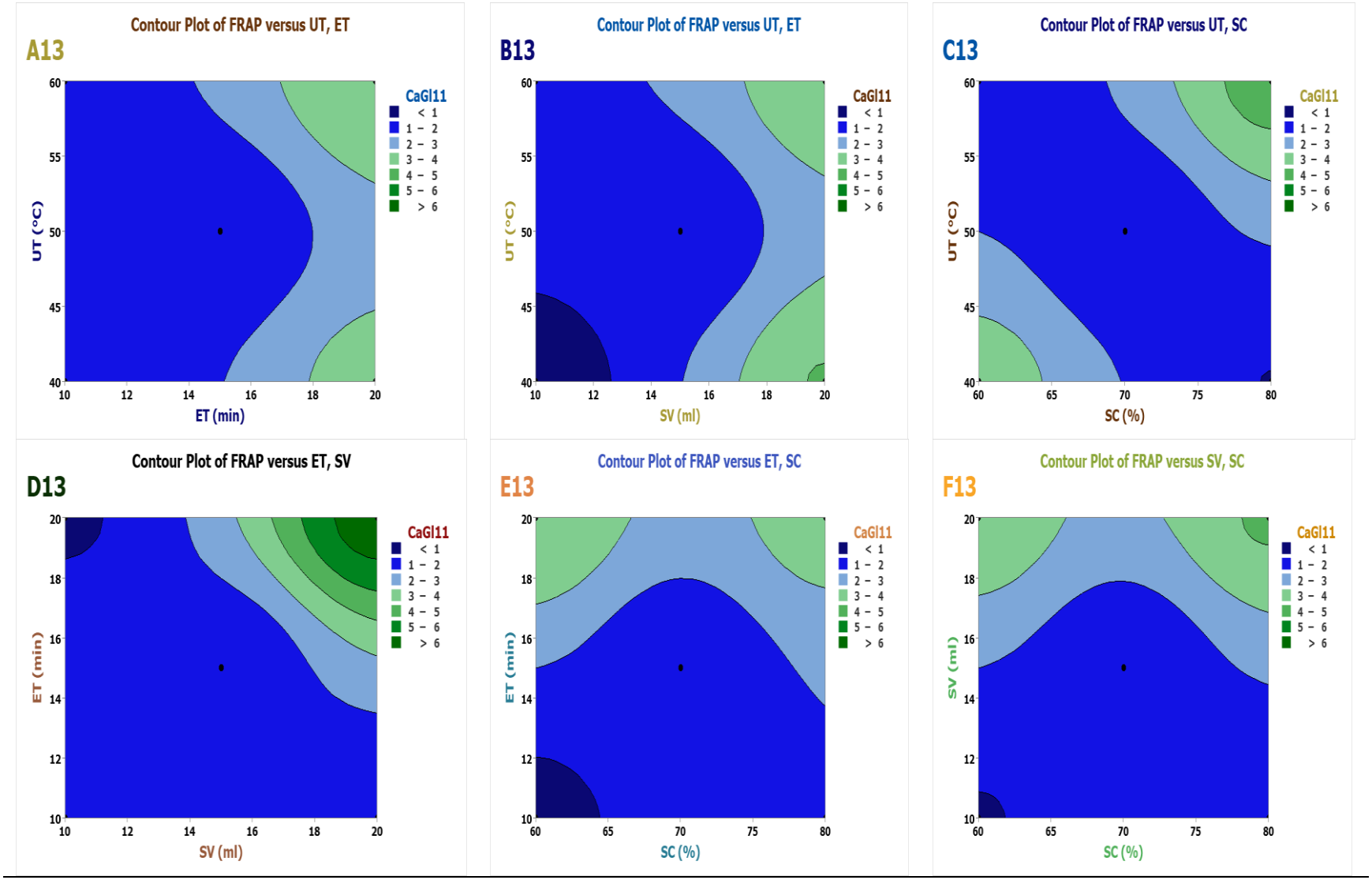


Figure 4.71 Contour plots of factors effects on FRAP potentials of African nutmeg peels using CaGl11

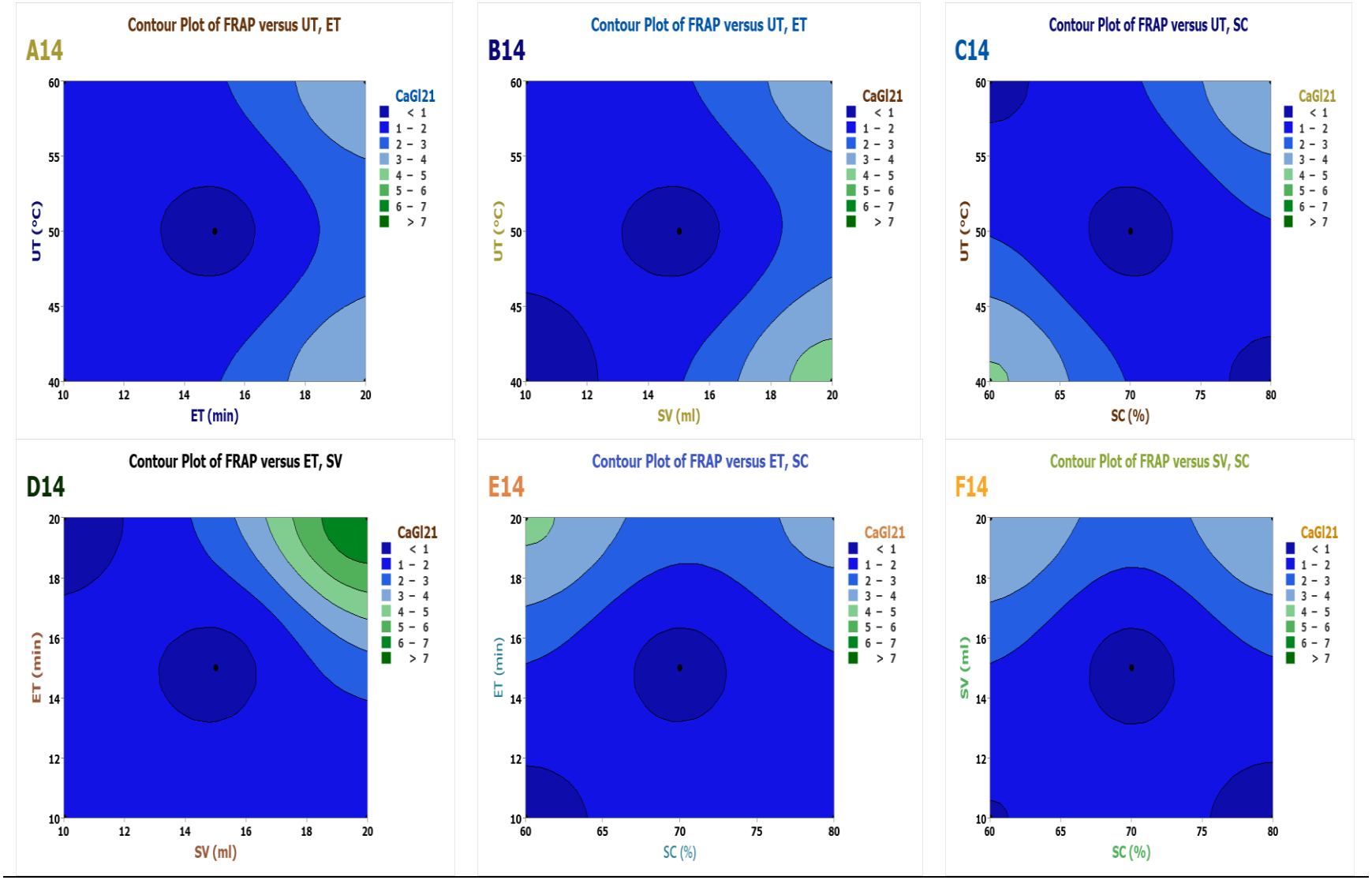


Figure 4.72 Contour plots of factors effects on FRAP potentials of African nutmeg peels extracted using CaGl21

4.6.3 Response surface methodology

Different factors affecting the efficiency of ultrasound-assisted extraction include the temperature of extraction, time of extraction, volume of solvent, and concentration of solvent. In order to optimize the extraction conditions, a comprehensive evaluation involving a four-factor, five-level, central composite design within the framework of response surface methodology (RSM) was employed, as detailed in **Table 3. 2**. The experiment's independent variables included the extraction temperature (UT), ranging from 30 to 70 ºC, the extraction time (ET), spanning 5 and 25 min, the solvent volume (SV), from 5 to 25 ml, and the solvent concentration (SC) which ranged from 50 to 90%. Experimental data were used to compute the coefficient of the polynomial equation that predicts response values. Regression equations for TPC, TFC, CUPRAC, FRAP, and DPPH calculated by response surface methodology for various responses are presented in **Table 4.10**. Analysis of variance showed that the experimental results could be well fitted with a full quadratic polynomial model for all parameters studied, except in CaSu11, CaFr21, CaXy11, and CaGc11 where linear plus interactions model perfectly fitted the TPC extraction. The analysis of variance model used for fitting the experimental results is presented in **Table 4.11**. Coefficients of determination (R^2) for TPC, TFC, CUPRAC, FRAP, and DPPH varied from 0.9977 to 1.000, 0.9985 to 1.000, 0.7004 to 0.9994, 0.7639 to 0.9999 and 0.9981 to 0.9999, respectively and are presented in **Table 4.12** with other statistical parameters calculated from ANOVA. The quadratic polynomial model, as well as the linear plus interactions models were found to be statistically significant with a non-significant lack of fit ($p < 0.05$) with respect to pure error among the parameters measured which showed that the models are statistically accurate for the data. The R^2 values closer to unity are an indication of better fitted model to experimental data, and contrary if the values of R^2 are lower, which shows that the independent variables are not predicting the values of responses accurately [122].

Table 4.10 Regression model equations for TPC, TFC, CUPRAC, FRAP, and DPPH of African nutmeg peels extracted with NADESs

NADESs			Model equation		Model
CaSu11	TPC	=	-610+20.4UT+96.0ET-44.6SV-8.46SC-1.475UT*ET-0.287UT*SV +0.115UT*SC+0.451ET*SV-0.498ET*SC+0.945SV*SC.....	**4.57**	Linear+ interaction
CaFr11	TPC	=	1829+61.4UT-7.5ET-39.7SV-88.5SC-0.191UT*UT+1.59ET*ET +4.29SV*SV+0.828SC*SC-0.468UT*ET-0.816UT*SV-0.246UT*SC +0.77ET*SV-0.498ET*SC- 0.543SV*SC.....	**4.58**	Full quadratic
CaFr12	TPC	=	-2111+52.6UT+17.3ET+102.6SV+1.2SC+0.075UT*UT+1.603ET*ET - 0.063SV*SV+0.112SC*SC-1.221UT*ET-1.281UT*SV-0.312UT*SC -0.400ET*SV- 0.015 ET*SC-0.146SV*SC.....	**4.59**	Full quadratic
CaFr21	TPC	=	-0+0.23UT+ 29.1ET+6.8 SV-5.87SC-0.271UT*ET-0.069UT*SV + 0.0737UT*SC-0.810ET*SV-0.062 ET*SC+0.214SV*SC.....	**4.60**	Linear + interaction
CaXy11	TPC	=	-1069+11.02UT+36.28ET+33.22SV+8.0SC-0.1436UT*ET-0.6877UT*SV +0.0226UT*SC+0.259ET*SV- 0.5071ET*SC+0.0386SV*SC..... .	**4.61**	Linear + interaction
CaXy12	TPC	=	172+0.66UT+18.65ET+2.74SV-0.65SC+0.1472UT*UT+0.879ET*ET +0.683SV*SV+0.1335SC*SC-0.2549UT*ET-0.5964 UT*SV -0.0411UT*SC-0.221ET*SV-0.4596ET*SC+0.2104 SV*SC.....	**4.62**	Full quadratic
CaXy21	TPC	=	523-11.74UT+12.67ET+3.39SV-10.55SC+0.1212UT*UT+0.284ET*ET +0.666SV*SV+0.0850SC*SC-0.1105UT*ET-0.3846UT*SV +0.1067UT*SC+0.195ET*SV-0.2915ET*SC-0.0549SV*SC.....	**4.63**	Full quadratic

Table 4.10 contd.

CaGr11	TPC	=	1004-1.96UT-38.3ET+2.7SV-20.15SC+0.0810UT*UT+1.749ET*ET +0.482SV*SV+0.1358SC*SC-0.201UT*ET-0.352UT*SV +0.0268UT*SC-0.113ET*SV-0.049ET*SC+0.12SV*SC	**4.64**	Full quadratic
CaGr12	TPC	=	1241-20.8UT-35.1ET+16.3SV-19.0SC+0.2804UT*UT+1.777ET*ET +1.569SV*SV+0.2016SC*SC+0.148UT*ET-0.755UT*SV +0.0393UT*SC-0.139ET*SV-0.376ET*SC-0.205SV*SC.....	**4.65**	Full quadratic
CaGr21	TPC	=	1868-36.76UT-6.9ET+16.1SV-32.91SC+0.3766UT*UT+0.741ET*ET +0.382SV*SV+0.2005SC*SC-0.281UT*ET-0.504UT*SV +0.1808UT*SC+0.153ET*SV-0.091ET*SC+0.022SV*SC.....	**4.66**	Full quadratic
CaGc11	TPC	=	-161+5.61UT+26ET+21.8SV-8.27SC-0.241UT*ET-0.445UT*SV +0.074UT*SC-.0ET*SV+0.019ET*SC+0.345SV*SC.....	**4.67**	Linear + interaction
CaGc21	TPC	=	748-0.90UT-29.0ET+22.3SV-20.04SC+0.1703UT*UT+1.068ET*ET +0.307SV*SV+0.1391SC*SC+0.012UT*ET-0.661UT*SV -0.0727UT*SC-0.637ET*SV+0.071ET*SC+0.255SV*SC.....	**4.68**	Full quadratic
CaGl11	TPC	=	1327-10.27UT-38.0ET+29.9SV-31.07SC+0.0272UT*UT+2.051ET*ET +0.827SV*SV+0.1776SC*SC-0.126UT*ET-0.705UT*SV +0.2823UT*SC-0.297ET*SV-0.225ET*SC-0.108SV*SC.....	**4.69**	Full quadratic
CaGl21	TPC	=	358-10.40UT+0.4ET+29.0SV-9.64SC+0.1517UT*UT+1.071ET*ET +0.533SV*SV+0.0950SC*SC+0.278UT*ET-0.785UT*SV +0.0432UT*SC-0.887ET*SV-0.499ET*SC+0.197SV*SC.....	**4.70**	Full quadratic

Table 4.10 contd.

CaSu11	TFC	=	1986+25.1UT-95.2ET-7.2SV-49.5SC+0.080UT*UT+1.02ET*ET +0.77SV*SV+0.133SC*SC-0.913UT*ET-1.920UT*SV -0.023UT*SC+1.28ET*SV+1.316ET*SC+1.202SV*SC.....	**4.71**	Full quadratic
CaFr11	TFC	=	-815+3.3UT+90.4ET+11.8SV+1.9SC-0.028UT*UT+0.97ET*ET +4.98SV*SV-0.267SC*SC-1.211 UT*ET-2.666UT*SV +0.715UT*SC-2.88ET*SV-0.456ET*SC+0.878 SV*SC.....	**4.72**	Full quadratic
CaFr12	TFC	=	-930-66.6UT+129ET+33SV+43.2SC+0.428UT*UT+0.231ET*ET -1.032SV*SV-0.240SC*SC-0.332UT*ET+0.140UT*SV +0.260UT*SC-1.69ET*SV-1.566ET*SC+0.644SV*SC.....	**4.73**	Full quadratic
CaFr21	TFC	=	-4442+38.19UT+95.8ET+90.6SV+67.61SC-0.4239UT*UT-1.239ET*ET -1.331SV*SV-0.4229SC*SC+0.169UT*ET-0.602UT*SV +0.1095UT*SC -1.113ET*SV-.809ET*SC+0.082SV*SC.....	**4.74**	Full quadratic
CaXy11	TFC	=	2263-35.6UT+126.0ET-41.7SV-63.7SC+0.1268UT*UT+0.922ET*ET +0.877SV*SV+0.3671SC*SC-1.232UT*ET+0.128UT*SV +0.593UT*SC-1.065ET*SV-1.216ET*SC+0.527SV*SC.....	**4.75**	Full quadratic
CaXy12	TFC	=	2792-54.4UT-99.4ET+133.1SV-44.7SC+0.709UT*UT+1.241ET*ET +1.232SV*SV+0.347SC*SC+0.304UT*ET-2.381UT*SV +0.040UT*SC+0.127ET*SV+0.486ET*SC-0.485SV*SC	**4.76**	Full quadratic
CaXy21	TFC	=	1282+7.5UT+10.3ET+0.3SV-45.9SC-0.0636UT*UT+1.303ET*ET +1.206SV*SV+0.3446SC*SC-0.410UT*ET-0.573UT*SV +0.183UT*SC+0.142ET*SV-0.451ET*SC-0.068SV*SC.....	**4.77**	Full quadratic

Table 4.10 contd.

CaGr11	TFC	=	396-21.4UT+42.0ET+58SV-17.5SC+0.156UT*UT+1.477ET*ET +1.142SV*SV+0.281SC*SC-0.130UT*ET-0.676UT*SV +0.265UT*SC+0.941ET*SV-1.388ET*SC-0.899SV*SC.....	**4.78**	Full quadratic
CaGr12	TFC	=	506-38UT+41.6ET+43.6SV-5.3SC+0.4238UT*UT+0.829ET*ET +0.829SV*SV+0.0986SC*SC-0.399UT*ET-1.061UT*SV +0.212UT*SC+0.401ET*SV-0.835ET*SC-0.189SV*SC.....	**4.79**	Full quadratic
CaGr21	TFC	=	2444-57.6UT-59.0ET+168.3SV-48.6SC +0.198UT*UT +1.280ET*ET +1.178SV*SV+ 0.246SC*SC +0.349UT*ET-1.442UT*SV +0.747UT*SC-0.583ET*SV+0.023ET*SC-1.571SV*SC.....	**4.80**	Full quadratic
CaGc11	TFC	=	-4829+90.4UT+11.9ET+448.6SV-10.4SC-1.296UT*UT-3.52ET*ET -3.19SV*SV-0.036SC*SC+2.287UT*ET-2.707UT*SV +0.567UT*SC-5.79ET*SV+0.795ET*SC-1.314SV*SC.....	**4.81**	Full quadratic
CaGc21	TFC	=	-5935+35.8UT+196.4ET+222.9SV+78.3SC-0.703UT*UT-2.353ET*ET -2.373SV*SV-0.713SC*SC+0.940UT*ET-1.9UT*SV +0.552UT*SC- 6.052ET*SV-1.237ET*SC+0.656SV*SC.....	**4.82**	Full quadratic
CaGl11	TFC	=	-485+28.2UT-35.9ET+19.5SV-2.3SC+0.075UT*UT+1.878ET*ET +2.998SV*SV+0.083SC*SC-0.401UT*ET-1.309UT*SV -0.16UT*SC-1.167ET*SV+0.117ET*SC-.127SV*SC.....	**4.83**	Full quadratic
CaGl21	TFC	=	290-1.5UT+12.8ET-27.4SV-6SC+0.204UT*UT+1.253ET*ET +1.319SV*SV+0.202SC*SC+0.642UT*ET-0.450UT*SV - 0.260UT*SC-0.389ET*SV-.034ET*SC+0.365SV*SC.....	**4.84**	Full quadratic

Table 4.10 contd.

CaSu11	CUPRAC	=	36.9-0.441UT-0.231ET-0.587SV-.532SC+0.00285UT*UT+0.03826ET*ET +0.03515SV*SV+0.00267SC*SC-0.0101UT*ET-0.00463UT*SV +0.00433UT*SC-0.0103ET*SV-0.00488ET*SC+0.00579 SV*SC.....	**4.85**	Full quadratic
CaFr11	CUPRAC	=	26-0.176UT-0.334ET-1.587SV-0.184SC+0.00282UT*UT+0.0507ET*ET +0.0798SV*SV+0.00127SC*SC-0.00585UT*ET-0.01381UT*SV +0.00182UT*SC-0.0168ET*SV-0.01232ET*SC+0.01121SV*SC.....	**4.86**	Full quadratic
CaFr12	CUPRAC	=	38.1-0.479UT-0.144ET-0.526SV-.572SC+0.00326UT*UT+0.03465ET*ET +0.03461SV*SV+0.00313SC*SC-0.00645UT*ET-0.00627UT*SV +0.00363UT*SC-0.0157ET*SV-.00587ET*SC+0.00778SV*SC.....	**4.87**	Full quadratic
CaFr21	CUPRAC	=	38.6-0.489UT-0.118ET-0.527SV-.584SC+0.00389UT*UT+0.03557ET*ET +0.03561SV*SV+0.00324SC*SC-0.00459UT*ET-0.00804UT*SV +0.00306UT*SC-0.0206ET*SV- 0.00664ET*SC+0.00946SV*SC.....	**4.88**	Full Quadratic
CaXy11	CUPRAC	=	34.5-0.408UT-0.021ET-0.651SV-0.522SC+0.0033UT*UT+0.03397ET*ET +0.03671SV*SV+0.00303SC*SC-0.00499UT*ET-0.00759UT*SV +0.00258UT*SC-0.0194 ET*SV- 0.00751ET*SC+0.01038SV*SC.....	**4.89**	Full quadratic
CaXy12	CUPRAC	=	35-0.437UT-0.068ET-0.565SV-0.522SC+0.00317UT*UT+0.03483ET*ET +0.03471SV*SV+0.00273SC*SC-0.00677UT*ET-0.00670UT*SV +0.00346UT*SC- 0.0173ET*SV-0.00621ET*SC+0.00871SV*SC.....	**4.90**	Full quadratic
CaXy21	CUPRAC	=	40.5-0.309UT-0.171ET-0.699SV-.735SC+0.00295UT*UT+0.03139ET*ET +0.03712SV*SV+0.00236SC*SC-0.00611UT*ET-0.01085UT*SV +0.00285UT*SC-0.0347ET*SV+0.00113ET*SC+0.01833SV*SC.....	**4.91**	Full quadratic

Table 4.10 contd.

CaGr11	CUPRAC	=	26.7-0.255UT+0.024ET-0.579SV-.427SC+0.00287UT*UT+0.03672ET*ET +0.03495SV*SV+0.00280SC*SC-0.00219UT*ET-0.00990UT*SV +0.00095UT*SC-0.02727ET*SV-0.00961ET*SC+0.01350SV*SC.....	**4.92**	Full quadratic
CaGr12	CUPRAC	=	30.8-0.458UT+0.305ET-0.910SV-.398SC+0.00436UT*UT+0.03358ET*ET +0.04795SV*SV+0.00239SC*SC-0.00515UT*ET-0.01067UT*SV +0.00284UT*SC-0.0216ET*SV-0.01139ET*SC+0.01098SV*SC.....	**4.93**	Full quadratic
CaGr21	CUPRAC	=	32.2-0.335UT-0.072ET-0.776SV-.473SC+0.00334UT*UT+0.03666ET*ET +0.04050SV*SV+0.00302SC*SC-0.00185UT*ET- 0.00883UT*SV +0.00112UT*SC-0.0257ET*SV-0.00863ET*SC+ 0.01283SV*SC.....	**4.94**	Full quadratic
CaGc11	CUPRAC	=	44.2-0.434UT-0.095ET-0.426SV-.791SC+0.00260UT*UT+0.03322ET*ET +0.03043SV*SV+0.00433SC*SC-0.00881UT*ET-0.00401UT*SV +0.00431UT*SC-0.0127ET*SV-0.00455ET*SC+0.00552SV*SC.....	**4.95**	Full quadratic
CaGc21	CUPRAC	=	36.9-0.449UT-0.152ET-0.585SV-.548SC+0.00280UT*UT+0.03516ET*ET +0.03366SV*SV+0.00286SC*SC-0.00803UT*ET-0.00443UT*SV +0.00398UT*SC-0.0129ET*SV-0.00530ET*SC+0.00691SV*SC.....	**4.96**	Full quadratic
CaGl11	CUPRAC	=	42.5-0.552UT-0.123ET-0.698SV-.617SC+0.00383UT*UT+0.03588ET*ET +0.03374SV*SV+0.00310SC*SC-0.00585UT*ET-0.00545UT*SV +0.00390UT*SC-0.0165ET*SV-0.00636ET*SC+0.00966SV*SC.....	**4.97**	Full quadratic
CaGl21	CUPRAC	=	39.9-0.441UT-0.083ET-0.625SV-.651SC+0.00314UT*UT+0.03781ET*ET +0.03575SV*SV+0.00358SC*SC-0.00796UT*ET-0.00695UT*SV + 0.00396UT*SC-0.0151ET*SV-0.00703ET*SC+0.00870SV*SC.....	**4.98**	Full quadratic

Table 4.10 contd.

CaSu11	FRAP	=	-8.4+0.337UT+0.829ET-1.508SV+0.109SC-0.00214UT*UT-0.0029ET*ET +0.0932SV*SV+0.00225 SC*SC-0.00799UT*ET-0.00994UT*SV +0.00085UT*SC+0.0427ET*SV-0.01365ET*SC-0.01487SV*SC.....	**4.99**	Full quadratic
CaFr11	FRAP	=	48.8 +0.302UT+1.080ET+0.962SV-2.100SC-.00100UT*UT+0.0023ET*ET +0.0265SV*SV+0.01822SC*SC-0.00444UT*ET-0.01691UT*SV +0.00195UT*SC+0.0303ET*SV-0.02024ET*SC- 0.01467SV*SC.....	**4.100**	Full quadratic
CaFr12	FRAP	=	0.5-0.085UT+1.051ET+0.681SV-.298SC+0.00140UT*UT+0.01142ET*ET +0.01073SV*SV+0.00312SC*SC-0.01086UT*ET-0.01292UT*SV +0.00363UT*SC+0.02114ET*SV-0.01580ET*SC-0.00683SV*SC.....	**4.101**	Full quadratic
CaFr21	FRAP	=	-0.49-0.127UT+1.164ET+0.85SV-0.303SC+0.0016UT*UT +0.01232ET*ET+0.0113SV*SV+0.00309SC*SC -0.01353UT*ET-0.01444UT*SV+0.00482UT*SC +0.024ET*SV-0.01659ET*SC-0.00901SV*SC	**4.102**	Full quadratic
CaXy11	FRAP	=	6.5-0.275UT+1.157ET+0.882SV-0.395SC +0.00166UT*UT +0.01045ET*ET +0.01195SV*SV +0.00281SC*SC -0.01479UT*ET-0.01327UT*SV+0.00692UT*SC +0.02258ET*SV-0.01404ET*SC- 0.01061SV*SC.....	**4.103**	Full quadratic
CaXy12	FRAP	=	25.2+0.159UT+0.846ET+0.553SV-1.166SC+0.00087UT*UT +0.00663ET*ET +0.00711SV*SV+0.00890SC*SC -0.01813UT*ET- 0.01577UT*SV+0.00283UT*SC +0.03339ET*SV-0.00772ET*SC-0.00393SV*SC.....	**4.104**	Full quadratic

Table 4.10 contd.

CaXy21	FRAP	=	7.9-0.270UT+1.662ET+0.227SV-0.447SC+0.00172UT*UT + 0.01213ET*ET+ 0.01727SV*SV+0.00319SC*SC - 0.01757UT*ET- 0.00818UT*SV+0.00660UT*SC +0.00892ET*SV- 0.01768ET*SC- 0.00394SV*SC.....	**4.105**	Full quadratic
CaGr11	FRAP	=	2.64-0.134UT+0.984ET+0.679SV-0.313SC+0.001158UT*UT +0.00996ET*ET+0.01027SV*SV+0.002605SC*SC - 0.01456UT*ET-0.01143UT*SV+ 0.00527UT*SC +0.02573ET*SV- 0.01276ET*SC- 0.00902SV*SC.....	**4.106**	Full quadratic
CaGr12	FRAP	=	42.5+0.160UT+1.541ET+0.627SV-1.713SC-0.00022UT*UT +0.00458ET*ET+0.00394SV*SV+0.01306SC*SC -0.00840UT*ET-0.01402UT*SV+0.00210UT*SC +0.00690ET*SV-0.01897ET*SC+0.00045SV*SC.....	**4.107**	Full quadratic
CaGr21	FRAP	=	-18.4+1.494UT+0.117ET-2.307SV-0.182SC+0.00062UT*UT +0.0092ET*ET+0.0808SV*SV+0.00204SC*SC -0.04042UT*ET-0.03591UT*SV-0.00766UT*SC +0.0836ET*SV+0.00888ET*SC+0.01378SV*SC.....	**4.108**	Full quadratic
CaGc11	FRAP	=	-4.2+0.120UT+0.967ET-0.986SV+0.052SC-0.00146UT*UT -0.00011ET*ET+0.05597SV*SV-0.00019SC*SC -0.01090UT*ET-0.00711UT*SV+0.00366UT*SC +0.01808ET*SV-0.00916ET*SC-0.00552SV*SC.....	**4.109**	Full quadratic
CaGc21	FRAP	=	6.4+0.111UT+0.302ET-0.631SV- 0.186SC-0.000694UT*UT +0.00246ET*ET+0.02548SV*SV+0.001509SC*SC -0.00464UT*ET-0.00175UT*SV+0.00053UT*SC +0.00639ET*SV-0.00342ET*SC+0.00027SV*SC.....	**4.110**	Full quadratic

Table 4.10 contd.

CaGl11	FRAP	=	1.3+0.207UT+0.252ET-1.029SV-0.046SC-0.00141UT*UT+0.00050ET*ET + 0.03694SV*SV+0.00128SC*SC-0.00245UT*ET+0.00036UT*SV -0.00069UT*SC+0.00779ET*SV- 0.00410ET*SC- 0.00027SV*SC.....	**4.111**	Full quadratic
CaGl21	FRAP	=	27.2+0.331UT+0.496ET-1.609SV-0.750SC-0.00289UT*UT -0.00995ET*ET+0.05419SV*SV+ 0.00502SC*SC -0.00327UT*ET+0.00033UT*SV-0.00014UT*SC +0.0023ET*SV-0.00105ET*SC+0.00246SV*SC.....	**4.112**	Full quadratic
CaSu11	DPPH	=	-1138 +14.62UT+30.25ET+1.67SV+16.88SC-0.1321UT*UT -0.3104ET*ET-0.3698SV*SV-0.1275SC*SC -0.3717UT*ET+0.1919UT*SV+0.0193UT*SC	**4.113**	Full quadratic
CaFr11	DPPH	=	-662+16.25UT+18.71ET+2.56SV+4.52SC-0.1126UT*UT -0.315ET*ET-0.070SV*SV-0.0293SC*SC -0.1555UT*ET-0.0317UT*SV-0.0149UT*SC.....	**4.114**	Full quadratic
CaFr12	DPPH	=	-1825+28.17UT+45.73ET+7.48SV+23.25SC-0.1810UT*UT -0.6751ET*ET-0.1639SV*SV-0.1573SC*SC -0.4851UT*ET-0.0662UT*SV-0.0270UT*SC.....	**4.115**	Full quadratic
CaFr21	DPPH	=	-1613+22.94UT+18.77ET+27.23SV+22.02SC-0.1460UT*UT -0.4610ET*ET-0.7156SV*SV-0.1270SC*SC -0.0727UT*ET-0.1384UT*SV- 0.0770UT*SC.....	**4.116**	Full quadratic
CaXy12	DPPH	=	-1175+15.29UT+27.55ET+25.34SV+14.00SC-0.1824UT*UT-.583ET*ET -0.753SV*SV-0.1331SC*SC-0.1452UT*ET-0.0790UT*SV+0.0872UT*SC...	**4.117**	Full quadratic

Table 4.10 contd.

CaGr11	DPPH	=	-1070+15.1UT+21.55ET+7.61SV+16.79SC-0.1488UT*UT-0.456ET*ET -0.446SV*SV-0.1267SC*SC-0.1262UT*ET+0.0823UT*SV+0.0042UT*SC	**4.118**	Full quadratic
CaGr12	DPPH	=	-1207+18.22UT+6.30ET+37.73SV+15.04SC- 0.0694UT*UT -0.4990ET*ET-0.3112SV*SV-0.0920SC*SC +0.1931UT*ET-0.5803UT*SV-0.0662UT*SC.....	**4.119**	Full quadratic
CaGr21	DPPH	=	-1882+28.05UT+25.57ET+32.67SV+23.70SC-0.1495UT*UT -0.5162ET*ET-0.6118SV*SV-0.1403SC*SC -0.1993UT*ET-0.2827UT*SV-0.0827UT*SC.....	**4.120**	Full quadratic
CaGc11	DPPH	=	-1185+17.24UT+13.16ET+19.62SV+16.87SC-0.1557UT*UT -0.349ET*ET-0.410SV*SV-0.1268SC*SC -0.0645UT*ET-0.1873UT*SV+0.0316UT*SC.....	**4.121**	Full quadratic
CaGc21	DPPH	=	-898 +13.41UT+10.61ET+6.34SV+15.72SC-0.0836UT*UT -0.2896ET*ET-0.4033SV*SV-0.0965SC*SC -0.0113UT*ET+0.0647UT*SV-0.0681UT*SC	**4.122**	Full quadratic
CaGl11	DPPH	=	-304+3.08UT+3.62ET+1.12SV+6.20SC+0.0028UT*UT -0.1005ET*ET- 0.0170SV*SV-0.0244SC*SC +0.0028UT*ET-0.0292UT*SV-0.0464UT*SC.....	**4.123**	Full quadratic
CaGl21	DPPH	=	-1978+29.58UT+34.52ET+28.89SV+24.33SC-0.1803UT*UT -0.7364ET*ET-0.6074SV*SV-0.1497SC*SC -0.2266UT*ET-0.2280UT*SV- 0.0680UT*SC.....	**4.124**	Full quadratic

Table 4.11 Analysis of variance model for fitting experimental results

NADESs	Model	TPC		TFC		CUPRAC		FRAP		DPPH	
		F-value	P-value	F-value	P-value	F-value	P-value	F-value	P-value	F-value	P-value
CaSu11	UT	3.18	0.079	15.12	**0.000**	9.81	**0.002**	9.67	**0.003**	0.11	0.741
	ET	6.44	**0.013**	0.03	0.868	3.21	0.077	0.21	0.647	39.82	**0.000**
	SV	36.53	**0.000**	16.51	**0.000**	107.44	**0.000**	46.84	**0.000**	0.22	0.640
	SC	12.02	**0.001**	4.19	**0.044**	9.40	**0.003**	2.05	0.157	0.00	0.981
	UT*UT	2.67	0.106	0.09	0.765	1.81	0.183	0.68	0.411	35.00	**0.000**
	ET*ET	2.58	0.112	0.92	0.342	20.37	**0.000**	0.08	0.777	12.08	**0.001**
	SV*SV	2.04	0.157	0.52	0.475	17.19	**0.000**	72.70	**0.000**	17.14	**0.000**
	SC*SC	1.04	0.312	0.25	0.618	1.58	0.212	0.76	0.386	32.58	**0.000**
	UT*ET	27.29	**0.000**	1.72	0.194	3.04	0.085	1.40	0.240	49.80	**0.000**
	UT*SV	1.04	0.312	7.59	**0.007**	0.62	0.432	2.17	0.145	13.27	**0.001**
	UT*SC	0.66	0.417	0.00	0.947	2.24	0.139	0.06	0.802	0.54	0.469
	ET*SV	0.64	0.427	0.84	0.362	0.79	0.378	9.98	**0.002**	ND	ND
	ET*SC	3.11	0.082	3.56	0.063	0.69	0.409	4.09	**0.047**	ND	ND
	SV*SC	11.21	**0.001**	2.98	0.089	1.00	0.320	4.85	**0.031**	ND	ND
CaFr11	UT	3.79	0.055	5.44	**0.022**	3.43	0.068	0.42	0.521	15.59	**0.000**
	ET	1.15	0.287	6.22	**0.015**	11.28	**0.001**	0.35	0.559	6.54	**0.015**
	SV	13.30	**0.000**	50.49	**0.000**	95.38	**0.000**	31.95	**0.000**	3.67	0.063
	SC	0.03	0.859	4.07	**0.047**	4.36	**0.040**	0.70	0.406	1.19	0.283
	UT*UT	0.47	0.497	0.01	0.928	0.89	0.349	0.14	0.714	10.42	**0.003**
	ET*ET	2.02	0.160	0.68	0.431	17.93	**0.000**	0.05	0.830	5.10	**0.030**
	SV*SV	14.68	**0.000**	16.67	**0.000**	44.44	**0.000**	5.31	**0.024**	0.25	0.620
	SC*SC	8.73	**0.004**	0.77	0.383	0.18	0.671	45.06	**0.000**	0.70	0.407
	UT*ET	0.41	0.526	2.30	0.134	0.51	0.476	0.39	0.533	3.57	0.066
	UT*SV	1.24	0.270	11.14	**0.001**	2.78	0.100	5.69	**0.020**	0.15	0.702
	UT*SC	0.45	0.504	3.21	0.077	0.20	0.657	0.30	0.584	0.13	0.720
	ET*SV	0.28	0.601	3.24	0.076	1.06	0.307	4.57	**0.036**	ND	ND
	ET*SC	0.46	0.499	0.33	0.570	2.21	0.141	8.15	**0.006**	ND	ND

Table 4.11 contd.

	SV*SC	0.55	0.462	1.21	0.275	1.88	0.174	4.28	**0.042**	ND	ND
CaFr12	UT	0.25	0.618	10.83	**0.002**	18.64	**0.000**	16.18	**0.000**	0.21	0.650
	ET	1.09	0.301	9.18	**0.003**	3.17	0.079	6.95	**0.010**	10.18	**0.003**
	SV	63.61	**0.000**	30.93	**0.000**	148.55	**0.000**	65.15	**0.000**	3.80	0.058
	SC	0.75	0.390	11.72	**0.001**	13.75	**0.000**	2.68	0.106	0.46	0.500
	UT*UT	0.39	0.536	3.15	0.080	3.02	0.086	1.62	0.208	62.54	**0.000**
	ET*ET	11.16	**0.001**	0.06	0.811	21.31	**0.000**	6.74	**0.011**	54.39	**0.000**
	SV*SV	0.02	0.896	1.14	0.289	21.26	**0.000**	5.32	**0.024**	3.21	0.081
	SC*SC	0.88	0.353	0.99	0.324	2.78	0.100	8.02	**0.006**	47.25	**0.000**
	UT*ET	15.10	**0.000**	0.28	0.601	1.59	0.212	14.28	**0.000**	80.73	**0.000**
	UT*SV	16.61	**0.000**	0.05	0.825	1.46	0.231	20.22	**0.000**	1.50	0.227
	UT*SC	3.59	0.051	0.68	0.413	2.01	0.161	6.39	**0.014**	1.00	0.323
	ET*SV	0.41	0.526	1.79	0.184	2.36	0.129	13.53	**0.000**	ND	ND
	ET*SC	0.00	0.963	6.14	**0.015**	18.64	**0.000**	30.21	**0.000**	ND	ND
	SV*SC	0.22	0.643	1.04	0.312	3.17	0.079	5.65	**0.020**	ND	ND
CaFr21	UT	0.35	0.555	22.22	**0.000**	10.10	**0.002**	17.19	**0.000**	1.79	0.189
	ET	0.75	0.389	23.54	**0.000**	1.33	0.252	5.74	**0.019**	17.88	**0.000**
	SV	37.05	**0.000**	55.97	**0.000**	107.26	**0.000**	66.71	**0.000**	14.19	**0.001**
	SC	0.04	0.850	21.41	**0.000**	7.44	**0.008**	1.26	0.265	6.71	**0.013**
	UT*UT	0.09	0.762	49.60	**0.000**	3.29	0.074	2.15	0.147	62.56	**0.000**
	ET*ET	0.53	0.470	26.51	**0.000**	17.21	**0.000**	7.93	**0.006**	39.01	**0.000**
	SV*SV	1.13	0.291	30.55	**0.000**	17.25	**0.000**	5.96	**0.017**	93.99	**0.000**
	SC*SC	0.57	0.451	49.37	**0.000**	2.28	0.135	7.98	**0.006**	47.35	**0.000**
	UT*ET	4.46	**0.034**	1.15	0.287	0.62	0.435	22.41	**0.000**	2.79	0.103
	UT*SV	0.30	0.586	14.60	**0.000**	1.83	0.180	25.50	**0.000**	10.11	**0.003**
	UT*SC	1.38	0.243	1.93	0.169	1.09	0.299	11.37	**0.001**	12.51	**0.001**
	ET*SV	10.45	**0.002**	12.46	**0.001**	3.10	0.082	17.62	**0.000**	ND	ND
	ET*SC	0.24	0.624	26.37	**0.000**	1.25	0.267	33.68	**0.000**	ND	ND
	SV*SC	2.91	0.092	0.27	0.603	2.61	0.110	9.92	**0.002**	ND	ND
CaXy11	UT	0.13	0.714	4.56	**0.036**	15.99	**0.000**	11.89	**0.001**	ND	ND

Table 4.11 contd.

	ET	12.44	**0.001**	22.88	**0.000**	2.60	0.111	11.22	**0.001**	ND	ND
	SV	57.23	**0.000**	39.54	**0.000**	141.50	**0.000**	40.81	**0.000**	ND	ND
	SC	34.38	**0.000**	54.29	**0.000**	12.68	**0.001**	3.46	0.067	ND	ND
	UT*UT	0.04	0.840	2.06	0.156	2.97	0.089	1.83	0.180	ND	ND
	ET*ET	1.38	0.244	6.80	**0.011**	19.62	**0.000**	4.51	**0.037**	ND	ND
	SV*SV	7.55	**0.008**	6.15	**0.015**	22.92	**0.000**	5.29	**0.024**	ND	ND
	SC*SC	0.01	0.929	17.24	**0.000**	2.50	0.118	5.24	**0.025**	ND	ND
	UT*ET	2.68	0.105	28.34	**0.000**	0.91	0.327	21.21	**0.000**	ND	ND
	UT*SV	61.59	**0.000**	0.31	0.582	3.44	0.067	17.09	**0.000**	ND	ND
	UT*SC	0.27	0.608	26.25	**0.000**	0.97	0.327	18.60	**0.000**	ND	ND
	ET*SV	2.18	0.144	5.29	**0.024**	3.44	0.067	12.37	**0.001**	ND	ND
	ET*SC	33.49	**0.000**	27.61	**0.000**	2.00	0.161	19.11	**0.000**	ND	ND
	SV*SC	0.19	0.661	5.18	**0.026**	3.93	0.051	10.92	**0.001**	ND	ND
CaXy12	UT	0.49	0.485	42.64	**0.000**	12.13	**0.001**	18.96	**0.000**	0.39	0.534
	ET	18.27	**0.000**	9.29	**0.003**	1.55	0.218	11.06	**0.001**	11.03	**0.002**
	SV	41.84	**0.000**	27.40	**0.000**	114.82	**0.000**	43.72	**0.000**	12.20	**0.001**
	SC	36.03	**0.000**	10.54	**0.002**	9.80	**0.002**	9.42	**0.003**	9.91	**0.003**
	UT*UT	17.75	**0.000**	17.52	**0.000**	2.36	0.129	0.39	0.537	27.87	**0.000**
	ET*ET	39.57	**0.000**	3.35	0.071	17.75	**0.000**	1.40	0.240	16.37	**0.000**
	SV*SV	23.89	**0.000**	3.30	0.073	17.63	**0.000**	1.45	0.233	15.63	**0.000**
	SC*SC	14.58	**0.000**	4.18	**0.044**	1.75	0.190	40.52	**0.000**	20.21	**0.000**
	UT*ET	7.76	**0.007**	0.47	0.496	1.44	0.234	24.66	**0.000**	3.60	0.065
	UT*SV	42.47	**0.000**	28.77	**0.000**	1.37	0.246	18.66	**0.000**	1.53	0.223
	UT*SC	0.80	0.373	0.03	0.858	1.50	0.224	2.40	0.126	0.02	0.901
	ET*SV	1.45	0.232	0.02	0.887	2.35	0.129	20.91	**0.000**	ND	ND
	ET*SC	25.21	**0.000**	1.20	0.277	1.18	0.281	4.47	**0.038**	ND	ND
	SV*SC	5.28	**0.024**	1.19	0.278	2.38	0.127	1.16	0.285	ND	ND
CaXy21	UT	1.42	0.237	0.86	0.357	8.84	**0.004**	3.09	0.083	ND	ND
	ET	6.77	**0.011**	0.07	0.788	0.26	0.615	3.06	0.085	ND	ND
	SV	21.14	**0.000**	9.24	**0.003**	186.36	**0.000**	55.94	**0.000**	ND	ND

Table 4.11 contd.

	SC	18.21	**0.000**	19.06	**0.000**	1.68	0.199	0.13	0.716	ND	ND
	UT*UT	13.66	**0.000**	0.63	0.431	1.98	0.164	2.13	0.149	ND	ND
	ET*ET	4.68	**0.034**	16.46	**0.000**	14.01	**0.000**	6.62	**0.012**	ND	ND
	SV*SV	25.80	**0.000**	14.09	**0.000**	19.60	**0.000**	12.01	**0.001**	ND	ND
	SC*SC	6.73	**0.011**	18.42	**0.000**	1.26	0.264	7.31	**0.008**	ND	ND
	UT*ET	1.66	0.202	3.79	0.055	1.14	0.289	32.55	**0.000**	ND	ND
	UT*SV	20.07	**0.000**	7.42	**0.008**	3.49	0.066	7.05	**0.010**	ND	ND
	UT*SC	6.18	**0.015**	3.04	0.085	0.99	0.323	18.38	**0.000**	ND	ND
	ET*SV	1.29	0.260	0.11	0.737	9.20	**0.003**	2.10	0.152	ND	ND
	ET*SC	11.53	**0.001**	4.60	**0.035**	0.04	0.846	32.96	**0.000**	ND	ND
	SV*SC	0.41	0.524	0.11	0.746	10.26	**0.002**	1.64	0.205	ND	ND
CaGr11	UT	0.21	0.645	0.27	0.603	17.10	**0.000**	18.44	**0.000**	11.03	**0.002**
	ET	0.75	0.391	1.61	0.209	2.75	0.117	6.96	**0.010**	12.20	**0.001**
	SV	31.52	**0.000**	13.90	**0.000**	161.58	**0.000**	83.48	**0.000**	9.91	**0.003**
	SC	5.22	**0.025**	0.42	0.521	12.51	**0.001**	1.59	0.212	7.47	**0.000**
	UT*UT	2.01	0.160	1.69	0.198	2.52	0.117	1.88	0.175	27.87	**0.000**
	ET*ET	58.69	**0.000**	9.45	**0.003**	25.73	**0.000**	8.69	**0.004**	16.37	**0.000**
	SV*SV	4.46	**0.038**	5.65	**0.020**	23.30	**0.000**	8.26	**0.005**	15.63	**0.000**
	SC*SC	5.66	**0.020**	5.48	**0.022**	2.39	0.126	9.51	**0.003**	20.21	**0.000**
	UT*ET	1.81	0.183	0.17	0.681	0.20	0.658	43.55	**0.000**	3.60	0.065
	UT*SV	5.55	**0.021**	4.63	**0.035**	3.90	0.052	26.81	**0.000**	1.53	0.223
	UT*SC	0.13	0.721	2.84	0.096	0.15	0.703	22.82	**0.000**	0.02	0.901
	ET*SV	0.14	0.707	2.24	0.139	7.62	**0.007**	33.98	**0.000**	ND	ND
	ET*SC	0.11	0.742	19.49	**0.000**	3.68	0.059	33.44	**0.000**	ND	ND
	SV*SC	0.74	0.392	8.18	**0.005**	7.46	**0.008**	16.72	**0.000**	ND	ND
CaGr12	UT	1.06	0.307	7.29	**0.009**	7.80	**0.007**	15.19	**0.000**	27.93	**0.000**
	ET	2.94	0.090	8.89	**0.004**	2.35	0.130	1.77	0.188	9.58	**0.004**
	SV	31.59	**0.000**	17.16	**0.000**	102.37	**0.000**	44.20	**0.000**	3.78	0.059
	SC	9.48	**0.003**	14.15	**0.000**	11.39	**0.001**	19.55	**0.000**	52.78	**0.000**
	UT*UT	13.51	**0.000**	20.88	**0.000**	4.96	**0.029**	0.03	0.861	13.23	**0.001**

Table 4.11 contd.

	ET*ET	33.93	**0.000**	4.99	**0.028**	18.41	**0.000**	0.88	0.352	42.72	**0.000**
	SV*SV	26.44	**0.000**	4.99	**0.028**	37.54	**0.000**	0.58	0.449	16.62	**0.000**
	SC*SC	6.99	**0.010**	1.13	0.291	1.49	0.226	113.80	**0.000**	23.25	**0.000**
	UT*ET	0.55	0.462	2.70	0.105	0.93	0.338	6.90	**0.010**	18.38	**0.000**
	UT*SV	14.29	**0.000**	19.08	**0.000**	3.88	0.053	19.21	**0.000**	166.08	**0.000**
	UT*SC	0.16	0.695	3.05	0.085	1.13	0.291	1.73	0.192	8.64	**0.006**
	ET*SV	0.12	0.728	0.68	0.412	4.07	**0.047**	1.17	0.284	ND	ND
	ET*SC	3.54	0.064	11.82	**0.001**	4.42	**0.039**	35.18	**0.000**	ND	ND
	SV*SC	1.05	0.308	0.61	0.438	4.22	**0.043**	0.02	0.889	ND	ND
CaGr21	UT	12.10	**0.001**	1.33	0.253	13.61	**0.000**	18.02	**0.000**	0.18	0.674
	ET	7.57	**0.007**	9.43	**0.003**	1.49	0.227	17.66	**0.000**	0.09	0.765
	SV	36.94	**0.000**	14.73	**0.000**	128.28	**0.000**	79.33	**0.000**	0.20	0.655
	SC	38.04	**0.000**	0.00	0.974	9.54	**0.003**	4.39	**0.040**	0.11	0.740
	UT*UT	61.90	**0.000**	1.58	0.212	2.71	0.104	0.05	0.822	38.51	**0.000**
	ET*ET	14.96	**0.000**	4.15	**0.045**	20.42	**0.000**	0.69	0.407	28.70	**0.000**
	SV*SV	3.98	0.050	3.52	0.065	24.91	**0.000**	48.24	**0.000**	40.31	**0.000**
	SC*SC	17.54	**0.000**	2.45	0.122	2.22	0.140	0.55	0.460	33.90	**0.000**
	UT*ET	5.03	**0.028**	0.72	0.399	0.11	0.739	31.64	**0.000**	12.30	**0.001**
	UT*SV	16.15	**0.000**	12.28	**0.001**	2.47	0.120	24.98	**0.000**	24.75	**0.000**
	UT*SC	8.32	**0.005**	13.19	**0.001**	0.16	0.688	4.54	**0.036**	8.46	**0.006**
	ET*SV	0.37	0.544	0.50	0.481	5.38	**0.023**	33.86	**0.000**	ND	ND
	ET*SC	0.53	0.470	0.00	0.955	2.36	0.128	1.53	0.221	ND	ND
	SV*SC	0.03	0.861	14.58	**0.000**	5.37	**0.023**	3.68	0.059	ND	ND
CaGc11	UT	0.38	0.542	3.39	0.070	6.94	**0.010**	8.77	**0.004**	0.12	0.730
	ET	0.04	0.849	2.70	0.105	0.97	0.317	3.29	0.074	0.76	0.387
	SV	28.45	**0.000**	36.79	**0.000**	97.71	**0.000**	63.94	**0.000**	11.51	**0.002**
	SC	1.21	0.274	2.64	0.108	3.41	0.069	0.78	0.380	5.22	**0.028**
	UT*UT	0.82	0.368	18.92	**0.000**	1.40	0.241	1.33	0.252	18.53	**0.000**
	ET*ET	1.89	0.174	8.72	**0.004**	14.21	**0.000**	0.00	0.983	5.80	**0.021**

Table 4.11 contd.

	SV*SV	0.42	0.518	7.19	**0.009**	11.92	**0.001**	110.11	**0.000**	8.03	**0.007**
	SC*SC	4.23	**0.043**	0.01	0.905	3.86	0.053	0.02	0.880	12.29	**0.001**
	UT*ET	1.45	0.232	8.59	**0.004**	2.15	0.147	10.93	**0.001**	0.57	0.454
	UT*SV	4.98	**0.029**	12.04	**0.001**	0.43	0.514	4.65	**0.034**	4.82	**0.034**
	UT*SC	0.55	0.461	2.11	0.150	2.05	0.156	4.92	**0.030**	0.55	0.463
	ET*SV	6.27	**0.014**	13.75	**0.000**	1.11	0.296	7.53	**0.008**	ND	ND
	ET*SC	0.01	0.923	1.04	0.312	0.56	0.458	7.72	**0.007**	ND	ND
	SV*SC	2.99	0.088	2.84	0.096	0.84	0.361	2.81	0.098	ND	ND
CaGc21	UT	5.10	**0.027**	28.76	**0.000**	12.69	**0.001**	3.90	0.052	59.85	**0.000**
	ET	0.66	0.419	1.41	0.239	2.18	0.144	0.00	0.999	23.57	**0.000**
	SV	34.90	**0.000**	9.50	**0.003**	126.23	**0.000**	75.88	**0.000**	81.70	**0.000**
	SC	1.41	0.239	1.99	0.162	11.87	**0.001**	0.24	0.623	73.84	**0.000**
	UT*UT	10.00	**0.002**	15.34	**0.000**	2.00	0.161	0.68	0.411	24.90	**0.000**
	ET*ET	24.60	**0.000**	10.74	**0.002**	19.76	**0.000**	0.54	0.466	18.68	**0.000**
	SV*SV	2.03	0.158	10.92	**0.001**	18.11	**0.000**	51.57	**0.000**	36.22	**0.000**
	SC*SC	6.67	**0.012**	15.77	**0.000**	2.09	0.152	3.23	0.076	33.20	**0.000**
	UT*ET	0.01	0.933	4.00	**0.049**	2.21	0.141	4.48	**0.038**	0.08	0.776
	UT*SV	21.99	**0.000**	16.33	**0.000**	0.66	0.421	0.64	0.427	2.68	0.110
	UT*SC	1.06	0.306	5.51	**0.022**	2.17	0.145	0.23	0.632	11.88	**0.001**
	ET*SV	5.10	**0.027**	41.43	**0.000**	1.43	0.235	2.13	0.149	ND	ND
	ET*SC	0.25	0.618	6.93	**0.010**	0.94	0.336	2.43	0.123	ND	ND
	SV*SC	3.28	0.074	1.94	0.167	1.64	0.204	0.02	0.901	ND	ND
CaGl11	UT	0.17	0.681	1.10	0.298	7.23	**0.009**	0.87	0.353	3.55	0.067
	ET	5.29	**0.024**	15.61	**0.000**	0.39	0.532	0.83	0.365	5.93	**0.020**
	SV	34.26	**0.000**	59.82	**0.000**	94.02	**0.000**	43.67	**0.000**	7.66	**0.009**
	SC	21.63	**0.000**	0.97	0.329	6.65	**0.012**	5.46	**0.022**	9.20	**0.004**
	UT*UT	0.21	0.645	0.49	0.485	3.05	0.085	1.11	0.296	0.02	0.880
	ET*ET	76.13	**0.000**	19.48	**0.000**	16.75	**0.000**	0.01	0.926	1.87	0.180
	SV*SV	12.36	**0.001**	49.63	**0.000**	14.81	**0.000**	42.56	**0.000**	0.05	0.819
	SC*SC	9.14	**0.003**	0.60	0.440	2.00	0.161	0.91	0.343	1.76	0.192

Table 4.11 contd.

	UT*ET	0.67	0.416	2.08	0.154	0.95	0.332	0.49	0.485	0.00	0.950
	UT*SV	21.01	**0.000**	22.07	**0.000**	0.81	0.372	0.01	0.919	0.45	0.505
	UT*SC	13.45	**0.000**	1.32	0.254	1.70	0.196	0.16	0.694	4.58	**0.039**
	ET*SV	0.93	0.338	4.39	**0.040**	1.89	0.173	1.24	0.269	ND	ND
	ET*SC	2.13	0.149	0.18	0.675	1.10	0.298	1.37	0.245	ND	ND
	SV*SC	0.49	0.484	0.21	0.649	2.60	0.111	0.01	0.940	ND	ND
CaGl21	UT	0.15	0.700	10.46	**0.002**	10.25	**0.002**	0.28	0.596	0.03	0.869
	ET	3.74	0.057	3.86	0.053	2.03	0.158	0.01	0.917	8.76	**0.005**
	SV	44.97	**0.000**	18.58	**0.000**	111.73	**0.000**	24.47	**0.000**	3.83	0.057
	SC	7.50	**0.008**	0.60	0.441	10.48	**0.002**	2.02	0.160	0.02	0.882
	UT*UT	11.97	**0.001**	4.00	**0.049**	2.33	0.131	1.74	0.192	65.62	**0.000**
	ET*ET	37.33	**0.000**	9.48	**0.003**	21.02	**0.000**	1.28	0.261	68.40	**0.000**
	SV*SV	9.23	**0.003**	10.51	**0.002**	18.79	**0.000**	34.11	**0.000**	46.55	**0.000**
	SC*SC	4.70	**0.033**	3.93	0.051	3.02	0.086	5.24	**0.025**	45.23	**0.000**
	UT*ET	5.85	**0.018**	5.81	**0.018**	2.00	0.162	0.33	0.570	18.62	**0.000**
	UT*SV	46.73	**0.000**	2.85	0.096	1.48	0.228	0.00	0.955	18.85	**0.000**
	UT*SC	0.57	0.454	3.81	0.055	1.98	0.164	0.00	0.960	6.70	**0.013**
	ET*SV	14.93	**0.000**	0.53	0.467	1.79	0.185	0.04	0.843	ND	ND
	ET*SC	18.90	**0.000**	15.06	**0.000**	1.51	0.222	0.03	0.855	ND	ND
	SV*SC	2.95	0.090	1.87	0.175	2.39	0.126	0.18	0.670	ND	ND

P-values in bold are statistically significant, ND = not determined.

Table 4.12 Coefficient of determination and other important analysis of variance statistical parameters for fitting experimental results

Model Terms	Runs	TPC	TFC	CUPRAC	FRAP	DPPH
%Model Contributions	1	99.99	99.95	72.13	99.99	99.98
% Error contributions		0.01	0.05	27.87	0.01	0.02
R^2 (%)		99.99	99.95	72.13	99.99	99.98
R^2(Adj) (%)		99.99	99.93	59.19	99.99	99.97
R^2(Pred) (%)		99.99	99.98	37.29	99.98	99.96
F-value		34416.33	4491.30	5.57	26356.39	11950.48
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	2	99.94	99.98	86.89	99.98	100
% Error contributions		0.06	0.02	13.11	0.02	0.0
R2 (%)		99.94	99.98	86.89	99.98	100
R2(Adj) (%)		99.92	99.97	80.81	99.97	100
R2(Pred) (%)		99.87	99.95	70.51	99.95	99.99
F-value		3751.46	9968.49	14.28	9791.32	84470.64
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	3	99.98	100	89.94	93.62	99.94
% Error contributions		0.02	0.00	10.06	6.38	0.06
R2 (%)		99.98	100	89.94	93.62	99.94
R2(Adj) (%)		99.97	100	85.28	90.66	99.91
R2(Pred) (%)		99.95	99.99	77.38	85.65	99.86
F-value		10163.27	64915	19.27	31.62	3437.39
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	4	99.99	99.97	96.38	76.39	ND
% Error contributions		0.01	0.03	3.62	23.61	ND
R2 (%)		99.99	99.97	96.38	76.39	ND
R2(Adj) (%)		99.98	99.96	94.70	65.43	ND
R2(Pred) (%)		99.97	99.94	91.85	46.87	ND
F-value		14886.62	8325.46	57.30	6.97	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	5	99.97	99.95	98.85	97.65	ND
% Error contributions		0.03	0.05	1.15	2.35	ND
R2 (%)		99.97	99.95	98.85	97.65	ND
R2(Adj) (%)		99.95	99.92	98.31	96.55	ND
R2(Pred) (%)		99.92	99.88	97.40	94.70	ND
F-value		6227.99	3596.91	184.56	83.36	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	6	99.98	100	99.17	99.98	ND
% Error contributions		0.02	0.00	0.83	0.02	ND
R2		99.98	100	99.17	99.98	ND
R2(Adj)		99.98	100	98.78	99.97	ND
R2(Pred)		99.96	100	98.12	99.95	ND
F-value		13651.40	110172.73	256.26	10556.76	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	7	99.79	99.97	99.94	99.99	99.99
% Error contributions		0.21	0.03	0.06	0.01	0.01
R2		99.79	99.97	99.94	99.99	99.99
R2(Adj)		99.69	99.96	99.92	99.98	99.99
R2(Pred)		99.53	99.93	99.87	99.98	99.99
F-value		1024.33	7367.53	3840.27	19934.74	35512.20

Table 4.12 contd.

P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	8	99.98	99.99	85.92	93.29	ND
% Error contributions		0.02	0.01	14.08	6.71	ND
R2		99.98	99.99	85.92	93.29	ND
R2(Adj)		99.98	99.99	79.39	90.17	ND
R2(Pred)		99.96	99.98	68.33	84.90	ND
F-value		13026.71	31970.44	13.15	29.94	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	9	99.98	99.99	96.22	95.52	ND
% Error contributions		0.02	0.01	3.78	4.48	ND
R2		99.98	99.99	96.22	95.52	ND
R2(Adj)		99.98	99.99	94.46	93.45	ND
R2(Pred)		99.96	99.98	91.49	89.93	ND
F-value		13375.18	26135.68	54.79	45.98	ND
P-value)		0.000	0.000	0.00	0.000	ND
% Model Contributions	10	99.99	99.99	99.90	99.99	ND
% Error contributions		0.01	0.01	0.10	0.01	ND
R2		99.99	99.99	99.90	99.99	ND
R2(Adj)		99.99	99.99	99.85	99.99	ND
R2(Pred)		99.98	99.98	99.77	99.98	ND
F-value		30232.00	22933.40	2090.88	24056.90	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	11	100.00	99.98	91.49	100	ND
% Error contributions		0.00	0.02	8.51	0.00	ND
R2		100.00	99.98	91.49	100	ND
R2(Adj)		100.00	99.98	87.54	99.99	ND
R2(Pred)		99.99	99.96	80.86	99.99	ND
F-value		64137.11	13236.08	23.17	60638.36	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	12	99.97	99.97	99.67	99.99	100
% Error contributions		0.03	0.03	0.33	0.01	0.0
R2		99.97	99.97	99.67	99.99	100
R2(Adj)		99.96	99.96	99.51	99.98	100
R2(Pred)		99.94	99.94	99.25	99.98	99.99
F-value		8036.19	7185.60	644.18	20697.27	75202.66
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	13	99.99	100	99.94	99.98	ND
% Error contributions		0.01	0.00	0.04	0.02	ND
R2		99.99	100	99.94	99.98	ND
R2(Adj)		99.99	100	99.91	99.98	ND
R2(Pred)		99.98	99.99	99.86	99.97	ND
F-value		22514.79	93801.79	3508.66	14220.97	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	14	99.96	99.97	98.41	99.94	ND
% Error contributions		0.04	0.03	1.59	0.06	ND
R2		99.96	99.97	98.41	99.94	ND
R2(Adj)		99.94	99.96	97.68	99.92	ND
R2(Pred)		99.91	99.94	96.43	99.88	ND
F-value		5503.70	8223.42	133.71	3896.83	ND
P-value)		0.000	0.000	0.000	0.000	ND

Table 4.12 contd.

% Model Contributions	15	99.99	99.98	93.76	84.57	ND
% Error contributions		0.01	0.02	6.24	15.43	ND
R2		99.99	99.98	93.76	84.57	ND
R2(Adj)		99.99	99.98	90.86	77.41	ND
R2(Pred)		99.98	99.96	85.96	65.29	ND
F-value		28951.29	13425.05	32.36	11.81	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	16	99.97	99.96	96.97	94.69	ND
% Error contributions		0.03	0.04	3.03	5.31	ND
R2		99.97	99.96	96.97	94.69	ND
R2(Adj)		99.96	99.95	95.57	92.23	ND
R2(Pred)		99.94	99.92	93.19	88.06	ND
F-value		7665.24	5998.51	69.03	38.43	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	17	99.99	99.90	99.40	99.97	99.97
% Error contributions		0.01	0.10	0.60	0.03	0.03
R2		99.99	99.90	99.40	99.97	99.97
R2(Adj)		99.99	99.85	99.13	99.95	99.96
R2(Pred)		99.98	99.77	98.66	99.93	99.94
F-value		24901.69	2140.47	359.03	6485.93	7929.57
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	18	99.91	99.98	92.99	99.68	99.99
% Error contributions		0.09	0.02	7.01	0.32	0.01
R2		99.91	99.98	92.99	99.68	99.99
R2(Adj)		99.86	99.98	89.73	99.54	99.99
R2(Pred)		99.79	99.96	84.22	99.29	99.98
F-value		2300.26	13304.94	28.55	679.71	21374.26
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	19	99.98	99.98	72.00	99.96	99.92
% Error contributions		0.02	0.02	28.00	0.04	0.08
R2		99.98	99.98	72.00	99.96	99.92
R2(Adj)		99.97	99.97	59.00	99.94	99.88
R2(Pred)		99.96	99.96	37.00	99.90	99.81
F-value		12247.47	11824.30	5.54	4920.45	2612.19
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	20	99.95	99.99	28.39	100	100
% Error contributions		0.05	0.01	71.61	0.00	0.00
R2		99.95	99.99	28.39	100	100
R2(Adj)		99.93	99.98	0.00	100	100
R2(Pred)		99.89	99.97	0.00	99.99	100
F-value		4448.50	17745.26	0.85	83737.43	116902.58
P-value)		0.000	0.000	0.605	0.000	0.000
% Model Contributions	21	99.97	99.99	87.28	92.91	ND
% Error contributions		0.03	0.01	12.72	7.09	ND
R2		99.97	99.99	87.28	92.91	ND
R2(Adj)		99.96	99.99	81.37	89.62	ND
R2(Pred)		99.94	99.98	71.38	84.05	ND
F-value		7678.46	23483.28	14.78	28.24	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	22	99.99	99.91	99.88	100	100

Table 4.12 contd.

% Error contributions		0.01	0.09	0.12	0.00	0.0
R2		99.99	99.91	99.88	100	100
R2(Adj)		99.98	99.87	99.82	99.99	99.99
R2(Pred)		99.97	99.80	99.72	99.99	99.99
F-value		19006.87	2395.42	1736.57	43636.73	47040.47
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	23	100.00	99.92	99.73	99.99	99.99
% Error contributions		0.00	0.08	0.27	0.01	0.01
R2		100.00	99.92	99.73	99.99	99.99
R2(Adj)		99.99	99.88	99.61	99.99	99.99
R2(Pred)		99.99	99.81	99.40	99.99	99.98
F-value		47656.50	2564.57	809.28	36824.12	27503.61
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	24	99.99	99.99	92.00	99.99	ND
% Error contributions		0.01	0.01	8.00	0.01	ND
R2		99.99	99.99	92.00	99.99	ND
R2(Adj)		99.99	99.99	88.29	99.98	ND
R2(Pred)		99.98	99.98	82.01	99.97	ND
F-value		23244.02	23769.47	24.78	17072.50	ND
P-value)		0.000	0.000	0.000	0.000	ND
% Model Contributions	25	99.99	99.98	70.04	100	99.99
% Error contributions		0.01	0.02	29.96	0.00	0.01
R2		99.99	99.98	70.04	100	99.99
R2(Adj)		99.99	99.97	56.13	99.99	99.98
R2(Pred)		99.99	99.95	32.59	99.99	99.97
F-value		33399.66	10464.59	5.03	53832.04	18943.33
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	26	99.96	99.85	93.19	96.10	99.99
% Error contributions		0.04	0.15	6.81	3.90	0.01
R2		99.96	99.85	93.19	96.10	99.99
R2(Adj)		99.94	99.78	90.03	94.28	99.99
R2(Pred)		99.91	99.67	84.67	91.22	99.99
F-value		5483.74	1460.33	29.47	53.01	33774.61
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	27	99.77	99.96	87.35	99.37	99.96
% Error contributions		0.23	0.04	12.65	0.63	0.04
R2		99.77	99.96	87.35	99.37	99.96
R2(Adj)		99.67	99.95	81.48	99.08	99.94
R2(Pred)		99.49	99.92	71.54	98.59	99.92
F-value		950.43	6042.35	14.87	340.57	5722.87
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	28	99.99	99.92	99.85	99.99	99.99
% Error contributions		0.01	0.08	0.15	0.01	0.01
R2		99.99	99.92	99.85	99.99	99.99
R2(Adj)		99.98	99.88	99.78	99.98	99.99
R2(Pred)		99.97	99.81	99.66	99.97	99.98
F-value		18173.65	2606.47	1429.26	17242.10	29998.34
P-value)		0.000	0.000	0.000	0.000	0.000

Table 4.12 contd.

% Model Contributions	29	99.99	99.85	99.91	99.99	99.98
% Error contributions		0.01	0.15	0.09	0.01	0.02
R2		99.99	99.85	99.91	99.99	99.98
R2(Adj)		99.99	99.78	99.87	99.99	99.97
R2(Pred)		99.99	99.66	99.80	99.98	99.95
F-value		38698.58	1412.10	2436.48	32097.95	10623.59
P-value)		0.000	0.000	0.000	0.000	0.000
% Model Contributions	30	99.97	99.93	99.94	99.59	99.99
% Error contributions		0.03	0.07	0.06	0.41	0.01
R2		99.97	99.93	99.94	99.59	99.99
R2(Adj)		99.96	99.90	99.91	99.40	99.98
R2(Pred)		99.94	99.85	99.86	99.08	99.97
F-value		7457.03	3200.60	3454.15	524.50	17016.13
P-value)		0.000	0.000	0.000	0.000	0.000

4.6.4 Antioxidant and antiradical scavenging activity of African nutmeg peels extracted using NADESs

The antioxidants measured as total polyphenolic content (TPC) and total flavonoids content (TFC), as well as the antiradical scavenging potentials of African nutmeg peels measured by CUPRAC, FRAP, and DPPH inhibition at different response conditions of experiment is presented in **Table 4. 13.** The results show that TPC varies from the lowest of 30.39±0.49 µgGAE/g in CaXy21 under extraction conditions of temperature, time, volume, and concentration of 40ºc, 20 min, 10 ml, and 80% (run 14) respectively, to the highest of 1373.4±7.88 µgGAE/g in CaFr11 under conditions of temperature, time, volume, and concentration of 50ºc, 15 min, 25 ml, and 70% (run 22) respectively. For TFC, the lowest yield was 56.901±0.45 µgQE/g obtained from CaGc11 under extraction conditions of temperature, time, volume, and concentration of 50ºc, 15 min, 5 ml, and 70% (run 30), respectively, and incidentally the highest yield of 1713±9.02 µgQE/g came from CaGc11 under conditions of 40ºc, 10 min, 20 ml, and 60% for temperature, time, volume, and concentration respectively (run 18). The CUPRAC antiradical activity ranged from 3.0895±0.01 µMTE/g in CaGc21to 26.3485±0.07 µMTE/g in CaFr11. The conditions that produced the lowest CUPRAC activity were temperature, time, volume, and concentration of 50ºc, 15 min, 5 ml, 70% (run 30) respectively, while the highest CUPRAC activity was observed at temperature, time, volume, and concentration of 50ºc, 15 min, 25 ml, 70% (run 22) respectively. CaFr12 gave the lowest FRAP power of 0.521±0.346 µMTE/g at temperature, time, volume, and concentration of

50ºc, 15 min, 5 ml, and 70% (run 30) respectively, while the highest FRAP power of 23.724±0.036 µMTE/g was obtained from CaGr21 at temperature, time, volume, and concentration of 40ºc, 20 min, 20 ml, and 80% (run 22), respectively. DPPH inhibition ranged from 0.49±0.2% in CaFr21 to 92±0.1% in CaFr11 respectively. The conditions in which the lowest and highest DPPH inhibition was observed include temperature, time, volume, and concentration from 50ºc, 15 min, 25 ml, and 70% (run 22) to 40ºc, 20 min, 10 ml, 60% (run 2), respectively.

Table 4.13 Antioxidant and antiradical scavenging activity of African nutmeg peels extracted using NADESs at different extraction conditions

NADES	RUN	Experimental conditions				Antioxidants		Antiradical scavenging Activity		
		UT (ºC)	ET (min)	SV (ml)	SC (%)	TPC (µgGAE/g)	TFC (µgQE/g)	CUPRAC (µMTE/g)	FRAP (µMTE/g)	DPPH (%)
CaSu11	1	60	20	10	80	149.67±0.28^{D}	58.720±3.61^{EF}	3.1137±0.01^{CD}	1.7310±0.01^{C}	26.7±0.1^{M}
CaFr11						352.78±1.72^{A}	291.02±0.78^{A}	3.1944±0.06^{B}	3.2131±0.01^{A}	77.2±0.3^{D}
CaFr12						179.09±0.75^{B}	61.328±0.78^{DE}	3.1702±0.01^{BC}	0.7490±0.00^{G}	29.2±0.0^{L}
CaFr21						60.294±0.49^{L}	61.068±1.19^{DE}	3.0976±0.01^{D}	0.8618±0.00^{F}	50.7±0.0^{G}
CaXy11						61.765±0.98^{K}	61.849±0.45^{D}	3.2025±0.04^{B}	1.7541±0.00^{B}	35.4±0.1^{I}
CaXy12						103.27±0.75^{H}	61.589±0.90^{D}	3.2752±0.04^{A}	0.8592±0.00^{F}	83.8±0.1^{B}
CaXy21						64.052±0.28^{J}	69.401±0.90^{C}	3.1060±0.00^{D}	1.2280±0.00^{D}	66.6±0.4^{E}
CaGr11						63.235±0.98^{J}	58.720±2.39^{EF}	3.1944±0.03^{B}	0.7310±0.00^{HI}	40.7±0.0^{H}
CaGr12						163.07±0.57^{C}	60.286±0.90^{DEF}	3.1944±0.03^{B}	0.7208±0.01^{I}	82.5±0.2^{C}
CaGr21						57.840±0.00^{M}	57.948±1.19^{F}	3.1702±0.03^{BC}	0.7182±0.00^{I}	31.5±0.3^{K}
CaGc11						135.29±0.85^{E}	129.04±1.97^{B}	3.1702±0.03^{BC}	0.7362±0.01^{H}	84.6±0.2^{A}
CaGc21						108.17±0.28^{G}	66.800±2.07^{C}	3.1137±0.01^{CD}	0.7208±0.01^{I}	54.3±0.2^{F}
CaGl11						113.20±0.00^{F}	58.203±0.78^{F}	3.1541±0.04^{BCD}	0.7208±0.01^{I}	40.9±0.2^{H}
CaGl21						67.320±0.28^{I}	59.245±1.63^{DEF}	3.1702±0.07^{BC}	0.8797±0.00^{E}	32.5±1.1^{J}
CaSu11	2	40	20	10	60	181.05±0.57^{B}	536.72±1.56^{C}	6.3404±0.03^{BC}	0.9849±0.01^{D}	90.4±0.2^{C}
CaFr11						275.49±0.98^{A}	563.80±3.25^{B}	6.3404±0.03^{BC}	0.3772±0.01^{J}	92.0±0.1^{A}
CaFr12						113.40±2.47^{D}	116.41±1.56^{HI}	6.2274±0.03^{DE}	0.7387±0.00^{G}	89.6±0.0^{D}
CaFr21						134.97±3.96^{C}	233.07±3.93^{D}	6.1789±0.03^{E}	0.7054±0.00^{I}	29.3±0.3^{J}
CaXy11						62.745±0.98^{K}	115.89±0.90^{HI}	6.2274±0.03^{DE}	1.3926±0.00^{B}	19.0±0.0^{M}
CaXy12						110.13±0.57^{E}	115.89±2.39^{HI}	6.3727±0.06^{B}	0.7182±0.01^{H}	89.2±0.2^{E}
CaXy21						68.300±2.83^{HIJ}	120.57±1.80^{GHI}	6.2435±0.06^{DE}	0.9515±0.01^{E}	49.7±0.3^{G}
CaGr11						70.588±0.98^{FGH}	224.22±7.16^{E}	6.2758±0.03^{CD}	0.7515±0.00^{F}	91.7±0.2^{B}
CaGr12						72.222±1.13^{F}	121.61±3.25^{GH}	6.3727±0.11^{B}	2.0592±0.01^{A}	16.5±0.1^{N}
CaGr21						71.242±1.13^{FG}	125.78±1.56^{G}	6.2274±0.03^{DE}	1.1746±0.01^{C}	28.2±0.1^{K}
CaGc11						67.320±0.57^{IJ}	187.76±2.39^{F}	6.3404±0.03^{BC}	0.7490±0.00^{FG}	36.3±0.2^{H}
CaGc21						66.013±1.13^{J}	764.84±8.27^{A}	6.2758±0.03^{CD}	0.7080±0.00^{HI}	81.9±0.1^{F}
CaGl11						68.954±1.50^{GHI}	121.61±2.39^{GH}	6.5665±0.03^{A}	0.7105±0.00^{HI}	27.5±0.2^{L}
CaGl21						71.895±1.13^{F}	115.36±2.39^{I}	6.3243±0.03^{BC}	0.9413±0.01^{E}	30.9±0.1^{I}
CaSu11	3	50	15	15	70	238.48±0.85^{B}	225.98±0.68^{E}	4.7069±0.04^{EF}	1.0619±0.01^{G}	77.8±0.1^{F}
CaFr11						149.02±2.36^{C}	368.95±0.68^{C}	4.8643±0.02^{AB}	1.1081±0.01^{D}	83.1±0.3^{E}
CaFr12						260.05±0.42^{A}	339.26±1.17^{D}	4.8886±0.04^{A}	1.0656±0.01^{FG}	89.0±0.1^{B}

Table 4.13 contd.

CaFr21						132.60±1.85^{D}	338.87±0.68^{D}	4.7553±0.04^{DE}	1.1081±0.01^{D}	86.8±0.1^{D}
CaXy11						93.380±1.95^{E}	88.480±2.03^{HI}	4.8038±0.06^{CD}	1.1196±0.01^{CD}	83.30±0.1^{E}
CaXy12						63.480±0.43^{I}	89.260±1.79^{GHI}	4.6463±0.02^{G}	1.0773±0.01^{EF}	91.3±0.2^{A}
CaXy21						52.451±0.43^{J}	90.820±1.17^{FGH}	4.8643±0.04^{AB}	1.1465±0.01^{A}	83.3±0.2^{E}
CaGr11						68.137±0.85^{H}	90.430±1.35^{FGHI}	4.8159±0.02^{BC}	1.1158±0.01^{CD}	83.8±0.3^{E}
CaGr12						71.324±0.74^{G}	91.211±0.68^{FG}	4.6463±0.04^{G}	1.0658±0.01^{FG}	88.1±0.9^{C}
CaGr21						47.059±1.28^{K}	91.210±1.79^{FG}	4.6705±0.02^{FG}	1.0658±0.01^{FG}	88.1±0.9^{C}
CaGc11						149.76±0.43^{C}	732.23±0.68^{A}	4.7553±0.02^{DE}	1.1350±0.01^{AB}	89.7±0.1^{B}
CaGc21						75.735±0.74^{F}	561.13±0.68^{B}	4.8159±0.04^{BC}	1.0889±0.01^{E}	90.9±0.0^{A}
CaGl11						50.735±1.28^{J}	88.086±0.68^{I}	4.7432±0.02^{E}	1.1235±0.01^{BC}	33.7±0.5^{G}
CaGl21						63.971±0.74^{I}	91.990±3.10^{F}	4.6220±0.00^{G}	1.1235±0.01^{BC}	89.2±0.8^{B}
CaSu11	4	50	15	15	70	252.70±0.43^{A}	222.07±3.10^{F}	4.8643±0.04^{B}	1.0965±0.01^{AB}	ND
CaFr11						160.29±0.74^{C}	368.56±0.00^{C}	4.7432±0.02^{CD}	1.1119±0.01^{A}	ND
CaFr12						250.49±0.43^{B}	337.30±2.95^{D}	4.6872±0.02^{EF}	1.0965±0.03^{AB}	ND
CaFr21						134.80±0.43^{E}	326.76±11.8^{E}	4.6705±0.02^{EF}	1.0619±0.01^{EF}	ND
CaXy11						97.549±1.12^{F}	90.430±0.68^{G}	4.7553±0.02^{C}	1.0658±0.01^{EF}	ND
CaXy12						51.961±0.85^{K}	90.430±1.79^{G}	4.8643±0.02^{B}	1.0658±0.01^{EF}	ND
CaXy21						58.578±0.85^{J}	94.73±4.44^{G}	4.7069±0.04^{DE}	1.0773±0.01^{CDE}	ND
CaGr11						68.137±0.43^{I}	91.600±1.79^{G}	4.8886±0.04^{B}	1.0850±0.02^{BCD}	ND
CaGr12						71.569±1.12^{H}	89.650±2.03^{G}	4.8522±0.02^{B}	1.0735±0.01^{CDEF}	ND
CaGr21						49.265±0.74^{L}	91.210±2.44^{G}	4.6705±0.02^{EF}	1.0889±0.01^{BC}	ND
CaGc11						145.83±0.85^{D}	735.74±3.00^{A}	5.1066±0.02^{A}	1.0700±0.00^{DEF}	ND
CaGc21						73.775±0.43^{G}	562.70±1.35^{B}	4.8522±0.02^{B}	1.0580±0.00^{F}	ND
CaGl11						52.700±2.58^{K}	90.040±1.79^{G}	4.8522±0.04^{B}	1.0658±0.01^{EF}	ND
CaGl21						68.382±0.43^{I}	91.990±3.10^{G}	4.6463±0.02^{F}	1.0619±0.01^{EF}	ND
CaSu11	5	40	10	10	60	40.196±0.85^{H}	59.770±2.07^{DEF}	3.2750±0.00^{B}	0.7541±0.009^{C}	ND
CaFr11						78.758±0.28^{B}	131.12±0.90^{C}	3.8485±0.03^{A}	1.0362±0.027^{A}	ND
CaFr12						164.05±1.58^{A}	60.026±1.19^{DEF}	3.1864±0.03^{CD}	0.8105±0.016^{B}	ND
CaFr21						37.750±0.00^{I}	60.807±1.19^{DE}	3.1702±0.03^{D}	0.7387±0.019^{CDE}	ND
CaXy11						54.248±0.75^{D}	59.240±1.97^{DEF}	3.1864±0.01^{CD}	0.7464±0.016^{CD}	ND
CaXy12						45.425±1.02^{FG}	58.460±2.51^{DEF}	3.0976±0.01^{G}	0.7541±0.016^{C}	ND
CaXy21						54.902±0.98^{D}	57.161±0.90^{F}	3.1137±0.03^{FG}	0.7336±0.016^{CDEF}	ND
CaGr11						51.634±0.75^{E}	58.200±2.71^{EF}	3.2267±0.04^{C}	0.7259±0.009^{DEF}	ND
CaGr12						52.124±0.57^{E}	61.590±2.96^{D}	3.1460±0.03^{DEF}	0.7464±0.018^{CD}	ND
CaGr21						32.680±0.28^{J}	60.810±2.51^{DE}	3.1621±0.01^{DE}	0.7259±0.012^{DEF}	ND
CaGc11						60.131±0.28^{C}	320.96±1.63^{A}	3.0975±0.03^{G}	0.7156±0.004^{EF}	ND

Table 4.13 contd.

CaGc21						44.281±0.28^{G}	156.64±2.07^{B}	3.1460±0.01^{DEF}	0.7105±0.004^{F}	ND
CaGl11						46.078±0.49^{F}	58.980±2.82^{DEF}	3.1218±0.01^{EFG}	0.7413±0.012^{CD}	ND
CaGl21						37.418±0.28^{I}	58.724±0.90^{DEF}	3.1702±0.03^{D}	0.7567±0.016^{C}	ND
CaSu11	6	60	20	10	60	145.72±0.75^{E}	72.526±0.45^{L}	3.1540±0.00^{G}	0.7439±0.008^{H}	ND
CaFr11						173.69±1.02^{B}	181.90±0.45^{E}	3.2270±0.21^{FG}	0.7336±0.004^{H}	ND
CaFr12						229.25±0.28^{A}	75.650±1.97^{K}	3.1702±0.03^{FG}	1.7003±0.009^{C}	ND
CaFr21						60.458±0.28^{I}	133.46±0.90^{F}	3.4771±0.01^{E}	1.1182±0.022^{E}	ND
CaXy11						106.70±0.57^{G}	85.286±0.45^{J}	3.2510±0.04^{FG}	1.1644±0.004^{D}	ND
CaXy12						76.471±0.49^{H}	62.370±0.45^{M}	3.2590±0.01^{F}	1.0233±0.004^{F}	ND
CaXy21						61.275±0.49^{I}	72.786±0.90^{L}	4.0342±0.03^{C}	2.1413±0.009^{B}	ND
CaGr11						42.974±1.72^{K}	117.32±0.45^{H}	4.6479±0.03^{B}	0.7695±0.004^{G}	ND
CaGr12						133.66±0.28^{F}	128.26±0.90^{G}	4.7610±0.03^{A}	2.2362±0.013^{A}	ND
CaGr21						51.634±1.02^{J}	92.057±0.45^{I}	3.1541±0.04^{G}	0.7413±0.009^{H}	ND
CaGc11						173.86±0.75^{B}	613.15±0.45^{B}	3.8570±0.00^{D}	0.7131±0.000^{I}	ND
CaGc21						159.80±0.49^{D}	492.06±0.90^{C}	3.4690±0.00^{E}	0.7105±0.004^{I}	ND
CaGl11						36.111±1.23^{L}	305.08±2.71^{D}	4.0020±0.00^{C}	0.7413±0.004^{H}	ND
CaGl21						162.91±1.58^{C}	637.89±0.78^{A}	3.1540±0.00^{G}	0.7413±0.009^{H}	ND
CaSu11	7	40	10	10	80	108.17±0.57^{D}	378.39±1.80^{C}	6.4696±0.03^{A}	7.7851±0.044^{A}	15.9±0.2^{G}
CaFr11						66.013±0.57^{J}	351.82±2.39^{D}	6.3080±0.00^{CD}	1.8262±0.027^{C}	19.7±0.3^{F}
CaFr12						168.63±0.98^{A}	546.61±1.80^{A}	6.3889±0.03^{B}	1.5390±0.018^{D}	14.6±0.1^{H}
CaFr21						96.405±1.50^{E}	222.66±1.56^{E}	6.2600±0.00^{DE}	1.4672±0.009^{FGH}	33.7±0.1^{D}
CaXy11						62.745±1.70^{K}	114.84±1.56^{I}	6.3889±0.03^{B}	1.4210±0.009^{I}	71.7±0.4^{A}
CaXy12						128.43±0.98^{B}	394.53±5.41^{B}	6.2758±0.03^{CDE}	1.4877±0.027^{EF}	11.2±0.1^{J}
CaXy21						62.745±1.70^{K}	114.81±0.19^{I}	ND	1.4210±0.009^{I}	ND
CaGr11						90.196±0.98^{F}	122.14±3.61^{GH}	6.1789±0.03^{F}	1.4467±0.036^{GHI}	23.8±0.1^{E}
CaGr12						117.32±1.50^{C}	120.05±0.90^{H}	6.2274±0.06^{EF}	1.5185±0.015^{DE}	12.0±0.2^{I}
CaGr21						68.63±0.00^{J}	120.57±0.90^{GH}	6.3243±0.03^{BCD}	1.4720±0.000^{FG}	4.40±0.2^{K}
CaGc11						82.026±0.57^{H}	126.82±0.90^{F}	6.3404±0.14^{BC}	1.5287±0.018^{D}	51.5±0.1^{B}
CaGc21						74.840±3.44^{I}	125.26±0.90^{FG}	6.5342±0.06^{A}	1.4774±0.009^{FG}	36.0±0.1^{C}
CaGl11						98.370±3.15^{E}	121.61±5.02^{FGH}	6.2600±0.00^{DE}	2.6774±0.009^{B}	35.8±0.1^{C}
CaGl21						86.928±0.57^{G}	122.66±5.41^{FGH}	6.1789±0.03^{F}	1.4364±0.009^{HI}	3.80±0.1^{L}
CaSu11	8	50	15	15	70	238.48±0.85^{B}	219.73±2.03^{E}	4.6584±0.06^{E}	1.1350±0.013^{AB}	ND
CaFr11						149.02±1.12^{C}	370.12±1.35^{C}	4.8643±0.02^{AB}	1.1119±0.007^{C}	ND
CaFr12						260.05±0.43^{A}	331.84±0.68^{D}	4.6950±0.00^{DE}	1.0656±0.007^{D}	ND
CaFr21						132.60±1.85^{D}	329.49±0.68^{D}	4.7553±0.04^{CD}	1.0773±0.018^{D}	ND

Table 4.13 contd.

CaXy11						93.380±1.95^{E}	88.480±2.03^{HI}	4.8038±0.06^{BC}	1.1196±0.007^{BC}	ND
CaXy12						63.480±0.43^{H}	88.870±2.71^{HI}	4.8643±0.02^{AB}	1.1312±0.007^{AB}	ND
CaXy21						52.451±0.43^{I}	86.520±2.71^{I}	4.8886±0.04^{A}	1.0656±0.013^{D}	ND
CaGr11						68.137±0.85^{G}	91.210±2.95^{GH}	4.8159±0.02^{BC}	1.0735±0.007^{D}	ND
CaGr12						69.853±0.74^{G}	92.380±1.35^{FG}	4.6463±0.04^{E}	1.0656±0.007^{D}	ND
CaGr21						46.569±1.12^{J}	91.210±1.79^{GH}	4.6705±0.02^{E}	1.0619±0.007^{D}	ND
CaGc11						149.27±1.27^{C}	744.34±1.35^{A}	4.6950±0.00^{DE}	1.0619±0.007^{D}	ND
CaGc21						75.735±0.74^{F}	561.52±0.68^{B}	4.7917±0.04^{C}	1.1427±0.013^{A}	ND
CaGl11						50.735±0.74^{I}	87.700±3.77^{I}	4.6705±0.02^{E}	1.1235±0.013^{BC}	ND
CaGl21						63.971±0.74^{H}	94.727±1.35^{F}	4.6705±0.08^{E}	1.1235±0.007^{BC}	ND
CaSu11	9	50	15	15	70	252.70±0.43^{A}	216.60±0.00^{F}	4.8643±0.04^{BC}	1.2465±0.007^{A}	ND
CaFr11						160.30±0.00^{C}	361.13±0.68^{C}	4.7432±0.02^{D}	1.2156±0.007^{B}	ND
CaFr12						250.49±0.43^{B}	329.49±0.68^{E}	4.6827±0.02^{E}	1.0965±0.027^{E}	ND
CaFr21						129.66±0.85^{E}	336.13±0.68^{D}	4.6705±0.04^{E}	1.0619±0.007^{F}	ND
CaXy11						95.100±1.85^{F}	91.210±4.12^{GHI}	4.7553±0.02^{D}	1.1004±0.013^{E}	ND
CaXy12						54.902±0.85^{J}	90.040±1.79^{HIJ}	4.8643±0.02^{BC}	1.1004±0.033^{E}	ND
CaXy21						52.696±0.85^{K}	86.914±0.68^{J}	4.7069±0.04^{DE}	1.0619±0.007^{F}	ND
CaGr11						68.137±0.85^{H}	94.727±1.35^{G}	5.1308±0.06^{A}	1.0696±0.012^{F}	ND
CaGr12						68.63±1.85^{H}	88.090±2.44^{IJ}	4.8522±0.02^{BC}	1.0619±0.007^{F}	ND
CaGr21						44.608±0.85^{L}	90.040±1.79^{HIJ}	4.8280±0.04^{C}	1.1542±0.013^{C}	ND
CaGc11						149.51±1.53^{D}	830.66±1.79^{A}	5.1066±0.02^{A}	1.0696±0.012^{F}	ND
CaGc21						75.000±0.74^{G}	536.52±5.54^{B}	4.8522±0.02^{BC}	1.1312±0.013^{CD}	ND
CaGl11						51.471±0.74^{K}	92.380±3.58^{GH}	4.9007±0.04^{B}	1.1119±0.007^{DE}	ND
CaGl21						63.235±1.27^{I}	90.430±0.68^{HIJ}	4.6705±0.02^{E}	1.1465±0.013^{C}	ND
CaSu11	10	40	10	20	80	187.26±1.70^{I}	376.82±0.90^{G}	6.2920±0.06^{I}	1.6467±0.018^{G}	ND
CaFr11						252.29±0.57^{E}	699.74±3.61^{C}	11.100±0.00^{A}	5.4005±0.018^{A}	ND
CaFr12						635.29±1.96^{A}	457.03±10.9^{E}	8.0685±0.06^{F}	2.7236±0.009^{D}	ND
CaFr21						130.72±2.04^{L}	442.45±0.90^{F}	7.2448±0.11^{G}	2.9595±0.018^{C}	ND
CaXy11						241.50±1.13^{F}	185.68±1.80^{L}	8.3592±0.11^{E}	1.4826±0.009^{K}	ND
CaXy12						278.11±1.13^{C}	463.80±1.80^{D}	7.1800±0.00^{G}	1.4260±0.000^{L}	ND
CaXy21						132.68±1.13^{L}	218.49±0.90^{K}	9.0052±0.06^{C}	1.8774±0.009^{E}	ND
CaGr11						220.59±0.98^{G}	271.61±1.80^{J}	9.5060±0.00^{B}	1.5390±0.009^{I}	ND
CaGr12						271.90±0.57^{D}	311.20±0.90^{H}	8.3753±0.06^{E}	5.0313±0.018^{B}	ND
CaGr21						189.87±1.50^{H}	131.51±0.90^{M}	8.8598±0.03^{D}	1.5851±0.009^{H}	ND
CaGc11						154.25±1.13^{K}	1131.5±0.90^{A}	5.8559±0.03^{K}	1.5133±0.018^{J}	ND
CaGc21						162.75±0.98^{J}	876.82±0.90^{B}	7.0350±0.00^{H}	1.6467±0.018^{G}	ND

Table 4.13 contd.

CaGl11						222.55±0.98^{G}	294.01±0.90^{I}	6.1789±0.03^{J}	1.6928±0.018^{F}	ND
CaGl21						287.30±0.00^{B}	185.68±1.80^{L}	6.9703±0.06^{H}	1.4723±0.027^{K}	ND
CaSu11	11	40	20	20	60	267.97±2.26^{C}	126.30±0.90^{E}	6.2920±0.03^{EF}	9.7595±0.036^{F}	ND
CaFr11						398.69±0.57^{B}	349.74±0.90^{B}	6.9541±0.03^{A}	10.031±0.009^{E}	ND
CaFr12						650.33±0.57^{A}	120.57±1.80^{GHI}	6.4212±0.03^{BCD}	10.267±0.018^{D}	ND
CaFr21						60.131±0.57^{L}	125.26±3.61^{EF}	6.3400±0.18^{DEF}	10.785±0.018^{B}	ND
CaXy11						122.55±1.70^{D}	115.37±0.90^{J}	6.3889±0.03^{CDE}	11.324±0.024^{A}	ND
CaXy12						92.484±1.50^{E}	120.57±0.90^{GHI}	6.2758±0.03^{F}	10.016±0.018^{E}	ND
CaXy21						64.379±0.57^{K}	121.62±0.90^{FGH}	6.3242±0.03^{DEF}	9.5133±0.036^{G}	ND
CaGr11						66.990±2.04^{J}	123.18±0.90^{EFG}	6.3404±0.03^{DEF}	9.2774±0.036^{H}	ND
CaGr12						70.588±0.98^{I}	114.32±1.80^{J}	6.5181±0.03^{B}	8.4364±0.018^{I}	ND
CaGr21						70.588±0.98^{I}	117.97±2.71^{HIJ}	6.2758±0.06^{F}	10.606±0.018^{C}	ND
CaGc11						74.510±0.00^{H}	645.05±0.90^{A}	6.2600±0.00^{F}	8.0467±0.009^{J}	ND
CaGc21						60.458±1.13^{L}	339.32±6.31^{C}	6.2758±0.03^{F}	2.8313±0.009^{K}	ND
CaGl11						78.758±0.57^{G}	117.45±0.90^{IJ}	6.2920±0.06^{EF}	1.4518±0.044^{L}	ND
CaGl21						83.66±0.57^{F}	186.20±0.90^{D}	6.4696±0.11^{BC}	1.4467±0.018^{L}	ND
CaSu11	12	60	20	20	60	316.01±6.89^{B}	119.53±2.71^{IJK}	6.3243±0.03^{C}	1.4672±0.009^{HI}	49.8±0.2^{E}
CaFr11						567.320±1.13^{A}	466.93±1.80^{B}	6.5342±0.06^{B}	5.9441±0.009^{A}	70.1±0.1^{C}
CaFr12						221.24±1.13^{D}	414.32±1.80^{C}	6.2920±0.11^{CDE}	1.9903±0.018^{C}	13.7±0.2^{M}
CaFr21						72.880±1.50^{J}	125.26±1.80^{H}	6.2435±0.03^{CDEF}	1.7595±0.018^{D}	21.5±0.1^{K}
CaXy11						104.58±0.57^{G}	115.37±0.90^{K}	6.1789±0.03^{F}	1.4979±0.024^{F}	49.3±0.0^{F}
CaXy12						67.320±1.50^{K}	121.09±2.71^{HIJ}	6.2110±0.00^{EF}	1.4621±0.009^{HI}	23.3±0.1^{J}
CaXy21						92.810±3.44^{H}	121.61±1.80^{HIJ}	9.1667±0.08^{A}	1.4774±0.018^{FGHI}	36.0±0.0^{G}
CaGr11						112.70±0.00^{F}	480.99±0.90^{A}	6.3081±0.08^{CD}	1.4928±0.009^{FG}	52.3±0.1^{D}
CaGr12						272.88±3.00^{C}	159.12±0.90^{G}	6.1789±0.03^{F}	1.4720±0.000^{GHI}	72.3±0.1^{B}
CaGr21						83.007±0.57^{I}	275.26±1.80^{E}	6.2758±0.03^{CDE}	3.2001±0.009^{B}	31.6±0.2^{I}
CaGc11						146.41±3.15^{E}	209.64±6.31^{F}	6.4696±0.03^{B}	1.4569±0.027^{I}	14.4±0.3^{L}
CaGc21						146.41±3.15^{E}	117.97±2.71^{JK}	6.2274±0.06^{DEF}	1.5390±0.009^{E}	90.9±0.3^{A}
CaGl11						72.220±2.04^{J}	124.22±5.41^{HI}	6.3243±0.03^{C}	1.4826±0.018^{FGH}	35.2±0.1^{H}
CaGl21						82.026±1.13^{I}	354.43±0.90^{D}	6.2435±0.03^{CDEF}	1.4980±0.009^{F}	11.8±0.1^{N}
CaSu11	13	60	10	10	80	262.09±0.75^{E}	383.72±0.45^{I}	4.2119±0.03^{J}	1.8080±0.004^{G}	ND
CaFr11						208.01±1.58^{I}	597.01±0.90^{B}	6.4970±0.00^{E}	3.7336±0.019^{A}	ND
CaFr12						322.71±0.28^{B}	284.51±0.90^{N}	4.1960±0.00^{J}	1.2618±0.009^{J}	ND
CaFr21						90.850±0.28^{M}	332.94±1.80^{K}	6.9008±0.03^{C}	2.1285±0.008^{D}	ND
CaXy11						281.54±0.28^{D}	427.47±0.45^{G}	5.8995±0.03^{F}	1.4310±0.024^{H}	ND

Table 4.13 contd.

CaXy12						232.52±0.75^{F}	470.44±0.45^{F}	5.6654±0.01^{G}	1.3156±0.009^{I}	ND
CaXy21						224.84±0.75^{G}	352.70±0.00^{J}	5.3747±0.03^{H}	2.3387±0.004^{C}	ND
CaGr11						210.46±2.04^{H}	671.75±0.45^{A}	6.5778±0.07^{D}	2.4285±0.015^{B}	ND
CaGr12						348.20±0.75^{A}	567.84±0.45^{D}	7.0785±0.04^{B}	1.9541±0.004^{F}	ND
CaGr21						310.29±0.49^{C}	590.50±0.45^{C}	8.0960±0.00^{A}	2.3464±0.004^{C}	ND
CaGc11						162.42±0.75^{K}	553.00±0.45^{E}	4.5995±0.01^{I}	0.7336±0.012^{L}	ND
CaGc21						115.85±0.28^{L}	325.91±0.45^{L}	3.9373±0.01^{K}	1.2490±0.009^{J}	ND
CaGl11						309.97±0.75^{C}	406.60±0.00^{H}	6.5375±0.07^{DE}	2.0280±0.000^{E}	ND
CaGl21						200.16±0.75^{J}	293.10±0.90^{M}	5.8753±0.06^{F}	1.1003±0.004^{K}	ND
CaSu11	14	40	20	10	80	147.55±0.98^{B}	72.526±0.45^{E}	3.1379±0.01^{FG}	0.7362±0.013^{F}	ND
CaFr11						140.20±0.49^{C}	205.34±0.45^{C}	3.5497±0.01^{A}	1.0105±0.004^{A}	ND
CaFr12						183.50±1.02^{A}	61.590±1.80^{F}	3.2187±0.01^{C}	0.7413±0.009^{EF}	ND
CaFr21						66.667±0.49^{E}	97.790±1.80^{D}	3.1460±0.03^{EFG}	0.8926±0.009^{C}	ND
CaXy11						50.817±0.28^{H}	70.180±1.80^{E}	3.1621±0.01^{DEF}	0.7515±0.000^{E}	ND
CaXy12						46.405±1.02^{I}	61.849±0.90^{F}	3.1379±0.01^{FG}	0.7182±0.004^{G}	ND
CaXy21						30.392±0.49^{M}	61.070±1.80^{F}	3.1300±0.00^{GH}	1.6721±0.009^{A}	ND
CaGr11						85.294±0.49^{D}	61.328±1.35^{F}	3.1864±0.01^{D}	0.7413±0.009^{EF}	ND
CaGr12						63.725±1.30^{F}	58.984±1.35^{F}	3.1621±0.01^{DEF}	0.7233±0.009^{G}	ND
CaGr21						58.007±0.28^{G}	61.070±2.26^{F}	3.2671±0.03^{B}	0.7182±0.004^{G}	ND
CaGc11						55.392±0.98^{H}	340.76±0.90^{A}	3.1060±0.00^{H}	0.7128±0.004^{G}	ND
CaGc21						41.176±0.49^{K}	299.09±1.80^{B}	3.2510±0.00^{B}	0.7131±0.000^{G}	ND
CaGl11						54.080±2.47^{H}	58.980±2.71^{F}	3.1702±0.03^{DE}	0.7669±0.008^{D}	ND
CaGl21						33.820±1.96^{L}	60.290±3.61^{F}	3.1379±0.01^{FG}	0.7131±0.000^{G}	ND
CaSu11	15	60	10	20	60	134.31±3.40^{D}	198.18±0.90^{D}	6.5342±0.03^{A}	1.5082±0.009^{BCD}	ND
CaFr11						225.16±1.50^{B}	118.49±0.90^{H}	6.3404±0.03^{BC}	1.5133±0.018^{ABC}	ND
CaFr12						695.42±2.83^{A}	123.70±1.80^{FG}	6.2435±0.03^{EFG}	1.4774±0.009^{E}	ND
CaFr21						109.80±0.98^{G}	145.57±1.80^{E}	6.2920±0.03^{CDE}	1.4877±0.027^{CDE}	ND
CaXy11						79.412±1.70^{I}	124.22±2.71^{F}	6.2758±0.03^{DEF}	1.5133±0.018^{ABC}	ND
CaXy12						105.88±0.98^{H}	121.61±3.61^{FGH}	6.2600±0.00^{EF}	1.4467±0.009^{F}	ND
CaXy21						61.438±0.57^{K}	121.09±5.41^{FGH}	6.2274±0.06^{FG}	1.4774±0.018^{E}	ND
CaGr11						112.42±1.50^{G}	120.57±1.80^{FGH}	6.3727±0.03^{B}	1.4467±0.009^{F}	ND
CaGr12						127.12±1.50^{E}	119.01±7.22^{GH}	6.2274±0.06^{FG}	1.5390±0.009^{A}	ND
CaGr21						116.34±1.13^{F}	123.18±0.90^{FGH}	6.2758±0.03^{DEF}	1.5287±0.018^{AB}	ND
CaGc11						166.67±0.98^{C}	826.82±1.80^{A}	6.5342±0.03^{A}	1.5390±0.009^{A}	ND
CaGc21						109.80±0.98^{G}	123.18±0.90^{FGH}	6.3243±0.03^{BCD}	1.4826±0.018^{DE}	ND
CaGl11						65.359±1.50^{J}	407.55±0.90^{B}	6.1951±0.03^{G}	1.4621±0.009^{EF}	ND

Table 4.13 contd.

CaGl21						64.706±0.98^{J}	265.37±0.90^{C}	6.2274±0.03^{FG}	1.5185±0.027^{AB}	ND
CaSu11	16	60	20	20	80	226.80±0.57^{B}	387.24±3.61^{B}	6.2435±0.06^{G}	1.5236±0.018^{B}	ND
CaFr11						63.072±0.57^{K}	124.74±0.90^{F}	6.1630±0.00^{H}	1.4774±0.009^{CD}	ND
CaFr12						276.47±0.98^{A}	122.14±4.51^{FGH}	6.4212±0.06^{CD}	1.4364±0.018^{FG}	ND
CaFr21						75.817±0.57^{I}	165.37±0.90^{E}	6.4050±0.00^{CDE}	1.4621±0.009^{DEF}	ND
CaXy11						89.87±2.26^{G}	124.74±4.51^{F}	6.4212±0.03^{CD}	1.4672±0.018^{CDE}	ND
CaXy12						59.477±0.57^{L}	117.45±1.80^{H}	6.3404±0.03^{F}	1.4672±0.018^{CDE}	ND
CaXy21						66.013±0.57^{J}	116.93±3.61^{H}	6.3566±0.05^{EF}	1.6467±0.018^{A}	ND
CaGr11						131.05±0.57^{D}	117.97±8.12^{GH}	6.2435±0.03^{G}	1.4262±0.0154^{G}	ND
CaGr12						129.09±1.13^{D}	123.70±1.80^{FG}	6.3889±0.03^{DEF}	1.4569±0.027^{DEF}	ND
CaGr21						177.45±0.98^{C}	119.53±5.41^{FGH}	6.4535±0.05^{BC}	1.4928±0.009^{C}	ND
CaGc11						112.42±2.04^{E}	689.32±1.80^{A}	6.3404±0.03^{F}	1.5287±0.018^{B}	ND
CaGc21						67.320±0.57^{J}	200.26±1.80^{D}	6.5020±0.00^{B}	1.4621±0.009^{DEF}	ND
CaGl11						109.80±0.98^{F}	121.09±2.71^{FGH}	6.9218±0.06^{A}	1.4467±0.009^{EFG}	ND
CaGl21						84.640±2.08^{H}	325.26±1.80^{C}	6.4212±0.03^{CD}	1.4826±0.009^{CD}	ND
CaSu11	17	60	10	10	60	267.97±0.57^{B}	62.630±0.90^{C}	3.2429±0.03^{B}	0.7541±0.004^{B}	26.1±0.2^{J}
CaFr11						368.97±0.28^{A}	199.87±0.45^{A}	4.1957±0.04^{A}	2.1849±0.004^{A}	68.1±0.1^{C}
CaFr12						237.09±1.98^{C}	59.245±0.45^{EF}	3.0895±0.01^{G}	0.7439±0.013^{BCD}	63.9±0.1^{D}
CaFr21						74.837±0.75^{J}	59.505±0.45^{DEF}	3.1379±0.01^{EF}	0.7362±0.013^{DEFG}	25.9±1.7^{J}
CaXy11						69.935±0.28^{L}	62.630±0.90^{C}	3.2025±0.04^{BC}	0.7285±0.000^{EFG}	37.8±0.4^{G}
CaXy12						90.686±1.30^{I}	61.068±0.90^{CDE}	3.0976±0.01^{FG}	0.7233±0.004^{G}	13.7±0.1^{L}
CaXy21						32.353±0.49^{N}	79.557±0.45^{B}	3.0975±0.03^{FG}	0.7387±0.004^{CDEF}	41.4±0.2^{F}
CaGr11						115.69±1.70^{F}	58.460±1.80^{F}	3.1944±0.01^{CD}	0.7541±0.004^{B}	30.1±0.3^{I}
CaGr12						153.10±2.04^{D}	61.590±1.80^{CD}	3.1300±0.00^{EFG}	0.7336±0.004^{DEFG}	85.6±0.0^{B}
CaGr21						100.65±0.28^{H}	58.460±1.80^{F}	3.1541±0.04^{DE}	0.7464±0.012^{BCD}	45.6±0.1^{E}
CaGc11						103.27±0.28^{G}	62.891±1.35^{C}	3.2106±0.03^{BC}	0.7259±0.004^{FG}	32.7±0.1^{H}
CaGc21						126.80±0.75^{E}	78.780±3.16^{B}	3.0895±0.01^{G}	0.7413±0.009^{BCDE}	91.8±0.1^{A}
CaGl11						72.222±0.57^{K}	59.245±1.19^{EF}	3.3114±0.03^{FG}	0.7515±0.013^{BC}	16.0±0.1^{K}
CaGl21						57.026±0.28^{M}	59.505±0.90^{DEF}	3.0895±0.01^{G}	0.7464±0.009^{BCD}	29.9±0.1^{I}
CaSu11	18	40	10	20	60	233.33±1.96^{F}	949.48±1.80^{F}	12.3902±0.06^{DEF}	2.8518±0.032^{A}	8.28±0.1^{I}
CaFr11						168.63±1.96^{H}	1543.2±18.0^{B}	12.3579±0.06^{EF}	1.6415±0.031^{B}	13.0±0.0^{H}
CaFr12						379.09±1.13^{A}	831.77±3.61^{G}	12.6163±0.10^{B}	1.5441±0.009^{C}	1.51±0.1^{K}
CaFr21						220.92±2.26^{G}	400.52±3.61^{J}	12.9716±0.06^{A}	1.4621±0.009^{EF}	1.40±0.1^{K}
CaXy11						124.84±2.26^{J}	243.23±7.22^{LM}	12.3579±0.06^{EF}	1.5236±0.018^{CD}	53.3±1.0^{B}
CaXy12						125.49±1.96^{J}	1030.73±1.80^{D}	12.4200±0.00^{CDEF}	1.4928±0.018^{DE}	1.35±0.0^{K}

Table 4.13 contd.

CaXy21						133.33±7.07^{I}	250.52±3.61^{L}	13.0685±0.11^{A}	1.5185±0.027^{CD}	7.38±0.0^{J}
CaGr11						222.22±2.26^{G}	414.06±5.41^{I}	12.4548±0.11^{CDE}	1.4774±0.009^{E}	20.6±0.2^{F}
CaGr12						332.68±1.13^{B}	308.85±7.22^{K}	12.3579±0.06^{EF}	1.4313±0.009^{F}	91.4±0.0^{A}
CaGr21						233.33±1.96^{F}	988.02±3.61^{E}	12.4871±0.11^{CD}	1.4877±0.031^{DE}	27.9±0.1^{E}
CaGc11						315.69±1.96^{C}	1713.0±9.02^{A}	12.5194±0.10^{BC}	1.4928±0.032^{DE}	31.4±0.0^{D}
CaGc21						294.12±3.40^{D}	1134.9±7.22^{C}	12.3579±0.06^{EF}	1.5339±0.015^{C}	32.3±0.0^{C}
CaGl11						296.08±3.92^{D}	525.52±9.02^{H}	12.4548±0.06^{CDE}	1.4928±0.018^{DE}	17.4±0.2^{G}
CaGl21						264.71±1.96^{E}	235.94±5.41^{M}	12.3300±0.00^{F}	1.4928±0.044^{DE}	1.57±0.3^{K}
CaSu11	19	60	10	20	80	728.10±3.00^{A}	247.40±3.61^{DE}	12.3902±0.06^{CDE}	2.9651±0.018^{C}	57.4±0.0^{A}
CaFr11						167.32±4.08^{I}	1246.4±14.4^{B}	12.3300±0.00^{E}	3.0980±0.000^{B}	23.0±0.1^{D}
CaFr12						406.54±3.00^{B}	1313.0±3.61^{A}	12.3300±0.00^{E}	2.9344±0.018^{CD}	24.9±0.1^{C}
CaFr21						241.83±1.13^{E}	252.60±1.80^{D}	12.4200±0.00^{CD}	2.9549±0.036^{C}	9.65±0.1^{H}
CaXy11						124.18±3.00^{J}	809.90±9.02^{C}	12.3902±0.11^{CDE}	2.8728±0.018^{E}	19.0±0.1^{E}
CaXy12						184.31±1.96^{H}	245.31±5.41^{DEF}	12.3300±0.00^{E}	2.8626±0.018^{EF}	9.16±0.0^{H}
CaXy21						121.60±0.00^{J}	243.23±7.22^{DEFG}	12.4225±0.10^{CD}	6.4220±0.000^{A}	14.9±0.1^{F}
CaGr11						220.26±3.00^{F}	236.98±7.22^{FGH}	12.4548±0.11^{BC}	2.8318±0.018^{F}	11.4±0.1^{G}
CaGr12						277.12±3.00^{C}	244.27±1.80^{DEF}	12.5517±0.06^{A}	2.8520±0.000^{EF}	2.66±0.0^{I}
CaGr21						198.04±1.96^{G}	243.23±7.22^{DEFG}	12.3300±0.00^{E}	2.9138±0.053^{D}	14.6±0.1^{F}
CaGc11						407.84±1.96^{B}	233.85±1.80^{GH}	12.3300±0.00^{E}	2.9651±0.036^{C}	55.2±1.3^{B}
CaGc21						238.56±1.13^{E}	247.40±3.61^{DE}	12.3579±0.06^{DE}	2.8626±0.018^{EF}	20.0±0.0^{E}
CaGl11						247.71±1.13^{D}	231.77±1.80^{H}	12.3300±0.00^{E}	2.8318±0.018^{F}	24.4±0.1^{C}
CaGl21						186.93±3.00^{H}	241.15±3.61^{EFGH}	12.5200±0.00^{AB}	2.8520±0.000^{EF}	2.90±0.1^{I}
CaSu11	20	40	20	20	80	598.04±3.92^{B}	1505.7±1.80^{A}	12.6809±0.06^{AB}	6.3805±0.018^{C}	75.6±0.1^{E}
CaFr11						313.07±2.26^{D}	1478.7±3.61^{B}	12.3579±0.06^{B}	2.8728±0.036^{I}	59.1±0.2^{J}
CaFr12						620.92±1.13^{A}	755.73±7.22^{D}	12.5200±0.00^{B}	3.0164±0.018^{DEF}	74.7±0.0^{F}
CaFr21						192.81±2.26^{I}	229.69±5.41^{I}	12.4548±0.11^{B}	2.9651±0.036^{FGH}	71.6±0.1^{G}
CaXy11						169.93±5.66^{J}	250.52±7.22^{G}	12.4548±0.06^{B}	2.8728±0.036^{I}	10.3±0.1^{N}
CaXy12						255.49±3.40^{G}	870.31±10.8^{C}	12.5840±0.11^{AB}	6.6779±0.036^{B}	65.6±0.1^{H}
CaXy21						152.94±6.79^{K}	249.48±3.61^{GH}	13.3500±1.78^{A}	2.9856±0.018^{EFG}	31.6±0.1^{L}
CaGr11						213.73±3.92^{H}	248.44±5.41^{GH}	12.4871±0.06^{B}	3.0267±0.036^{DE}	54.8±0.0^{K}
CaGr12						242.48±8.16^{F}	304.69±10.8^{F}	12.3579±0.06^{B}	3.0370±0.000^{DE}	76.1±0.0^{D}
CaGr21						194.12±1.96^{I}	246.35±1.80^{GH}	12.4200±0.00^{B}	23.724±0.036^{A}	86.9±0.0^{A}
CaGc11						335.29±1.96^{C}	253.65±1.80^{G}	12.3579±0.06^{B}	2.9241±0.018^{HI}	83.6±0.1^{B}
CaGc21						289.54±1.13^{E}	240.10±1.80^{H}	12.4871±0.06^{B}	2.9241±0.018^{HI}	24.4±0.1^{M}
CaGl11						198.04±1.96^{I}	526.56±5.41^{E}	12.3902±0.06^{B}	2.9549±0.036^{GH}	60.3±0.1^{I}
CaGl21						152.94±1.96^{K}	245.31±5.41^{GH}	12.6486±0.06^{AB}	3.0574±0.071^{D}	76.6±0.2^{C}

Table 4.13 contd.

CaSu11	21	50	15	15	70	238.48±0.85^{B}	233.63±0.68^{F}	4.7069±0.04^{DE}	1.1350±0.013^{B}	ND
CaFr11						156.37±2.36^{C}	363.09±1.35^{C}	4.8643±0.02^{AB}	1.1081±0.007^{D}	ND
CaFr12						260.05±0.85^{A}	315.43±1.35^{E}	4.8643±0.04^{AB}	1.1235±0.007^{BC}	ND
CaFr21						132.60±1.85^{E}	329.10±0.68^{D}	4.7553±0.04^{CD}	1.0850±0.007^{E}	ND
CaXy11						93.380±1.95^{F}	88.480±2.03^{HI}	4.8038±0.06^{BC}	1.1196±0.007^{CD}	ND
CaXy12						63.480±1.12^{J}	88.870±2.71^{HI}	4.8643±0.02^{AB}	1.1312±0.007^{ABC}	ND
CaXy21						52.450±2.25^{K}	86.520±2.71^{I}	4.8886±0.04^{A}	1.1312±0.013^{ABC}	ND
CaGr11						68.137±0.43^{I}	91.210±2.95^{GH}	4.8159±0.02^{BC}	1.0773±0.007^{EF}	ND
CaGr12						71.324±0.74^{H}	90.430±4.74^{H}	4.6705±0.02^{EF}	1.0658±0.007^{F}	ND
CaGr21						47.304±0.85^{L}	91.602±1.35^{GH}	4.6705±0.02^{EF}	1.0658±0.007^{F}	ND
CaGc11						149.27±0.74^{D}	725.59±0.68^{A}	4.8159±0.08^{BC}	1.0735±0.007^{EF}	ND
CaGc21						75.735±0.74^{G}	521.68±1.35^{B}	4.7553±0.02^{CD}	1.1427±0.013^{A}	ND
CaGl11						50.735±1.47^{K}	88.090±3.38^{HI}	4.6705±0.02^{EF}	1.1235±0.013^{BC}	ND
CaGl21						63.725±1.12^{J}	94.727±1.35^{G}	4.6342±0.02^{F}	1.1235±0.007^{BC}	ND
CaSu11	22	50	15	25	70	236.93±1.42^{D}	302.73±6.77^{EFG}	15.8107±0.14^{CD}	20.3090±0.022^{A}	27.4±0.2^{D}
CaFr11						1373.4±7.88^{A}	1279.3±13.5^{A}	26.3485±0.07^{A}	12.5910±0.044^{D}	83.3±0.1^{A}
CaFr12						231.21±1.42^{D}	345.70±6.77^{D}	15.4877±0.14^{FG}	3.7449±0.044^{JK}	73.6±0.3^{B}
CaFr21						198.33±2.45^{G}	292.32±15.8^{G}	15.6500±0.00^{DEF}	3.7833±0.022^{IJ}	0.49±0.2^{N}
CaXy11						208.33±8.49^{F}	288.41±2.26^{G}	15.9320±0.28^{C}	3.6939±0.044^{KL}	2.32±0.1^{M}
CaXy12						204.25±1.42^{FG}	297.53±11.3^{EFG}	15.7300±0.14^{DE}	3.6423±0.039^{L}	6.03±0.1^{L}
CaXy21						178.10±3.74^{H}	304.04±2.26^{EFG}	16.4163±0.07^{B}	4.6167±0.044^{H}	9.94±0.1^{I}
CaGr11						215.50±3.74^{E}	313.15±4.51^{E}	15.8107±0.07^{CD}	3.7833±0.044^{IJ}	11.2±0.1^{H}
CaGr12						399.51±2.45^{B}	301.43±4.51^{EFG}	15.8107±0.07^{CD}	3.8603±0.022^{I}	29.9±0.3^{C}
CaGr21						156.86±2.45^{J}	292.32±2.26^{G}	16.3356±0.14^{B}	16.206±0.022^{B}	14.7±0.2^{F}
CaGc11						178.10±3.74^{H}	690.76±4.51^{B}	15.6089±0.07^{EFG}	10.800±0.000^{E}	6.50±0.0^{K}
CaGc21						169.94±1.42^{I}	296.22±9.02^{FG}	15.4877±0.07^{FG}	7.0654±0.067^{G}	25.8±0.1^{E}
CaGl11						258.17±1.42^{C}	641.30±22.6^{C}	15.4474±0.07^{G}	10.309±0.089^{F}	7.15±0.3^{J}
CaGl21						201.80±3.74^{FG}	310.55±6.77^{EF}	15.4474±0.07^{G}	13.950±0.067^{C}	13.8±0.4^{G}
CaSu11	23	70	15	15	70	163.97±0.74^{H}	90.820±2.03^{DEF}	4.8401±0.13^{FG}	1.0889±0.007^{GH}	26.0±0.3^{H}
CaFr11						576.93±0.43^{A}	324.80±3.38^{A}	7.9046±0.02^{A}	5.5580±0.000^{A}	76.9±0.6^{C}
CaFr12						370.74±1.95^{B}	91.990±4.06^{CDEF}	4.6827±0.02^{H}	1.0735±0.007^{H}	20.6±0.2^{K}
CaFr21						203.43±1.12^{E}	90.430±3.38^{DEF}	5.0703±0.02^{E}	1.1427±0.013^{D}	26.8±0.3^{G}
CaXy11						89.216±1.70^{M}	94.727±0.68^{C}	4.7069±0.02^{H}	1.3196±0.013^{C}	20.2±0.1^{K}
CaXy12						143.38±1.47^{I}	93.945±1.35^{CD}	4.7674±0.06^{GH}	1.1158±0.020^{EF}	8.54±0.4^{L}
CaXy21						138.73±0.43^{J}	86.523±0.68^{G}	4.7674±0.06^{GH}	1.1427±0.007^{D}	71.8±0.0^{D}
CaGr11						123.78±0.85^{K}	90.039±0.68^{EFG}	4.8765±0.06^{F}	1.1119±0.007^{EF}	25.5±0.3^{I}

Table 4.13 contd.

CaGr12						189.95±0.43^{F}	91.602±1.35^{CDEF}	6.1361±0.04^{B}	1.0889±0.007^{GH}	78.9±0.3^{B}
CaGr21						273.28±0.43^{C}	93.160±2.03^{CDE}	4.7069±0.02^{H}	1.1235±0.007^{E}	34.7±0.2^{E}
CaGc11						91.912±0.74^{L}	173.63±1.35^{B}	5.3609±0.02^{C}	1.0889±0.007^{GH}	29.2±0.1^{F}
CaGc21						229.41±0.74^{D}	93.555±0.68^{CDE}	4.8401±0.06^{FG}	1.1004±0.013^{FG}	81.8±0.1^{A}
CaGl11						82.108±0.85^{N}	89.258±1.35^{FG}	5.2277±0.04^{D}	1.0735±0.007^{H}	25.7±0.4^{HI}
CaGl21						182.11±1.12^{G}	91.600±3.38^{CDEF}	4.7553±0.04^{GH}	1.4465±0.018^{B}	23.6±0.1^{J}
CaSu11	24	50	15	15	70	252.70±1.12^{A}	218.95±2.71^{F}	4.8643±0.04^{B}	1.0773±0.007^{GH}	ND
CaFr11						160.29±1.47^{B}	364.26±0.68^{C}	4.7432±0.02^{DEF}	4.6273±0.013^{A}	ND
CaFr12						251.96±0.43^{A}	315.04±0.68^{E}	4.8159±0.02^{BCD}	1.0965±0.027^{EFG}	ND
CaFr21						129.41±1.27^{D}	329.49±0.68^{D}	4.7553±0.10^{CDE}	1.0619±0.007^{H}	ND
CaXy11						96.57±0.43^{E}	91.210±4.12^{GHI}	4.8280±0.04^{BC}	1.1196±0.007^{CD}	ND
CaXy12						61.520±0.43^{J}	90.040±1.79^{HI}	4.8643±0.04^{B}	1.0889±0.013^{FG}	ND
CaXy21						52.696±0.43^{K}	92.383+0.68^{GH}	4.7069±0.04^{EF}	1.1081±0.013^{DEF}	ND
CaGr11						67.402±0.43^{H}	94.727±1.35^{G}	5.1672±0.06^{A}	1.1542±0.013^{B}	ND
CaGr12						72.304±0.43^{G}	88.090±2.44^{I}	4.8038±0.06^{BCD}	1.1119±0.013^{CDE}	ND
CaGr21						45.588±1.27^{L}	90.040±1.79^{HI}	4.6705±0.02^{F}	1.0889±0.007^{C}	ND
CaGc11						148.28±0.43^{C}	830.66±1.79^{A}	5.1066±0.02^{A}	1.1620±0.000^{B}	ND
CaGc21						75.490±0.43^{F}	536.52±5.54^{B}	4.8280±0.02^{BC}	1.1312±0.013^{C}	ND
CaGl11						51.716±0.43^{K}	92.380±3.58^{GH}	4.8280±0.04^{BC}	1.1119±0.007^{CDE}	ND
CaGl21						63.480±0.85^{I}	91.211±0.68^{GHI}	4.7674±0.06^{CDE}	1.1312±0.013^{C}	ND
CaSu11	25	50	15	15	90	306.37±2.25^{B}	185.55±9.47^{HI}	9.4380±0.08^{BCD}	4.3162±0.027^{C}	17.4±0.3^{I}
CaFr11						884.31±0.85^{A}	195.70±8.12^{G}	9.5107±0.04^{BC}	13.209±0.027^{A}	81.4±0.1^{A}
CaFr12						148.04±0.85^{G}	290.23±1.35^{E}	9.3653±0.04^{CD}	2.3854±0.027^{F}	22.4±0.4^{F}
CaFr21						98.040±2.25^{L}	187.11±1.35^{H}	9.5349±0.13^{B}	2.2623±0.013^{G}	29.6±0.1^{D}
CaXy11						121.08±3.70^{JK}	370.70±1.35^{C}	9.4380±0.08^{BCD}	2.2162±0.027^{H}	18.7±0.3^{H}
CaXy12						119.10±0.00^{K}	299.61±5.41^{D}	9.4380±0.08^{BCD}	8.1392±0.023^{B}	5.83±0.2^{L}
CaXy21						123.53±2.94^{J}	398.05±2.71^{B}	9.3411±0.04^{D}	2.2700±0.013^{G}	33.6±0.0^{C}
CaGr11						133.33±1.70^{H}	186.33±4.06^{HI}	9.4138±0.04^{BCD}	2.1854±0.040^{HI}	12.5±0.1^{K}
CaGr12						254.41±1.47^{C}	182.42±5.41^{HI}	9.3411±0.04^{D}	3.8238±0.040^{D}	24.9±0.1^{E}
CaGr21						205.90±0.00^{D}	219.92±1.35^{F}	9.2926±0.04^{D}	2.2080±0.000^{H}	25.3±0.1^{E}
CaGc11						187.75±2.25^{E}	1269.9±1.35^{A}	9.2926±0.04^{D}	2.1469±0.013^{I}	20.2±0.0^{G}
CaGc21						167.16±0.85^{F}	180.08±5.41^{HI}	9.3411±0.08^{D}	2.1620±0.000^{I}	46.4±0.1^{B}
CaGl11						169.61±0.85^{F}	178.52±6.77^{I}	9.5591±0.17^{AB}	3.1235±0.013^{E}	22.6±0.2^{F}
CaGl21						128.43±2.25^{I}	180.86±2.71^{HI}	9.7045±0.17^{A}	2.2777±0.023^{G}	16.6±0.4^{J}
CaSu11	26	50	25	15	70	103.92±1.70^{K}	178.52±2.71^{FG}	9.2926±0.04^{GH}	2.1390±0.000^{G}	51.1±0.3^{C}
CaFr11						190.69±3.06^{G}	183.20±6.77^{EFG}	9.3411±0.04^{FG}	2.1700±0.013^{G}	44.2±0.1^{D}

Table 4.13 contd.

CaFr12						409.31±3.06^{A}	347.27±5.41^{C}	9.3411±0.04^{FG}	2.1700±0.013^{G}	15.5±0.0^{K}
CaFr21						181.86±2.25^{H}	183.20±6.77^{EFG}	9.4380±0.08^{DE}	2.2931±0.013^{BCD}	40.7±0.0^{E}
CaXy11						93.140±3.06^{L}	180.08±1.35^{FG}	9.2440±0.00^{H}	2.1469±0.013^{G}	75.9±0.1^{A}
CaXy12						161.76±1.47^{J}	177.73±5.41^{G}	9.4138±0.04^{EF}	2.4085±0.013^{A}	22.0±0.1^{I}
CaXy21						100.980±1.7^{K}	398.05±2.71^{B}	9.2440±0.00^{H}	2.2392±0.027^{EF}	23.5±0.4^{H}
CaGr11						362.75±4.49^{B}	252.73±5.41^{D}	9.6560±0.08^{B}	2.2239±0.013^{F}	24.0±0.3^{G}
CaGr12						349.51±2.25^{C}	184.77±2.71^{EFG}	9.2926±0.08^{GH}	2.1390±0.000^{G}	40.7±0.1^{E}
CaGr21						171.08±2.25^{I}	180.86±2.71^{FG}	9.4864±0.08^{DE}	2.3162±0.013^{B}	14.5±0.0^{L}
CaGc11						294.61±2.25^{D}	502.73±8.12^{A}	9.8498±0.04^{A}	2.2780±0.000^{CD}	25.9±0.1^{F}
CaGc21						228.92±1.70^{F}	186.33±4.06^{EF}	9.5107±0.08^{CD}	2.2623±0.027^{DE}	72.9±0.0^{B}
CaGl11						352.94±1.47^{C}	189.45±2.71^{E}	9.5833±0.04^{BC}	2.3008±0.040^{BC}	17.3±0.2^{J}
CaGl21						246.57±2.25^{E}	178.52±2.71^{FG}	9.2440±0.00^{H}	2.2392±0.027^{EF}	7.96±0.1^{M}
CaSu11	27	30	15	15	70	150.98±2.25^{C}	180.86±2.71^{EFG}	9.3653±0.04^{CDE}	2.1777±0.013^{FG}	5.93±0.1^{K}
CaFr11						93.630±2.25^{FG}	188.67±4.06^{D}	9.3895±0.13^{CD}	2.1700±0.013^{FG}	12.4±0.4^{F}
CaFr12						100.00±1.47^{E}	862.89±5.41^{A}	9.6318±0.04^{B}	2.1931±0.013^{DEFG}	3.15±0.4^{L}
CaFr21						90.200±2.25^{GH}	186.33±4.06^{DE}	9.7045±0.04^{AB}	2.2162±0.013^{DE}	29.1±0.3^{C}
CaXy11						87.750±8.10^{H}	180.86±2.71^{EFG}	9.6560±0.17^{B}	2.2008±0.013^{DEF}	7.70±0.2^{I}
CaXy12						108.82±1.47^{D}	586.33±2.71^{B}	9.7045±0.04^{AB}	2.8392±0.053^{A}	6.68±0.1^{J}
CaXy21						100.98±1.70^{E}	173.83±1.35^{G}	9.8256±0.13^{A}	2.1931±0.013^{DEFG}	1.13±0.2^{M}
CaGr11						151.47±2.55^{C}	179.30±4.06^{EFG}	9.3895±0.13^{CD}	2.2008±0.013^{DEF}	9.08±0.1^{G}
CaGr12						279.90±0.85^{A}	444.14±8.12^{C}	9.4138±0.08^{CD}	2.1850±0.000^{EFG}	35.2±0.4^{B}
CaGr21						148.04±0.85^{C}	179.30±4.06^{EFG}	9.4864±0.04^{C}	2.1620±0.000^{G}	15.9±0.5^{D}
CaGc11						163.73±2.25^{B}	176.17±2.71^{FG}	9.3653±0.04^{CDE}	2.2238±0.027^{D}	12.9±0.3^{E}
CaGc21						93.137±0.85^{FG}	186.33±4.06^{DE}	9.2440±0.00^{E}	2.3315±0.027^{C}	36.4±0.3^{A}
CaGl11						95.100±3.70^{F}	176.95±8.12^{FG}	9.7045±0.04^{AB}	2.1620±0.000^{G}	36.6±0.3^{A}
CaGl21						103.92±1.70^{E}	182.42±5.41^{DEF}	9.3170±0.00^{DE}	2.6930±0.000^{B}	8.19±0.1^{H}
CaSu11	28	50	5	15	70	490.69±3.70^{B}	233.20±4.06^{D}	10.2859±0.08^{B}	2.2469±0.027^{CD}	24.5±0.6^{I}
CaFr11						950.98±2.25^{A}	545.70±1.35^{A}	15.8333±0.08^{A}	6.8315±0.013^{A}	72.1±0.2^{B}
CaFr12						302.45±2.25^{C}	311.33±5.41^{C}	9.2926±0.08^{G}	2.2623±0.013^{C}	17.9±0.2^{L}
CaFr21						95.590±4.41^{K}	184.77±1.35^{EFG}	9.3411±0.08^{FG}	2.2469±0.013^{CD}	39.8±0.4^{F}
CaXy11						109.80±6.63^{J}	178.52±1.35^{HI}	9.2684±0.04^{G}	2.1315±0.013^{H}	77.8±0.1^{A}
CaXy12						148.53±1.47^{H}	183.20±6.77^{FGH}	9.4864±0.04^{E}	2.1777±0.013^{F}	22.6±0.3^{J}
CaXy21						98.530±2.98^{K}	173.83±1.35^{I}	9.2684±0.04^{G}	2.1469±0.013^{GH}	1.13±0.2^{M}
CaGr11						197.55±2.25^{F}	187.11±2.71^{EF}	9.6560±0.17^{D}	2.1546±0.027^{FGH}	38.4±0.1^{G}
CaGr12						251.47±1.47^{D}	177.73±5.41^{HI}	9.4864±0.04^{E}	2.2239±0.013^{DE}	29.2±0.1^{H}
CaGr21						97.059±1.47^{K}	189.45±1.35^{E}	9.3653±0.04^{EFG}	2.3085±0.013^{B}	52.5±0.0^{E}

Table 4.13 contd.

CaGc11						100.00±1.47^{K}	180.08±1.35^{GH}	9.4380±0.04^{EF}	2.1777±0.013^{F}	71.1±0.2^{C}
CaGc21						171.08±2.25^{G}	185.55±2.71^{EFG}	9.3653±0.04^{EFG}	2.2162±0.027^{E}	54.3±0.1^{D}
CaGl11						212.75±3.06^{E}	392.58±4.06^{B}	9.4622±0.13^{EF}	2.1620±0.000^{FG}	22.7±0.2^{J}
CaGl21						132.40±0.00^{I}	183.20±5.41^{FGH}	9.8740±0.04^{C}	2.2320±0.000^{DE}	20.8±0.1^{K}
CaSu11	29	50	15	15	50	237.50±1.47^{D}	129.10±1.35^{C}	4.6220±0.00^{G}	1.2312±0.020^{E}	18.3±0.3^{K}
CaFr11						601.47±0.74^{A}	125.98±2.03^{D}	6.5480±0.00^{B}	4.9465±0.000^{B}	74.6±0.3^{A}
CaFr12						332.84±1.12^{B}	130.27±0.68^{C}	4.8401±0.06^{C}	1.1273±0.020^{FG}	20.2±0.3^{J}
CaFr21						178.16±1.53^{F}	90.430±0.68^{HI}	4.7190±0.02^{E}	1.1427±0.007^{F}	41.5±0.1^{F}
CaXy11						48.04±1.85^{N}	97.070±0.68^{E}	4.7069±0.02^{E}	1.1119±0.007^{GH}	25.4±0.2^{I}
CaXy12						122.06±1.47^{J}	90.430±1.35^{HI}	4.6827±0.02^{E}	1.1196±0.007^{FG}	48.8±0.1^{D}
CaXy21						87.250±1.85^{L}	188.87±0.68^{A}	4.7796±0.02^{D}	1.1196±0.013^{FG}	11.6±0.1^{L}
CaGr11						185.78±1.12^{E}	183.01±1.25^{B}	4.7917±0.02^{D}	1.1427±0.013^{F}	39.7±1.0^{G}
CaGr12						152.45±1.12^{G}	93.160±2.03^{FG}	4.6342±0.02^{G}	5.0350±0.007^{A}	71.1±0.3^{B}
CaGr21						74.510±0.85^{M}	91.211±1.35^{GH}	4.6463±0.02^{FG}	1.1081±0.013^{GH}	32.7±0.1^{H}
CaGc11						248.53±0.74^{C}	88.090±3.38^{I}	6.8144±0.02^{A}	1.0889±0.013^{H}	45.1±0.3^{E}
CaGc21						130.39±0.85^{H}	91.990±2.03^{FGH}	4.7917±0.02^{D}	1.5158±0.013^{D}	61.4±0.1^{C}
CaGl11						127.94±0.74^{I}	93.945±1.35^{F}	4.7917±0.02^{D}	1.1312±0.007^{FG}	18.0±0.1^{K}
CaGl21						112.26±1.12^{K}	91.602±0.68^{FGH}	4.7190±0.02^{E}	4.0965±0.033^{C}	39.7±0.1^{G}
CaSu11	30	50	15	5	70	95.750±1.98^{D}	58.203±1.35^{FGH}	3.1460±0.03^{EF}	1.6926±0.022^{E}	36.3±0.1^{H}
CaFr11						308.82±0.49^{A}	252.47±2.26^{A}	4.6479±0.01^{B}	1.3490±0.009^{F}	82.0±0.4^{A}
CaFr12						147.22±1.50^{C}	60.286±0.45^{FGH}	3.1379±0.01^{EF}	0.5210±0.346^{I}	62.1±0.1^{D}
CaFr21						66.010±2.04^{I}	57.420±0.00^{GH}	3.1379±0.03^{EF}	0.7105±0.004^{H}	29.1±0.6^{J}
CaXy11						36.765±0.49^{L}	61.068±0.45^{EFG}	3.1298±0.02^{F}	1.0464±0.004^{G}	ND
CaXy12						66.830±0.75^{I}	61.589±0.45^{EF}	3.1460±0.01^{EF}	1.6772±0.009^{E}	ND
CaXy21						97.876±1.50^{D}	248.31±0.90^{B}	3.2429±0.03^{D}	0.7592±0.013^{H}	ND
CaGr11						90.359±1.72^{F}	59.770±2.71^{FGH}	3.1460±0.03^{EF}	0.7618±0.022^{H}	53.3±0.1^{E}
CaGr12						159.80±1.77^{B}	61.070±2.26^{EFG}	5.8430±0.04^{A}	0.7233±0.004^{H}	77.5±0.1^{C}
CaGr21						39.542±0.28^{K}	57.682±0.45^{GH}	3.2833±0.01^{C}	2.2336±0.009^{C}	33.1±0.3^{I}
CaGc11						93.140±2.45^{E}	56.901±0.45^{H}	3.1218±0.03^{FG}	5.0823±0.013^{A}	78.2±0.1^{B}
CaGc21						77.778±0.57^{G}	71.740±4.51^{D}	3.0895±0.01^{G}	2.0054±0.013^{D}	78.6±0.4^{B}
CaGl11						62.582±0.57^{J}	164.71±2.96^{C}	3.1702±0.01^{E}	0.7336±0.004^{H}	49.6±0.2^{F}
CaGl21						69.444±0.75^{H}	64.450±4.06^{E}	3.2590±0.01^{CD}	2.9387±0.004^{B}	40.8±0.1^{G}

Means that do not share superscript within same experimental conditions and parameters are significantly different, ND = not determined, UT = ultrasound temperature, ET = extraction time, SV = solvent volume, SC = solvent concentration.

4.6.4.1 Effect of Factors on Total polyphenol content (TPC)

The total phenolic content of extracts was measured using Follin–Ciocalteu's reagent, which assesses phenolic oxidation and the subsequent interaction with phosphomolybdic-phosphotungstic acid complexes. The total phenolic content of the extracts is presented in **Table 4.13,** expressed as equivalents of gallic acid (GAE), with values spanning from 30.392±0.49 µgGAE/g to 1373.4±7.88 µgGAE/g. The highest TPC extract was obtained from CaFr11 as shown in run 22, which has operating conditions of ultrasound temperature, extraction time, solvent volume, and solvent concentration set at 50°C, 15 min, 25 ml, and 70%, respectively. The lowest TPC was obtained from CaXy21 in run 14 with conditions of ultrasound temperature, extraction time, solvent volume, and solvent concentration set at 40°c, 20 min, 20 ml, and 80%, respectively. Regression analysis (**Table 4.10**) shows that full quadratic model fits TPC extraction with factors conditions in the synthesized NADESs, except in CaSu11, CaFr21, CaXy11, and CaGc11, where linear plus interaction model fits the data. Analysis of variance pareto chart (**Figure 4.73**) shows significant factors and factor combination affecting TPC extraction from African nutmeg peels, and how they relate with each other for the synthesized NADESs, thus:

A. CaSu11- SV > UT*ET > SC > SV*SC > ET.
B. CaFr11- SV*SV > SV > SC*SC.
C. CaFr12- SV > UT*SV > UT*ET > ET*ET.
D. CaFr21- SV > ET*SV > UT*ET;
E. CaXy11- UT*SV > SV > SC > ET.
F. CaXy12- UT*SV > SV > ET*ET > SC > ET*SC > SV*SV > ET > UT*UT >SC*SC > UT*ET > SV*SC.
G. CaXy21- SV*SV > SV > UT*SV > SC > UT*UT > ET*SC > ET > SC*SC > UT*SC > ET*ET.
H. CaGr11- ET*ET > SV > SC*SC > UT*SV > SC > SV*SV.
I. CaGr12 – ET*ET > SV > SV*SV > UT*SV > UT*UT > SC > SC*SC.
J. CaGr21- UT*UT > SC > SV > SC*SC > UT*SV > ET*ET > UT >UT*SC > ET > UT*ET.
K. CaGc11- SV > ET*SV > UT*SV.
L. CaGc21- SV > ET*ET > UT*SV > UT*UT > SC*SC > ET*SV > UT.
M. CaGl11- ET*ET >SV > SC > UT*SV > UT*SC > SV*SV > SC*SC > ET.
N. CaGl21- UT*SV > SV > ET*ET > ET*SC > ET*SV > UT*UT > SV*SV > SC > UT*ET > SC*SC.

As can be seen from **Figure 4.73**, volume, and interaction of volume with other factors appear to exert the most significant variation on TPC extraction from African nutmeg peels, because their significance is seen in all the synthesized NADESs while temperature seems to affect the least variation because its significance is only observed in CaGr21 and CaGc21.

Three-dimensional surface plots of the effects of two factors interaction on TPC extraction from African nutmeg peels are presented in **Figure 4.74** to **Figure 4.87** for the synthesized NADESs, respectively. From the plots, the conditions necessary to maximize TPC extraction are as follows:

1. CaSu11- UT (50ºc), ET (5 min), SV (24 ml), and SC (75%), TPC ≥ 400 µgGAE/g.

2. CaFr11 - UT (50ºc), ET (24 min), SV (24 ml), and SC (70%), TPC ≥ 1200 µgGAE/g.
3. CaFr12 - UT (60ºc), ET (24 min), SV (18 ml), and SC (70%), TPC ≥ 400 µgGAE/g.
4. CaFr21- UT (70ºc), ET (15 min), SV (24 ml), and SC (70%), TPC ≥ 180 µgGAE/g.
5. CaXy11- UT (75ºc), ET (24 min), SV (24 ml), and SC (70%), TPC ≥ 200 µgGAE/g.
6. CaXy12- UT (75ºc), ET (20 min), SV (24 ml), and SC (70%), TPC ≥200 µgGAE/g.
7. CaXy21 – UT (75ºc), ET (24 min), SV (24 ml), and SC (70%), TPC ≥150 µgGAE/g.
8. CaGr11 – UT (75ºc), ET (24 min), SV (15 ml), and SC (70%), TPC ≥250 µgGAE/g.
9. CaGr12 – UT (75ºc), ET (24 min), SV (15 ml), and SC (70%), TPC ≥300 µgGAE/g.
10. CaGr21 – UT (75ºc), ET (15 min), SV (15 min), and SC (70%), TPC ≥200 µgGAE/g.
11. CaGc11- UT (50ºc), ET (24 min), SV (15 ml), and SC (70%), TPC ≥200 µgGAE/g.
12. CaGc21 – UT (70ºc), ET (24 min), SV (15 ml), and SC (70%), TPC ≥200 µgGAE/g.
13. CaGl11 – UT (75ºc), ET (24 min), SV (15 ml), and SC (70%), TPC ≥ 250 µgGAE/g.
14. CaGl21 – UT (70º), ET (24 min), SV (15 ml), and SC (70%), TPC ≥200 µgGAE/g.

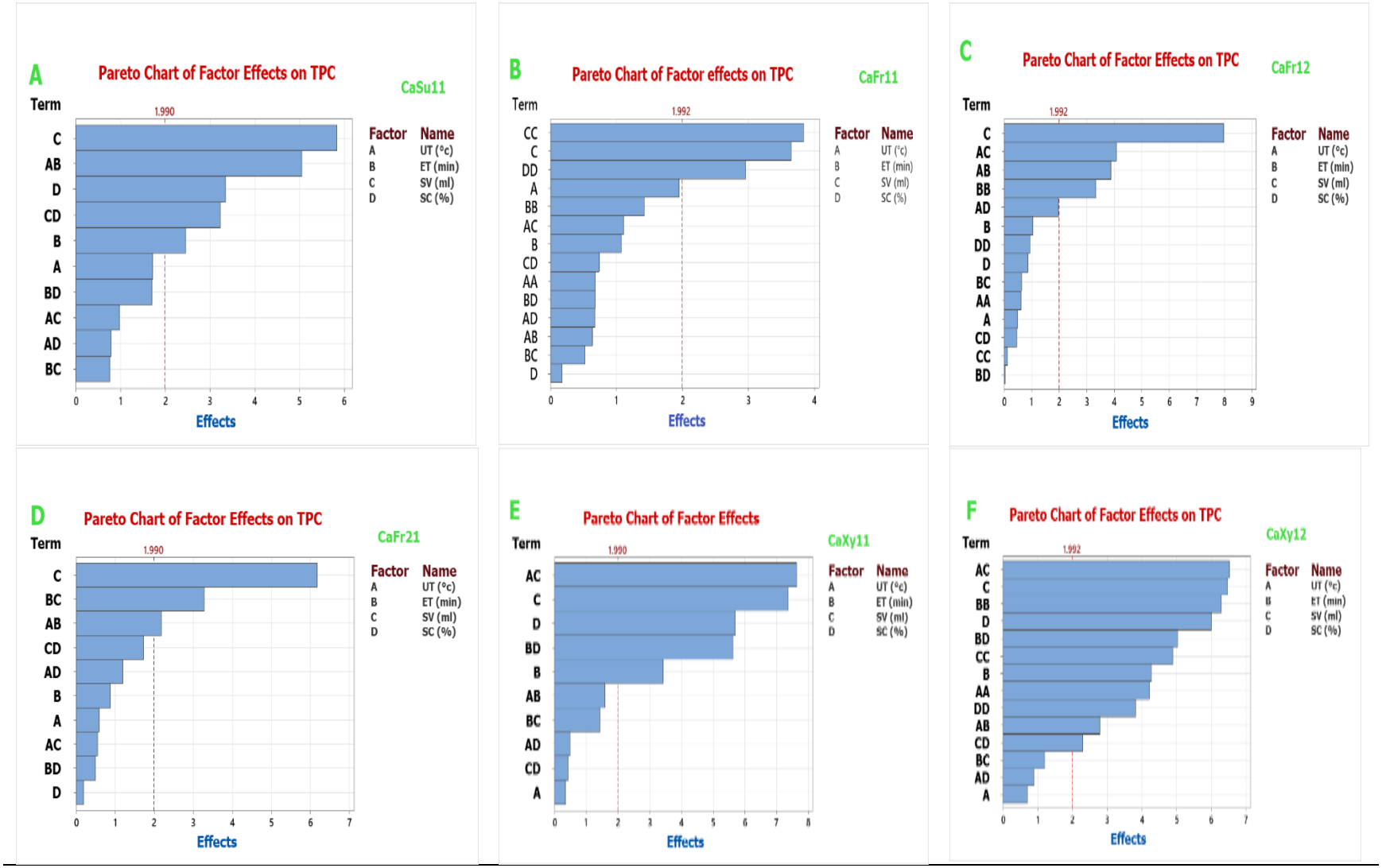


Figure 4.73 Pareto plots of significance factors and factor interactions on TPC of African nutmeg peels extracted using the synthesized NADESs

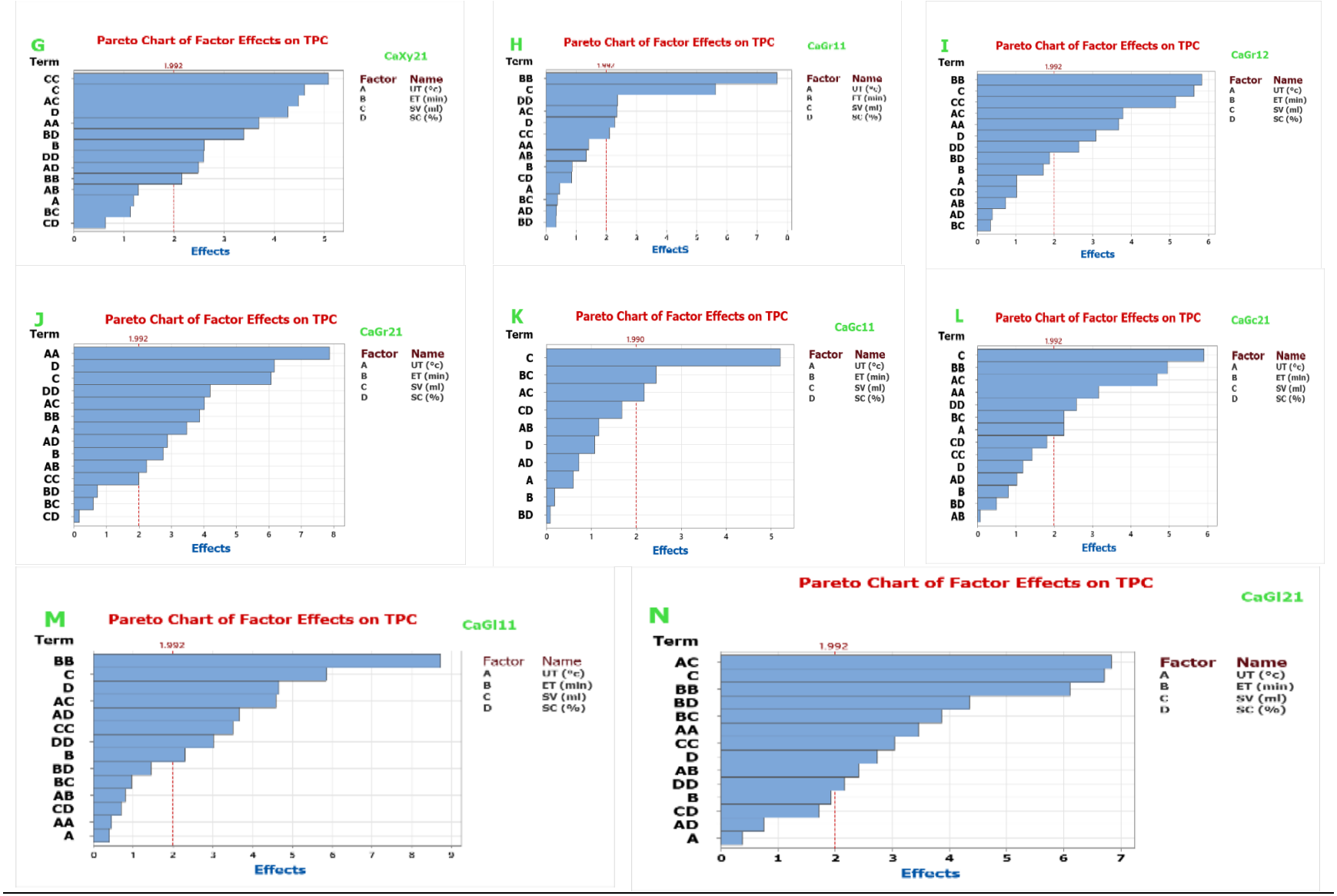


Figure 4.73 contd.

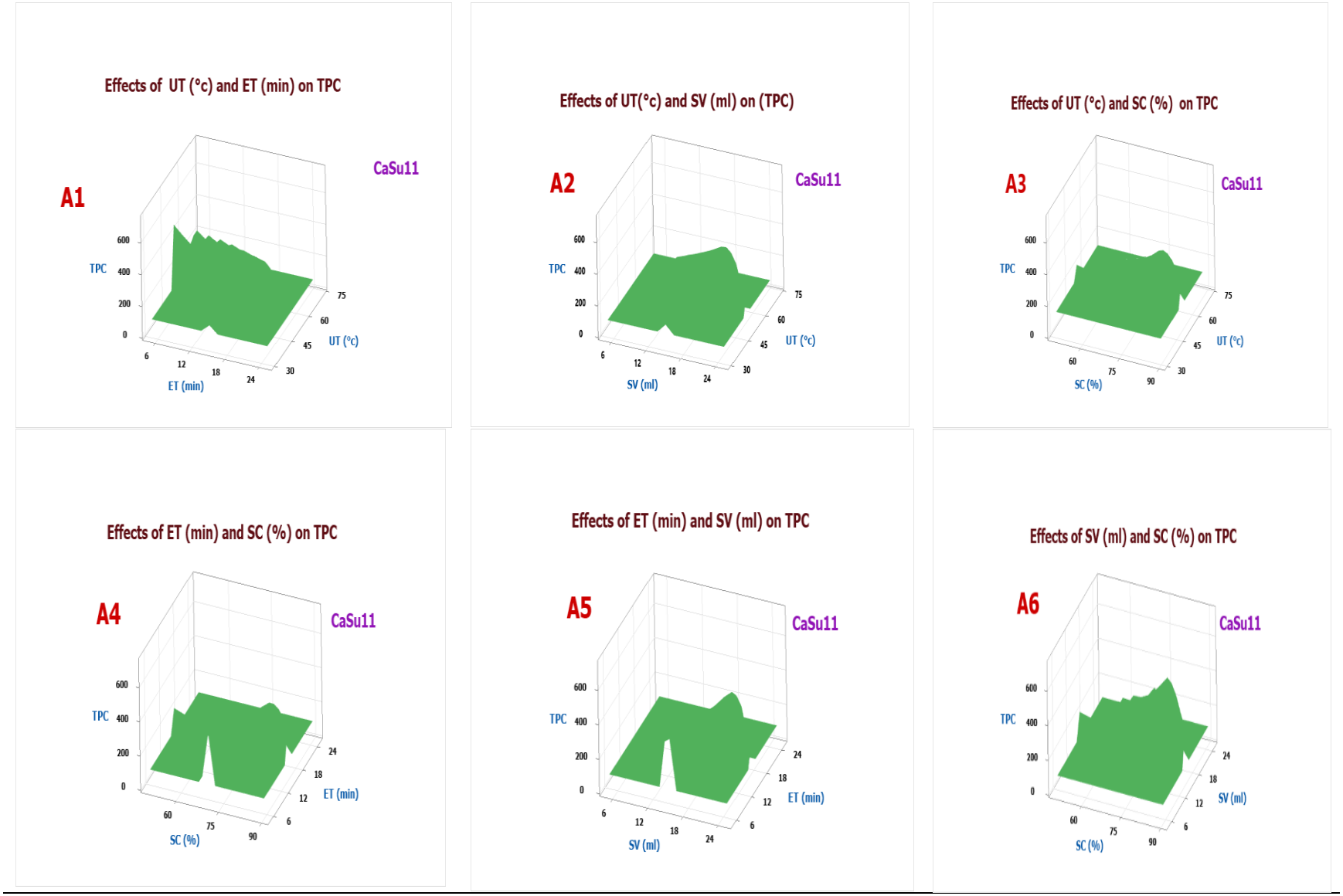


Figure 4.74 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaSu11

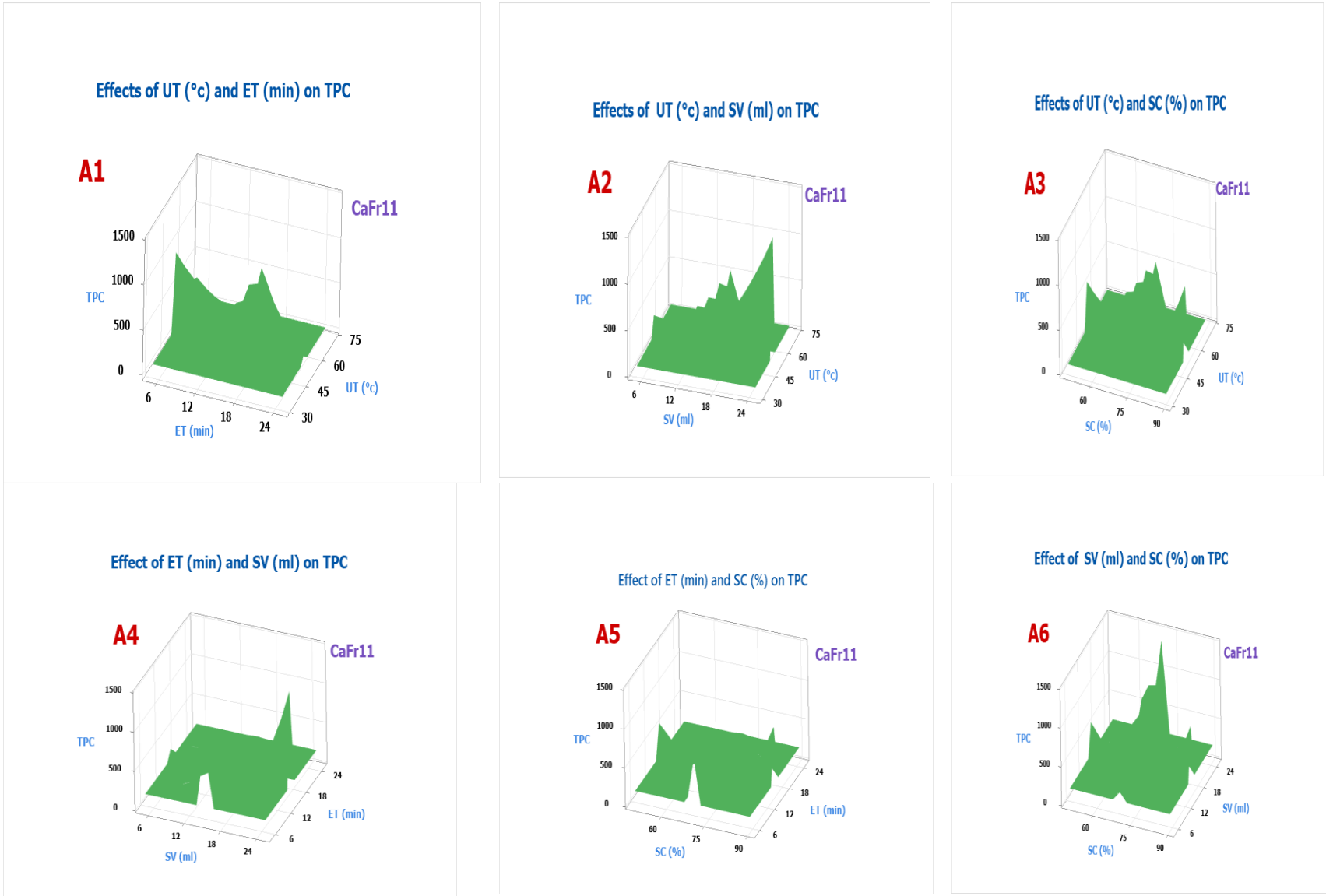


Figure 4.75 Three-dimensional surface plot of factors effects on TPC extraction from African nutmeg peels using CaFr11

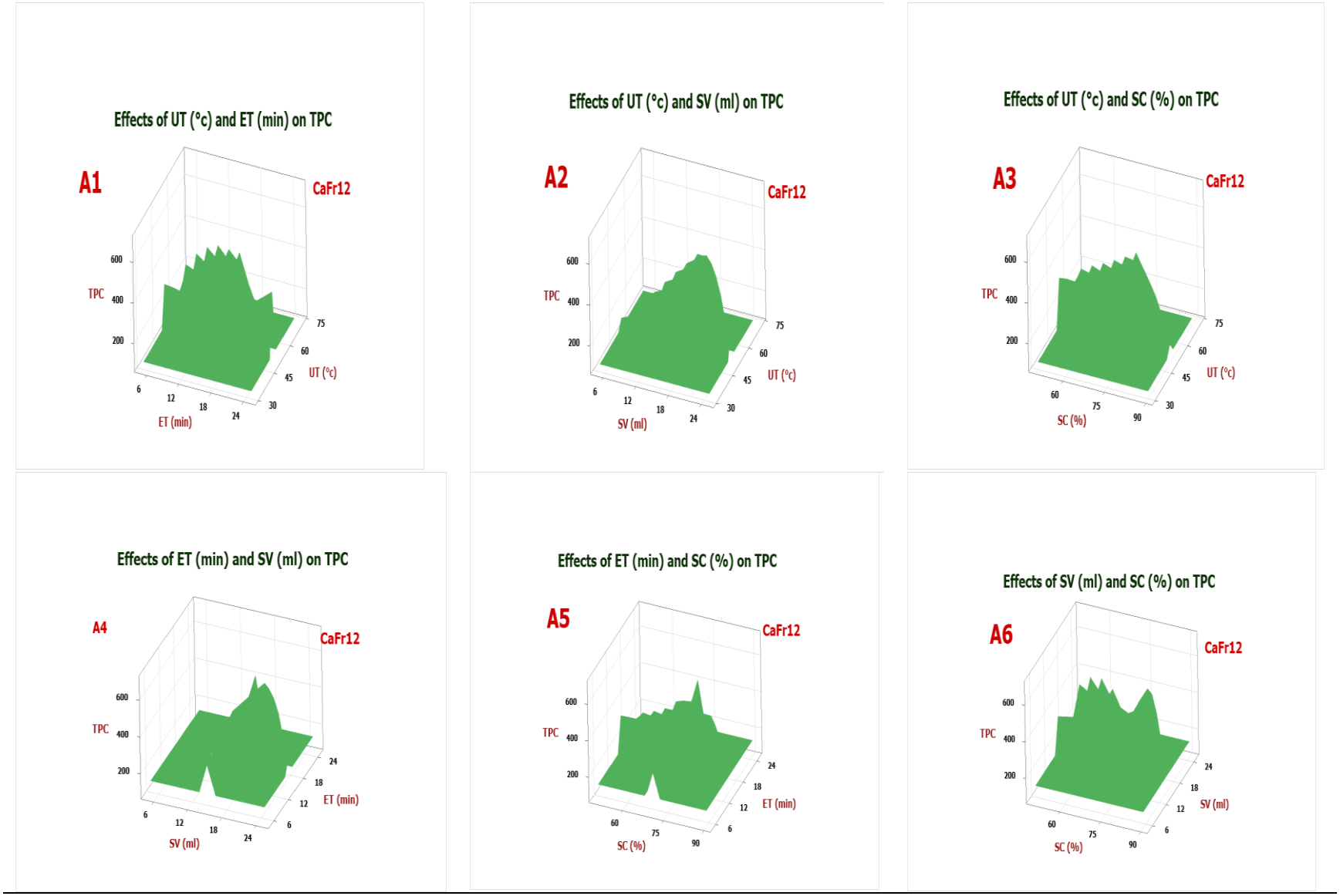


Figure 4.76 Three-dimensional surface plot of factors effects on TPC extraction from African nutmeg peels using CaFr12

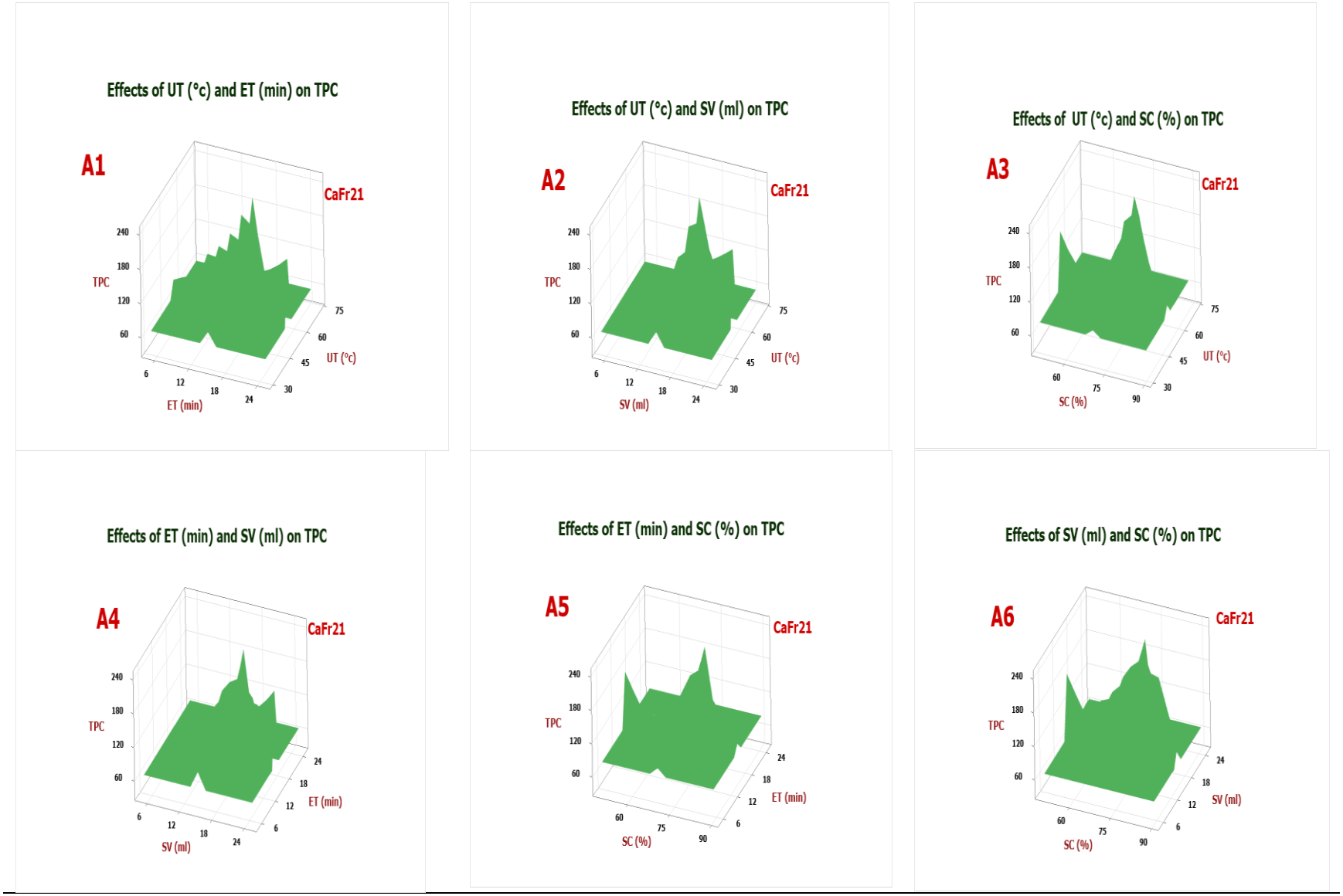


Figure 4.77 Three-dimensional surface plot of factors effects on TPC extraction from African nutmeg peels using CaFr21

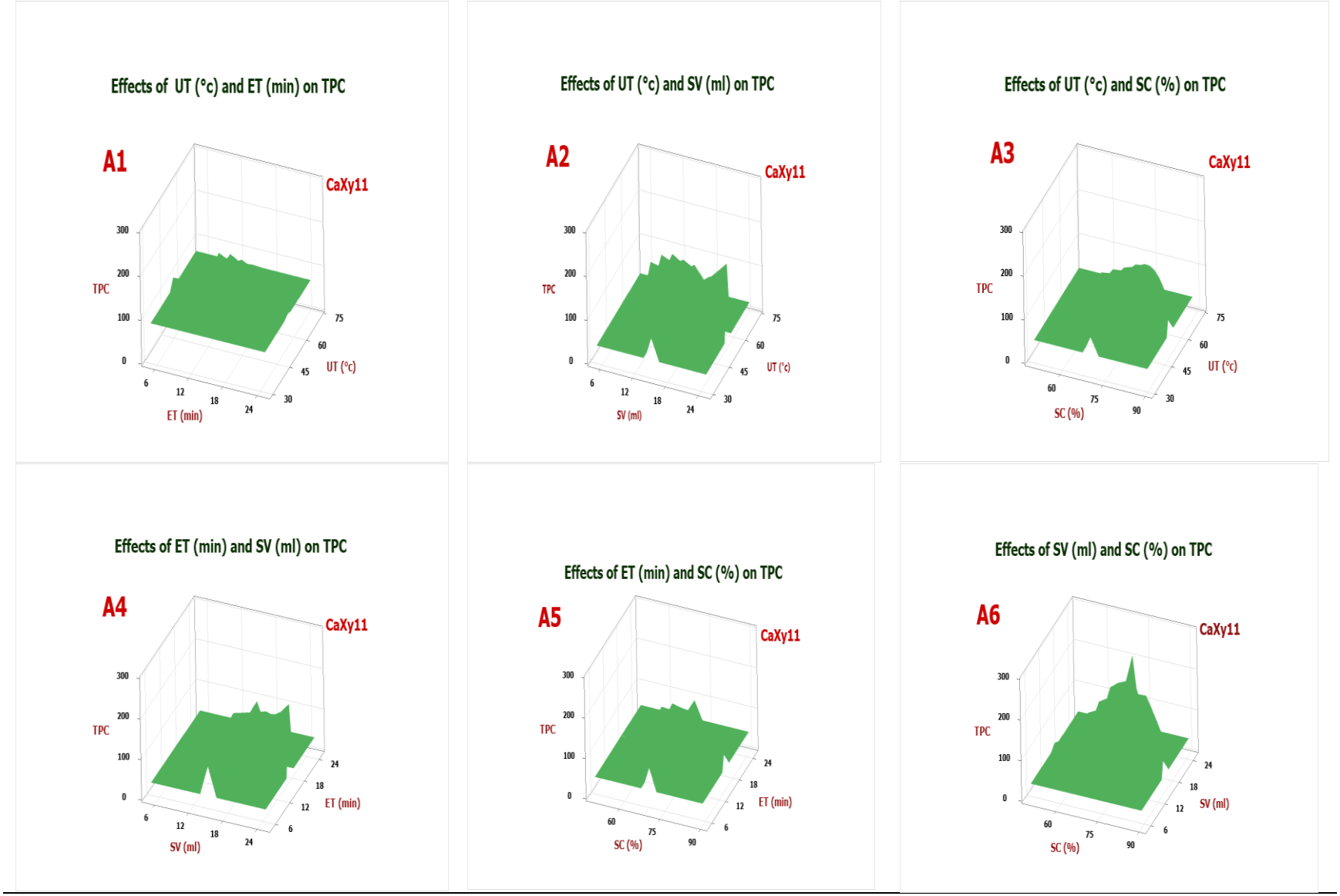


Figure 4.78 Three-dimensional surface plot of factors effects on TPC extraction from African nutmeg peels using CaXy11

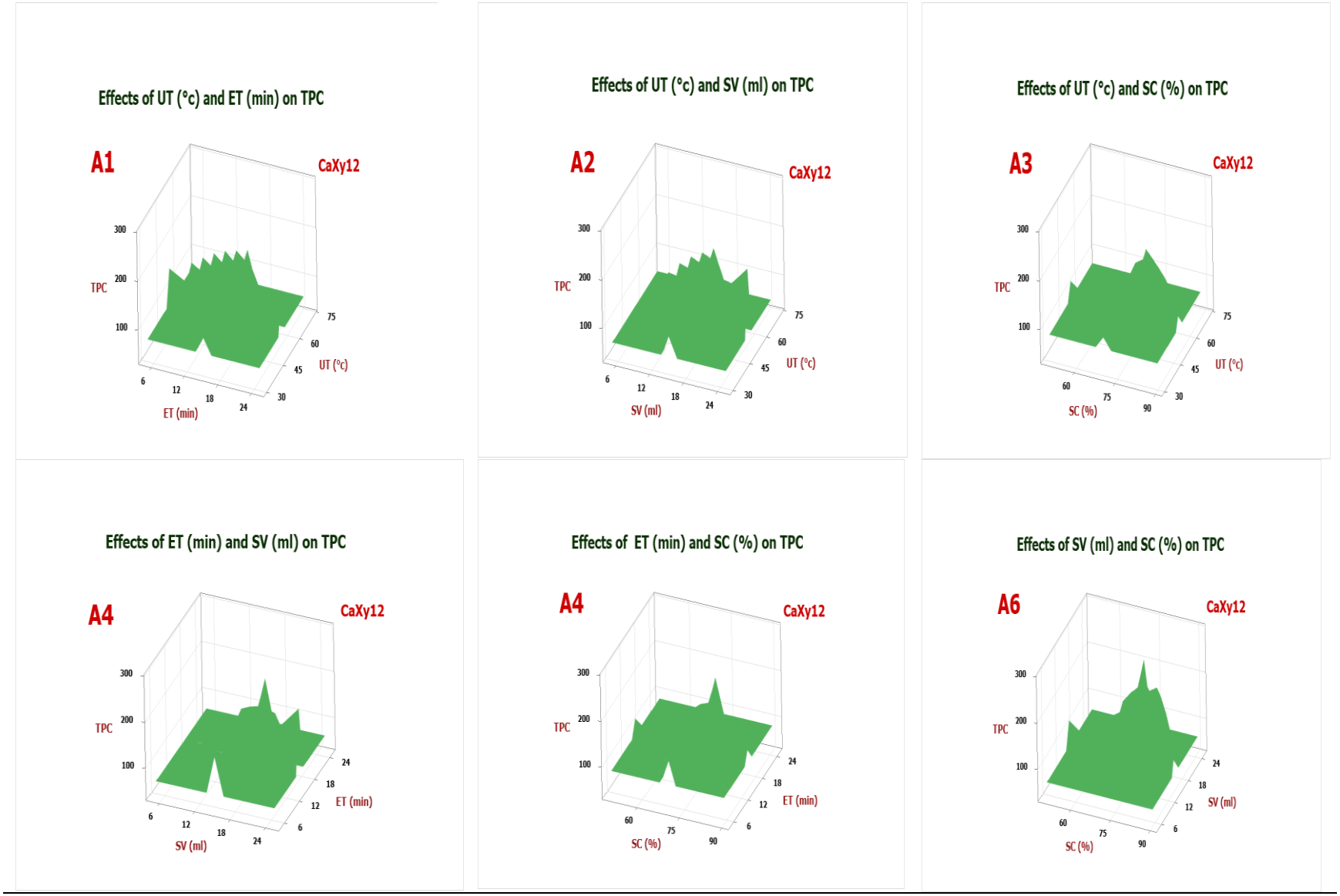


Figure 4.79 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaXy12

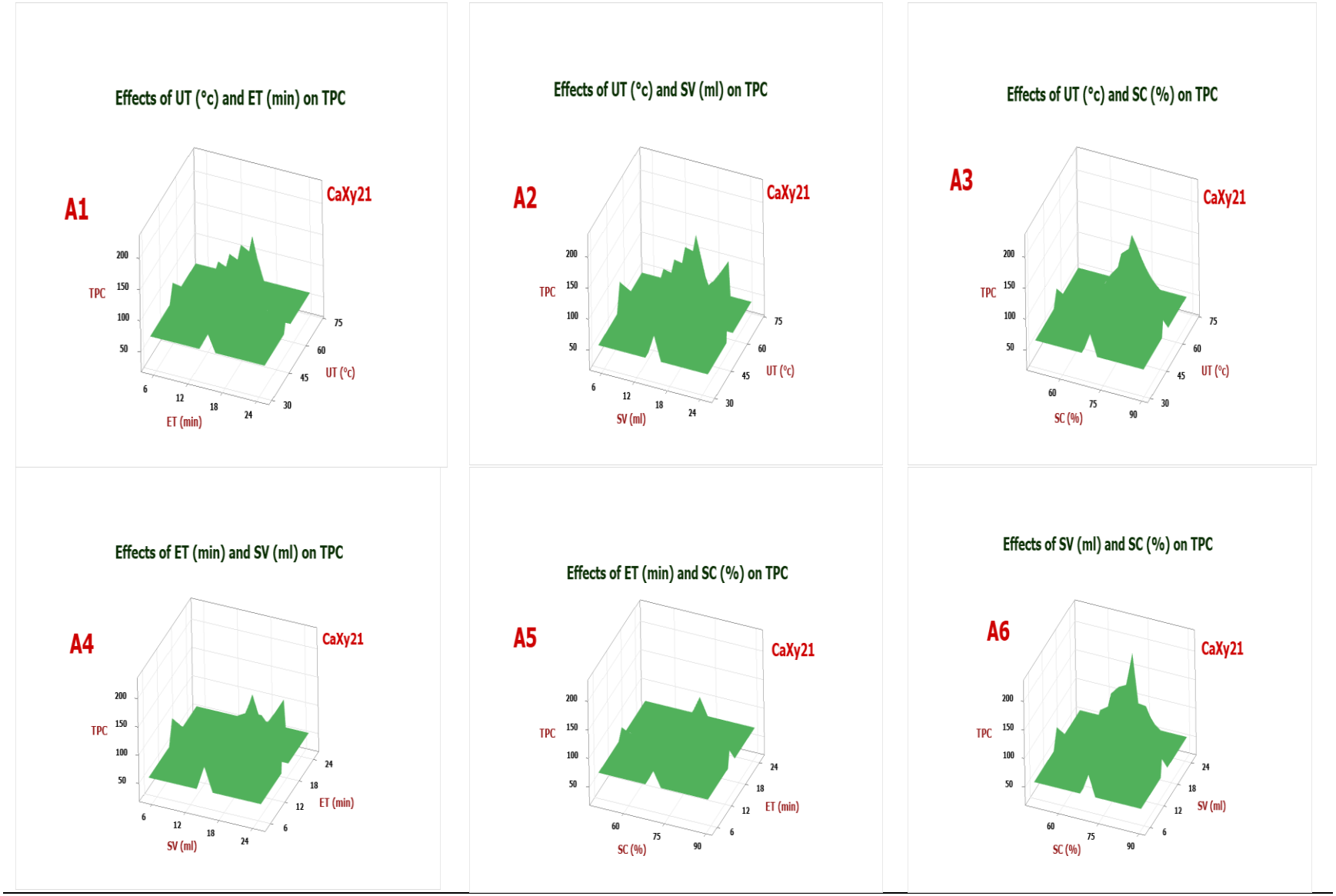


Figure 4.80 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaXy21

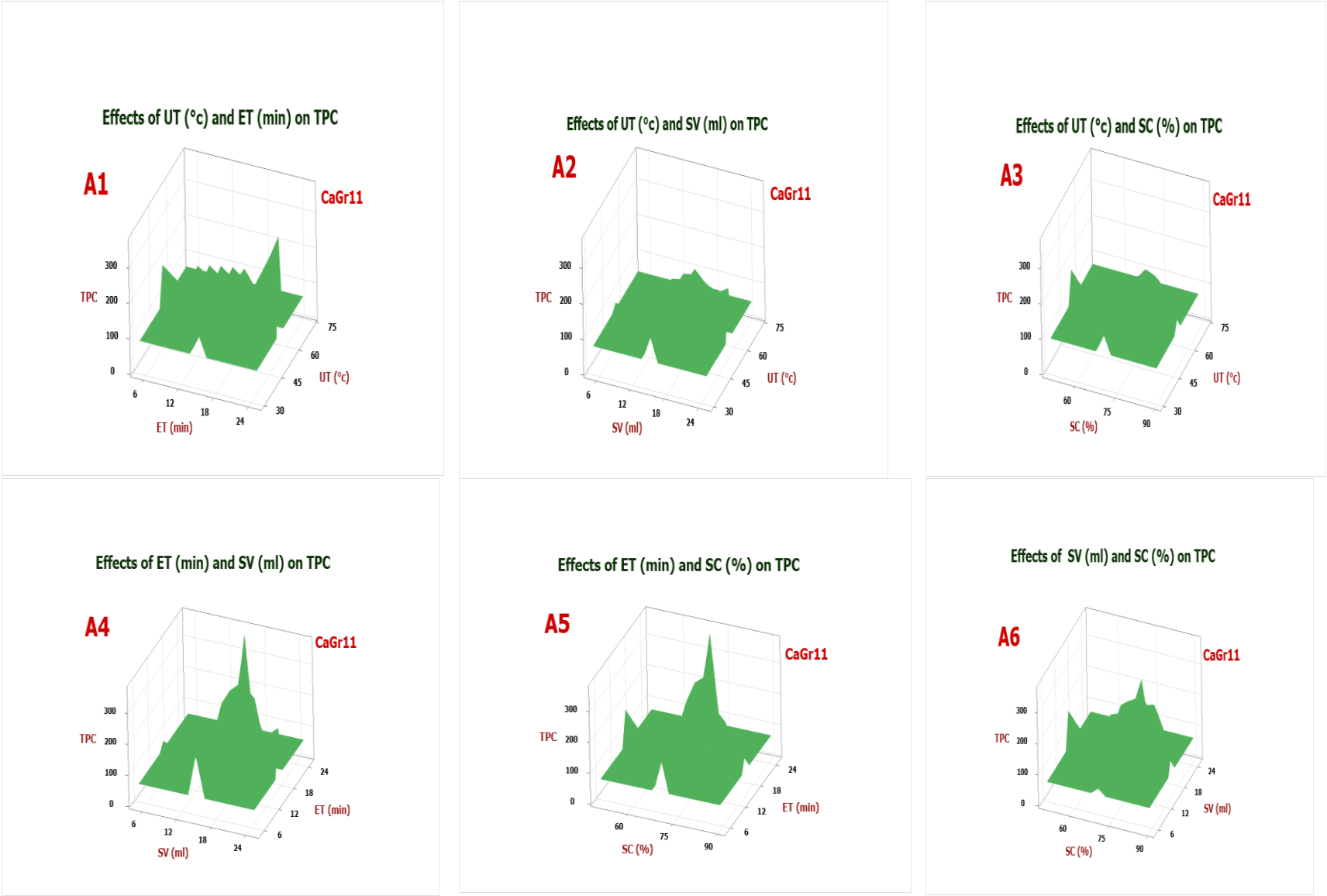


Figure 4.81 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels Using CaGr11

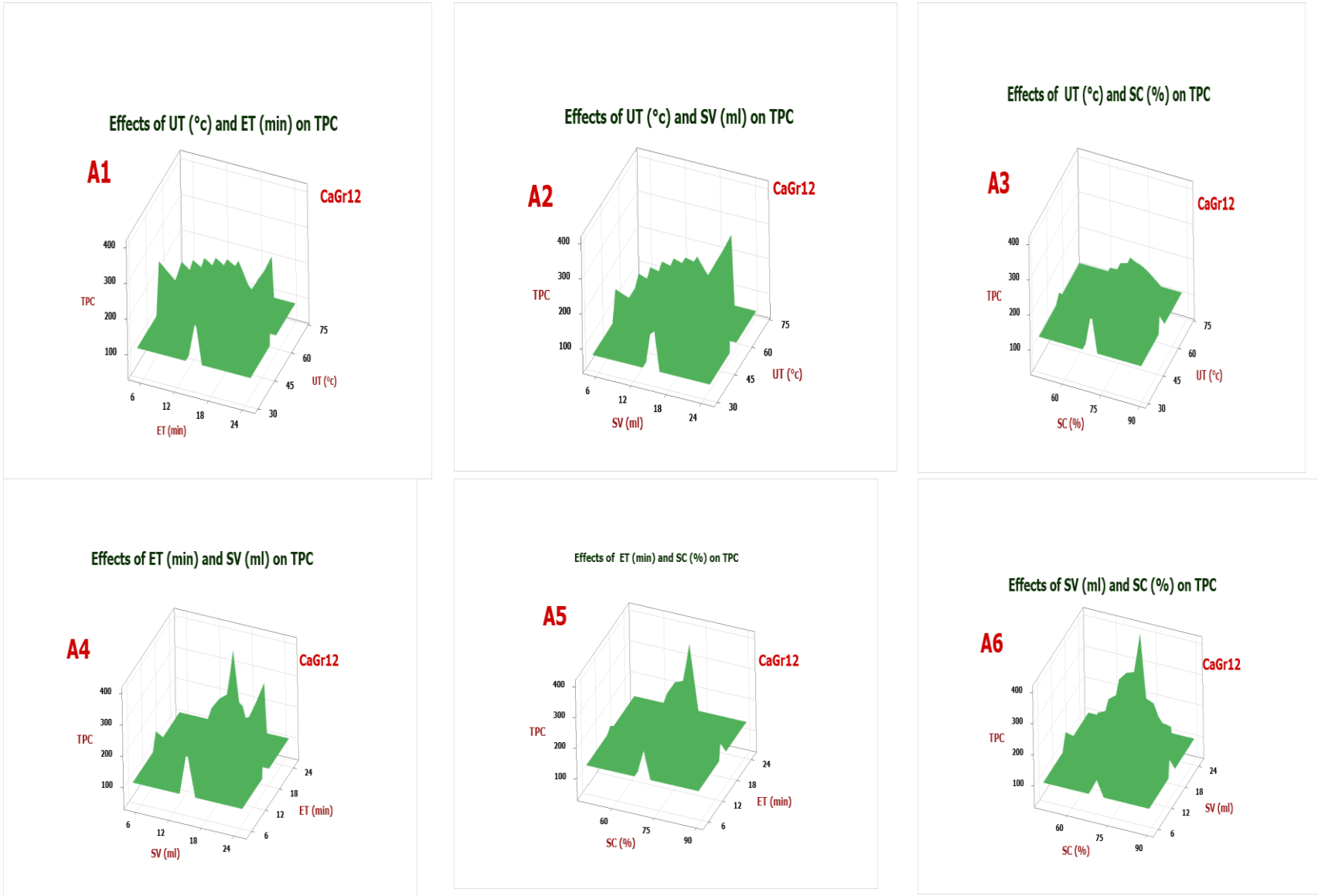


Figure 4.82 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGr12.

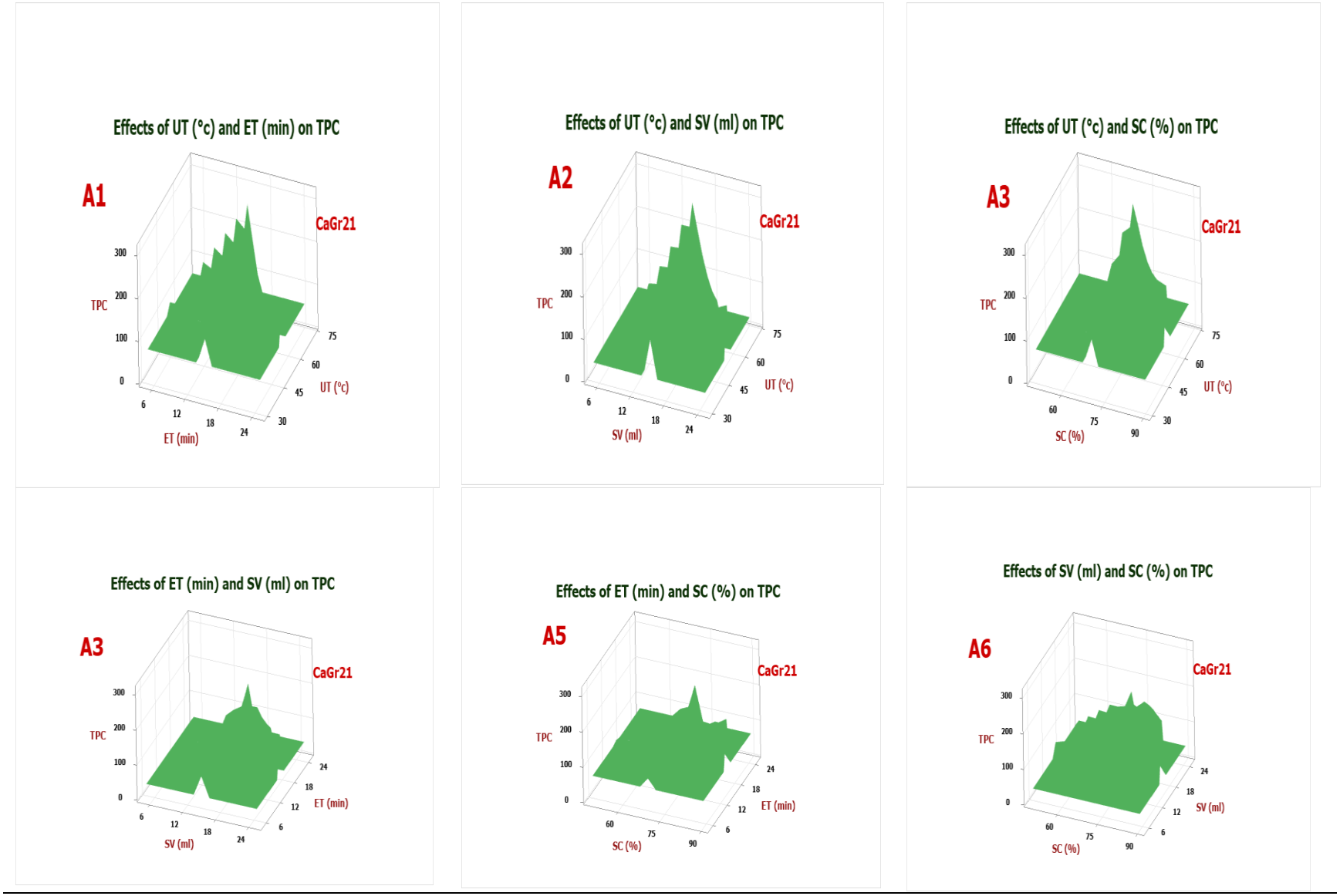


Figure 4.83 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGr21

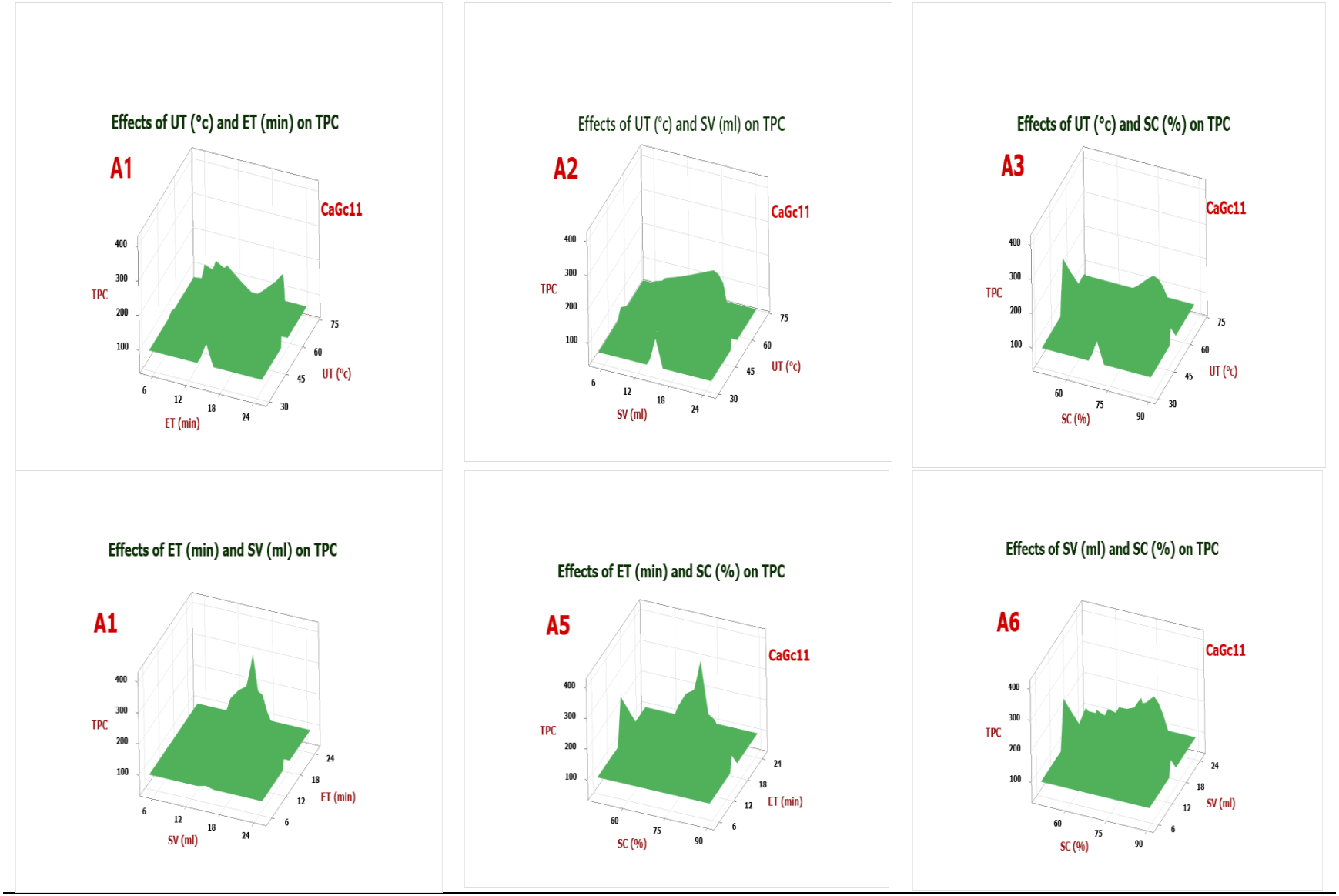


Figure 4.84 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGc11.

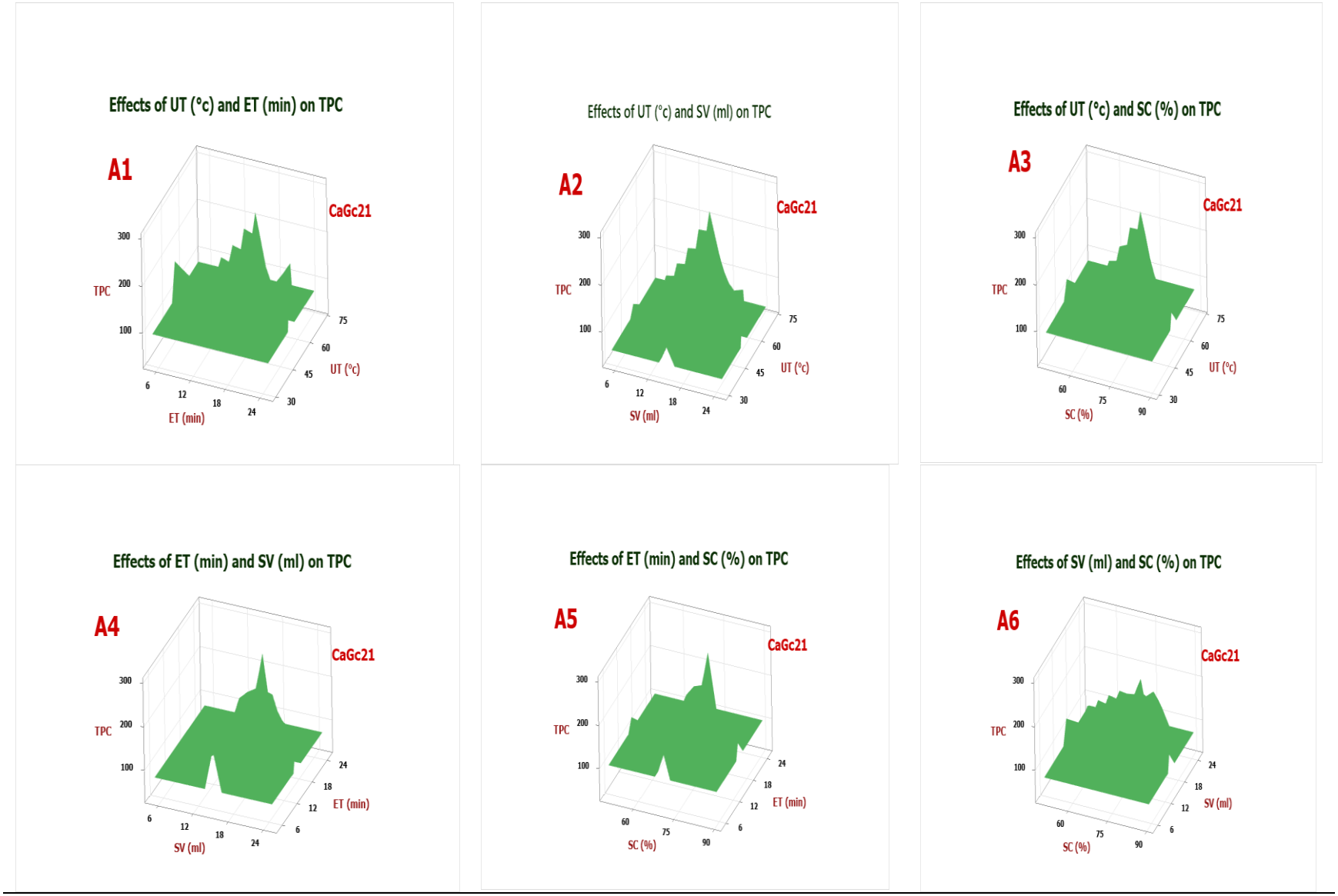


Figure 4.85 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGc21

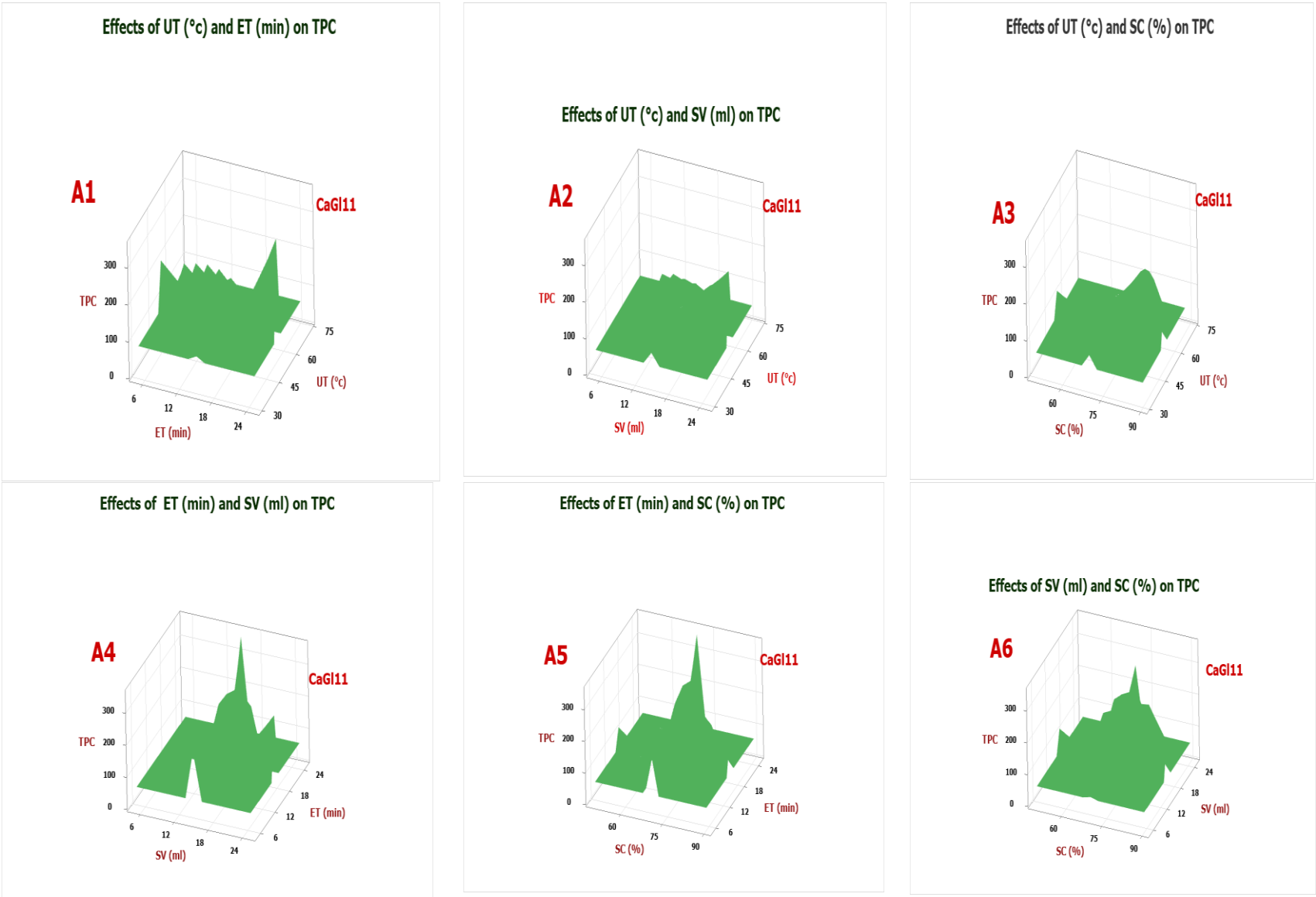


Figure 4.86 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGl11

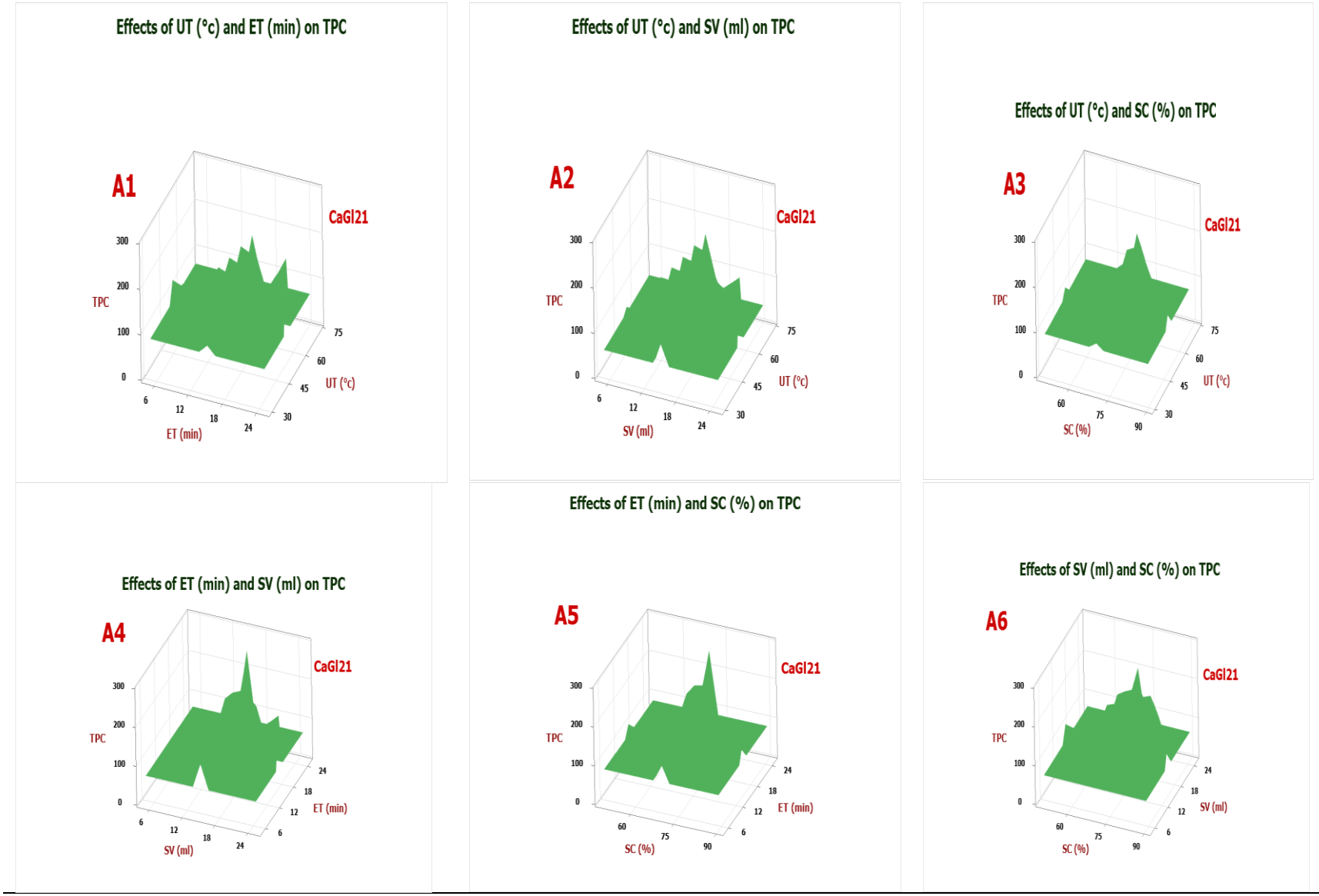


Figure 4.87 Three-dimensional surface plots of factors effects on TPC extraction from African nutmeg peels using CaGl21.

4.6.4.2 Effect of Factors on Total Flavonoid content (TFC)

The total flavonoid content was measured as a quercetin equivalent per gram of samples on a dry weight basis. The maximum and minimum flavonoid contents were 1713±9.02 µgQE/g and 56.901±0.45 µg QE/g respectively and were obtained from the same solvent (CaGc11) at different operating conditions. The maximum extract was obtained in run number 18 with operating conditions of temperature, time, volume, and concentration set as 40°c, 10 min, 20 ml, and 60%, respectively, while the minimum TFC was obtained in run number 30 with temperature, time, volume, and concentration of 50°c, 15 min, 5 ml, 70% respectively, and are shown in **Table 4.13**. The regression equation shows that the full quadratic model was adequate to fit TFC extraction at factor conditions for all the studied NADESs (**Table 4.10**). Pareto charts (**Figure 4.88**) of the analysis shows the factors and factor combinations that significantly affect TFC extraction from African nutmeg peels and how they relate with each other for the synthesized NADESs, and are outlined as follows:

A. CaSu11 - SV > UT > UT*SV > SC.
B. CaFr11- SV > SV*SV > UT*SV > ET > UT > SC.
C. CaFr12 - SV > SC > UT > SC*SC.
D. CaFr21 - SV > UT*UT > SC*SC > SV*SV > ET*ET > ET*SC > ET > UT > SC > UT*SV > ET*SV.
E. CaXy11 - SC > SV > UT*ET > ET*SC >ET > SC*SC > ET*ET > SV*SV > ET*SV > SV*SC > UT.
F. CaXy12 - UT > UT*SV > SV > UT*UT > SC > ET > SC*SC.
G. CaXy21- SC > SC*SC > ET*ET > SV*SV > SV > UT*SV > ET*SC.
H. CaGr11- ET*SC > SC > SV > ET*ET > SV*SC > SV*SV > SC*SC > UT*SV.
I. CaGr12 – UT*UT > UT*SV > SV > SC > ET*SC > ET > UT > ET*ET > SV*SV.
J. CaGr21- SV > SV*SC > UT*SC > UT*SV > ET > ET*ET.
K. CaGc11- SV > UT*UT > ET*SV > UT*SV > ET*ET > UT*ET > SV*SV.
L. CaGc21- ET*SV > UT > UT*SV > SC*SC > UT*UT > SV*SV > ET*ET > SV > ET*SC >UT*SC > UT*ET.
M. CaGl11- SV > SV*SV > UT*SV > ET*ET > ET > ET*SV.
N. CaGl21- SV > ET*SC > SV*SV > UT > ET*ET > UT*ET > UT*UT > SC*SC.

From the outline above, solvent volume (SV) shows to be the factor with the most significant effects on antioxidant extraction from African nutmeg peels. Three-dimensional surface plots of the effects of two factors on TFC extraction from African nutmeg peels are presented in Figure 4.89 to Figure 4.102 for the synthesized NADESs, respectively. From the plots, the conditions necessary to maximize TFC extraction are as follows:

A. CaSu11- UT (45ºc), ET (18 min), SV (18 ml), and SC (75%), TPC ≥ 500 µgQE/g.
B. CaFr11 - UT (45ºc), ET (18 min), SV (20 ml), and SC (75%), TPC ≥ 500 µgQE/g.
C. CaFr12 - UT (45ºc), ET (20 min), SV (18 ml), and SC (75%), TPC ≥ 300 µgQE/g.
D. CaFr21- UT (45ºc), ET (20 min), SV (18 ml), and SC (75%), TPC ≥ 250 µgQE/g.
E. CaXy11- UT (60ºc), ET (18 min), SV (18 ml), and SC (80%), TPC ≥ 200 µgQE/g.
F. CaXy12- UT (40ºc), ET (12 min), SV (18 ml), and SC (80%), TPC ≥200 µgQE/g.
G. CaXy21 – UT (60ºc), ET (20 min), SV (20 ml), and SC (80%), TPC ≥200 µgQE/g.
H. CaGr11 – UT (60ºc), ET (12 min), SV (20 ml), and SC (80%), TPC ≥200 µgQE/g.
I. CaGr12 – UT (45ºc), ET (12 min), SV (23 ml), and SC (75%), TPC ≥200 µgQE/g.
J. CaGr21 – UT (35ºc), ET (12 min), SV (20 min), and SC (60%), TPC ≥300 µgQE/g.
K. CaGc11- UT (60ºc), ET (18 min), SV (18 ml), and SC (80%), TPC ≥500 µgQE/g.
L. CaGc21 – UT (45ºc), ET (12 min), SV (18 ml), and SC (60%), TPC ≥350 µgQE/g.
M. CaGl11 – UT (50ºc), ET (12 min), SV (20 ml), and SC (60%), TPC ≥ 500 µgQE/g.
N. CaGl21 – UT (65ºc), ET (18 min), SV (18 ml), and SC (60%), TPC ≥400 µgQE/g.

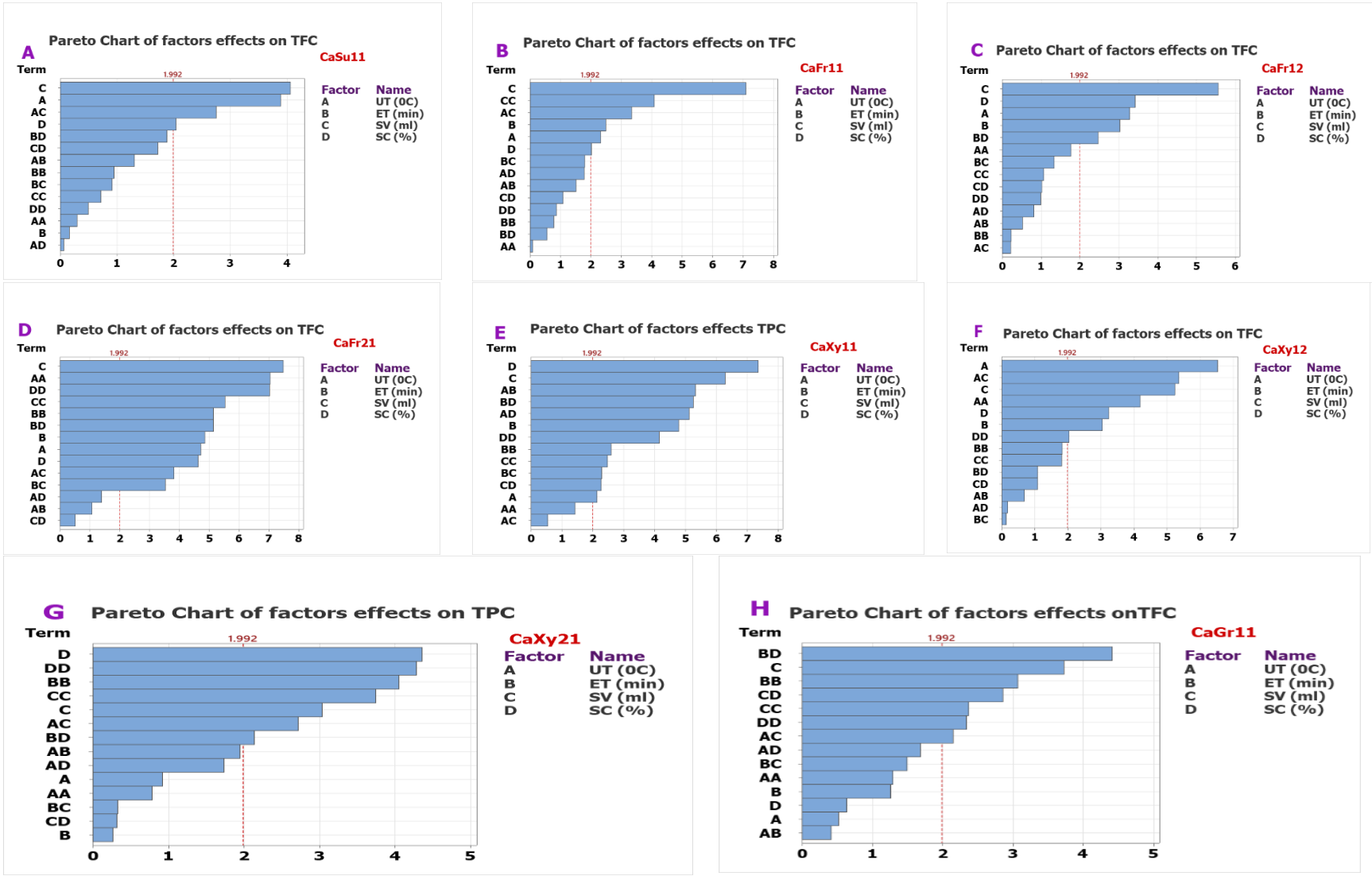


Figure 4.88 Pareto charts of factor effects on TFC extraction from African nutmeg peels using synthesized NADESs

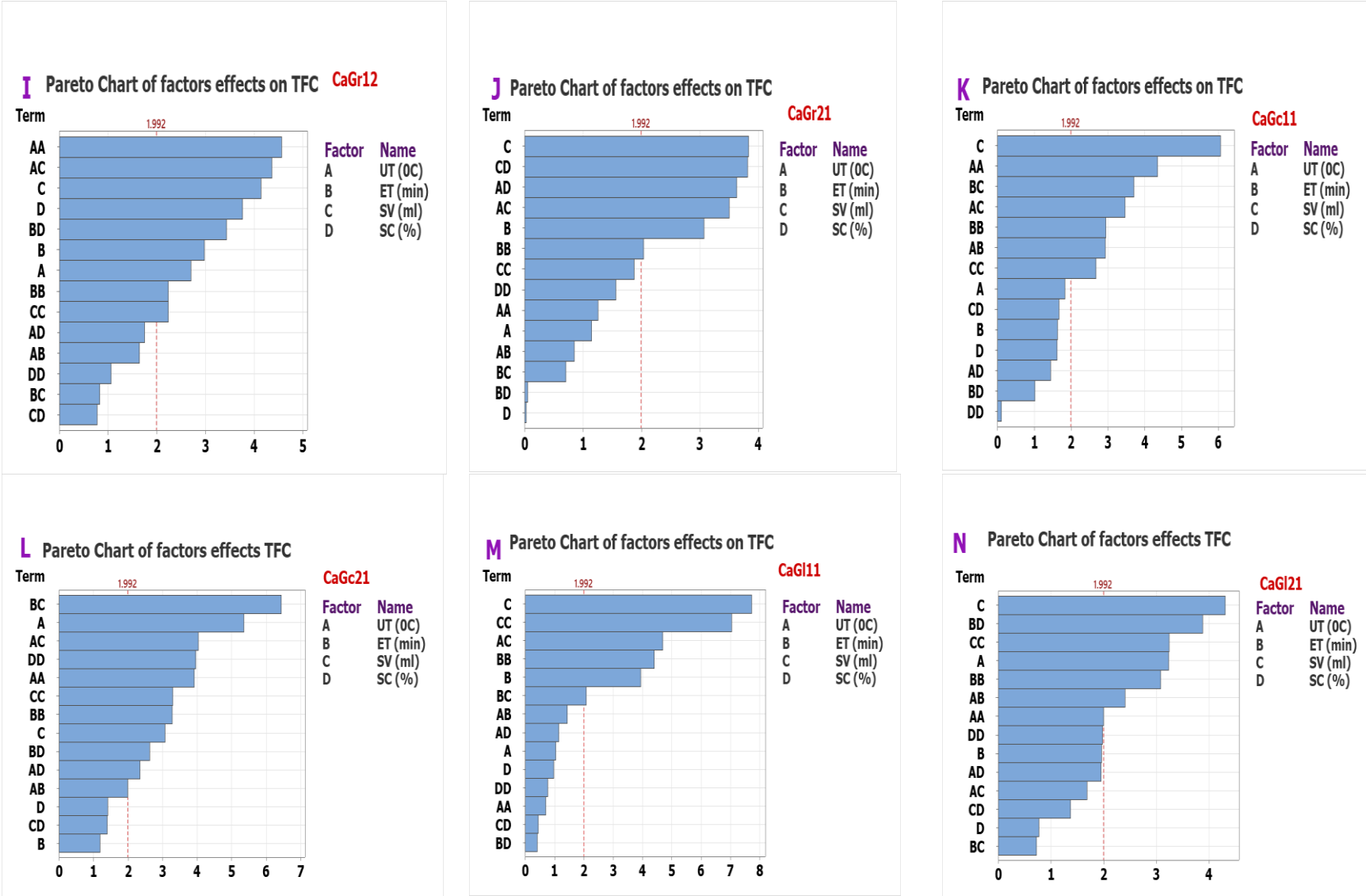


Figure 4.88 contd.

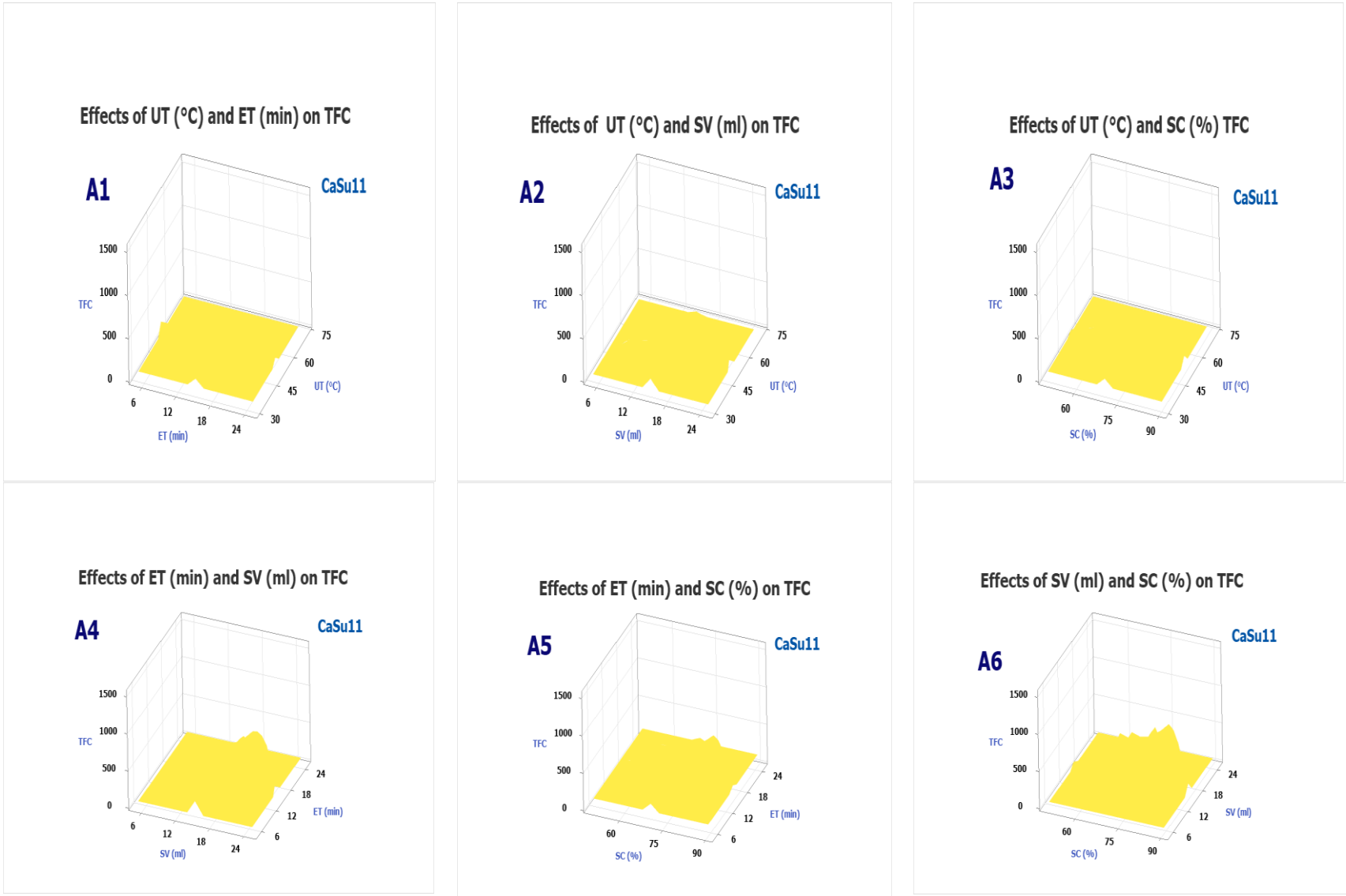


Figure 4.89 Three-dimensional surface plots of Factors effects on TFC extraction from African nutmeg peels using CaSu11

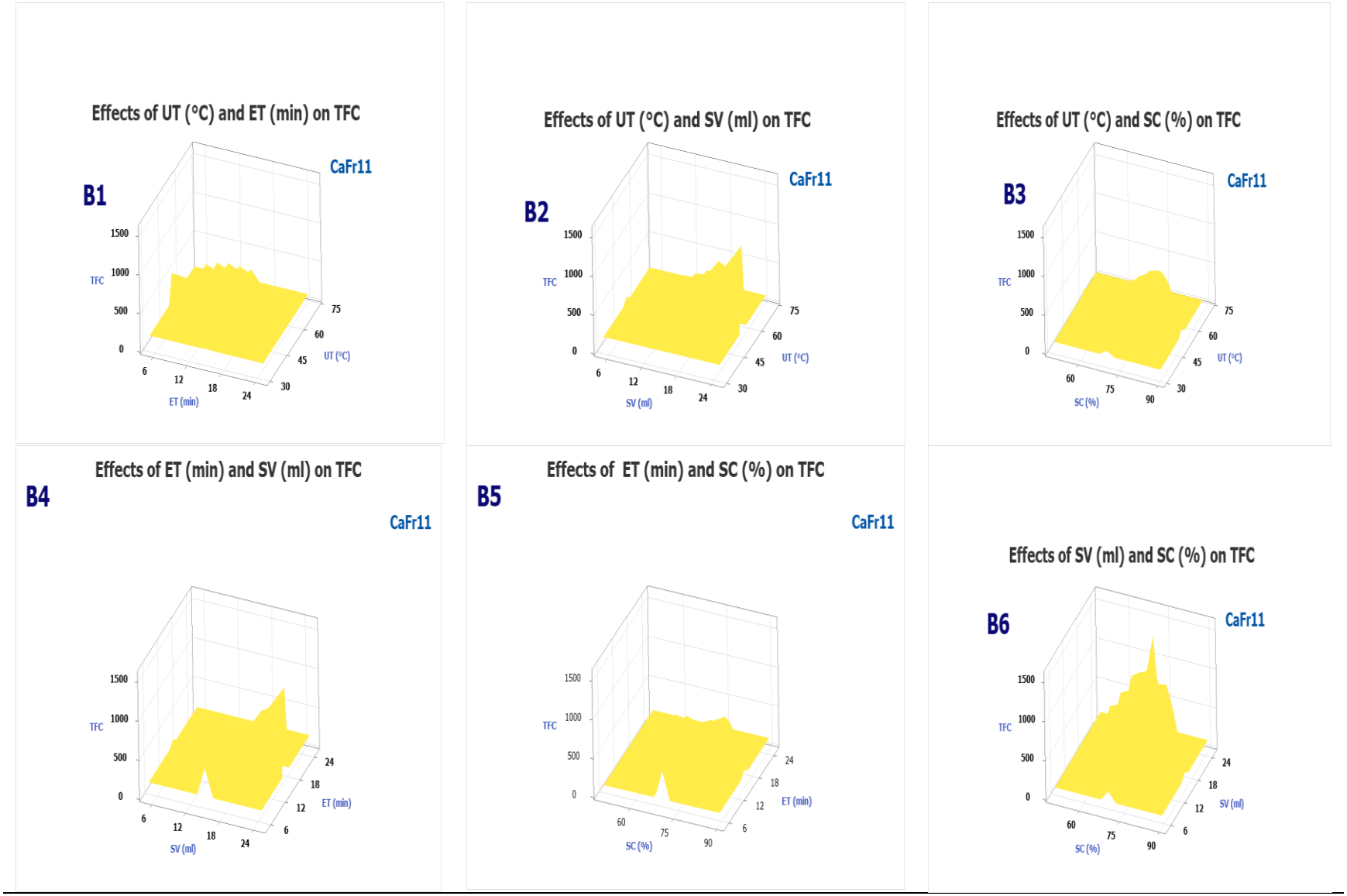


Figure 4.90 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaFr11.

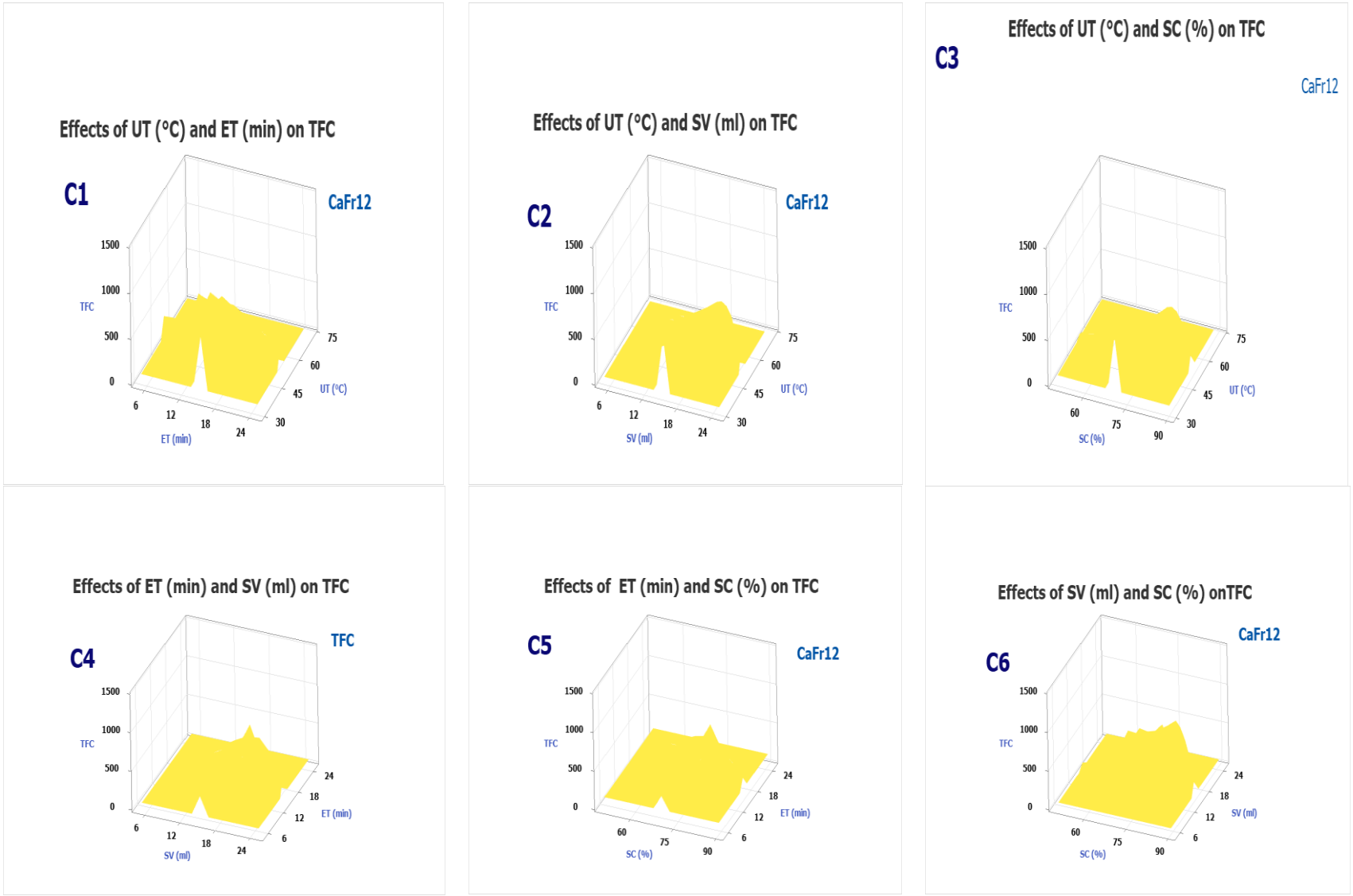


Figure 4.91 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaFr12.

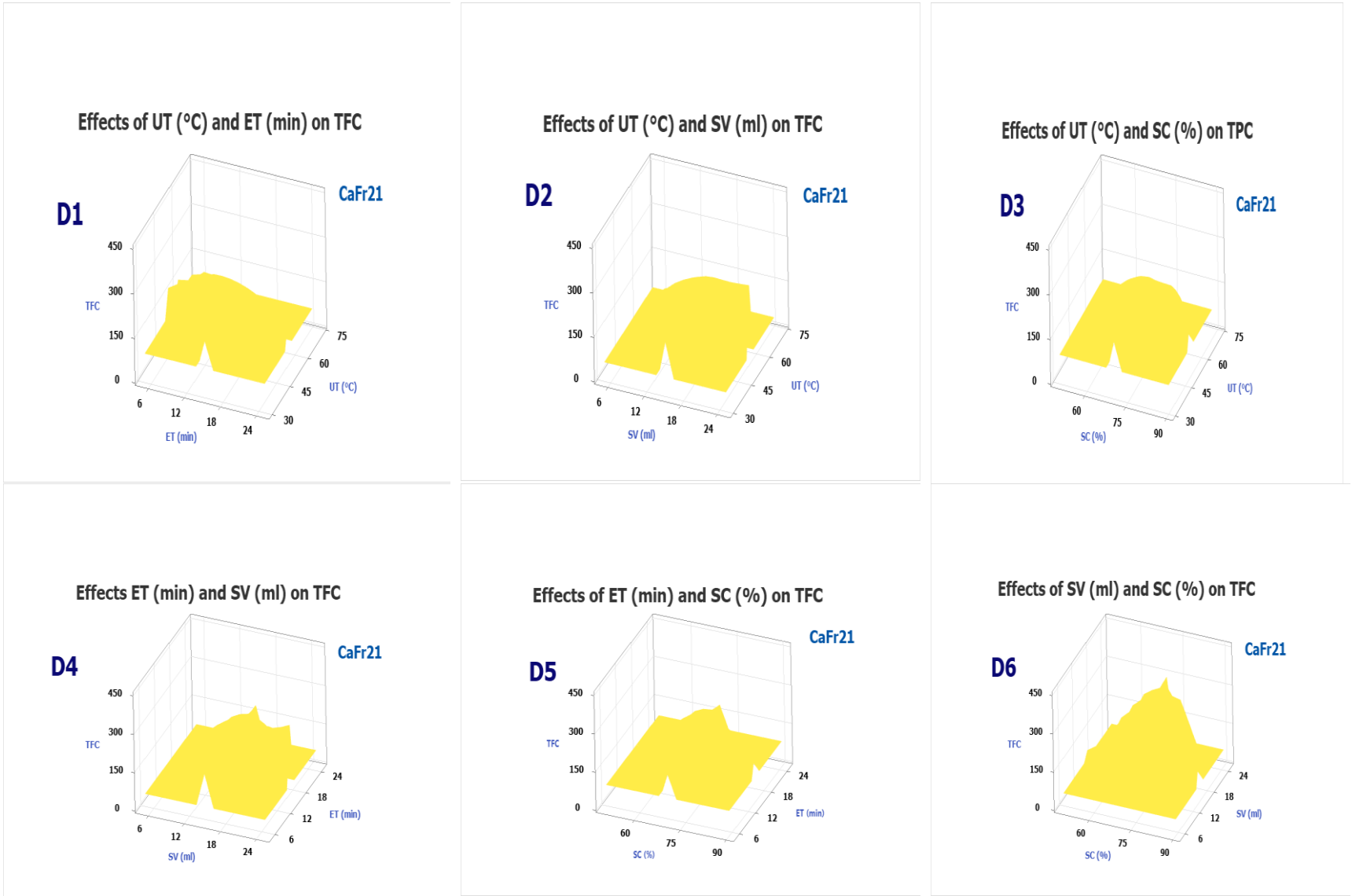


Figure 4.92 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaFr21

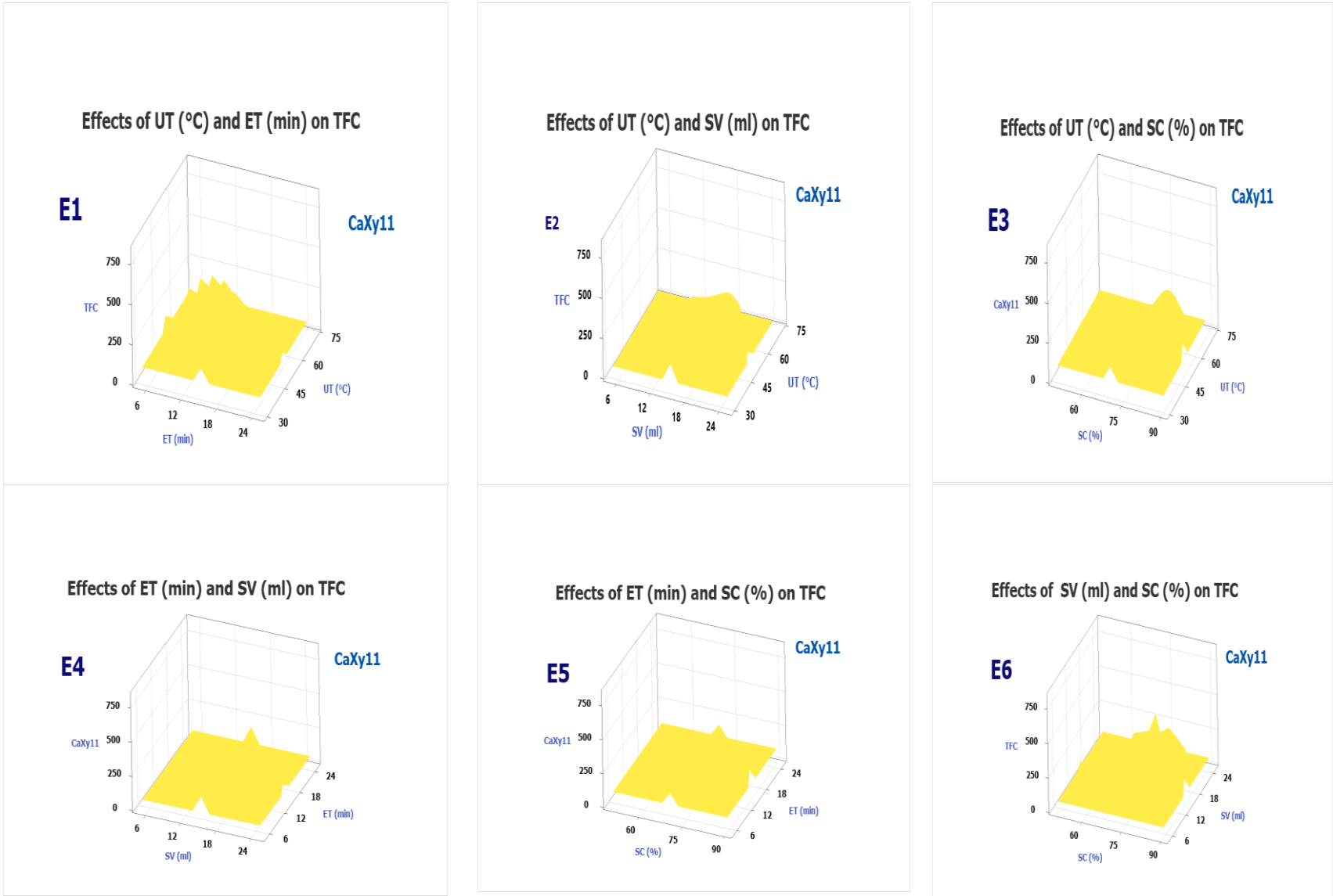


Figure 4.93 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaXy11

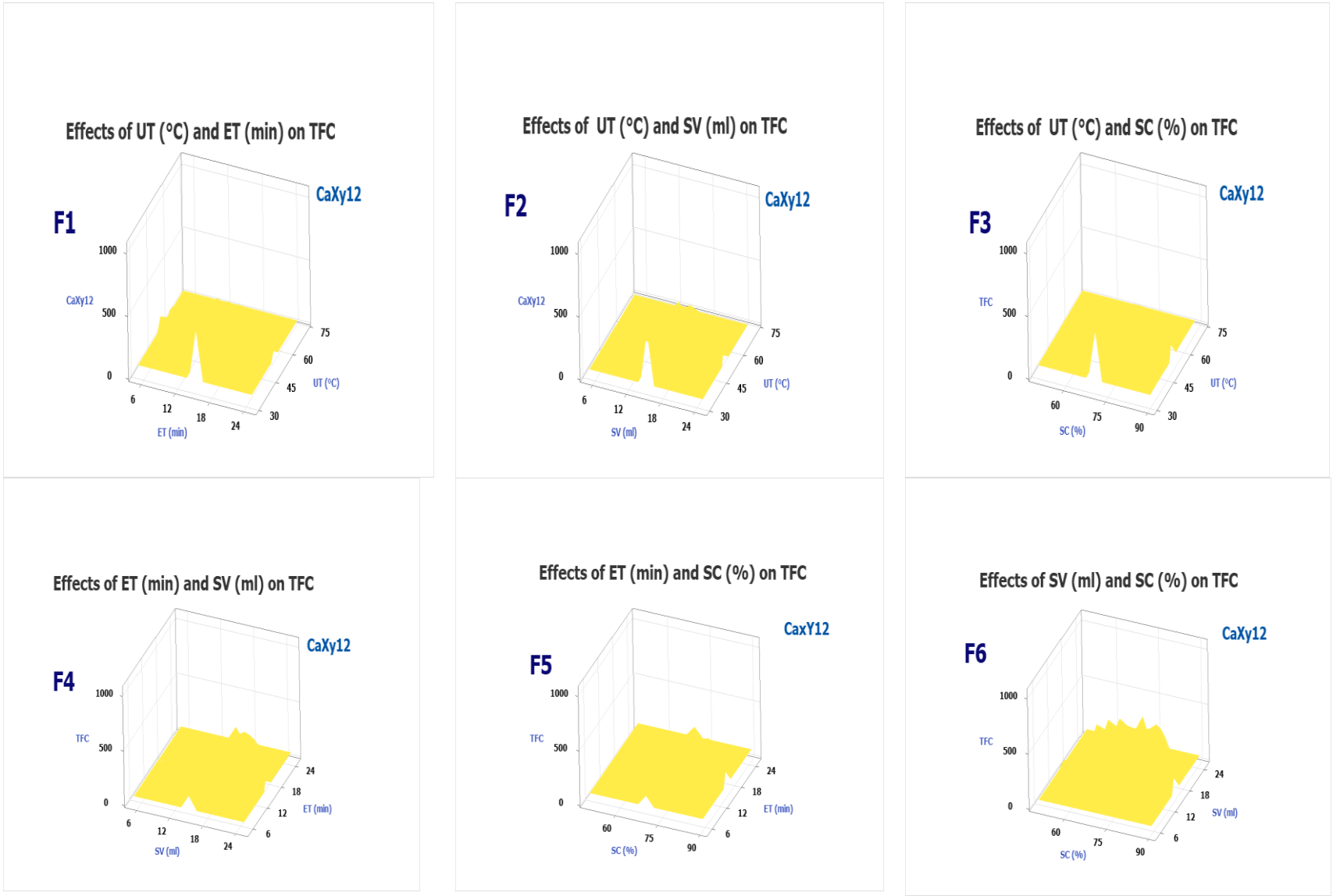


Figure 4.94 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaXy12

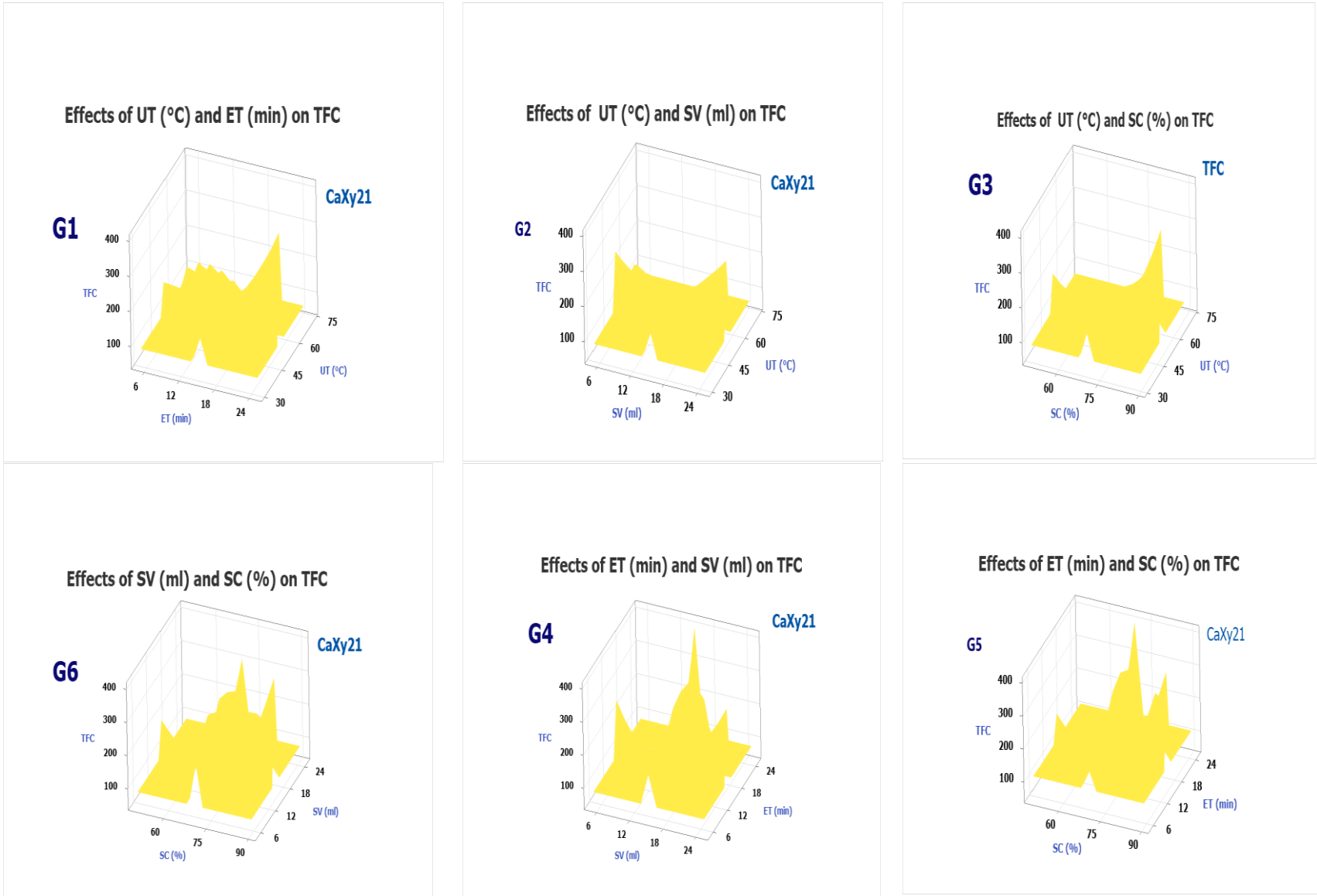


Figure 4.95 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaXy21

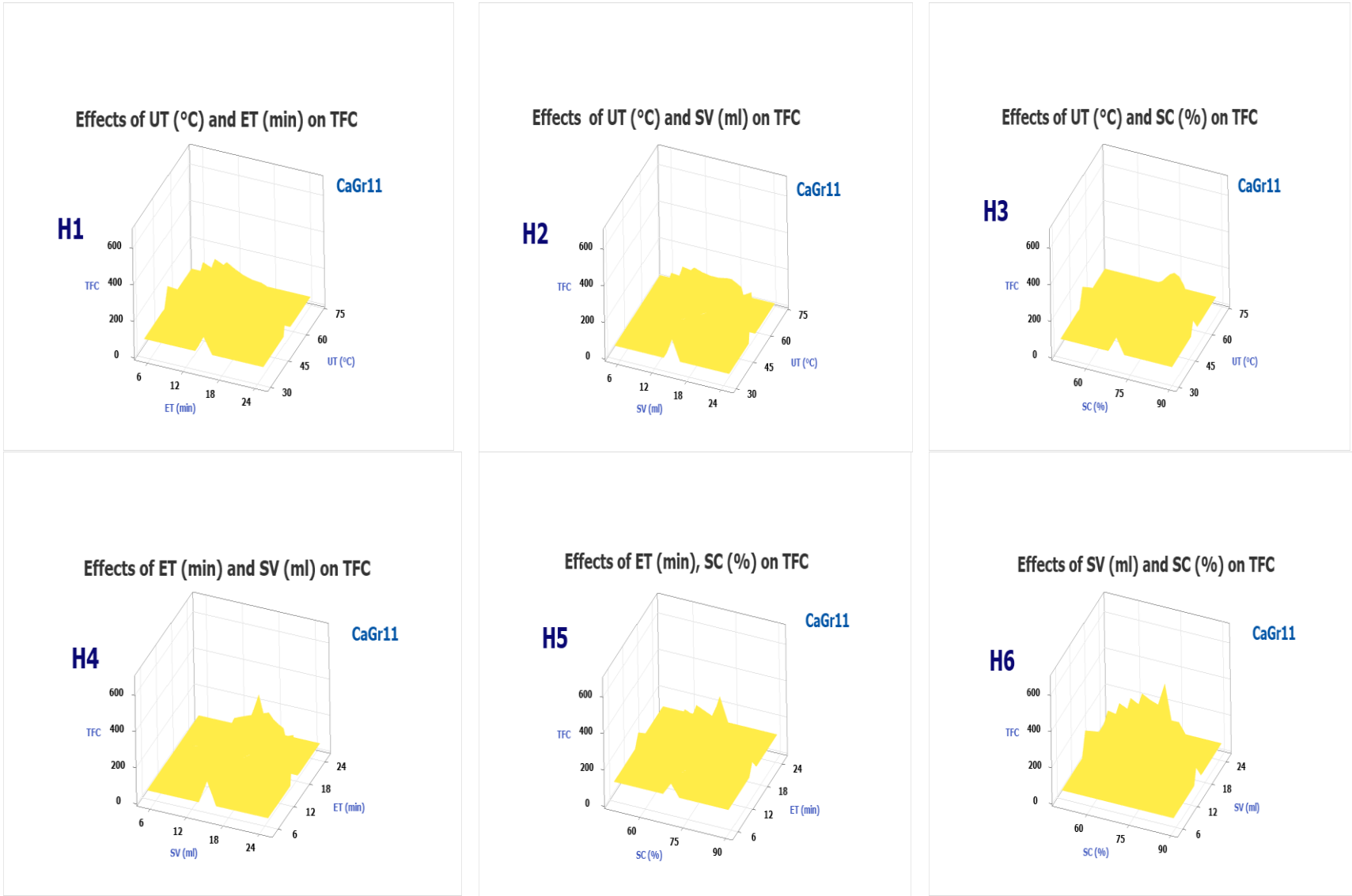


Figure 4.96 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGr11

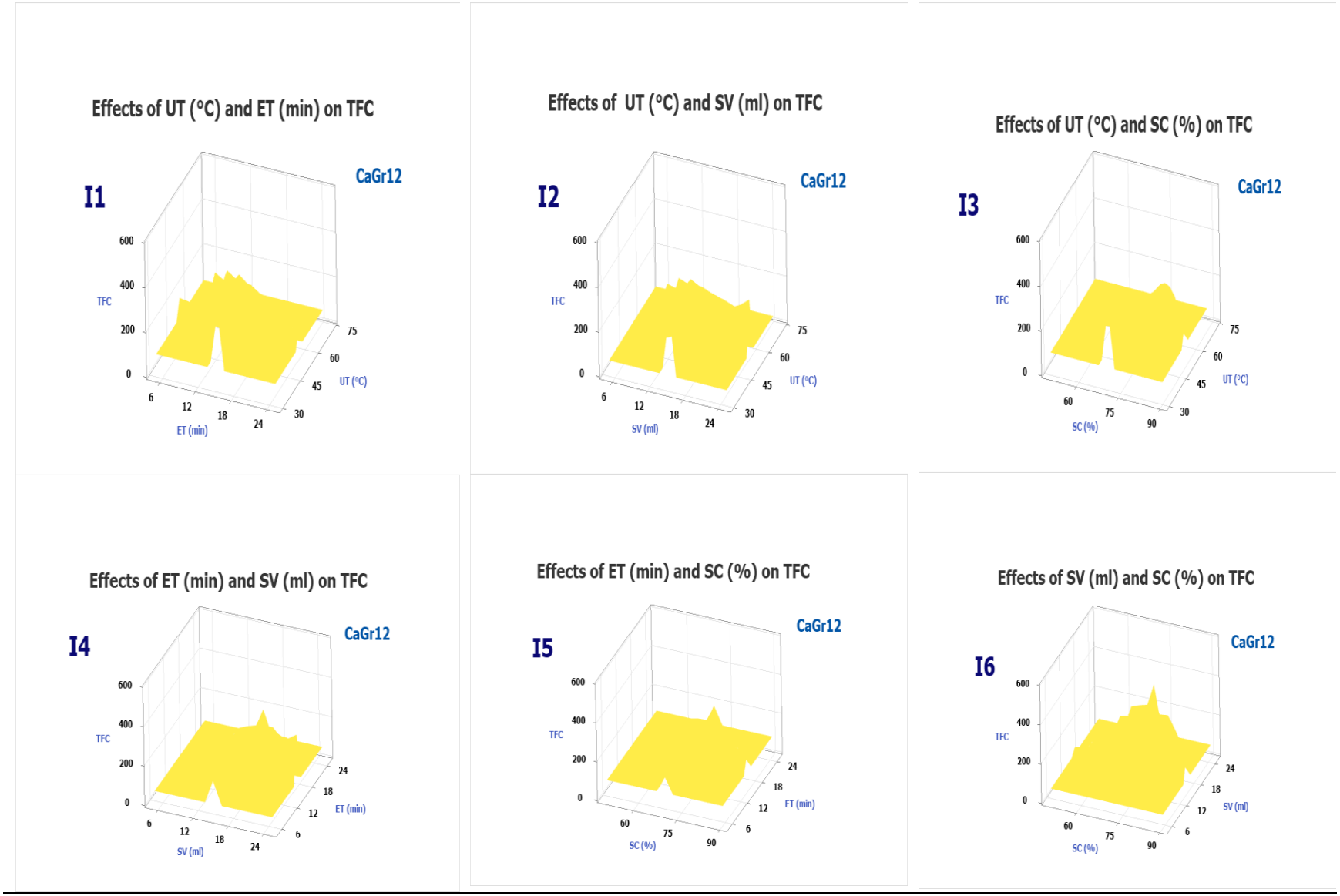


Figure 4.97 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGr12

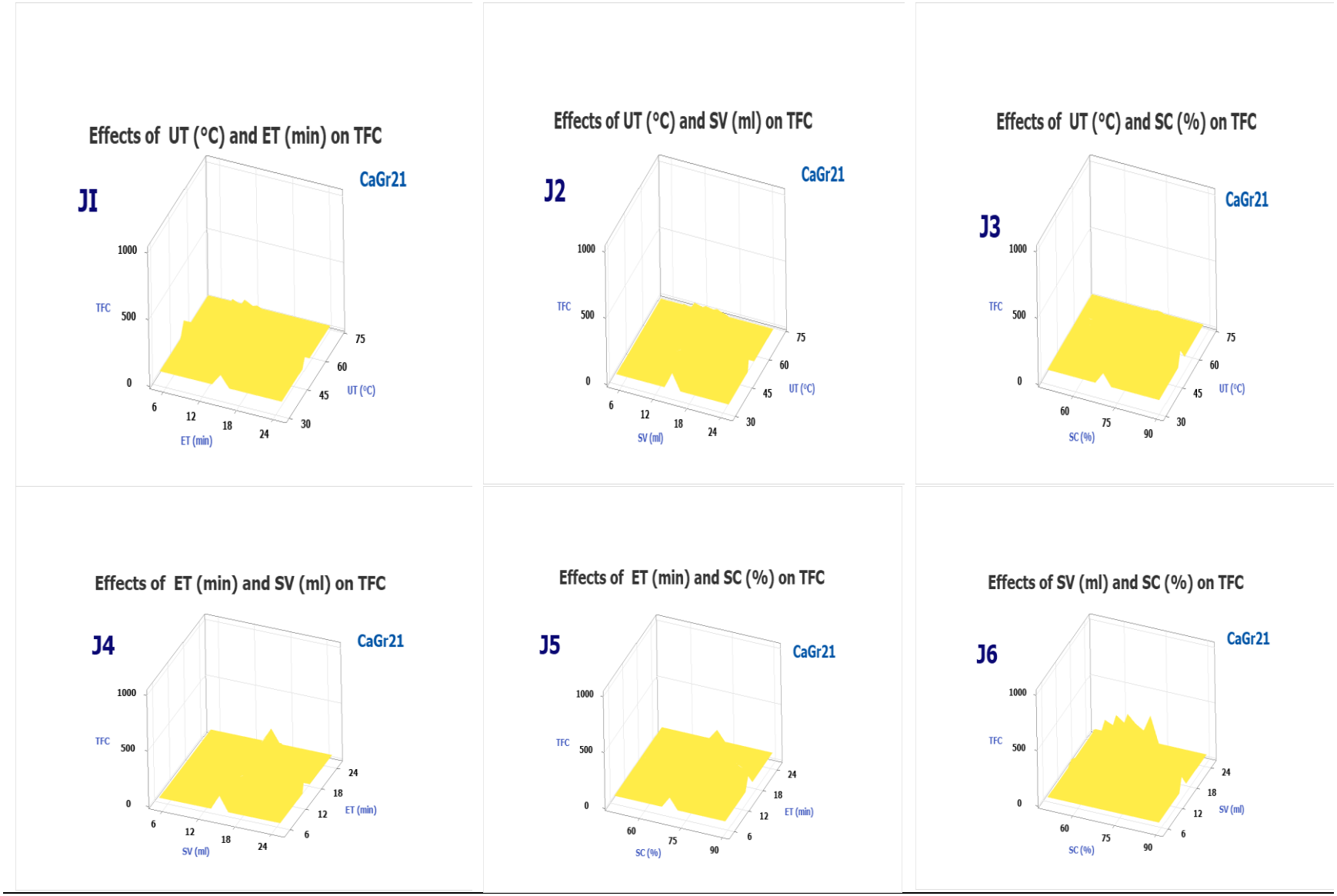


Figure 4.98 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGr21

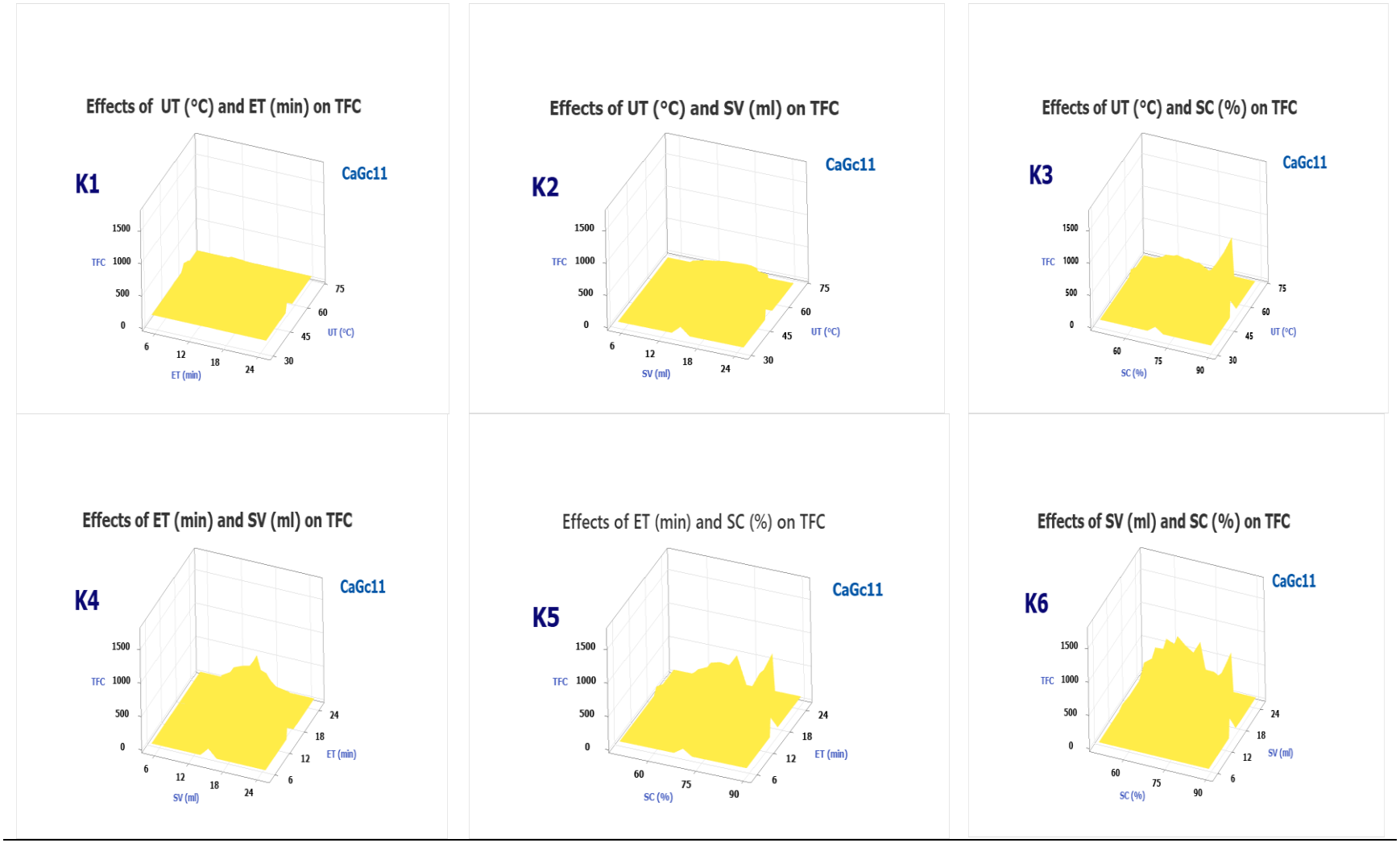


Figure 4.99 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGC11

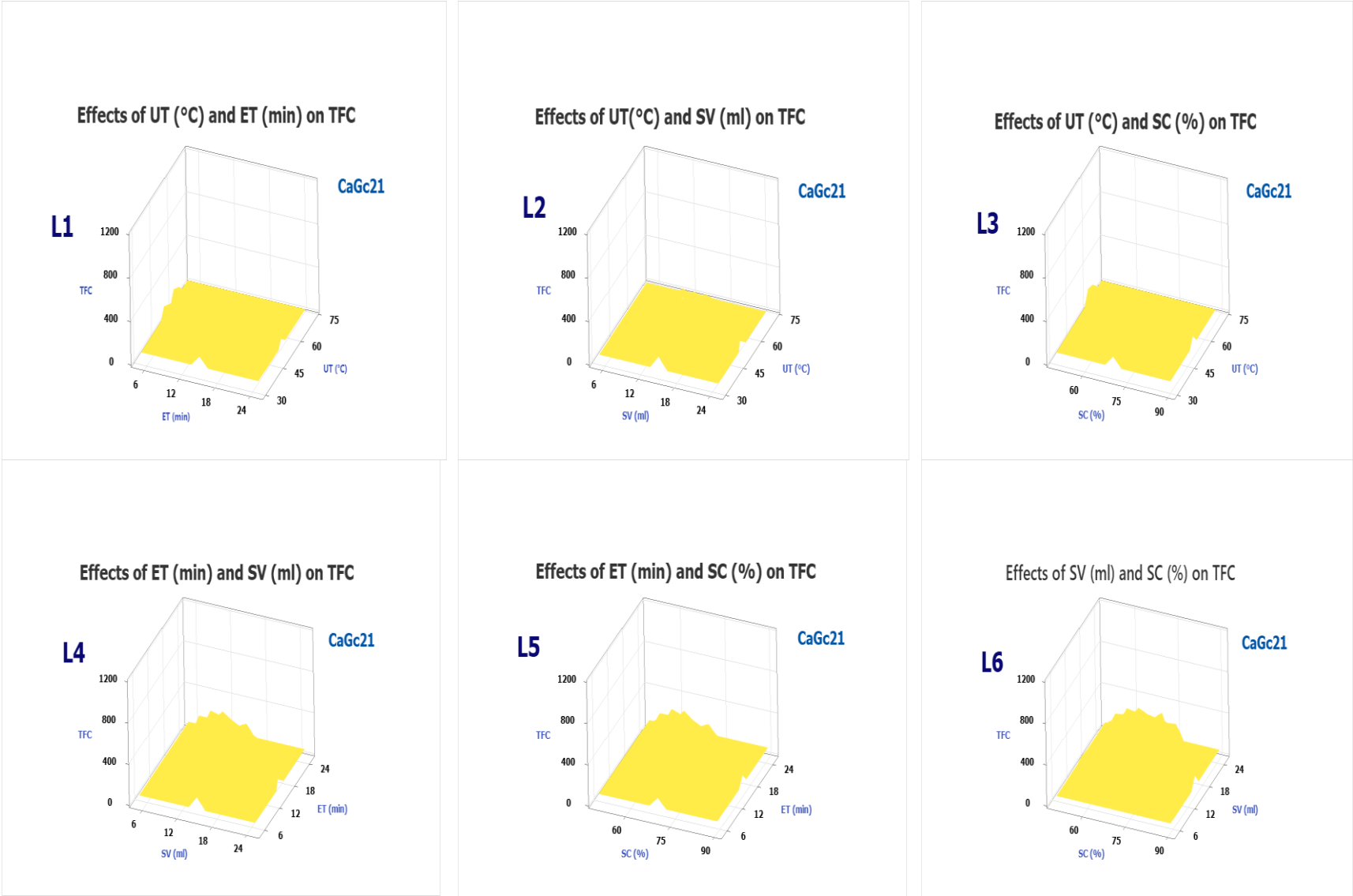


Figure 4.100Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGc21

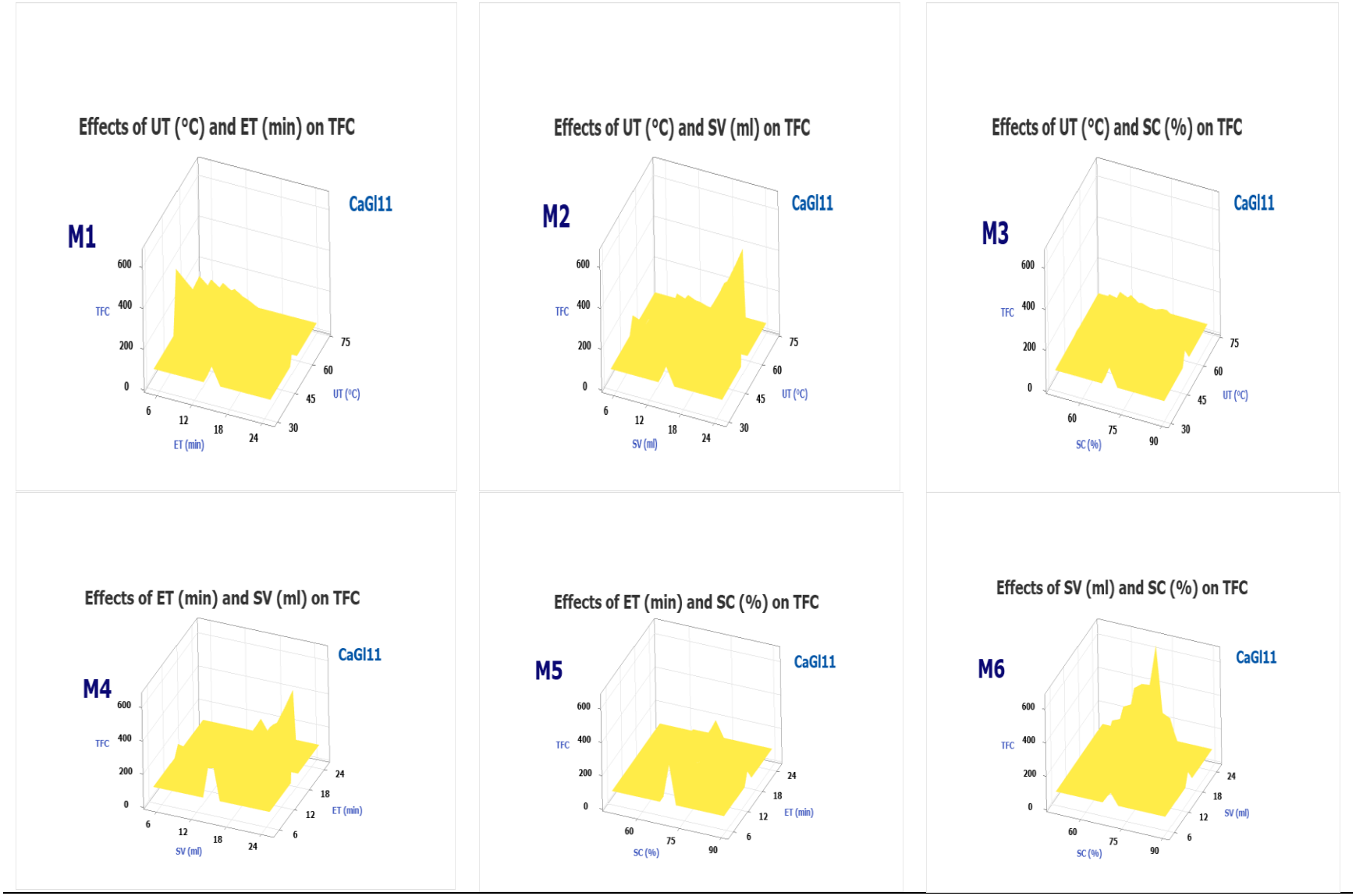


Figure 4.101Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGl11

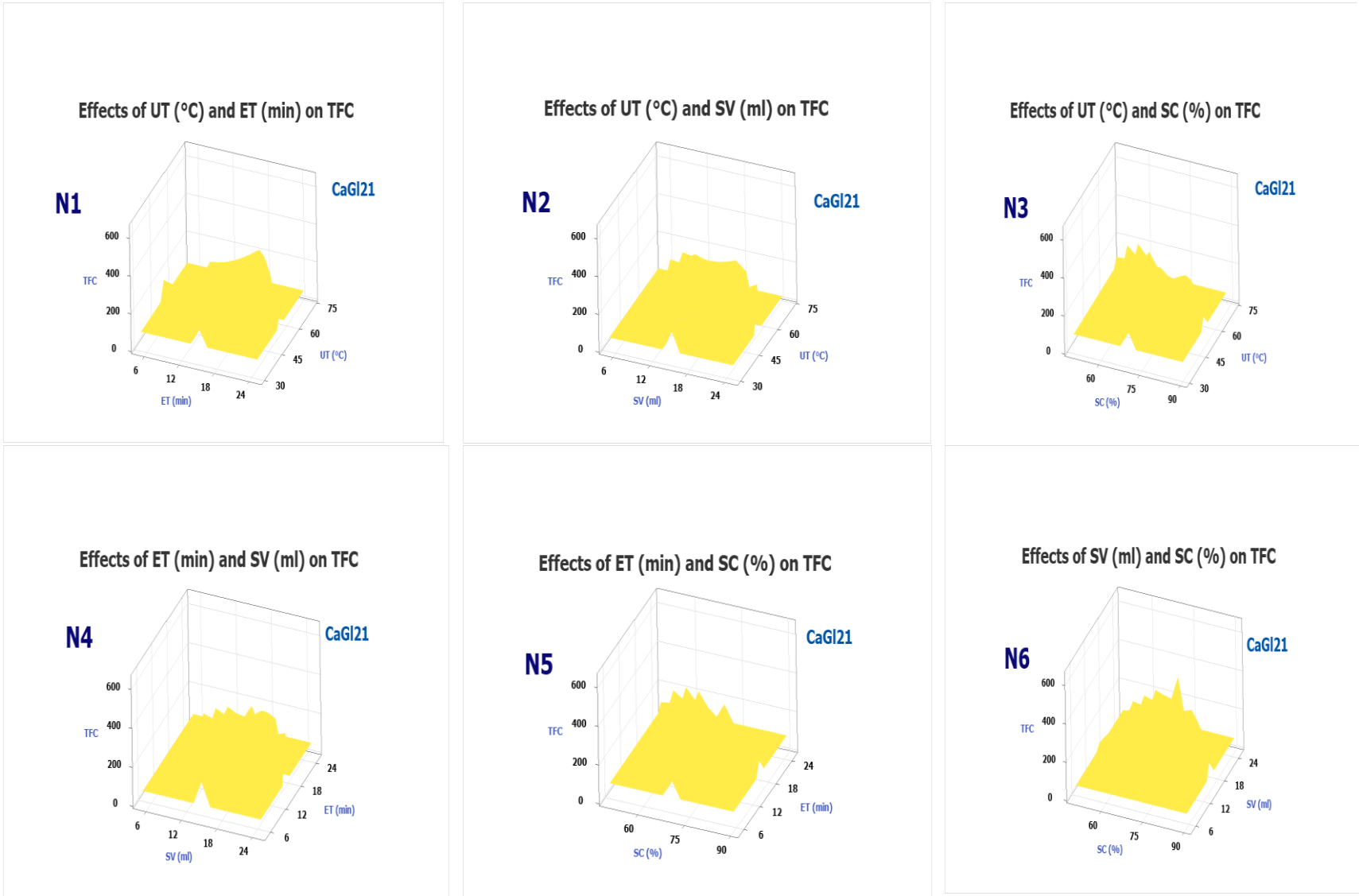


Figure 4.102 Three-dimensional surface plots of factors effects on TFC extraction from African nutmeg peels using CaGl21

4.6.4.3 Effects of Factors on Antiradical scavenging activity

The antiradical scavenging activity of the extracts using different levels of independent variables was measured based on CUPRAC, FRAP, and DPPH inhibition methods. The results obtained for CUPRAC and DPPH were reported in micro mole of Trolox equivalent per gram (µMTE/g) of sample in dry weight, while DPPH was reported as percentage of inhibition. The results for the three methods are presented in **Table 4.13**.

4.6.4.3.1 Effects of Factors on Cupric Ion-Reducing Antioxidant Capacity (CUPRAC) Assay

The highest CUPRAC activity was 26.2785±0.07 µMTE/g obtained in run 22 from CaFr11 under extraction temperature, extraction time, solvent volume, and solvent concentration of 50°c, 15 min, 25 ml, and 70% respectively, while the lowest CUPRAC activity was 3.0895±0.01 µMTE/g obtained in run 17 from CaFr11, CaGc21, and CaGl21 at temperature, time, volume, and concentration of 40ºc, 10 min, 20 ml, 60%, respectively. Also, at temperature, time, volume, and concentration of 50ºc, 15 min, 5 ml, 70% (run 30), respectively, CaGc21 produced 3.0895±0.01 µMTE/g CUPRAC effects. The regression equations show that the full quadratic model was adequate to fit the CUPRAC capacity at factor conditions for all the studied NADESs (**Table 4.10**). Pareto charts (**Figure 4.103**) of the analysis show the factors and factor combinations with significant effects on CUPRAC capacity of African nutmeg peels and how they relate with each other for the synthesized NADESs, and are delineated as follows:

A. CaSu11 - SV > ET*ET > SV*SV > UT > SC.
B. CaFr11- SV > SV*SV > ET*ET > ET > SC.
C. CaFr12 - SV > ET*ET > SV*SV > UT > SC.
D. CaFr21 - SV > SV*SV > ET*ET > UT > SC.
E. CaXy11 - SV > SV*SV > ET*ET > UT > SC.
F. CaXy12 - SV > ET*ET > SV*SV > UT > SC.
G. CaXy21- SV > SV*SV > ET*ET > SV*SC > ET*SV >UT.
H. CaGr11- SV > ET*ET > SV*SV > UT > SC > ET*SV > SV*SC.
I. CaGr12– SV >SV*SV > ET*ET > SC > UT > UT*UT > ET*SC > SV*SC > ET*SV > UT*SV.

J. CaGr21- SV > ET*ET > SV*SCV> UT > SC > ET*SV > SV*SC.

K. CaGc11- SV > ET*ET > SV*SV > UT.

L. CaGc21- SV > ET*ET > SV*SV > UT >SC.

M. CaGl11- SV > ET*ET > SV*SV > UT > SC.

N. CaGl21- SV > ET*ET > SV*SV > SC > UT.

From the outline above, solvent volume (SV) can be deduced as the factor with the most significant effects on CUPRAC capacity of African nutmeg peels, followed by squared extraction time, the squared solvent volume, and so on. Three-dimensional surface plots of the effects of two factors on CUPRAC antiradical scavenging capacity of African nutmeg peels are shown in Figure 4.104 to Figure 4.117 for the synthesized NADESs, and the maximizing conditions for CUPRAC activity surprisingly appears to be the same for all the synthesized and is given as UT (60ºc), ET (18-24 min), SV (18-24 ml), and SC (70%), $10 \leq TPC \leq 15$ µMTE/g.

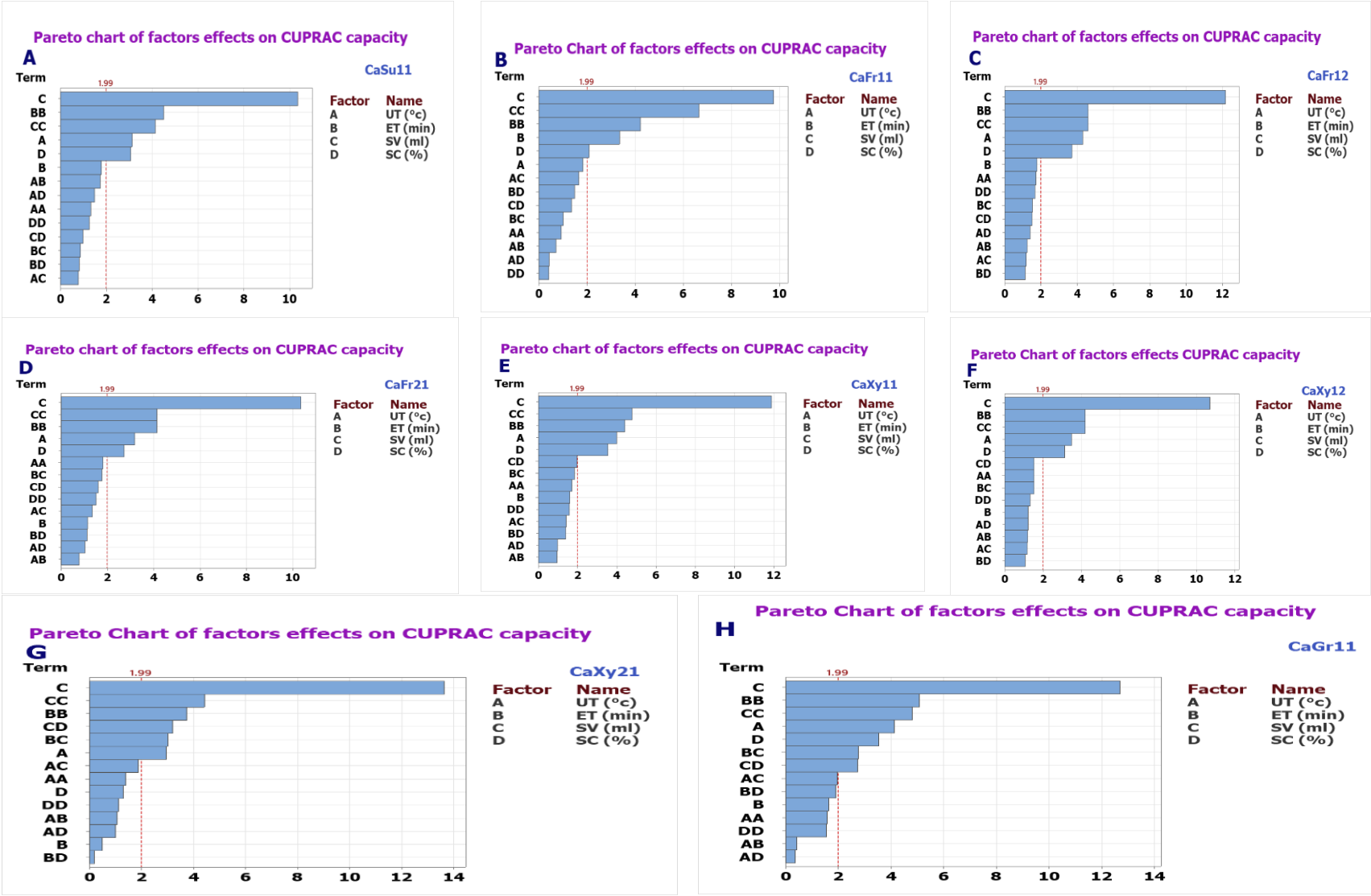


Figure 4.103 Pareto charts of factors effects on CUPRAC capacity of African nutmeg peels extracted with synthesized NADESs

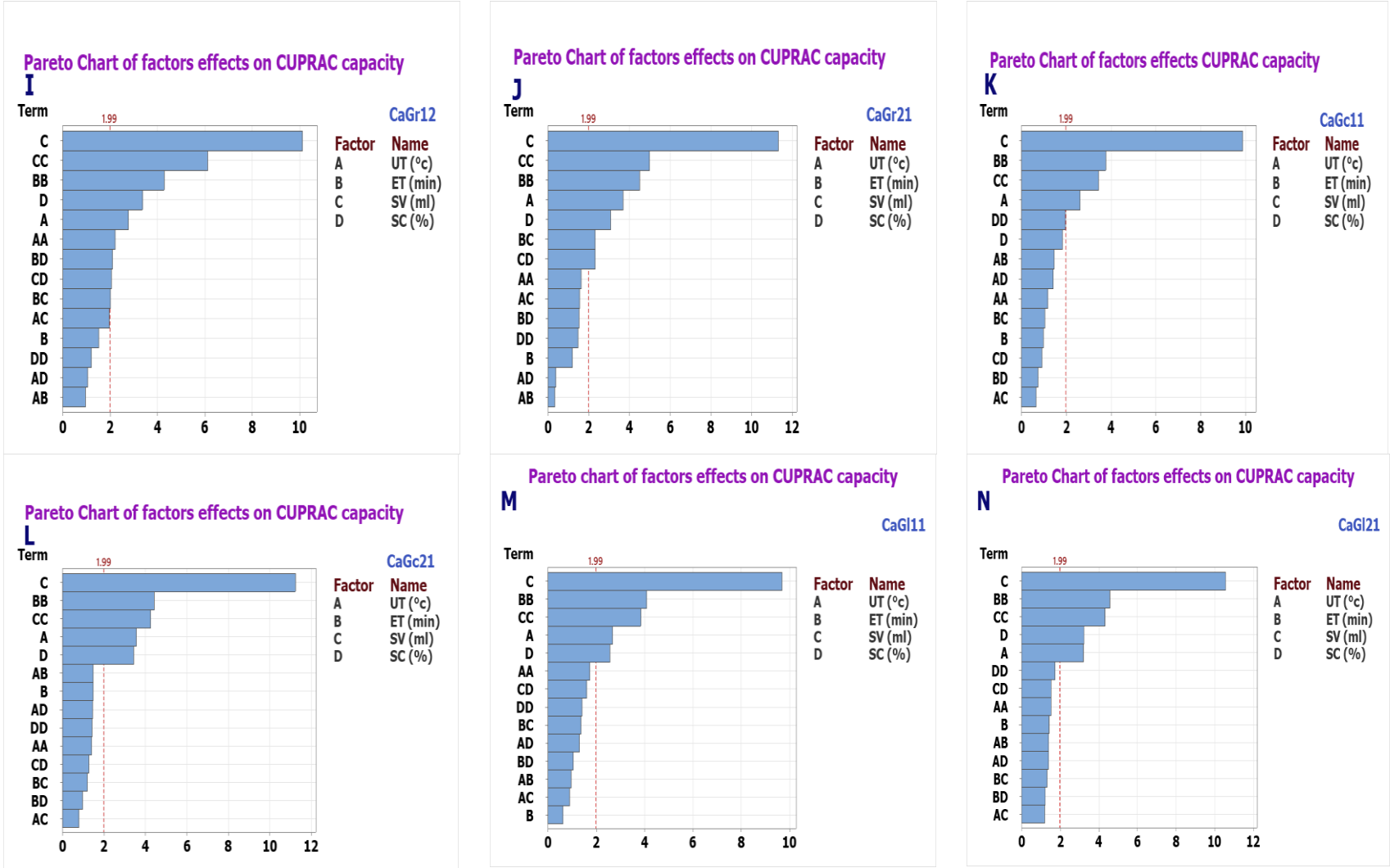


Figure 4.103 contd.

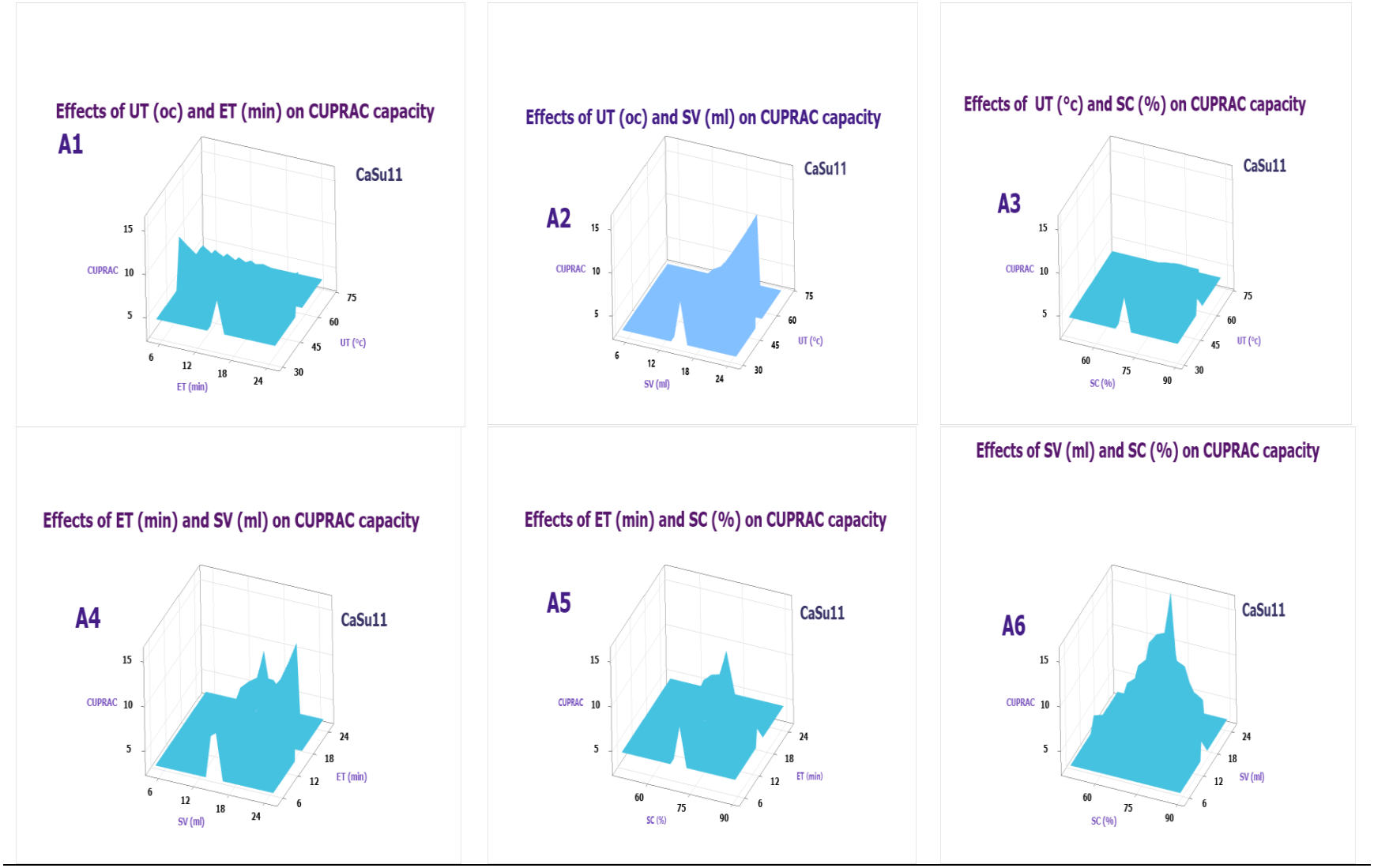


Figure 4.104 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaSu11.

Figure 4.105 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaFr11.

Figure 4.106 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaFr12.

Figure 4.107 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaFr21.

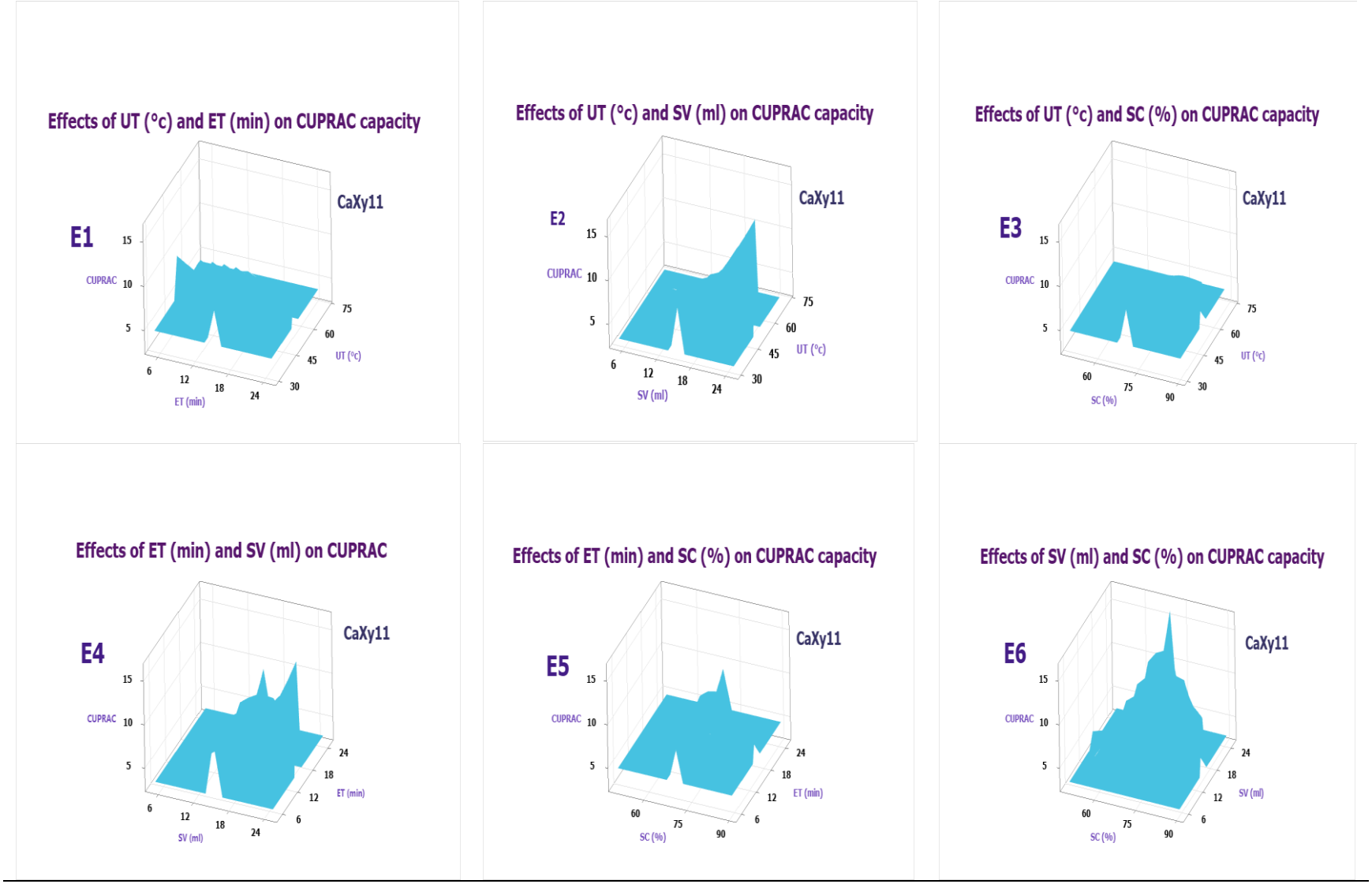


Figure 4.108 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaXy11.

Figure 4.109 Three-dimensional surface plots of factors effects on CUPRAC capacity from African nutmeg peels extracted using CaXy12.

Figure 4.110 Three-dimensional surface plots of factors effects on CUPRAC capacity from African nutmeg peels extracted using CaXy21.

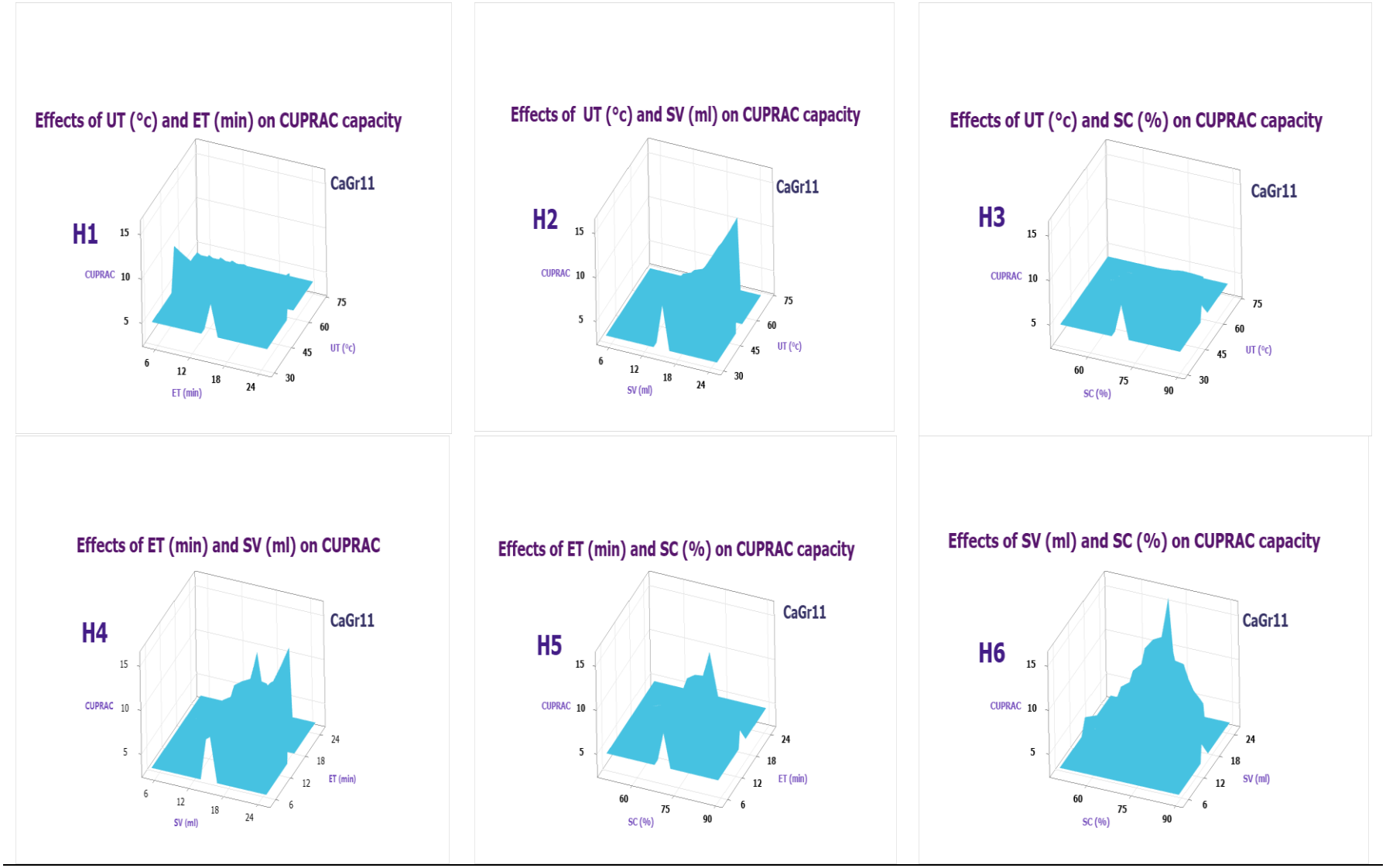


Figure 4.111 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGr11

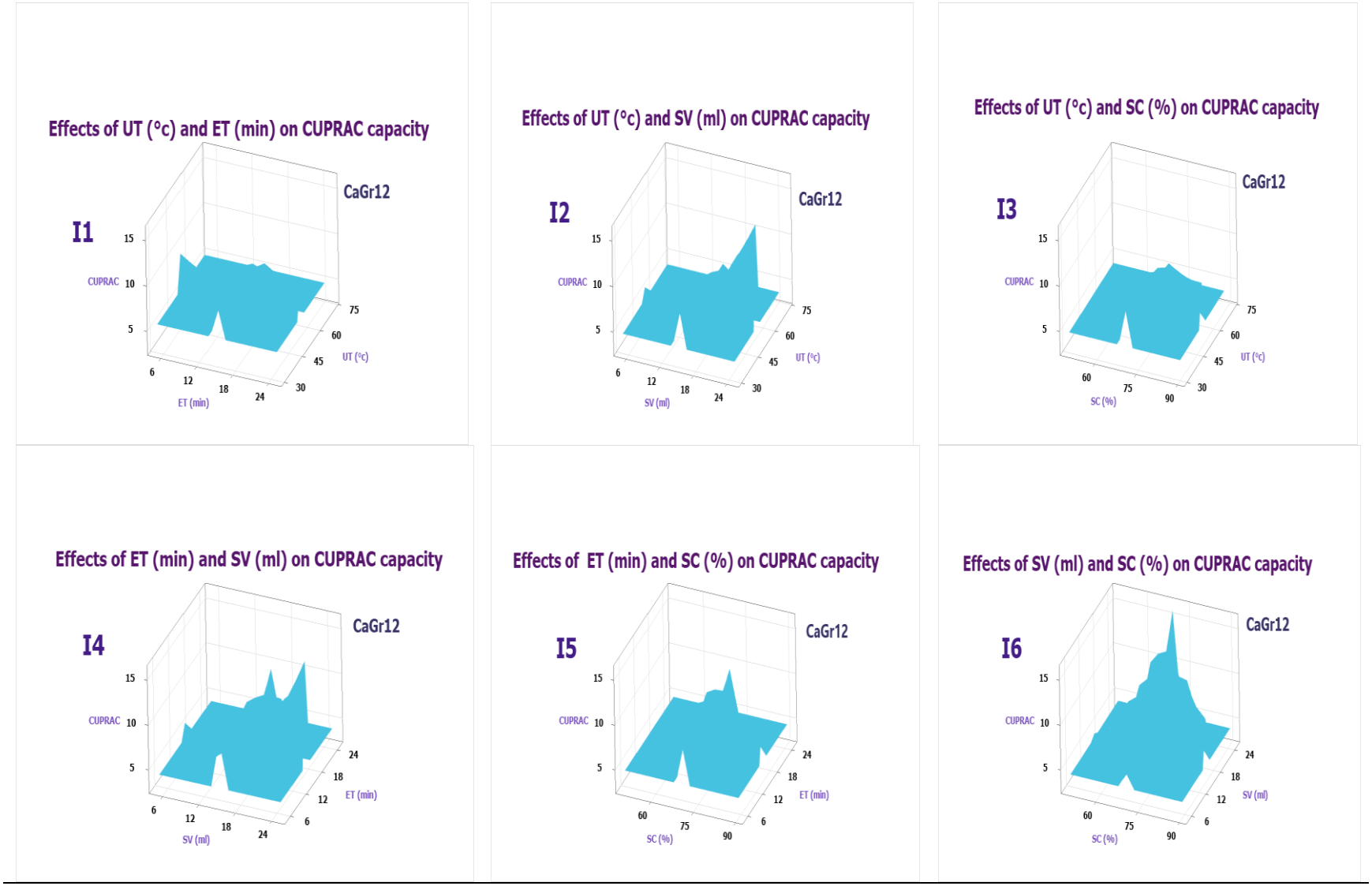


Figure 4.112 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGr12.

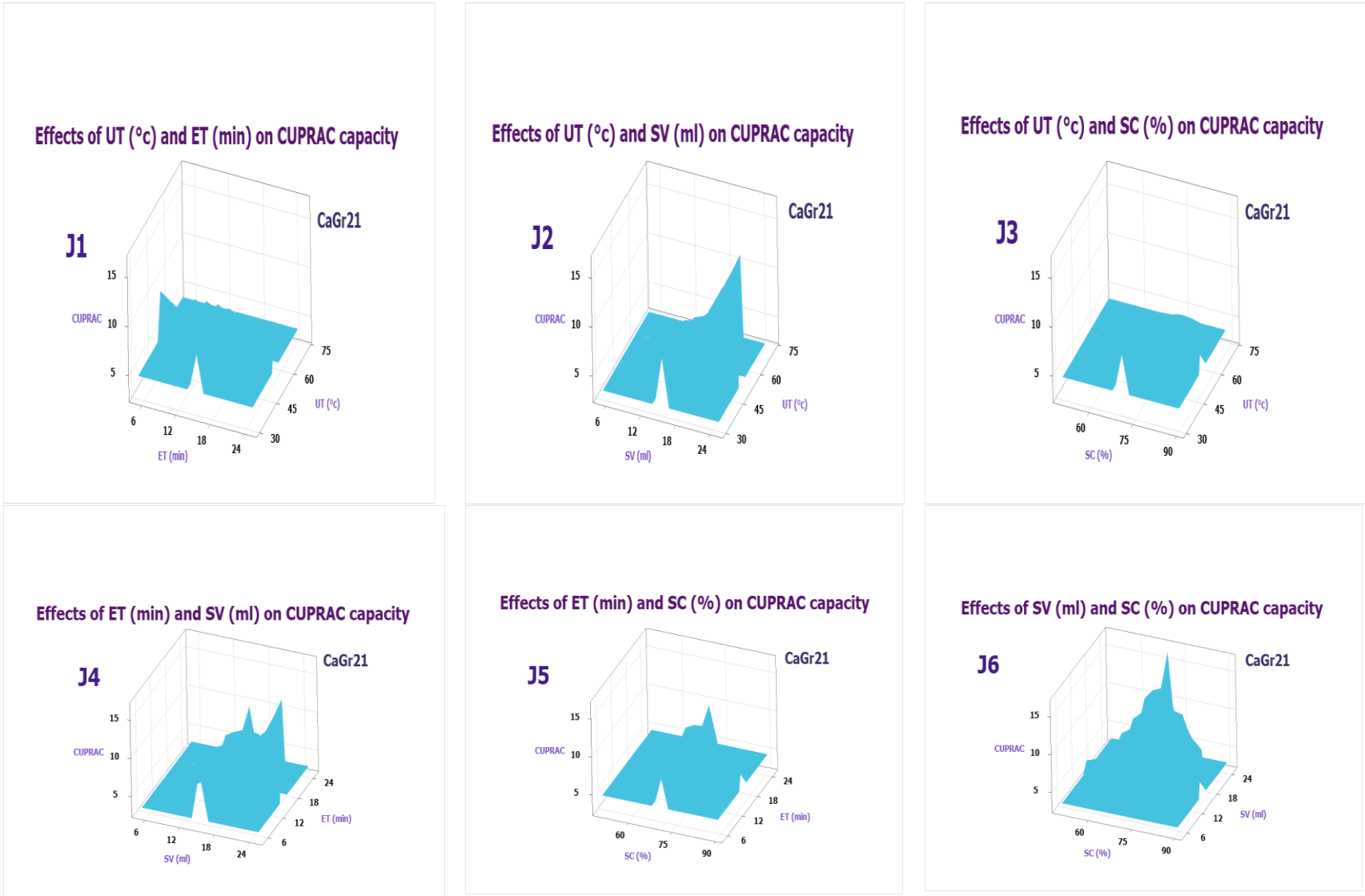


Figure 4.113 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGr21.

Figure 4.114 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGc11.

Figure 4.115 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGc21.

Figure 4.116 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGl11.

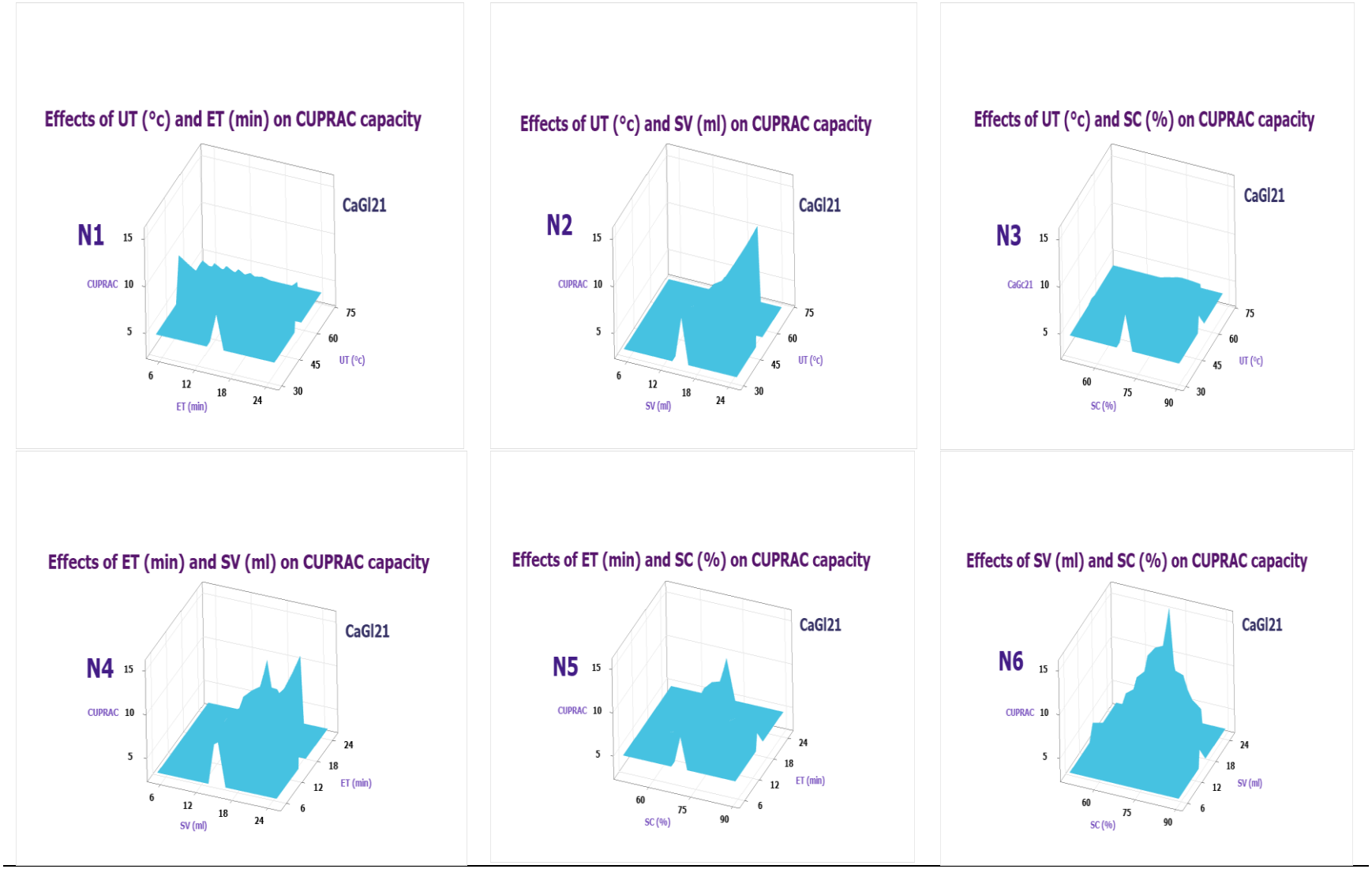


Figure 4.117 Three-dimensional surface plots of factors effects on CUPRAC capacity of African nutmeg peels extracted using CaGc21

4.6.4.3.2 Effects of Factors on Ferric-Reducing Antioxidant Power (FRAP) Assay

The highest FRAP power of 20.3090±0.022 µMTE/g was obtained in run 22 from CaSu11 under extraction temperature, extraction time, solvent volume, and solvent concentration of 50°c, 15 min, 25 ml, and 70% respectively, while the lowest was 0.5210±0.346 µMTE/g obtained in run 30 from CaFr12 under conditions of temperature, time, volume, and concentration of 50ºc, 15 min, 5ml, 70%, respectively. The regression equations show that full quadratic model was adequate to fit the FRAP power at factor conditions for all the studied NADESs (**Table 4.10**). Pareto charts (**Figure 4.118**) of the analysis show the factors and factor combinations with significant effects on FRAP power of African nutmeg peels and how they relate with each other for the synthesized NADESs, and are listed as follows:

A. CaSu11 – SV*SV > SV > ET*SV > UT > SV*SC > ET*SC.
B. CaFr11- SC*SC > SV > ET*SC > UT*SV >SV*SV > ET*SV > SV*SC.
C. CaFr12 - SV > ET*SC > UT*SV > UT > UT*ET > ET*SV > SC*SC > ET > ET*ET > UT*SC > SV*SC > SV*SV.
D. CaFr21 - SV > ET*SC > UT*SV >UT*ET > ET*SV > UT > UT*SC > SV*SC > SC*SC >ET*ET >SV*SV > ET.
E. CaXy11 - SV > UT*ET > ET*SC > UT*SC > UT*SV >ET*SV >UT > ET > UT*SC > SV*SV > SC*SC > ET*ET.
F. CaXy12 - SV > SC*SC > UT*ET > ET*SV > UT > UT*SV > ET >SC > ET*SC.
G. CaXy21- SV > ET*SC > UT*ET > UT*SC >SV*SV > SC*SC > UT*SV >ET*ET.
H. CaGr11- SV > ET*SC > ET*SV > ET*SC > UT*SV > UT*SC > UT > SV*SC > SC*SC >ET*ET > SV*SV > ET.
I. CaGr12 – SC*SC >SV >ET*SC > SC > UT*SV > UT > UT*ET.
J. CaGr21- SV > SV*SV > ET*SV> UT*ET > UT*SV > UT > ET > UT*SC > SC.
K. CaGc11- SV*SV > SV > UT*ET > UT > ET*SC > ET*SV > UT*SC > UT*SV.
L. CaGc21- SV > SV*SV > UT*ET.
M. CaGl11- SV > SV*SV > SC.
N. CaGl21- SV*SV > SV > SC*SC.

From the outline above, solvent volume (SV) has once again shown to be the factor with the most significant effects on FRAP power of African nutmeg peels, as other factors trail behind. Three-

dimensional surface plots of the effects of factors on FRAP power of African nutmeg peels extracted using different NADESs are shown in **Figure 4.119** to **Figure 4.132** respectively, and the conditions for maximizing FRAP power indicated below:

A. CaSu11- UT (60ºc), ET (18-20 min), SV (18-22 ml), and SC (75%), FRAP ≥ 10 µMTE/g.

B. CaFr11-UT (60ºc), ET (18-22 min), SV (18-22 ml), and SC (55-80%), FRAP ≥ 15µMTE/g.

C. CaFr12 - UT (60ºc), ET (18 min), SV (18 ml), and SC (75%), FRAP ≥ 4 µMTE/g.

D. CaFr21- UT (60ºc), ET (20 min), SV (18 ml), and SC (75%), FRAP ≥ 3 µMTE/g.

E. CaXy11- UT (60ºc), ET (20 min), SV (20 ml), and SC (70%), FRAP ≥ 3 µMTE/g.

F. CaXy12- UT (60ºc), ET (20 min), SV (20 ml), and SC (80%), FRAP ≥4 µMTE/g.

G. CaXy21 – UT (60ºc), ET (20 min), SV (20-24 ml), and SC (70%), FRAP ≥4 µMTE/g.

H. CaGr11 – UT (60ºc), ET (20 min), SV (22 ml), and SC (70%), FRAP ≥4 µMTE/g.

I. CaGr12 – UT (60ºc), ET (20 min), SV (18 ml), and SC (55-60%), FRAP ≥10 µMTE/g.

J. CaGr21 – UT (60ºc), ET (20 min), SV (20 min), and SC (65%), FRAP ≥15 µMTE/g.

K. CaGc11- UT (60ºc), ET (20 min), SV (22 ml), and SC (65%), FRAP ≥8 µMTE/g.

L. CaGc21 – UT (60ºc), ET (20min), SV (24 ml), and SC (70%), FRAP ≥6 µMTE/g.

M. CaGl11–UT (60-65ºc), ET (20-22 min), SV (20-24 ml), and SC (60-75%), FRAP ≥ 5 µMTE/g.

N. CaGl21 – UT (60-70ºc), ET (20-24 min), SV (18-24 ml), and SC (60-80%), FRAP ≥6 µMTE/g.

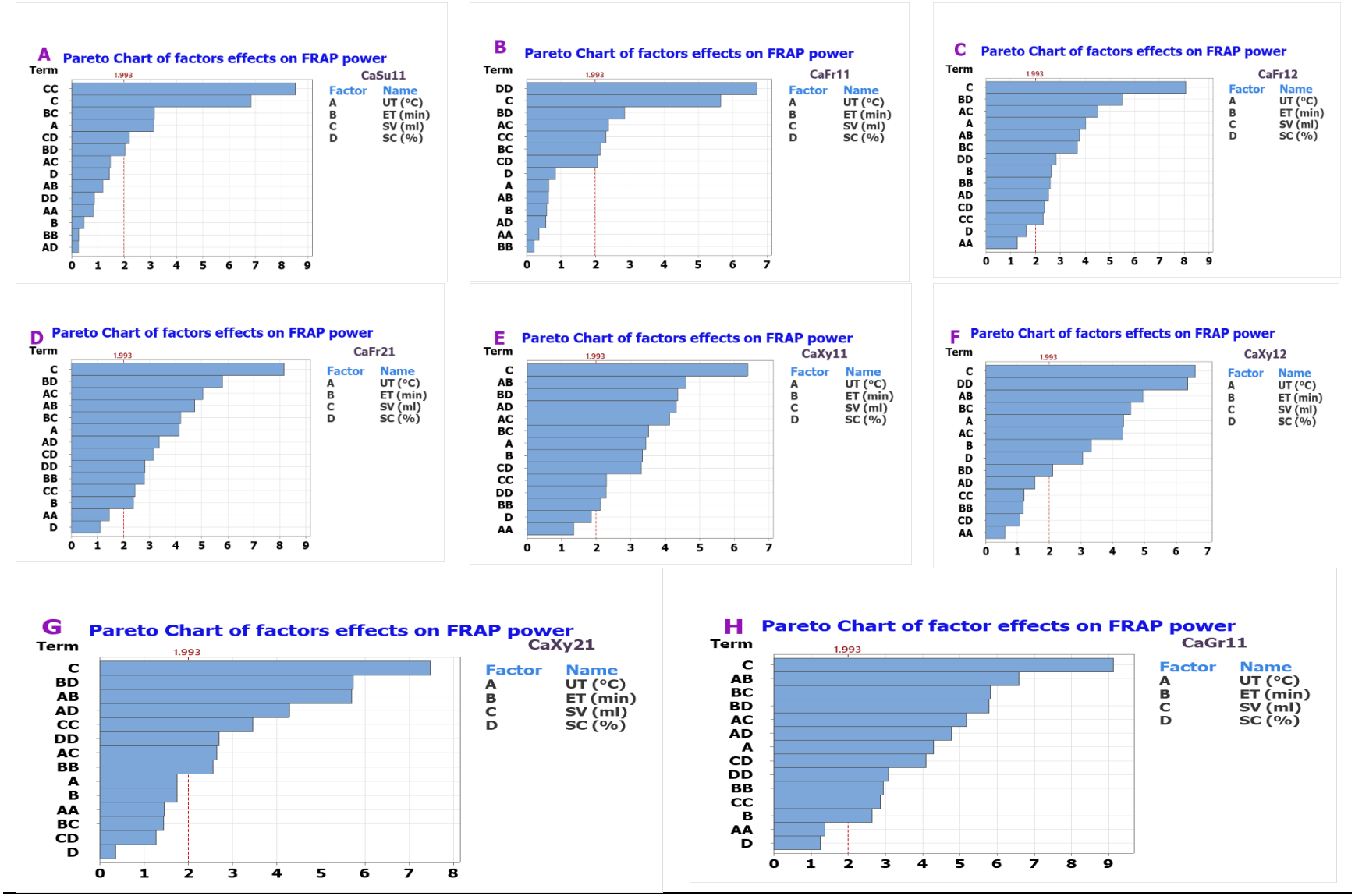


Figure 4.118 Pareto charts of factors effects on FRAP power of African nutmeg peels extracted using synthesized NADESs

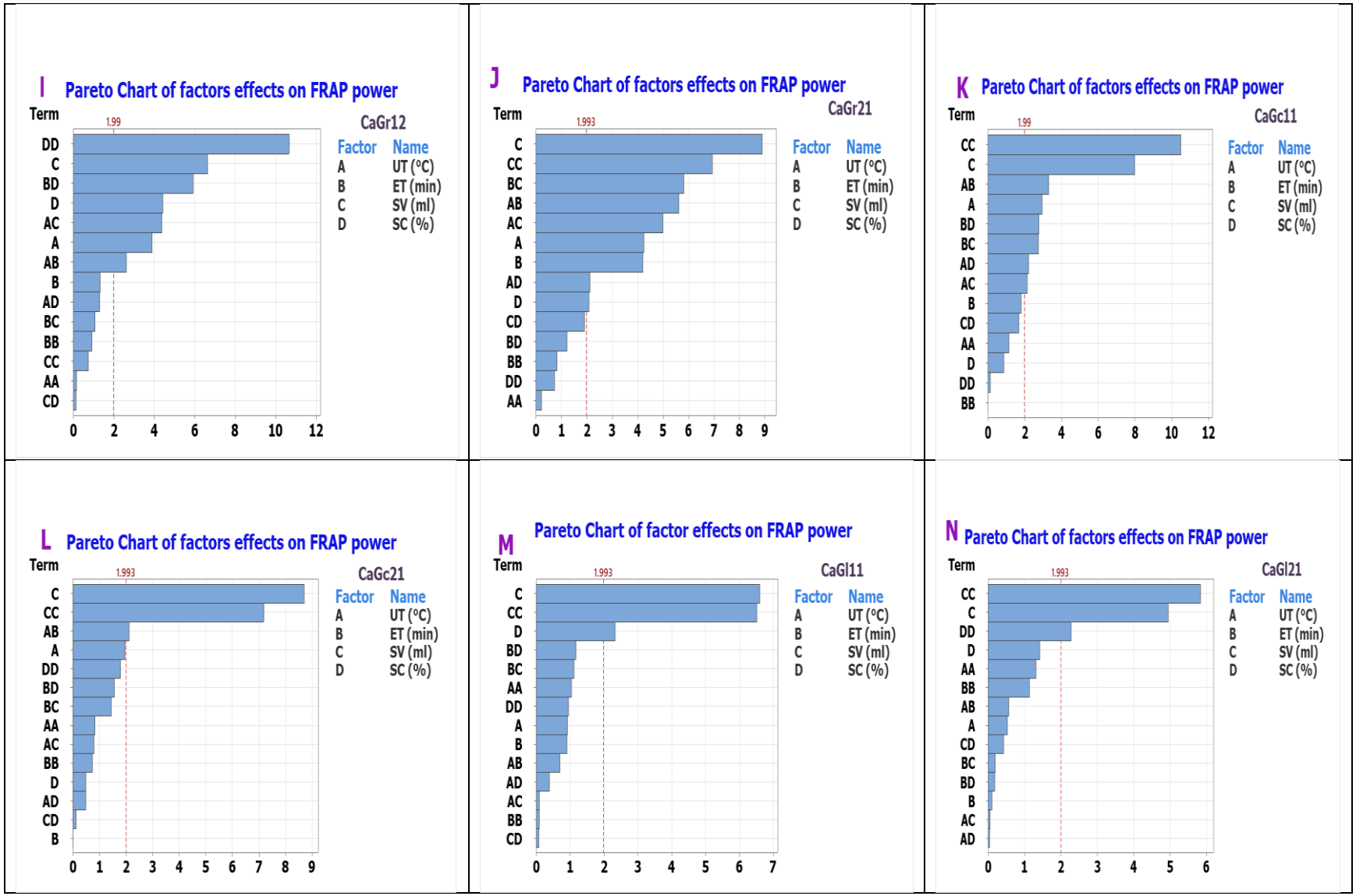


Figure 4.118 contd.

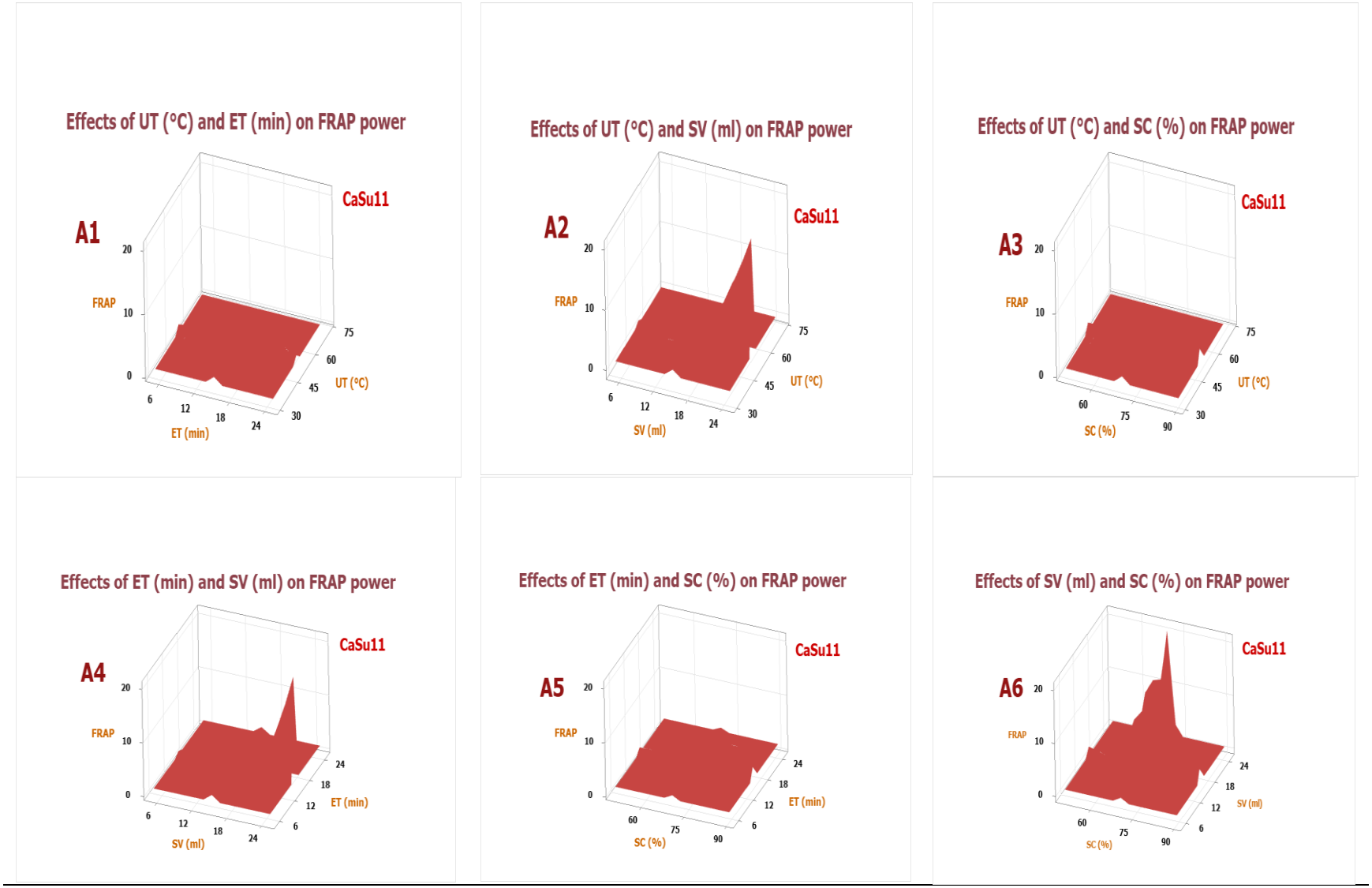


Figure 4.119 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaSu11.

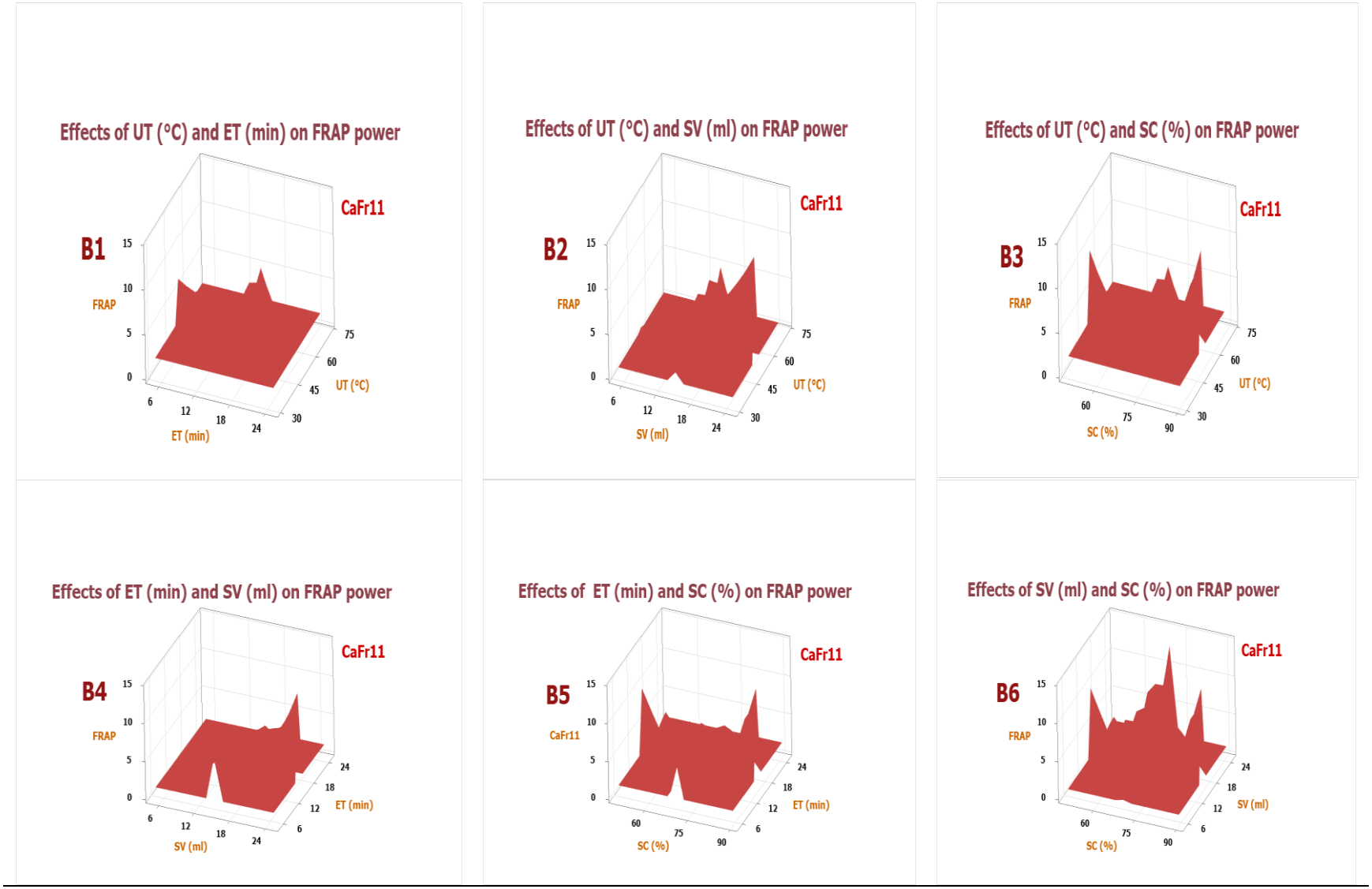


Figure 4.120 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaFr11.

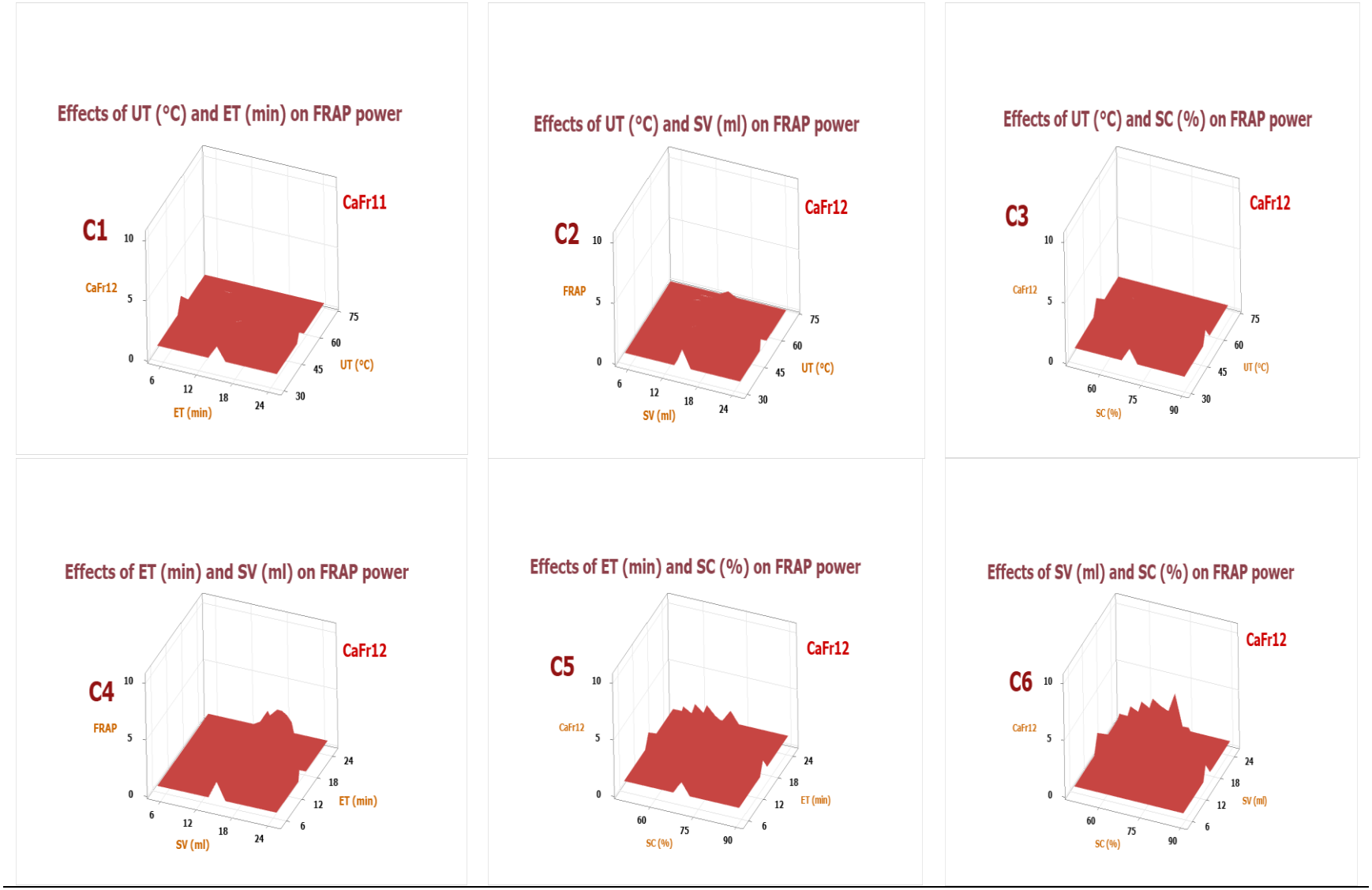


Figure 4.121 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaFr12.

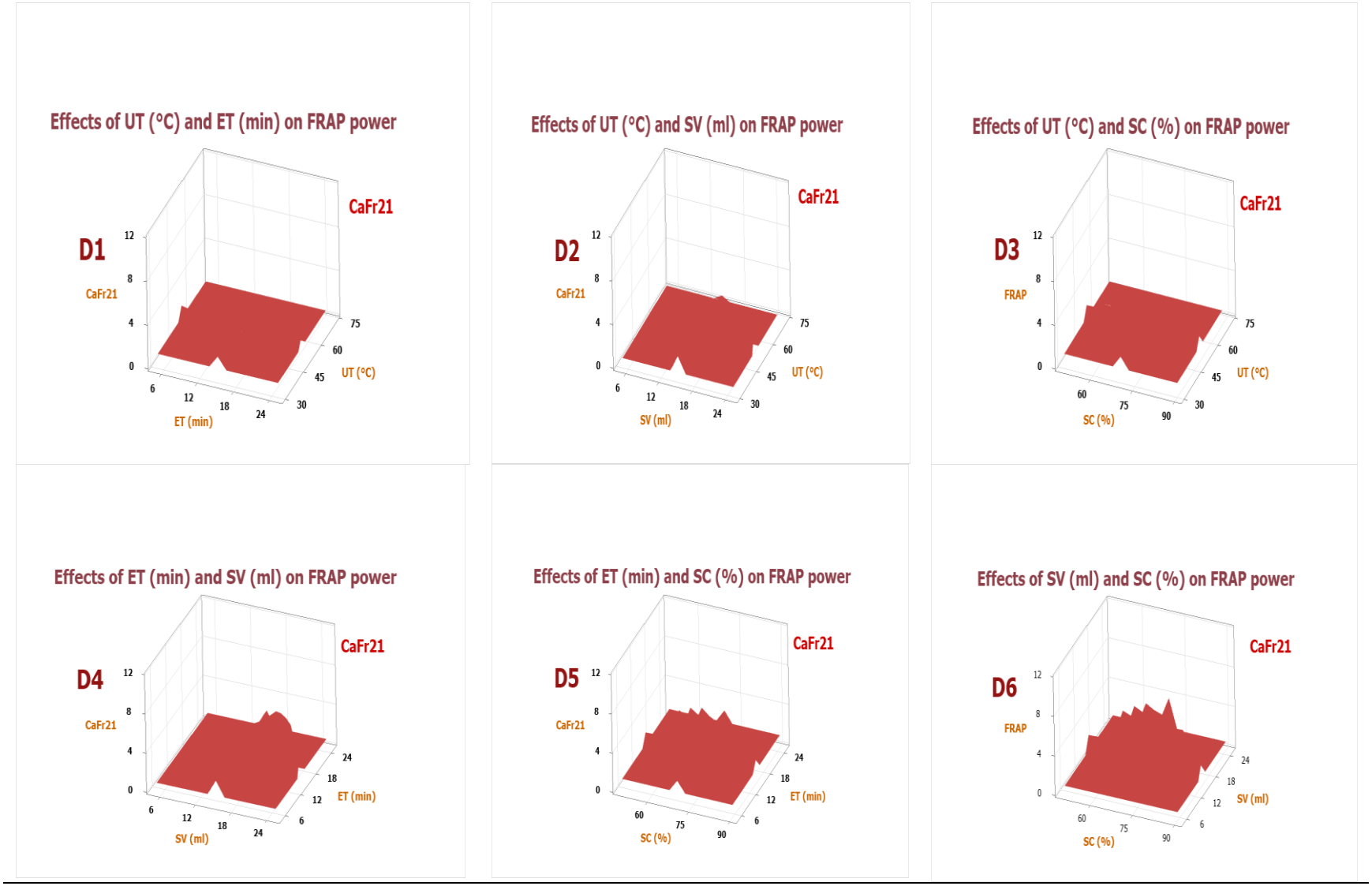


Figure 4.122 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaFr21.

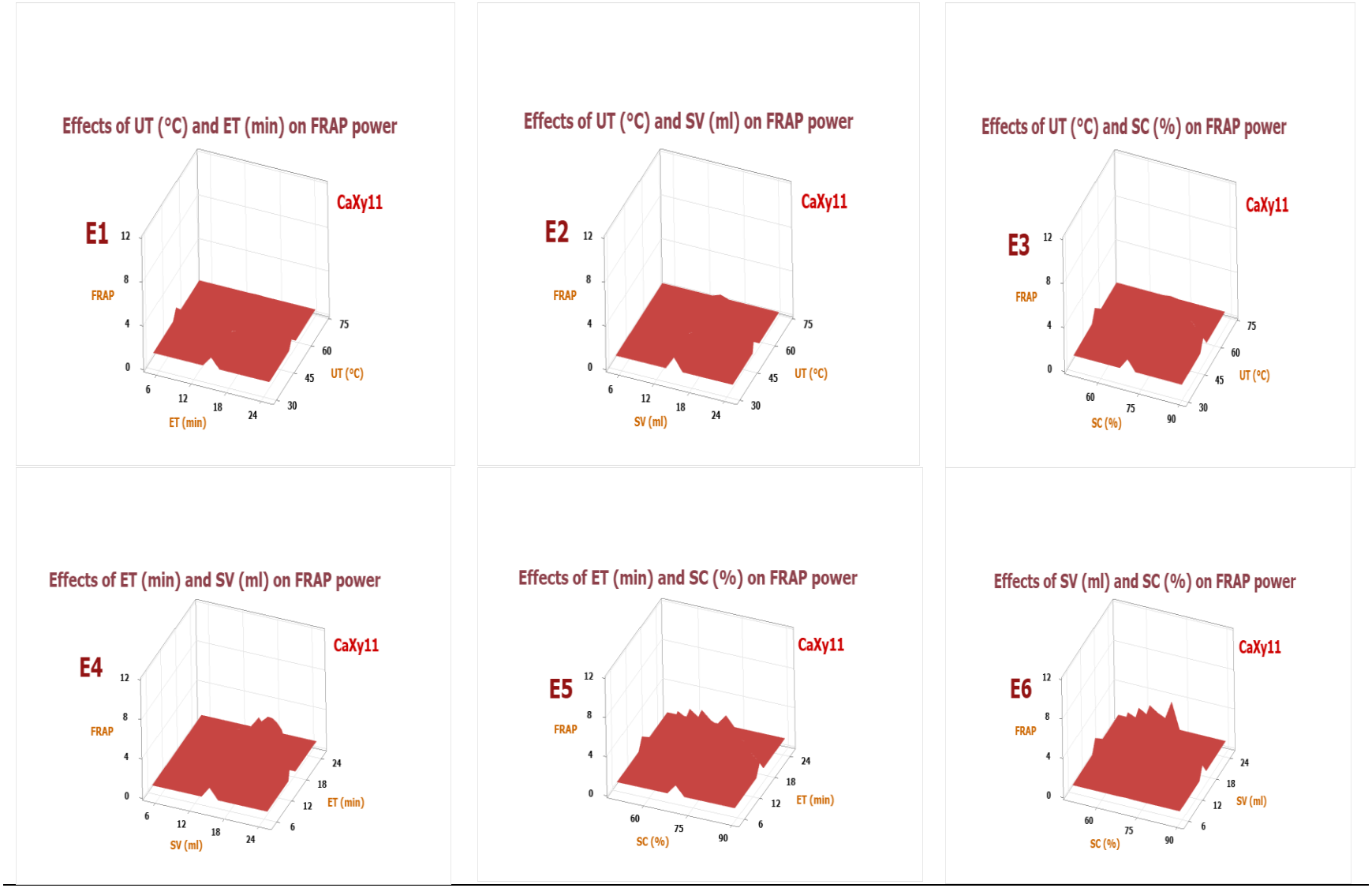


Figure 4.123 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaXy11

Figure 4.124 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaXy12.

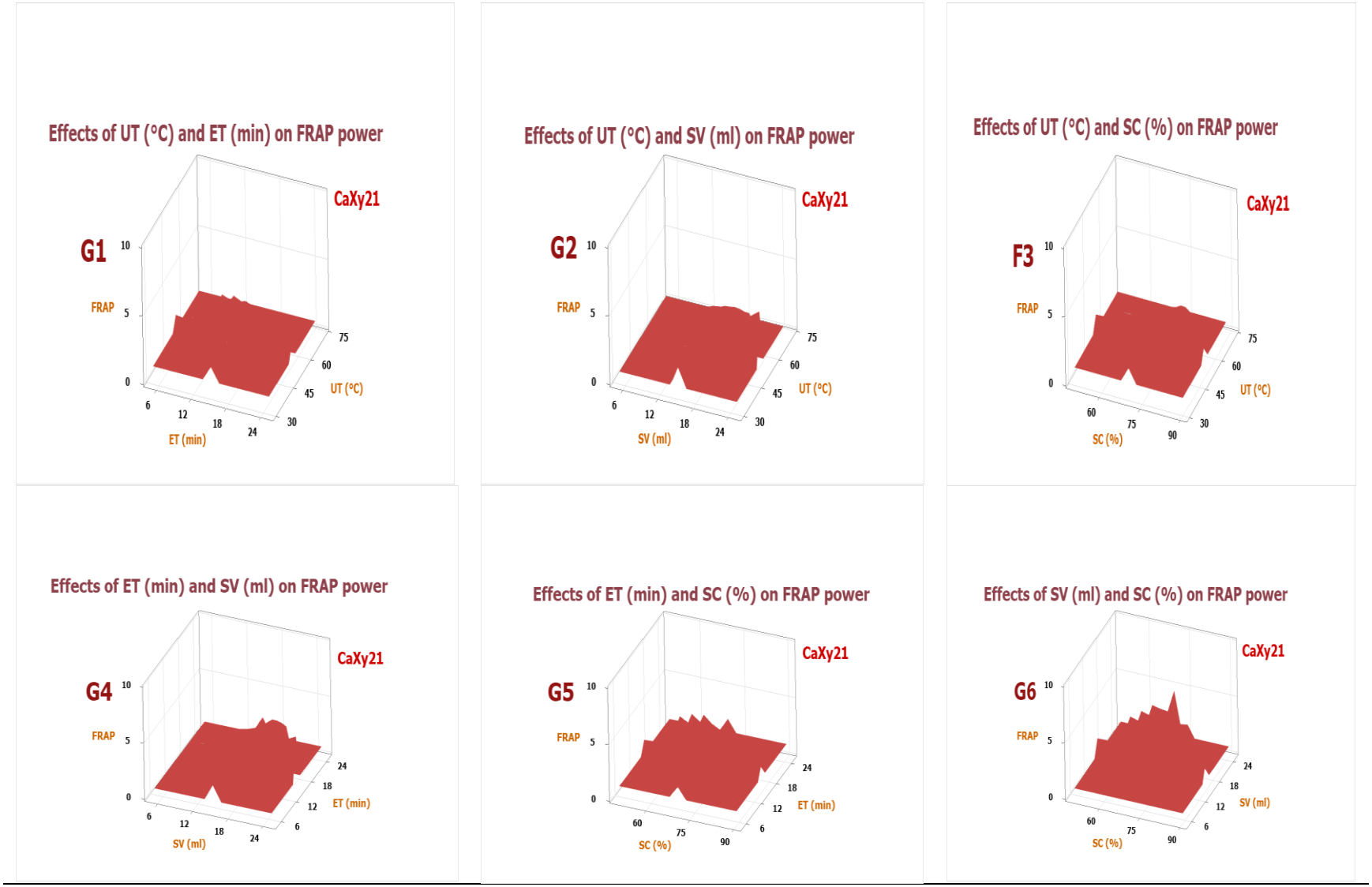


Figure 4.125 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaXy21.

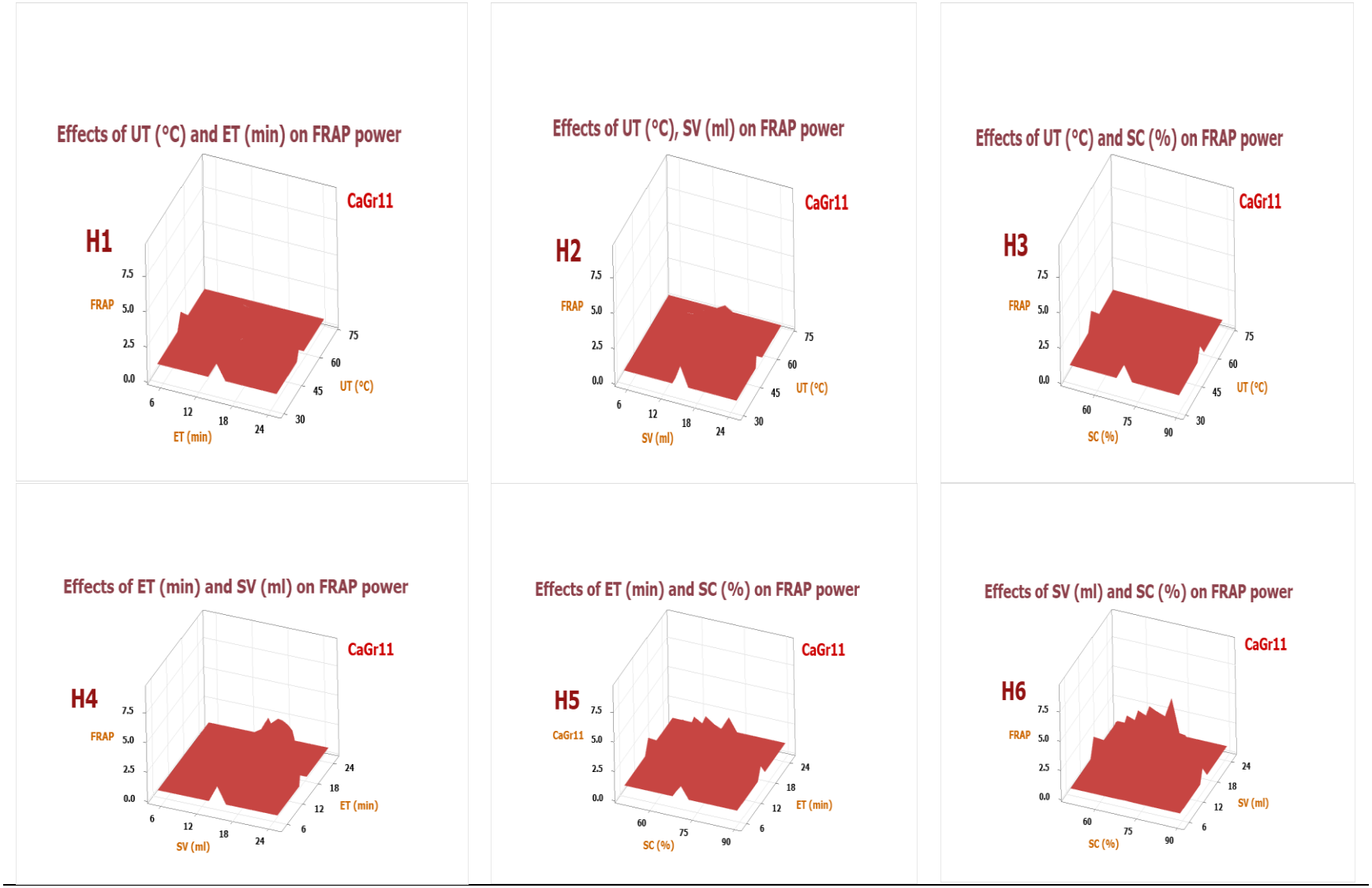


Figure 54.126 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGr11.

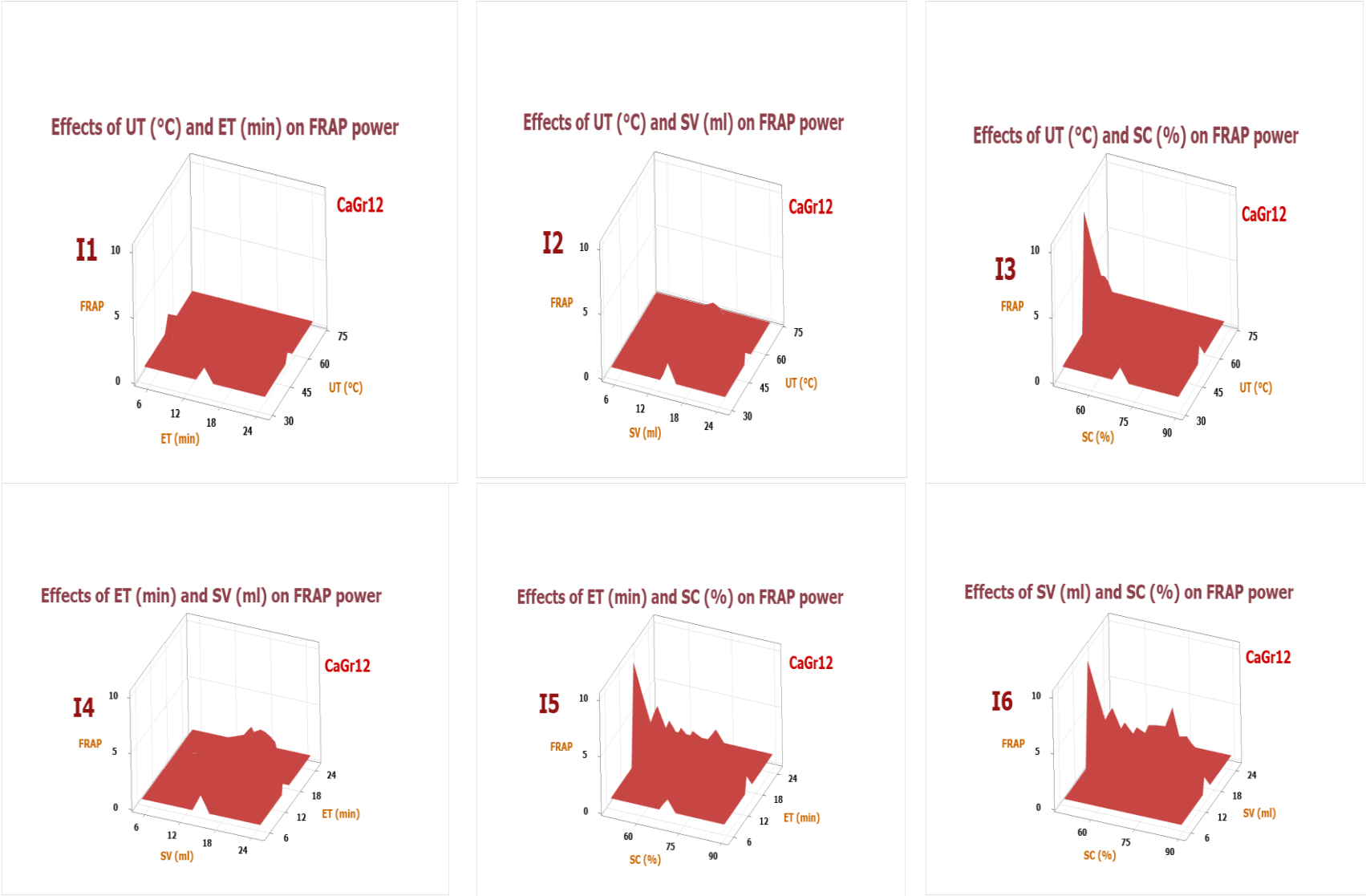


Figure 4.127 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGr12.

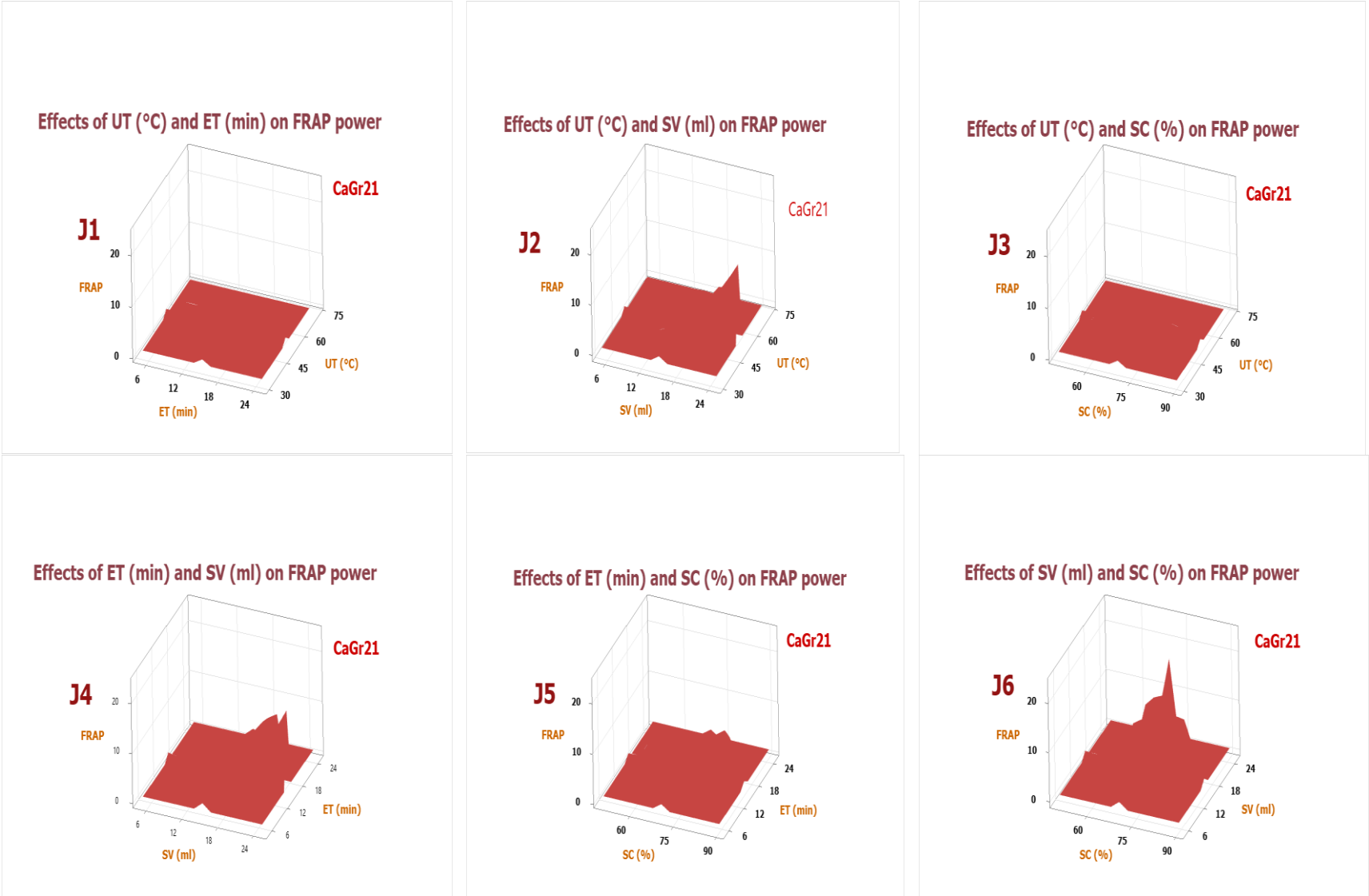


Figure 4.128 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGr21.

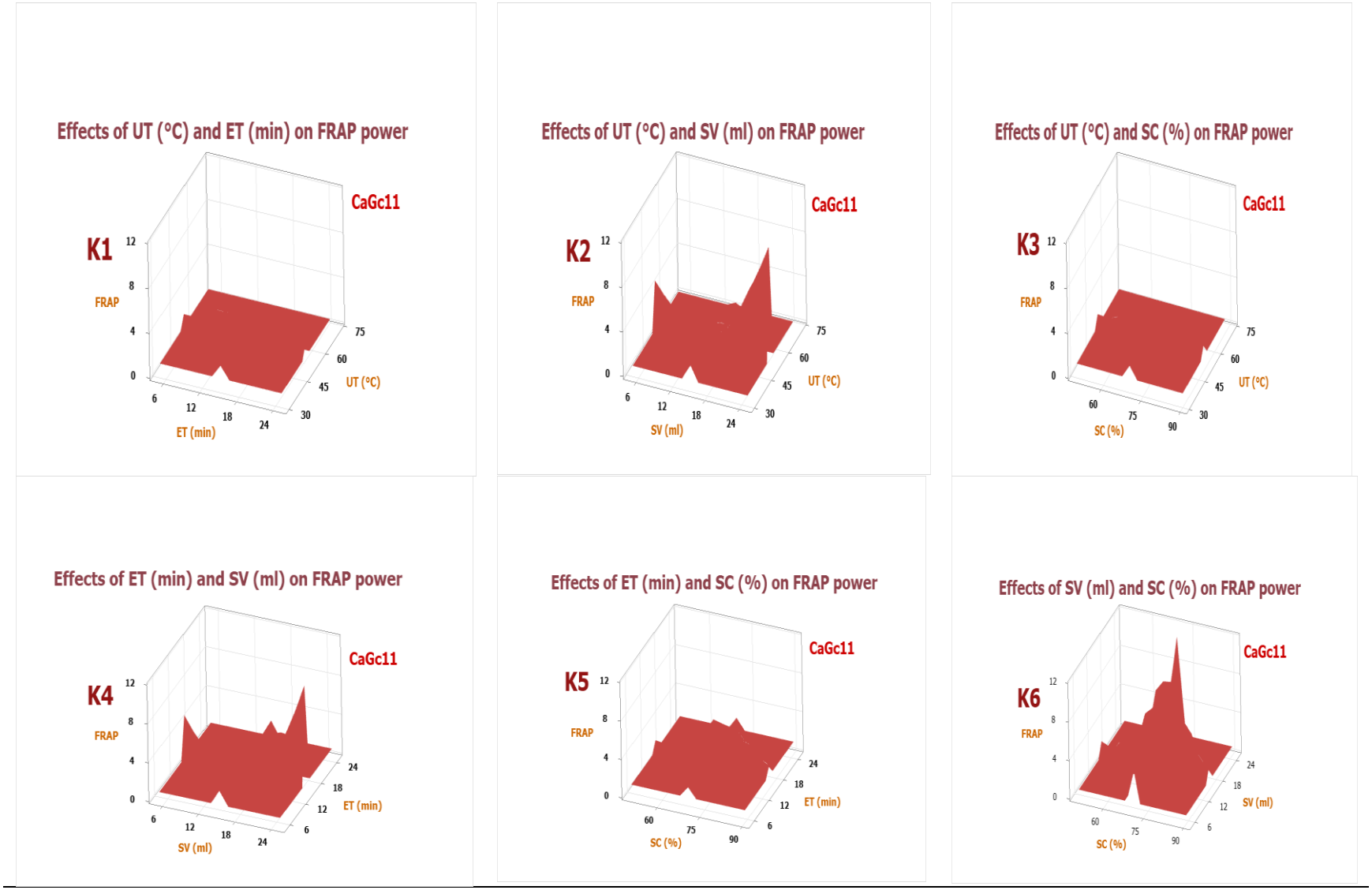


Figure 4.129 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGc11.

Figure 4.130 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGc21.

Figure 4.131 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGl11.

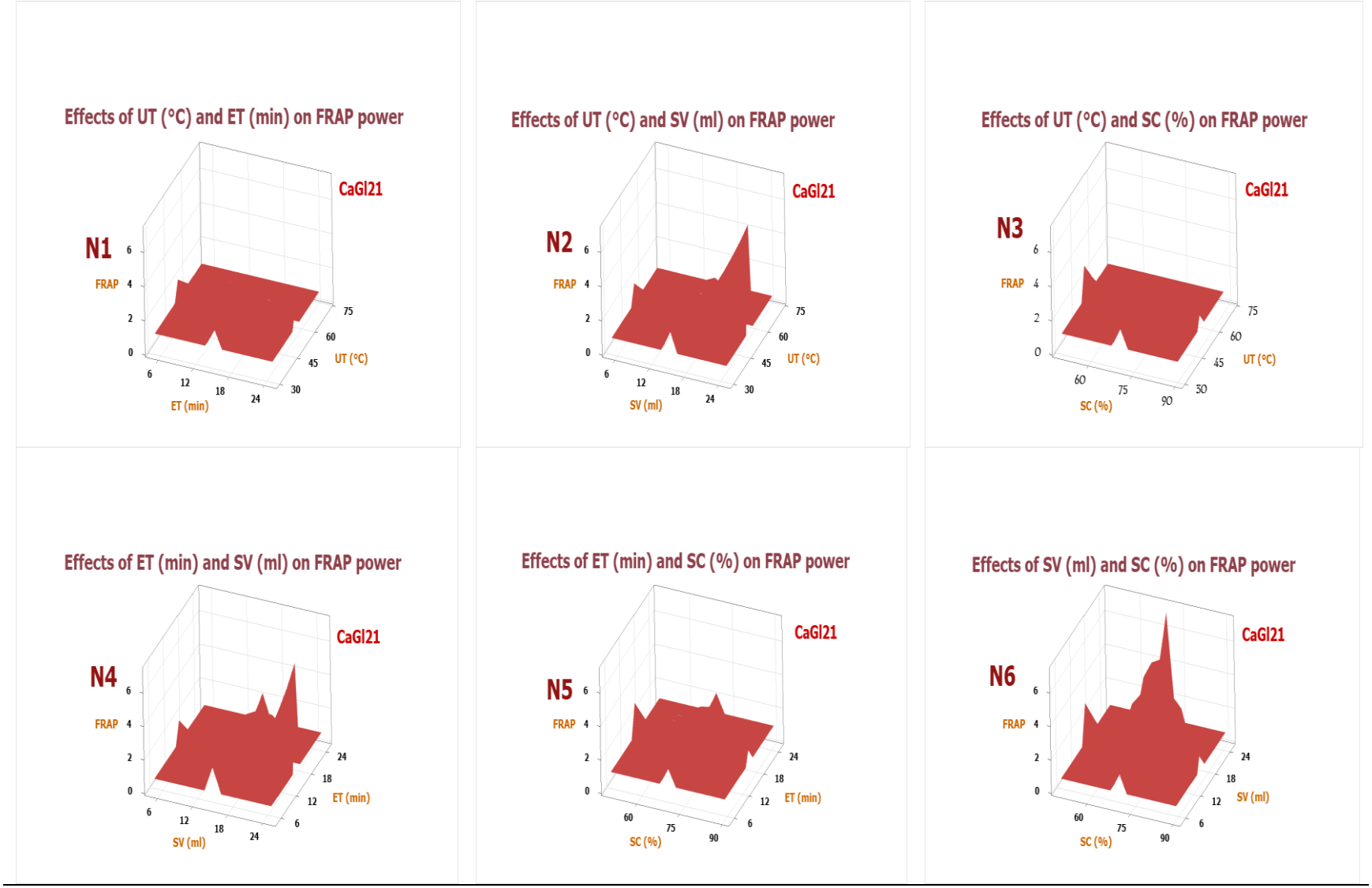


Figure 4.132 Three-dimensional surface plots of factors effects on FRAP power of African nutmeg peels extracted using CaGl21.

4.6.4.3.3. Effects of Factors on 2,2-diphenil-1-picrylhydrazyl (DPPH) Radical Scavenging Assay

The percentage inhibition measured by DPPH gave the maximum percentage inhibition of 92 from CaFr11 in run number 2 under extraction temperature, extraction time, solvent volume, and solvent concentration of 40°c, 20 min, 10 ml, and 60% respectively, while the minimum inhibition of 1.13 was observed from CaXy21 under two different sets of conditions, specifically, runs 27 and 28 with extraction temperature, extraction time, solvent volume, and percentage concentration of solvent of 30°c, 15 min, 15ml, and 70%, and 50°c, 5 min, 15ml, and 70%, respectively **Table 4.14**. The regression equations show that full quadratic model was adequate to fit the DPPH inhibition at factor conditions for all the studied NADESs (**Table 4.10**). Pareto charts (**Figure 4.133**) of the analysis show the factors and factor combinations with significant effects on DPPH inhibition of African nutmeg peels and how they relate with each other for the synthesized NADESs, and are shown below:

A. CaSu11 – UT*ET > ET > UT*UT > SC*SC > SV*SV > UT*SV > ET*ET.
B. CaFr11- UT > UT*UT > ET > ET*ET.
C. CaFr12 – UT*ET > UT*UT > ET*ET > SC*SC > ET.
D. CaFr21 – SV*SV > UT*UT > SC*SC > ET*ET > ET > SV > UT*SC > UT*SV > SC.
E. CaXy11 – SV*SV > UT*UT > SC*SC > UT*ET > ET >UT*SC >SC.
F. CaXy12 – SV*SV > UT*UT > ET > ET*ET > SC*SC.
G. CaXy21- SV*SV > ET*ET > UT > SC*SC >ET > UT*UT > UT*SV.
H. CaGr11- UT*UT > SC*SC > ET*ET > SV*SV > SV > ET > SC.
I. CaGr12 – UT*SV >SC >ET*ET > UT >SC*SC > UT*ET > SV*SV > ET > UT*SC.
J. CaGr21- SV*SV > UT*UT > SC*SC > ET*ET > UT*SV > UT*ET > UT*SC.
K. CaGc11- UT*UT > SC*SC > SV > SV*SV > ET*ET > SC > UT*SV.
L. CaGc21- SV > SC > UT > SV*SV > SC*SC > UT*UT > ET > ET*ET > UT*SC.
M. CaGl11- SC > SV > ET > UT*SC.
N. CaGl21- ET*ET > UT*UT > SV*SV > SC*SC > UT*SV > UT*ET > ET > UT*SC.

From the outline above, temperature (UT), and volume (SV) factors either as main or interactions have maximizing effects on DPPH inhibition in six solvents each, while time (ET), and concentration (SC) factors either as main or interaction have maximizing effects on DPPH inhibition in one solvent each. Three-dimensional surface plots of the effects of factors on

percentage DPPH inhibition of African nutmeg peels extracted using different NADESs are shown in **Figure 4.134** to **Figure 4.147** respectively, and the conditions for maximizing DPPH inhibition are indicated as follows:

A. CaSu11- UT (60-70ºc), ET (18-24 min), SV (18-24 ml), and SC (60-80%), DPPH ≥ 50 %.
B. CaFr11-UT (60-70ºc), ET (18-24 min), SV (18-24 ml), and SC (60-75%), DPPH ≥ 60%.
C. CaFr12 - UT (45-60ºc), ET (18-24 min), SV (18-24 ml), and SC (60-75%), DPPH ≥ 50 %.
D. CaFr21- UT (45-60ºc), ET (12-18 min), SV (12-18 ml), and SC (60-75%), DPPH ≥ 25%.
E. CaXy11- UT (45-60ºc), ET (12-18 min), SV (12-18 ml), and SC (60-70%), DPPH ≥ 25%.
F. CaXy12- UT (45-60ºc), ET (18-20 min), SV (12-18 ml), and SC (60-70%), DPPH ≥ 25%.
G. CaXy21 – UT (60-70ºc), ET (12-18 min), SV (12-18 ml), and SC (60-70%), DPPH ≥ 50%.
H. CaGr11 – UT (45-60ºc), ET (18-24 min), SV (12-18 ml), and SC (60-70%), DPPH ≥ 25%.
I. CaGr12 – UT (60-70ºc), ET (12-18 min), SV (6-18 ml), and SC (55-65%), DPPH ≥50%.
J. CaGr21 – UT (60-65ºc), ET (12-18 min), SV (6-18 ml), and SC (60-70%), DPPH ≥25%.
K. CaGc11- UT (60-70ºc), ET (6-12 min), SV (6-12 ml), and SC (70-80%), DPPH ≥ 50%.
L. CaGc21 – UT (60-70ºc), ET (12-18min), SV (12-18 ml), and SC (55-70%), DPPH ≥60%.
M. CaGl11–UT (60-65ºc), ET (15-18 min), SV (6-12 ml), and SC (70-75%), DPPH ≥ 40%.
N. CaGl21 – UT (60-65ºc), ET (15-18 min), SV (15-18 ml), and SC (75-80%), DPPH ≥25%.

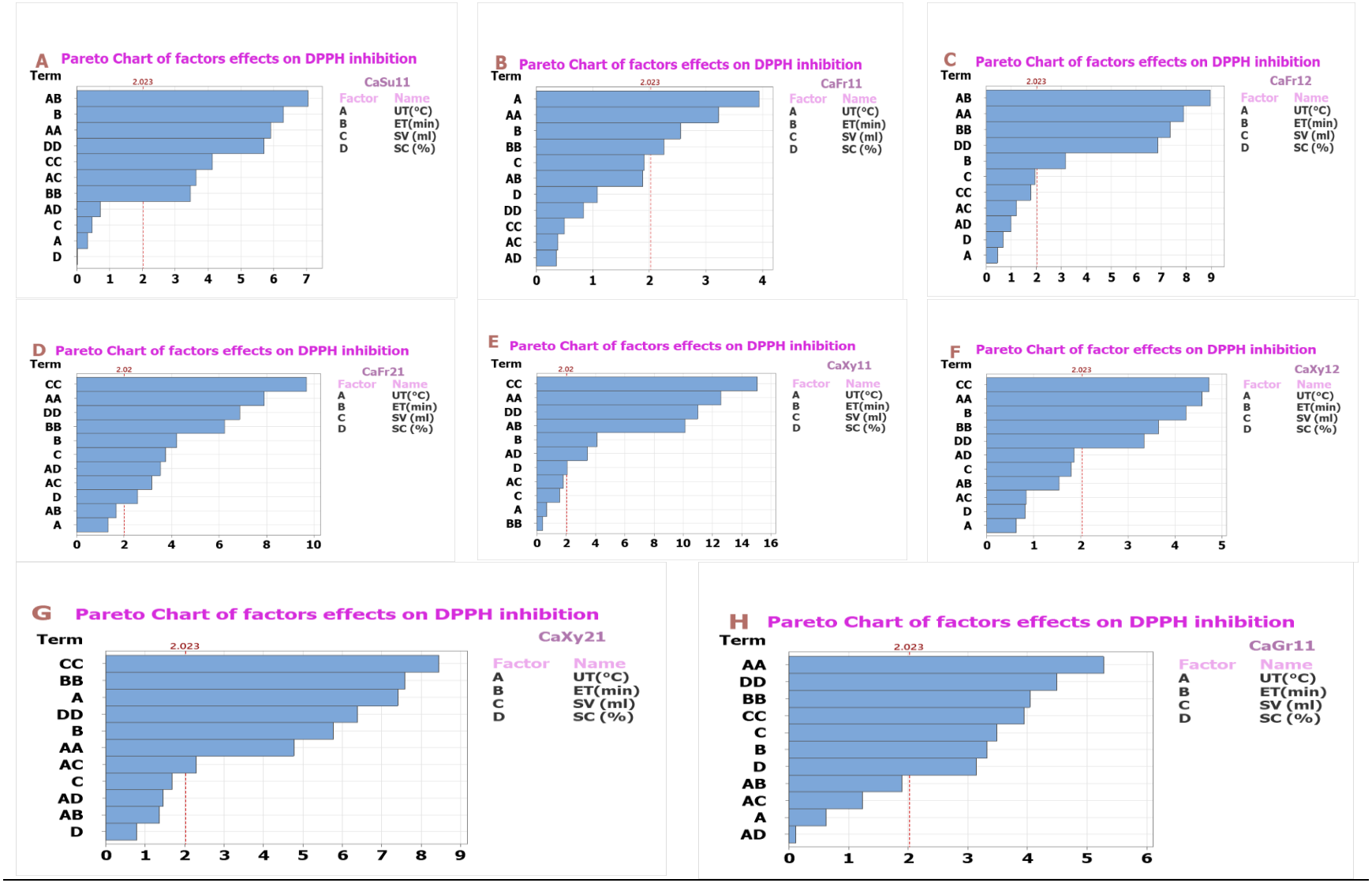


Figure 4.133 Pareto charts of factors effects on DPPH inhibition of African nutmeg peels extracted using different NADESs

Figure 4.133 contd.

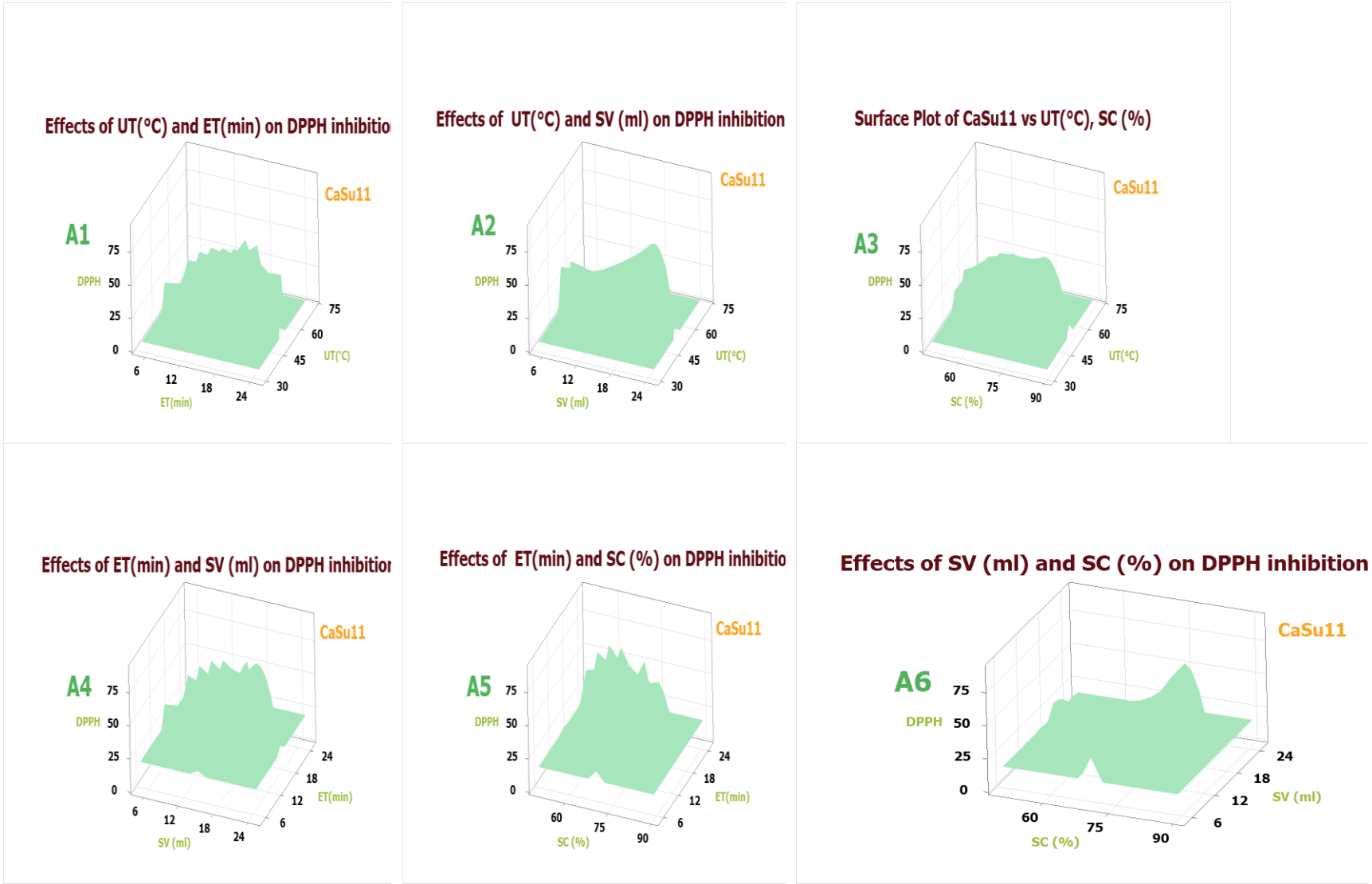


Figure 4.134 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using Casu11.

Figure 4.135Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaFr11.

Figure 4.136 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaFr12.

Figure 4.137 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaFr21.

Figure 4.138 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaXy11.

Figure 4.139 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaXy12.

Figure 4.140 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaXy21.

Figure 4.141 Three-dimensional surface plots of factros effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGr11.

Figure 4.142 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGr12.

Figure 4.143 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGr21.

Figure 4.144 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGc11.

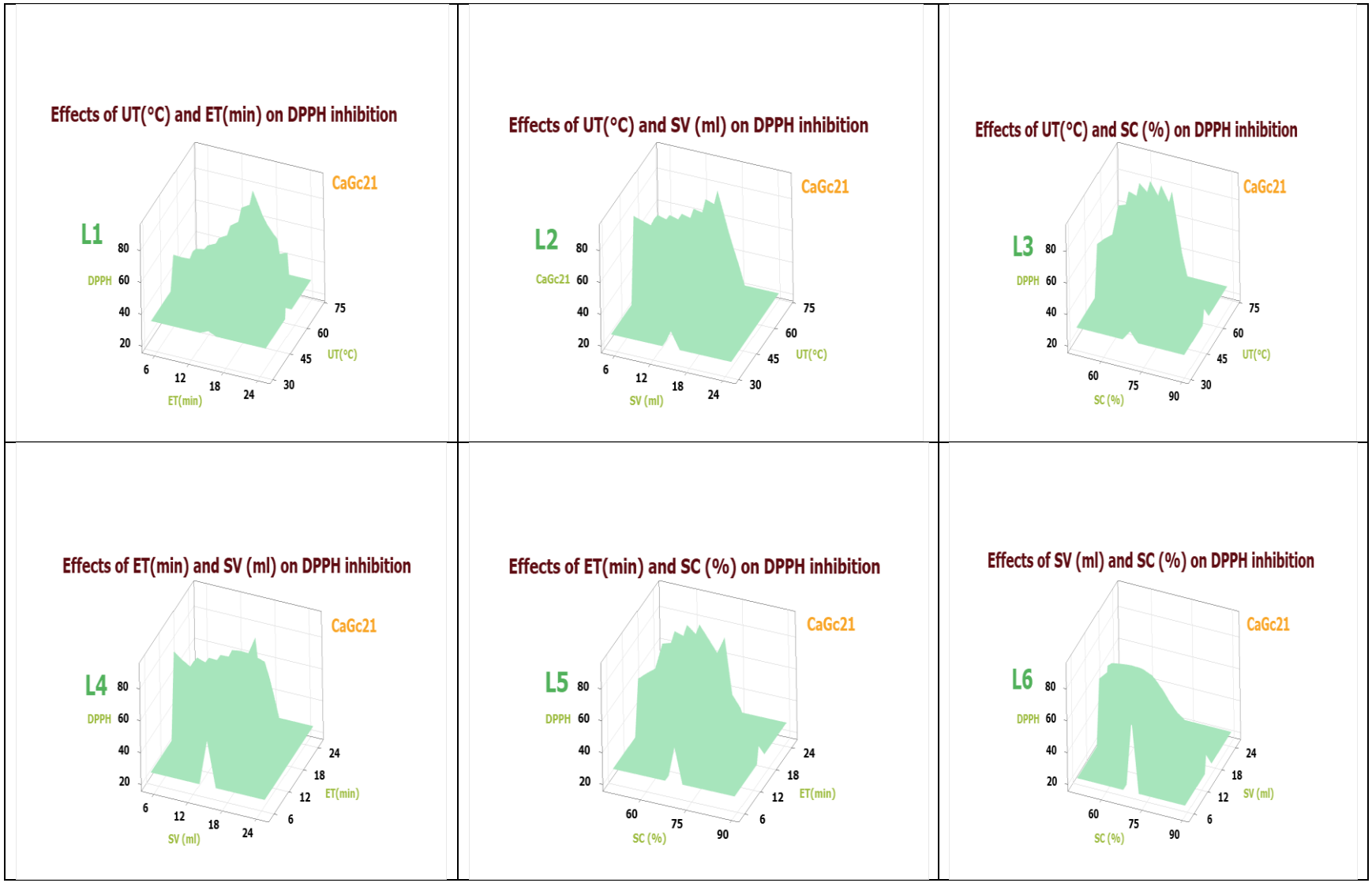


Figure 4.145 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGc21.

Figure 4.146 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGl11.

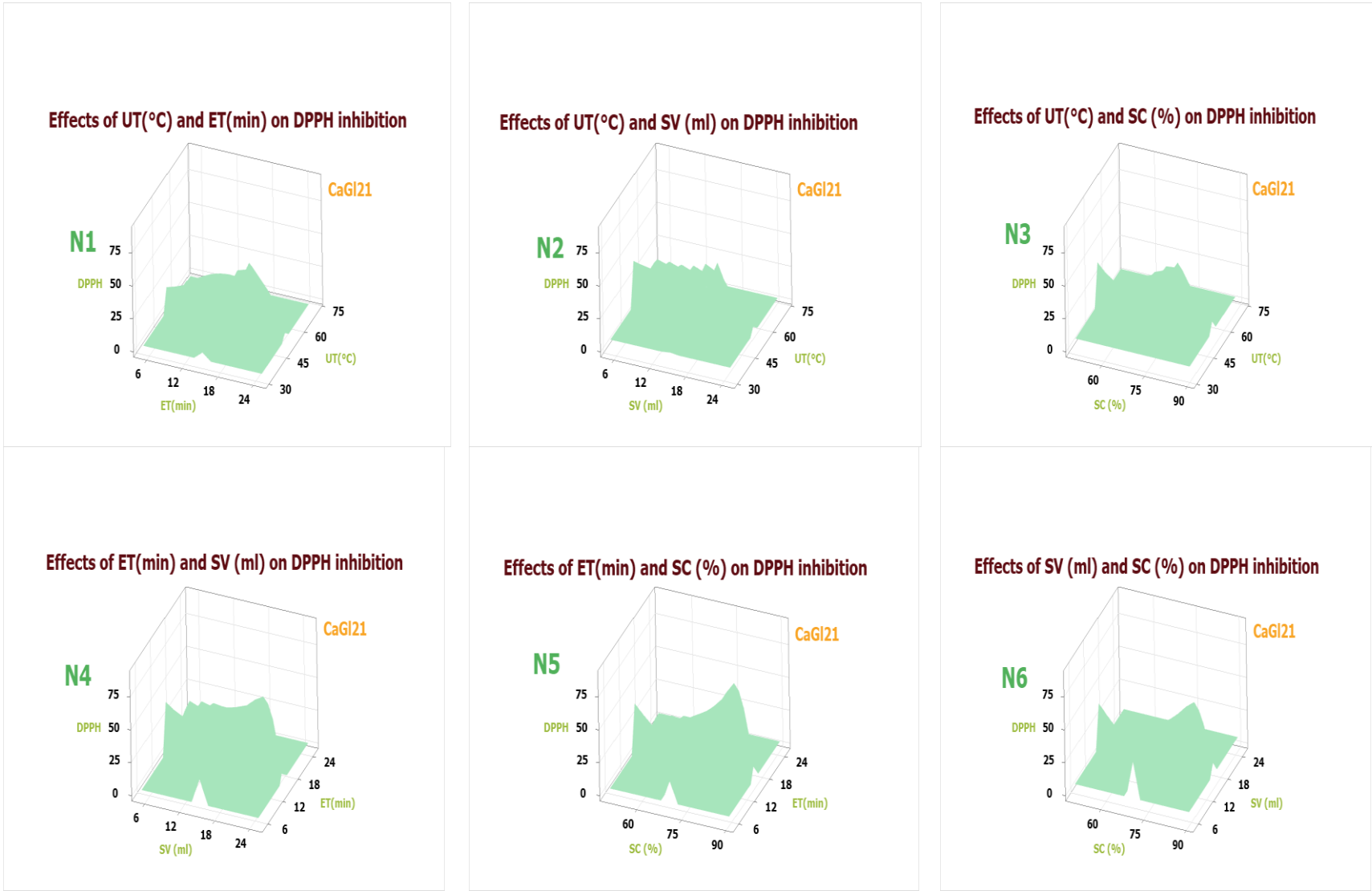


Figure 4.147 Three-dimensional surface plots of factors effects on percentage DPPH inhibition of African nutmeg peels extracted using CaGl21.

4.6.5 Optimization of extraction, validation of model, and comparison with hydro-extraction

Numeric optimization of responses was carried out by desirability function using Minitab software. Optimization was carried out with the goal set to maximize the total phenolic content, total flavonoid content, and the antiradical scavenging activity using the independent variables of temperature, time, volume, and concentration of solvents in the ranges that were used in the rotatable central composite response surface experiments. Five different solutions were calculated by Minitab software with different levels of independent variables with good desirability. The solution with maximum desirability and predicted conditions is presented in **Table 4. 14.**

Table 4.14 Maximum desirability and predicted conditions for numeric optimization of TPC, TFC, CUPRAC, FRAP, and DPPH of African nutmeg peels.

Parameters	**Factors**				**Maximum desirability**
	UT (ºc)	**ET (min)**	**SV (ml)**	**SC (%)**	
TPC	44.9495 **(45)**	5	25	90	0.993634
TFC	30	5	25	85.5556 **(90)**	0.900334
CUPRAC	30	5	25	90	1.000000
FRAP	42.9293 **(45)**	25	25	50	0.960543
DPPH	50.6061 **(50)**	16.3131 **(15)**	13.8889 **(15)**	69.3939 **(70)**	0.931252

The predicted conditions were applied to the samples, however, due to limitations of instrument, the values in bold were used in place of the actual predicted values. The Fitted responses with standard errors of fits, the experimental responses with standard deviations obtained under the predicted conditions are presented in **Table 4.15**. Water as the greenest solvent was used to compare the performance of the NADESs in this study and the results at the optimized conditions are presented in **Figure 4.148** to **Figure 4.152** for TPC, TFC, CUPRAC, FRAP, and DPPH studies, respectively.

Table 4.15 Optimized antioxidant and antiradical scavenging properties of African nutmeg peels extracts by UAE-NADESs techniques: predicted (fitted) and experimental values.

Solvents	TPC (µgGAE/g)		TFC (µgQE/g)		CUPRAC (µMTE/g)		FRAP (µMTE/g)		DPPH (%)	
	Fitted	Experimental	Fitted	Experimental	Fitted	Experimental	Fitted	Experimental	Fitted	Experimental
CaSu11	732±128	860.02±4.7^{B}	1061±373	1176.0±13^{F}	23.27±3.1	24.76±0.39^{H}	26.28±3.1	26.17±0.17^{A}	79.18±7.3	72.24±0.15^{J}
CaFr11	1269±332	1290.9±5.6^{A}	2329±427	2398.7±23^{A}	38.03±4.4	38.46±0.44^{A}	26.05±3.3	26.15±0.11^{B}	86.40±11	73.55±0.24^{I}
CaFr12	711±142	748.64±12^{C}	1449±338	1446.0±12^{C}	26.20±2.8	26.24±0.31^{F}	16.75±1.3	17.31±0.12^{G}	89.65±7.4	84.19±0.35^{F}
CaFr21	272.9±56.8	281.05±18^{L}	437.5±84.3	442.13±8.7^{L}	27.71±3.1	25.15±0.34^{G}	18.07±1.3	18.45±0.08^{E}	87.68±6.0	84.26±0.36^{F}
CaXy11	375.±39.7	365.20±11^{K}	607±124	618.27±10^{J}	28.34±2.8	24.71±0.49^{H}	18.12±1.5	19.21±0.13^{D}	81.81±4.2	64.78±0.25^{K}
CaXy12	577.1±41.5	588.78±9.4^{F}	1694±237	1777.1±10^{B}	25.96±3.0	28.92±0.53^{E}	17.11±1.7	18.13±0.11^{F}	94.20±13	97.42±0.40^{A}
CaXy21	294.8±38.9	289.76±6.7^{L}	551±112	584.85±19^{K}	28.58±3.1	29.53±0.55^{D}	15.82±1.4	16.19±0.11^{I}	85.25±6.9	64.19±0.33^{L}
CaGr11	507.7±67.7	539.76±16^{G}	621±168	633.85±20^{I}	31.72±2.7	32.29±0.52^{B}	16.41±1.0	17.04±0.09^{H}	86.43±9.2	83.55±0.25^{G}
CaGr12	748.5±90.5	754.63±7.1^{C}	828±130	869.57±12^{H}	29.92±2.9	29.89±0.32^{CD}	17.07±1.5	18.52±0.18^{E}	90.52±6.2	89.71±0.31^{C}
CaGr21	393.6±56.8	396.24±9.7^{J}	681±220	632.60±10^{I}	31.45±3.0	29.92±0.37^{C}	26.59±3.3	26.21±0.12^{C}	86.42±7.8	80.93±0.20^{H}
CaGc11	498.8±90.5	475.22±8.6^{I}	1330±417	1354.4±15^{D}	22.16±3.2	22.78±0.43^{J}	16.30±1.5	17.21±0.22^{G}	89.70±12	86.08±0.15^{E}
CaGc21	499.3±63.9	502.72±7.5^{H}	1224±251	1341.4±8.8^{E}	24.02±2.9	23.89±0.50^{I}	7.92±1.0	7.59±0.14^{M}	95.98±5.4	90.05±0.23^{B}
CaGl11	626.8±69.7	660.13±7.6^{E}	1224±149	1448.6±10^{C}	25.29±3.2	25.40±0.15^{G}	8.11±1.6	8.59±0.13^{L}	34.98±6.0	34.77±0.24^{M}
CaGl21	649.6±52.0	688.45±7.8^{D}	1003±142	1025.4±9.4^{G}	25.99±3.0	25.50±0.52^{G}	10.64±2.7	11.59±0.14^{K}	89.29±7.2	86.49±0.27^{D}
Water	-	144.34±8.0^{M}	-	589.63±11^{K}	-	22.81±0.46^{J}	-	12.07±0.14^{J}	-	11.69±0.24^{N}

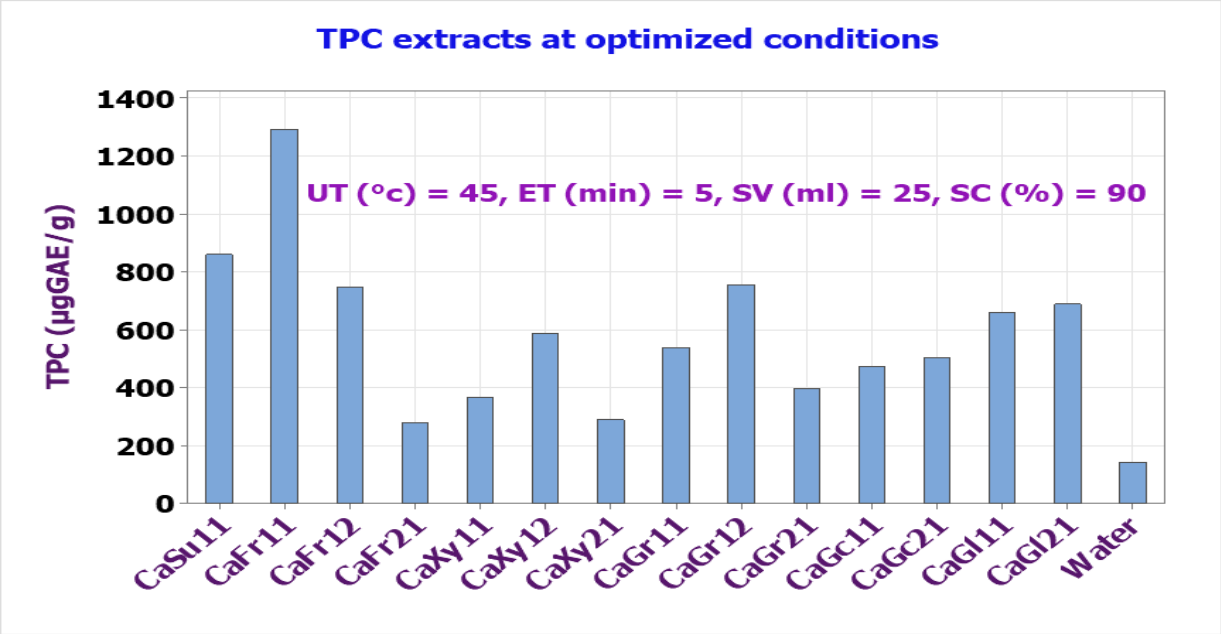


Figure 4.148 The total phenolic contents of African nutmeg peels at optimized extraction conditions with synthesized NADESs compared with water.

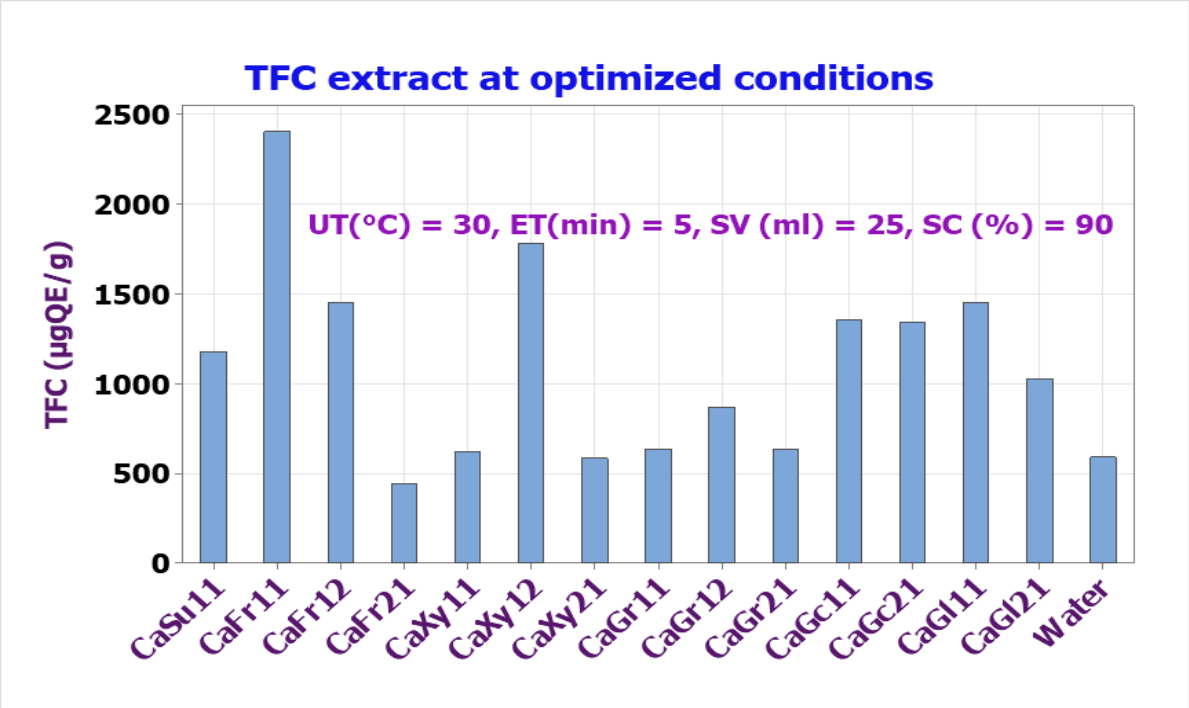


Figure 4.149The total flavonoid contents of African nutmeg peels at optimized extraction conditions with synthesized NADESs compared with water.

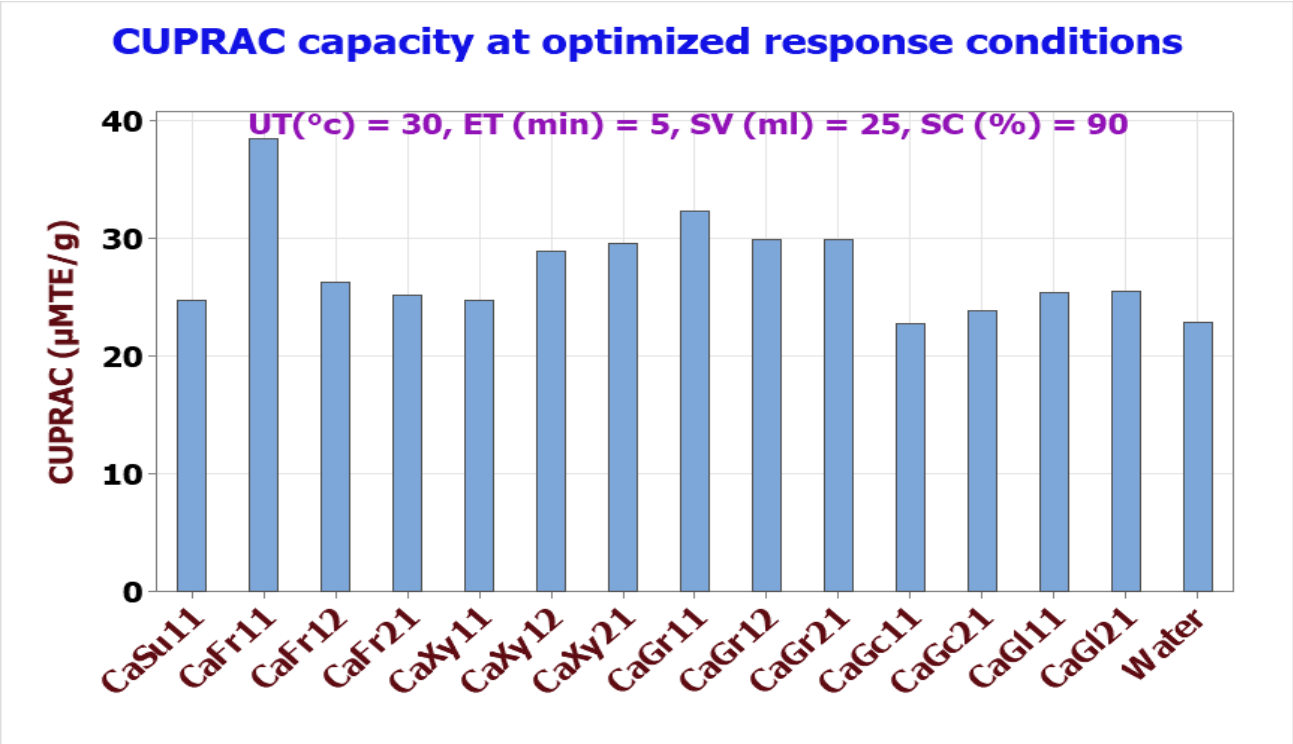


Figure 4.150 CUPRAC capacity of African nutmeg peels at optimized extraction conditions using synthesized NADESs and compared with water.

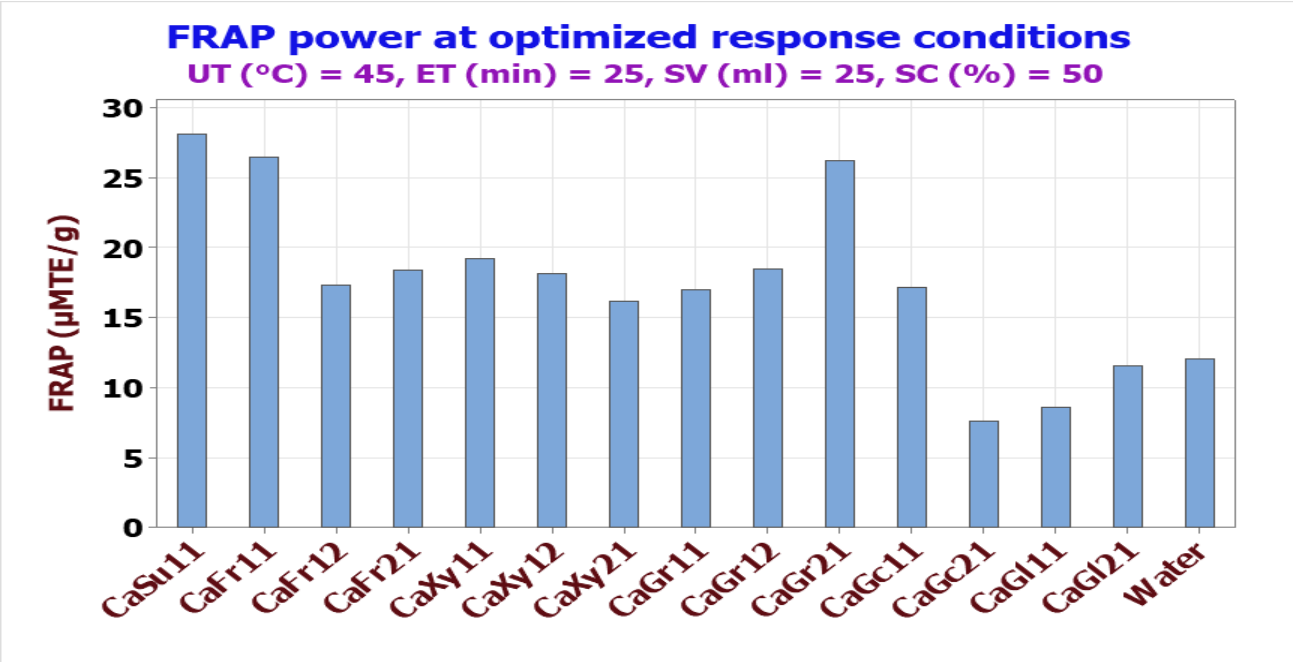


Figure 4.151 FRAP power of African nutmeg peels at optimized extraction conditions using synthesized NADESs and compared with water.

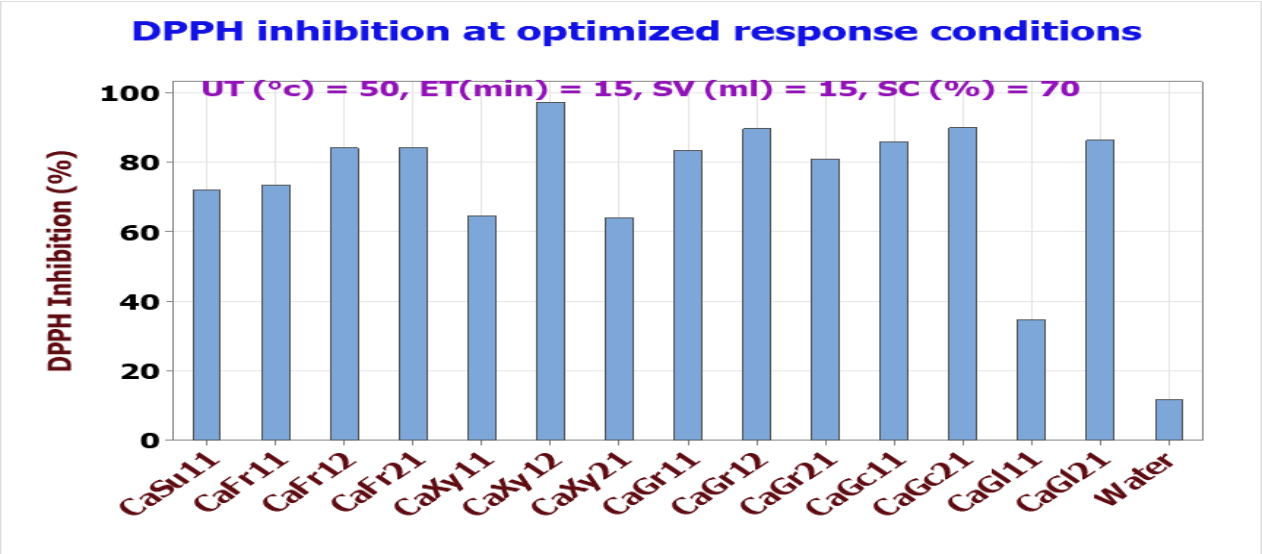


Figure 4.152 DPPH inhibition of African nutmeg peels at optimized extraction conditions using the synthesized NADESs and compared with water.

CHAPTER FIVE

DISCUSSIONS

5.1. Synthesis of natural acidic deep eutectic solvents (NADESs)

NADES is a homogeneous mixture that forms a superlattice when combined at a specific molar ratio. The joint superlattice melted at eutectic temperatures below the melting point of its components. DES formations have mostly been designed with ChCl as HBA. Most studies that used glycerol as the HBD in DES used it at molar ratios not exceeding (1:3) of the HBA[123 124]. Higher glycerol molar ratios (1:6 and 1:8) produce viscous liquids that are challenging to handle and have few practical applications in the industry [125]. The formation of a transparent liquid at a certain molar ratio suggests that the DESs were affected by the interaction of hydrogen bonding between the HBA and the HBD [126]. The freezing point of DES is lowered due to hydrogen bonding between the HBA and the HBD, resulting in a liquid form [127].

In the study, the amount of citric acid was insufficient to form appropriate hydrogen bonding with sucrose, glycine, and glucose at molar ratio of 1:2 respectively. As a result, the formed solutions solidified into white mass on cooling. At 2:1 molar ratio, the NADES formed with sucrose was extremely viscous like a gel and could not be used for extraction application and was discarded. It is therefore imperative to note that a critical factor is to establish the ideal HBA to HBD molar ratio that will produce a stable liquid-phase mixture on standing.

Heating and stirring was the primary method used by most researchers in the synthesis of deep eutectic solvents (DESs) including NADES[128 129 107 130 109 113]. Due to high energy consumption, as well as longer duration of synthesis time (between 6-24 h) in heating and stirring (HS) technique, more novel approaches are being explored. For instance, microwave [114 113 131], freeze-drying[132 133 98], rotary evaporation [133], extrusion[113] and ultrasonication[134].

Application of ultrasound to the mixture caused acoustic cavitation by generating, growing, and eventually collapse of the bubbles. As ultrasound waves were propagated, the bubbles oscillated and collapsed causing thermal, mechanical, and chemical effects. Mechanical effects include collapsed pressure, turbulence, and shear stresses, while the chemical effects include ionization of

bonds and an increase in hydrogen bonding potentials to form. The locally produced alternating positive and negative pressures caused the expansion of the mixture resulting in bond rupture and realignment. Ultrasound causes hydrolysis of water inside the oscillating bubbles leading to the formation of H^+ and OH^- that were captured in the chemical reaction by the rearrangement of HBA and HBD to form the NADESs. When cavitation is generated, OH radicals are released, that is why chemical effect is obtained in the solution.

Temperature and time played significant roles in ultrasound-assisted synthesis the NADESs. At 50ºc temperature, the HBA and HBD were unable to form the desired solvent at different time intervals. At 90ºc, the formed solvents with sugar based HBDs were very dark in colour which was suspected to be the effects of caramelization of the sugars. The caramelization effect was also observed when the temperature was 70ºc and the time prolonged above 80 min. In their study with choline chloride based NADES, Hsieh *et al* [134] employed ultrasound-assisted technique with frequency of 40kHz, 300 W power, and synthesis time of 5h. The temperature was not controlled but measured to be 50ºc at the end of the synthesis time. Based on their findings, 50ºc could also be used for the synthesis of citric acid based NADESs but will require such a long time. Therefore, thermal effects in addition to the cavitation and mechanical effects, significantly influence ultrasound-assisted synthesis (UAS)[135], making temperature and time important variables UAS of NADESs. While extraction studies utilizing the properties of ultrasonic waves exist in volumes, there is a dearth of knowledge on the use of ultrasonication for the preparation of NADES.

5.2 Physical Properties of NADESs

The current study shows that NADESs can be prepared and synthesized from citric acids (Ca), sugars, amino acids, and sugar alcohols. Ca + Su (sucrose) mole ratio 1:1; Ca + Fr (fructose) mole ratios (1:1, 1:2, and 2:1); Ca + Xy (xylitol) mole ratios (1:1, 1:2, and 2:1); Ca + Gr (glycerol) mole ratios (1:1, 1:2, and 2:1); Ca + Gc (glycine) mole ratios (1:1 and 2:1); and Ca + Gl (glucose) mole ratios (1:1 and 2:1) were synthesized in the study. The water activity of NADESs in different proportions were determined at 25°c, which ranged from 0.71 to 0.83 (**Table 4.2**). With the increase of Ca content, the water activity of NADES decreases slightly, which indicates that the carboxyl group of citric acid has stronger hydrophilicity than hydroxyl group, so it has little effect

on the water activity of NADES. The basic physical properties of NADESs at 25°c were measured, including density, viscosity and pH, to provide reference for the application of the synthesized NADESs to extraction of bioactive compounds from plant materials. The densities of NADESs were shown in **Table 4.2** and can be seen to range from 1.2818 to 1.3768 g/cm^3, which is greater than the density of water.

5.2.1 Density

The density of solvent is critical for its diffusion and miscibility with other liquids. The density of NADES is crucial in chemical processes involving extraction, fluid mechanics and mass transfer. The high density of NADES may be advantageous for phase separation, even though it may impact on handling and mixing processes. The densities of the synthesized NADESs at 25ºC are presented in Figure 4.1 and shows that the densities of fructose-based NADES are higher than those of glucose irrespective of molar ratios of the HBD. The densities obtained in this study are similar with those obtained from choline chloride-based NADESs (1.00–1.35 g/cm^3)[85 136 137], and glycolic acid based NADESs (1.3528-1.3741 g/cm^3)[112]. NADESs have higher densities than water due to their varying degrees of hydrogen bonding in the formulation [138 139]. The arrangement and packing of DES molecules significantly impact their density [140]. According to Abbott et al., DES mixtures like ionic liquid counterpart, contain holes whose size controls the density of the solvent [141]. NADESs formed from sugars (sucrose, fructose, and glucose) had higher densities than those formed from sugar alcohols (xylitol, and glycerol) indicating that the HBD functional groups substantially impacted the properties. Although the densities of DESs decreases dramatically as the chain length of HBDs increases in the case of choline chloride-based NADES[136 137], the contrary was observed in this study.

5.2.2 Water activity

Water activity is an important and critical thermodynamic property used to predict shelf-life of food products, microbial activity, microbial growth, solute to solute interactions, etc. It is defined as the ratio of the fugacity of water in a system at a given temperature to the fugacity of pure water at the same temperature. In food products, water activity can be manipulated by addition or

reduction of electrolyte solution to achieve the desired goal[142]. Water activity also provide treasured data with respect to solute-to-solute and solute-to solvent interacts, an important factor for extraction processes [143]. In the present work, the water activity of the synthesized NADESs were measured with a digital water activity meter at 25°c and the result presented in **Table 4.2.** There is a paucity of information in the literature with regards to water activity of NADESs, however, it could be seen from data obtained about some ternary mixtures of choline chloride based NADESs with sugars and water that the present NADESs have lower water activity than those ternary mixtures. For example, Behboudi, *et al*., provided water activity data for choline chloride: urea + sucrose+ water, choline chloride: ethylene glycol + sucrose + water, and choline chloride: glycerol +sucrose+ water as 0.942-0.988, 0.949-0.974, and 0.98-0.982 respectively [144]. Their result was far too high to be compared with the result obtained in the current study: 0.71-0.83. The discrepancies in the results could be explained from the dilution effects of water on the ternary mixtures of water and NADESs as against the concentrated NADESs in the present work. In the present study, it could be discovered that water activity is influenced by the molar ratios of the HBD in the structure, **Figure 4.2**. The higher the ratio of the HBA in the NADESs structure, the lower the water activity, hence, CaFr11, CaXy11, CaGr11, and CaGl11 have higher water activities than CaFr21, CaXy21, CaGr21, and CaGl21 respectively. This observation could be used in tuning the synthesis of NADESs for a given purpose, such as application in formulation of preservatives.

5.2.3 Viscosity

Dynamic viscosity measures the resistance of fluid to flow and the molecular bond strength of the fluid. The viscosities of the NADESs for all functional groups of HBD at different molar ratios are shown in **Table 4.2**. The viscosities obtained in this study were 0.0131- 0.3545 pa.s, which are similar to those obtained by Sazali *et al*., (0.235-0.453 pa.s, using choline chloride: glycerol; and 0.04-0.06 pa.s, using choline chloride: lactic acid)[145], and Liu *et al* (0.207-2.66 pa.s using choline chloride: glycerol at the same molar ration)[146]. Similarly, Francisco *et al*., obtained choline chloride: lactic acid viscosities of 0.3–0.7 Pa.s at 1:1.3–1:5 mole ratios [147]. Kang *et al*, also obtained similar viscosities for different molar ratios of glycolic acid: l-proline based NADESs[112]. Due to their dense hydrogen-bond networks, NADESs have higher viscosities than water, molten salts

and other molecular solvents. This is due to inhibiting free mobility species within the DES[148]. Higher viscosities are also caused by electrostatic interactions, van der Waals forces, ion sizes and void volumes. In this study, the role of HBD chemical structure and functional groups in the properties of NADESs is demonstrated. Carboxylic acid and hydroxyl groups, in addition to the alkyl chain length, affect viscosity, with more hydroxyl groups and longer hydrocarbon chains resulting in higher viscosities[149] as can be seen in **Figure 4.3**. Alcalde *et al*., observed that water dilutes the hydrogen bonding between choline chloride and lactic acid, but only at concentrations greater than 10%, accordingly, increasing the HBD molar ratio will increase the viscosity[150].

5.2.4 PH

The pH of NADESs is very important for chemical analysis, extraction processes, catalysis, biological activity and metal treatment. The pH of NADES can affect process engineering, as it involves operational conditions and materials of construction[151] [145]. The pH is dictated by the acidity and basicity of HBA and HBD and their combined acidity and basicity [152]. The pH values of the synthesized NADESs at 25°c are shown in **Table 4. 2**. The pH of all the synthesized NADESs are below pH 2 except CaGc11 and CaGc21 whose pH values are above pH 2. It should be noted that CaGc11 (citric acid: glycine, 1:1), CaGc21 (citric acid: glycine, 2:1) are the only samples that were synthesized using amino acid as HBD. Amino acids have fewer hydroxyl group in its' molecular structure when compared to sugars and sugar alcohols. The limited number of hydroxyl groups in the structure of Gc as HBD may have influenced the resultant NADESs to be less acidic, that is higher pH value. There is significant difference between the pH of CaFr12 (citric acid and fructose, 1:2) and CaXy12 (citric acid: xylitol, 1:2). This may be explained by the similar numbers of hydroxyl groups in the respective molecules of CaFr12 and CaXy12.

The pH is also affected not only by the HBD groups but also by the molar ratio of HBA to HBD. For instance, the pH values of CaFr12 (citric acid: fructose, 1:2), CaXy12 (citric acid: xylitol, 1:2), and CaGr12 (citric acid: glycerol, 1:2) respectively were all higher than those of CaFr21 (citric acid: fructose, 2:1), CaXy21 (citric acid: xylitol, 2:1), and CaGr21 (citric acid: glycerol, 2:1) respectively **Figure 4.4**. This may be explained using the hole theory of Abbott, *et al*.,[141]. In this case, there are more free hydrogen bond donating groups from two moles of fructose, xylitol, and

glycerol that need to be accepted by the HBA but couldn't because there are not a free bonding sites from the one mole of the citric acid thereby creating more acidic environment.

Overall, DES prepared using organic acids either as a HBA or HBD tend to have extremely high acidity because of HBA: HBD hydrogen bonding [140]. In their study, Skulcova *et al* [152] obtained pH values from 4.1- 4.5 using choline chloride and glycerol at 1:2 M ratio and at temperatures from 25ºC to 60ºC. The pH of DES synthesized with choline chloride and lactic acid varied between 0.99 and 1.8 for molar ratios of 1:5 and 1:10 under similar conditions [152]. The pH of choline chloride: lactic acid DES and choline chloride: glycerol DES were significantly impacted by the type of HBD used, with the first DES containing an acid and the second containing an alcohol [151].

Lemaouni, *et al* suggested that the trend of pH with molar ratios caused by functional group addition to HBDs is not always correlated for some DESs, instead, molecular-level interactions between HBA and HBD significantly affect the pH of DESs[153]. The pH changes of DESs with different molar ratios are significant because they indicate differences in the nature and applications of DES. Studies on DES pH and their dependence on temperature with changes in HBD have been elucidated by several scholars. For example, Skulcova, *et al* showed that the pH of choline chloride: fructose decreased as temperature increased[152]. Kareem *et al*, showed that DESs using triphenyl phosphonium salt derivatives produced slight increase in pH with temperature when glycerol was used as the HBD [154]. Prior knowledge of the acidity/basicity of DESs based on HBA and HBD choices and their molar ratios via pH and temperature dependence is critical, particularly in algal fractionation, which involves diverse compounds, such as proteins, polysaccharides, cellulose and lipids. For example, algal solubilization is favoured at a pH of less than 7 [155]. A pH below 2 did not affect hemicellulose solubility but enhanced cellulose solubilization[156]. These studies have established the significance of HBD selection and its molar ratios, especially in algal biomass-derived production.

5.3 Storage Stability of NDESs

The physical properties of the synthesized NADESs stored in a desiccator at 25°c for 90 days is presented in **Table 4.3** and depicts that the NADESs were stable. The result agrees with Zhang *et al* who studied the stability of choline chloride carboxylic acid-based DES prepared using three methods of heating and stirring, rotary evaporation, and freeze drying techniques, and observed

that the stability of DESs is dependent on the preparation method used, the type of HBA/HBD, the ratio of HBA/HBD, and the volume of impurities in the preparation[111]. According to the authors, when the HBA/HBD molar ratio was 2:1, many of the DESs from the heating method were easily converted into crystals. They also noted that choline chloride-glycolic acid and choline chloride-pyruvic acid with a molar ratio of 1:1 show poor physical stability indicated by the appearance of birefringence under the microscope. DESs formed by choline-chloride-glycolic acid, choline-chloride-lactic acid, choline-chloride-pyruvic acid, choline-chloride-malonic acid, choline-chloride-citric acid, or choline-chloride-ketoglutaric acid at 1:2 molar ratios remained in liquid form irrespective of preparation methods. However, only choline chloride-glycolic acid, choline chloride-pyruvic acid, and choline-chloride-lactic acid remained stable at the molar ratio of 1:5. Furthermore, they suggested that the stability difference among DESs may be influenced by the number and ability of the acid to provide hydrogen bonds. Accordingly, due to the involvement of temperature, pressure, and moisture brought by different methods, the final mixtures produced by different preparation methods may not be the same composition and may affect the physical stability of the solvents. They stated that the stability of DESs prepared by rotary evaporation was higher than those prepared by the freeze-drying or heating methods because the residual water dissolved in the DESs prepared by rotary evaporation led to a larger melting point depression, and thus increased stability. With reference to methods, they found the stability of DESs prepared by heating was similar to those prepared by freeze-drying, except in choline-chloride-glycolic acid (1:1), choline-chloride-glycolic acid (2:1), and choline-chloride-pyruvic acid (1:1) where there was slight higher water content in those DESs prepared by freeze-drying methods than those prepared by the heating method[111]. Residual water as impurity has a greater influence on the physical stability of the solvent DES because of significant shifts in the mole fraction, thereby affecting the molecular interactions.

Gomez *et al* studied the stability of lactic acid−glucose, citric acid−glucose, and citric acid-fructose based NADESs at different mole ratios using microwave assisted technique, and the conventional heating and stirring method. They concluded that the NADESs synthesized by microwave was more stable than those synthesized by the heating technique[113]. Therefore, it may be concluded that the novel synthesis methods produced more stable solvents because they contain less

impurities in the form of moisture, as well as the lower temperature and shorter time of synthesis with the novel techniques.

5.4 Instrumentation and Characterization

The charge delocalization of HBA and HBD occurring through hydrogen bonding is responsible for the formation of DESs. The NADESs prepared by combining citric acid with glycine shows changes in the FTIR spectra when compared to others indicated by a second peak following the OH peak identified as amide stretching (3300-3200 cm^{-1}). **Figure 4.5** presents the spectra of the NADESs (CaSu11– CaGl21) and shows the absence of intensive OH stretching bands at wavenumber between 3800 and 3400 cm^{-1}, indicating a very low water content solvent [157]. However, the NADESs FTIR spectra showed OH stretching bands at wavenumbers (3305; 3327; 3287; 3375; 3321; 3298; 3385; 3358; 3286; 3367; 3373; 3392; 3321; 3371 cm^{-1}) for CaSu11; CaFr11; CaFr12; CaFr21; CaXy11; CaXy12; CaXy21; CaGr11; CaGr12; CaGr21; CaGc11; CaGc21; CaGl11; and CaGl21 respectively. According to the literature, changes in stretching vibration of NADES at the wavenumber of 3300 cm^{-1} are the main indication of hydrogen bonding formation between hydrogen bond acceptor, and hydrogen bond donor [157] [157]; [158]; [159]. These results confirm the synthesis of NADES with the increase and strengthening of hydrogen bonds. The presence of characteristic functional groups indicated in FT-IR spectra were OH (3500–3200 cm^{-1}), CH (3000–2500 cm^{-1}), RCOOR (1710–1730 cm^{-1}), C=C allyl stretching (1615–1682 cm^{-1}), =CH**2** bending (1416–1485 cm^{-1}), C–O (1112–1000 cm^{-1}), C=C allyl wagging vibration and =CH**2** wagging vibration (1000–727 cm^{-1}), groups. The results obtained were in agreement with the result obtained by Silva *et al*.[159], and Rashid *et al*., [160] with choline chloride based NADESs. NADES prepared by a combination of individual components reveals alteration in the infra-red spectra when differentiated with the separate components. The broader peaks seen at 3000–3500 cm^{-1} accords to more O–H bond formation between individual components in NADES. According to [158] changes in the band stretching between 3000 and 3500 are the main evidence of hydrogen bond formation between the individual components, which confirms the synthesis of NADES. The FT-IR spectra of CaGc11 and CaGc21, show two distinct functional peaks at 3373 cm^{-1} to 3392 cm^{-1} indicating OH stretching from the citric acid and 3207 cm^{-1} to 3230 cm^{-1} indicating amide N-H bond from amino acid glycine, respectively. The number of bonds in each of the NADESs formed

are indicated by the number of peaks in each individual solvent, however, the most important indication of the formation of eutectic solvent is the presence of H-bonds in the molecule. In the present study, the presence of H-bonds indicated by peaks feature prominently among all the synthesized solvents, an indication of the formation of NADES.

5.5. Chemometric Analysis

Chemometrics is the branch of chemistry concerned with the analysis of chemical data and extracting information from data, ensuring that experimental data contain maximum information from the design of experiments. It is how to get chemically relevant information out of measured chemical data, and how to represent and display this information, and how to get such information into data. Chemometrics is also the discipline of analytical chemistry concerned with the application of statistics, mathematics, and other methods of formal logic to the generation and analysis of chemical data. It is the chemical discipline that uses mathematical, statistical and other methods employing formal logic (i) to design or select optimal measurement procedures and experiments, and (ii) to provide maximum relevant chemical information by analyzing chemical data. In the study, chemometric analysis of the principal components was performed by Minitab and shows the similarities and differences among the groups as well as the relationship between the variables (physical properties and FTIR peaks)[161 162]. **Figure 4.6** demonstrates the loading plot of the physical properties and FTIR peaks of the solvents. Variations in the data set were described by principal components (PCs), where generally two PCs (PC1 and PC2) are sufficient. The model illustrated total variation of 98.99% (25.81% and 73.18% for PC1 and PC2, respectively). The score plot of PCA of the first two components showed a separation of the solvents into four main groups **Figure 4.7** with one solvent depicting an outlier characteristic, and one other solvent that could not fit into any of the four groups. Group 1 at the top left of the quadrant comprise of CaGr11, CaFr21, and CaXy12. Group 2 at the top right contains CaGl21, and CaXy11. Group 3 at the bottom right has the highest number of solvents, CaFr12, CaGr21, CaGl11, and CaSu11, while group 4 has CaFr11, CaXy21, and CaGr12. Two striking observations were the inclusion of each of the HBD molecules at different mole ratios in different groups except the solvent developed from glycine as HBD. While CaGc21 displays an outlier characteristic, CaGc11 almost fit into all

the groups. The observation may be explained as aligning with the tunability of NADES. Each group may have similar performance attributes such as good extraction capacity, more hydrophilicity, etc. However, this conclusion needs to be investigated further through application of the solvents to different processes.

5.6 Application of NADESs for extraction of bioactive compounds

The synthesized NADESs were applied in ultrasound-assisted extraction of bioactive compounds (polyphenols and flavonoids) from the peels of African nutmeg (*Monodora myristica* (Gaertn.) Dunal*)*. High-intensity ultrasound has been applied as an economically feasible technology for the extraction of thermolabile compounds[56]. Ultrasound-assisted extraction has been efficiently used in the extraction of total phenolic compounds from plants including fruits and vegetable materials[163]. A fast rise in temperature of the reaction system was observed when long extraction time was used. Therefore, it is extremely important to pay attention to the temperature factor during the extraction process to avoid thermally degrading the extracts[55].

In combination with ultrasonication, different types of NADESs have been synthesized and used in extraction of bioactive compounds from plants, animals, algae, and microbial biomass in recent years[129 164 165 166 167]. In the present work, a comprehensive study of extraction of bioactive polyphenols and flavonoids using UAE-NADESs was undertaken, and the antiradical scavenging potential elucidated.

5.6.1 Factorial experiments for UAE-NADESs extraction of bioactive compounds from African nutmeg peels.

The extraction of TPC and TFC compounds from African Nutmeg peels was carried out by many factors at a time (MFAT) experimental technique. Specifically, a 2^4 fractional factorial experiment with eight (8) conners and two (2) center points was used for the process. The experiments were replicated three times at each of the points for a total of 30 experimental runs. MFAT design was chosen over OFAT (one factor at a time) for this study because, there are obvious advantages the former has over the latter including simultaneous determination of interactions effects, conduct of fewer experiments to elucidate causality, reduction of experimental time, experimental conditions

as true representation of actual process, reduction of cost, etc. The MFAT model gave 85-99% adequacy for TPC, and 99-100% for TFC (**Table 4.5**). The significant impact of temperature, solvent concentration, and ultrasound application time on the extraction efficiency, as revealed by the MFAT analysis, underscores the necessity of optimizing these parameters to achieve the maximum yield of phenolic and flavonoid compounds. This optimization aligns with recent studies demonstrating the importance of such parameters in enhancing the extraction process. Recent advancements in the field suggest the integration of in silico models and response surface methodology (RSM) for further optimization, aligning with the observations on solvent behaviour and the presence of significant curvatures, indicating a potential for even finer tuning of the extraction process [168 169]. The high degree of model adequacy may be linked to the capture of all necessary components (linear, interactions, curvatures, and errors) inherent in the process, unlike in the case of OFAT, which examines only the linear effects of the model. Accordingly, all the parameters (TPC, TFC, CUPRAC, FRAP) displayed linear plus interaction regression model (**Tables 4.6 and 4.8)** thereby soliciting further validation with a more robust design such as response surface methodology (RSM). Furthermore, the analysis of variance pareto charts (**Figures 4.8-4.11**) show all factors (temperature, time, volume, and concentration) as statistically significant among all the NADESs, with a nonsignificant lack of fit with respect to pure error. UAE experiments in the literature have been designed and executed using the OFAT technique [170 171 172 173 174 175 176 177], possibly because the OFAT design is simple to design and execute. However, the reliability and accuracy of the outcome of the OFAT cannot be compared with those of an MFAT experiment.

5.6.1.1 Model performance on extraction of polyphenols and flavonoids from African Nutmeg peels

Antioxidants can slow or prevent the oxidation process. These substances can significantly slow or inhibit the oxidation of easily oxidizable substances even at low concentrations. Phenols and polyphenolic compounds, such as flavonoids, are widely found in many food products derived from plant sources, and they have been shown to possess significant antioxidant activities (AOA). Phenols have also been implicated in the survival of plants under extreme conditions. Consequently, the presence of phenolic compounds in the extracts suggested their important role in the plant. Several studies have successfully correlated the phenolic content with AOA[178]. The

findings, particularly the enhanced extraction efficiencies and antioxidant activities observed under the multifactorial conditions, further corroborate the critical role of phenolic and flavonoid compounds in contributing to the AOA of African Nutmeg peels, emphasizing the potential of NADESs in extracting these bioactive compounds [179]. The phenolic and flavonoid contents in the extracts indicate that African Nutmeg peels are a rich source of phenolic and flavonoid compounds. Additionally, the synthesized NADESs are excellent solvents for the extraction of phenolic compounds and TFCs from African Nutmeg peels. The maximum flavonoid content was found in the extract of CaGc11 (897.3 µgQE/g), while the minimum flavonoid content was extracted in CaXy11 (172.1 µg QE/g). These values are much greater than those obtained from extracts from other wastes, such as apple pomace and grape pomace [180 158 115 181], using choline chloride-based NADESs.

5.6.1.2 Effects of experimental factors on polyphenols and flavonoids extraction from African nutmeg peels extracts using NADESs.

The effects of the experimental factors on TPC and TFC extraction (**Figure 4.13 and Figure 4.14**) show that the NADESs extract higher phenolic compounds under different conditions. Sugar based NADESs (CaSu11, CaFr11, CaFr12, and CaFr21), except glucose-based ones (CaGl11 and CaGl21) favour lower temperatures, longer times, larger volumes, and lower concentrations (**Figure 4.13D) (**UT=40°C, ET=20 min, SV=20 ml, SC=60%). Glucose-based NADES, along with glycerol-based ones (CaGr11, CaGr12, and CaGr21), as well as glycine-based NADESs (CaGc11 and CaGc21) prefer higher temperature, shorter time, smaller volume, and higher concentration (**Figure 4.13F**) (UT=60°C, ET=10 min, SV=10 ml, SC=80%), while xylitol-based solvents (CaXy11, CaXy12, CaXy21) prefer something in-between (**Figure 4.13B**) (UT=40°C, ET=10 min, SV=20 ml, SC=80%) for higher TPC extraction**.** On the other hand, the TFC extractions show similar variability among the NADESs. For instance, while glycine-based (CaGc11, CaGC21) and fructose-based (CaFr11, CaFr12, and CaFr21) were in favoured of lower temperature, and larger volume (**Figure 4.14B**) (UT=40°C, ET=10 min, SV=20 ml, SC=80%), sucrose-based and glycerol-based NADESs settled for higher temperature and smaller volume (**Figure 4.14F**) (UT=60°C, ET=10 min, SV=10 ml, SC=80%), glucose-based (CaGl11 and CaGl21) depicted entirely different scenarios. CaGl11 favors (**Figure 4.14G**) (UT=60°C, ET=10

min, SV=20 ml, SC=60%) and CaGl21 goes for (**Figure 4.14H**) (UT=60°C, ET=20 min, SV=10 ml, SC=60%). NADESs.

The significance of the experimental factors on the extraction of phenolic compounds from African Nutmeg plants showed that each of the NADESs was significantly affected by different factors and factor combinations and are depicted by contour plots shown in **Figures 4.15 -4.28** for TPC, and **Figures 4.29-4.42** for TFC, respectively, and found to be statistically significant ($p < 0.05$). The independent variables UT, ET, SV, and SC had mixed effects on each of the NADESs. Several factors were negatively correlated with the TPC in some solvents but had almost no effect on others. For example, UT was negatively correlated with CaFr11 but had almost no effect on CaSu11, CaFr12, or CaFr21. In addition, the interaction between UT and SC was significant for all the tested NADESs except for CaGc21. NADESs are more viscous than most conventional solvents, such as water, possibly because their extraction efficiency improves with temperature. A higher temperature will increase the kinetic energy of the solvent, thereby allowing it to penetrate the sample matrix to release the molecules of interest. A higher temperature will also tend to improve the solvation capacity of the solvent. The extraction of TPC and TFC from plants and other food wastes by other researchers using deep eutectic solvents and ultrasonic techniques was considered to compare the results from the current study. For example, Ahmad *et al*. obtained a TPC of 53.6-87.01 µgGAE/g from coffee beans using lactic acid-sucrose-based NADES and ultrasonication[182], whereas 229.7-311.5 µgGAE/g were obtained from African nutmeg peels using citric acid-sucrose-based NADES and ultrasonication. In the case of Ahmad *et al*., the authors used the OFAT technique with the extraction temperature held constant at 40°C, extraction time at 15 min and extraction solvent at 10 ml. The authors did not report on the concentration of the solvent. The experimental conditions employed by Ahmed *et al* maybe inadequate or African nutmeg peels samples may contain higher amount of phenolics than coffee beans or citric acid-sucrose based NADESs has better extracting power than lactic acid-sucrose based NADESs. Any of the above conditions could explain to lower value of phenolics from Ahmed *et al*, requiring further investigation which is outside the scope of current study. Oktaviyanti *et al*. performed TFC extraction from Javanese Ixora plant with ultrasonic assistance using various DESs. They reported a threefold increase when employing the choline chloride-oxalic acid based DES combination compared to ethanol derived organic solvents[183]. In a comparative study, Zheng *et al*. evaluated

flavonoid extraction from millet bran using an ultrasonic-assisted DES and conventional ethanol extraction. One study revealed that the TFC yield was twice as high when using green technology and green solvents[184]. In a study of DESs prepared with citric acid: malic acid: water (1:1:10), the TFC values of the persimmon pulp were determined, and the value was calculated as 2.5 mg QE/g[185]. Choline chloride-based solvents formed from 10 different plant varieties were used to obtain TFCs from yellow scale plants. The maximum efficiency was obtained when acetic acid was used in combination with HBD[186]. Furthermore, similar to the current research, the positive impact of extending the sonication time on the TFC yield was reported by Xu *et al*. in a study involving lemon peels [123]. The absence of any extraction studies using DESs related to African nutmeg waste in the literature has demonstrated the originality of this study. Besides, the observations in this study were in agreement with several other studies employing UAE-NADESs in extraction of phenolic and flavonoid compounds from other sample matrices[187 179 158].

5.6.1.3 Effects of experimental factors on antiradical scavenging activity of African nutmeg peels extracts using NADESs.

The effects of the experimental factors on antiradical scavenging potentials of African nutmeg peels measured with CUPRAC and FRAP techniques shows that antiradical power of African nutmeg peels is highly influenced by the concentration of the NADESs. The antiradical scavenging activities of the extracts determined by the CUPRAC and FRAP method followed similar patterns in comparison with extraction of phenolics, therefore, higher CUPRAC and FRAP activities were observed under low temperatures. However, while CUPRAC activities requires higher concentration and shorter time, FRAP action was enhanced with lower concentration but longer time as shown **Figure 4.43B** (UT=40°C, ET=10 min, SV=20 ml, SC=80%) and **Figure 4.44D** (UT=40°C, ET=20 min, SV=20 ml, SC=60%) for CUPRAC and FRAP, respectively. Considering these observations, it is evident that further exploration into the tunability of NADES and the application of advanced optimization methodologies could significantly contribute to the refinement and enhancement of ultrasound-assisted extraction processes. Such advancements not only promise to elevate the efficiency and sustainability of extracting valuable phytochemicals

from plant materials but also offer a pathway towards the development of green extraction technologies. Factors effects were further investigated and observed that the factors and their interactions follow the same pattern in CUPRAC and FRAP as they do in TPC and TFC interaction thereby validating the experimental model. The factors effects for CUPRAC and FRAP depicted with contour plots are shown in **Figures 4.45-4.58** and **Figures 4.59- 4.72** respectively for the 14 synthesized NADESs used in the study.

5.6.1.4 The behaviour of NADESs at different experimental conditions.

The use of NADESs responsive to ionic strength for sustainable extraction of bioactive molecules from plants highlights an innovative approach that was mimicked in this study, potentially enhancing the extraction efficiency and environmental sustainability of the process. The behaviour of the solvents (**Figure 4.12**) used for the extraction was studied to determine the appropriate design for further optimization studies. All the solvents except CaFr11 have important curvatures. The presence of curvature is an important indication that factorial design is inadequate for modelling the optimization of the process. As a result, further optimization of the process was carried out with a rotatable central composite response surface methodology (RCCRSM). However, curvature could be used to determine the tunability of the solvent. Moreover, the tunability of the solvents enable the application of these solvents in different operations, such as extraction, electroplating, analysis, and enzymatic activities [188]. An important observation from the results is that sucrose- and glucose-based NADESs have concave curvatures, while fructose-based NADESs have convex curvatures, which agrees with the rotation of the sugars in solution. Furthermore, there was the absence of orthogonality among the NADESs behaviour, limiting the choice of optimization to center composite design[122]

5.6.2 Rotatable Central Composite Response Surface Methodology for Optimization of Extraction of antioxidant and antiradical scavenging potential of African nutmeg peels

It has already been established that the practical application of extraction of bioactive compounds with NADES is more suitable than organic solvents for use in food and pharmaceutical products [187] [160] [189]. Therefore, citric acid-based NADESs were investigated for efficient extraction of

phenolic compounds using a multifactorial modelling as a screening study for further optimization. The 14 synthesized NADESs were found to be suitable for extracting bioactive compounds from African nutmeg peels prompting further optimization study using rotatable central composite response surface methodology. The behavior of phenolic compounds with more tendency towards acidic NADESs was seen as the basis for increase in the extraction efficiency of phenolic and antioxidant compounds [190]. Extraction with NADESs coupled with ultrasonication techniques have been reported by different authors [191] [192] [193] [194] [195]. Bertolo *et al*. prepared NADESs with choline chloride as HBA and glucose, sucrose, glycerol, lactic acid, and citric acid as HBDs and reported that choline chloride-lactic acid (ChCl-LA) as the best solvent for extracting bioactive, and phenolic compounds from pomegranate peel waste using NADES coupled with ultrasonic bath [195]. They used various NADES based on choline chloride containing glucose, sucrose, glycerol, citric acid, and lactic acid. Based on the results obtained by these researchers, it was found that the phenolic content of compounds extracted by ChCl-LA was significantly higher than other NADES and ethanolic solutions. They attributed this to a more acidic pH of lactic acid than other solvents. Also, Obluchinskaya *et al*.[194], Olfat *et al*.[196], and Koraqi *et al*.[192] studied the extraction of bioactive compounds from arctic Brown seaweed, red seaweed, and damask rose by NADESs coupled with ultrasonication, respectively, and reported that NADESs based on lactic acid coupled with ultrasonic bath led to a better extraction of phenolic and bioactive compounds. The current study finds similarity of efficiency between citric acid-fructose based NADESs to the ChCl-LA based NADES of the afore mentioned authors in TPC extraction. Therefore, it may be appropriate to assert that the acidic condition plays a crucial role in the extraction of phenolic compounds using NADESs coupled to ultrasonic technique.

5.6.2.1 Factor effects on antioxidant and antiradical scavenging properties of African nutmeg peels extracted with UAE-NADESs.

The rotatable central composite response surface methodology (RCCRSM) design to optimize the bioactive compounds extraction from African nutmeg peels using NADESs coupled to ultrasound bath, reveals highly efficient results for TPC, TFC, CUPRAC, FRAP, and DPPH as shown in **Table 4.13**. Evaluation by RCCRSM shows variation of model in TPC modelling where a second-order polynomial (full quadratic) model fits 10 out of the 14 NADESs studied (**Table 4.10**), and

linear plus interaction model fits the remaining 4. In the cases of TFC, CUPRAC, FRAP, and DPPH, the full quadratic model fits all the 14 studied NADESs with appropriate statistical parameters for data analysis. The ANOVA for the model responses using Fisher's statistical tests (*F*-test) and probability (*p*-value) shows the statistical significance of factors and interactions indicated in bold (**Table 4.11**). Accordingly, **Table 4.12** indicates a good fit of the models for reasonable prediction of data in the experimental range. The models are significant, and the data fits well with the proposed models highlighted with high R^2 (0.9977-1.00) for TPC, (0.998-1.00) for TFC, (0.7004- 0.9994) for CUPRAC, (0.7639 -1.000) for FRAP, and (0.9992-1.000) for DPPH, respectively, and non-significant Lack of Fit (p = 0.000) among the studied parameters. The performance is similar to the result obtained by Sahin and Samlı in a UAE- EtOH extraction of polyphenols from olive leaf extracts with a model performance of 0.9797 with respect to DPPH inhibition was obtained[197], better than the model developed by Bi *et al* to extract flavonoids with alcohol-based DESs[198]. Other studies that optimized a response surface UAE-NADESs extraction of bioactive compounds with model fits similar to the current study include[199 200].

5.6.2.1.1 Ultrasonic temperature (UT)

Theoretically, the ideal ultrasonic temperatures using NADES ranged from room temperature to about 60 °C[198]. Increasing the ultrasonic temperature can reduce the viscosity; however, if the temperature continues to increase, the yield of the heat-sensitive target substance may be decrease or denatured. In addition, the use of high temperature in the extraction process will increase energy consumption, which violates the principle of green extraction[201]. In this study, the effects of temperature could be observed from 30-60ºc, after which no significant effects are observed for extraction of TPC (**Figures 4.74- 4.87**), TFC (**Figures 4.89-4.102**) and antiradical scavenging (**Figures 4.102-4.117**) CUPRAC, (**Figures 4.119-4.132**) FRAP, and (**Figures 4.134-4.147**) DPPH, respectively. Therefore, 30–60 °C, represents the most effective temperature range for UAE-NADESs application for extraction of bioactive compounds from African nutmeg peels.

5.6.2.1.2 Extraction time

The mechanism of the UAE process could be determined in two main stages. Stage one was the dissolution of soluble components on surfaces of the plant matrix occurs, which could be taken as

‘‘washing’’, while stage two was mass transfer of the solute from the plant matrix into the solvent by diffusion and osmotic processes, and could be taken as ‘‘slow extraction’’[198]. These two phenomena are clearly observed in the process. Washing happened at the beginning of the extraction with a rapid increase in extracts among the NADESs. However, after about 15 min, the slow extraction was observed by a low rise in the amounts of extracts. Depending on the parameters studied, 12-20 minutes appeared to have maximized effects on the process. The total phenolic content from all NADESs increased steadily as a function of time (**Figures 4.74-4.87**). There was a tendency to drop the scavenging effects by FRAP capacity after 24 min. This can be explained by the heating effect of overexposure to ultrasound treatment for longer extraction time, which leads to the degradation of the bioactive compounds of the extracts, thereby affecting their scavenging property, even though the extended ultrasonic time could result in a higher extract yield. It is also obvious that spending much longer time is an impractical situation from the economic point of view.

5.6.2.1.3 Solvent volume

By decreasing the volume of solvent, the amounts of extracts and their total polyphenol both decreased across the NADESs, while the antiradical scavenging activities of the related extracts show no alteration. The increase of the yields with the increase of solvent volume is consistent with mass transfer principles, as the concentration gradient which is the driving force is higher when a lower solid to solvent ratio (higher solvent volume) is used, leading to higher diffusion. The same effects was observed for pectin extraction from apple pomace [202], orange peels[203], and Olive leaf[198]. On the other hand, consuming less solvent for the extraction is extremely reasonable and practical state from the economical point of view.

5.6.2.1.4 Solvent concentration

While 90% NADESs as extraction solvent was distinguished by the highest level of extract yield, pure water showed the poorest yield across. In addition, pure water extracts were found to be significantly different ($p < 0.001$) from the extracts obtained by the NADESs. Regarding total polyphenols, the best performance was achieved by using 90% of NADESs as extractant under the

optimized extraction conditions **Figure 4.148 and Figure 4.149**. Although pure water (0% NADESs) is the most polar solvent of all, it did not yield the best results with respect to extract and total phenolic content from African nutmeg peels using UAE-NADESs. This phenomenon might be attributed to the lower viscosity of water than those of the synthesized NADESs, which is a matter of ultrasonic cavitation dislodge the bonding mechanism. 90% CaFr11 showed the greatest yield of extract and total phenolic content, because of its many hydrogen bonds functional groups observed from FTIR spectroscopy. Accordingly, water (10%) may act as the plant swelling agent, while NADESs (90%) is believed to disrupt the bonding between the solutes and plant matrices. Therefore, the 90% NADESs exhibited the best performance to extract polyphenols from the African nutmeg peels. Another explanation might be the high dielectric constant of water, which leads to increased polarity indices of NADESs with its water solution. Generally, NADESs extracts had higher scavenging capacity **Figures 4.150-152**. On the other hand, pure water extracts exhibited relatively lower scavenging capacity. Degradation of polyphenols might occur by hydrolysis with water, and by oxidation of the antioxidant components with formed peroxyl and hydroxyl radicals[197].

5.6.3.1 Effects of UAE-NADESs on TPC and TFC extraction from of African nutmeg peels

In the presence of a solvent (NADES), the cavitation phenomenon occurs by exposing the African nutmeg peels to ultrasound waves. Cavitation is microbubbles that are formed by the application of ultrasonic waves. Ultrasound waves, due to the cycle of compression and rarefaction, cause the formation, growth, and implosion of bubbles. As the bubbles explode, the tissue matrix of the peel collapses. The cycle of compression and rarefaction is directly related to the solvent volume, so that at higher volumes, the rate of cavitation will be higher. Therefore, as a result of increasing the solvent volume, the ultrasound cavitation increases leading to increased tissue disruption and ultimate increase in TPC extraction [204 205 206]. The two main steps on which the UAE process is based are the washing and the slow extraction mechanisms. In the washing stage, the soluble compounds on the surface or close to the surface are washed and extracted by solvent, which is accompanied by a rapid increase in the extraction slope, while during the slow extraction stage, soluble materials are slowly extracted from the sample matrix into the solvent by both diffusion and osmotic phenomena. At the slow extraction stage, temperature plays a role as it helps in

diffusion and osmosis through increased molecular mobility. At this mechanism, sufficient time to extract bioactive compounds from the target matrix is required[197]. Therefore, providing sufficient time will cause the most bioactive compounds to be extracted and thus increase the extraction efficiency. However, prolonging the time may lead to polyphenol degradation. The concentration of the solvent increases by reducing the amount of water added to the NADES. Increasing the solvent concentration causes the mass transfer more rapidly and the phenolic compounds in the African nutmeg peels to diffuse into the solvent[207]. This may be because higher solvent concentration means availability of more hydrogen bond species for interaction with the bioactive molecules leaving the sample matrix into the solvent. higher concentration of NADESs will increase the content of hydrophilic compounds, because of the acidic nature of solvents.

5.7 Optimization of UAE-NADESs extraction of antioxidant and antiradical scavenging potentials of African nutmeg peels by RSM

Table 4.14 shows the maximum desirability values for TPC, TFC, and antiradical scavenging properties measured with CUPRAC, FRAP, and DPPH inhibition of the African nutmeg peels extracts. The Predicted and experimental values obtained using the optimized response conditions for TPC (UT = 45ºc, ET = 5 min, SV = 25 ml, SC = 90%), TFC (UT = 30ºc, ET = 5 min, SV = 25 ml, SC = 90%), CUPRAC (UT = 30ºc, ET = 5 min, SV = 25 ml, SC = 90%), FRAP (UT = 45ºc, ET = 25 min, SV = 25 ml, SC = 50%), and DPPH (UT = 50ºc, ET = 15 min, SV = 15 ml, SC = 70%) are presented in Table 4.16. The performance of the synthesized NADESs at optimized conditions were compared with the performance of pure water at the same conditions and are presented in Figure 4.148 for TPC, Figure 4.149 for TFC, Figure 4.150 for CUPRAC, Figure 4. 151 for FRAP, and Figure 4.152 for DPPH, respectively.

Comparison of the performance shows that TPC and TFC compounds extracted by the UAE-NADESs method at optimized conditions were higher than those extracted with water (greenest solvent) at the same conditions **Figures 4.148** and **Figure 4.149**. The total phenol content of the bioactive compound extracted by the UAE optimal method with eutectic solvents showed a better performance than water among all the formed NADESs. The combination of ultrasonic process and eutectic solvent, probably due to its role in improving the mass transfer process of bioactive compounds from the African nutmeg peels, will cause more bioactive and phenolic compounds to

be extracted and will increase the total phenol content [208]. The UAE-NADESs, due to their role in the stability of solutes, prevents the degradation of these compounds during the extraction process and thus increases the extraction efficiency. In this extraction process, due to the formation of strong hydrogen bonds between solutes and NADES molecules, the stability of the target compounds may increase against adverse environmental conditions (oxidative degradation) [209]. Also, during the UAE process, the high solubility of NADES may confer a significant advantage for the extraction and stability of bioactive compounds (polyphenols, flavonoids), at such shorter extraction time than conventional extraction processes [210]. Macchioni et al. reported similar results for extracting phenolic compounds from common hops using NADES and UAE [211]. They stated that the extraction efficiency of phenolic compounds by lactic acid-based eutectic solvents is higher than the conventional extraction method using ethanol 80 %. They attributed this behavior to the improvement of the mass transfer process by the UAE method and the increase in the stability of phenolic compounds induced by eutectic solvents [211].

In the case of the antiradical scavenging activity (CUPRAC, FRAP, and DPPH) of the extracts at optimized conditions (**Figure 4.150, Figure 4.151**, and **Figure 4.152**), CUPRAC shows that all UAE-NADESs were significantly higher than UAE-water (22.81± 0.46 µMTE/g) except in UAE-CaGc11(22.78±0.43 µMTE/g) where former performed better but at no statistical significance ($p < 0.05$). UAE-water performed significantly higher than UAE-CaGl11, UAE-CaGl21, and UAE-CaGc21 using FRAP test, but significantly lower in all other UAE-NADESs studied ($p < 0.05$). However, DPPH inhibitions performed significantly better in all UAE-NADESs than in UAE-water ($p < 0.05$). The free radical scavenging activity of DPPH, CUPRAC and FRAP of UAE coupled with NADES may probably be connected to the content of higher phenolic compounds extracted by the UAE method using eutectic solvents. These bioactive (nutraceuticals) have various antioxidant and biological activities in food and biological systems due to their structural properties [212 213]. The hydrogen donating capability and reduction ability of phenolic compounds cause the oxidation chain reaction to be broken, and these compounds are referred to as potent antioxidants [196]. These findings are consistent with the results of other researchers. Mansinhos *et al.* studied the extraction of phenolic compounds from butterfly lavender leaf with UAE and NADES, and found that the combination of UAE and NADES resulted in higher antioxidant activity compared to conventional methods [214]. They stated that scavenging of DPPH free radicals

by UAE-NADES methods was greater than that of extracts obtained by conventional methods, and attributed the higher antioxidant activity to the content of higher phenolic compounds in the UAE method [214].

CHAPTER SIX

SUMMARY AND CONCLUSIONS

6.1 Summary

- Fourteen neoteric deep eutectic solvents (NADESs) were synthesized with ultrasonic assistance using citric acid as HBA and sucrose, fructose, xylitol, glycerol, glycine, and glucose as HBDs, and different molar ratios.
- The physicochemical properties and bonding functional groups of the NADESs were evaluated and confirmed to meet the characteristics of deep eutectic solvents.
- Shelf stability of the NADESs was studied over a ninety-day period and was found to be stable at ambient conditions for the storage period.
- Extraction of bioactive compounds from African nutmeg peels using the NADESs coupled to ultrasonication at different conditions of temperature, time, volume and concentration was studied, optimized and compared with water extracts at the optimized conditions.
- The results obtained confirmed that NADESs are better solvents for extraction of polyphenols and flavonoids from African nutmeg peels, with better antioxidant and antiradical scavenging power than water extracts.

6.2 Conclusions

Ultrasound assisted technique was developed to synthesize fourteen natural acidic deep eutectic solvents (NADESs) using citric acid and different plant secondary metabolites. The physicochemical properties and storage stability of solvents were characterized using both physical property and chemical bond energies. The physical properties obtained had similar trends with choline chloride based NADESs. H-bonding was established from the functional peak frequency of FTIR spectroscopy indicating the formation of eutectic solvents. The NADESs formed were shelf stable over a 90 day storage.

The synthesized NADESs coupled with ultrasonication were applied to extract bioactive compounds from African nutmeg (*M. myristica)* peels, and the antioxidant and antiradical scavenging power of the extracts evaluated in vitro, along with the extraction conditions. A

screening process follows a multifactorial experimental design with a 2^4 fractional factorial consisting of four factors (ultrasound temperature, extraction time, solvent volume, and solvent concentration) at low and high levels with a central point to simultaneously study the effects of the factors and their interactions as conditions in a prototypical extraction setting. All the solvents were very effective at extracting TPCs and TFCs, with high antiradical scavenging activity prompting further optimization of the process with a rotatable central composite response surface methodology to achieve maximum extractions.

The extraction process was optimized to obtain maximum bioactive compounds from African nutmeg (*M. myristica)* peels representing a typical agrifood waste. The optimized extraction process exhibited volume and concentration dependency. That was expected because higher volumes provide wider areas for cavitation activity of ultrasonic waves which leads to biomolecule release from sample matrix. Shorter time and medium temperature with a high solvent volume is also ideal for selective extraction of polyphenols. However, a high temperature may be necessary for viscous solvents to lower the viscosity of the solvent to increase the surface area available for interaction. The comparative analysis with water extracts under the optimized conditions revealed a significant difference and correlates with industrial scalability and environmental impact. Specifically, the application of NADESs, characterized by their biodegradability and low toxicity, underscores a pivotal advancement towards sustainable and eco-friendly extraction technologies. This highlights NADES' practical applicability in enhancing the yield and quality of bioactive extractions, thereby promoting a greener approach in the phytochemical industry.

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APPENDICES

Appendix 1.1: pH data for synthesized NADESs measured on day 1, day 45, and day 90.

Solvents	HBA	HBD	HBA: HBD Ratio	pH (day 1)	pH (day 1)	pH (day 1)	pH (day 45)	pH (day 45)	pH (day 45)	pH (day 90)	pH (day 90)	pH (day 90)
CaSu11	Citric acid	sucrose	1:1	1.92	1.92	1.92	2.01	2.02	2.02	2.02	2.00	2.03
CaFr11	Citric acid	fructose	1:1	1.75	1.74	1.76	1.89	1.90	1.90	1.86	1.86	1.86
CaFr12	Citric acid	fructose	1:2	1.90	1.91	1.89	1.89	1.88	1.90	1.95	1.97	1.93
CaFr21	Citric acid	fructose	2:1	1.84	1.84	1.84	1.73	1.72	1.73	1.75	1.77	1.76
CaXy11	Citric acid	xylitol	1:1	1.85	1.90	1.80	1.88	1.88	1.87	1.91	1.92	1.90
CaXy12	Citric acid	xylitol	1:2	1.90	1.87	1.93	1.91	1.90	1.92	1.95	1.95	1.96
CaXy21	Citric acid	xylitol	2:1	1.89	1.92	1.87	1.74	1.70	1.76	1.79	1.79	1.80
CaGr11	Citric acid	glycerol	1:1	1.67	1.70	1.66	1.82	1.80	1.83	1.88	1.88	1.87
CaGr12	Citric acid	glycerol	1:2	1.86	1.88	1.85	1.88	1.88	1.89	1.92	1.92	1.92
CaGr21	Citric acid	glycerol	2:1	1.78	1.79	1.77	1.60	1.62	1.58	1.77	1.77	1.77
CaGc11	Citric acid	glycine	1:1	2.61	2.65	2.58	2.67	2.66	2.68	2.61	2.62	2.60
CaGc21	Citric acid	glycine	2:1	2.39	2.38	2.40	2.37	2.35	2.37	2.43	2.46	2.40
CaGl11	Citric acid	glucose	1:1	1.82	1.81	1.81	1.87	1.87	1.88	1.86	1.88	1.84
CaGl21	Citric acid	glucose	2:1	1.71	1.71	1.70	1.70	1.70	1.69	1.71	1.70	1.72

Appendix 1.2: water activity data for synthesized NADESs measured on day 1, day 45, and day 90

Solvents	HBA	HBD	HBA: HBD Ratio	Water activity (day 1)	Water activity (day 1)	Water activity (day 1)	Water activity (day 45)	Water activity (day 45)	Water activity (day 45)	Water activity (day90)	Water activity (day90)	Water activity (day90)
CaSu11	Citric acid	sucrose	1:1	0.73	0.72	0.74	0.70	0.69	0.71	0.70	0.71	0.70
CaFr11	Citric acid	fructose	1:1	0.77	0.77	0.78	0.78	0.77	0.79	0.76	0.75	0.77
CaFr12	Citric acid	fructose	1:2	0.76	0.75	0.77	0.70	0.72	0.68	0.71	0.71	0.71
CaFr21	Citric acid	fructose	2:1	0.72	0.71	0.73	0.69	0.69	0.69	0.70	0.69	0.71
CaXy11	Citric acid	xylitol	1:1	0.78	0.79	0.77	0.77	0.78	0.76	0.78	0.78	0.78
CaXy12	Citric acid	xylitol	1:2	0.76	0.77	0.75	0.73	0.73	0.73	0.73	0.73	0.73
CaXy21	Citric acid	xylitol	2:1	0.72	0.72	0.73	0.71	0.71	0.71	0.72	0.72	0.72
CaGr11	Citric acid	glycerol	1:1	0.79	0.79	0.79	0.79	0.80	0.78	0.78	0.78	0.78
CaGr12	Citric acid	glycerol	1:2	0.77	0.76	0.78	0.75	0.75	0.75	0.74	0.74	0.74
CaGr21	Citric acid	glycerol	2:1	0.77	0.78	0.76	0.73	0.73	0.73	0.72	0.72	0.72
CaGc11	Citric acid	glycine	1:1	0.83	0.84	0.82	0.83	0.83	0.83	0.83	0.83	0.83
CaGc21	Citric acid	glycine	2:1	0.81	0.81	0.81	0.76	0.76	0.77	0.76	0.76	0.76
CaGl11	Citric acid	glucose	1:1	0.77	0.76	0.78	0.76	0.75	0.78	0.76	0.76	0.76
CaGl21	Citric acid	glucose	2:1	0.71	0.70	0.72	0.69	0.69	0.70	0.71	0.71	0.71

Appendix 1.3: Viscosity data of synthesized NADESs measured on day 1, day 45, and day 90.

Solvents	HBA	HBD	HBA: HBD Ratio	Viscosity (day 1)	Viscosity (day 1)	Viscosity (day 1)	Viscosity (day 45)	Viscosity (day 45)	Viscosity (day 45)	Viscosity (day 90)	Viscosity (day 90)	Viscosity (day 90)
CaSu11	Citric acid	Sucrose	1:1	0.3546	0.3542	0.3548	0.3378	0.3370	0.3378	0.3129	0.3127	0.3131
CaFr11	Citric acid	Fructose	1:1	0.0805	0.0806	0.0804	0.0888	0.0884	0.0886	0.0984	0.0982	0.0980
CaFr12	Citric acid	Fructose	1:2	0.1797	0.1795	0.1798	0.1806	0.1804	0.1808	0.1819	0.1819	0.1819
CaFr21	Citric acid	Fructose	2:1	0.1221	0.1220	0.1222	0.1343	0.1347	0.1344	0.1401	0.1401	0.1400
CaXy11	Citric acid	Xylitol	1:1	0.0269	0.0269	0.0270	0.0272	0.0275	0.0273	0.0284	0.0286	0.029
CaXy12	Citric acid	Xylitol	1:2	0.0804	0.0808	0.0806	0.0960	0.0959	0.0960	0.1053	0.1054	0.1055
CaXy21	Citric acid	Xylitol	2:1	0.0872	0.0871	0.0870	0.0841	0.0843	0.0841	0.0828	0.0828	0.0828
CaGr11	Citric acid	Glycerol	1:1	0.0130	0.0131	0.0131	0.0136	0.0138	0.0136	0.0144	0.0144	0.0144
CaGr12	Citric acid	Glycerol	1:2	0.0191	0.0191	0.0191	0.0443	0.0443	0.0443	0.0739	0.0739	0.0739
CaGr21	Citric acid	Glycerol	2:1	0.0520	0.0525	0.0530	0.0481	0.0483	0.0481	0.0447	0.0447	0.0447
CaGc11	Citric acid	Glycine	1:1	0.0204	0.0204	0.0204	0.0320	0.0319	0.0320	0.0414	0.0418	0.0416
CaGc21	Citric acid	Glycine	2:1	0.0740	0.0760	0.0780	0.0742	0.0740	0.0740	0.0727	0.0727	0.0727
CaGl11	Citric acid	Glucose	1:1	0.0437	0.0439	0.0437	0.0471	0.0472	0.0471	0.0501	0.0501	0.0501
CaGl21	Citric acid	Glucose	2:1	0.1311	0.1313	0.1315	0.1061	0.1061	0.1061	0.0953	0.0959	0.0956

Appendix 1.4: Density data of synthesized NADESs measured on day 1, day 45, and day 90.

Solvents	HBA	HBD	HBA: HBD Ratio	Density (day 1)	Density (day 1)	Density (day 1)	Density (day 45)	Density (day 45)	Density (day 45)	Density (day 90)	Density (day 90)	Density (day 90)
CaSu11	Citric acid	Sucrose	1:1	1.3768	1.3770	1.3766	1.3609	1.3670	1.3608	1.3600	1.3590	1.3595
CaFr11	Citric acid	Fructose	1:1	1.3290	1.3293	1.3296	1.3201	1.3203	1.3200	1.3142	1.3142	1.3142
CaFr12	Citric acid	Fructose	1:2	1.3760	1.3768	1.3776	1.3373	1.3374	1.3375	1.3140	1.3146	1.3140
CaFr21	Citric acid	Fructose	2:1	1.3768	1.3768	1.3768	1.3604	1.3607	1.3610	1.3595	1.3595	1.3595
CaXy11	Citric acid	Xylitol	1:1	1.2818	1.2822	1.2814	1.2709	1.2709	1.2709	1.2689	1.2689	1.2689
CaXy12	Citric acid	Xylitol	1:2	1.2826	1.2818	1.2810	1.2972	1.2972	1.2972	1.3180	1.3184	1.3182
CaXy21	Citric acid	Xylitol	2:1	1.3291	1.3295	1.3293	1.3200	1.3200	1.3200	1.3182	1.3182	1.3182
CaGr11	Citric acid	Glycerol	1:1	1.2348	1.2344	1.2340	1.2206	1.2206	1.2206	1.2272	1.2277	1.2270
CaGr12	Citric acid	Glycerol	1:2	1.2350	1.2338	1.2344	1.2797	1.2794	1.2794	1.3182	1.3182	1.3182
CaGr21	Citric acid	Glycerol	2:1	1.3293	1.3290	1.3296	1.3021	1.3021	1.3021	1.2724	1.2730	1.2727
CaGc11	Citric acid	Glycine	1:1	1.3292	1.3297	1.3290	1.3048	1.3045	1.3045	1.2727	1.2727	1.2727
CaGc21	Citric acid	Glycine	2:1	1.3297	1.3290	1.3292	1.3214	1.3214	1.3214	1.3180	1.3180	1.3186
CaGl11	Citric acid	Glucose	1:1	1.2818	1.2814	1.2822	1.2800	1.2818	1.2800	1.2729	1.2725	1.2727
CaGl21	Citric acid	Glucose	2:1	1.3296	1.3293	1.3290	1.3203	1.3202	1.3201	1.3180	1.3183	1.3180

Appendix 2.1 factorial experiment TPC run 1

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	5	Blank B	A	0.026					
F	6	Sample X1	A	0.379	0.353	CaSu11	15.3431373	0.1534314	153.43137
F	7	Sample X1	A	0.373	0.347	CaSu11	15.0490196	0.1504902	150.4902
F	8	Sample X1	A	0.376	0.35	CaSu11	15.1960784	0.1519608	151.96078
C	9	Blank B	A	0.024					
C	10	Sample X1	A	0.659	0.635	CaFr11	29.1666667	0.2916667	291.66667
C	11	Sample X1	A	0.654	0.63	CaFr11	28.9215686	0.2892157	289.21569
C	12	Sample X1	A	0.652	0.628	CaFr11	28.8235294	0.2882353	288.23529
D	1	Blank B	B	0.025					
D	2	Sample X1	B	0.643	0.618	CaFr12	28.3333333	0.2833333	283.33333
D	3	Sample X1	B	0.644	0.619	CaFr12	28.3823529	0.2838235	283.82353
D	4	Sample X1	B	0.643	0.618	CaFr12	28.3333333	0.2833333	283.33333
D	5	Blank B	C	0.028					
D	6	Sample X1	C	0.306	0.278	CaFr21	11.6666667	0.1166667	116.66667
D	7	Sample X1	C	0.304	0.276	CaFr21	11.5686275	0.1156863	115.68627
D	8	Sample X1	C	0.303	0.275	CaFr21	11.5196078	0.1151961	115.19608
D	9	Blank B	D	0.014					
D	10	Sample X1	D	0.274	0.26	CaXy11	10.7843137	0.1078431	107.84314
D	11	Sample X1	D	0.279	0.265	CaXy11	11.0294118	0.1102941	110.29412
D	12	Sample X1	D	0.278	0.264	CaXy11	10.9803922	0.1098039	109.80392
E	1	Blank B	E	0.019					
E	2	Sample X1	E	0.244	0.225	CaXy12	9.06862745	0.0906863	90.686275
E	3	Sample X1	E	0.241	0.222	CaXy12	8.92156863	0.0892157	89.215686
E	4	Sample X1	E	0.247	0.228	CaXy12	9.21568627	0.0921569	92.156863
E	5	Blank B	F	0.013					
E	6	Sample X1	F	0.294	0.281	CaXy21	11.8137255	0.1181373	118.13725
E	7	Sample X1	F	0.298	0.285	CaXy21	12.0098039	0.120098	120.09804
E	8	Sample X1	F	0.298	0.285	CaXy21	12.0098039	0.120098	120.09804
F	9	Blank B	B	0.018					
F	10	Sample X1	B	0.242	0.224	CaGr11	9.01960784	0.0901961	90.196078
F	11	Sample X1	B	0.243	0.225	CaGr11	9.06862745	0.0906863	90.686275
F	12	Sample X1	B	0.241	0.223	CaGr11	8.97058824	0.0897059	89.705882
G	1	Blank B	C	0.019					
G	2	Sample X1	C	0.257	0.238	CaGr12	9.70588235	0.0970588	97.058824
G	3	Sample X1	C	0.252	0.233	CaGr12	9.46078431	0.0946078	94.607843
G	4	Sample X1	C	0.255	0.236	CaGr12	9.60784314	0.0960784	96.078431

Appendix 2.1 contd.

G	5	Blank B	D	0.018					
G	6	Sample X1	D	0.192	0.174	CaGr21	6.56862745	0.0656863	65.686275
G	7	Sample X1	D	0.197	0.179	CaGr21	6.81372549	0.0681373	68.137255
G	8	Sample X1	D	0.192	0.174	CaGr21	6.56862745	0.0656863	65.686275
E	9	Blank B	G	0.018					
E	10	Sample X1	G	0.255	0.237	CaGc11	9.65686275	0.0965686	96.568627
E	11	Sample X1	G	0.252	0.234	CaGc11	9.50980392	0.095098	95.098039
E	12	Sample X1	G	0.259	0.241	CaGc11	9.85294118	0.0985294	98.529412
F	1	Blank B	H	0.018					
F	2	Sample X1	H	0.219	0.201	CaGc21	7.89215686	0.0789216	78.921569
F	3	Sample X1	H	0.217	0.199	CaGc21	7.79411765	0.0779412	77.941176
F	4	Sample X1	H	0.217	0.199	CaGc21	7.79411765	0.0779412	77.941176
G	9	Blank B	E	0.017					
G	10	Sample X1	E	0.24	0.223	CaGl11	8.97058824	0.0897059	89.705882
G	11	Sample X1	E	0.24	0.223	CaGl11	8.97058824	0.0897059	89.705882
G	12	Sample X1	E	0.243	0.226	CaGl11	9.11764706	0.0911765	91.176471
H	1	Blank B	F	0.018					
H	2	Sample X1	F	0.205	0.187	CaGl21	7.20588235	0.0720588	72.058824
H	3	Sample X1	F	0.205	0.187	CaGl21	7.20588235	0.0720588	72.058824
H	4	Sample X1	F	0.205	0.187	CaGl21	7.20588235	0.0720588	72.058824

Appendix 2.2 factorial experiment TPC, run 2.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	9	Blank B	C	0.023					
F	10	Sample X1	C	0.556	0.533	CaSu11	24.1666667	0.483333333	483.33333
F	11	Sample X1	C	0.555	0.532	CaSu11	24.1176471	0.482352941	482.35294
F	12	Sample X1	C	0.555	0.532	CaSu11	24.1176471	0.482352941	482.35294
G	1	Blank B	D	0.054					
G	2	Sample X1	D	0.976	0.922	CaFr11	43.2352941	0.864705882	864.70588
G	3	Sample X1	D	0.971	0.917	CaFr11	42.9901961	0.859803922	859.80392
G	4	Sample X1	D	0.975	0.921	CaFr11	43.1862745	0.86372549	863.72549
G	5	Blank B	E	0.028					
G	6	Sample X1	E	0.997	0.969	CaFr12	45.5392157	0.910784314	910.78431
G	7	Sample X1	E	0.99	0.962	CaFr12	45.1960784	0.903921569	903.92157
G	8	Sample X1	E	0.996	0.968	CaFr12	45.4901961	0.909803922	909.80392
G	9	Blank B	F	0.028					
G	10	Sample X1	F	0.396	0.368	CaFr21	16.0784314	0.321568627	321.56863

Appendix 2.2 contd.

G	11	Sample X1	F	0.394	0.366	CaFr21	15.9803922	0.319607843	319.60784
G	12	Sample X1	F	0.398	0.37	CaFr21	16.1764706	0.323529412	323.52941
A	1	Blank B	A	0.019					
A	2	Sample X1	A	0.267	0.248	CaXy11	10.1960784	0.203921569	203.92157
A	3	Sample X1	A	0.269	0.25	CaXy11	10.2941176	0.205882353	205.88235
A	4	Sample X1	A	0.267	0.248	CaXy11	10.1960784	0.203921569	203.92157
A	5	Blank B	B	0.012					
A	6	Sample X1	B	0.251	0.239	CaXy12	9.75490196	0.195098039	195.09804
A	7	Sample X1	B	0.256	0.244	CaXy12	10	0.2	200
A	8	Sample X1	B	0.251	0.239	CaXy12	9.75490196	0.195098039	195.09804
A	9	Blank B	C	0.019					
A	10	Sample X1	C	0.187	0.168	CaXy21	6.2745098	0.125490196	125.4902
A	11	Sample X1	C	0.185	0.166	CaXy21	6.17647059	0.123529412	123.52941
A	12	Sample X1	C	0.181	0.162	CaXy21	5.98039216	0.119607843	119.60784
B	1	Blank B	D	0.019					
B	2	Sample X1	D	0.188	0.169	CaGr11	6.32352941	0.126470588	126.47059
B	3	Sample X1	D	0.189	0.17	CaGr11	6.37254902	0.12745098	127.45098
B	4	Sample X1	D	0.186	0.167	CaGr11	6.2254902	0.124509804	124.5098
B	5	Blank B	E	0.014					
B	6	Sample X1	E	0.202	0.188	CaGr12	7.25490196	0.145098039	145.09804
B	7	Sample X1	E	0.206	0.192	CaGr12	7.45098039	0.149019608	149.01961
B	8	Sample X1	E	0.2	0.186	CaGr12	7.15686275	0.143137255	143.13725
B	9	Blank B	F	0.019					
B	10	Sample X1	F	0.181	0.162	CaGr21	5.98039216	0.119607843	119.60784
B	11	Sample X1	F	0.186	0.167	CaGr21	6.2254902	0.124509804	124.5098
B	12	Sample X1	F	0.189	0.17	CaGr21	6.37254902	0.12745098	127.45098
C	1	Blank B	G	0.018					
C	2	Sample X1	G	0.201	0.183	CaGc11	7.00980392	0.140196078	140.19608
C	3	Sample X1	G	0.201	0.183	CaGc11	7.00980392	0.140196078	140.19608
C	4	Sample X1	G	0.205	0.187	CaGc11	7.20588235	0.144117647	144.11765
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.197	0.111	CaGc21	3.48039216	0.069607843	69.607843
C	7	Sample X1	H	0.19	0.104	CaGc21	3.1372549	0.062745098	62.745098
C	8	Sample X1	H	0.196	0.11	CaGc21	3.43137255	0.068627451	68.627451
H	1	Blank B	G	0.019					
H	2	Sample X1	G	0.207	0.188	CaGl11	7.25490196	0.145098039	145.09804
H	3	Sample X1	G	0.209	0.19	CaGl11	7.35294118	0.147058824	147.05882
H	4	Sample X1	G	0.202	0.183	CaGl11	7.00980392	0.140196078	140.19608
H	5	Blank B	H	0.018					
H	6	Sample X1	H	0.213	0.195	CaGl21	7.59803922	0.151960784	151.96078
H	7	Sample X1	H	0.219	0.201	CaGl21	7.89215686	0.157843137	157.84314
H	8	Sample X1	H	0.213	0.195	CaGl21	7.59803922	0.151960784	151.96078

Appendix 2.3 factorial experiment TPC run 3

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	1	Blank B	H	0.311					
F	2	Sample X1	H	0.928	0.617	CaSu11	28.28431373	0.282843137	282.843137
F	3	Sample X1	H	0.929	0.618	CaSu11	28.33333333	0.283333333	283.333333
F	4	Sample X1	H	0.928	0.617	CaSu11	28.28431373	0.282843137	282.843137
F	5	Blank B	A	0.298					
F	6	Sample X1	A	1.252	0.954	CaFr11	44.80392157	0.448039216	448.039216
F	7	Sample X1	A	1.258	0.96	CaFr11	45.09803922	0.450980392	450.980392
F	8	Sample X1	A	1.253	0.955	CaFr11	44.85294118	0.448529412	448.529412
F	9	Blank B	B	0.297					
F	10	Sample X1	B	0.968	0.671	CaFr12	30.93137255	0.309313725	309.313725
F	11	Sample X1	B	0.961	0.664	CaFr12	30.58823529	0.305882353	305.882353
F	12	Sample X1	B	0.967	0.67	CaFr12	30.88235294	0.308823529	308.823529
G	1	Blank B	C	0.294					
G	2	Sample X1	C	0.659	0.365	CaFr21	15.93137255	0.159313725	159.313725
G	3	Sample X1	C	0.655	0.361	CaFr21	15.73529412	0.157352941	157.352941
G	4	Sample X1	C	0.655	0.361	CaFr21	15.73529412	0.157352941	157.352941
G	5	Blank B	D	0.105					
G	6	Sample X1	D	0.731	0.626	CaXy11	28.7254902	0.287254902	287.254902
G	7	Sample X1	D	0.733	0.628	CaXy11	28.82352941	0.288235294	288.235294
G	8	Sample X1	D	0.733	0.628	CaXy11	28.82352941	0.288235294	288.235294
G	9	Blank B	E	0.109					
G	10	Sample X1	E	0.658	0.549	CaXy12	24.95098039	0.249509804	249.509804
G	11	Sample X1	E	0.65	0.541	CaXy12	24.55882353	0.245588235	245.588235
G	12	Sample X1	E	0.652	0.543	CaXy12	24.65686275	0.246568627	246.568627
H	1	Blank B	F	0.105					
H	2	Sample X1	F	0.703	0.598	CaXy21	27.35294118	0.273529412	273.529412
H	3	Sample X1	F	0.706	0.601	CaXy21	27.5	0.275	275
H	4	Sample X1	F	0.708	0.603	CaXy21	27.59803922	0.275980392	275.980392
E	1	Blank B	E	0.095					
E	2	Sample X1	E	0.751	0.656	CaGr11	30.19607843	0.301960784	301.960784
E	3	Sample X1	E	0.753	0.658	CaGr11	30.29411765	0.302941176	302.941176
E	4	Sample X1	E	0.759	0.664	CaGr11	30.58823529	0.305882353	305.882353
E	5	Blank B	F	0.103					
E	6	Sample X1	F	0.885	0.782	CaGr12	36.37254902	0.36372549	363.72549
E	7	Sample X1	F	0.882	0.779	CaGr12	36.2254902	0.362254902	362.254902
E	8	Sample X1	F	0.883	0.78	CaGr12	36.2745098	0.362745098	362.745098
E	9	Blank B	G	0.078					
E	10	Sample X1	G	0.753	0.675	CaGr21	31.12745098	0.31127451	311.27451

Appendix 2.3 contd.

E	11	Sample X1	G	0.756	0.678	CaGr21	31.2745098	0.312745098	312.745098
E	12	Sample X1	G	0.757	0.679	CaGr21	31.32352941	0.313235294	313.235294
H	5	Blank B	G	0.086					
H	6	Sample X1	G	0.461	0.375	CaGc11	16.42156863	0.164215686	164.215686
H	7	Sample X1	G	0.462	0.376	CaGc11	16.47058824	0.164705882	164.705882
H	8	Sample X1	G	0.469	0.383	CaGc11	16.81372549	0.168137255	168.137255
H	9	Blank B	H	0.082					
H	10	Sample X1	H	0.634	0.552	CaGc21	25.09803922	0.250980392	250.980392
H	11	Sample X1	H	0.633	0.551	CaGc21	25.04901961	0.250490196	250.490196
H	12	Sample X1	H	0.635	0.553	CaGc21	25.14705882	0.251470588	251.470588
C	1	Blank B	G	0.112					
C	2	Sample X1	G	0.825	0.713	CaGl11	32.99019608	0.329901961	329.901961
C	3	Sample X1	G	0.827	0.715	CaGl11	33.08823529	0.330882353	330.882353
C	4	Sample X1	G	0.825	0.713	CaGl11	32.99019608	0.329901961	329.901961
C	5	Blank B	H	0.093					
C	6	Sample X1	H	0.646	0.553	CaGl21	25.14705882	0.251470588	251.470588
C	7	Sample X1	H	0.641	0.548	CaGl21	24.90196078	0.249019608	249.019608
C	8	Sample X1	H	0.641	0.548	CaGl21	24.90196078	0.249019608	249.019608

Appendix 2.4 factorial experiment TPC, RUN 4.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	5	Blank B	A	0.256					
F	6	Sample X1	A	0.613	0.357	CaSu11	15.5392157	0.15539216	155.39216
F	7	Sample X1	A	0.618	0.362	CaSu11	15.7843137	0.15784314	157.84314
F	8	Sample X1	A	0.619	0.363	CaSu11	15.8333333	0.15833333	158.33333
F	9	Blank B	B	0.251					
F	10	Sample X1	B	0.891	0.64	CaFr11	29.4117647	0.29411765	294.11765
F	11	Sample X1	B	0.897	0.646	CaFr11	29.7058824	0.29705882	297.05882
F	12	Sample X1	B	0.898	0.647	CaFr11	29.754902	0.29754902	297.54902
F	5	Blank B	A	0.211					
F	6	Sample X1	A	0.851	0.64	CaFr12	29.4117647	0.29411765	294.11765
F	7	Sample X2	A	0.856	0.645	CaFr12	29.6568627	0.29656863	296.56863
F	8	Sample X3	A	0.859	0.648	CaFr12	29.8039216	0.29803922	298.03922
F	9	Blank B	B	0.25					
F	10	Sample X1	B	0.447	0.197	CaFr21	7.69607843	0.07696078	76.960784
F	11	Sample X2	B	0.443	0.193	CaFr21	7.5	0.075	75
F	12	Sample X3	B	0.44	0.19	CaFr21	7.35294118	0.07352941	73.529412
G	1	Blank B	C	0.112					

Appendix 2.4 contd.

G	2	Sample X1	C	0.581	0.469	CaXy11	21.0294118	0.21029412	210.29412
G	3	Sample X2	C	0.585	0.473	CaXy11	21.2254902	0.2122549	212.2549
G	4	Sample X3	C	0.583	0.471	CaXy11	21.127451	0.21127451	211.27451
G	5	Blank B	D	0.116					
G	6	Sample X1	D	0.355	0.239	CaXy12	9.75490196	0.09754902	97.54902
G	7	Sample X2	D	0.359	0.243	CaXy12	9.95098039	0.0995098	99.509804
G	8	Sample X3	D	0.352	0.236	CaXy12	9.60784314	0.09607843	96.078431
G	9	Blank B	E	0.113					
G	10	Sample X1	E	0.167	0.054	CaXy21	6.8627451	0.06862745	68.627451
G	11	Sample X2	E	0.167	0.054	CaXy21	6.8627451	0.06862745	68.627451
G	12	Sample X3	E	0.167	0.054	CaXy21	6.8627451	0.06862745	68.627451
H	1	Blank B	F	0.097					
H	2	Sample X1	F	0.268	0.171	CaGr11	6.42156863	0.06421569	64.215686
H	3	Sample X2	F	0.261	0.164	CaGr11	6.07843137	0.06078431	60.784314
H	4	Sample X3	F	0.265	0.168	CaGr11	6.2745098	0.0627451	62.745098
H	5	Blank B	G	0.096					
H	6	Sample X1	G	0.431	0.335	CaGr12	14.4607843	0.14460784	144.60784
H	7	Sample X2	G	0.434	0.338	CaGr12	14.6078431	0.14607843	146.07843
H	8	Sample X3	G	0.431	0.335	CaGr12	14.4607843	0.14460784	144.60784
H	9	Blank B	H	0.098					
H	10	Sample X1	H	0.271	0.173	CaGr21	6.51960784	0.06519608	65.196078
H	11	Sample X2	H	0.274	0.176	CaGr21	6.66666667	0.06666667	66.666667
H	12	Sample X3	H	0.275	0.177	CaGr21	6.71568627	0.06715686	67.156863
A	1	Blank B	A	0.073					
A	2	Sample X1	A	0.494	0.421	CaGc11	18.6764706	0.18676471	186.76471
A	3	Sample X1	A	0.493	0.42	CaGc11	18.627451	0.18627451	186.27451
A	4	Sample X1	A	0.491	0.418	CaGc11	18.5294118	0.18529412	185.29412
A	5	Blank B	B	0.078					
A	6	Sample X1	B	0.455	0.377	CaGc21	16.5196078	0.16519608	165.19608
A	7	Sample X1	B	0.458	0.38	CaGc21	16.6666667	0.16666667	166.66667
A	8	Sample X1	B	0.459	0.381	CaGc21	16.7156863	0.16715686	167.15686
A	9	Blank B	C	0.082					
A	10	Sample X1	C	0.23	0.148	CaGl11	5.29411765	0.05294118	52.941176
A	11	Sample X1	C	0.233	0.151	CaGl11	5.44117647	0.05441176	54.411765
A	12	Sample X1	C	0.232	0.15	CaGl11	5.39215686	0.05392157	53.921569
B	1	Blank B	D	0.081					
B	2	Sample X1	D	0.472	0.391	CaGl21	17.2058824	0.17205882	172.05882
B	3	Sample X1	D	0.477	0.396	CaGl21	17.4509804	0.1745098	174.5098
B	4	Sample X1	D	0.471	0.39	CaGl21	17.1568627	0.17156863	171.56863

Appendix 2.5 factorial experiment TPC, run 5.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.155					
A	2	Sample X1	A	0.535	0.38	CaSu11	16.6666667	0.25	250
A	3	Sample X1	A	0.533	0.378	CaSu11	16.5686275	0.248529412	248.52941
A	4	Sample X1	A	0.533	0.378	CaSu11	16.5686275	0.248529412	248.52941
A	1	Blank B	A	0.414					
A	2	Sample X1	A	0.689	0.275	CaFr11	11.5196078	0.172794118	172.79412
A	3	Sample X1	A	0.683	0.269	CaFr11	11.2254902	0.168382353	168.38235
A	4	Sample X1	A	0.688	0.274	CaFr11	11.4705882	0.172058824	172.05882
H	1	Blank B	F	0.289					
H	2	Sample X1	F	0.687	0.398	CaFr12	17.5490196	0.263235294	263.23529
H	3	Sample X1	F	0.682	0.393	CaFr12	17.3039216	0.259558824	259.55882
H	4	Sample X1	F	0.689	0.4	CaFr12	17.6470588	0.264705882	264.70588
A	9	Blank B	C	0.233					
A	10	Sample X1	C	0.466	0.233	CaFr21	9.46078431	0.141911765	141.91176
A	11	Sample X1	C	0.463	0.23	CaFr21	9.31372549	0.139705882	139.70588
A	12	Sample X1	C	0.461	0.228	CaFr21	9.21568627	0.138235294	138.23529
B	1	Blank B	D	0.098					
B	2	Sample X1	D	0.274	0.176	CaXy11	6.66666667	0.1	100
B	3	Sample X1	D	0.278	0.18	CaXy11	6.8627451	0.102941176	102.94118
B	4	Sample X1	D	0.273	0.175	CaXy11	6.61764706	0.099264706	99.264706
B	5	Blank B	E	0.12					
B	6	Sample X1	E	0.251	0.131	CaXy12	4.46078431	0.066911765	66.911765
B	7	Sample X1	E	0.255	0.135	CaXy12	4.65686275	0.069852941	69.852941
B	8	Sample X1	E	0.253	0.133	CaXy12	4.55882353	0.068382353	68.382353
B	9	Blank B	F	0.098					
B	10	Sample X1	F	0.219	0.121	CaXy21	3.97058824	0.059558824	59.558824
B	11	Sample X1	F	0.211	0.113	CaXy21	3.57843137	0.053676471	53.676471
B	12	Sample X1	F	0.219	0.121	CaXy21	3.97058824	0.059558824	59.558824
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.233	0.142	CaGr11	5	0.075	75
A	11	Sample X1	C	0.238	0.147	CaGr11	5.24509804	0.078676471	78.676471
A	12	Sample X1	C	0.233	0.142	CaGr11	5	0.075	75
B	1	Blank B	D	0.102					
B	2	Sample X1	D	0.243	0.141	CaGr12	4.95098039	0.074264706	74.264706
B	3	Sample X1	D	0.248	0.146	CaGr12	5.19607843	0.077941176	77.941176
B	4	Sample X1	D	0.246	0.144	CaGr12	5.09803922	0.076470588	76.470588

Appendix 2.5 contd.

B	5	Blank B	E	0.093					
B	6	Sample X1	E	0.177	0.084	CaGr21	2.15686275	0.032352941	32.352941
B	7	Sample X1	E	0.172	0.079	CaGr21	1.91176471	0.028676471	28.676471
B	8	Sample X1	E	0.171	0.078	CaGr21	1.8627451	0.027941176	27.941176
C	1	Blank B	G	0.081					
C	2	Sample X1	G	0.329	0.248	CaGc11	10.1960784	0.152941176	152.94118
C	3	Sample X1	G	0.328	0.247	CaGc11	10.1470588	0.152205882	152.20588
C	4	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.239	0.153	CaGc21	5.53921569	0.083088235	83.088235
C	7	Sample X1	H	0.237	0.151	CaGc21	5.44117647	0.081617647	81.617647
C	8	Sample X1	H	0.231	0.145	CaGc21	5.14705882	0.077205882	77.205882
E	9	Blank B	G	0.108					
E	10	Sample X1	G	0.224	0.116	CaGl11	3.7254902	0.055882353	55.882353
E	11	Sample X1	G	0.225	0.117	CaGl11	3.7745098	0.056617647	56.617647
E	12	Sample X1	G	0.222	0.114	CaGl11	3.62745098	0.054411765	54.411765
F	1	Blank B	H	0.084					
F	2	Sample X1	H	0.212	0.128	CaGl21	4.31372549	0.064705882	64.705882
F	3	Sample X1	H	0.215	0.131	CaGl21	4.46078431	0.066911765	66.911765
F	4	Sample X1	H	0.216	0.132	CaGl21	4.50980392	0.067647059	67.647059

Appendix 2.6 factorial experiment TPC, run 6

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	5	Blank B	B	0.015					
A	6	Sample X1	B	0.463	0.448	CaSu11	20	0.4	400
A	7	Sample X1	B	0.469	0.454	CaSu11	20.29412	0.405882353	405.88235
A	8	Sample X1	B	0.468	0.453	CaSu11	20.2451	0.404901961	404.90196
C	9	Blank B	A	0.015					
C	10	Sample X1	A	0.456	0.441	CaFr11	19.65686	0.393137255	393.13725
C	11	Sample X1	A	0.452	0.437	CaFr11	19.46078	0.389215686	389.21569
C	12	Sample X1	A	0.457	0.442	CaFr11	19.70588	0.394117647	394.11765
D	1	Blank B	B	0.015					
D	2	Sample X1	B	0.593	0.578	CaFr12	26.37255	0.52745098	527.45098
D	3	Sample X1	B	0.592	0.577	CaFr12	26.32353	0.526470588	526.47059
D	4	Sample X1	B	0.591	0.576	CaFr12	26.27451	0.525490196	525.4902
D	5	Blank B	C	0.013					
D	6	Sample X1	C	0.369	0.356	CaFr21	15.4902	0.309803922	309.80392

Appendix 2.6 contd.

D	7	Sample X1	C	0.366	0.353	CaFr21	15.34314	0.306862745	306.86275
D	8	Sample X1	C	0.366	0.353	CaFr21	15.34314	0.306862745	306.86275
D	9	Blank B	D	0.014					
D	10	Sample X1	D	0.247	0.233	CaXy11	9.460784	0.189215686	189.21569
D	11	Sample X1	D	0.247	0.233	CaXy11	9.460784	0.189215686	189.21569
D	12	Sample X1	D	0.243	0.229	CaXy11	9.264706	0.185294118	185.29412
E	1	Blank B	E	0.012					
E	2	Sample X1	E	0.227	0.215	CaXy12	8.578431	0.171568627	171.56863
E	3	Sample X1	E	0.226	0.214	CaXy12	8.529412	0.170588235	170.58824
E	4	Sample X1	E	0.227	0.215	CaXy12	8.578431	0.171568627	171.56863
E	5	Blank B	F	0.013					
E	6	Sample X1	F	0.204	0.191	CaX21	7.401961	0.148039216	148.03922
E	7	Sample X1	F	0.205	0.192	CaXy21	7.45098	0.149019608	149.01961
E	8	Sample X1	F	0.201	0.188	CaXy21	7.254902	0.145098039	145.09804
B	9	Blank B	F	0.019					
B	10	Sample X1	F	0.277	0.258	CaGr11	10.68627	0.21372549	213.72549
B	11	Sample X1	F	0.279	0.26	CaGr11	10.78431	0.215686275	215.68627
B	12	Sample X1	F	0.276	0.257	CaGr11	10.63725	0.212745098	212.7451
C	1	Blank B	G	0.019					
C	2	Sample X1	G	0.278	0.259	CaGr12	10.73529	0.214705882	214.70588
C	3	Sample X1	G	0.276	0.257	CaGr12	10.63725	0.212745098	212.7451
C	4	Sample X1	G	0.272	0.253	CaGr12	10.44118	0.208823529	208.82353
C	5	Blank B	H	0.019					
C	6	Sample X1	H	0.358	0.339	CaGr21	14.65686	0.293137255	293.13725
C	7	Sample X1	H	0.359	0.34	CaGr21	14.70588	0.294117647	294.11765
C	8	Sample X1	H	0.351	0.332	CaGr21	14.31373	0.28627451	286.27451
E	9	Blank B	G	0.018					
E	10	Sample X1	G	0.254	0.236	CaGc11	9.607843	0.192156863	192.15686
E	11	Sample X1	G	0.253	0.235	CaGc11	9.558824	0.191176471	191.17647
E	12	Sample X1	G	0.251	0.233	CaGc11	9.460784	0.189215686	189.21569
F	1	Blank B	H	0.018					
F	2	Sample X1	H	0.197	0.179	CaGc21	6.813725	0.13627451	136.27451
F	3	Sample X1	H	0.194	0.176	CaGc21	6.666667	0.133333333	133.33333
F	4	Sample X1	H	0.194	0.176	CaGc21	6.666667	0.133333333	133.33333
G	9	Blank B	A	0.016					
G	10	Sample X1	A	0.268	0.252	CaGl11	10.39216	0.207843137	207.84314
G	11	Sample X1	A	0.265	0.249	CaGl11	10.2451	0.204901961	204.90196
G	12	Sample X1	A	0.261	0.245	CaGl11	10.04902	0.200980392	200.98039
H	1	Blank B	B	0.018					
H	2	Sample X1	B	0.226	0.208	CaGl21	8.235294	0.164705882	164.70588
H	3	Sample X1	B	0.221	0.203	CaGl21	7.990196	0.159803922	159.80392
H	4	Sample X1	B	0.226	0.208	CaGl21	8.235294	0.164705882	164.70588

Appendix 2.7 factorial experiment TPC run 7

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
C	9	Blank B	A	0.261					
C	10	Sample X1	A	0.516	0.255	CaSu11	10.5392157	0.210784314	210.784314
C	11	Sample X1	A	0.511	0.25	CaSu11	10.2941176	0.205882353	205.882353
C	12	Sample X1	A	0.519	0.258	CaSu11	10.6862745	0.21372549	213.72549
A	1	Blank B	A	0.291					
A	2	Sample X1	A	0.812	0.521	CaFr11	23.5784314	0.471568627	471.568627
A	3	Sample X1	A	0.816	0.525	CaFr11	23.7745098	0.475490196	475.490196
A	4	Sample X1	A	0.817	0.526	CaFr11	23.8235294	0.476470588	476.470588
A	5	Blank B	B	0.25					
A	6	Sample X1	B	0.946	0.696	CaFr12	32.1568627	0.643137255	643.137255
A	7	Sample X1	B	0.94	0.69	CaFr12	31.8627451	0.637254902	637.254902
A	8	Sample X1	B	0.942	0.692	CaFr12	31.9607843	0.639215686	639.215686
A	9	Blank B	C	0.28					
A	10	Sample X1	C	0.515	0.235	CaFr21	9.55882353	0.191176471	191.176471
A	11	Sample X1	C	0.514	0.234	CaFr21	9.50980392	0.190196078	190.196078
A	12	Sample X1	C	0.513	0.233	CaFr21	9.46078431	0.189215686	189.215686
	1	Blank B	D	0.102					
B	2	Sample X1	D	0.473	0.371	CaXy11	16.2254902	0.324509804	324.509804
B	3	Sample X1	D	0.473	0.371	CaXy11	16.2254902	0.324509804	324.509804
B	4	Sample X1	D	0.479	0.377	CaXy11	16.5196078	0.330392157	330.392157
B	5	Blank B	E	0.127					
B	6	Sample X1	E	0.469	0.342	CaXy12	14.8039216	0.296078431	296.078431
B	7	Sample X1	E	0.467	0.34	CaXy12	14.7058824	0.294117647	294.117647
B	8	Sample X1	E	0.466	0.339	CaXy12	14.6568627	0.293137255	293.137255
B	9	Blank B	F	0.108					
B	10	Sample X1	F	0.394	0.286	CaXy21	12.0588235	0.241176471	241.176471
B	11	Sample X1	F	0.392	0.284	CaXy21	11.9607843	0.239215686	239.215686
B	12	Sample X1	F	0.394	0.286	CaXy21	12.0588235	0.241176471	241.176471
D	1	Blank B	B	0.093					
D	2	Sample X1	B	0.387	0.294	CaGr11	12.4509804	0.249019608	249.019608
D	3	Sample X1	B	0.389	0.296	CaGr11	12.5490196	0.250980392	250.980392
D	4	Sample X1	B	0.388	0.295	CaGr11	12.5	0.25	250
D	5	Blank B	C	0.094					
D	6	Sample X1	C	0.415	0.321	CaGr12	13.7745098	0.275490196	275.490196
D	7	Sample X1	C	0.413	0.319	CaGr12	13.6764706	0.273529412	273.529412
D	8	Sample X1	C	0.417	0.323	CaGr12	13.872549	0.27745098	277.45098

Appendix 2.7 contd.

D	9	Blank B	D	0.085					
D	10	Sample X1	D	0.349	0.264	CaGr21	10.9803922	0.219607843	219.607843
D	11	Sample X1	D	0.347	0.262	CaGr21	10.8823529	0.217647059	217.647059
D	12	Sample X1	D	0.342	0.257	CaGr21	10.6372549	0.212745098	212.745098
C	1	Blank B	G	0.082					
C	2	Sample X1	G	0.285	0.203	CaGc11	7.99019608	0.159803922	159.803922
C	3	Sample X1	G	0.287	0.205	CaGc11	8.08823529	0.161764706	161.764706
C	4	Sample X1	G	0.286	0.204	CaGc11	8.03921569	0.160784314	160.784314
C	5	Blank B	H	0.087					
C	6	Sample X1	H	0.337	0.25	CaGc21	10.2941176	0.205882353	205.882353
C	7	Sample X1	H	0.332	0.245	CaGc21	10.0490196	0.200980392	200.980392
C	8	Sample X1	H	0.335	0.248	CaGc21	10.1960784	0.203921569	203.921569
H	5	Blank B	G	0.109					
H	6	Sample X1	G	0.389	0.28	CaGl11	11.7647059	0.235294118	235.294118
H	7	Sample X1	G	0.381	0.272	CaGl11	11.372549	0.22745098	227.45098
H	8	Sample X1	G	0.382	0.273	CaGl11	11.4215686	0.228431373	228.431373
H	9	Blank B	H	0.086					
H	10	Sample X1	H	0.434	0.348	CaGl21	15.0980392	0.301960784	301.960784
H	11	Sample X1	H	0.433	0.347	CaGl21	15.0490196	0.300980392	300.980392
H	12	Sample X1	H	0.431	0.345	CaGl21	14.9509804	0.299019608	299.019608

Appendix 2.8 factorial experiment TPC run 8

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.212					
A	2	Sample X1	A	0.573	0.361	CaSu11	15.7352941	0.15735294	157.3529412
A	3	Sample X1	A	0.575	0.363	CaSu11	15.8333333	0.15833333	158.3333333
A	4	Sample X1	A	0.571	0.359	CaSu11	15.6372549	0.15637255	156.372549
E	1	Blank B	A	0.262					
E	2	Sample X1	A	0.756	0.494	CaFr11	22.254902	0.22254902	222.5490196
E	3	Sample X1	A	0.758	0.496	CaFr11	22.3529412	0.22352941	223.5294118
E	4	Sample X1	A	0.752	0.49	CaFr11	22.0588235	0.22058824	220.5882353
E	5	Blank B	B	0.261					
E	6	Sample X1	B	0.684	0.423	CaFr12	18.7745098	0.1877451	187.745098
E	7	Sample X1	B	0.683	0.422	CaFr12	18.7254902	0.1872549	187.254902
E	8	Sample X1	B	0.686	0.425	CaFr12	18.872549	0.18872549	188.7254902
E	9	Blank B	C	0.26					
E	10	Sample X1	C	0.347	0.087	CaFr21	2.30392157	0.02303922	23.03921569

Appendix 2.8 contd.

E	11	Sample X1	C	0.344	0.084	CaFr21	2.15686275	0.02156863	21.56862745
E	12	Sample X1	C	0.341	0.081	CaFr21	2.00980392	0.02009804	20.09803922
F	1	Blank B	D	0.106					
F	2	Sample X1	D	0.259	0.153	CaXy11	5.53921569	0.05539216	55.39215686
F	3	Sample X1	D	0.256	0.15	CaXy11	5.39215686	0.05392157	53.92156863
F	4	Sample X1	D	0.256	0.15	CaXy11	5.39215686	0.05392157	53.92156863
F	5	Blank B	E	0.102					
F	6	Sample X1	E	0.23	0.128	CaXy12	4.31372549	0.04313725	43.1372549
F	7	Sample X1	E	0.23	0.128	CaXy12	4.31372549	0.04313725	43.1372549
F	8	Sample X1	E	0.231	0.129	CaXy12	4.3627451	0.04362745	43.62745098
F	9	Blank B	F	0.101					
F	10	Sample X1	F	0.21	0.109	CaXy21	3.38235294	0.03382353	33.82352941
F	11	Sample X1	F	0.212	0.111	CaXy21	3.48039216	0.03480392	34.80392157
F	12	Sample X1	F	0.21	0.109	CaXy21	3.38235294	0.03382353	33.82352941
A	5	Blank B	B	0.089					
A	6	Sample X1	B	0.305	0.216	CaGr11	8.62745098	0.08627451	86.2745098
A	7	Sample X1	B	0.301	0.212	CaGr11	8.43137255	0.08431373	84.31372549
A	8	Sample X1	B	0.308	0.219	CaGr11	8.7745098	0.0877451	87.74509804
A	9	Blank B	C	0.084					
A	10	Sample X1	C	0.277	0.193	CaGr12	7.5	0.075	75
A	11	Sample X1	C	0.275	0.191	CaGr12	7.40196078	0.07401961	74.01960784
A	12	Sample X1	C	0.276	0.192	CaGr12	7.45098039	0.07450980	74.50980392
B	1	Blank B	D	0.081					
B	2	Sample X1	D	0.247	0.166	CaGr21	6.17647059	0.06176471	61.76470588
B	3	Sample X1	D	0.249	0.168	CaGr21	6.2745098	0.0627451	62.74509804
B	4	Sample X1	D	0.262	0.181	CaGr21	6.91176471	0.06911765	69.11764706
G	1	Blank B	G	0.083					
G	2	Sample X1	G	0.234	0.151	CaGc11	5.44117647	0.05441176	54.41176471
G	3	Sample X1	G	0.238	0.155	CaGc11	5.6372549	0.05637255	56.37254902
G	4	Sample X1	G	0.236	0.153	CaGc11	5.53921569	0.05539216	55.39215686
G	5	Blank B	H	0.083					
G	6	Sample X1	H	0.219	0.136	CaGc21	4.70588235	0.04705882	47.05882353
G	7	Sample X1	H	0.215	0.132	CaGc21	4.50980392	0.04509804	45.09803922
G	8	Sample X1	H	0.217	0.134	CaGc21	4.60784314	0.04607843	46.07843137
B	5	Blank B	E	0.081					
B	6	Sample X1	E	0.265	0.184	CaGl11	7.05882353	0.07058824	70.58823529
B	7	Sample X1	E	0.262	0.181	CaGl11	6.91176471	0.06911765	69.11764706
B	8	Sample X1	E	0.265	0.184	CaGl11	7.05882353	0.07058824	70.58823529
B	9	Blank B	F	0.084					
B	10	Sample X1	F	0.199	0.115	CaGl21	3.67647059	0.03676471	36.76470588
B	11	Sample X1	F	0.193	0.109	CaGl21	3.38235294	0.03382353	33.82352941
B	12	Sample X1	F	0.197	0.113	CaGl21	3.57843137	0.03578431	35.78431373

Appendix 2.9 factorial experiment TPC run 9.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
G	1	Blank B	C	0.016					
G	2	Sample X1	C	0.691	0.675	CaSu11	31.12745098	0.46691176	466.9118
G	3	Sample X1	C	0.691	0.675	CaSu11	31.12745098	0.46691176	466.9118
G	4	Sample X1	C	0.691	0.675	CaSu11	31.12745098	0.46691176	466.9118
A	11	Blank B	A	0.057					
A	12	Sample X1	A	0.765	0.708	CaFr11	32.74509804	0.49117647	491.1765
B	11	Sample X1	A	0.763	0.706	CaFr11	32.64705882	0.48970588	489.7059
B	12	Sample X1	A	0.767	0.71	CaFr11	32.84313725	0.49264706	492.6471
C	11	Blank B	B	0.014					
C	12	Sample X1	B	0.588	0.574	CaFr12	26.17647059	0.39264706	392.6471
D	11	Sample X1	B	0.589	0.575	CaFr12	26.2254902	0.39338235	393.3824
D	12	Sample X1	B	0.589	0.575	CaFr12	26.2254902	0.39338235	393.3824
G	5	Blank B	D	0.017					
G	6	Sample X1	D	0.321	0.304	CaFr21	12.94117647	0.19411765	194.1176
G	7	Sample X1	D	0.324	0.307	CaFr21	13.08823529	0.19632353	196.3235
G	8	Sample X1	D	0.324	0.307	CaFr21	13.08823529	0.19632353	196.3235
C	1	Blank B	A	0.018					
C	2	Sample X1	A	0.294	0.276	CaXy11	11.56862745	0.17352941	173.5294
C	3	Sample X1	A	0.297	0.279	CaXy11	11.71568627	0.17573529	175.7353
C	4	Sample X1	A	0.296	0.278	CaXy11	11.66666667	0.175	175
C	9	Blank B	B	0.018					
C	10	Sample X1	B	0.121	0.103	CaXy12	3.088235294	0.04632353	46.32353
C	11	Sample X1	B	0.123	0.105	CaXy12	3.18627451	0.04779412	47.79412
C	12	Sample X1	B	0.126	0.108	CaXy12	3.333333333	0.05	50
D	1	Blank B	C	0.018					
D	2	Sample X1	C	0.228	0.21	CaXy21	8.333333333	0.125	125
D	3	Sample X1	C	0.228	0.21	CaXy21	8.333333333	0.125	125
D	4	Sample X1	C	0.228	0.21	CaXy21	8.333333333	0.125	125
D	5	Blank B	D	0.018					
D	6	Sample X1	D	0.243	0.225	CaGr11	9.068627451	0.13602941	136.0294
D	7	Sample X1	D	0.246	0.228	CaGr11	9.215686275	0.13823529	138.2353
D	8	Sample X1	D	0.246	0.228	CaGr11	9.215686275	0.13823529	138.2353
D	9	Blank B	E	0.018					
D	10	Sample X1	E	0.275	0.257	CaGr12	10.6372549	0.15955882	159.5588
D	11	Sample X1	E	0.271	0.253	CaGr12	10.44117647	0.15661765	156.6176
D	12	Sample X1	E	0.273	0.255	CaGr12	10.53921569	0.15808824	158.0882
E	1	Blank B	F	0.018					
E	2	Sample X1	F	0.241	0.223	CaGr21	8.970588235	0.13455882	134.5588

Appendix 2.9 contd.

E	3	Sample X1	F	0.241	0.223	CaGr21	8.970588235	0.13455882	134.5588
E	4	Sample X1	F	0.249	0.231	CaGr21	9.362745098	0.14044118	140.4412
E	5	Blank B	G	0.018					
E	6	Sample X1	G	0.254	0.236	CaGc11	9.607843137	0.14411765	144.1176
E	7	Sample X1	G	0.252	0.234	CaGc11	9.509803922	0.14264706	142.6471
E	8	Sample X1	G	0.257	0.239	CaGc11	9.754901961	0.14632353	146.3235
E	9	Blank B	H	0.018					
E	10	Sample X1	H	0.188	0.17	CaGc21	6.37254902	0.09558824	95.58824
E	11	Sample X1	H	0.184	0.166	CaGc21	6.176470588	0.09264706	92.64706
E	12	Sample X1	H	0.183	0.165	CaGc21	6.12745098	0.09191176	91.91176
F	1	Blank B	A	0.017					
F	2	Sample X1	A	0.305	0.288	CaGl11	12.15686275	0.18235294	182.3529
F	3	Sample X1	A	0.301	0.284	CaGl11	11.96078431	0.17941176	179.4118
F	4	Sample X1	A	0.308	0.291	CaGl11	12.30392157	0.18455882	184.5588
F	5	Blank B	B	0.017					
F	6	Sample X1	B	0.221	0.204	CaGl21	8.039215686	0.12058824	120.5882
F	7	Sample X1	B	0.229	0.212	CaGl21	8.431372549	0.12647059	126.4706
F	8	Sample X1	B	0.22	0.203	CaGl21	7.990196078	0.11985294	119.8529

Appendix 2.10 factorial experiment TPC run 10.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	5	Blank B	F	0.277					
E	6	Sample X1	F	0.462	0.185	CaSu11	7.10784314	0.14215686	142.156863
E	7	Sample X1	F	0.468	0.191	CaSu11	7.40196078	0.14803922	148.039216
E	8	Sample X1	F	0.462	0.185	CaSu11	7.10784314	0.14215686	142.156863
F	5	Blank B	A	0.439					
F	6	Sample X1	A	0.726	0.287	CaFr11	12.1078431	0.24215686	242.156863
F	7	Sample X1	A	0.727	0.288	CaFr11	12.1568627	0.24313725	243.137255
F	8	Sample X1	A	0.726	0.287	CaFr11	12.1078431	0.24215686	242.156863
F	9	Blank B	B	0.196					
F	10	Sample X1	B	1.022	0.826	CaFr12	38.5294118	0.77058824	770.588235
F	11	Sample X1	B	1.027	0.831	CaFr12	38.7745098	0.7754902	775.490196
F	12	Sample X1	B	1.027	0.831	CaFr12	38.7745098	0.7754902	775.490196
G	1	Blank B	C	0.26					
G	2	Sample X1	C	0.413	0.153	CaFr21	5.53921569	0.11078431	110.784314
G	3	Sample X1	C	0.411	0.151	CaFr21	5.44117647	0.10882353	108.823529
G	4	Sample X1	C	0.416	0.156	CaFr21	5.68627451	0.11372549	113.72549

Appendix 2.10 contd.

G	5	Blank B	D	0.098					
G	6	Sample X1	D	0.229	0.131	CaXy11	4.46078431	0.08921569	89.2156863
G	7	Sample X1	D	0.227	0.129	CaXy11	4.3627451	0.0872549	87.254902
G	8	Sample X1	D	0.221	0.123	CaXy11	4.06862745	0.08137255	81.372549
G	9	Blank B	E	0.111					
G	10	Sample X1	E	0.264	0.153	CaXy12	5.53921569	0.11078431	110.784314
G	11	Sample X1	E	0.261	0.15	CaXy12	5.39215686	0.10784314	107.843137
G	12	Sample X1	E	0.262	0.151	CaXy12	5.44117647	0.10882353	108.823529
H	1	Blank B	F	0.101					
H	2	Sample X1	F	0.204	0.103	CaXy21	3.08823529	0.06176471	61.7647059
H	3	Sample X1	F	0.203	0.102	CaXy21	3.03921569	0.06078431	60.7843137
H	4	Sample X1	F	0.207	0.106	CaXy21	3.23529412	0.06470588	64.7058824
C	9	Blank B	A	0.078					
C	10	Sample X1	A	0.254	0.176	CaGr11	6.66666667	0.13333333	133.333333
C	11	Sample X1	A	0.253	0.175	CaGr11	6.61764706	0.13235294	132.352941
C	12	Sample X1	A	0.251	0.173	CaGr11	6.51960784	0.13039216	130.392157
D	1	Blank B	B	0.093					
D	2	Sample X1	B	0.265	0.172	CaGr12	6.47058824	0.12941176	129.411765
D	3	Sample X1	B	0.264	0.171	CaGr12	6.42156863	0.12843137	128.431373
D	4	Sample X1	B	0.269	0.176	CaGr12	6.66666667	0.13333333	133.333333
D	5	Blank B	C	0.088					
D	6	Sample X1	C	0.256	0.168	CaGr21	6.2745098	0.1254902	125.490196
D	7	Sample X1	C	0.256	0.168	CaGr21	6.2745098	0.1254902	125.490196
D	8	Sample X1	C	0.258	0.17	CaGr21	6.37254902	0.12745098	127.45098
H	5	Blank B	G	0.086					
H	6	Sample X1	G	0.309	0.223	CaGc11	8.97058824	0.17941176	179.411765
H	7	Sample X1	G	0.305	0.219	CaGc11	8.7745098	0.1754902	175.490196
H	8	Sample X1	G	0.303	0.217	CaGc11	8.67647059	0.17352941	173.529412
H	9	Blank B	H	0.082					
H	10	Sample X1	H	0.233	0.151	CaGc21	5.44117647	0.10882353	108.823529
H	11	Sample X1	H	0.236	0.154	CaGc21	5.58823529	0.11176471	111.764706
H	12	Sample X1	H	0.233	0.151	CaGc21	5.44117647	0.10882353	108.823529
D	9	Blank B	D	0.104					
D	10	Sample X1	D	0.219	0.115	CaGl11	3.67647059	0.07352941	73.5294118
D	11	Sample X1	D	0.215	0.111	CaGl11	3.48039216	0.06960784	69.6078431
D	12	Sample X1	D	0.218	0.114	CaGl11	3.62745098	0.07254902	72.5490196
E	1	Blank B	E	0.081					
E	2	Sample X1	E	0.178	0.097	CaGl21	2.79411765	0.05588235	55.8823529
E	3	Sample X1	E	0.174	0.093	CaGl21	2.59803922	0.05196078	51.9607843
E	4	Sample X1	E	0.174	0.093	CaGl21	2.59803922	0.05196078	51.9607843

Appendix 3.1 factorial experiment TFC run 1

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.065				
E	10	Sample X1	A	0.313	0.248	CaSu11	18.789063	281.8359
E	11	Sample X1	A	0.315	0.25	CaSu11	18.945313	284.1797
E	12	Sample X1	A	0.313	0.248	CaSu11	18.789063	281.8359
C	1	Blank B	A	0.09				
C	2	Sample X1	A	0.462	0.372	CaFr11	28.476563	427.1484
C	3	Sample X1	A	0.462	0.372	CaFr11	28.476563	427.1484
C	4	Sample X1	A	0.463	0.373	CaFr11	28.554688	428.3203
C	5	Blank B	B	0.059				
C	6	Sample X1	B	0.412	0.353	CaFr12	26.992188	404.8828
C	7	Sample X1	B	0.412	0.353	CaFr12	26.992188	404.8828
C	8	Sample X1	B	0.416	0.357	CaFr12	27.304688	409.5703
C	9	Blank B	C	0.074				
C	10	Sample X1	C	0.405	0.331	CaFr21	25.273438	379.1016
C	11	Sample X1	C	0.401	0.327	CaFr21	24.960938	374.4141
C	12	Sample X1	C	0.405	0.331	CaFr21	25.273438	379.1016
D	1	Blank B	D	0.045				
D	2	Sample X1	D	0.154	0.109	CaXy11	7.9296875	118.9453
D	3	Sample X1	D	0.151	0.106	CaXy11	7.6953125	115.4297
D	4	Sample X1	D	0.151	0.106	CaXy11	7.6953125	115.4297
D	5	Blank B	E	0.055				
D	6	Sample X1	E	0.268	0.213	CaXy12	16.054688	240.8203
D	7	Sample X1	E	0.268	0.213	CaXy12	16.054688	240.8203
D	8	Sample X1	E	0.269	0.214	CaXy12	16.132813	241.9922
D	9	Blank B	F	0.057				
D	10	Sample X1	F	0.216	0.159	CaXy21	11.835938	177.5391
D	11	Sample X1	F	0.213	0.156	CaXy21	11.601563	174.0234
D	12	Sample X1	F	0.213	0.156	CaXy21	11.601563	174.0234
F	1	Blank B	B	0.056				
F	2	Sample X1	B	0.183	0.127	CaGr11	9.3359375	140.0391
F	3	Sample X1	B	0.185	0.129	CaGr11	9.4921875	142.3828
F	4	Sample X1	B	0.185	0.129	CaGr11	9.4921875	142.3828
F	5	Blank B	C	0.05				
F	6	Sample X1	C	0.155	0.105	CaGr12	7.6171875	114.2578
F	7	Sample X1	C	0.152	0.102	CaGr12	7.3828125	110.7422
F	8	Sample X1	C	0.152	0.102	CaGr12	7.3828125	110.7422
F	9	Blank B	D	0.063				
F	10	Sample X1	D	0.166	0.103	CaGr21	7.4609375	111.9141

Appendix 3.1 contd.

F	11	Sample X1	D	0.169	0.106	CaGr21	7.6953125	115.4297
F	12	Sample X1	D	0.169	0.106	CaGr21	7.6953125	115.4297
G	1	Blank B	E	0.054				
G	2	Sample X1	E	0.953	0.899	CaGc11	69.648438	1044.727
G	3	Sample X1	E	0.951	0.897	CaGc11	69.492188	1042.383
G	4	Sample X1	E	0.951	0.897	CaGc11	69.492188	1042.383
G	5	Blank B	F	0.05				
G	6	Sample X1	F	0.587	0.537	CaGc21	41.367188	620.5078
G	7	Sample X1	F	0.589	0.539	CaGc21	41.523438	622.8516
G	8	Sample X1	F	0.589	0.539	CaGc21	41.523438	622.8516
E	1	Blank B	G	0.059				
E	2	Sample X1	G	0.196	0.137	CaGl11	10.117188	151.7578
E	3	Sample X1	G	0.196	0.137	CaGl11	10.117188	151.7578
E	4	Sample X1	G	0.198	0.139	CaGl11	10.273438	154.1016
E	5	Blank B	H	0.061				
E	6	Sample X1	H	0.345	0.284	CaGl21	21.601563	324.0234
E	7	Sample X1	H	0.345	0.284	CaGl21	21.601563	324.0234
E	8	Sample X1	H	0.346	0.285	CaGl21	21.679688	325.1953

Appendix 3.2 factorial experiment TFC run 2.

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC(µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.063				
C	10	Sample X1	A	0.247	0.184	CaSu11	13.7890625	275.78125
C	11	Sample X1	A	0.248	0.185	CaSu11	13.8671875	277.34375
C	12	Sample X1	A	0.247	0.184	CaSu11	13.7890625	275.78125
A	1	Blank B	A	0.071				
A	2	Sample X1	A	0.195	0.124	CaFr11	9.1015625	182.03125
A	3	Sample X1	A	0.191	0.12	CaFr11	8.7890625	175.78125
A	4	Sample X1	A	0.194	0.123	CaFr11	9.0234375	180.46875
A	5	Blank B	B	0.057				
A	6	Sample X1	B	0.151	0.094	CaFr12	6.7578125	135.15625
A	7	Sample X1	B	0.155	0.098	CaFr12	7.0703125	141.40625
A	8	Sample X1	B	0.153	0.096	CaFr12	6.9140625	138.28125
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.202	0.15	CaFr21	11.1328125	222.65625
A	11	Sample X1	C	0.204	0.152	CaFr21	11.2890625	225.78125
A	12	Sample X1	C	0.208	0.156	CaFr21	11.6015625	232.03125
B	1	Blank B	D	0.05				

Appendix 3.2 contd.

B	2	Sample X1	D	0.131	0.081	CaXy11	5.7421875	114.84375
B	3	Sample X1	D	0.136	0.086	CaXy11	6.1328125	122.65625
B	4	Sample X1	D	0.139	0.089	CaXy11	6.3671875	127.34375
B	5	Blank B	E	0.049				
B	6	Sample X1	E	0.123	0.074	CaXy12	5.1953125	103.90625
B	7	Sample X1	E	0.127	0.078	CaXy12	5.5078125	110.15625
B	8	Sample X1	E	0.122	0.073	CaXy12	5.1171875	102.34375
B	9	Blank B	F	0.048				
B	10	Sample X1	F	0.133	0.085	CaXy21	6.0546875	121.09375
B	11	Sample X1	F	0.137	0.089	CaXy21	6.3671875	127.34375
B	12	Sample X1	F	0.131	0.083	CaXy21	5.8984375	117.96875
D	1	Blank B	B	0.059				
D	2	Sample X1	B	0.171	0.112	CaGr11	8.1640625	163.28125
D	3	Sample X1	B	0.175	0.116	CaGr11	8.4765625	169.53125
D	4	Sample X1	B	0.173	0.114	CaGr11	8.3203125	166.40625
D	5	Blank B	C	0.056				
D	6	Sample X1	C	0.157	0.101	CaGr12	7.3046875	146.09375
D	7	Sample X1	C	0.155	0.099	CaGr12	7.1484375	142.96875
D	8	Sample X1	C	0.157	0.101	CaGr12	7.3046875	146.09375
D	9	Blank B	D	0.059				
D	10	Sample X1	D	0.166	0.107	CaGr21	7.7734375	155.46875
D	11	Sample X1	D	0.169	0.11	CaGr21	8.0078125	160.15625
D	12	Sample X1	D	0.165	0.106	CaGr21	7.6953125	153.90625
E	1	Blank B	E	0.063				
E	2	Sample X1	E	0.792	0.729	CaGc11	56.3671875	1127.34375
E	3	Sample X1	E	0.791	0.728	CaGc11	56.2890625	1125.78125
E	4	Sample X1	E	0.792	0.729	CaGc11	56.3671875	1127.34375
E	5	Blank B	F	0.052				
E	6	Sample X1	F	0.145	0.093	CaGc21	6.6796875	133.59375
E	7	Sample X1	F	0.148	0.096	CaGc21	6.9140625	138.28125
E	8	Sample X1	F	0.149	0.097	CaGc21	6.9921875	139.84375
C	1	Blank B	G	0.089				
C	2	Sample X1	G	0.532	0.443	CaGl11	34.0234375	680.46875
C	3	Sample X1	G	0.533	0.444	CaGl11	34.1015625	682.03125
C	4	Sample X1	G	0.536	0.447	CaGl11	34.3359375	686.71875
C	5	Blank B	H	0.058				
C	6	Sample X1	H	0.315	0.257	CaGl21	19.4921875	389.84375
C	7	Sample X1	H	0.315	0.257	CaGl21	19.4921875	389.84375
C	8	Sample X1	H	0.311	0.253	CaGl21	19.1796875	383.59375

Appendix 3.3 factorial experiment TFC run 3

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.055				
C	10	Sample X1	A	0.493	0.438	CaSu11	33.6328125	672.65625
C	11	Sample X1	A	0.494	0.439	CaSu11	33.7109375	674.21875
C	12	Sample X1	A	0.499	0.444	CaSu11	34.1015625	682.03125
A	1	Blank B	A	0.051				
A	2	Sample X1	A	0.855	0.804	CaFr11	62.2265625	1244.53125
A	3	Sample X1	A	0.855	0.804	CaFr11	62.2265625	1244.53125
A	4	Sample X1	A	0.852	0.801	CaFr11	61.9921875	1239.84375
A	5	Blank B	B	0.055				
A	6	Sample X1	B	0.407	0.352	CaFr12	26.9140625	538.28125
A	7	Sample X1	B	0.407	0.352	CaFr12	26.9140625	538.28125
A	8	Sample X1	B	0.408	0.353	CaFr12	26.9921875	539.84375
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.402	0.35	CaFr21	26.7578125	535.15625
A	11	Sample X1	C	0.402	0.35	CaFr21	26.7578125	535.15625
A	12	Sample X1	C	0.404	0.352	CaFr21	26.9140625	538.28125
B	1	Blank B	D	0.057				
B	2	Sample X1	D	0.257	0.2	CaXy11	15.0390625	300.78125
B	3	Sample X1	D	0.254	0.197	CaXy11	14.8046875	296.09375
B	4	Sample X1	D	0.254	0.197	CaXy11	14.8046875	296.09375
B	5	Blank B	E	0.049				
B	6	Sample X1	E	0.632	0.583	CaXy12	44.9609375	899.21875
B	7	Sample X1	E	0.635	0.586	CaXy12	45.1953125	903.90625
B	8	Sample X1	E	0.637	0.588	CaXy12	45.3515625	907.03125
B	9	Blank B	F	0.044				
B	10	Sample X1	F	0.261	0.217	CaXy21	16.3671875	327.34375
B	11	Sample X1	F	0.265	0.221	CaXy21	16.6796875	333.59375
B	12	Sample X1	F	0.262	0.218	CaXy21	16.4453125	328.90625
D	1	Blank B	B	0.057				
D	2	Sample X1	B	0.285	0.228	CaGr11	17.2265625	344.53125
D	3	Sample X1	B	0.289	0.232	CaGr11	17.5390625	350.78125
D	4	Sample X1	B	0.289	0.232	CaGr11	17.5390625	350.78125
D	5	Blank B	C	0.057				
D	6	Sample X1	C	0.314	0.257	CaGr12	19.4921875	389.84375
D	7	Sample X1	C	0.313	0.256	CaGr12	19.4140625	388.28125
D	8	Sample X1	C	0.314	0.257	CaGr12	19.4921875	389.84375
D	9	Blank B	D	0.06				
D	10	Sample X1	D	0.211	0.151	CaGr21	11.2109375	224.21875

Appendix 3.3 contd.

D	11	Sample X1	D	0.211	0.151	CaGr21	11.2109375	224.21875
D	12	Sample X1	D	0.212	0.152	CaGr21	11.2890625	225.78125
E	1	Blank B	E	0.059				
E	2	Sample X1	E	0.981	0.922	CaGc11	71.4453125	1428.90625
E	3	Sample X1	E	0.984	0.925	CaGc11	71.6796875	1433.59375
E	4	Sample X1	E	0.983	0.924	CaGc11	71.6015625	1432.03125
E	5	Blank B	F	0.052				
E	6	Sample X1	F	0.689	0.637	CaGc21	49.1796875	983.59375
E	7	Sample X1	F	0.689	0.637	CaGc21	49.1796875	983.59375
E	8	Sample X1	F	0.683	0.631	CaGc21	48.7109375	974.21875
C	1	Blank B	G	0.066				
C	2	Sample X1	G	0.312	0.246	CaGl11	18.6328125	372.65625
C	3	Sample X1	G	0.311	0.245	CaGl11	18.5546875	371.09375
C	4	Sample X1	G	0.312	0.246	CaGl11	18.6328125	372.65625
C	5	Blank B	H	0.052				
C	6	Sample X1	H	0.234	0.182	CaGl21	13.6328125	272.65625
C	7	Sample X1	H	0.232	0.18	CaGl21	13.4765625	269.53125
C	8	Sample X1	H	0.232	0.18	CaGl21	13.4765625	269.53125

Appendix 3.4 factorial experiment TFC run 4

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.055				
C	10	Sample X1	A	0.215	0.16	CaSu11	11.914063	119.1406
C	11	Sample X1	A	0.216	0.161	CaSu11	11.992188	119.9219
C	12	Sample X1	A	0.215	0.16	CaSu11	11.914063	119.1406
A	1	Blank B	A	0.075				
A	2	Sample X1	A	0.414	0.339	CaFr11	25.898438	258.9844
A	3	Sample X1	A	0.413	0.338	CaFr11	25.820313	258.2031
A	4	Sample X1	A	0.413	0.338	CaFr11	25.820313	258.2031
A	5	Blank B	B	0.057				
A	6	Sample X1	B	0.216	0.159	CaFr12	11.835938	118.3594
A	7	Sample X1	B	0.216	0.159	CaFr12	11.835938	118.3594
A	8	Sample X1	B	0.212	0.155	CaFr12	11.523438	115.2344
A	9	Blank B	C	0.051				
A	10	Sample X1	C	0.248	0.197	CaFr21	14.804688	148.0469
A	11	Sample X1	C	0.248	0.197	CaFr21	14.804688	148.0469
A	12	Sample X1	C	0.245	0.194	CaFr21	14.570313	145.7031

Appendix 3.4 contd.

B	1	Blank B	D	0.048				
B	2	Sample X1	D	0.194	0.146	CaXy11	10.820313	108.2031
B	3	Sample X1	D	0.194	0.146	CaXy11	10.820313	108.2031
B	4	Sample X1	D	0.198	0.15	CaXy11	11.132813	111.3281
B	5	Blank B	E	0.053				
B	6	Sample X1	E	0.151	0.098	CaXy12	7.0703125	70.70313
B	7	Sample X1	E	0.157	0.104	CaXy12	7.5390625	75.39063
B	8	Sample X1	E	0.157	0.104	CaXy12	7.5390625	75.39063
B	9	Blank B	F	0.045				
B	10	Sample X1	F	0.188	0.143	CaXy21	10.585938	105.8594
B	11	Sample X1	F	0.182	0.137	CaXy21	10.117188	101.1719
B	12	Sample X1	F	0.182	0.137	CaXy21	10.117188	101.1719
D	1	Blank B	B	0.072				
D	2	Sample X1	B	0.174	0.102	CaGr11	7.3828125	73.82813
D	3	Sample X1	B	0.172	0.1	CaGr11	7.2265625	72.26563
D	4	Sample X1	B	0.172	0.1	CaGr11	7.2265625	72.26563
D	5	Blank B	C	0.054				
D	6	Sample X1	C	0.158	0.104	CaGr12	7.5390625	75.39063
D	7	Sample X1	C	0.158	0.104	CaGr12	7.5390625	75.39063
D	8	Sample X1	C	0.159	0.105	CaGr12	7.6171875	76.17188
D	9	Blank B	D	0.049				
D	10	Sample X1	D	0.183	0.134	Gr21	9.8828125	98.82813
D	11	Sample X1	D	0.183	0.134	Gr21	9.8828125	98.82813
D	12	Sample X1	D	0.181	0.132	Gr21	9.7265625	97.26563
E	1	Blank B	E	0.057				
E	2	Sample X1	E	0.732	0.675	CaGc11	52.148438	521.4844
E	3	Sample X1	E	0.733	0.676	CaGc11	52.226563	522.2656
E	4	Sample X1	E	0.732	0.675	CaGc11	52.148438	521.4844
E	5	Blank B	F	0.064				
E	6	Sample X1	F	0.917	0.853	CaGc21	66.054688	660.5469
E	7	Sample X1	F	0.918	0.854	CaGc21	66.132813	661.3281
E	8	Sample X1	F	0.917	0.853	CaGc21	66.054688	660.5469
C	1	Blank B	G	0.057				
C	2	Sample X1	G	0.188	0.131	CaGl11	9.6484375	96.48438
C	3	Sample X1	G	0.187	0.13	CaGl11	9.5703125	95.70313
C	4	Sample X1	G	0.187	0.13	CaGl11	9.5703125	95.70313
C	5	Blank B	H	0.051				
C	6	Sample X1	H	0.188	0.137	CaGl21	10.117188	101.1719
C	7	Sample X1	H	0.188	0.137	CaGl21	10.117188	101.1719
C	8	Sample X1	H	0.186	0.135	CaGl21	9.9609375	99.60938

Appendix 3.5 factorial experiment TFC run 5.

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.061				
E	10	Sample X1	A	0.216	0.155	CaSu11	11.5234375	115.234375
E	11	Sample X1	A	0.216	0.155	CaSu11	11.5234375	115.234375
E	12	Sample X1	A	0.214	0.153	CaSu11	11.3671875	113.671875
C	1	Blank B	A	0.078				
C	2	Sample X1	A	0.369	0.291	CaFr11	22.1484375	221.484375
C	3	Sample X1	A	0.367	0.289	CaFr11	21.9921875	219.921875
C	4	Sample X1	A	0.367	0.289	CaFr11	21.9921875	219.921875
C	5	Blank B	B	0.06				
C	6	Sample X1	B	0.234	0.174	CaFr12	13.0078125	130.078125
C	7	Sample X1	B	0.232	0.172	CaFr12	12.8515625	128.515625
C	8	Sample X1	B	0.234	0.174	CaFr12	13.0078125	130.078125
C	9	Blank B	C	0.054				
C	10	Sample X1	C	0.283	0.229	CaFr21	17.3046875	173.046875
C	11	Sample X1	C	0.283	0.229	CaFr21	17.3046875	173.046875
C	12	Sample X1	C	0.281	0.227	CaFr21	17.1484375	171.484375
D	1	Blank B	D	0.061				
D	2	Sample X1	D	0.227	0.166	CaXy11	12.3828125	123.828125
D	3	Sample X1	D	0.228	0.167	CaXy11	12.4609375	124.609375
D	4	Sample X1	D	0.226	0.165	CaXy11	12.3046875	123.046875
D	5	Blank B	E	0.057				
D	6	Sample X1	E	0.165	0.108	CaXy12	7.8515625	78.515625
D	7	Sample X1	E	0.162	0.105	CaXy12	7.6171875	76.171875
D	8	Sample X1	E	0.164	0.107	CaXy12	7.7734375	77.734375
D	9	Blank B	F	0.05				
D	10	Sample X1	F	0.202	0.152	CaXy21	11.2890625	112.890625
D	11	Sample X1	F	0.204	0.154	CaXy21	11.4453125	114.453125
D	12	Sample X1	F	0.205	0.155	CaXy21	11.5234375	115.234375
F	1	Blank B	B	0.056				
F	2	Sample X1	B	0.274	0.218	CaGr11	16.4453125	164.453125
F	3	Sample X1	B	0.273	0.217	CaGr11	16.3671875	163.671875
F	4	Sample X1	B	0.274	0.218	CaGr11	16.4453125	164.453125
F	5	Blank B	C	0.046				
F	6	Sample X1	C	0.265	0.219	CaGr12	16.5234375	165.234375
F	7	Sample X1	C	0.269	0.223	CaGr12	16.8359375	168.359375
F	8	Sample X1	C	0.267	0.221	CaGr12	16.6796875	166.796875
F	9	Blank B	D	0.041				
F	10	Sample X1	D	0.217	0.176	CaGr21	13.1640625	131.640625

Appendix 3.5 contd.

F	11	Sample X1	D	0.216	0.175	CaGr21	13.0859375	130.859375
F	12	Sample X1	D	0.214	0.173	CaGr21	12.9296875	129.296875
G	1	Blank B	E	0.056				
G	2	Sample X1	E	0.929	0.873	CaGc11	67.6171875	676.171875
G	3	Sample X1	E	0.93	0.874	CaGc11	67.6953125	676.953125
G	4	Sample X1	E	0.931	0.875	CaGc11	67.7734375	677.734375
G	5	Blank B	F	0.045				
G	6	Sample X1	F	0.713	0.668	CaGc21	51.6015625	516.015625
G	7	Sample X1	F	0.713	0.668	CaGc21	51.6015625	516.015625
G	8	Sample X1	F	0.714	0.669	CaGc21	51.6796875	516.796875
E	1	Blank B	G	0.058				
E	2	Sample X1	G	0.482	0.424	CaGl11	32.5390625	325.390625
E	3	Sample X1	G	0.482	0.424	CaGl11	32.5390625	325.390625
E	4	Sample X1	G	0.483	0.425	CaGl11	32.6171875	326.171875
E	5	Blank B	H	0.05				
E	6	Sample X1	H	0.923	0.873	CaGl21	67.6171875	676.171875
E	7	Sample X1	H	0.924	0.874	CaGl21	67.6953125	676.953125
E	8	Sample X1	H	0.923	0.873	CaGl21	67.6171875	676.171875

Appendix 3.6 factorial experiment TFC run 6

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.06				
A	2	Sample X1	A	0.924	0.864	CaSu11	66.9140625	669.140625
A	3	Sample X1	A	0.924	0.864	CaSu11	66.9140625	669.140625
A	4	Sample X1	A	0.923	0.863	CaSu11	66.8359375	668.359375
E	9	Blank B	A	0.057				
E	10	Sample X1	A	0.888	0.831	CaFr11	64.3359375	643.359375
E	11	Sample X1	A	0.888	0.831	CaFr11	64.3359375	643.359375
E	12	Sample X1	A	0.882	0.825	CaFr11	63.8671875	638.671875
F	1	Blank B	B	0.06				
F	2	Sample X1	B	0.666	0.606	CaFr12	46.7578125	467.578125
F	3	Sample X1	B	0.663	0.603	CaFr12	46.5234375	465.234375
F	4	Sample X1	B	0.666	0.606	CaFr12	46.7578125	467.578125
F	5	Blank B	C	0.056				
F	6	Sample X1	C	0.571	0.515	CaFr21	39.6484375	396.484375
F	7	Sample X1	C	0.574	0.518	CaFr21	39.8828125	398.828125
F	8	Sample X1	C	0.574	0.518	CaFr21	39.8828125	398.828125

Appendix 3.6 contd.

F	9	Blank B	D	0.055				
F	10	Sample X1	D	0.715	0.66	CaXy11	50.9765625	509.765625
F	11	Sample X1	D	0.715	0.66	CaXy11	50.9765625	509.765625
F	12	Sample X1	D	0.716	0.661	CaXy11	51.0546875	510.546875
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.766	0.711	CaXy12	54.9609375	549.609375
G	3	Sample X1	E	0.768	0.713	CaXy12	55.1171875	551.171875
G	4	Sample X1	E	0.766	0.711	CaXy12	54.9609375	549.609375
G	5	Blank B	F	0.056				
G	6	Sample X1	F	0.585	0.529	CaXy21	40.7421875	407.421875
G	7	Sample X1	F	0.586	0.53	CaXy21	40.8203125	408.203125
G	8	Sample X1	F	0.583	0.527	CaXy21	40.5859375	405.859375
A	5	Blank B	B	0.052				
A	6	Sample X1	B	0.997	0.945	CaGr11	73.2421875	732.421875
A	7	Sample X1	B	0.997	0.945	CaGr11	73.2421875	732.421875
A	8	Sample X1	B	0.998	0.946	CaGr11	73.3203125	733.203125
A	9	Blank B	C	0.046				
A	10	Sample X1	C	0.914	0.868	CaGr12	67.2265625	672.265625
A	11	Sample X1	C	0.917	0.871	CaGr12	67.4609375	674.609375
A	12	Sample X1	C	0.917	0.871	CaGr12	67.4609375	674.609375
B	1	Blank B	D	0.054				
B	2	Sample X1	D	0.927	0.873	CaGr21	67.6171875	676.171875
B	3	Sample X1	D	0.926	0.872	CaGr21	67.5390625	675.390625
B	4	Sample X1	D	0.925	0.871	CaGr21	67.4609375	674.609375
B	5	Blank B	E	0.047				
B	6	Sample X1	E	0.833	0.786	CaGc11	60.8203125	608.203125
B	7	Sample X1	E	0.832	0.785	CaGc11	60.7421875	607.421875
B	8	Sample X1	E	0.832	0.785	CaGc11	60.7421875	607.421875
B	9	Blank B	F	0.045				
B	10	Sample X1	F	0.539	0.494	CaGc21	38.0078125	380.078125
B	11	Sample X1	F	0.538	0.493	CaGc21	37.9296875	379.296875
B	12	Sample X1	F	0.538	0.493	CaGc21	37.9296875	379.296875
G	9	Blank B	G	0.069				
G	10	Sample X1	G	0.764	0.695	CaGl11	53.7109375	537.109375
G	11	Sample X1	G	0.769	0.7	CaGl11	54.1015625	541.015625
G	12	Sample X1	G	0.768	0.699	CaGl11	54.0234375	540.234375
H	1	Blank B	H	0.062				
H	2	Sample X1	H	0.638	0.576	CaGl21	44.4140625	444.140625
H	3	Sample X1	H	0.634	0.572	CaGl21	44.1015625	441.015625
H	4	Sample X1	H	0.636	0.574	CaGl21	44.2578125	442.578125

Appendix 3.7 factorial experiment TFC run 7

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.068				
E	10	Sample X1	A	0.496	0.428	CaSu11	32.8515625	657.03125
E	11	Sample X1	A	0.498	0.43	CaSu11	33.0078125	660.15625
E	12	Sample X1	A	0.492	0.424	CaSu11	32.5390625	650.78125
C	1	Blank B	A	0.076				
C	2	Sample X1	A	0.193	0.117	CaFr11	8.5546875	171.09375
C	3	Sample X1	A	0.196	0.12	CaFr11	8.7890625	175.78125
C	4	Sample X1	A	0.194	0.118	CaFr11	8.6328125	172.65625
C	5	Blank B	B	0.056				
C	6	Sample X1	B	0.185	0.129	CaFr12	9.4921875	189.84375
C	7	Sample X1	B	0.184	0.128	CaFr12	9.4140625	188.28125
C	8	Sample X1	B	0.187	0.131	CaFr12	9.6484375	192.96875
C	9	Blank B	C	0.056				
C	10	Sample X1	C	0.244	0.188	CaFr21	14.1015625	282.03125
C	11	Sample X1	C	0.242	0.186	CaFr21	13.9453125	278.90625
C	12	Sample X1	C	0.241	0.185	CaFr21	13.8671875	277.34375
D	1	Blank B	D	0.059				
D	2	Sample X1	D	0.172	0.113	CaXy11	8.2421875	164.84375
D	3	Sample X1	D	0.178	0.119	CaXy11	8.7109375	174.21875
D	4	Sample X1	D	0.178	0.119	CaXy11	8.7109375	174.21875
D	5	Blank B	E	0.052				
D	6	Sample X1	E	0.144	0.092	CaXy12	6.6015625	132.03125
D	7	Sample X1	E	0.146	0.094	CaXy12	6.7578125	135.15625
D	8	Sample X1	E	0.144	0.092	CaXy12	6.6015625	132.03125
D	9	Blank B	F	0.057				
D	10	Sample X1	F	0.158	0.101	CaXy21	7.3046875	146.09375
D	11	Sample X1	F	0.158	0.101	CaXy21	7.3046875	146.09375
D	12	Sample X1	F	0.151	0.094	CaXy21	6.7578125	135.15625
F	1	Blank B	B	0.063				
F	2	Sample X1	B	0.172	0.109	CaGr11	7.9296875	158.59375
F	3	Sample X1	B	0.173	0.11	CaGr11	8.0078125	160.15625
F	4	Sample X1	B	0.173	0.11	CaGr11	8.0078125	160.15625
F	5	Blank B	C	0.051				
F	6	Sample X1	C	0.145	0.094	CaGr12	6.7578125	135.15625
F	7	Sample X1	C	0.149	0.098	CaGr12	7.0703125	141.40625
F	8	Sample X1	C	0.147	0.096	CaGr12	6.9140625	138.28125
F	9	Blank B	D	0.055				
F	10	Sample X1	D	0.185	0.13	CaGr21	9.5703125	191.40625

Appendix 3.7 contd.

F	11	Sample X1	D	0.181	0.126	CaGr21	9.2578125	185.15625
F	12	Sample X1	D	0.183	0.128	CaGr21	9.4140625	188.28125
G	1	Blank B	E	0.061				
G	2	Sample X1	E	0.781	0.72	CaGc11	55.6640625	1113.28125
G	3	Sample X1	E	0.787	0.726	CaGc11	56.1328125	1122.65625
G	4	Sample X1	E	0.789	0.728	CaGc11	56.2890625	1125.78125
G	5	Blank B	F	0.051				
G	6	Sample X1	F	0.246	0.195	CaGc21	14.6484375	292.96875
G	7	Sample X1	F	0.243	0.192	CaGc21	14.4140625	288.28125
G	8	Sample X1	F	0.246	0.195	CaGc21	14.6484375	292.96875
E	1	Blank B	G	0.058				
E	2	Sample X1	G	0.152	0.094	CaGl11	6.7578125	135.15625
E	3	Sample X1	G	0.152	0.094	CaGl11	6.7578125	135.15625
E	4	Sample X1	G	0.155	0.097	CaGl11	6.9921875	139.84375
E	5	Blank B	H	0.059				
E	6	Sample X1	H	0.474	0.415	CaGl21	31.8359375	636.71875
E	7	Sample X1	H	0.474	0.415	CaGl21	31.8359375	636.71875
E	8	Sample X1	H	0.471	0.412	CaGl21	31.6015625	632.03125

Appendix 3.8 factorial experiment TFC run 8

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.072				
A	2	Sample X1	A	0.181	0.109	CaSu11	7.9296875	158.59375
A	3	Sample X1	A	0.183	0.111	CaSu11	8.0859375	161.71875
A	4	Sample X1	A	0.184	0.112	CaSu11	8.1640625	163.28125
E	9	Blank B	A	0.077				
E	10	Sample X1	A	0.383	0.306	CaFr11	23.3203125	466.40625
E	11	Sample X1	A	0.385	0.308	CaFr11	23.4765625	469.53125
E	12	Sample X1	A	0.389	0.312	CaFr11	23.7890625	475.78125
F	1	Blank B	B	0.061				
F	2	Sample X1	B	0.172	0.111	CaFr12	8.0859375	161.71875
F	3	Sample X1	B	0.175	0.114	CaFr12	8.3203125	166.40625
F	4	Sample X1	B	0.177	0.116	CaFr12	8.4765625	169.53125
F	5	Blank B	C	0.021				
F	6	Sample X1	C	0.1	0.079	CaFr21	5.5859375	111.71875
F	7	Sample X1	C	0.102	0.081	CaFr21	5.7421875	114.84375
F	8	Sample X1	C	0.102	0.081	CaFr21	5.7421875	114.84375

Appendix 3.8 contd.

F	9	Blank B	D	0.027				
F	10	Sample X1	D	0.093	0.066	CaXy11	4.5703125	91.40625
F	11	Sample X1	D	0.098	0.071	CaXy11	4.9609375	99.21875
F	12	Sample X1	D	0.099	0.072	CaXy11	5.0390625	100.78125
G	1	Blank B	E	0.053				
G	2	Sample X1	E	0.128	0.075	CaXy12	5.2734375	105.46875
G	3	Sample X1	E	0.127	0.074	CaXy12	5.1953125	103.90625
G	4	Sample X1	E	0.124	0.071	CaXy12	4.9609375	99.21875
G	5	Blank B	F	0.047				
G	6	Sample X1	F	0.132	0.085	CaXy21	6.0546875	121.09375
G	7	Sample X1	F	0.133	0.086	CaXy21	6.1328125	122.65625
G	8	Sample X1	F	0.137	0.09	CaXy21	6.4453125	128.90625
A	5	Blank B	B	0.064				
A	6	Sample X1	B	0.138	0.074	CaGr11	5.1953125	103.90625
A	7	Sample X1	B	0.138	0.074	CaGr11	5.1953125	103.90625
A	8	Sample X1	B	0.138	0.074	CaGr11	5.1953125	103.90625
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.131	0.079	CaGr12	5.5859375	111.71875
A	11	Sample X1	C	0.132	0.08	CaGr12	5.6640625	113.28125
A	12	Sample X1	C	0.134	0.082	CaGr12	5.8203125	116.40625
B	1	Blank B	D	0.061				
B	2	Sample X1	D	0.146	0.085	CaGr21	6.0546875	121.09375
B	3	Sample X1	D	0.143	0.082	CaGr21	5.8203125	116.40625
B	4	Sample X1	D	0.143	0.082	CaGr21	5.8203125	116.40625
B	5	Blank B	E	0.062				
B	6	Sample X1	E	0.736	0.674	CaGc11	52.0703125	1041.40625
B	7	Sample X1	E	0.737	0.675	CaGc11	52.1484375	1042.96875
B	8	Sample X1	E	0.735	0.673	CaGc11	51.9921875	1039.84375
B	9	Blank B	F	0.049				
B	10	Sample X1	F	0.326	0.277	CaGc21	21.0546875	421.09375
B	11	Sample X1	F	0.326	0.277	CaGc21	21.0546875	421.09375
B	12	Sample X1	F	0.326	0.277	CaGc21	21.0546875	421.09375
G	9	Blank B	G	0.043				
G	10	Sample X1	G	0.135	0.092	CaGl11	6.6015625	132.03125
G	11	Sample X1	G	0.133	0.09	CaGl11	6.4453125	128.90625
G	12	Sample X1	G	0.136	0.093	CaGl11	6.6796875	133.59375
H	1	Blank B	H	0.048				
H	2	Sample X1	H	0.102	0.054	CaGl21	3.6328125	72.65625
H	3	Sample X1	H	0.103	0.055	CaGl21	3.7109375	74.21875
H	4	Sample X1	H	0.101	0.053	CaGl21	3.5546875	71.09375

Appendix 3.9 factorial experiment TFC run 9.

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.065				
A	2	Sample X1	A	0.313	0.248	CaSu11	18.7890625	281.8359375
A	3	Sample X1	A	0.315	0.25	CaSu11	18.9453125	284.1796875
A	4	Sample X1	A	0.313	0.248	CaSu11	18.7890625	281.8359375
E	9	Blank B	A	0.09				
E	10	Sample X1	A	0.462	0.372	CaFr11	28.4765625	427.1484375
E	11	Sample X1	A	0.462	0.372	CaFr11	28.4765625	427.1484375
E	12	Sample X1	A	0.463	0.373	CaFr11	28.5546875	428.3203125
F	1	Blank B	B	0.059				
F	2	Sample X1	B	0.412	0.353	CaFr12	26.9921875	404.8828125
F	3	Sample X1	B	0.412	0.353	CaFr12	26.9921875	404.8828125
F	4	Sample X1	B	0.416	0.357	CaFr12	27.3046875	409.5703125
F	5	Blank B	C	0.074				
F	6	Sample X1	C	0.405	0.331	CaFr21	25.2734375	379.1015625
F	7	Sample X1	C	0.401	0.327	CaFr21	24.9609375	374.4140625
F	8	Sample X1	C	0.405	0.331	CaFr21	25.2734375	379.1015625
F	9	Blank B	D	0.045				
F	10	Sample X1	D	0.154	0.109	CaXy11	7.9296875	118.9453125
F	11	Sample X1	D	0.151	0.106	CaXy11	7.6953125	115.4296875
F	12	Sample X1	D	0.151	0.106	CaXy11	7.6953125	115.4296875
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.268	0.213	CaXy12	16.0546875	240.8203125
G	3	Sample X1	E	0.268	0.213	CaXy12	16.0546875	240.8203125
G	4	Sample X1	E	0.269	0.214	CaXy12	16.1328125	241.9921875
G	5	Blank B	F	0.057				
G	6	Sample X1	F	0.216	0.159	CaXy21	11.8359375	177.5390625
G	7	Sample X1	F	0.213	0.156	CaXy21	11.6015625	174.0234375
G	8	Sample X1	F	0.213	0.156	CaXy21	11.6015625	174.0234375
A	5	Blank B	B	0.056				
A	6	Sample X1	B	0.183	0.127	CaGr11	9.3359375	140.0390625
A	7	Sample X1	B	0.185	0.129	CaGr11	9.4921875	142.3828125
A	8	Sample X1	B	0.185	0.129	CaGr11	9.4921875	142.3828125
A	9	Blank B	C	0.05				
A	10	Sample X1	C	0.155	0.105	CaGr12	7.6171875	114.2578125
A	11	Sample X1	C	0.152	0.102	CaGr12	7.3828125	110.7421875
A	12	Sample X1	C	0.152	0.102	CaGr12	7.3828125	110.7421875
B	1	Blank B	D	0.063				
B	2	Sample X1	D	0.166	0.103	CaGr21	7.4609375	111.9140625

Appendix 3.9 contd.

B	3	Sample X1	D	0.169	0.106	CaGr21	7.6953125	115.4296875
B	4	Sample X1	D	0.169	0.106	CaGr21	7.6953125	115.4296875
B	5	Blank B	E	0.054				
B	6	Sample X1	E	0.953	0.899	CaGc11	69.6484375	1044.726563
B	7	Sample X1	E	0.951	0.897	CaGc11	69.4921875	1042.382813
B	8	Sample X1	E	0.951	0.897	CaGc11	69.4921875	1042.382813
B	9	Blank B	F	0.05				
B	10	Sample X1	F	0.587	0.537	CaGc21	41.3671875	620.5078125
B	11	Sample X1	F	0.589	0.539	CaGc21	41.5234375	622.8515625
B	12	Sample X1	F	0.589	0.539	CaGc21	41.5234375	622.8515625
G	9	Blank B	G	0.059				
G	10	Sample X1	G	0.196	0.137	CaGl11	10.1171875	151.7578125
G	11	Sample X1	G	0.196	0.137	CaGl11	10.1171875	151.7578125
G	12	Sample X1	G	0.198	0.139	CaGl11	10.2734375	154.1015625
H	1	Blank B	H	0.061				
H	2	Sample X1	H	0.345	0.284	CaGl21	21.6015625	324.0234375
H	3	Sample X1	H	0.345	0.284	CaGl21	21.6015625	324.0234375
H	4	Sample X1	H	0.346	0.285	CaGl21	21.6796875	325.1953125

Appendix 3.10 factorial experiment TFC run 10

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.058				
E	10	Sample X1	A	0.161	0.103	CaSu11	7.4609375	74.609375
E	11	Sample X1	A	0.162	0.104	CaSu11	7.5390625	75.390625
E	12	Sample X1	A	0.161	0.103	CaSu11	7.4609375	74.609375
C	1	Blank B	A	0.074				
C	2	Sample X1	A	0.302	0.228	CaFr11	17.2265625	172.265625
C	3	Sample X1	A	0.302	0.228	CaFr11	17.2265625	172.265625
C	4	Sample X1	A	0.301	0.227	CaFr11	17.1484375	171.484375
C	5	Blank B	B	0.058				
C	6	Sample X1	B	0.154	0.096	CaFr12	6.9140625	69.140625
C	7	Sample X1	B	0.151	0.093	CaFr12	6.6796875	66.796875
C	8	Sample X1	B	0.151	0.093	CaFr12	6.6796875	66.796875
C	9	Blank B	C	0.052				
C	10	Sample X1	C	0.168	0.116	CaFr21	8.4765625	84.765625
C	11	Sample X1	C	0.166	0.114	CaFr21	8.3203125	83.203125
C	12	Sample X1	C	0.167	0.115	CaFr21	8.3984375	83.984375

Appendix 3.10 contd.

D	1	Blank B	D	0.058				
D	2	Sample X1	D	0.138	0.08	CaXy11	5.6640625	56.640625
D	3	Sample X1	D	0.138	0.08	CaXy11	5.6640625	56.640625
D	4	Sample X1	D	0.139	0.081	CaXy11	5.7421875	57.421875
D	5	Blank B	E	0.055				
D	6	Sample X1	E	0.145	0.09	CaXy12	6.4453125	64.453125
D	7	Sample X1	E	0.141	0.086	CaXy12	6.1328125	61.328125
D	8	Sample X1	E	0.146	0.091	CaXy12	6.5234375	65.234375
D	9	Blank B	F	0.05				
D	10	Sample X1	F	0.13	0.08	CaXy21	5.6640625	56.640625
D	11	Sample X1	F	0.13	0.08	CaXy21	5.6640625	56.640625
D	12	Sample X1	F	0.13	0.08	CaXy21	5.6640625	56.640625
F	1	Blank B	B	0.057				
F	2	Sample X1	B	0.137	0.08	CaGr11	5.6640625	56.640625
F	3	Sample X1	B	0.133	0.076	CaGr11	5.3515625	53.515625
F	4	Sample X1	B	0.137	0.08	CaGr11	5.6640625	56.640625
F	5	Blank B	C	0.049				
F	6	Sample X1	C	0.138	0.089	CaGr12	6.3671875	63.671875
F	7	Sample X1	C	0.137	0.088	CaGr12	6.2890625	62.890625
F	8	Sample X1	C	0.138	0.089	CaGr12	6.3671875	63.671875
F	9	Blank B	D	0.042				
F	10	Sample X1	D	0.135	0.093	CaGr21	6.6796875	66.796875
F	11	Sample X1	D	0.135	0.093	CaGr21	6.6796875	66.796875
F	12	Sample X1	D	0.136	0.094	CaGr21	6.7578125	67.578125
G	1	Blank B	E	0.067				
G	2	Sample X1	E	0.533	0.466	CaGc11	35.8203125	358.203125
G	3	Sample X1	E	0.537	0.47	CaGc11	36.1328125	361.328125
G	4	Sample X1	E	0.536	0.469	CaGc11	36.0546875	360.546875
G	5	Blank B	F	0.048				
G	6	Sample X1	F	0.305	0.257	CaGc21	19.4921875	194.921875
G	7	Sample X1	F	0.304	0.256	CaGc21	19.4140625	194.140625
G	8	Sample X1	F	0.305	0.257	CaGc21	19.4921875	194.921875
E	1	Blank B	G	0.063				
E	2	Sample X1	G	0.15	0.087	CaGl11	6.2109375	62.109375
E	3	Sample X1	G	0.153	0.09	CaGl11	6.4453125	64.453125
E	4	Sample X1	G	0.153	0.09	CaGl11	6.4453125	64.453125
E	5	Blank B	H	0.054				
E	6	Sample X1	H	0.146	0.092	CaGl21	6.6015625	66.015625
E	7	Sample X1	H	0.146	0.092	CaGl21	6.6015625	66.015625
E	8	Sample X1	H	0.148	0.094	CaGl21	6.7578125	67.578125

Appendix 4.1 factorial experiment CUPRAC run 1

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.102					
D	2	Sample X1	J	0.112	0.01	CaSu11	0.114341085	0.001715116	1.715116279
D	3	Sample X1	J	0.114	0.012	CaSu11	0.119186047	0.001787791	1.787790698
D	4	Sample X1	J	0.112	0.01	CaSu11	0.114341085	0.001715116	1.715116279
A	1	Blank B	A	0.106					
A	2	Sample X1	A	0.12	0.014	CaFr11	0.124031008	0.001860465	1.860465116
A	3	Sample X1	A	0.119	0.013	CaFr11	0.121608527	0.001824128	1.824127907
A	4	Sample X1	A	0.119	0.013	CaFr11	0.121608527	0.001824128	1.824127907
A	5	Blank B	B	0.103					
A	6	Sample X1	B	0.131	0.028	CaFr12	0.157945736	0.002369186	2.369186047
A	7	Sample X1	B	0.132	0.029	CaFr12	0.160368217	0.002405523	2.405523256
A	8	Sample X1	B	0.132	0.029	CaFr12	0.160368217	0.002405523	2.405523256
A	9	Blank B	C	0.107					
A	10	Sample X1	C	0.114	0.007	CaFr21	0.107073643	0.001606105	1.606104651
A	11	Sample X1	C	0.116	0.009	CaFr21	0.111918605	0.001678779	1.67877907
A	12	Sample X1	C	0.114	0.007	CaFr21	0.107073643	0.001606105	1.606104651
B	1	Blank B	D	0.093					
B	2	Sample X1	D	0.107	0.014	CaXy11	0.124031008	0.001860465	1.860465116
B	3	Sample X1	D	0.107	0.014	CaXy11	0.124031008	0.001860465	1.860465116
B	4	Sample X1	D	0.105	0.012	CaXy11	0.119186047	0.001787791	1.787790698
B	5	Blank B	E	0.096					
B	6	Sample X1	E	0.106	0.01	CaXy12	0.114341085	0.001715116	1.715116279
B	7	Sample X1	E	0.109	0.013	CaXy12	0.121608527	0.001824128	1.824127907
B	8	Sample X1	E	0.109	0.013	CaXy12	0.121608527	0.001824128	1.824127907
B	9	Blank B	F	0.09					
B	10	Sample X1	F	0.093	0.003	CaXy21	0.097383721	0.001460756	1.460755814
B	11	Sample X1	F	0.091	0.001	CaXy21	0.09253876	0.001388081	1.388081395
B	12	Sample X1	F	0.091	0.001	CaXy21	0.09253876	0.001388081	1.388081395
C	1	Blank B	G	0.095					
C	2	Sample X1	G	0.12	0.025	CaGr11	0.150678295	0.002260174	2.260174419
C	3	Sample X1	G	0.121	0.026	CaGr11	0.153100775	0.002296512	2.296511628
C	4	Sample X1	G	0.12	0.025	CaGr11	0.150678295	0.002260174	2.260174419
C	5	Blank B	H	0.101					
C	6	Sample X1	H	0.103	0.002	CaGr12	0.09496124	0.001424419	1.424418605
C	7	Sample X1	H	0.103	0.002	CaGr12	0.09496124	0.001424419	1.424418605
C	8	Sample X1	H	0.105	0.004	CaGr12	0.099806202	0.001497093	1.497093023
C	9	Blank B	I	0.08					
C	10	Sample X1	I	0.101	0.021	CaGr21	0.140988372	0.002114826	2.114825581

Appendix 4.1 contd.

C	11	Sample X1	I	0.101	0.021	CaGr21	0.140988372	0.002114826	2.114825581
C	12	Sample X1	I	0.101	0.021	CaGr21	0.140988372	0.002114826	2.114825581
D	5	Blank B	K	0.084					
D	6	Sample X1	K	0.112	0.028	CaGc11	0.157945736	0.002369186	2.369186047
D	7	Sample X1	K	0.108	0.024	CaGc11	0.148255814	0.002223837	2.223837209
D	8	Sample X1	K	0.108	0.024	CaGc11	0.148255814	0.002223837	2.223837209
D	9	Blank B	L	0.065					
D	10	Sample X1	L	0.108	0.043	CaGc21	0.194282946	0.002914244	2.914244186
D	11	Sample X1	L	0.111	0.046	CaGc21	0.201550388	0.003023256	3.023255814
D	12	Sample X1	L	0.108	0.043	CaGc21	0.194282946	0.002914244	2.914244186
E	1	Blank B	M	0.091					
E	2	Sample X1	M	0.119	0.028	CaGl11	0.157945736	0.002369186	2.369186047
E	3	Sample X1	M	0.114	0.023	CaGl11	0.145833333	0.0021875	2.1875
E	4	Sample X1	M	0.115	0.024	CaGl11	0.148255814	0.002223837	2.223837209
E	5	Blank B	N	0.09					
E	6	Sample X1	N	0.114	0.024	CaGl21	0.148255814	0.002223837	2.223837209
E	7	Sample X1	N	0.119	0.029	CaGl21	0.160368217	0.002405523	2.405523256
E	8	Sample X1	N	0.119	0.029	CaGl21	0.160368217	0.002405523	2.405523256

Appendix 4.2 factorial experiment CUPRAC run 2

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.096					
D	2	Sample X1	J	0.124	0.028	CaSu11	0.15794574	0.00315891	3.158915
D	3	Sample X1	J	0.127	0.031	CaSu11	0.16521318	0.00330426	3.304264
D	4	Sample X1	J	0.124	0.028	CaSu11	0.15794574	0.00315891	3.158915
A	1	Blank B	A	0.1					
A	2	Sample X1	A	0.147	0.047	CaFr11	0.20397287	0.00407946	4.079457
A	3	Sample X1	A	0.147	0.047	CaFr11	0.20397287	0.00407946	4.079457
A	4	Sample X1	A	0.147	0.047	CaFr11	0.20397287	0.00407946	4.079457
A	5	Blank B	B	0.088					
A	6	Sample X1	B	0.162	0.074	CaFr12	0.26937984	0.0053876	5.387597
A	7	Sample X1	B	0.162	0.074	CaFr12	0.26937984	0.0053876	5.387597
A	8	Sample X1	B	0.161	0.073	CaFr12	0.26695736	0.00533915	5.339147
A	9	Blank B	C	0.094					
A	10	Sample X1	C	0.127	0.033	CaFr21	0.17005814	0.00340116	3.401163
A	11	Sample X1	C	0.127	0.033	CaFr21	0.17005814	0.00340116	3.401163
A	12	Sample X1	C	0.126	0.032	CaFr21	0.16763566	0.00335271	3.352713

Appendix 4.2 contd.

B	1	Blank B	D	0.073					
B	2	Sample X1	D	0.102	0.029	CaXy11	0.16036822	0.00320736	3.207364
B	3	Sample X1	D	0.102	0.029	CaXy11	0.16036822	0.00320736	3.207364
B	4	Sample X1	D	0.109	0.036	CaXy11	0.17732558	0.00354651	3.546512
B	5	Blank B	E	0.083					
B	6	Sample X1	E	0.112	0.029	CaXy12	0.16036822	0.00320736	3.207364
B	7	Sample X1	E	0.113	0.03	CaXy12	0.1627907	0.00325581	3.255814
B	8	Sample X1	E	0.113	0.03	CaXy12	0.1627907	0.00325581	3.255814
B	9	Blank B	F	0.064					
B	10	Sample X1	F	0.092	0.028	CaXy21	0.15794574	0.00315891	3.158915
B	11	Sample X1	F	0.092	0.028	CaXy21	0.15794574	0.00315891	3.158915
B	12	Sample X1	F	0.094	0.03	CaXy21	0.1627907	0.00325581	3.255814
C	1	Blank B	G	0.079					
C	2	Sample X1	G	0.113	0.034	CaGr11	0.17248062	0.00344961	3.449612
C	3	Sample X1	G	0.113	0.034	CaGr11	0.17248062	0.00344961	3.449612
C	4	Sample X1	G	0.114	0.035	CaGr11	0.1749031	0.00349806	3.498062
C	5	Blank B	H	0.088					
C	6	Sample X1	H	0.104	0.016	CaGr12	0.12887597	0.00257752	2.577519
C	7	Sample X1	H	0.109	0.021	CaGr12	0.14098837	0.00281977	2.819767
C	8	Sample X1	H	0.109	0.021	CaGr12	0.14098837	0.00281977	2.819767
C	9	Blank B	I	0.08					
C	10	Sample X1	I	0.113	0.033	CaGr21	0.17005814	0.00340116	3.401163
C	11	Sample X1	I	0.109	0.029	CaGr21	0.16036822	0.00320736	3.207364
C	12	Sample X1	I	0.108	0.028	CaGr21	0.15794574	0.00315891	3.158915
D	5	Blank B	K	0.108					
D	6	Sample X1	K	0.15	0.042	CaGc11	0.19186047	0.00383721	3.837209
D	7	Sample X1	K	0.15	0.042	CaGc11	0.19186047	0.00383721	3.837209
D	8	Sample X1	K	0.151	0.043	CaGc11	0.19428295	0.00388566	3.885659
D	9	Blank B	L	0.081					
D	10	Sample X1	L	0.123	0.042	CaGc21	0.19186047	0.00383721	3.837209
D	11	Sample X1	L	0.123	0.042	CaGc21	0.19186047	0.00383721	3.837209
D	12	Sample X1	L	0.128	0.047	CaGc21	0.20397287	0.00407946	4.079457
E	1	Blank B	M	0.095					
E	2	Sample X1	M	0.112	0.017	CaGl11	0.13129845	0.00262597	2.625969
E	3	Sample X1	M	0.107	0.012	CaGl11	0.11918605	0.00238372	2.383721
E	4	Sample X1	M	0.107	0.012	CaGl11	0.11918605	0.00238372	2.383721
E	5	Blank B	N	0.1					
E	6	Sample X1	N	0.101	0.001	CaGl21	0.09253876	0.00185078	1.850775
E	7	Sample X1	N	0.107	0.007	CaGl21	0.10707364	0.00214147	2.141473
E	8	Sample X1	N	0.101	0.001	CaGl21	0.09253876	0.00185078	1.850775

Appendix 4.3 factorial experiment CUPRAC run 3

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.098					
D	2	Sample X1	J	0.172	0.074	CaSu11	0.2693798	0.0053876	5.387597
D	3	Sample X1	J	0.17	0.072	CaSu11	0.2645349	0.0052907	5.290698
D	4	Sample X1	J	0.17	0.072	CaSu11	0.2645349	0.0052907	5.290698
A	1	Blank B	A	0.126					
A	2	Sample X1	A	0.326	0.2	CaFr11	0.5746124	0.0114922	11.49225
A	3	Sample X1	A	0.328	0.202	CaFr11	0.5794574	0.0115891	11.58915
A	4	Sample X1	A	0.328	0.202	CaFr11	0.5794574	0.0115891	11.58915
A	5	Blank B	B	0.113					
A	6	Sample X1	B	0.244	0.131	CaFr12	0.4074612	0.0081492	8.149225
A	7	Sample X1	B	0.243	0.13	CaFr12	0.4050388	0.0081008	8.100775
A	8	Sample X1	B	0.243	0.13	CaFr12	0.4050388	0.0081008	8.100775
A	9	Blank B	C	0.11					
A	10	Sample X1	C	0.256	0.146	CaFr21	0.4437984	0.008876	8.875969
A	11	Sample X1	C	0.258	0.148	CaFr21	0.4486434	0.0089729	8.972868
A	12	Sample X1	C	0.256	0.146	CaFr21	0.4437984	0.008876	8.875969
B	1	Blank B	D	0.074					
B	2	Sample X1	D	0.212	0.138	CaXy11	0.4244186	0.0084884	8.488372
B	3	Sample X1	D	0.218	0.144	CaXy1	0.4389535	0.0087791	8.77907
B	4	Sample X1	D	0.218	0.144	CaXy1	0.4389535	0.0087791	8.77907
B	5	Blank B	E	0.08					
B	6	Sample X1	E	0.193	0.113	CaXy12	0.3638566	0.0072771	7.277132
B	7	Sample X1	E	0.191	0.111	CaXy12	0.3590116	0.0071802	7.180233
B	8	Sample X1	E	0.191	0.111	CaXy12	0.3590116	0.0071802	7.180233
B	9	Blank B	F	0.064					
B	10	Sample X1	F	0.212	0.148	CaXy21	0.4486434	0.0089729	8.972868
B	11	Sample X1	F	0.214	0.15	CaXy21	0.4534884	0.0090698	9.069767
B	12	Sample X1	F	0.212	0.148	CaXy21	0.4486434	0.0089729	8.972868
C	1	Blank B	G	0.087					
C	2	Sample X1	G	0.246	0.159	CaGr11	0.4752907	0.0095058	9.505814
C	3	Sample X1	G	0.246	0.159	CaGr11	0.4752907	0.0095058	9.505814
C	4	Sample X1	G	0.246	0.159	CaGr11	0.4752907	0.0095058	9.505814
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.243	0.137	CaGr12	0.4219961	0.0084399	8.439922
C	7	Sample X1	H	0.241	0.135	CaGr12	0.4171512	0.008343	8.343023
C	8	Sample X1	H	0.241	0.135	CaGr12	0.4171512	0.008343	8.343023

Appendix 4.3 contd.

C	9	Blank B	I	0.061					
C	10	Sample X1	I	0.206	0.145	CaGr21	0.441376	0.0088275	8.827519
C	11	Sample X1	I	0.207	0.146	CaGr21	0.4437984	0.008876	8.875969
C	12	Sample X1	I	0.207	0.146	CaGr21	0.4437984	0.008876	8.875969
D	5	Blank B	K	0.076					
D	6	Sample X1	K	0.16	0.084	CaGC11	0.2936047	0.0058721	5.872093
D	7	Sample X1	K	0.161	0.085	CaGC11	0.2960271	0.0059205	5.920543
D	8	Sample X1	K	0.16	0.084	CaGC11	0.2936047	0.0058721	5.872093
D	9	Blank B	L	0.066					
D	10	Sample X1	L	0.174	0.108	CaGc21	0.3517442	0.0070349	7.034884
D	11	Sample X1	L	0.174	0.108	CaGc21	0.3517442	0.0070349	7.034884
D	12	Sample X1	L	0.174	0.108	CaGc21	0.3517442	0.0070349	7.034884
F	1	Blank B	M	0.075					
E	2	Sample X1	M	0.166	0.091	CaGl11	0.310562	0.0062112	6.21124
E	3	Sample X1	M	0.164	0.089	CaGl11	0.3057171	0.0061143	6.114341
E	4	Sample X1	M	0.164	0.089	CaGl11	0.3057171	0.0061143	6.114341
E	5	Blank B	N	0.066					
E	6	Sample X1	N	0.172	0.106	CaGl21	0.3468992	0.006938	6.937984
E	7	Sample X1	N	0.174	0.108	CaGl21	0.3517442	0.0070349	7.034884
E	8	Sample X1	N	0.172	0.106	CaGl21	0.3468992	0.006938	6.937984

Appendix 4.4 factorial experiment CUPRAC run 4

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/ml)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.09					
D	2	Sample X1	J	0.12	0.03	CaSu11	0.1627907	0.00162791	1.627907
D	3	Sample X1	J	0.118	0.028	CaSu11	0.15794574	0.00157946	1.579457
D	4	Sample X1	J	0.118	0.028	CaSu11	0.15794574	0.00157946	1.579457
A	1	Blank B	A	0.089					
A	2	Sample X1	A	0.198	0.109	CaFr11	0.35416667	0.00354167	3.541667
A	3	Sample X1	A	0.199	0.11	CaFr11	0.35658915	0.00356589	3.565891
A	4	Sample X1	A	0.198	0.109	CaFr11	0.35416667	0.00354167	3.541667
A	5	Blank B	B	0.085					
A	6	Sample X1	B	0.148	0.063	CaFr12	0.24273256	0.00242733	2.427326
A	7	Sample X1	B	0.148	0.063	CaFr12	0.24273256	0.00242733	2.427326
A	8	Sample X1	B	0.149	0.064	CaFr12	0.24515504	0.00245155	2.45155
A	9	Blank B	C	0.097					
A	10	Sample X1	C	0.141	0.044	CaFr21	0.19670543	0.00196705	1.967054

Appendix 4.4 contd.

A	11	Sample X1	C	0.139	0.042	CaFr21	0.19186047	0.0019186	1.918605
A	12	Sample X1	C	0.139	0.042	CaFr21	0.19186047	0.0019186	1.918605
B	1	Blank B	D	0.074					
B	2	Sample X1	D	0.118	0.044	CaXy11	0.19670543	0.00196705	1.967054
B	3	Sample X1	D	0.118	0.044	CaXy11	0.19670543	0.00196705	1.967054
B	4	Sample X1	D	0.115	0.041	CaXy11	0.18943798	0.00189438	1.89438
B	5	Blank B	E	0.081					
B	6	Sample X1	E	0.113	0.032	CaXy12	0.16763566	0.00167636	1.676357
B	7	Sample X1	E	0.114	0.033	CaXy12	0.17005814	0.00170058	1.700581
B	8	Sample X1	E	0.113	0.032	CaXy12	0.16763566	0.00167636	1.676357
B	9	Blank B	F	0.078					
B	10	Sample X1	F	0.11	0.032	CaXy21	0.16763566	0.00167636	1.676357
B	11	Sample X1	F	0.11	0.032	CaXy21	0.16763566	0.00167636	1.676357
B	12	Sample X1	F	0.11	0.032	CaXy21	0.16763566	0.00167636	1.676357
C	1	Blank B	G	0.08					
C	2	Sample X1	G	0.131	0.051	CaGr11	0.21366279	0.00213663	2.136628
C	3	Sample X1	G	0.129	0.049	CaGr11	0.20881783	0.00208818	2.088178
C	4	Sample X1	G	0.129	0.049	CaGr11	0.20881783	0.00208818	2.088178
C	5	Blank B	H	0.08					
C	6	Sample X1	H	0.12	0.04	CaGr12	0.1870155	0.00187016	1.870155
C	7	Sample X1	H	0.119	0.039	CaGr12	0.18459302	0.00184593	1.84593
C	8	Sample X1	H	0.119	0.039	CaGr12	0.18459302	0.00184593	1.84593
C	9	Blank B	I	0.065					
C	10	Sample X1	I	0.112	0.047	CaGr21	0.20397287	0.00203973	2.039729
C	11	Sample X1	I	0.114	0.049	CaGr21	0.20881783	0.00208818	2.088178
C	12	Sample X1	I	0.112	0.047	CaGr21	0.20397287	0.00203973	2.039729
D	5	Blank B	K	0.08					
D	6	Sample X1	K	0.121	0.041	CaGc11	0.18943798	0.00189438	1.89438
D	7	Sample X1	K	0.121	0.041	CaGc11	0.18943798	0.00189438	1.89438
D	8	Sample X1	K	0.121	0.041	CaGc11	0.18943798	0.00189438	1.89438
D	9	Blank B	L	0.066					
D	10	Sample X1	L	0.093	0.027	CaGc21	0.15552326	0.00155523	1.555233
D	11	Sample X1	L	0.093	0.027	CaGc21	0.15552326	0.00155523	1.555233
D	12	Sample X1	L	0.093	0.027	CaGc21	0.15552326	0.00155523	1.555233
E	1	Blank B	M	0.086					
E	2	Sample X1	M	0.121	0.035	CaGl11	0.1749031	0.00174903	1.749031
E	3	Sample X1	M	0.119	0.033	CaGl11	0.17005814	0.00170058	1.700581
E	4	Sample X1	M	0.119	0.033	CaGl11	0.17005814	0.00170058	1.700581
E	5	Blank B	N	0.07					
E	6	Sample X1	N	0.1	0.03	CaGl21	0.1627907	0.00162791	1.627907
E	7	Sample X1	N	0.101	0.029	CaGl21	0.16036822	0.00160368	1.603682
E	8	Sample X1	N	0.1	0.029	CaGl21	0.16036822	0.00160368	1.603682

Appendix 4.5 factorial experiment CUPRAC run 5

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.096					
D	2	Sample X1	J	0.159	0.063	CaSu11	0.2427326	0.0024273	2.427326
D	3	Sample X1	J	0.159	0.063	CaSu11	0.2427326	0.0024273	2.427326
D	4	Sample X1	J	0.159	0.063	CaSu11	0.2427326	0.0024273	2.427326
A	1	Blank B	A	0.163					
A	2	Sample X1	A	0.206	0.043	CaFr11	0.1942829	0.0019428	1.942829
A	3	Sample X1	A	0.204	0.041	CaFr11	0.189438	0.0018944	1.89438
A	4	Sample X1	A	0.204	0.041	CaFr11	0.189438	0.0018944	1.89438
A	5	Blank B	B	0.098					
A	6	Sample X1	B	0.161	0.063	CaFr12	0.2427326	0.0024273	2.427326
A	7	Sample X1	B	0.163	0.065	CaFr12	0.2475775	0.0024758	2.475775
A	8	Sample X1	B	0.161	0.063	CaFr12	0.2427326	0.0024273	2.427326
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.198	0.107	CaFr21	0.3493217	0.0034932	3.493217
A	11	Sample X1	C	0.197	0.106	CaFr21	0.3468992	0.003469	3.468992
A	12	Sample X1	C	0.197	0.106	CaFr21	0.3468992	0.003469	3.468992
B	1	Blank B	D	0.078					
B	2	Sample X1	D	0.154	0.075	CaXy11	0.2718023	0.002718	2.718023
B	3	Sample X1	D	0.157	0.079	CaXy11	0.2814922	0.0028149	2.814922
B	4	Sample X1	D	0.154	0.076	CaXy11	0.2742248	0.0027422	2.742248
B	5	Blank B	E	0.097					
B	6	Sample X1	E	0.184	0.087	CaXy12	0.3008721	0.0030087	3.008721
B	7	Sample X1	E	0.185	0.088	CaXy12	0.3032946	0.0030329	3.032946
B	8	Sample X1	E	0.184	0.087	CaXy12	0.3008721	0.0030087	3.008721
B	9	Blank B	F	0.071					
B	10	Sample X1	F	0.202	0.131	CaXy21	0.4074612	0.0040746	4.074612
B	11	Sample X1	F	0.201	0.13	CaXy21	0.4050388	0.0040504	4.050388
B	12	Sample X1	F	0.201	0.13	CaXy21	0.4050388	0.0040504	4.050388
C	1	Blank B	G	0.076					
C	2	Sample X1	G	0.23	0.154	CaGr11	0.4631783	0.0046318	4.631783
C	3	Sample X1	G	0.232	0.156	CaGr11	0.4680233	0.0046802	4.680233
C	4	Sample X1	G	0.23	0.154	CaGr11	0.4631783	0.0046318	4.631783
C	5	Blank B	H	0.072					
C	6	Sample X1	H	0.254	0.182	CaGr12	0.5310078	0.0053101	5.310078
C	7	Sample X1	H	0.254	0.182	CaGr12	0.5310078	0.0053101	5.310078
C	8	Sample X1	H	0.256	0.184	CaGr12	0.5358527	0.0053585	5.358527
C	9	Blank B	I	0.062					
C	10	Sample X1	I	0.145	0.083	CaGr21	0.2911822	0.0029118	2.911822

Appendix 4.5 contd.

C	11	Sample X1	I	0.145	0.081	CaGr21	0.2863372	0.0028634	2.863372
C	12	Sample X1	I	0.146	0.084	CaGr21	0.2936047	0.002936	2.936047
D	5	Blank B	K	0.067					
D	6	Sample X1	K	0.189	0.122	CaGc11	0.3856589	0.0038566	3.856589
D	7	Sample X1	K	0.189	0.122	CaGc11	0.3856589	0.0038566	3.856589
D	8	Sample X1	K	0.189	0.122	CaGc11	0.3856589	0.0038566	3.856589
D	9	Blank B	L	0.058					
D	10	Sample X1	L	0.164	0.106	CaGc21	0.3468992	0.003469	3.468992
D	11	Sample X1	L	0.164	0.106	CaGc21	0.3468992	0.003469	3.468992
D	12	Sample X1	L	0.164	0.106	CaGc21	0.3468992	0.003469	3.468992
E	1	Blank B	M	0.072					
E	2	Sample X1	M	0.22	0.128	CaGl11	0.4001938	0.0040019	4.001938
E	3	Sample X1	M	0.22	0.128	CaGl11	0.4001938	0.0040019	4.001938
E	4	Sample X1	M	0.22	0.128	CaGl11	0.4001938	0.0040019	4.001938
E	5	Blank B	N	0.067					
E	6	Sample X1	N	0.16	0.093	CaGl21	0.315407	0.0031541	3.15407
E	7	Sample X1	N	0.16	0.093	CaGl21	0.315407	0.0031541	3.15407
E	8	Sample X1	N	0.16	0.093	CaGl21	0.315407	0.0031541	3.15407

Appendix 4.6 factorial experiment CUPRAC run 6

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.091					
D	2	Sample X1	J	0.227	0.136	CaSu11	0.41957364	0.00419574	4.195736
D	3	Sample X1	J	0.229	0.138	CaSu11	0.4244186	0.00424419	4.244186
D	4	Sample X1	J	0.227	0.136	CaSu11	0.41957364	0.00419574	4.195736
A	1	Blank B	A	0.126					
A	2	Sample X1	A	0.383	0.257	CaFr11	0.7126938	0.00712694	7.126938
A	3	Sample X1	A	0.383	0.257	CaFr11	0.7126938	0.00712694	7.126938
A	4	Sample X1	A	0.385	0.259	CaFr11	0.71753876	0.00717539	7.175388
A	5	Blank B	B	0.082					
A	6	Sample X1	B	0.224	0.142	CaFr12	0.43410853	0.00434109	4.341085
A	7	Sample X1	B	0.224	0.142	CaFr12	0.43410853	0.00434109	4.341085
A	8	Sample X1	B	0.228	0.146	CaFr12	0.44379845	0.00443798	4.437984
A	9	Blank B	C	0.095					
A	10	Sample X1	C	0.367	0.272	CaFr21	0.74903101	0.00749031	7.49031
A	11	Sample X1	C	0.362	0.267	CaFr21	0.7369186	0.00736919	7.369186

Appendix 4.6 contd.

A	12	Sample X1	C	0.362	0.267	CaFr21	0.7369186	0.00736919	7.369186
B	1	Blank B	D	0.073					
B	2	Sample X1	D	0.285	0.212	CaXy11	0.60368217	0.00603682	6.036822
B	3	Sample X1	D	0.285	0.213	CaXy11	0.60610465	0.00606105	6.061047
B	4	Sample X1	D	0.284	0.212	CaXy11	0.60368217	0.00603682	6.036822
B	5	Blank B	E	0.079					
B	6	Sample X1	E	0.302	0.223	CaXy12	0.63032946	0.00630329	6.303295
B	7	Sample X1	E	0.301	0.222	CaXy12	0.62790698	0.00627907	6.27907
B	8	Sample X1	E	0.302	0.223	CaXy12	0.63032946	0.00630329	6.303295
B	9	Blank B	F	0.076					
B	10	Sample X1	F	0.28	0.204	CaXy21	0.58430233	0.00584302	5.843023
B	11	Sample X1	F	0.284	0.208	CaXy21	0.59399225	0.00593992	5.939922
B	12	Sample X1	F	0.284	0.208	CaXy21	0.59399225	0.00593992	5.939922
C	1	Blank B	G	0.085					
C	2	Sample X1	G	0.332	0.226	CaGr11	0.6375969	0.00637597	6.375969
C	3	Sample X1	G	0.331	0.246	CaGr11	0.68604651	0.00686047	6.860465
C	4	Sample X1	G	0.331	0.231	CaGr11	0.6497093	0.00649709	6.497093
C	5	Blank B	H	0.096					
C	6	Sample X1	H	0.374	0.278	CaGr12	0.76356589	0.00763566	7.635659
C	7	Sample X1	H	0.373	0.277	CaGr12	0.76114341	0.00761143	7.611434
C	8	Sample X1	H	0.373	0.277	CaGr12	0.76114341	0.00761143	7.611434
C	9	Blank B	I	0.069					
C	10	Sample X1	I	0.429	0.36	CaGr21	0.9622093	0.00962209	9.622093
C	11	Sample X1	I	0.426	0.357	CaGr21	0.95494186	0.00954942	9.549419
C	12	Sample X1	I	0.426	0.357	CaGr21	0.95494186	0.00954942	9.549419
D	5	Blank B	K	0.078					
D	6	Sample X1	K	0.238	0.16	CaGc11	0.47771318	0.00477713	4.777132
D	7	Sample X1	K	0.235	0.157	CaGc11	0.47044574	0.00470446	4.704457
D	8	Sample X1	K	0.238	0.16	CaGc11	0.47771318	0.00477713	4.777132
D	9	Blank B	L	0.074					
D	10	Sample X1	L	0.211	0.137	CaGc21	0.42199612	0.00421996	4.219961
D	11	Sample X1	L	0.218	0.144	CaGc21	0.43895349	0.00438953	4.389535
D	12	Sample X1	L	0.218	0.144	CaGc21	0.43895349	0.00438953	4.389535
E	1	Blank B	M	0.081					
E	2	Sample X1	M	0.321	0.24	CaGl11	0.67151163	0.00671512	6.715116
E	3	Sample X1	M	0.321	0.24	CaGl11	0.67151163	0.00671512	6.715116
E	4	Sample X1	M	0.322	0.241	CaGl11	0.67393411	0.00673934	6.739341
E	5	Blank B	N	0.069					
E	6	Sample X1	N	0.303	0.234	CaGl21	0.65697674	0.00656977	6.569767
E	7	Sample X1	N	0.302	0.233	CaGl21	0.65455426	0.00654554	6.545543
E	8	Sample X1	N	0.303	0.234	CaGl21	0.65697674	0.00656977	6.569767

Appendix 4.7 factorial experiment CUPRAC run 7

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.112					
D	2	Sample X1	J	0.131	0.019	CaSu11	0.1361434	0.0027229	2.722868
D	3	Sample X1	J	0.132	0.02	CaSu11	0.1385659	0.0027713	2.771318
D	4	Sample X1	J	0.132	0.02	CaSu11	0.1385659	0.0027713	2.771318
A	1	Blank B	A	0.127					
A	2	Sample X1	A	0.137	0.01	CaFr11	0.1143411	0.0022868	2.286822
A	3	Sample X1	A	0.137	0.01	CaFr11	0.1143411	0.0022868	2.286822
A	4	Sample X1	A	0.137	0.01	CaFr11	0.1143411	0.0022868	2.286822
A	5	Blank B	B	0.1					
A	6	Sample X1	B	0.184	0.084	CaFr12	0.2936047	0.0058721	5.872093
A	7	Sample X1	B	0.186	0.086	CaFr12	0.2984496	0.0029845	5.968992
A	8	Sample X1	B	0.186	0.086	CaFr12	0.2984496	0.0029845	5.968992
A	9	Blank B	C	0.117					
A	10	Sample X1	C	0.175	0.058	CaFr21	0.2306202	0.0046124	4.612403
A	11	Sample X1	C	0.175	0.058	CaFr21	0.2306202	0.0046124	4.612403
A	12	Sample X1	C	0.175	0.058	CaFr21	0.2306202	0.0046124	4.612403
B	1	Blank B	D	0.076					
B	2	Sample X1	D	0.141	0.065	CaXy11	0.2475775	0.0049516	4.95155
B	3	Sample X1	D	0.141	0.065	CaXy11	0.2475775	0.0049516	4.95155
B	4	Sample X1	D	0.142	0.066	CaXy11	0.25	0.005	5
B	5	Blank B	E	0.107					
B	6	Sample X1	E	0.121	0.014	CaXy12	0.124031	0.0012403	2.48062
B	7	Sample X1	E	0.121	0.014	CaXy12	0.124031	0.0024806	2.48062
B	8	Sample X1	E	0.121	0.014	CaXy12	0.124031	0.0024806	2.48062
B	9	Blank B	F	0.079					
B	10	Sample X1	F	0.134	0.055	CaXy21	0.2233527	0.0044671	4.467054
B	11	Sample X1	F	0.134	0.055	CaXy21	0.2233527	0.0044671	4.467054
B	12	Sample X1	F	0.131	0.052	CaXy21	0.2160853	0.0043217	4.321705
C	1	Blank B	G	0.087					
C	2	Sample X1	G	0.111	0.024	CaGr11	0.1482558	0.0029651	2.965116
C	3	Sample X1	G	0.111	0.024	CaGr11	0.1482558	0.0029651	2.965116
C	4	Sample X1	G	0.111	0.024	CaGr11	0.1482558	0.0029651	2.965116
C	5	Blank B	H	0.088					
C	6	Sample X1	H	0.144	0.056	CaGr12	0.2257752	0.0045155	4.515504
C	7	Sample X1	H	0.144	0.056	CaGr12	0.2257752	0.0045155	4.515504
C	8	Sample X1	H	0.149	0.061	CaGr12	0.2378876	0.0047578	4.757752
C	9	Blank B	I	0.065					
C	10	Sample X1	I	0.137	0.072	CaGr21	0.2645349	0.0052907	5.290698

Appendix 4.7 contd.

C	11	Sample X1	I	0.138	0.073	CaGr21	0.2669574	0.0053391	5.339147
C	12	Sample X1	I	0.138	0.073	CaGr21	0.2669574	0.0053391	5.339147
D	5	Blank B	K	0.077					
D	6	Sample X1	K	0.126	0.049	CaGc11	0.2088178	0.0041764	4.176357
D	7	Sample X1	K	0.126	0.049	CaGc11	0.2088178	0.0041764	4.176357
D	8	Sample X1	K	0.128	0.051	CaGc11	0.2136628	0.0042733	4.273256
D	9	Blank B	L	0.054					
D	10	Sample X1	L	0.138	0.084	CaGc21	0.2936047	0.0058721	5.872093
D	11	Sample X1	L	0.138	0.084	CaGc21	0.2936047	0.0058721	5.872093
D	12	Sample X1	L	0.132	0.078	CaGc21	0.2790698	0.0055814	5.581395
E	1	Blank B	M	0.052					
E	2	Sample X1	M	0.161	0.109	CaGl11	0.3541667	0.0070833	7.083333
E	3	Sample X1	M	0.166	0.114	CaGl11	0.3662791	0.0073256	7.325581
E	4	Sample X1	M	0.161	0.109	CaGl11	0.3541667	0.0070833	7.083333
E	5	Blank B	N	0.053					
E	6	Sample X1	N	0.121	0.068	CaGl21	0.254845	0.0050969	5.096899
E	7	Sample X1	N	0.123	0.07	CaGl21	0.2596899	0.0051938	5.193798
E	8	Sample X1	N	0.123	0.07	CaGl21	0.2596899	0.0051938	5.193798

Appendix 4.8 factorial experiment CUPRAC run 8

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.093					
D	2	Sample X1	J	0.131	0.038	CaSu11	0.18217054	0.0036434	3.643411
D	3	Sample X1	J	0.132	0.039	CaSu11	0.18459302	0.0036919	3.69186
D	4	Sample X1	J	0.132	0.039	CaSu11	0.18459302	0.0036919	3.69186
A	1	Blank B	A	0.095					
A	2	Sample X1	A	0.202	0.107	CaFr11	0.34932171	0.0069864	6.986434
A	3	Sample X1	A	0.201	0.106	CaFr11	0.34689922	0.006938	6.937984
A	4	Sample X1	A	0.201	0.106	CaFr11	0.34689922	0.006938	6.937984
A	5	Blank B	B	0.093					
A	6	Sample X1	B	0.158	0.065	CaFr12	0.24757752	0.0049516	4.95155
A	7	Sample X1	B	0.157	0.064	CaFr12	0.24515504	0.0049031	4.903101
A	8	Sample X1	B	0.158	0.065	CaFr12	0.24757752	0.0049516	4.95155
A	9	Blank B	C	0.083					
A	10	Sample X1	C	0.155	0.072	CaFr21	0.26453488	0.0052907	5.290698
A	11	Sample X1	C	0.154	0.071	CaFr21	0.2621124	0.0052422	5.242248

Appendix 4.8 contd.

A	12	Sample X1	C	0.154	0.071	CaFr21	0.2621124	0.0052422	5.242248
B	1	Blank B	D	0.052					
B	2	Sample X1	D	0.103	0.051	CaXy11	0.21366279	0.0042733	4.273256
B	3	Sample X1	D	0.108	0.056	CaXy11	0.22577519	0.0045155	4.515504
B	4	Sample X1	D	0.103	0.051	CaXy11	0.21366279	0.0042733	4.273256
B	5	Blank B	E	0.071					
B	6	Sample X1	E	0.103	0.032	CaXy12	0.16763566	0.0033527	3.352713
B	7	Sample X1	E	0.103	0.032	CaXy12	0.16763566	0.0033527	3.352713
B	8	Sample X1	E	0.103	0.032	CaXy12	0.16763566	0.0033527	3.352713
B	9	Blank B	F	0.067					
B	10	Sample X1	F	0.116	0.049	CaXy21	0.20881783	0.0041764	4.176357
B	11	Sample X1	F	0.119	0.052	CaXy21	0.21608527	0.0043217	4.321705
B	12	Sample X1	F	0.119	0.052	CaXy21	0.21608527	0.0043217	4.321705
C	1	Blank B	G	0.059					
C	2	Sample X1	G	0.099	0.04	CaGr11	0.1870155	0.0037403	3.74031
C	3	Sample X1	G	0.095	0.036	CaGr11	0.17732558	0.0035465	3.546512
C	4	Sample X1	G	0.099	0.04	CaGr11	0.1870155	0.0037403	3.74031
C	5	Blank B	H	0.103					
C	6	Sample X1	H	0.144	0.041	CaGr12	0.18943798	0.0037888	3.78876
C	7	Sample X1	H	0.144	0.041	CaGr12	0.18943798	0.0037888	3.78876
C	8	Sample X1	H	0.145	0.042	CaGr12	0.19186047	0.0038372	3.837209
C	9	Blank B	I	0.073					
C	10	Sample X1	I	0.111	0.038	CaGr21	0.18217054	0.0036434	3.643411
C	11	Sample X1	I	0.116	0.043	CaGr21	0.19428295	0.0038857	3.885659
C	12	Sample X1	I	0.116	0.043	CaGr21	0.19428295	0.0038857	3.885659
D	5	Blank B	K	0.073					
D	6	Sample X1	K	0.125	0.052	CaGc11	0.21608527	0.0043217	4.321705
D	7	Sample X1	K	0.124	0.051	CaGc11	0.21366279	0.0042733	4.273256
D	8	Sample X1	K	0.124	0.051	CaGc11	0.21366279	0.0042733	4.273256
D	9	Blank B	L	0.071					
D	10	Sample X1	L	0.101	0.03	CaGc21	0.1627907	0.0032558	3.255814
D	11	Sample X1	L	0.103	0.032	CaGc21	0.16763566	0.0033527	3.352713
D	12	Sample X1	L	0.103	0.032	CaGc21	0.16763566	0.0033527	3.352713
E	1	Blank B	M	0.082					
E	2	Sample X1	M	0.113	0.031	CaGl11	0.16521318	0.0033043	3.304264
E	3	Sample X1	M	0.114	0.032	CaGl11	0.16763566	0.0033527	3.352713
E	4	Sample X1	M	0.114	0.032	CaGl11	0.16763566	0.0033527	3.352713
E	5	Blank B	N	0.078					
E	6	Sample X1	N	0.128	0.05	CaGl21	0.21124031	0.0042248	4.224806
E	7	Sample X1	N	0.127	0.049	CaGl21	0.20881783	0.0041764	4.176357
E	8	Sample X1	N	0.127	0.049	CaGl21	0.20881783	0.0041764	4.176357

Appendix 4.9 factorial experiment CUPRAC run 9

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.108					
D	2	Sample X1	J	0.168	0.06	CaSu11	0.235465116	0.003531977	3.531977
D	3	Sample X1	J	0.168	0.06	CaSu11	0.235465116	0.003531977	3.531977
D	4	Sample X1	J	0.169	0.061	CaSu11	0.237887597	0.003568314	3.568314
A	1	Blank B	A	0.133					
A	2	Sample X1	A	0.207	0.074	CaFr11	0.269379845	0.004040698	4.040698
A	3	Sample X1	A	0.206	0.073	CaFr11	0.266957364	0.00400436	4.00436
A	4	Sample X1	A	0.206	0.073	CaFr11	0.266957364	0.00400436	4.00436
A	5	Blank B	B	0.091					
A	6	Sample X1	B	0.182	0.091	CaFr12	0.310562016	0.00465843	4.65843
A	7	Sample X1	B	0.183	0.092	CaFr12	0.312984496	0.004694767	4.694767
A	8	Sample X1	B	0.183	0.092	CaFr12	0.312984496	0.004694767	4.694767
A	9	Blank B	C	0.102					
A	10	Sample X1	C	0.181	0.079	CaFr21	0.281492248	0.004222384	4.222384
A	11	Sample X1	C	0.184	0.082	CaFr21	0.28875969	0.004331395	4.331395
A	12	Sample X1	C	0.184	0.082	CaFr21	0.28875969	0.004331395	4.331395
B	1	Blank B	D	0.072					
B	2	Sample X1	D	0.117	0.045	CaXy11	0.199127907	0.002986919	2.986919
B	3	Sample X1	D	0.117	0.045	CaXy11	0.199127907	0.002986919	2.986919
B	4	Sample X1	D	0.118	0.046	CaXy11	0.201550388	0.003023256	3.023256
B	5	Blank B	E	0.085					
B	6	Sample X1	E	0.112	0.027	CaXy12	0.155523256	0.002332849	2.332849
B	7	Sample X1	E	0.111	0.026	CaXy12	0.153100775	0.002296512	2.296512
B	8	Sample X1	E	0.112	0.027	CaXy12	0.155523256	0.002332849	2.332849
B	9	Blank B	F	0.071					
B	10	Sample X1	F	0.124	0.053	CaXy21	0.218507752	0.003277616	3.277616
B	11	Sample X1	F	0.121	0.05	CaXy21	0.21124031	0.003168605	3.168605
B	12	Sample X1	F	0.121	0.05	CaXy21	0.21124031	0.003168605	3.168605
C	1	Blank B	G	0.064					
C	2	Sample X1	G	0.167	0.103	CaGr11	0.339631783	0.005094477	5.094477
C	3	Sample X1	G	0.163	0.099	CaGr11	0.32994186	0.004949128	4.949128
C	4	Sample X1	G	0.163	0.099	CaGr11	0.32994186	0.004949128	4.949128
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.139	0.053	CaGr12	0.218507752	0.003277616	3.277616
C	7	Sample X1	H	0.139	0.053	CaGr12	0.218507752	0.003277616	3.277616
C	8	Sample X1	H	0.139	0.053	CaGr12	0.218507752	0.003277616	3.277616
C	9	Blank B	I	0.074					
C	10	Sample X1	I	0.144	0.07	CaGr21	0.259689922	0.003895349	3.895349

Appendix 4.9 contd.

C	11	Sample X1	I	0.142	0.068	CaGr21	0.254844961	0.003822674	3.822674
C	12	Sample X1	I	0.142	0.068	CaGr21	0.254844961	0.003822674	3.822674
D	5	Blank B	K	0.063					
D	6	Sample X1	K	0.168	0.105	CaGc11	0.344476744	0.005167151	5.167151
D	7	Sample X1	K	0.166	0.103	CaGc11	0.339631783	0.005094477	5.094477
D	8	Sample X1	K	0.166	0.103	CaGc11	0.339631783	0.005094477	5.094477
D	9	Blank B	L	0.08					
D	10	Sample X1	L	0.135	0.055	CaGc21	0.223352713	0.003350291	3.350291
D	11	Sample X1	L	0.136	0.056	CaGc21	0.225775194	0.003386628	3.386628
D	12	Sample X1	L	0.136	0.056	CaGc21	0.225775194	0.003386628	3.386628
E	1	Blank B	M	0.095					
E	2	Sample X1	M	0.132	0.037	CaGl11	0.179748062	0.002696221	2.696221
E	3	Sample X1	M	0.134	0.039	CaGl11	0.184593023	0.002768895	2.768895
E	4	Sample X1	M	0.134	0.039	CaGl11	0.184593023	0.002768895	2.768895
E	5	Blank B	N	0.082					
E	6	Sample X1	N	0.103	0.021	CaGl21	0.140988372	0.002114826	2.114826
E	7	Sample X1	N	0.101	0.019	CaGl21	0.136143411	0.002042151	2.042151
E	8	Sample X1	N	0.101	0.019	CaGl21	0.136143411	0.002042151	2.042151

Appendix 4.10 factorial experiment CUPRAC run 10

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (mMTE/L)	CUPRAC (mMTE/g)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.091					
D	2	Sample X1	J	0.174	0.083	CaSu11	0.29118217	0.00291182	2.911822
D	3	Sample X1	J	0.179	0.088	CaSu11	0.30329457	0.00303295	3.032946
D	4	Sample X1	J	0.179	0.088	CaSu11	0.30329457	0.00303295	3.032946
A	1	Blank B	A	0.111					
A	2	Sample X1	A	0.234	0.123	CaFr11	0.3880814	0.00388081	3.880814
A	3	Sample X1	A	0.232	0.121	CaFr11	0.38323643	0.00383236	3.832364
A	4	Sample X1	A	0.232	0.121	CaFr11	0.38323643	0.00383236	3.832364
A	5	Blank B	B	0.087					
A	6	Sample X1	B	0.163	0.076	CaFr12	0.27422481	0.00274225	2.742248
A	7	Sample X1	B	0.163	0.076	CaFr12	0.27422481	0.00274225	2.742248
A	8	Sample X1	B	0.161	0.074	CaFr12	0.26937984	0.0026938	2.693798
A	9	Blank B	C	0.082					
A	10	Sample X1	C	0.154	0.072	CaFr21	0.26453488	h28*10/1000	2.645349
A	11	Sample X1	C	0.158	0.076	CaFr21	0.27422481	0.00274225	2.742248
A	12	Sample X1	C	0.154	0.072	CaFr21	0.26453488	0.00264535	2.645349

Appendix4.10 contd.

B	1	Blank B	D	0.07					
B	2	Sample X1	D	0.124	0.054	CaXy11	0.22093023	0.0022093	2.209302
B	3	Sample X1	D	0.123	0.053	CaXy11	0.21850775	0.00218508	2.185078
B	4	Sample X1	D	0.123	0.053	CaXy11	0.21850775	0.00218508	2.185078
B	5	Blank B	E	0.095					
B	6	Sample X1	E	0.112	0.017	CaXy12	0.13129845	0.00131298	1.312984
B	7	Sample X1	E	0.112	0.017	CaXy12	0.13129845	0.00131298	1.312984
B	8	Sample X1	E	0.116	0.021	CaXy12	0.14098837	0.00140988	1.409884
B	9	Blank B	F	0.07					
B	10	Sample X1	F	0.123	0.053	CaXy21	0.21850775	0.00218508	2.185078
B	11	Sample X1	F	0.124	0.054	CaXy21	0.22093023	0.0022093	2.209302
B	12	Sample X1	F	0.123	0.053	CaXy21	0.21850775	0.00218508	2.185078
C	1	Blank B	G	0.073					
C	2	Sample X1	G	0.122	0.049	CaGr11	0.20881783	0.00208818	2.088178
C	3	Sample X1	G	0.129	0.056	CaGr11	0.22577519	0.00225775	2.257752
C	4	Sample X1	G	0.129	0.056	CaGr11	0.22577519	0.00225775	2.257752
C	5	Blank B	H	0.088					
C	6	Sample X1	H	0.131	0.043	CaGr12	0.19428295	0.00194283	1.942829
C	7	Sample X1	H	0.134	0.046	CaGr12	0.20155039	0.0020155	2.015504
C	8	Sample X1	H	0.131	0.043	CaGr12	0.19428295	0.00194283	1.942829
C	9	Blank B	I	0.07					
C	10	Sample X1	I	0.123	0.053	CaGr21	0.21850775	0.00218508	2.185078
C	11	Sample X1	I	0.124	0.054	CaGr21	0.22093023	0.0022093	2.209302
C	12	Sample X1	I	0.123	0.053	CaGr21	0.21850775	0.00218508	2.185078
D	5	Blank B	K	0.075					
D	6	Sample X1	K	0.135	0.06	CaGc11	0.23546512	0.00235465	2.354651
D	7	Sample X1	K	0.135	0.06	CaGc11	0.23546512	0.00235465	2.354651
D	8	Sample X1	K	0.139	0.064	CaGc11	0.24515504	0.00245155	2.45155
D	9	Blank B	L	0.073					
D	10	Sample X1	L	0.125	0.052	CaGc21	0.21608527	0.00216085	2.160853
D	11	Sample X1	L	0.125	0.052	CaGc21	0.21608527	0.00216085	2.160853
D	12	Sample X1	L	0.126	0.053	CaGc21	0.21850775	0.00218508	2.185078
E	1	Blank B	M	0.091					
E	2	Sample X1	M	0.112	0.021	CaGl11	0.14098837	0.00140988	1.409884
E	3	Sample X1	M	0.113	0.022	CaGl11	0.14341085	0.00143411	1.434109
E	4	Sample X1	M	0.113	0.022	CaGl11	0.14341085	0.00143411	1.434109
E	5	Blank B	N	0.08					
E	6	Sample X1	N	0.134	0.054	CaGl21	0.22093023	0.0022093	2.209302
E	7	Sample X1	N	0.139	0.059	CaGl21	0.23304264	0.00233043	2.330426
E	8	Sample X1	N	0.134	0.054	CaGl21	0.22093023	0.0022093	2.209302

Appendix 5.1 factorial experiment FRAP run 1

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	1.083				
D	2	Sample X1	J	1.234	0.151	CaSu11	117.461538	1.761923
D	3	Sample X1	J	1.234	0.151	CaSu11	117.461538	1.761923
D	4	Sample X1	J	1.236	0.153	CaSu11	119	1.785
A	1	Blank B	A	1.55				
A	2	Sample X1	A	2.194	0.644	CaFr11	496.692308	7.450385
A	3	Sample X1	A	2.192	0.642	CaFr11	495.153846	7.427308
A	4	Sample X1	A	2.194	0.644	CaFr11	496.692308	7.450385
A	5	Blank B	B	1.038				
A	6	Sample X1	B	1.443	0.405	CaFr12	312.846154	4.692692
A	7	Sample X1	B	1.446	0.408	CaFr12	315.153846	4.727308
A	8	Sample X1	B	1.443	0.405	CaFr12	312.846154	4.692692
A	9	Blank B	C	1.037				
A	10	Sample X1	C	1.381	0.344	CaFr21	265.923077	3.988846
A	11	Sample X1	C	1.381	0.344	CaFr21	265.923077	3.988846
A	12	Sample X1	C	1.382	0.345	CaFr21	266.692308	4.000385
B	1	Blank B	D	1.034				
B	2	Sample X1	D	1.385	0.351	CaXy11	271.307692	4.069615
B	3	Sample X1	D	1.387	0.353	CaXy11	272.846154	4.092692
B	4	Sample X1	D	1.385	0.351	CaXy11	271.307692	4.069615
B	5	Blank B	E	1.039				
B	6	Sample X1	E	1.207	0.168	CaXy12	130.538462	1.958077
B	7	Sample X1	E	1.207	0.168	CaXy12	130.538462	1.958077
B	8	Sample X1	E	1.209	0.17	CaXy12	132.076923	1.981154
B	9	Blank B	F	1.03				
B	10	Sample X1	F	1.276	0.246	CaXy21	190.538462	2.858077
B	11	Sample X1	F	1.277	0.247	CaXy21	191.307692	2.869615
B	12	Sample X1	F	1.276	0.246	CaXy21	190.538462	2.858077
C	1	Blank B	G	1.021				
C	2	Sample X1	G	1.245	0.224	CaGr11	173.615385	2.604231
C	3	Sample X1	G	1.243	0.222	CaGr11	172.076923	2.581154
C	4	Sample X1	G	1.245	0.224	CaGr11	173.615385	2.604231
C	5	Blank B	H	1.02				
C	6	Sample X1	H	1.201	0.181	CaGr12	140.538462	2.108077
C	7	Sample X1	H	1.201	0.181	CaGr12	140.538462	2.108077
C	8	Sample X1	H	1.2	0.18	CaGr12	139.769231	2.096538
C	9	Blank B	I	1.02				

Appendix 5.1 contd.

C	10	Sample X1	I	1.198	0.178	CaGr21	138.230769	2.073462
C	11	Sample X1	I	1.197	0.177	CaGr21	137.461538	2.061923
C	12	Sample X1	I	1.197	0.177	CaGr21	137.461538	2.061923
D	5	Blank B	K	1.014				
D	6	Sample X1	K	1.065	0.051	CaGc11	40.5384615	0.608077
D	7	Sample X1	K	1.065	0.051	CaGc11	40.5384615	0.608077
D	8	Sample X1	K	1.065	0.051	CaGc11	40.5384615	0.608077
D	9	Blank B	L	1.014				
D	10	Sample X1	L	1.067	0.053	CaGc21	42.0769231	0.631154
D	11	Sample X1	L	1.067	0.053	CaGc21	42.0769231	0.631154
D	12	Sample X1	L	1.066	0.052	CaGc21	41.3076923	0.619615
E	1	Blank B	M	1.011				
E	2	Sample X1	M	1.105	0.094	CaGl11	73.6153846	1.104231
E	3	Sample X1	M	1.104	0.093	CaGl11	72.8461538	1.092692
E	4	Sample X1	M	1.105	0.094	CaGl11	73.6153846	1.104231
E	5	Blank B	N	1.013				
E	6	Sample X1	N	1.076	0.063	CaGl21	49.7692308	0.746538
E	7	Sample X1	N	1.078	0.065	CaGl21	51.3076923	0.769615
E	8	Sample X1	N	1.074	0.061	CaGl21	48.2307692	0.723462

Appendix 5.2 factorial experiment FRAP run 2

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	0.554				
D	2	Sample X1	J	0.637	0.083	CaSu11	65.1538462	1.303077
D	3	Sample X1	J	0.638	0.084	CaSu11	65.9230769	1.318462
D	4	Sample X1	J	0.638	0.084	CaSu11	65.9230769	1.318462
A	1	Blank B	A	0.705				
A	2	Sample X1	A	0.783	0.078	CaFr11	61.3076923	1.226154
A	3	Sample X1	A	0.781	0.076	CaFr11	59.7692308	1.195385
A	4	Sample X1	A	0.783	0.078	CaFr11	61.3076923	1.226154
A	5	Blank B	B	0.704				
A	6	Sample X1	B	0.756	0.052	CaFr12	41.3076923	0.826154
A	7	Sample X1	B	0.755	0.051	CaFr12	40.5384615	0.810769
A	8	Sample X1	B	0.755	0.051	CaFr12	40.5384615	0.810769
A	9	Blank B	C	0.737				
A	10	Sample X1	C	0.805	0.068	CaFr21	53.6153846	1.072308
A	11	Sample X1	C	0.807	0.07	CaFr21	55.1538462	1.103077

Appendix 5.2 contd.

A	12	Sample X1	C	0.807	0.07	CaFr21	55.1538462	1.103077
B	1	Blank B	D	0.628				
B	2	Sample X1	D	0.696	0.068	CaXy11	53.6153846	1.072308
B	3	Sample X1	D	0.694	0.066	CaXy11	52.0769231	1.041538
B	4	Sample X1	D	0.694	0.066	CaXy11	52.0769231	1.041538
B	5	Blank B	E	0.602				
B	6	Sample X1	E	0.653	0.051	CaXy12	40.5384615	0.810769
B	7	Sample X1	E	0.658	0.056	CaXy12	44.3846154	0.887692
B	8	Sample X1	E	0.658	0.056	CaXy12	44.3846154	0.887692
B	9	Blank B	F	0.607				
B	10	Sample X1	F	0.652	0.045	CaXy21	35.9230769	0.718462
B	11	Sample X1	F	0.652	0.045	CaXy21	35.9230769	0.718462
B	12	Sample X1	F	0.656	0.049	CaXy21	39	0.78
C	1	Blank B	G	0.573				
C	2	Sample X1	G	0.618	0.045	CaGr11	35.9230769	0.718462
C	3	Sample X1	G	0.618	0.045	CaGr11	35.9230769	0.718462
C	4	Sample X1	G	0.616	0.043	CaGr11	34.3846154	0.687692
C	5	Blank B	H	0.509				
C	6	Sample X1	H	0.557	0.048	CaGr12	38.2307692	0.764615
C	7	Sample X1	H	0.557	0.048	CaGr12	38.2307692	0.764615
C	8	Sample X1	H	0.556	0.047	CaGr12	37.4615385	0.749231
C	9	Blank B	I	0.484				
C	10	Sample X1	I	0.564	0.08	CaGr21	62.8461538	1.256923
C	11	Sample X1	I	0.561	0.077	CaGr21	60.5384615	1.210769
C	12	Sample X1	I	0.561	0.077	CaGr21	60.5384615	1.210769
D	5	Blank B	K	0.303				
D	6	Sample X1	K	0.424	0.121	CaGc11	94.3846154	1.887692
D	7	Sample X1	K	0.422	0.119	CaGc11	92.8461538	1.856923
D	8	Sample X1	K	0.422	0.119	CaGc11	92.8461538	1.856923
D	9	Blank B	L	0.346				
D	10	Sample X1	L	0.446	0.1	CaGc21	78.2307692	1.564615
D	11	Sample X1	L	0.446	0.1	CaGc21	78.2307692	1.564615
D	12	Sample X1	L	0.444	0.098	CaGc21	76.6923077	1.533846
E	1	Blank B	M	0.353				
E	2	Sample X1	M	0.41	0.057	CaGl11	45.1538462	0.903077
E	3	Sample X1	M	0.408	0.055	CaGl11	43.6153846	0.872308
E	4	Sample X1	M	0.41	0.057	CaGl11	45.1538462	0.903077
E	5	Blank B	N	0.329				
E	6	Sample X1	N	0.374	0.045	CaGl21	35.9230769	0.718462
E	7	Sample X1	N	0.374	0.045	CaGl21	35.9230769	0.718462
E	8	Sample X1	N	0.376	0.047	CaGl21	37.4615385	0.749231

Appendix 5.3 factorial experiment FRAP run 3

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	0.558				
D	2	Sample X1	J	0.664	0.106	CaSu11	82.84615385	1.656923
D	3	Sample X1	J	0.668	0.11	CaSu11	85.92307692	1.718462
D	4	Sample X1	J	0.664	0.106	CaSu11	82.84615385	1.656923
A	1	Blank B	A	0.869				
A	2	Sample X1	A	1.345	0.476	CaFr11	367.4615385	7.349231
A	3	Sample X1	A	1.345	0.476	CaFr11	367.4615385	7.349231
A	4	Sample X1	A	1.348	0.479	CaFr11	369.7692308	7.395385
A	5	Blank B	B	0.791				
A	6	Sample X1	B	0.984	0.193	CaFr12	149.7692308	2.995385
A	7	Sample X1	B	0.984	0.193	CaFr12	149.7692308	2.995385
A	8	Sample X1	B	0.987	0.196	CaFr12	152.0769231	3.041538
A	9	Blank B	C	0.792				
A	10	Sample X1	C	1.044	0.252	CaFr21	195.1538462	3.903077
A	11	Sample X1	C	1.048	0.256	CaFr21	198.2307692	3.964615
A	12	Sample X1	C	1.045	0.253	CaFr21	195.9230769	3.918462
B	1	Blank B	D	0.792				
B	2	Sample X1	D	0.844	0.052	CaXy11	41.30769231	0.826154
B	3	Sample X1	D	0.844	0.052	CaXy11	41.30769231	0.826154
B	4	Sample X1	D	0.849	0.057	CaXy11	45.15384615	0.903077
B	5	Blank B	E	0.686				
B	6	Sample X1	E	0.788	0.102	CaXy12	79.76923077	1.595385
B	7	Sample X1	E	0.788	0.102	CaXy12	79.76923077	1.595385
B	8	Sample X1	E	0.787	0.101	CaXy12	79	1.58
B	9	Blank B	F	0.678				
B	10	Sample X1	F	0.815	0.137	CaXy21	106.6923077	2.133846
B	11	Sample X1	F	0.815	0.137	CaXy21	106.6923077	2.133846
B	12	Sample X1	F	0.819	0.141	CaXy21	109.7692308	2.195385
C	1	Blank B	G	0.651				
C	2	Sample X1	G	0.749	0.098	CaGr11	76.69230769	1.533846
C	3	Sample X1	G	0.749	0.098	CaGr11	76.69230769	1.533846
C	4	Sample X1	G	0.741	0.09	CaGr11	70.53846154	1.410769
C	5	Blank B	H	0.608				
C	6	Sample X1	H	0.942	0.334	CaGr12	258.2307692	5.164615
C	7	Sample X1	H	0.942	0.334	CaGr12	258.2307692	5.164615
C	8	Sample X1	H	0.949	0.341	CaGr12	263.6153846	5.272308
C	9	Blank B	I	0.566				
C	10	Sample X1	I	0.686	0.12	CaGr21	93.61538462	1.872308

Appendix 5.3 contd.

C	11	Sample X1	I	0.687	0.121	CaGr21	94.38461538	1.887692
C	12	Sample X1	I	0.688	0.122	CaGr21	95.15384615	1.903077
D	5	Blank B	K	0.462				
D	6	Sample X1	K	0.538	0.076	CaGc11	59.76923077	1.195385
D	7	Sample X1	K	0.538	0.076	CaGc11	59.76923077	1.195385
D	8	Sample X1	K	0.537	0.075	CaGc11	59	1.18
D	9	Blank B	L	0.468				
D	10	Sample X1	L	0.573	0.105	CaGc21	82.07692308	1.641538
D	11	Sample X1	L	0.571	0.103	CaGc21	80.53846154	1.610769
D	12	Sample X1	L	0.573	0.105	CaGc21	82.07692308	1.641538
E	1	Blank B	M	0.528				
E	2	Sample X1	M	0.633	0.105	CaGl11	82.07692308	1.641538
E	3	Sample X1	M	0.633	0.105	CaGl11	82.07692308	1.641538
E	4	Sample X1	M	0.632	0.104	CaGl11	81.30769231	1.626154
E	5	Blank B	N	0.437				
E	6	Sample X1	N	0.527	0.09	CaGl21	70.53846154	1.410769
E	7	Sample X1	N	0.523	0.086	CaGl21	67.46153846	1.349231
E	8	Sample X1	N	0.527	0.09	CaGl21	70.53846154	1.410769

Appendix 5.4 factorial experiment FRAP run 4

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	0.559				
D	2	Sample X1	J	0.644	0.085	CaSu11	66.6923077	0.666923
D	3	Sample X1	J	0.644	0.085	CaSu11	66.6923077	0.666923
D	4	Sample X1	J	0.647	0.088	CaSu11	69	0.69
A	1	Blank B	A	0.924				
A	2	Sample X1	A	1.073	0.149	CaFr11	115.923077	1.159231
A	3	Sample X1	A	1.073	0.149	CaFr11	115.923077	1.159231
A	4	Sample X1	A	1.076	0.152	CaFr11	118.230769	1.182308
A	5	Blank B	B	0.717				
A	6	Sample X1	B	0.877	0.16	CaFr12	124.384615	1.243846
A	7	Sample X1	B	0.878	0.161	CaFr12	125.153846	1.251538
A	8	Sample X1	B	0.877	0.16	CaFr12	124.384615	1.243846
A	9	Blank B	C	0.793				
A	10	Sample X1	C	0.955	0.162	CaFr21	125.923077	1.259231
A	11	Sample X1	C	0.954	0.161	CaFr21	125.153846	1.251538

Appendix 5.4 contd.

A	12	Sample X1	C	0.954	0.161	CaFr21	125.153846	1.251538
B	1	Blank B	D	0.709				
B	2	Sample X1	D	0.773	0.064	CaXy11	50.5384615	0.505385
B	3	Sample X1	D	0.773	0.064	CaXy11	50.5384615	0.505385
B	4	Sample X1	D	0.773	0.064	CaXy11	50.5384615	0.505385
B	5	Blank B	E	0.627				
B	6	Sample X1	E	0.713	0.086	CaXy12	67.4615385	0.674615
B	7	Sample X1	E	0.713	0.086	CaXy12	67.4615385	0.674615
B	8	Sample X1	E	0.712	0.085	CaXy12	66.6923077	0.666923
B	9	Blank B	F	0.679				
B	10	Sample X1	F	0.909	0.23	CaXy21	178.230769	1.782308
B	11	Sample X1	F	0.909	0.23	CaXy21	178.230769	1.782308
B	12	Sample X1	F	0.906	0.227	CaXy21	175.923077	1.759231
C	1	Blank B	G	0.583				
C	2	Sample X1	G	0.641	0.058	CaGr11	45.9230769	0.459231
C	3	Sample X1	G	0.641	0.058	CaGr11	45.9230769	0.459231
C	4	Sample X1	G	0.639	0.056	CaGr11	44.3846154	0.443846
C	5	Blank B	H	0.564				
C	6	Sample X1	H	0.619	0.055	CaGr12	43.6153846	0.436154
C	7	Sample X1	H	0.615	0.051	CaGr12	40.5384615	0.405385
C	8	Sample X1	H	0.619	0.055	CaGr12	43.6153846	0.436154
C	9	Blank B	I	0.576				
C	10	Sample X1	I	0.632	0.056	CaGr21	44.3846154	0.443846
C	11	Sample X1	I	0.632	0.056	CaGr21	44.3846154	0.443846
C	12	Sample X1	I	0.631	0.055	CaGr21	43.6153846	0.436154
D	5	Blank B	K	0.372				
D	6	Sample X1	K	0.462	0.09	CaGc11	70.5384615	0.705385
D	7	Sample X1	K	0.462	0.09	CaGc11	70.5384615	0.705385
D	8	Sample X1	K	0.462	0.09	CaGc11	70.5384615	0.705385
D	9	Blank B	L	0.488				
D	10	Sample X1	L	0.535	0.047	CaGc21	37.4615385	0.374615
D	11	Sample X1	L	0.538	0.05	CaGc21	39.7692308	0.397692
D	12	Sample X1	L	0.536	0.048	CaGc21	38.2307692	0.382308
E	1	Blank B	M	0.401				
E	2	Sample X1	M	0.442	0.041	CaGl11	32.8461538	0.328462
E	3	Sample X1	M	0.442	0.041	CaGl11	32.8461538	0.328462
E	4	Sample X1	M	0.449	0.048	CaGl11	38.2307692	0.382308
E	5	Blank B	N	0.407				
E	6	Sample X1	N	0.449	0.042	CaGl21	33.6153846	0.336154
E	7	Sample X1	N	0.449	0.042	CaGl21	33.6153846	0.336154
E	8	Sample X1	N	0.448	0.041	CaGl21	32.8461538	0.328462

Appendix 5.5 factorial experiment FRAP run 5

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.483				
D	2	Sample X1	J	0.618	0.135	CaSu11	105.1538462	1.051538
D	3	Sample X1	J	0.618	0.135	CaSu11	105.1538462	1.051538
D	4	Sample X1	J	0.619	0.136	CaSu11	105.9230769	1.059231
A	1	Blank B	A	0.754				
A	2	Sample X1	A	1.003	0.249	CaFr11	192.8461538	1.928462
A	3	Sample X1	A	1.002	0.248	CaFr11	192.0769231	1.920769
A	4	Sample X1	A	1.003	0.249	CaFr11	192.8461538	1.928462
A	5	Blank B	B	0.85				
A	6	Sample X1	B	1.076	0.226	CaFr12	175.1538462	1.751538
A	7	Sample X1	B	1.075	0.225	CaFr12	174.3846154	1.743846
A	8	Sample X1	B	1.075	0.225	CaFr12	174.3846154	1.743846
A	9	Blank B	C	0.056				
A	10	Sample X1	C	0.278	0.222	CaFr21	172.0769231	1.720769
A	11	Sample X1	C	0.273	0.217	CaFr21	168.2307692	1.682308
A	12	Sample X1	C	0.278	0.222	CaFr21	172.0769231	1.720769
B	1	Blank B	D	0.793				
B	2	Sample X1	D	0.998	0.205	CaXy11	159	1.59
B	3	Sample X1	D	0.996	0.203	CaXy11	157.4615385	1.574615
B	4	Sample X1	D	0.996	0.203	CaXy11	157.4615385	1.574615
B	5	Blank B	E	0.707				
B	6	Sample X1	E	0.957	0.25	CaXy12	193.6153846	1.936154
B	7	Sample X1	E	0.954	0.247	CaXy12	191.3076923	1.913077
B	8	Sample X1	E	0.954	0.247	CaXy12	191.3076923	1.913077
B	9	Blank B	F	0.621				
B	10	Sample X1	F	0.922	0.301	CaXy21	232.8461538	2.328462
B	11	Sample X1	F	0.921	0.3	CaXy21	232.0769231	2.320769
B	12	Sample X1	F	0.922	0.301	CaXy21	232.8461538	2.328462
C	1	Blank B	G	0.609				
C	2	Sample X1	G	0.688	0.079	CaGr11	62.07692308	0.620769
C	3	Sample X1	G	0.687	0.078	CaGr11	61.30769231	0.613077
C	4	Sample X1	G	0.687	0.078	CaGr11	61.30769231	0.613077
C	5	Blank B	H	0.338				
C	6	Sample X1	H	0.636	0.298	CaGr12	230.5384615	2.305385
C	7	Sample X1	H	0.638	0.3	CaGr12	232.0769231	2.320769
C	8	Sample X1	H	0.638	0.3	CaGr12	232.0769231	2.320769
C	9	Blank B	I	0.553				
C	10	Sample X1	I	0.615	0.062	CaGr21	49	0.49

Appendix 5.5 contd.

C	11	Sample X1	I	0.614	0.061	CaGr21	48.23076923	0.482308
C	12	Sample X1	I	0.614	0.061	CaGr21	48.23076923	0.482308
D	5	Blank B	K	0.368				
D	6	Sample X1	K	0.464	0.096	CaGc11	75.15384615	0.751538
D	7	Sample X1	K	0.465	0.097	CaGc11	75.92307692	0.759231
D	8	Sample X1	K	0.465	0.097	CaGc11	75.92307692	0.759231
D	9	Blank B	L	0.375				
D	10	Sample X1	L	0.465	0.09	CaGc21	70.53846154	0.705385
D	11	Sample X1	L	0.462	0.087	CaGc21	68.23076923	0.682308
D	12	Sample X1	L	0.465	0.09	CaGc21	70.53846154	0.705385
E	1	Blank B	M	0.411				
E	2	Sample X1	M	0.595	0.184	CaGl11	142.8461538	1.428462
E	3	Sample X1	M	0.595	0.184	CaGl11	142.8461538	1.428462
E	4	Sample X1	M	0.591	0.18	CaGl11	139.7692308	1.397692
E	5	Blank B	N	0.401				
E	6	Sample X1	N	0.535	0.134	CaGl21	104.3846154	1.043846
E	7	Sample X1	N	0.533	0.132	CaGl21	102.8461538	1.028462
E	8	Sample X1	N	0.535	0.134	CaGl21	104.3846154	1.043846

Appendix 5.6 Factorial experiment FRAP run 6

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	0.575				
D	2	Sample X1	J	0.833	0.258	CaSu11	199.769231	1.997692
D	3	Sample X1	J	0.839	0.264	CaSu11	204.384615	2.043846
D	4	Sample X1	J	0.833	0.258	CaSu11	199.769231	1.997692
A	1	Blank B	A	0.791				
A	2	Sample X1	A	1.346	0.555	CaFr11	428.230769	4.282308
A	3	Sample X1	A	1.345	0.554	CaFr11	427.461538	4.274615
A	4	Sample X1	A	1.347	0.556	CaFr11	429	4.29
A	5	Blank B	B	0.789				
A	6	Sample X1	B	1.006	0.217	CaFr12	168.230769	1.682308
A	7	Sample X1	B	1.009	0.22	CaFr12	170.538462	1.705385
A	8	Sample X1	B	1.006	0.217	CaFr12	168.230769	1.682308
A	9	Blank B	C	0.749				
A	10	Sample X1	C	1.065	0.316	CaFr21	244.384615	2.443846
A	11	Sample X1	C	1.064	0.315	CaFr21	243.615385	2.436154

Appendix 5.6 contd.

A	12	Sample X1	C	1.065	0.316	CaFr21	244.384615	2.443846
B	1	Blank B	D	0.677				
B	2	Sample X1	D	0.898	0.221	CaXy11	171.307692	1.713077
B	3	Sample X1	D	0.894	0.217	CaXy11	168.230769	1.682308
B	4	Sample X1	D	0.894	0.217	CaXy11	168.230769	1.682308
B	5	Blank B	E	0.691				
B	6	Sample X1	E	0.874	0.183	CaXy12	142.076923	1.420769
B	7	Sample X1	E	0.876	0.185	CaXy12	143.615385	1.436154
B	8	Sample X1	E	0.874	0.183	CaXy12	142.076923	1.420769
B	9	Blank B	F	0.624				
B	10	Sample X1	F	0.951	0.327	CaXy21	252.846154	2.528462
B	11	Sample X1	F	0.954	0.33	CaXy21	255.153846	2.551538
B	12	Sample X1	F	0.954	0.33	CaXy21	255.153846	2.551538
C	1	Blank B	G	0.625				
C	2	Sample X1	G	0.958	0.333	CaGr11	257.461538	2.574615
C	3	Sample X1	G	0.959	0.334	CaGr11	258.230769	2.582308
C	4	Sample X1	G	0.958	0.333	CaGr11	257.461538	2.574615
C	5	Blank B	H	0.62				
C	6	Sample X1	H	0.884	0.264	CaGr12	204.384615	2.043846
C	7	Sample X1	H	0.884	0.264	CaGr12	204.384615	2.043846
C	8	Sample X1	H	0.885	0.265	CaGr12	205.153846	2.051538
C	9	Blank B	I	0.543				
C	10	Sample X1	I	0.879	0.336	CaGr21	259.769231	2.597692
C	11	Sample X1	I	0.878	0.335	CaGr21	259	2.59
C	12	Sample X1	I	0.879	0.336	CaSu11	259.769231	2.597692
D	5	Blank B	K	0.464				
D	6	Sample X1	K	0.555	0.091	CaGc11	71.3076923	0.713077
D	7	Sample X1	K	0.555	0.091	CaGc11	71.3076923	0.713077
D	8	Sample X1	K	0.559	0.095	CaGc11	74.3846154	0.743846
D	9	Blank B	L	0.463				
D	10	Sample X1	L	0.636	0.173	CaGc21	134.384615	1.343846
D	11	Sample X1	L	0.638	0.175	CaGc21	135.923077	1.359231
D	12	Sample X1	L	0.638	0.175	CaGc21	135.923077	1.359231
E	1	Blank B	M	0.509				
E	2	Sample X1	M	0.796	0.287	CaGl11	222.076923	2.220769
E	3	Sample X1	M	0.792	0.283	CaGl11	219	2.19
E	4	Sample X1	M	0.796	0.287	CaGl11	222.076923	2.220769
E	5	Blank B	N	0.458				
E	6	Sample X1	N	0.625	0.167	CaGl21	129.769231	1.297692
E	7	Sample X1	N	0.625	0.167	CaGl21	129.769231	1.297692
E	8	Sample X1	N	0.626	0.168	CaGl21	130.538462	1.305385

Appendix 5.7 factorial experiment run 7

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
	1	Blank B	J	0.063				
D	2	Sample X1	J	0.562	0.499	CaSu11	385.15385	7.703076923
D	3	Sample X1	J	0.565	0.502	CaSu11	387.46154	7.749230769
D	4	Sample X1	J	0.562	0.499	CaSu11	385.15385	7.703076923
A	1	Blank B	A	0.089				
A	2	Sample X1	A	0.894	0.805	CaFr11	620.53846	12.41076923
A	3	Sample X1	A	0.89	0.801	CaFr11	617.46154	12.34923077
A	4	Sample X1	A	0.89	0.801	CaFr11	617.46154	12.34923077
A	5	Blank B	B	0.079				
A	6	Sample X1	B	0.798	0.719	CaFr12	554.38462	11.08769231
A	7	Sample X1	B	0.796	0.717	CaFr12	552.84615	11.05692308
A	8	Sample X1	B	0.796	0.717	CaFr12	552.84615	11.05692308
A	9	Blank B	C	0.075				
A	10	Sample X1	C	0.901	0.826	CaFr21	636.69231	12.73384615
A	11	Sample X1	C	0.901	0.826	CaFr21	636.69231	12.73384615
A	12	Sample X1	C	0.902	0.827	CaFr21	637.46154	12.74923077
B	1	Blank B	D	0.069				
B	2	Sample X1	D	0.756	0.687	CaXy11	529.76923	10.59538462
B	3	Sample X1	D	0.755	0.686	CaXy11	529	10.58
B	4	Sample X1	D	0.753	0.684	CaXy11	527.46154	10.54923077
B	5	Blank B	E	0.067				
B	6	Sample X1	E	0.673	0.606	CaXy12	467.46154	9.349230769
B	7	Sample X1	E	0.672	0.605	CaXy12	466.69231	9.333846154
B	8	Sample X1	E	0.675	0.608	CaXy12	469	9.38
B	9	Blank B	F	0.068				
B	10	Sample X1	F	0.713	0.645	CaXy21	497.46154	9.949230769
B	11	Sample X1	F	0.715	0.647	CaXy21	499	9.98
B	12	Sample X1	F	0.715	0.647	CaXy21	499	9.98
C	1	Blank B	G	0.062				
C	2	Sample X1	G	0.657	0.595	CaGr11	459	9.949230769
C	3	Sample X1	G	0.659	0.597	CaGr11	460.53846	9.98
C	4	Sample X1	G	0.658	0.596	CaGr11	459.76923	9.98
C	5	Blank B	H	0.057				
C	6	Sample X1	H	0.629	0.572	CaGr12	441.30769	8.826153846
C	7	Sample X1	H	0.629	0.572	CaGr12	441.30769	8.826153846
C	8	Sample X1	H	0.629	0.572	CaGr12	441.30769	8.826153846
C	9	Blank B	I	0.059				
C	10	Sample X1	I	0.587	0.528	CaGr21	407.46154	8.826153846

Appendix 5.7 contd.

C	11	Sample X1	I	0.585	0.526	CaGr21	405.92308	8.826153846
C	12	Sample X1	I	0.585	0.526	CaSu11	405.92308	8.826153846
D	5	Blank B	K	0.052				
D	6	Sample X1	K	0.456	0.404	CaGc11	312.07692	6.241538462
D	7	Sample X1	K	0.458	0.406	CaGc11	313.61538	6.272307692
D	8	Sample X1	K	0.454	0.402	CaGc11	310.53846	6.210769231
D	9	Blank B	L	0.046				
D	10	Sample X1	L	0.434	0.388	CaGc21	299.76923	5.995384615
D	11	Sample X1	L	0.434	0.388	CaGc21	299.76923	5.995384615
D	12	Sample X1	L	0.433	0.387	CaGc21	299	5.98
E	1	Blank B	M	0.049				
E	2	Sample X1	M	0.472	0.423	CaGl11	326.69231	6.533846154
E	3	Sample X1	M	0.475	0.426	CaGl11	329	6.58
E	4	Sample X1	M	0.475	0.426	CaGl11	329	6.58
E	5	Blank B	N	0.048				
E	6	Sample X1	N	0.448	0.4	CaGl21	309	6.18
E	7	Sample X1	N	0.443	0.395	CaGl21	305.15385	6.103076923
E	8	Sample X1	N	0.448	0.4	CaGl21	309	6.18

Appendix 5.8 factorial experiment FRAP run 8

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.59				
D	2	Sample X1	J	1.257	0.667	CaSu11	514.3846154	10.28769
D	3	Sample X1	J	1.257	0.667	CaSu11	514.3846154	10.28769
D	4	Sample X1	J	1.254	0.664	CaSu11	512.0769231	10.24154
A	1	Blank B	A	0.903				
A	2	Sample X1	A	1.584	0.681	CaFr11	525.1538462	10.50308
A	3	Sample X1	A	1.584	0.681	CaFr11	525.1538462	10.50308
A	4	Sample X1	A	1.589	0.686	CaFr11	529	10.58
A	5	Blank B	B	0.828				
A	6	Sample X1	B	1.536	0.708	CaFr12	545.9230769	10.91846
A	7	Sample X1	B	1.536	0.708	CaFr12	545.9230769	10.91846
A	8	Sample X1	B	1.538	0.71	CaFr12	547.4615385	10.94923
A	9	Blank B	C	0.817				
A	10	Sample X1	C	1.569	0.752	CaFr21	579.7692308	11.59538
A	11	Sample X1	C	1.561	0.744	CaFr21	573.6153846	11.47231

Appendix 5.8 contd.

A	12	Sample X1	C	1.569	0.752	CaFr21	579.7692308	11.59538
B	1	Blank B	D	0.426				
B	2	Sample X1	D	1.388	0.962	CaXy11	741.3076923	14.82615
B	3	Sample X1	D	1.385	0.959	CaXy11	739	14.78
B	4	Sample X1	D	1.384	0.958	CaXy11	738.2307692	14.76462
B	5	Blank B	E	0.727				
B	6	Sample X1	E	1.397	0.67	CaXy12	516.6923077	10.33385
B	7	Sample X1	E	1.397	0.67	CaXy12	516.6923077	10.33385
B	8	Sample X1	E	1.398	0.671	CaXy12	517.4615385	10.34923
B	9	Blank B	F	0.703				
B	10	Sample X1	F	1.341	0.638	CaXy21	492.0769231	9.841538
B	11	Sample X1	F	1.342	0.639	CaXy21	492.8461538	9.856923
B	12	Sample X1	F	1.34	0.637	CaXy21	491.3076923	9.826154
C	1	Blank B	G	0.664				
C	2	Sample X1	G	1.285	0.621	CaGr11	479	9.58
C	3	Sample X1	G	1.285	0.621	CaGr11	479	9.58
C	4	Sample X1	G	1.283	0.619	CaGr11	477.4615385	9.549231
C	5	Blank B	H	0.698				
C	6	Sample X1	H	1.343	0.645	CaGr12	497.4615385	9.949231
C	7	Sample X1	H	1.345	0.647	CaGr12	499	9.98
C	8	Sample X1	H	1.343	0.645	CaGr12	497.4615385	9.949231
C	9	Blank B	I	0.542				
C	10	Sample X1	I	1.269	0.727	CaGr21	560.5384615	11.21077
C	11	Sample X1	I	1.261	0.719	CaGr21	554.3846154	11.08769
C	12	Sample X1	I	1.269	0.727	CaSu11	560.5384615	11.21077
D	5	Blank B	K	0.572				
D	6	Sample X1	K	1.161	0.589	CaGc11	454.3846154	9.087692
D	7	Sample X1	K	1.161	0.589	CaGc11	454.3846154	9.087692
D	8	Sample X1	K	1.16	0.588	CaGc11	453.6153846	9.072308
D	9	Blank B	L	1.274				
D	10	Sample X1	L	1.476	0.202	CaGc21	156.6923077	3.133846
D	11	Sample X1	L	1.477	0.203	CaGc21	157.4615385	3.149231
D	12	Sample X1	L	1.476	0.202	CaGc21	156.6923077	3.133846
E	1	Blank B	M	1.159				
E	2	Sample X1	M	1.578	0.419	CaGl11	323.6153846	6.472308
E	3	Sample X1	M	1.573	0.414	CaGl11	319.7692308	6.395385
E	4	Sample X1	M	1.579	0.42	CaGl11	324.3846154	6.487692
E	5	Blank B	N	1.2				
E	6	Sample X1	N	1.665	0.465	CaGl21	359	7.18
E	7	Sample X1	N	1.669	0.469	CaGl21	362.0769231	7.241538
E	8	Sample X1	N	1.665	0.465	CaGl21	359	7.18

Appendix 5.9 factorial experiment FRAP run 9

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	1.083				
D	2	Sample X1	J	1.235	0.152	CaSu11	118.2307692	1.7734615
D	3	Sample X1	J	1.235	0.152	CaSu11	118.2307692	1.7734615
D	4	Sample X1	J	1.236	0.153	CaSu11	119	1.785
A	1	Blank B	A	1.551				
A	2	Sample X1	A	2.195	0.644	CaFr11	496.6923077	7.4503846
A	3	Sample X1	A	2.197	0.646	CaFr11	498.2307692	7.4734615
A	4	Sample X1	A	2.194	0.643	CaFr11	495.9230769	7.4388462
A	5	Blank B	B	1.038				
A	6	Sample X1	B	1.441	0.403	CaFr12	311.3076923	4.6696154
A	7	Sample X1	B	1.446	0.408	CaFr12	315.1538462	4.7273077
A	8	Sample X1	B	1.443	0.405	CaFr12	312.8461538	4.6926923
A	9	Blank B	C	1.037				
A	10	Sample X1	C	1.38	0.343	CaFr21	265.1538462	3.9773077
A	11	Sample X1	C	1.38	0.343	CaFr21	265.1538462	3.9773077
A	12	Sample X1	C	1.382	0.345	CaFr21	266.6923077	4.0003846
B	1	Blank B	D	1.039				
B	2	Sample X1	D	1.385	0.346	CaXy11	267.4615385	4.0119231
B	3	Sample X1	D	1.387	0.348	CaXy11	269	4.035
B	4	Sample X1	D	1.385	0.346	CaXy11	267.4615385	4.0119231
B	5	Blank B	E	1.038				
B	6	Sample X1	E	1.207	0.169	CaXy12	131.3076923	1.9696154
B	7	Sample X1	E	1.207	0.169	CaXy12	131.3076923	1.9696154
B	8	Sample X1	E	1.209	0.171	CaXy12	132.8461538	1.9926923
B	9	Blank B	F	1.031				
B	10	Sample X1	F	1.276	0.245	CaXy21	189.7692308	2.8465385
B	11	Sample X1	F	1.277	0.246	CaXy21	190.5384615	2.8580769
B	12	Sample X1	F	1.274	0.243	CaXy21	188.2307692	2.8234615
C	1	Blank B	G	1.021				
C	2	Sample X1	G	1.245	0.224	CaGr11	173.6153846	2.6042308
C	3	Sample X1	G	1.243	0.222	CaGr11	172.0769231	2.5811538
C	4	Sample X1	G	1.245	0.224	CaGr11	173.6153846	2.6042308
C	5	Blank B	H	1.02				
C	6	Sample X1	H	1.201	0.181	CaGr12	140.5384615	2.1080769
C	7	Sample X1	H	1.201	0.181	CaGr12	140.5384615	2.1080769
C	8	Sample X1	H	1.2	0.18	CaGr12	139.7692308	2.0965385
C	9	Blank B	I	1.02				
C	10	Sample X1	I	1.198	0.178	CaGr21	138.2307692	2.0734615

Appendix 5.9 contd.

C	11	Sample X1	I	1.197	0.177	CaGr21	137.4615385	2.0619231
C	12	Sample X1	I	1.197	0.177	CaSu11	137.4615385	2.0619231
D	5	Blank B	K	1.014				
D	6	Sample X1	K	1.065	0.051	CaGc11	40.53846154	0.6080769
D	7	Sample X1	K	1.065	0.051	CaGc11	40.53846154	0.6080769
D	8	Sample X1	K	1.065	0.051	CaGc11	40.53846154	0.6080769
D	9	Blank B	L	1.014				
D	10	Sample X1	L	1.067	0.053	CaGc21	42.07692308	0.6311538
D	11	Sample X1	L	1.067	0.053	CaGc21	42.07692308	0.6311538
D	12	Sample X1	L	1.066	0.052	CaGc21	41.30769231	0.6196154
E	1	Blank B	M	1.011				
E	2	Sample X1	M	1.105	0.094	CaGl11	73.61538462	1.1042308
E	3	Sample X1	M	1.104	0.093	CaGl11	72.84615385	1.0926923
E	4	Sample X1	M	1.105	0.094	CaGl11	73.61538462	1.1042308
E	5	Blank B	N	1.013				
E	6	Sample X1	N	1.076	0.063	CaGl21	49.76923077	0.7465385
E	7	Sample X1	N	1.078	0.065	CaGl21	51.30769231	0.7696154
E	8	Sample X1	N	1.074	0.061	CaGl21	48.23076923	0.7234615

Appendix 5.10 factorial experiment FRAP run 10

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/L)	FRAP (µMTE/g)
D	1	Blank B	J	0.021				
D	2	Sample X1	J	0.184	0.163	CaSu11	126.6923077	1.26692308
D	3	Sample X1	J	0.186	0.165	CaSu11	128.2307692	1.28230769
D	4	Sample X1	J	0.184	0.163	CaSu11	126.6923077	1.26692308
A	1	Blank B	A	0.049				
A	2	Sample X1	A	0.662	0.613	CaFr11	472.8461538	4.72846154
A	3	Sample X1	A	0.663	0.614	CaFr11	473.6153846	4.73615385
A	4	Sample X1	A	0.662	0.613	CaFr11	472.8461538	4.72846154
A	5	Blank B	B	0.047				
A	6	Sample X1	B	0.521	0.474	CaFr12	365.9230769	3.65923077
A	7	Sample X1	B	0.523	0.476	CaFr12	367.4615385	3.67461538
A	8	Sample X1	B	0.521	0.474	CaFr12	365.9230769	3.65923077
A	9	Blank B	C	0.045				
A	10	Sample X1	C	0.435	0.39	CaFr21	301.3076923	3.01307692
A	11	Sample X1	C	0.436	0.391	CaFr21	302.0769231	3.02076923
A	12	Sample X1	C	0.435	0.39	CaFr21	301.3076923	3.01307692

Appendix 5.10 contd.

B	1	Blank B	D	0.036				
B	2	Sample X1	D	0.317	0.281	CaXy11	217.4615385	2.17461538
B	3	Sample X1	D	0.317	0.281	CaXy11	217.4615385	2.17461538
B	4	Sample X1	D	0.316	0.28	CaXy11	216.6923077	2.16692308
B	5	Blank B	E	0.031				
B	6	Sample X1	E	0.307	0.276	CaXy12	213.6153846	2.13615385
B	7	Sample X1	E	0.309	0.278	CaXy12	215.1538462	2.15153846
B	8	Sample X1	E	0.309	0.278	CaXy12	215.1538462	2.15153846
B	9	Blank B	F	0.028				
B	10	Sample X1	F	0.274	0.246	CaXy21	190.5384615	1.90538462
B	11	Sample X1	F	0.276	0.248	CaXy21	192.0769231	1.92076923
B	12	Sample X1	F	0.274	0.246	CaXy21	190.5384615	1.90538462
C	1	Blank B	G	0.023				
C	2	Sample X1	G	0.268	0.245	CaGr11	189.7692308	1.89769231
C	3	Sample X1	G	0.261	0.238	CaGr11	184.3846154	1.84384615
C	4	Sample X1	G	0.268	0.245	CaGr11	189.7692308	1.89769231
C	5	Blank B	H	0.026				
C	6	Sample X1	H	0.257	0.231	CaGr12	179	1.79
C	7	Sample X1	H	0.257	0.231	CaGr12	179	1.79
C	8	Sample X1	H	0.253	0.227	CaGr12	175.9230769	1.75923077
C	9	Blank B	I	0.022				
C	10	Sample X1	I	0.081	0.059	CaGr21	46.69230769	0.46692308
C	11	Sample X1	I	0.083	0.061	CaGr21	48.23076923	0.48230769
C	12	Sample X1	I	0.081	0.059	CaSu11	46.69230769	0.46692308
D	5	Blank B	K	0.024				
D	6	Sample X1	K	0.098	0.074	CaGc11	58.23076923	0.58230769
D	7	Sample X1	K	0.098	0.074	CaGc11	58.23076923	0.58230769
D	8	Sample X1	K	0.097	0.073	CaGc11	57.46153846	0.57461538
D	9	Blank B	L	0.014				
D	10	Sample X1	L	0.063	0.049	CaGc21	39	0.39
D	11	Sample X1	L	0.065	0.051	CaGc21	40.53846154	0.40538462
D	12	Sample X1	L	0.065	0.051	CaGc21	40.53846154	0.40538462
E	1	Blank B	M	0.011				
E	2	Sample X1	M	0.073	0.062	CaGl11	49	0.49
E	3	Sample X1	M	0.075	0.064	CaGl11	50.53846154	0.50538462
E	4	Sample X1	M	0.073	0.062	CaGl11	49	0.49
E	5	Blank B	N	0.012				
E	6	Sample X1	N	0.131	0.119	CaGl21	92.84615385	0.92846154
E	7	Sample X1	N	0.132	0.12	CaGl21	93.61538462	0.93615385
E	8	Sample X1	N	0.131	0.119	CaGl21	92.84615385	0.92846154

Appendix 6.1 RCCDRSM TPC run 1

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.181					
A	2	Sample X1	A	0.526	0.345	CaSu11	14.95098	0.14951	149.5098
A	3	Sample X1	A	0.527	0.346	CaSu11	15	0.15	150
A	4	Sample X1	A	0.526	0.345	CaSu11	14.95098	0.14951	149.5098
A	5	Blank B	B	0.075					
A	6	Sample X1	B	0.835	0.76	CaFr11	35.29412	0.352941	352.9412
A	7	Sample X1	B	0.838	0.763	CaFr11	35.44118	0.354412	354.4118
A	8	Sample X1	B	0.831	0.756	CaFr11	35.09804	0.35098	350.9804
A	9	Blank B	C	0.209					
A	10	Sample X1	C	0.614	0.405	CaFr12	17.89216	0.178922	178.9216
A	11	Sample X1	C	0.613	0.404	CaFr12	17.84314	0.178431	178.4314
A	12	Sample X1	C	0.616	0.407	CaFr12	17.9902	0.179902	179.902
B	1	Blank B	D	0.171					
B	2	Sample X1	D	0.333	0.162	CaFr21	5.980392	0.059804	59.80392
B	3	Sample X1	D	0.334	0.163	CaFr21	6.029412	0.060294	60.29412
B	4	Sample X1	D	0.335	0.164	CaFr21	6.078431	0.060784	60.78431
A	1	Blank B	A	0.1					
A	2	Sample X1	A	0.264	0.164	CaXy11	6.078431	0.060784	60.78431
A	3	Sample X1	A	0.266	0.166	CaXy11	6.176471	0.061765	61.76471
A	4	Sample X1	A	0.268	0.168	CaXy11	6.27451	0.062745	62.7451
B	5	Blank B	E	0.116					
B	6	Sample X1	E	0.368	0.252	CaXy12	10.39216	0.103922	103.9216
B	7	Sample X1	E	0.365	0.249	CaXy12	10.2451	0.102451	102.451
B	8	Sample X1	E	0.367	0.251	CaXy12	10.34314	0.103431	103.4314
A	1	Blank B	A	0.088					
A	2	Sample X1	A	0.258	0.17	CaXy21	6.372549	0.063725	63.72549
A	3	Sample X1	A	0.259	0.171	CaXy21	6.421569	0.064216	64.21569
A	4	Sample X1	A	0.259	0.171	CaXy21	6.421569	0.064216	64.21569
B	9	Blank B	F	0.115					
B	10	Sample X1	F	0.282	0.167	CaGr11	6.22549	0.062255	62.2549
B	11	Sample X1	F	0.286	0.171	CaGr11	6.421569	0.064216	64.21569
B	12	Sample X1	F	0.284	0.169	CaGr11	6.323529	0.063235	63.23529
C	1	Blank B	G	0.088					
C	2	Sample X1	G	0.462	0.374	CaGr12	16.37255	0.163725	163.7255
C	3	Sample X1	G	0.46	0.372	CaGr12	16.27451	0.162745	162.7451
C	4	Sample X1	G	0.46	0.372	CaGr12	16.27451	0.162745	162.7451
C	5	Blank B	H	0.091					

Appendix 6.1 contd.

C	6	Sample X1	H	0.249	0.158	CaGr21	5.784314	0.057843	57.84314
C	7	Sample X1	H	0.249	0.158	CaGr21	5.784314	0.057843	57.84314
C	8	Sample X1	H	0.249	0.158	CaGr21	5.784314	0.057843	57.84314
C	9	Blank B	I	0.112					
C	10	Sample X1	I	0.426	0.314	CaGc11	13.43137	0.134314	134.3137
C	11	Sample X1	I	0.429	0.317	CaGc11	13.57843	0.135784	135.7843
C	12	Sample X1	I	0.429	0.317	CaGc11	13.57843	0.135784	135.7843
D	1	Blank B	J	0.093					
D	2	Sample X1	J	0.354	0.261	CaGc21	10.83333	0.108333	108.3333
D	3	Sample X1	J	0.354	0.261	CaGc21	10.83333	0.108333	108.3333
D	4	Sample X1	J	0.353	0.26	CaGc21	10.78431	0.107843	107.8431
D	5	Blank B	K	0.099					
D	6	Sample X1	K	0.37	0.271	CaGl11	11.32353	0.113235	113.2353
D	7	Sample X1	K	0.37	0.271	CaGl11	11.32353	0.113235	113.2353
D	8	Sample X1	K	0.37	0.271	CaGl11	11.32353	0.113235	113.2353
D	9	Blank B	L	0.09					
D	10	Sample X1	L	0.267	0.177	CaGl21	6.715686	0.067157	67.15686
D	11	Sample X1	L	0.267	0.177	CaGl21	6.715686	0.067157	67.15686
D	12	Sample X1	L	0.268	0.178	CaGl21	6.764706	0.067647	67.64706

Appendix 6.2 RCCDRSM TPC run 2

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.154					
A	2	Sample X1	A	0.378	0.224	CaSu11	9.019607843	0.1803922	180.392157
A	3	Sample X1	A	0.379	0.225	CaSu11	9.068627451	0.1813725	181.372549
A	4	Sample X1	A	0.379	0.225	CaSu11	9.068627451	0.1813725	181.372549
A	5	Blank B	B	0.204					
A	6	Sample X1	B	0.524	0.32	CaFr11	13.7254902	0.2745098	274.509804
A	7	Sample X1	B	0.525	0.321	CaFr11	13.7745098	0.2754902	275.490196
A	8	Sample X1	B	0.526	0.322	CaFr11	13.82352941	0.2764706	276.470588
A	9	Blank B	C	0.199					
A	10	Sample X1	C	0.352	0.153	CaFr12	5.539215686	0.1107843	110.784314
A	11	Sample X1	C	0.355	0.156	CaFr12	5.68627451	0.1137255	113.72549
A	12	Sample X1	C	0.357	0.158	CaFr12	5.784313725	0.1156863	115.686275
B	1	Blank B	D	0.018					
B	2	Sample X1	D	0.198	0.18	CaFr21	6.862745098	0.1372549	137.254902
B	3	Sample X1	D	0.198	0.18	CaFr21	6.862745098	0.1372549	137.254902

Appendix 6.3 RCCDRSM TPC run 3

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.155					
A	2	Sample X1	A	0.52	0.365	CaSu11	15.931373	0.2389706	238.97059
A	3	Sample X1	A	0.518	0.363	CaSu11	15.833333	0.2375	237.5
A	4	Sample X1	A	0.52	0.365	CaSu11	15.931373	0.2389706	238.97059
A	1	Blank B	A	0.414					
A	2	Sample X1	A	0.659	0.245	CaFr11	10.04902	0.1507353	150.73529
A	3	Sample X1	A	0.653	0.239	CaFr11	9.754902	0.1463235	146.32353
A	4	Sample X1	A	0.658	0.244	CaFr11	10	0.15	150
H	1	Blank B	F	0.289					
H	2	Sample X1	F	0.683	0.394	CaFr12	17.352941	0.2602941	260.29412
H	3	Sample X1	F	0.682	0.393	CaFr12	17.303922	0.2595588	259.55882
H	4	Sample X1	F	0.683	0.394	CaFr12	17.352941	0.2602941	260.29412
A	9	Blank B	C	0.233					
A	10	Sample X1	C	0.456	0.223	CaFr21	8.9705882	0.1345588	134.55882
A	11	Sample X1	C	0.453	0.22	CaFr21	8.8235294	0.1323529	132.35294
A	12	Sample X1	C	0.451	0.218	CaFr21	8.7254902	0.1308824	130.88235
B	1	Blank B	D	0.098					
B	2	Sample X1	D	0.264	0.166	CaXy11	6.1764706	0.0926471	92.647059
B	3	Sample X1	D	0.268	0.17	CaXy11	6.372549	0.0955882	95.588235
B	4	Sample X1	D	0.263	0.165	CaXy11	6.127451	0.0919118	91.911765
B	5	Blank B	E	0.12					
B	6	Sample X1	E	0.246	0.126	CaXy12	4.2156863	0.0632353	63.235294
B	7	Sample X1	E	0.246	0.126	CaXy12	4.2156863	0.0632353	63.235294
B	8	Sample X1	E	0.247	0.127	CaXy12	4.2647059	0.0639706	63.970588
B	9	Blank B	F	0.098					
B	10	Sample X1	F	0.209	0.111	CaXy21	3.4803922	0.0522059	52.205882
B	11	Sample X1	F	0.21	0.112	CaXy21	3.5294118	0.0529412	52.941176
B	12	Sample X1	F	0.209	0.111	CaXy21	3.4803922	0.0522059	52.205882
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.223	0.132	CaGr11	4.5098039	0.0676471	67.647059
A	11	Sample X1	C	0.223	0.132	CaGr11	4.5098039	0.0676471	67.647059
A	12	Sample X1	C	0.225	0.134	CaGr11	4.6078431	0.0691176	69.117647
B	1	Blank B	D	0.102					
B	2	Sample X1	D	0.239	0.137	CaGr12	4.754902	0.0713235	71.323529
B	3	Sample X1	D	0.238	0.136	CaGr12	4.7058824	0.0705882	70.588235
B	4	Sample X1	D	0.24	0.138	CaGr12	4.8039216	0.0720588	72.058824
B	5	Blank B	E	0.069					

Appendix 6.3 contd.

B	6	Sample X1	E	0.174	0.105	CaGr21	3.1862745	0.0477941	47.794118
B	7	Sample X1	E	0.174	0.105	CaGr21	3.1862745	0.0477941	47.794118
B	8	Sample X1	E	0.171	0.102	CaGr21	3.0392157	0.0455882	45.588235
C	1	Blank B	G	0.081					
C	2	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	3	Sample X1	G	0.324	0.243	CaGc11	9.9509804	0.1492647	149.26471
C	4	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.229	0.143	CaGc21	5.0490196	0.0757353	75.735294
C	7	Sample X1	H	0.228	0.142	CaGc21	5	0.075	75
C	8	Sample X1	H	0.23	0.144	CaGc21	5.0980392	0.0764706	76.470588
E	9	Blank B	G	0.108					
E	10	Sample X1	G	0.218	0.11	CaGl11	3.4313725	0.0514706	51.470588
E	11	Sample X1	G	0.215	0.107	CaGl11	3.2843137	0.0492647	49.264706
E	12	Sample X1	G	0.218	0.11	CaGl11	3.4313725	0.0514706	51.470588
F	1	Blank B	H	0.084					
F	2	Sample X1	H	0.212	0.128	CaGl21	4.3137255	0.0647059	64.705882
F	3	Sample X1	H	0.211	0.127	CaGl21	4.2647059	0.0639706	63.970588
F	4	Sample X1	H	0.21	0.126	CaGl21	4.2156863	0.0632353	63.235294

Appendix 6.4 RCCDRSM TPD run 4

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
G	1	Blank B	C	0.264					
G	2	Sample X1	C	0.648	0.384	CaSu11	16.8627451	0.252941176	252.9411765
G	3	Sample X1	C	0.647	0.383	CaSu11	16.8137255	0.252205882	252.2058824
G	4	Sample X1	C	0.648	0.384	CaSu11	16.8627451	0.252941176	252.9411765
A	11	Blank B	A	0.507					
A	12	Sample X1	A	0.765	0.258	CaFr11	10.6862745	0.160294118	160.2941176
B	11	Sample X1	A	0.764	0.257	CaFr11	10.6372549	0.159558824	159.5588235
B	12	Sample X1	A	0.766	0.259	CaFr11	10.7352941	0.161029412	161.0294118
C	11	Blank B	B	0.208					
C	12	Sample X1	B	0.588	0.38	CaFr12	16.6666667	0.25	250
D	11	Sample X1	B	0.589	0.381	CaFr12	16.7156863	0.250735294	250.7352941
D	12	Sample X1	B	0.589	0.381	CaFr12	16.7156863	0.250735294	250.7352941
G	5	Blank B	D	0.093					
G	6	Sample X1	D	0.316	0.223	CaFr21	8.97058824	0.134558824	134.5588235

Appendix 6.4 contd.

G	7	Sample X1	D	0.317	0.224	CaFr21	9.01960784	0.135294118	135.2941176
G	8	Sample X1	D	0.316	0.223	CaFr21	8.97058824	0.134558824	134.5588235
C	1	Blank B	A	0.103					
C	2	Sample X1	A	0.274	0.171	CaXy11	6.42156863	0.096323529	96.32352941
C	3	Sample X1	A	0.277	0.174	CaXy11	6.56862745	0.098529412	98.52941176
C	4	Sample X1	A	0.276	0.173	CaXy11	6.51960784	0.097794118	97.79411765
C	9	Blank B	B	0.006					
C	10	Sample X1	B	0.118	0.112	CaXy12	3.52941176	0.052941176	52.94117647
C	11	Sample X1	B	0.116	0.11	CaXy12	3.43137255	0.051470588	51.47058824
C	12	Sample X1	B	0.116	0.11	CaXy12	3.43137255	0.051470588	51.47058824
D	1	Blank B	C	0.089					
D	2	Sample X1	C	0.208	0.119	CaXy21	3.87254902	0.058088235	58.08823529
D	3	Sample X1	C	0.21	0.121	CaXy21	3.97058824	0.059558824	59.55882353
D	4	Sample X1	C	0.208	0.119	CaXy21	3.87254902	0.058088235	58.08823529
D	5	Blank B	D	0.108					
D	6	Sample X1	D	0.24	0.132	CaGr11	4.50980392	0.067647059	67.64705882
D	7	Sample X1	D	0.241	0.133	CaGr11	4.55882353	0.068382353	68.38235294
D	8	Sample X1	D	0.241	0.133	CaGr11	4.55882353	0.068382353	68.38235294
D	9	Blank B	E	0.129					
D	10	Sample X1	E	0.268	0.139	CaGr12	4.85294118	0.072794118	72.79411765
D	11	Sample X1	E	0.265	0.136	CaGr12	4.70588235	0.070588235	70.58823529
D	12	Sample X1	E	0.266	0.137	CaGr12	4.75490196	0.071323529	71.32352941
E	1	Blank B	F	0.13					
E	2	Sample X1	F	0.236	0.106	CaGr21	3.23529412	0.048529412	48.52941176
E	3	Sample X1	F	0.238	0.108	CaGr21	3.33333333	0.05	50
E	4	Sample X1	F	0.237	0.107	CaGr21	3.28431373	0.049264706	49.26470588
E	5	Blank B	G	0.008					
E	6	Sample X1	G	0.245	0.237	CaGc11	9.65686275	0.144852941	144.8529412
E	7	Sample X1	G	0.247	0.239	CaGc11	9.75490196	0.146323529	146.3235294
E	8	Sample X1	G	0.247	0.239	CaGc11	9.75490196	0.146323529	146.3235294
E	9	Blank B	H	0.043					
E	10	Sample X1	H	0.183	0.14	CaGc21	4.90196078	0.073529412	73.52941176
E	11	Sample X1	H	0.184	0.141	CaGc21	4.95098039	0.074264706	74.26470588
E	12	Sample X1	H	0.183	0.14	CaGc21	4.90196078	0.073529412	73.52941176
F	1	Blank B	A	0.183					
F	2	Sample X1	A	0.295	0.112	CaGl11	3.52941176	0.052941176	52.94117647
F	3	Sample X1	A	0.291	0.108	CaGl11	3.33333333	0.05	50
F	4	Sample X1	A	0.298	0.115	CaGl11	3.67647059	0.055147059	55.14705882
F	5	Blank B	B	0.077					
F	6	Sample X1	B	0.211	0.134	CaGl21	4.60784314	0.069117647	69.11764706
F	7	Sample X1	B	0.209	0.132	CaGl21	4.50980392	0.067647059	67.64705882
F	8	Sample X1	B	0.21	0.133	CaGl21	4.55882353	0.068382353	68.38235294

Appendix 6.5 RCCDRSM TPC run 5

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	5	Blank B	A	0.26					
F	6	Sample X1	A	0.381	0.121	CaSu11	3.970588235	0.039705882	39.7058824
F	7	Sample X1	A	0.384	0.124	CaSu11	4.117647059	0.041176471	41.1764706
F	8	Sample X1	A	0.381	0.121	CaSu11	3.970588235	0.039705882	39.7058824
C	9	Blank B	A	0.431					
C	10	Sample X1	A	0.631	0.2	CaFr11	7.843137255	0.078431373	78.4313725
C	11	Sample X1	A	0.632	0.201	CaFr11	7.892156863	0.078921569	78.9215686
C	12	Sample X1	A	0.632	0.201	CaFr11	7.892156863	0.078921569	78.9215686
D	1	Blank B	B	0.252					
D	2	Sample X1	B	0.623	0.371	CaFr12	16.2254902	0.162254902	162.254902
D	3	Sample X1	B	0.629	0.377	CaFr12	16.51960784	0.165196078	165.196078
D	4	Sample X1	B	0.628	0.376	CaFr12	16.47058824	0.164705882	164.705882
D	5	Blank B	C	0.184					
D	6	Sample X1	C	0.301	0.117	CaFr21	3.774509804	0.037745098	37.745098
D	7	Sample X1	C	0.301	0.117	CaFr21	3.774509804	0.037745098	37.745098
D	8	Sample X1	C	0.301	0.117	CaFr21	3.774509804	0.037745098	37.745098
D	9	Blank B	D	0.104					
D	10	Sample X1	D	0.253	0.149	CaXy11	5.343137255	0.053431373	53.4313725
D	11	Sample X1	D	0.256	0.152	CaXy11	5.490196078	0.054901961	54.9019608
D	12	Sample X1	D	0.255	0.151	CaXy11	5.441176471	0.054411765	54.4117647
E	1	Blank B	E	0.099					
E	2	Sample X1	E	0.234	0.135	CaXy12	4.656862745	0.046568627	46.5686275
E	3	Sample X1	E	0.231	0.132	CaXy12	4.509803922	0.045098039	45.0980392
E	4	Sample X1	E	0.23	0.131	CaXy12	4.460784314	0.044607843	44.6078431
E	5	Blank B	F	0.132					
E	6	Sample X1	F	0.284	0.152	CaXy21	5.490196078	0.054901961	54.9019608
E	7	Sample X1	F	0.286	0.154	CaXy21	5.588235294	0.055882353	55.8823529
E	8	Sample X1	F	0.282	0.15	CaXy21	5.392156863	0.053921569	53.9215686
F	9	Blank B	B	0.086					
F	10	Sample X1	B	0.23	0.144	CaGr11	5.098039216	0.050980392	50.9803922
F	11	Sample X1	B	0.233	0.147	CaGr11	5.245098039	0.05245098	52.4509804
F	12	Sample X1	B	0.231	0.145	CaGr11	5.147058824	0.051470588	51.4705882
G	1	Blank B	C	0.095					
G	2	Sample X1	C	0.24	0.145	CaGr12	5.147058824	0.051470588	51.4705882
G	3	Sample X1	C	0.242	0.147	CaGr12	5.245098039	0.05245098	52.4509804
G	4	Sample X1	C	0.242	0.147	CaGr12	5.245098039	0.05245098	52.4509804
G	5	Blank B	D	0.087					
G	6	Sample X1	D	0.194	0.107	CaGr21	3.284313725	0.032843137	32.8431373

Appendix 6.5 contd.

G	7	Sample X1	D	0.193	0.106	CaGr21	3.235294118	0.032352941	32.3529412
G	8	Sample X1	D	0.194	0.107	CaGr21	3.284313725	0.032843137	32.8431373
E	9	Blank B	G	0.086					
E	10	Sample X1	G	0.248	0.162	CaGc11	5.980392157	0.059803922	59.8039216
E	11	Sample X1	G	0.249	0.163	CaGc11	6.029411765	0.060294118	60.2941176
E	12	Sample X1	G	0.249	0.163	CaGc11	6.029411765	0.060294118	60.2941176
F	1	Blank B	H	0.084					
F	2	Sample X1	H	0.215	0.131	CaGc21	4.460784314	0.044607843	44.6078431
F	3	Sample X1	H	0.214	0.13	CaGc21	4.411764706	0.044117647	44.1176471
F	4	Sample X1	H	0.214	0.13	CaGc21	4.411764706	0.044117647	44.1176471
G	9	Blank B	E	0.107					
G	10	Sample X1	E	0.24	0.133	CaGl11	4.558823529	0.045588235	45.5882353
G	11	Sample X1	E	0.241	0.134	CaGl11	4.607843137	0.046078431	46.0784314
G	12	Sample X1	E	0.242	0.135	CaGl11	4.656862745	0.046568627	46.5686275
H	1	Blank B	F	0.082					
H	2	Sample X1	F	0.198	0.116	CaGl21	3.725490196	0.037254902	37.254902
H	3	Sample X1	F	0.198	0.116	CaGl21	3.725490196	0.037254902	37.254902
H	4	Sample X1	F	0.199	0.117	CaGl21	3.774509804	0.037745098	37.745098

Appendix 6.6 RCCDRSM TPC run 6

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	5	Blank B	A	0.256					
F	6	Sample X1	A	0.593	0.337	CaSu11	14.5588235	0.14558824	145.58824
F	7	Sample X1	A	0.595	0.339	CaSu11	14.6568627	0.14656863	146.56863
F	8	Sample X1	A	0.592	0.336	CaSu11	14.5098039	0.14509804	145.09804
F	9	Blank B	B	0.451					
F	10	Sample X1	B	0.843	0.392	CaFr11	17.254902	0.17254902	172.54902
F	11	Sample X1	B	0.847	0.396	CaFr11	17.4509804	0.1745098	174.5098
F	12	Sample X1	B	0.846	0.395	CaFr11	17.4019608	0.17401961	174.01961
F	5	Blank B	A	0.311					
F	6	Sample X1	A	0.819	0.508	CaFr12	22.9411765	0.22941176	229.41176
F	7	Sample X2	A	0.818	0.507	CaFr12	22.8921569	0.22892157	228.92157
F	8	Sample X3	A	0.819	0.508	CaFr12	22.9411765	0.22941176	229.41176
F	9	Blank B	B	0.25					
F	10	Sample X1	B	0.413	0.163	CaFr21	6.02941176	0.06029412	60.294118
F	11	Sample X2	B	0.413	0.163	CaFr21	6.02941176	0.06029412	60.294118
F	12	Sample X3	B	0.414	0.164	CaFr21	6.07843137	0.06078431	60.784314
G	1	Blank B	C	0.112					

Appendix 6.6 contd.

G	2	Sample X1	C	0.371	0.259	CaXy11	10.7352941	0.10735294	107.35294
G	3	Sample X2	C	0.369	0.257	CaXy11	10.6372549	0.10637255	106.37255
G	4	Sample X3	C	0.369	0.257	CaXy11	10.6372549	0.10637255	106.37255
G	5	Blank B	D	0.136					
G	6	Sample X1	D	0.333	0.197	CaXy12	7.69607843	0.07696078	76.960784
G	7	Sample X2	D	0.332	0.196	CaXy12	7.64705882	0.07647059	76.470588
G	8	Sample X3	D	0.331	0.195	CaXy12	7.59803922	0.07598039	75.980392
G	9	Blank B	E	0.103					
G	10	Sample X1	E	0.267	0.164	CaXy21	6.07843137	0.06078431	60.784314
G	11	Sample X2	E	0.268	0.165	CaXy21	6.12745098	0.06127451	61.27451
G	12	Sample X3	E	0.269	0.166	CaXy21	6.17647059	0.06176471	61.764706
H	1	Blank B	F	0.097					
H	2	Sample X1	F	0.228	0.131	CaGr11	4.46078431	0.04460784	44.607843
H	3	Sample X2	F	0.221	0.124	CaGr11	4.11764706	0.04117647	41.176471
H	4	Sample X3	F	0.225	0.128	CaGr11	4.31372549	0.04313725	43.137255
H	5	Blank B	G	0.096					
H	6	Sample X1	G	0.409	0.313	CaGr12	13.3823529	0.13382353	133.82353
H	7	Sample X2	G	0.409	0.313	CaGr12	13.3823529	0.13382353	133.82353
H	8	Sample X3	G	0.408	0.312	CaGr12	13.3333333	0.13333333	133.33333
H	9	Blank B	H	0.088					
H	10	Sample X1	H	0.231	0.143	CaGr21	5.04901961	0.0504902	50.490196
H	11	Sample X2	H	0.234	0.146	CaGr21	5.19607843	0.05196078	51.960784
H	12	Sample X3	H	0.235	0.147	CaGr21	5.24509804	0.05245098	52.45098
A	1	Blank B	A	0.073					
A	2	Sample X1	A	0.469	0.396	CaGc11	17.4509804	0.1745098	174.5098
A	3	Sample X1	A	0.466	0.393	CaGc11	17.3039216	0.17303922	173.03922
A	4	Sample X1	A	0.468	0.395	CaGc11	17.4019608	0.17401961	174.01961
A	5	Blank B	B	0.078					
A	6	Sample X1	B	0.443	0.365	CaGc21	15.9313725	0.15931373	159.31373
A	7	Sample X1	B	0.445	0.367	CaGc21	16.0294118	0.16029412	160.29412
A	8	Sample X1	B	0.444	0.366	CaGc21	15.9803922	0.15980392	159.80392
A	9	Blank B	C	0.102					
A	10	Sample X1	C	0.218	0.116	CaGl11	3.7254902	0.0372549	37.254902
A	11	Sample X1	C	0.213	0.111	CaGl11	3.48039216	0.03480392	34.803922
A	12	Sample X1	C	0.216	0.114	CaGl11	3.62745098	0.03627451	36.27451
B	1	Blank B	D	0.081					
B	2	Sample X1	D	0.452	0.371	CaGl21	16.2254902	0.1622549	162.2549
B	3	Sample X1	D	0.457	0.376	CaGl21	16.4705882	0.16470588	164.70588
B	4	Sample X1	D	0.451	0.37	CaGl21	16.1764706	0.16176471	161.76471

Appendix 6.7 RCCDRSM TPC run 7

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/)
E	1	Blank B	A	0.097					
E	2	Sample X1	A	0.247	0.15	CaSu11	5.39215686	0.10784314	107.84314
E	3	Sample X1	A	0.248	0.151	CaSu11	5.44117647	0.10882353	108.82353
E	4	Sample X1	A	0.247	0.15	CaSu11	5.39215686	0.10784314	107.84314
E	5	Blank B	B	0.124					
E	6	Sample X1	B	0.231	0.107	CaFr11	3.28431373	0.06568627	65.686275
E	7	Sample X1	B	0.232	0.108	CaFr11	3.33333333	0.06666667	66.666667
E	8	Sample X1	B	0.231	0.107	CaFr11	3.28431373	0.06568627	65.686275
E	9	Blank B	C	0.268					
E	10	Sample X1	C	0.481	0.213	CaFr12	8.48039216	0.16960784	169.60784
E	11	Sample X1	C	0.479	0.211	CaFr12	8.38235294	0.16764706	167.64706
E	12	Sample X1	C	0.48	0.212	CaFr12	8.43137255	0.16862745	168.62745
F	1	Blank B	D	0.015					
F	2	Sample X1	D	0.155	0.14	CaFr21	4.90196078	0.09803922	98.039216
F	3	Sample X1	D	0.153	0.138	CaFr21	4.80392157	0.09607843	96.078431
F	4	Sample X1	D	0.152	0.137	CaFr21	4.75490196	0.09509804	95.098039
A	9	Blank B	C	0.039					
A	10	Sample X1	C	0.141	0.102	CaXy11	3.03921569	0.06078431	60.784314
A	11	Sample X1	C	0.144	0.105	CaXy11	3.18627451	0.06372549	63.72549
A	12	Sample X1	C	0.144	0.105	CaXy11	3.18627451	0.06372549	63.72549
F	5	Blank B	E	0.023					
F	6	Sample X1	E	0.193	0.17	CaXy12	6.37254902	0.12745098	127.45098
F	7	Sample X1	E	0.194	0.171	CaXy12	6.42156863	0.12843137	128.43137
F	8	Sample X1	E	0.195	0.172	CaXy12	6.47058824	0.12941176	129.41176
F	9	Blank B	F	0.018					
F	10	Sample X1	F	0.149	0.131	CaGr11	4.46078431	0.08921569	89.215686
F	11	Sample X1	F	0.151	0.133	CaGr11	4.55882353	0.09117647	91.176471
F	12	Sample X1	F	0.15	0.132	CaGr11	4.50980392	0.09019608	90.196078
G	1	Blank B	G	0.012					
G	2	Sample X1	G	0.172	0.16	CaGr12	5.88235294	0.11764706	117.64706
G	3	Sample X1	G	0.173	0.161	CaGr12	5.93137255	0.11862745	118.62745
G	4	Sample X1	G	0.17	0.158	CaGr12	5.78431373	0.11568627	115.68627
G	5	Blank B	H	0.001					
G	6	Sample X1	H	0.111	0.11	CaGr21	3.43137255	0.06862745	68.627451
G	7	Sample X1	H	0.111	0.11	CaGr21	3.43137255	0.06862745	68.627451
G	8	Sample X1	H	0.111	0.11	CaGr21	3.43137255	0.06862745	68.627451
G	9	Blank B	I	0.015					

Appendix 6.7 contd.

G	10	Sample X1	I	0.138	0.123	CaGc11	4.06862745	0.08137255	81.372549
G	11	Sample X1	I	0.139	0.124	CaGc11	4.11764706	0.08235294	82.352941
G	12	Sample X1	I	0.139	0.124	CaGc11	4.11764706	0.08235294	82.352941
H	1	Blank B	J	0.008					
H	2	Sample X1	J	0.121	0.113	CaGc21	3.57843137	0.07156863	71.568627
H	3	Sample X1	J	0.128	0.12	CaGc21	3.92156863	0.07843137	78.431373
H	4	Sample X1	J	0.124	0.116	CaGc21	3.7254902	0.0745098	74.509804
H	5	Blank B	K	0.004					
H	6	Sample X1	K	0.143	0.139	CaGl11	4.85294118	0.09705882	97.058824
H	7	Sample X1	K	0.142	0.138	CaGl11	4.80392157	0.09607843	96.078431
H	8	Sample X1	K	0.148	0.144	CaGl11	5.09803922	0.10196078	101.96078
H	9	Blank B	L	0.001					
H	10	Sample X1	L	0.13	0.129	CaGl21	4.3627451	0.0872549	87.254902
H	11	Sample X1	L	0.129	0.128	CaGl21	4.31372549	0.08627451	86.27451
H	12	Sample X1	L	0.13	0.129	CaGl21	4.3627451	0.0872549	87.254902

Appendix 6.8 RCCDRSM TPC run 8.

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.155					
A	2	Sample X1	A	0.52	0.365	CaSu11	15.931373	0.2389706	238.970588
A	3	Sample X1	A	0.518	0.363	CaSu11	15.833333	0.2375	237.5
A	4	Sample X1	A	0.52	0.365	CaSu11	15.931373	0.2389706	238.970588
A	1	Blank B	A	0.414					
A	2	Sample X1	A	0.657	0.243	CaFr11	9.9509804	0.1492647	149.264706
A	3	Sample X1	A	0.655	0.241	CaFr11	9.8529412	0.1477941	147.794118
A	4	Sample X1	A	0.658	0.244	CaFr11	10	0.15	150
H	1	Blank B	F	0.289					
H	2	Sample X1	F	0.683	0.394	CaFr12	17.352941	0.2602941	260.294118
H	3	Sample X1	F	0.682	0.393	CaFr12	17.303922	0.2595588	259.558824
H	4	Sample X1	F	0.683	0.394	CaFr12	17.352941	0.2602941	260.294118
A	9	Blank B	C	0.233					
A	10	Sample X1	C	0.456	0.223	CaFr21	8.9705882	0.1345588	134.558824
A	11	Sample X1	C	0.453	0.22	CaFr21	8.8235294	0.1323529	132.352941
A	12	Sample X1	C	0.451	0.218	CaFr21	8.7254902	0.1308824	130.882353
B	1	Blank B	D	0.098					
B	2	Sample X1	D	0.264	0.166	CaXy11	6.1764706	0.0926471	92.6470588
B	3	Sample X1	D	0.268	0.17	CaXy11	6.372549	0.0955882	95.5882353
B	4	Sample X1	D	0.263	0.165	CaXy11	6.127451	0.0919118	91.9117647

Appendix 6.8 contd.

B	5	Blank B	E	0.12					
B	6	Sample X1	E	0.246	0.126	CaXy12	4.2156863	0.0632353	63.235294
B	7	Sample X1	E	0.246	0.126	CaXy12	4.2156863	0.0632353	63.2352941
B	8	Sample X1	E	0.247	0.127	CaXy12	4.2647059	0.0639706	63.9705882
B	9	Blank B	F	0.098					
B	10	Sample X1	F	0.209	0.111	CaXy21	3.4803922	0.0522059	52.2058824
B	11	Sample X1	F	0.21	0.112	CaXy21	3.5294118	0.0529412	52.9411765
B	12	Sample X1	F	0.209	0.111	CaXy21	3.4803922	0.0522059	52.2058824
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.223	0.132	CaGr11	4.5098039	0.0676471	67.6470588
A	11	Sample X1	C	0.223	0.132	CaGr11	4.5098039	0.0676471	67.6470588
A	12	Sample X1	C	0.225	0.134	CaGr11	4.6078431	0.0691176	69.1176471
B	1	Blank B	D	0.102					
B	2	Sample X1	D	0.237	0.135	CaGr12	4.6568627	0.0698529	69.8529412
B	3	Sample X1	D	0.238	0.136	CaGr12	4.7058824	0.0705882	70.5882353
B	4	Sample X1	D	0.236	0.134	CaGr12	4.6078431	0.0691176	69.1176471
B	5	Blank B	E	0.07					
B	6	Sample X1	E	0.175	0.105	CaGr21	3.1862745	0.0477941	47.7941176
B	7	Sample X1	E	0.172	0.102	CaGr21	3.0392157	0.0455882	45.5882353
B	8	Sample X1	E	0.173	0.103	CaGr21	3.0882353	0.0463235	46.3235294
C	1	Blank B	G	0.081					
C	2	Sample X1	G	0.322	0.241	CaGc11	9.8529412	0.1477941	147.794118
C	3	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	4	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.229	0.143	CaGc21	5.0490196	0.0757353	75.7352941
C	7	Sample X1	H	0.228	0.142	CaGc21	5	0.075	75
C	8	Sample X1	H	0.23	0.144	CaGc21	5.0980392	0.0764706	76.4705882
E	9	Blank B	G	0.108					
E	10	Sample X1	G	0.216	0.108	CaGl11	3.3333333	0.05	50
E	11	Sample X1	G	0.217	0.109	CaGl11	3.3823529	0.0507353	50.7352941
E	12	Sample X1	G	0.218	0.11	CaGl11	3.4313725	0.0514706	51.4705882
F	1	Blank B	H	0.084					
F	2	Sample X1	H	0.212	0.128	CaGl21	4.3137255	0.0647059	64.7058824
F	3	Sample X1	H	0.21	0.126	CaGl21	4.2156863	0.0632353	63.2352941
F	4	Sample X1	H	0.211	0.127	CaGl21	4.2647059	0.0639706	63.9705882

Appendix 6.9 RCCDRSM TPC run 9

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
G	1	Blank B	C	0.264					
G	2	Sample X1	C	0.647	0.383	CaSu11	16.8137255	0.25220588	252.20588
G	3	Sample X1	C	0.648	0.384	CaSu11	16.8627451	0.25294118	252.94118
G	4	Sample X1	C	0.648	0.384	CaSu11	16.8627451	0.25294118	252.94118
A	11	Blank B	A	0.507					
A	12	Sample X1	A	0.765	0.258	CaFr11	10.6862745	0.16029412	160.29412
B	11	Sample X1	A	0.765	0.258	CaFr11	10.6862745	0.16029412	160.29412
B	12	Sample X1	A	0.765	0.258	CaFr11	10.6862745	0.16029412	160.29412
C	11	Blank B	B	0.208					
C	12	Sample X1	B	0.588	0.38	CaFr12	16.6666667	0.25	250
D	11	Sample X1	B	0.589	0.381	CaFr12	16.7156863	0.25073529	250.73529
D	12	Sample X1	B	0.589	0.381	CaFr12	16.7156863	0.25073529	250.73529
G	5	Blank B	D	0.1					
G	6	Sample X1	D	0.317	0.217	CaFr21	8.67647059	0.13014706	130.14706
G	7	Sample X1	D	0.315	0.215	CaFr21	8.57843137	0.12867647	128.67647
G	8	Sample X1	D	0.317	0.217	CaFr21	8.67647059	0.13014706	130.14706
C	1	Blank B	A	0.113					
C	2	Sample X1	A	0.28	0.167	CaXy11	6.2254902	0.09338235	93.382353
C	3	Sample X1	A	0.285	0.172	CaXy11	6.47058824	0.09705882	97.058824
C	4	Sample X1	A	0.282	0.169	CaXy11	6.32352941	0.09485294	94.852941
C	9	Blank B	B	0.002					
C	10	Sample X1	B	0.118	0.116	CaXy12	3.7254902	0.05588235	55.882353
C	11	Sample X1	B	0.116	0.114	CaXy12	3.62745098	0.05441176	54.411765
C	12	Sample X1	B	0.116	0.114	CaXy12	3.62745098	0.05441176	54.411765
D	1	Blank B	C	0.097					
D	2	Sample X1	C	0.208	0.111	CaXy21	3.48039216	0.05220588	52.205882
D	3	Sample X1	C	0.21	0.113	CaXy21	3.57843137	0.05367647	53.676471
D	4	Sample X1	C	0.208	0.111	CaXy21	3.48039216	0.05220588	52.205882
D	5	Blank B	D	0.108					
D	6	Sample X1	D	0.242	0.134	CaGr11	4.60784314	0.06911765	69.117647
D	7	Sample X1	D	0.24	0.132	CaGr11	4.50980392	0.06764706	67.647059
D	8	Sample X1	D	0.24	0.132	CaGr11	4.50980392	0.06764706	67.647059
D	9	Blank B	E	0.133					
D	10	Sample X1	E	0.269	0.136	CaGr12	4.70588235	0.07058824	70.588235
D	11	Sample X1	E	0.264	0.131	CaGr12	4.46078431	0.06691176	66.911765
D	12	Sample X1	E	0.266	0.133	CaGr12	4.55882353	0.06838235	68.382353
E	1	Blank B	F	0.135					

Appendix 6.9 contd.

E	2	Sample X1	F	0.235	0.1	CaGr21	2.94117647	0.04411765	44.117647
E	3	Sample X1	F	0.237	0.102	CaGr21	3.03921569	0.04558824	45.588235
E	4	Sample X1	F	0.235	0.1	CaGr21	2.94117647	0.04411765	44.117647
E	5	Blank B	G	0.003					
E	6	Sample X1	G	0.244	0.241	CaGc11	9.85294118	0.14779412	147.79412
E	7	Sample X1	G	0.248	0.245	CaGc11	10.0490196	0.15073529	150.73529
E	8	Sample X1	G	0.247	0.244	CaGc11	10	0.15	150
E	9	Blank B	H	0.043					
E	10	Sample X1	H	0.186	0.143	CaGc21	5.04901961	0.07573529	75.735294
E	11	Sample X1	H	0.184	0.141	CaGc21	4.95098039	0.07426471	74.264706
E	12	Sample X1	H	0.185	0.142	CaGc21	5	0.075	75
F	1	Blank B	A	0.173					
F	2	Sample X1	A	0.283	0.11	CaGl11	3.43137255	0.05147059	51.470588
F	3	Sample X1	A	0.282	0.109	CaGl11	3.38235294	0.05073529	50.735294
F	4	Sample X1	A	0.284	0.111	CaGl11	3.48039216	0.05220588	52.205882
F	5	Blank B	B	0.084					
F	6	Sample X1	B	0.209	0.125	CaGl21	4.16666667	0.0625	62.5
F	7	Sample X1	B	0.209	0.125	CaGl21	4.16666667	0.0625	62.5
F	8	Sample X1	B	0.212	0.128	CaGl21	4.31372549	0.06470588	64.705882

Appendix 6.10 RCCDRSM TPC run 10

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
C	9	Blank B	A	0.261					
C	10	Sample X1	A	0.491	0.23	CaSu11	9.3137255	0.1862745	186.27451
C	11	Sample X1	A	0.491	0.23	CaSu11	9.3137255	0.1862745	186.27451
C	12	Sample X1	A	0.494	0.233	CaSu11	9.4607843	0.1892157	189.215686
A	1	Blank B	A	0.491					
A	2	Sample X1	A	0.788	0.297	CaFr11	12.598039	0.2519608	251.960784
A	3	Sample X1	A	0.789	0.298	CaFr11	12.647059	0.2529412	252.941176
A	4	Sample X1	A	0.788	0.297	CaFr11	12.598039	0.2519608	251.960784
A	5	Blank B	B	0.25					
A	6	Sample X1	B	0.936	0.686	CaFr12	31.666667	0.6333333	633.333333
A	7	Sample X1	B	0.94	0.69	CaFr12	31.862745	0.6372549	637.254902
A	8	Sample X1	B	0.938	0.688	CaFr12	31.764706	0.6352941	635.294118
A	9	Blank B	C	0.28					
A	10	Sample X1	C	0.455	0.175	CaFr21	6.6176471	0.1323529	132.352941
A	11	Sample X1	C	0.454	0.174	CaFr21	6.5686275	0.1313725	131.372549

Appendix 6.10 contd.

A	12	Sample X1	C	0.451	0.171	CaFr21	6.4215686	0.1284314	128.431373
B	1	Blank B	D	0.102					
B	2	Sample X1	D	0.389	0.287	CaXy11	12.107843	0.2421569	242.156863
B	3	Sample X1	D	0.387	0.285	CaXy11	12.009804	0.2401961	240.196078
B	4	Sample X1	D	0.389	0.287	CaXy11	12.107843	0.2421569	242.156863
B	5	Blank B	E	0.127					
B	6	Sample X1	E	0.45	0.323	CaXy12	13.872549	0.277451	277.45098
B	7	Sample X1	E	0.45	0.323	CaXy12	13.872549	0.277451	277.45098
B	8	Sample X1	E	0.452	0.325	CaXy12	13.970588	0.2794118	279.411765
B	9	Blank B	F	0.108					
B	10	Sample X1	F	0.284	0.176	CaXy21	6.6666667	0.1333333	133.333333
B	11	Sample X1	F	0.282	0.174	CaXy21	6.5686275	0.1313725	131.372549
B	12	Sample X1	F	0.284	0.176	CaXy21	6.6666667	0.1333333	133.333333
D	1	Blank B	B	0.093					
D	2	Sample X1	B	0.357	0.264	CaGr11	10.980392	0.2196078	219.607843
D	3	Sample X1	B	0.359	0.266	CaGr11	11.078431	0.2215686	221.568627
D	4	Sample X1	B	0.358	0.265	CaGr11	11.029412	0.2205882	220.588235
D	5	Blank B	C	0.094					
D	6	Sample X1	C	0.412	0.318	CaGr12	13.627451	0.272549	272.54902
D	7	Sample X1	C	0.411	0.317	CaGr12	13.578431	0.2715686	271.568627
D	8	Sample X1	C	0.411	0.317	CaGr12	13.578431	0.2715686	271.568627
D	9	Blank B	D	0.085					
D	10	Sample X1	D	0.319	0.234	CaGr21	9.5098039	0.1901961	190.196078
D	11	Sample X1	D	0.319	0.232	CaGr21	9.4117647	0.1882353	188.235294
D	12	Sample X1	D	0.32	0.235	CaGr21	9.5588235	0.1911765	191.176471
C	1	Blank B	G	0.082					
C	2	Sample X1	G	0.28	0.198	CaGc11	7.745098	0.154902	154.901961
C	3	Sample X1	G	0.28	0.198	CaGc11	7.745098	0.154902	154.901961
C	4	Sample X1	G	0.278	0.196	CaGc11	7.6470588	0.1529412	152.941176
C	5	Blank B	H	0.087					
C	6	Sample X1	H	0.294	0.207	CaGc21	8.1862745	0.1637255	163.72549
C	7	Sample X1	H	0.292	0.205	CaGc21	8.0882353	0.1617647	161.764706
C	8	Sample X1	H	0.293	0.206	CaGc21	8.1372549	0.1627451	162.745098
H	5	Blank B	G	0.109					
H	6	Sample X1	G	0.375	0.266	CaGl11	11.078431	0.2215686	221.568627
H	7	Sample X1	G	0.374	0.267	CaGl11	11.127451	0.222549	222.54902
H	8	Sample X1	G	0.373	0.268	CaGl11	11.176471	0.2235294	223.529412
H	9	Blank B	H	0.086					
H	10	Sample X1	H	0.419	0.333	CaGl21	14.362745	0.2872549	287.254902
H	11	Sample X1	H	0.419	0.333	CaGl21	14.362745	0.2872549	287.254902
H	12	Sample X1	H	0.419	0.333	CaGl21	14.362745	0.2872549	287.254902

Appendix 6.11 RCCDRSM TPC run 11

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	9	Blank B	C	0.233					
F	10	Sample X1	C	0.549	0.316	CaSu11	13.5294118	0.2705882	270.5882353
F	11	Sample X1	C	0.545	0.312	CaSu11	13.3333333	0.2666667	266.6666667
F	12	Sample X1	C	0.545	0.312	CaSu11	13.3333333	0.2666667	266.6666667
G	1	Blank B	D	0.524					
G	2	Sample X1	D	0.971	0.447	CaFr11	19.9509804	0.3990196	399.0196078
G	3	Sample X1	D	0.971	0.447	CaFr11	19.9509804	0.3990196	399.0196078
G	4	Sample X1	D	0.97	0.446	CaFr11	19.9019608	0.3980392	398.0392157
G	5	Blank B	E	0.288					
G	6	Sample X1	E	0.991	0.703	CaFr12	32.5	0.65	650
G	7	Sample X1	E	0.991	0.703	CaFr12	32.5	0.65	650
G	8	Sample X1	E	0.992	0.704	CaFr12	32.5490196	0.6509804	650.9803922
G	9	Blank B	F	0.285					
G	10	Sample X1	F	0.386	0.101	CaFr21	2.99019608	0.0598039	59.80392157
G	11	Sample X1	F	0.386	0.101	CaFr21	2.99019608	0.0598039	59.80392157
G	12	Sample X1	F	0.387	0.102	CaFr21	3.03921569	0.0607843	60.78431373
A	1	Blank B	A	0.09					
A	2	Sample X1	A	0.254	0.164	CaXy11	6.07843137	0.1215686	121.5686275
A	3	Sample X1	A	0.254	0.164	CaXy11	6.07843137	0.1215686	121.5686275
A	4	Sample X1	A	0.257	0.167	CaXy11	6.2254902	0.1245098	124.5098039
A	5	Blank B	B	0.112					
A	6	Sample X1	B	0.245	0.133	CaXy12	4.55882353	0.0911765	91.17647059
A	7	Sample X1	B	0.246	0.134	CaXy12	4.60784314	0.0921569	92.15686275
A	8	Sample X1	B	0.248	0.136	CaXy12	4.70588235	0.0941176	94.11764706
A	9	Blank B	C	0.076					
A	10	Sample X1	C	0.182	0.106	CaXy21	3.23529412	0.0647059	64.70588235
A	11	Sample X1	C	0.182	0.106	CaXy21	3.23529412	0.0647059	64.70588235
A	12	Sample X1	C	0.181	0.105	CaXy21	3.18627451	0.0637255	63.7254902
B	1	Blank B	D	0.076					
B	2	Sample X1	D	0.182	0.106	CaGr11	3.23529412	0.0647059	64.70588235
B	3	Sample X1	D	0.185	0.109	CaGr11	3.38235294	0.0676471	67.64705882
B	4	Sample X1	D	0.186	0.11	CaGr11	3.43137255	0.0686275	68.62745098
B	5	Blank B	E	0.084					
B	6	Sample X1	E	0.195	0.111	CaGr12	3.48039216	0.0696078	69.60784314
B	7	Sample X1	E	0.196	0.112	CaGr12	3.52941176	0.0705882	70.58823529
B	8	Sample X1	E	0.197	0.113	CaGr12	3.57843137	0.0715686	71.56862745
B	9	Blank B	F	0.07					

Appendix 6.11 contd.

B	10	Sample X1	F	0.181	0.111	CaGr21	3.48039216	0.0696078	69.60784314
B	11	Sample X1	F	0.182	0.112	CaGr21	3.52941176	0.0705882	70.58823529
B	12	Sample X1	F	0.183	0.113	CaGr21	3.57843137	0.0715686	71.56862745
C	1	Blank B	G	0.083					
C	2	Sample X1	G	0.199	0.116	CaGc11	3.7254902	0.0745098	74.50980392
C	3	Sample X1	G	0.199	0.116	CaGc11	3.7254902	0.0745098	74.50980392
C	4	Sample X1	G	0.199	0.116	CaGc11	3.7254902	0.0745098	74.50980392
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.187	0.101	CaGc21	2.99019608	0.0598039	59.80392157
C	7	Sample X1	H	0.189	0.103	CaGc21	3.08823529	0.0617647	61.76470588
C	8	Sample X1	H	0.187	0.101	CaGc21	2.99019608	0.0598039	59.80392157
H	1	Blank B	G	0.079					
H	2	Sample X1	G	0.199	0.12	CaGl11	3.92156863	0.0784314	78.43137255
H	3	Sample X1	G	0.199	0.12	CaGl11	3.92156863	0.0784314	78.43137255
H	4	Sample X1	G	0.2	0.121	CaGl11	3.97058824	0.0794118	79.41176471
H	5	Blank B	H	0.067					
H	6	Sample X1	H	0.193	0.126	CaGl21	4.21568627	0.0843137	84.31372549
H	7	Sample X1	H	0.192	0.125	CaGl21	4.16666667	0.0833333	83.33333333
H	8	Sample X1	H	0.192	0.125	CaGl21	4.16666667	0.0833333	83.33333333

Appendix 6.12 RCCDRSM TPC run 12

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	1	Blank B	A	0.226					
E	2	Sample X1	A	0.581	0.355	CaSu11	15.44117647	0.308823529	308.8235294
E	3	Sample X1	A	0.589	0.363	CaSu11	15.83333333	0.316666667	316.6666667
E	4	Sample X1	A	0.585	0.369	CaSu11	16.12745098	0.32254902	322.5490196
E	5	Blank B	B	0.314					
E	6	Sample X1	B	0.932	0.618	CaFr11	28.33333333	0.566666667	566.6666667
E	7	Sample X1	B	0.934	0.62	CaFr11	28.43137255	0.568627451	568.627451
E	8	Sample X1	B	0.932	0.618	CaFr11	28.33333333	0.566666667	566.6666667
E	9	Blank B	C	0.356					
E	10	Sample X1	C	0.621	0.265	CaFr12	11.02941176	0.220588235	220.5882353
E	11	Sample X1	C	0.623	0.267	CaFr12	11.12745098	0.22254902	222.5490196
E	12	Sample X1	C	0.621	0.265	CaFr12	11.02941176	0.220588235	220.5882353
F	1	Blank B	D	0.307					
F	2	Sample X1	D	0.42	0.113	CaFr21	3.578431373	0.071568627	71.56862745
F	3	Sample X1	D	0.421	0.114	CaFr21	3.62745098	0.07254902	72.54901961

Appendix 6.12 contd.

F	4	Sample X1	D	0.423	0.116	CaFr21	3.725490196	0.074509804	74.50980392
B	1	Blank B	D	0.103					
B	2	Sample X1	D	0.249	0.146	CaXy11	5.196078431	0.103921569	103.9215686
B	3	Sample X1	D	0.25	0.147	CaXy11	5.245098039	0.104901961	104.9019608
B	4	Sample X1	D	0.25	0.147	CaXy11	5.245098039	0.104901961	104.9019608
F	5	Blank B	E	0.15					
F	6	Sample X1	E	0.259	0.109	CaXy12	3.382352941	0.067647059	67.64705882
F	7	Sample X1	E	0.258	0.107	CaXy12	3.284313725	0.065686275	65.68627451
F	8	Sample X1	E	0.26	0.11	CaXy12	3.431372549	0.068627451	68.62745098
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.226	0.135	CaXy21	4.656862745	0.093137255	93.1372549
A	11	Sample X1	C	0.222	0.131	CaXy21	4.460784314	0.089215686	89.21568627
A	12	Sample X1	C	0.229	0.138	CaXy21	4.803921569	0.096078431	96.07843137
F	9	Blank B	F	0.124					
F	10	Sample X1	F	0.279	0.155	CaGr11	5.637254902	0.112745098	112.745098
F	11	Sample X1	F	0.279	0.155	CaGr11	5.637254902	0.112745098	112.745098
F	12	Sample X1	F	0.279	0.155	CaGr11	5.637254902	0.112745098	112.745098
G	1	Blank B	G	0.148					
G	2	Sample X1	G	0.469	0.321	CaGr12	13.7745098	0.275490196	275.4901961
G	3	Sample X1	G	0.467	0.319	CaGr12	13.67647059	0.273529412	273.5294118
G	4	Sample X1	G	0.463	0.315	CaGr12	13.48039216	0.269607843	269.6078431
G	5	Blank B	H	0.086					
G	6	Sample X1	H	0.211	0.125	CaGr21	4.166666667	0.083333333	83.33333333
G	7	Sample X1	H	0.21	0.124	CaGr21	4.117647059	0.082352941	82.35294118
G	8	Sample X1	H	0.211	0.125	CaGr21	4.166666667	0.083333333	83.33333333
G	9	Blank B	I	0.094					
G	10	Sample X1	I	0.281	0.187	CaGc11	7.205882353	0.144117647	144.1176471
G	11	Sample X1	I	0.282	0.188	CaGc11	7.254901961	0.145098039	145.0980392
G	12	Sample X1	I	0.287	0.193	CaGc11	7.5	0.15	150
H	1	Blank B	J	0.108					
H	2	Sample X1	J	0.306	0.198	CaGc21	7.745098039	0.154901961	144.1176471
H	3	Sample X1	J	0.306	0.198	CaGc21	7.745098039	0.154901961	145.0980392
H	4	Sample X1	J	0.304	0.196	CaGc21	7.647058824	0.152941176	150
H	5	Blank B	K	0.13					
H	6	Sample X1	K	0.246	0.116	CaGl11	3.725490196	0.074509804	74.50980392
H	7	Sample X1	K	0.243	0.113	CaGl11	3.578431373	0.071568627	71.56862745
H	8	Sample X1	K	0.242	0.112	CaGl11	3.529411765	0.070588235	70.58823529
H	9	Blank B	L	0.087					
H	10	Sample X1	L	0.21	0.123	CaGl21	4.068627451	0.081372549	81.37254902
H	11	Sample X1	L	0.21	0.123	CaGl21	4.068627451	0.081372549	81.37254902
H	12	Sample X1	L	0.212	0.125	CaGl21	4.166666667	0.083333333	83.33333333

Appendix 6.13 RCCDRSM TPC run 13

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
F	1	Blank B	H	0.311					
F	2	Sample X1	H	0.887	0.576	CaSu11	26.2745098	0.2627451	262.745098
F	3	Sample X1	H	0.884	0.573	CaSu11	26.127451	0.2612745	261.27451
F	4	Sample X1	H	0.886	0.575	CaSu11	26.2254902	0.2622549	262.254902
F	5	Blank B	A	0.48					
F	6	Sample X1	A	0.942	0.462	CaFr11	20.6862745	0.2068627	206.862745
F	7	Sample X1	A	0.948	0.468	CaFr11	20.9803922	0.2098039	209.803922
F	8	Sample X1	A	0.943	0.463	CaFr11	20.7352941	0.2073529	207.352941
F	9	Blank B	B	0.267					
F	10	Sample X1	B	0.966	0.699	CaFr12	32.3039216	0.3230392	323.039216
F	11	Sample X1	B	0.965	0.698	CaFr12	32.254902	0.322549	322.54902
F	12	Sample X1	B	0.965	0.698	CaFr12	32.254902	0.322549	322.54902
G	1	Blank B	C	0.294					
G	2	Sample X1	C	0.519	0.225	CaFr21	9.06862745	0.0906863	90.6862745
G	3	Sample X1	C	0.52	0.226	CaFr21	9.11764706	0.0911765	91.1764706
G	4	Sample X1	C	0.519	0.225	CaFr21	9.06862745	0.0906863	90.6862745
G	5	Blank B	D	0.105					
G	6	Sample X1	D	0.719	0.614	CaXy11	28.1372549	0.2813725	281.372549
G	7	Sample X1	D	0.719	0.614	CaXy11	28.1372549	0.2813725	281.372549
G	8	Sample X1	D	0.72	0.615	CaXy11	28.1862745	0.2818627	281.862745
G	9	Blank B	E	0.139					
G	10	Sample X1	E	0.655	0.516	CaXy12	23.3333333	0.2333333	233.333333
G	11	Sample X1	E	0.653	0.514	CaXy12	23.2352941	0.2323529	232.352941
G	12	Sample X1	E	0.652	0.513	CaXy12	23.1862745	0.2318627	231.862745
H	1	Blank B	F	0.105					
H	2	Sample X1	F	0.604	0.499	CaXy21	22.5	0.225	225
H	3	Sample X1	F	0.602	0.497	CaXy21	22.4019608	0.2240196	224.019608
H	4	Sample X1	F	0.605	0.5	CaXy21	22.5490196	0.2254902	225.490196
E	1	Blank B	E	0.095					
E	2	Sample X1	E	0.561	0.466	CaGr11	20.8823529	0.2088235	208.823529
E	3	Sample X1	E	0.563	0.468	CaGr11	20.9803922	0.2098039	209.803922
E	4	Sample X1	E	0.569	0.474	CaGr11	21.2745098	0.2127451	212.745098
E	5	Blank B	F	0.103					
E	6	Sample X1	F	0.855	0.752	CaGr12	34.9019608	0.3490196	349.019608
E	7	Sample X1	F	0.852	0.749	CaGr12	34.754902	0.347549	347.54902
E	8	Sample X1	F	0.853	0.75	CaGr12	34.8039216	0.3480392	348.039216
E	9	Blank B	G	0.078					

Appendix 6.13 contd.

E	10	Sample X1	G	0.75	0.672	CaGr21	30.9803922	0.3098039	309.803922
E	11	Sample X1	G	0.752	0.674	CaGr21	31.0784314	0.3107843	310.784314
E	12	Sample X1	G	0.751	0.673	CaGr21	31.0294118	0.3102941	310.294118
H	5	Blank B	G	0.086					
H	6	Sample X1	G	0.457	0.371	CaGc11	16.2254902	0.1622549	162.254902
H	7	Sample X1	G	0.456	0.37	CaGc11	16.1764706	0.1617647	161.764706
H	8	Sample X1	G	0.459	0.373	CaGc11	16.3235294	0.1632353	163.235294
H	9	Blank B	H	0.082					
H	10	Sample X1	H	0.358	0.276	CaGc21	11.5686275	0.1156863	115.686275
H	11	Sample X1	H	0.359	0.277	CaGc21	11.6176471	0.1161765	116.176471
H	12	Sample X1	H	0.358	0.276	CaGc21	11.5686275	0.1156863	115.686275
C	1	Blank B	G	0.112					
C	2	Sample X1	G	0.783	0.671	CaGl11	30.9313725	0.3093137	309.313725
C	3	Sample X1	G	0.786	0.674	CaGl11	31.0784314	0.3107843	310.784314
C	4	Sample X1	G	0.784	0.672	CaGl11	30.9803922	0.3098039	309.803922
C	5	Blank B	H	0.093					
C	6	Sample X1	H	0.543	0.45	CaGl21	20.0980392	0.2009804	200.980392
C	7	Sample X1	H	0.541	0.448	CaGl21	20	0.2	200
C	8	Sample X1	H	0.54	0.447	CaGl21	19.9509804	0.1995098	199.509804

Appendix 6.14 RCCDRSM TPC run 14

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.212					
A	2	Sample X1	A	0.553	0.341	CaSu11	14.75490196	0.14754902	147.54902
A	3	Sample X1	A	0.555	0.343	CaSu11	14.85294118	0.14852941	148.52941
A	4	Sample X1	A	0.551	0.339	CaSu11	14.65686275	0.14656863	146.56863
E	1	Blank B	A	0.426					
E	2	Sample X1	A	0.753	0.327	CaFr11	14.06862745	0.14068627	140.68627
E	3	Sample X1	A	0.751	0.325	CaFr11	13.97058824	0.13970588	139.70588
E	4	Sample X1	A	0.752	0.326	CaFr11	14.01960784	0.14019608	140.19608
E	5	Blank B	B	0.261					
E	6	Sample X1	B	0.677	0.416	CaFr12	18.43137255	0.18431373	184.31373
E	7	Sample X1	B	0.673	0.412	CaFr12	18.23529412	0.18235294	182.35294
E	8	Sample X1	B	0.676	0.415	CaFr12	18.38235294	0.18382353	183.82353
E	9	Blank B	C	0.16					
E	10	Sample X1	C	0.335	0.175	CaFr21	6.617647059	0.06617647	66.176471
E	11	Sample X1	C	0.336	0.176	CaFr21	6.666666667	0.06666667	66.666667

Appendix 6.14 contd.

E	12	Sample X1	C	0.337	0.177	CaFr21	6.715686275	0.06715686	67.156863
F	1	Blank B	D	0.106					
F	2	Sample X1	D	0.249	0.143	CaXy11	5.049019608	0.0504902	50.490196
F	3	Sample X1	D	0.25	0.144	CaXy11	5.098039216	0.05098039	50.980392
F	4	Sample X1	D	0.25	0.144	CaXy11	5.098039216	0.05098039	50.980392
F	5	Blank B	E	0.092					
F	6	Sample X1	E	0.229	0.137	CaXy12	4.754901961	0.04754902	47.54902
F	7	Sample X1	E	0.226	0.134	CaXy12	4.607843137	0.04607843	46.078431
F	8	Sample X1	E	0.225	0.133	CaXy12	4.558823529	0.04558824	45.588235
F	9	Blank B	F	0.101					
F	10	Sample X1	F	0.203	0.102	CaXy21	3.039215686	0.03039216	30.392157
F	11	Sample X1	F	0.202	0.101	CaXy21	2.990196078	0.02990196	29.901961
F	12	Sample X1	F	0.204	0.103	CaXy21	3.088235294	0.03088235	30.882353
A	5	Blank B	B	0.089					
A	6	Sample X1	B	0.303	0.214	CaGr11	8.529411765	0.08529412	85.294118
A	7	Sample X1	B	0.302	0.213	CaGr11	8.480392157	0.08480392	84.803922
A	8	Sample X1	B	0.304	0.215	CaGr11	8.578431373	0.08578431	85.784314
A	9	Blank B	C	0.094					
A	10	Sample X1	C	0.261	0.167	CaGr12	6.225490196	0.0622549	62.254902
A	11	Sample X1	C	0.265	0.171	CaGr12	6.421568627	0.06421569	64.215686
A	12	Sample X1	C	0.266	0.172	CaGr12	6.470588235	0.06470588	64.705882
B	1	Blank B	D	0.091					
B	2	Sample X1	D	0.249	0.158	CaGr21	5.784313725	0.05784314	57.843137
B	3	Sample X1	D	0.249	0.158	CaGr21	5.784313725	0.05784314	57.843137
B	4	Sample X1	D	0.25	0.159	CaGr21	5.833333333	0.05833333	58.333333
G	1	Blank B	G	0.083					
G	2	Sample X1	G	0.235	0.151	CaGc11	5.441176471	0.05441176	54.411765
G	3	Sample X1	G	0.237	0.155	CaGc11	5.637254902	0.05637255	56.372549
G	4	Sample X1	G	0.236	0.153	CaGc11	5.539215686	0.05539216	55.392157
G	5	Blank B	H	0.083					
G	6	Sample X1	H	0.206	0.123	CaGc21	4.068627451	0.04068627	40.686275
G	7	Sample X1	H	0.208	0.125	CaGc21	4.166666667	0.04166667	41.666667
G	8	Sample X1	H	0.207	0.124	CaGc21	4.117647059	0.04117647	41.176471
B	5	Blank B	E	0.11					
B	6	Sample X1	E	0.26	0.145	CaGl11	5.147058824	0.05147059	51.470588
B	7	Sample X1	E	0.262	0.151	CaGl11	5.441176471	0.05441176	54.411765
B	8	Sample X1	E	0.26	0.155	CaGl11	5.637254902	0.05637255	56.372549
B	9	Blank B	F	0.084					
B	10	Sample X1	F	0.192	0.105	CaGl21	3.18627451	0.03186275	31.862745
B	11	Sample X1	F	0.193	0.109	CaGl21	3.382352941	0.03382353	33.823529
B	12	Sample X1	F	0.194	0.113	CaGl21	3.578431373	0.03578431	35.784314

Appendix 6.15 RCCDRSM TPC run 15

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	5	Blank B	F	0.277					
E	6	Sample X1	F	0.452	0.175	CaSu11	6.617647059	0.132352941	132.3529412
E	7	Sample X1	F	0.458	0.181	CaSu11	6.911764706	0.138235294	138.2352941
E	8	Sample X1	F	0.452	0.175	CaSu11	6.617647059	0.132352941	132.3529412
F	5	Blank B	A	0.439					
F	6	Sample X1	A	0.71	0.271	CaFr11	11.32352941	0.226470588	226.4705882
F	7	Sample X1	A	0.707	0.268	CaFr11	11.17647059	0.223529412	223.5294118
F	8	Sample X1	A	0.709	0.27	CaFr11	11.2745098	0.225490196	225.4901961
F	9	Blank B	B	0.196					
F	10	Sample X1	B	0.942	0.746	CaFr12	34.60784314	0.692156863	692.1568627
F	11	Sample X1	B	0.947	0.751	CaFr12	34.85294118	0.697058824	697.0588235
F	12	Sample X1	B	0.947	0.751	CaFr12	34.85294118	0.697058824	697.0588235
G	1	Blank B	C	0.26					
G	2	Sample X1	C	0.413	0.153	CaFr21	5.539215686	0.110784314	110.7843137
G	3	Sample X1	C	0.411	0.151	CaFr21	5.441176471	0.108823529	108.8235294
G	4	Sample X1	C	0.412	0.152	CaFr21	5.490196078	0.109803922	109.8039216
G	5	Blank B	D	0.098					
G	6	Sample X1	D	0.217	0.119	CaXy11	3.87254902	0.07745098	77.45098039
G	7	Sample X1	D	0.22	0.122	CaXy11	4.019607843	0.080392157	80.39215686
G	8	Sample X1	D	0.22	0.122	CaXy11	4.019607843	0.080392157	80.39215686
G	9	Blank B	E	0.111					
G	10	Sample X1	E	0.258	0.147	CaXy12	5.245098039	0.104901961	104.9019608
G	11	Sample X1	E	0.259	0.148	CaXy12	5.294117647	0.105882353	105.8823529
G	12	Sample X1	E	0.26	0.149	CaXy12	5.343137255	0.106862745	106.8627451
H	1	Blank B	F	0.101					
H	2	Sample X1	F	0.204	0.103	CaXy21	3.088235294	0.061764706	61.76470588
H	3	Sample X1	F	0.203	0.102	CaXy21	3.039215686	0.060784314	60.78431373
H	4	Sample X1	F	0.204	0.103	CaXy21	3.088235294	0.061764706	61.76470588
C	9	Blank B	A	0.078					
C	10	Sample X1	A	0.233	0.155	CaGr11	5.637254902	0.112745098	112.745098
C	11	Sample X1	A	0.231	0.153	CaGr11	5.539215686	0.110784314	110.7843137
C	12	Sample X1	A	0.234	0.156	CaGr11	5.68627451	0.11372549	113.7254902
D	1	Blank B	B	0.093					
D	2	Sample X1	B	0.261	0.168	CaGr12	6.274509804	0.125490196	125.4901961
D	3	Sample X1	B	0.264	0.171	CaGr12	6.421568627	0.128431373	128.4313725
D	4	Sample X1	B	0.263	0.17	CaGr12	6.37254902	0.12745098	127.4509804
D	5	Blank B	C	0.088					

Appendix 6.15 contd.

D	6	Sample X1	C	0.246	0.158	CaGr21	5.784313725	0.115686275	115.6862745
D	7	Sample X1	C	0.246	0.158	CaGr21	5.784313725	0.115686275	115.6862745
D	8	Sample X1	C	0.248	0.16	CaGr21	5.882352941	0.117647059	117.6470588
H	5	Blank B	G	0.086					
H	6	Sample X1	G	0.296	0.21	CaGc11	8.333333333	0.166666667	166.6666667
H	7	Sample X1	G	0.295	0.209	CaGc11	8.284313725	0.165686275	165.6862745
H	8	Sample X1	G	0.297	0.211	CaGc11	8.382352941	0.167647059	167.6470588
H	9	Blank B	H	0.082					
H	10	Sample X1	H	0.234	0.152	CaGc21	5.490196078	0.109803922	109.8039216
H	11	Sample X1	H	0.235	0.153	CaGc21	5.539215686	0.110784314	110.7843137
H	12	Sample X1	H	0.233	0.151	CaGc21	5.441176471	0.108823529	108.8235294
D	9	Blank B	D	0.104					
D	10	Sample X1	D	0.209	0.105	CaGl11	3.18627451	0.06372549	63.7254902
D	11	Sample X1	D	0.212	0.108	CaGl11	3.333333333	0.066666667	66.66666667
D	12	Sample X1	D	0.211	0.107	CaGl11	3.284313725	0.065686275	65.68627451
E	1	Blank B	E	0.071					
E	2	Sample X1	E	0.176	0.105	CaGl21	3.18627451	0.06372549	63.7254902
E	3	Sample X1	E	0.177	0.106	CaGl21	3.235294118	0.064705882	64.70588235
E	4	Sample X1	E	0.178	0.107	CaGl21	3.284313725	0.065686275	65.68627451

Appendix 6.16 RCCDRSM TPC run 16

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	5	Blank B	B	0.152					
A	6	Sample X1	B	0.423	0.271	CaSu11	11.3235294	0.2264706	226.47059
A	7	Sample X1	B	0.423	0.271	CaSu11	11.3235294	0.2264706	226.47059
A	8	Sample X1	B	0.424	0.272	CaSu11	11.372549	0.227451	227.45098
C	9	Blank B	A	0.308					
C	10	Sample X1	A	0.412	0.104	CaFr11	3.1372549	0.0627451	62.745098
C	11	Sample X1	A	0.412	0.104	CaFr11	3.1372549	0.0627451	62.745098
C	12	Sample X1	A	0.413	0.105	CaFr11	3.18627451	0.0637255	63.72549
D	1	Blank B	B	0.25					
D	2	Sample X1	B	0.573	0.323	CaFr12	13.872549	0.277451	277.45098
D	3	Sample X1	B	0.572	0.322	CaFr12	13.8235294	0.2764706	276.47059
D	4	Sample X1	B	0.571	0.321	CaFr12	13.7745098	0.2754902	275.4902
D	5	Blank B	C	0.241					
D	6	Sample X1	C	0.359	0.118	CaFr21	3.82352941	0.0764706	76.470588
D	7	Sample X1	C	0.358	0.117	CaFr21	3.7745098	0.0754902	75.490196
D	8	Sample X1	C	0.358	0.117	CaFr21	3.7745098	0.0754902	75.490196

Appendix 6.16 contd.

D	9	Blank B	D	0.104					
D	10	Sample X1	D	0.237	0.133	CaXy11	4.55882353	0.0911765	91.176471
D	11	Sample X1	D	0.237	0.133	CaXy11	4.55882353	0.0911765	91.176471
D	12	Sample X1	D	0.233	0.129	CaXy11	4.3627451	0.0872549	87.254902
E	1	Blank B	E	0.126					
E	2	Sample X1	E	0.227	0.101	CaXy12	2.99019608	0.0598039	59.803922
E	3	Sample X1	E	0.226	0.1	CaXy12	2.94117647	0.0588235	58.823529
E	4	Sample X1	E	0.227	0.101	CaXy12	2.99019608	0.0598039	59.803922
E	5	Blank B	F	0.093					
E	6	Sample X1	F	0.2	0.107	CaX21	3.28431373	0.0656863	65.686275
E	7	Sample X1	F	0.2	0.107	CaXy21	3.28431373	0.0656863	65.686275
E	8	Sample X1	F	0.201	0.108	CaXy21	3.33333333	0.0666667	66.666667
B	9	Blank B	F	0.097					
B	10	Sample X1	F	0.271	0.174	CaGr11	6.56862745	0.1313725	131.37255
B	11	Sample X1	F	0.271	0.174	CaGr11	6.56862745	0.1313725	131.37255
B	12	Sample X1	F	0.27	0.173	CaGr11	6.51960784	0.1303922	130.39216
C	1	Blank B	G	0.097					
C	2	Sample X1	G	0.268	0.171	CaGr12	6.42156863	0.1284314	128.43137
C	3	Sample X1	G	0.268	0.171	CaGr12	6.42156863	0.1284314	128.43137
C	4	Sample X1	G	0.27	0.173	CaGr12	6.51960784	0.1303922	130.39216
C	5	Blank B	H	0.098					
C	6	Sample X1	H	0.318	0.22	CaGr21	8.82352941	0.1764706	176.47059
C	7	Sample X1	H	0.319	0.221	CaGr21	8.87254902	0.177451	177.45098
C	8	Sample X1	H	0.32	0.222	CaGr21	8.92156863	0.1784314	178.43137
E	9	Blank B	G	0.087					
E	10	Sample X1	G	0.244	0.157	CaGc11	5.73529412	0.1147059	114.70588
E	11	Sample X1	G	0.24	0.153	CaGc11	5.53921569	0.1107843	110.78431
E	12	Sample X1	G	0.241	0.154	CaGc11	5.58823529	0.1117647	111.76471
F	1	Blank B	H	0.083					
F	2	Sample X1	H	0.191	0.108	CaGc21	3.33333333	0.0666667	66.666667
F	3	Sample X1	H	0.192	0.109	CaGc21	3.38235294	0.0676471	67.647059
F	4	Sample X1	H	0.192	0.109	CaGc21	3.38235294	0.0676471	67.647059
G	9	Blank B	A	0.106					
G	10	Sample X1	A	0.257	0.151	CaGl11	5.44117647	0.1088235	108.82353
G	11	Sample X1	A	0.259	0.153	CaGl11	5.53921569	0.1107843	110.78431
G	12	Sample X1	A	0.258	0.152	CaGl11	5.49019608	0.1098039	109.80392
H	1	Blank B	B	0.088					
H	2	Sample X1	B	0.216	0.128	CaGl21	4.31372549	0.0862745	86.27451
H	3	Sample X1	B	0.211	0.123	CaGl21	4.06862745	0.0813725	81.372549
H	4	Sample X1	B	0.216	0.128	CaGl21	4.31372549	0.0862745	86.27451

Appendix 6.17 RCCDRSM TPC run 17

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.173					
A	2	Sample X1	A	0.761	0.588	CaSu11	26.862745	0.26862745	268.62745
A	3	Sample X1	A	0.759	0.586	CaSu11	26.764706	0.26764706	267.64706
A	4	Sample X1	A	0.759	0.586	CaSu11	26.764706	0.26764706	267.64706
A	5	Blank B	B	0.128					
A	6	Sample X1	B	0.921	0.793	CaFr11	36.911765	0.36911765	369.11765
A	7	Sample X1	B	0.92	0.792	CaFr11	36.862745	0.36862745	368.62745
A	8	Sample X1	B	0.92	0.792	CaFr11	36.862745	0.36862745	368.62745
A	9	Blank B	C	0.302					
A	10	Sample X1	C	0.822	0.52	CaFr12	23.529412	0.23529412	235.29412
A	11	Sample X1	C	0.825	0.523	CaFr12	23.676471	0.23676471	236.76471
A	12	Sample X1	C	0.83	0.528	CaFr12	23.921569	0.23921569	239.21569
B	1	Blank B	D	0.099					
B	2	Sample X1	D	0.29	0.191	CaFr21	7.4019608	0.07401961	74.019608
B	3	Sample X1	D	0.292	0.193	CaFr21	7.5	0.075	75
B	4	Sample X1	D	0.293	0.194	CaFr21	7.5490196	0.0754902	75.490196
B	5	Blank B	E	0.094					
B	6	Sample X1	E	0.277	0.183	CaXy11	7.0098039	0.07009804	70.098039
B	7	Sample X1	E	0.277	0.183	CaXy11	7.0098039	0.07009804	70.098039
B	8	Sample X1	E	0.276	0.182	CaXy11	6.9607843	0.06960784	69.607843
B	5	Blank B	E	0.108					
B	6	Sample X1	E	0.335	0.227	CaXy12	9.1666667	0.09166667	91.666667
B	7	Sample X1	E	0.334	0.226	CaXy12	9.1176471	0.09117647	91.176471
B	8	Sample X1	E	0.33	0.222	CaXy12	8.9215686	0.08921569	89.215686
B	1	Blank B	D	0.081					
B	2	Sample X1	D	0.186	0.105	CaX21	3.1862745	0.03186275	31.862745
B	3	Sample X1	D	0.188	0.107	CaXy21	3.2843137	0.03284314	32.843137
B	4	Sample X1	D	0.187	0.106	CaXy21	3.2352941	0.03235294	32.352941
B	9	Blank B	F	0.099					
B	10	Sample X1	F	0.371	0.272	CaGr11	11.372549	0.11372549	113.72549
B	11	Sample X1	F	0.377	0.278	CaGr11	11.666667	0.11666667	116.66667
B	12	Sample X1	F	0.377	0.278	CaGr11	11.666667	0.11666667	116.66667
C	1	Blank B	G	0.102					
C	2	Sample X1	G	0.459	0.357	CaGr12	15.539216	0.15539216	155.39216
C	3	Sample X1	G	0.451	0.349	CaGr12	15.147059	0.15147059	151.47059
C	4	Sample X1	G	0.453	0.351	CaGr12	15.245098	0.15245098	152.45098
C	5	Blank B	H	0.105					

Appendix 6.17 contd.

C	6	Sample X1	H	0.35	0.245	CaGr21	10.04902	0.1004902	100.4902
C	7	Sample X1	H	0.35	0.245	CaGr21	10.04902	0.1004902	100.4902
C	8	Sample X1	H	0.351	0.246	CaGr21	10.098039	0.10098039	100.98039
C	9	Blank B	I	0.096					
C	10	Sample X1	I	0.346	0.25	CaGc11	10.294118	0.10294118	102.94118
C	11	Sample X1	I	0.347	0.251	CaGc11	10.343137	0.10343137	103.43137
C	12	Sample X1	I	0.347	0.251	CaGc11	10.343137	0.10343137	103.43137
D	1	Blank B	J	0.101					
D	2	Sample X1	J	0.398	0.297	CaGc21	12.598039	0.12598039	125.98039
D	3	Sample X1	J	0.401	0.3	CaGc21	12.745098	0.12745098	127.45098
D	4	Sample X1	J	0.4	0.299	CaGc21	12.696078	0.12696078	126.96078
D	5	Blank B	K	0.106					
D	6	Sample X1	K	0.292	0.186	CaGl11	7.1568627	0.07156863	71.568627
D	7	Sample X1	K	0.294	0.188	CaGl11	7.254902	0.07254902	72.54902
D	8	Sample X1	K	0.294	0.188	CaGl11	7.254902	0.07254902	72.54902
D	9	Blank B	L	0.108					
D	10	Sample X1	L	0.264	0.156	CaGl21	5.6862745	0.05686275	56.862745
D	11	Sample X1	L	0.264	0.156	CaGl21	5.6862745	0.05686275	56.862745
D	12	Sample X1	L	0.265	0.157	CaGl21	5.7352941	0.05735294	57.352941

Appendix 6.18 RCCDRSM TPC run 18

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.165					
A	2	Sample X1	A	0.323	0.158	CaSu11	5.7843137	0.2313725	231.372549
A	3	Sample X1	A	0.324	0.159	CaSu11	5.8333333	0.2333333	233.333333
A	4	Sample X1	A	0.325	0.16	CaSu11	5.8823529	0.2352941	235.294118
A	5	Blank B	B	0.213					
A	6	Sample X1	B	0.339	0.126	CaFr11	4.2156863	0.1686275	168.627451
A	7	Sample X1	B	0.338	0.125	CaFr11	4.1666667	0.1666667	166.666667
A	8	Sample X1	B	0.34	0.127	CaFr11	4.2647059	0.1705882	170.588235
A	9	Blank B	C	0.214					
A	10	Sample X1	C	0.447	0.233	CaFr12	9.4607843	0.3784314	378.431373
A	11	Sample X1	C	0.447	0.233	CaFr12	9.4607843	0.3784314	378.431373
A	12	Sample X1	C	0.448	0.234	CaFr12	9.5098039	0.3803922	380.392157
B	1	Blank B	D	0.194					
B	2	Sample X1	D	0.346	0.152	CaFr21	5.4901961	0.2196078	219.607843

Appendix 6.18 contd.

B	3	Sample X1	D	0.348	0.154	CaFr21	5.5882353	0.2235294	223.529412
B	4	Sample X1	D	0.346	0.152	CaFr21	5.4901961	0.2196078	219.607843
B	9	Blank B	F	0.057					
B	10	Sample X1	F	0.16	0.103	CaXy11	3.0882353	0.1235294	123.529412
B	11	Sample X1	F	0.16	0.103	CaXy11	3.0882353	0.1235294	123.529412
B	12	Sample X1	F	0.162	0.105	CaXy11	3.1862745	0.127451	127.45098
B	5	Blank B	E	0.123					
B	6	Sample X1	E	0.228	0.105	CaXy12	3.1862745	0.127451	127.45098
B	7	Sample X1	E	0.227	0.104	CaXy12	3.1372549	0.1254902	125.490196
B	8	Sample X1	E	0.226	0.103	CaXy12	3.0882353	0.1235294	123.529412
B	5	Blank B	E	0.026					
B	6	Sample X1	E	0.138	0.112	CaX21	3.5294118	0.1411765	141.176471
B	7	Sample X1	E	0.133	0.107	CaXy21	3.2843137	0.1313725	131.372549
B	8	Sample X1	E	0.131	0.105	CaXy21	3.1862745	0.127451	127.45098
B	9	Blank B	F	0.103					
B	10	Sample X1	F	0.257	0.154	CaGr11	5.5882353	0.2235294	223.529412
B	11	Sample X1	F	0.257	0.154	CaGr11	5.5882353	0.2235294	223.529412
B	12	Sample X1	F	0.255	0.152	CaGr11	5.4901961	0.2196078	219.607843
C	1	Blank B	G	0.085					
C	2	Sample X1	G	0.294	0.209	CaGr12	8.2843137	0.3313725	331.372549
C	3	Sample X1	G	0.295	0.21	CaGr12	8.3333333	0.3333333	333.333333
C	4	Sample X1	G	0.295	0.21	CaGr12	8.3333333	0.3333333	333.333333
C	5	Blank B	H	0.082					
C	6	Sample X1	H	0.241	0.159	CaGr21	5.8333333	0.2333333	233.333333
C	7	Sample X1	H	0.242	0.16	CaGr21	5.8823529	0.2352941	235.294118
C	8	Sample X1	H	0.24	0.158	CaGr21	5.7843137	0.2313725	231.372549
C	9	Blank B	I	0.093					
C	10	Sample X1	I	0.293	0.2	CaGc11	7.8431373	0.3137255	313.72549
C	11	Sample X1	I	0.295	0.202	CaGc11	7.9411765	0.3176471	317.647059
C	12	Sample X1	I	0.294	0.201	CaGc11	7.8921569	0.3156863	315.686275
D	1	Blank B	J	0.084					
D	2	Sample X1	J	0.276	0.192	CaGc21	7.4509804	0.2980392	298.039216
D	3	Sample X1	J	0.273	0.189	CaGc21	7.3039216	0.2921569	292.156863
D	4	Sample X1	J	0.273	0.189	CaGc21	7.3039216	0.2921569	292.156863
D	5	Blank B	K	0.087					
D	6	Sample X1	K	0.28	0.193	CaGl11	7.5	0.3	300
D	7	Sample X1	K	0.278	0.191	CaGl11	7.4019608	0.2960784	296.078431
D	8	Sample X1	K	0.276	0.189	CaGl11	7.3039216	0.2921569	292.156863
D	9	Blank B	L	0.077					
D	10	Sample X1	L	0.251	0.174	CaGl21	6.5686275	0.2627451	262.745098
D	11	Sample X1	L	0.253	0.176	CaGl21	6.6666667	0.2666667	266.666667
D		Sample X1	L	0.252	0.175	CaGl21	6.6176471	0.2647059	264.705882

Appendix 6.19 RCCDRSM TPC run 19

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	1	Blank B	A	0.138					
E	2	Sample X1	A	0.549	0.411	CaSu11	18.186275	0.727451	727.45098
E	3	Sample X1	A	0.548	0.41	CaSu11	18.137255	0.7254902	725.4902
E	4	Sample X1	A	0.551	0.413	CaSu11	18.284314	0.7313725	731.37255
E	5	Blank B	B	0.189					
E	6	Sample X1	B	0.315	0.126	CaFr11	4.2156863	0.1686275	168.62745
E	7	Sample X1	B	0.316	0.127	CaFr11	4.2647059	0.1705882	170.58824
E	8	Sample X1	B	0.312	0.123	CaFr11	4.0686275	0.1627451	162.7451
E	9	Blank B	C	0.163					
E	10	Sample X1	C	0.409	0.246	CaFr12	10.098039	0.4039216	403.92157
E	11	Sample X1	C	0.412	0.249	CaFr12	10.245098	0.4098039	409.80392
E	12	Sample X1	C	0.41	0.247	CaFr12	10.147059	0.4058824	405.88235
F	1	Blank B	D	0.131					
F	2	Sample X1	D	0.294	0.163	CaFr21	6.0294118	0.2411765	241.17647
F	3	Sample X1	D	0.294	0.163	CaFr21	6.0294118	0.2411765	241.17647
F	4	Sample X1	D	0.295	0.164	CaFr21	6.0784314	0.2431373	243.13725
C	1	Blank B	G	0.052					
C	2	Sample X1	G	0.154	0.102	CaXy11	3.0392157	0.1215686	121.56863
C	3	Sample X1	G	0.157	0.105	CaXy11	3.1862745	0.127451	127.45098
C	4	Sample X1	G	0.155	0.103	CaXy11	3.0882353	0.1235294	123.52941
F	5	Blank B	E	0.132					
F	6	Sample X1	E	0.266	0.134	CaXy12	4.6078431	0.1843137	184.31373
F	7	Sample X1	E	0.265	0.133	CaXy12	4.5588235	0.1823529	182.35294
F	8	Sample X1	E	0.267	0.135	CaXy12	4.6568627	0.1862745	186.27451
B	9	Blank B	F	0.01					
B	10	Sample X1	F	0.112	0.102	CaX21	3.0392157	0.1215686	121.56863
B	11	Sample X1	F	0.112	0.102	CaXy21	3.0392157	0.1215686	121.56863
B	12	Sample X1	F	0.112	0.102	CaXy21	3.0392157	0.1215686	121.56863
F	9	Blank B	F	0.117					
F	10	Sample X1	F	0.271	0.154	CaGr11	5.5882353	0.2235294	223.52941
F	11	Sample X1	F	0.268	0.151	CaGr11	5.4411765	0.2176471	217.64706
F	12	Sample X1	F	0.269	0.152	CaGr11	5.4901961	0.2196078	219.60784
G	1	Blank B	G	0.125					
G	2	Sample X1	G	0.308	0.183	CaGr12	7.0098039	0.2803922	280.39216
G	3	Sample X1	G	0.305	0.18	CaGr12	6.8627451	0.2745098	274.5098
G	4	Sample X1	G	0.306	0.181	CaGr12	6.9117647	0.2764706	276.47059
G	5	Blank B	H	0.105					

Appendix 6.19 contd.

G	6	Sample X1	H	0.247	0.142	CaGr21	5	0.2	200
G	7	Sample X1	H	0.245	0.14	CaGr21	4.9019608	0.1960784	196.07843
G	8	Sample X1	H	0.246	0.141	CaGr21	4.9509804	0.1980392	198.03922
G	9	Blank B	I	0.093					
G	10	Sample X1	I	0.341	0.248	CaGc11	10.196078	0.4078431	407.84314
G	11	Sample X1	I	0.34	0.247	CaGc11	10.147059	0.4058824	405.88235
G	12	Sample X1	I	0.342	0.249	CaGc11	10.245098	0.4098039	409.80392
H	1	Blank B	J	0.111					
H	2	Sample X1	J	0.272	0.161	CaGc21	5.9313725	0.2372549	237.2549
H	3	Sample X1	J	0.273	0.162	CaGc21	5.9803922	0.2392157	239.21569
H	4	Sample X1	J	0.273	0.162	CaGc21	5.9803922	0.2392157	239.21569
H	5	Blank B	K	0.113					
H	6	Sample X1	K	0.28	0.167	CaGl11	6.2254902	0.2490196	249.01961
H	7	Sample X1	K	0.279	0.166	CaGl11	6.1764706	0.2470588	247.05882
H	8	Sample X1	K	0.279	0.166	CaGl11	6.1764706	0.2470588	247.05882
H	9	Blank B	L	0.113					
H	10	Sample X1	L	0.25	0.137	CaGl21	4.754902	0.1901961	190.19608
H	11	Sample X1	L	0.248	0.135	CaGl21	4.6568627	0.1862745	186.27451
H	12	Sample X1	L	0.247	0.134	CaGl21	4.6078431	0.1843137	184.31373

Appendix 6.20 RCCDRSM TPC run 20

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.128					
A	2	Sample X1	A	0.471	0.343	CaSu11	14.852941	0.5941176	594.11765
A	3	Sample X1	A	0.475	0.347	CaSu11	15.04902	0.6019608	601.96078
A	4	Sample X1	A	0.473	0.345	CaSu11	14.95098	0.5980392	598.03922
A	5	Blank B	B	0.165					
A	6	Sample X1	B	0.366	0.201	CaFr11	7.8921569	0.3156863	315.68627
A	7	Sample X1	B	0.364	0.199	CaFr11	7.7941176	0.3117647	311.76471
A	8	Sample X1	B	0.364	0.199	CaFr11	7.7941176	0.3117647	311.76471
A	9	Blank B	C	0.203					
A	10	Sample X1	C	0.56	0.357	CaFr12	15.539216	0.6215686	621.56863
A	11	Sample X1	C	0.56	0.357	CaFr12	15.539216	0.6215686	621.56863
A	12	Sample X1	C	0.559	0.356	CaFr12	15.490196	0.6196078	619.60784
B	1	Blank B	D	0.191					
B	2	Sample X1	D	0.328	0.137	CaFr21	4.754902	0.1901961	190.19608
B	3	Sample X1	D	0.33	0.139	CaFr21	4.8529412	0.1941176	194.11765

Appendix 6.20 contd.

B	4	Sample X1	D	0.33	0.139	CaFr21	4.8529412	0.1941176	194.11765
C	5	Blank B	H	0.011					
C	6	Sample X1	H	0.141	0.13	CaXy11	4.4117647	0.1764706	176.47059
C	7	Sample X1	H	0.136	0.125	CaXy11	4.1666667	0.1666667	166.66667
C	8	Sample X1	H	0.136	0.125	CaXy11	4.1666667	0.1666667	166.66667
B	5	Blank B	E	0.166					
B	6	Sample X1	E	0.323	0.157	CaXy12	5.7352941	0.2294118	229.41176
B	7	Sample X1	E	0.32	0.154	CaXy12	5.5882353	0.2235294	223.52941
B	8	Sample X1	E	0.32	0.154	CaXy12	5.5882353	0.2235294	223.52941
C	1	Blank B	G	0.009					
C	2	Sample X1	G	0.125	0.116	CaX21	3.7254902	0.1490196	149.01961
C	3	Sample X1	G	0.131	0.122	CaXy21	4.0196078	0.1607843	160.78431
C	4	Sample X1	G	0.125	0.116	CaXy21	3.7254902	0.1490196	149.01961
B	9	Blank B	F	0.106					
B	10	Sample X1	F	0.257	0.151	CaGr11	5.4411765	0.2176471	217.64706
B	11	Sample X1	F	0.255	0.149	CaGr11	5.3431373	0.2137255	213.72549
B	12	Sample X1	F	0.253	0.147	CaGr11	5.245098	0.2098039	209.80392
C	1	Blank B	G	0.111					
C	2	Sample X1	G	0.278	0.167	CaGr12	6.2254902	0.2490196	249.01961
C	3	Sample X1	G	0.27	0.159	CaGr12	5.8333333	0.2333333	233.33333
C	4	Sample X1	G	0.276	0.165	CaGr12	6.127451	0.245098	245.09804
C	5	Blank B	H	0.112					
C	6	Sample X1	H	0.251	0.139	CaGr21	4.8529412	0.1941176	194.11765
C	7	Sample X1	H	0.25	0.138	CaGr21	4.8039216	0.1921569	192.15686
C	8	Sample X1	H	0.252	0.14	CaGr21	4.9019608	0.1960784	196.07843
C	9	Blank B	I	0.079					
C	10	Sample X1	I	0.29	0.211	CaGc11	8.3823529	0.3352941	335.29412
C	11	Sample X1	I	0.289	0.21	CaGc11	8.3333333	0.3333333	333.33333
C	12	Sample X1	I	0.291	0.212	CaGc11	8.4313725	0.3372549	337.2549
D	1	Blank B	J	0.092					
D	2	Sample X1	J	0.28	0.188	CaGc21	7.254902	0.2901961	290.19608
D	3	Sample X1	J	0.279	0.187	CaGc21	7.2058824	0.2882353	288.23529
D	4	Sample X1	J	0.28	0.188	CaGc21	7.254902	0.2901961	290.19608
D	5	Blank B	K	0.118					
D	6	Sample X1	K	0.26	0.142	CaGl11	5	0.2	200
D	7	Sample X1	K	0.258	0.14	CaGl11	4.9019608	0.1960784	196.07843
D	8	Sample X1	K	0.259	0.141	CaGl11	4.9509804	0.1980392	198.03922
D	9	Blank B	L	0.136					
D	10	Sample X1	L	0.254	0.118	CaGl21	3.8235294	0.1529412	152.94118
D	11	Sample X1	L	0.253	0.117	CaGl21	3.7745098	0.1509804	150.98039
D	12	Sample X1	L	0.255	0.119	CaGl21	3.872549	0.154902	154.90196

Appendix 6.21 RCCDRSM TPC run 21

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.155					
A	2	Sample X1	A	0.52	0.365	CaSu11	15.93137	0.2389706	238.9705882
A	3	Sample X1	A	0.518	0.363	CaSu11	15.83333	0.2375	237.5
A	4	Sample X1	A	0.52	0.365	CaSu11	15.93137	0.2389706	238.9705882
A	1	Blank B	A	0.404					
A	2	Sample X1	A	0.659	0.255	CaFr11	10.53922	0.1580882	158.0882353
A	3	Sample X1	A	0.653	0.249	CaFr11	10.2451	0.1536765	153.6764706
A	4	Sample X1	A	0.658	0.254	CaFr11	10.4902	0.1573529	157.3529412
H	1	Blank B	F	0.289					
H	2	Sample X1	F	0.682	0.393	CaFr12	17.30392	0.2595588	259.5588235
H	3	Sample X1	F	0.682	0.393	CaFr12	17.30392	0.2595588	259.5588235
H	4	Sample X1	F	0.684	0.395	CaFr12	17.40196	0.2610294	261.0294118
A	9	Blank B	C	0.233					
A	10	Sample X1	C	0.456	0.223	CaFr21	8.970588	0.1345588	134.5588235
A	11	Sample X1	C	0.453	0.22	CaFr21	8.823529	0.1323529	132.3529412
A	12	Sample X1	C	0.451	0.218	CaFr21	8.72549	0.1308824	130.8823529
B	1	Blank B	D	0.098					
B	2	Sample X1	D	0.264	0.166	CaXy11	6.176471	0.0926471	92.64705882
B	3	Sample X1	D	0.268	0.17	CaXy11	6.372549	0.0955882	95.58823529
B	4	Sample X1	D	0.263	0.165	CaXy11	6.127451	0.0919118	91.91176471
B	5	Blank B	E	0.12					
B	6	Sample X1	E	0.246	0.126	CaXy12	4.215686	0.0632353	63.23529412
B	7	Sample X1	E	0.245	0.125	CaXy12	4.166667	0.0625	62.5
B	8	Sample X1	E	0.248	0.128	CaXy12	4.313725	0.0647059	64.70588235
B	9	Blank B	F	0.098					
B	10	Sample X1	F	0.206	0.108	CaXy21	3.333333	0.05	50
B	11	Sample X1	F	0.21	0.112	CaXy21	3.529412	0.0529412	52.94117647
B	12	Sample X1	F	0.212	0.114	CaXy21	3.627451	0.0544118	54.41176471
A	9	Blank B	C	0.091					
A	10	Sample X1	C	0.223	0.132	CaGr11	4.509804	0.0676471	67.64705882
A	11	Sample X1	C	0.224	0.133	CaGr11	4.558824	0.0683824	68.38235294
A	12	Sample X1	C	0.224	0.133	CaGr11	4.558824	0.0683824	68.38235294
B	1	Blank B	D	0.102					
B	2	Sample X1	D	0.239	0.137	CaGr12	4.754902	0.0713235	71.32352941
B	3	Sample X1	D	0.238	0.136	CaGr12	4.705882	0.0705882	70.58823529
B	4	Sample X1	D	0.24	0.138	CaGr12	4.803922	0.0720588	72.05882353
B	5	Blank B	E	0.069					

Appendix 6.21 contd.

B	6	Sample X1	E	0.174	0.105	CaGr21	3.186275	0.0477941	47.79411765
B	7	Sample X1	E	0.172	0.103	CaGr21	3.088235	0.0463235	46.32352941
B	8	Sample X1	E	0.174	0.105	CaGr21	3.186275	0.0477941	47.79411765
C	1	Blank B	G	0.081					
C	2	Sample X1	G	0.324	0.243	CaGc11	9.95098	0.1492647	149.2647059
C	3	Sample X1	G	0.323	0.242	CaGc11	9.901961	0.1485294	148.5294118
C	4	Sample X1	G	0.325	0.244	CaGc11	10	0.15	150
C	5	Blank B	H	0.086					
C	6	Sample X1	H	0.229	0.143	CaGc21	5.04902	0.0757353	75.73529412
C	7	Sample X1	H	0.228	0.142	CaGc21	5	0.075	75
C	8	Sample X1	H	0.23	0.144	CaGc21	5.098039	0.0764706	76.47058824
E	9	Blank B	G	0.108					
E	10	Sample X1	G	0.217	0.109	CaGl11	3.382353	0.0507353	50.73529412
E	11	Sample X1	G	0.215	0.107	CaGl11	3.284314	0.0492647	49.26470588
E	12	Sample X1	G	0.219	0.111	CaGl11	3.480392	0.0522059	52.20588235
F	1	Blank B	H	0.084					
F	2	Sample X1	H	0.212	0.128	CaGl21	4.313725	0.0647059	64.70588235
F	3	Sample X1	H	0.209	0.125	CaGl21	4.166667	0.0625	62.5
F	4	Sample X1	H	0.211	0.127	CaGl21	4.264706	0.0639706	63.97058824

Appendix 6.22 RCCDRSM TPC run 22

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	1	Blank B	A	0.183					
E	2	Sample X1	A	0.32	0.137	CaSu11	4.75490196	0.2377451	237.745098
E	3	Sample X1	A	0.319	0.136	CaSu11	4.70588235	0.23529412	235.2941176
E	4	Sample X1	A	0.32	0.137	CaSu11	4.75490196	0.2377451	237.745098
E	5	Blank B	B	0.248					
E	6	Sample X1	B	0.846	0.598	CaFr11	27.3529412	1.36764706	1367.647059
E	7	Sample X1	B	0.852	0.604	CaFr11	27.6470588	1.38235294	1382.352941
E	8	Sample X1	B	0.847	0.599	CaFr11	27.4019608	1.37009804	1370.098039
E	9	Blank B	C	0.259					
E	10	Sample X1	C	0.393	0.134	CaFr12	4.60784314	0.23039216	230.3921569
E	11	Sample X1	C	0.393	0.134	CaFr12	4.60784314	0.23039216	230.3921569
E	12	Sample X1	C	0.394	0.135	CaFr12	4.65686275	0.23284314	232.8431373
F	1	Blank B	D	0.115					
F	2	Sample X1	D	0.237	0.122	CaFr21	4.01960784	0.20098039	200.9803922
F	3	Sample X1	D	0.235	0.12	CaFr21	3.92156863	0.19607843	196.0784314

Appendix 6.22 contd.

F	4	Sample X1	D	0.236	0.121	CaFr21	3.97058824	0.19852941	198.5294118
C	9	Blank B	I	0.012					
C	10	Sample X1	I	0.135	0.123	CaXy11	4.06862745	0.20343137	203.4313725
C	11	Sample X1	I	0.141	0.129	CaXy11	4.3627451	0.21813725	218.1372549
C	12	Sample X1	I	0.135	0.123	CaXy11	4.06862745	0.20343137	203.4313725
F	5	Blank B	E	0.027					
F	6	Sample X1	E	0.151	0.124	CaXy12	4.11764706	0.20588235	205.8823529
F	7	Sample X1	E	0.15	0.123	CaXy12	4.06862745	0.20343137	203.4313725
F	8	Sample X1	E	0.15	0.123	CaXy12	4.06862745	0.20343137	203.4313725
C	5	Blank B	H	0.019					
C	6	Sample X1	H	0.132	0.113	CaXy21	3.57843137	0.17892157	178.9215686
C	7	Sample X1	H	0.133	0.114	CaXy21	3.62745098	0.18137255	181.372549
C	8	Sample X1	H	0.13	0.111	CaXy21	3.48039216	0.17401961	174.0196078
F	9	Blank B	F	0.019					
F	10	Sample X1	F	0.128	0.109	CaGr11	4.31372549	0.21568627	215.6862745
F	11	Sample X1	F	0.13	0.111	CaGr11	4.41176471	0.22058824	220.5882353
F	12	Sample X1	F	0.127	0.108	CaGr11	4.26470588	0.21323529	213.2352941
G	1	Blank B	G	0.104					
G	2	Sample X1	G	0.306	0.202	CaGr12	7.94117647	0.39705882	397.0588235
G	3	Sample X1	G	0.308	0.204	CaGr12	8.03921569	0.40196078	401.9607843
G	4	Sample X1	G	0.307	0.203	CaGr12	7.99019608	0.3995098	399.5098039
G	5	Blank B	H	0.005					
G	6	Sample X1	H	0.109	0.104	CaGr21	3.1372549	0.15686275	156.8627451
G	7	Sample X1	H	0.11	0.105	CaGr21	3.18627451	0.15931373	159.3137255
G	8	Sample X1	H	0.108	0.103	CaGr21	3.08823529	0.15441176	154.4117647
H	1	Blank B	J	0.033					
H	2	Sample X1	J	0.147	0.114	CaGc11	3.62745098	0.18137255	181.372549
H	3	Sample X1	J	0.146	0.113	CaGc11	3.57843137	0.17892157	178.9215686
H	4	Sample X1	J	0.144	0.111	CaGc11	3.48039216	0.17401961	174.0196078
H	5	Blank B	K	0.043					
H	6	Sample X1	K	0.152	0.109	CaGc21	3.38235294	0.16911765	169.1176471
H	7	Sample X1	K	0.152	0.109	CaGc21	3.38235294	0.16911765	169.1176471
H	8	Sample X1	K	0.153	0.11	CaGc21	3.43137255	0.17156863	171.5686275
H	9	Blank B	L	0.016					
H	10	Sample X1	L	0.161	0.145	CaGl11	5.14705882	0.25735294	257.3529412
H	11	Sample X1	L	0.161	0.145	CaGl11	5.14705882	0.25735294	257.3529412
H	12	Sample X1	L	0.162	0.146	CaGl11	5.19607843	0.25980392	259.8039216
G	9	Blank B	I	0.019					
G	10	Sample X1	I	0.143	0.124	CaGl21	4.11764706	0.20588235	205.8823529
G	11	Sample X1	I	0.141	0.122	CaGl21	4.01960784	0.20098039	200.9803922
G	12	Sample X1	I	0.14	0.121	CaGl21	3.97058824	0.19852941	198.5294118

Appendix 6.23 RCCDRSM TPC run 23

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.164					
A	2	Sample X1	A	0.427	0.263	CaSu11	10.9313725	0.16397059	163.970588
A	3	Sample X1	A	0.428	0.264	CaSu11	10.9803922	0.16470588	164.705882
A	4	Sample X1	A	0.426	0.262	CaSu11	10.8823529	0.16323529	163.235294
A	5	Blank B	B	0.137					
A	6	Sample X1	B	0.962	0.825	CaFr11	38.4803922	0.57720588	577.205882
A	7	Sample X1	B	0.962	0.825	CaFr11	38.4803922	0.57720588	577.205882
A	8	Sample X1	B	0.961	0.824	CaFr11	38.4313725	0.57647059	576.470588
A	9	Blank B	C	0.29					
A	10	Sample X1	C	0.81	0.52	CaFr12	23.5294118	0.35294118	352.941176
A	11	Sample X1	C	0.806	0.516	CaFr12	23.3333333	0.35	350
A	12	Sample X1	C	0.805	0.515	CaFr12	23.2843137	0.34926471	349.264706
B	1	Blank B	D	0.17					
B	2	Sample X1	D	0.488	0.318	CaFr21	13.627451	0.20441176	204.411765
B	3	Sample X1	D	0.487	0.317	CaFr21	13.5784314	0.20367647	203.676471
B	4	Sample X1	D	0.485	0.315	CaFr21	13.4803922	0.20220588	202.205882
D	1	Blank B	J	0.106					
D	2	Sample X1	J	0.266	0.16	CaXy11	5.88235294	0.08823529	88.2352941
D	3	Sample X1	J	0.266	0.16	CaXy11	5.88235294	0.08823529	88.2352941
D	4	Sample X1	J	0.27	0.164	CaXy11	6.07843137	0.09117647	91.1764706
B	5	Blank B	E	0.144					
B	6	Sample X1	E	0.381	0.237	CaXy12	9.65686275	0.14485294	144.852941
B	7	Sample X1	E	0.377	0.233	CaXy12	9.46078431	0.14191176	141.911765
B	8	Sample X1	E	0.379	0.235	CaXy12	9.55882353	0.14338235	143.382353
C	9	Blank B	I	0.081					
C	10	Sample X1	I	0.31	0.229	CaXy21	9.26470588	0.13897059	138.970588
C	11	Sample X1	I	0.31	0.229	CaXy21	9.26470588	0.13897059	138.970588
C	12	Sample X1	I	0.309	0.228	CaXy21	9.21568627	0.13823529	138.235294
B	9	Blank B	F	0.091					
B	10	Sample X1	F	0.3	0.209	CaGr11	8.28431373	0.12426471	124.264706
B	11	Sample X1	F	0.298	0.207	CaGr11	8.18627451	0.12279412	122.794118
B	12	Sample X1	F	0.3	0.209	CaGr11	8.28431373	0.12426471	124.264706
C	1	Blank B	G	0.095					
C	2	Sample X1	G	0.394	0.299	CaGr12	12.6960784	0.19044118	190.441176
C	3	Sample X1	G	0.393	0.298	CaGr12	12.6470588	0.18970588	189.705882
C	4	Sample X1	G	0.393	0.298	CaGr12	12.6470588	0.18970588	189.705882
C	5	Blank B	H	0.112					

Appendix 6.23 contd.

C	6	Sample X1	H	0.524	0.412	CaGr21	18.2352941	0.27352941	273.529412
C	7	Sample X1	H	0.524	0.412	CaGr21	18.2352941	0.27352941	273.529412
C	8	Sample X1	H	0.523	0.411	CaGr21	18.1862745	0.27279412	272.794118
C	9	Blank B	I	0.012					
C	10	Sample X1	I	0.176	0.164	CaGc11	6.07843137	0.09117647	91.1764706
C	11	Sample X1	I	0.177	0.165	CaGc11	6.12745098	0.09191176	91.9117647
C	12	Sample X1	I	0.178	0.166	CaGc11	6.17647059	0.09264706	92.6470588
D	1	Blank B	J	0.106					
D	2	Sample X1	J	0.457	0.351	CaGc21	15.245098	0.22867647	228.676471
D	3	Sample X1	J	0.459	0.353	CaGc21	15.3431373	0.23014706	230.147059
D	4	Sample X1	J	0.458	0.352	CaGc21	15.2941176	0.22941176	229.411765
D	5	Blank B	K	0.076					
D	6	Sample X1	K	0.229	0.153	CaGl11	5.53921569	0.08308824	83.0882353
D	7	Sample X1	K	0.227	0.151	CaGl11	5.44117647	0.08161765	81.6176471
D	8	Sample X1	K	0.227	0.151	CaGl11	5.44117647	0.08161765	81.6176471
D	9	Blank B	L	0.088					
D	10	Sample X1	L	0.374	0.286	CaGl21	12.0588235	0.18088235	180.882353
D	11	Sample X1	L	0.377	0.289	CaGl21	12.2058824	0.18308824	183.088235
D	12	Sample X1	L	0.376	0.288	CaGl21	12.1568627	0.18235294	182.352941

Appendix 6.24 RCCDRSM TPC run 24

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µg/GAE/g)
G	1	Blank B	C	0.264					
G	2	Sample X1	C	0.649	0.385	CaSu11	16.91176471	0.253676471	253.676471
G	3	Sample X1	C	0.646	0.382	CaSu11	16.76470588	0.251470588	251.470588
G	4	Sample X1	C	0.648	0.384	CaSu11	16.8627451	0.252941176	252.941176
A	11	Blank B	A	0.507					
A	12	Sample X1	A	0.765	0.258	CaFr11	10.68627451	0.160294118	160.294118
B	11	Sample X1	A	0.763	0.256	CaFr11	10.58823529	0.158823529	158.823529
B	12	Sample X1	A	0.767	0.26	CaFr11	10.78431373	0.161764706	161.764706
C	11	Blank B	B	0.206					
C	12	Sample X1	B	0.588	0.382	CaFr12	16.76470588	0.251470588	251.470588
D	11	Sample X1	B	0.589	0.383	CaFr12	16.81372549	0.252205882	252.205882
D	12	Sample X1	B	0.589	0.383	CaFr12	16.81372549	0.252205882	252.205882
G	5	Blank B	D	0.1					
G	6	Sample X1	D	0.317	0.217	CaFr21	8.676470588	0.130147059	130.147059
G	7	Sample X1	D	0.317	0.217	CaFr21	8.676470588	0.130147059	130.147059

Appendix 6.24 contd.

G	8	Sample X1	D	0.314	0.214	CaFr21	8.529411765	0.127941176	127.941176
C	1	Blank B	A	0.125					
C	2	Sample X1	A	0.297	0.172	CaXy11	6.470588235	0.097058824	97.0588235
C	3	Sample X1	A	0.296	0.171	CaXy11	6.421568627	0.096323529	96.3235294
C	4	Sample X1	A	0.296	0.171	CaXy11	6.421568627	0.096323529	96.3235294
C	9	Blank B	B	0.003					
C	10	Sample X1	B	0.127	0.124	CaXy12	4.117647059	0.061764706	61.7647059
C	11	Sample X1	B	0.127	0.124	CaXy12	4.117647059	0.061764706	61.7647059
C	12	Sample X1	B	0.126	0.123	CaXy12	4.068627451	0.061029412	61.0294118
D	1	Blank B	C	0.096					
D	2	Sample X1	C	0.208	0.112	CaXy21	3.529411765	0.052941176	52.9411765
D	3	Sample X1	C	0.207	0.111	CaXy21	3.480392157	0.052205882	52.2058824
D	4	Sample X1	C	0.208	0.112	CaXy21	3.529411765	0.052941176	52.9411765
D	5	Blank B	D	0.109					
D	6	Sample X1	D	0.241	0.132	CaGr11	4.509803922	0.067647059	67.6470588
D	7	Sample X1	D	0.24	0.131	CaGr11	4.460784314	0.066911765	66.9117647
D	8	Sample X1	D	0.241	0.132	CaGr11	4.509803922	0.067647059	67.6470588
D	9	Blank B	E	0.118					
D	10	Sample X1	E	0.257	0.139	CaGr12	4.852941176	0.072794118	72.7941176
D	11	Sample X1	E	0.256	0.138	CaGr12	4.803921569	0.072058824	72.0588235
D	12	Sample X1	E	0.256	0.138	CaGr12	4.803921569	0.072058824	72.0588235
E	1	Blank B	F	0.135					
E	2	Sample X1	F	0.236	0.101	CaGr21	2.990196078	0.044852941	44.8529412
E	3	Sample X1	F	0.236	0.101	CaGr21	2.990196078	0.044852941	44.8529412
E	4	Sample X1	F	0.239	0.104	CaGr21	3.137254902	0.047058824	47.0588235
E	5	Blank B	G	0.006					
E	6	Sample X1	G	0.248	0.242	CaGc11	9.901960784	0.148529412	148.529412
E	7	Sample X1	G	0.248	0.242	CaGc11	9.901960784	0.148529412	148.529412
E	8	Sample X1	G	0.247	0.241	CaGc11	9.852941176	0.147794118	147.794118
E	9	Blank B	H	0.043					
E	10	Sample X1	H	0.186	0.143	CaGc21	5.049019608	0.075735294	75.7352941
E	11	Sample X1	H	0.186	0.143	CaGc21	5.049019608	0.075735294	75.7352941
E	12	Sample X1	H	0.185	0.142	CaGc21	5	0.075	75
F	1	Blank B	A	0.173					
F	2	Sample X1	A	0.283	0.11	CaGl11	3.431372549	0.051470588	51.4705882
F	3	Sample X1	A	0.284	0.111	CaGl11	3.480392157	0.052205882	52.2058824
F	4	Sample X1	A	0.283	0.11	CaGl11	3.431372549	0.051470588	51.4705882
F	5	Blank B	B	0.084					
F	6	Sample X1	B	0.211	0.127	CaGl21	4.264705882	0.063970588	63.9705882
F	7	Sample X1	B	0.209	0.125	CaGl21	4.166666667	0.0625	62.5
F	8	Sample X1	B	0.211	0.127	CaGl21	4.264705882	0.063970588	63.9705882

APPENDIX 6.25 RCCDRSM TPC run 25

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µg/GAE/g)
A	1	Blank B	A	0.185					
A	2	Sample X1	A	0.432	0.247	CaSu11	10.14705882	0.30441176	304.41176
A	3	Sample X1	A	0.435	0.25	CaSu11	10.29411765	0.30882353	308.82353
A	4	Sample X1	A	0.433	0.248	CaSu11	10.19607843	0.30588235	305.88235
A	5	Blank B	B	0.164					
A	6	Sample X1	B	0.805	0.641	CaFr11	29.46078431	0.88382353	883.82353
A	7	Sample X1	B	0.805	0.641	CaFr11	29.46078431	0.88382353	883.82353
A	8	Sample X1	B	0.806	0.642	CaFr11	29.50980392	0.88529412	885.29412
A	9	Blank B	C	0.297					
A	10	Sample X1	C	0.437	0.14	CaFr12	4.901960784	0.14705882	147.05882
A	11	Sample X1	C	0.438	0.141	CaFr12	4.950980392	0.14852941	148.52941
A	12	Sample X1	C	0.438	0.141	CaFr12	4.950980392	0.14852941	148.52941
B	1	Blank B	D	0.075					
B	2	Sample X1	D	0.18	0.105	CaFr21	3.18627451	0.09558824	95.588235
B	3	Sample X1	D	0.182	0.107	CaFr21	3.284313725	0.09852941	98.529412
B	4	Sample X1	D	0.183	0.108	CaFr21	3.333333333	0.1	100
D	5	Blank B	K	0.01					
D	6	Sample X1	K	0.13	0.12	CaXy11	3.921568627	0.11764706	117.64706
D	7	Sample X1	K	0.132	0.122	CaXy11	4.019607843	0.12058824	120.58824
D	8	Sample X1	K	0.135	0.125	CaXy11	4.166666667	0.125	125
B	5	Blank B	E	0.043					
B	6	Sample X1	E	0.164	0.121	CaXy12	3.970588235	0.11911765	119.11765
B	7	Sample X1	E	0.164	0.121	CaXy12	3.970588235	0.11911765	119.11765
B	8	Sample X1	E	0.164	0.121	CaXy12	3.970588235	0.11911765	119.11765
D	1	Blank B	J	0.011					
D	2	Sample X1	J	0.135	0.124	CaXy21	4.117647059	0.12352941	123.52941
D	3	Sample X1	J	0.133	0.122	CaXy21	4.019607843	0.12058824	120.58824
D	4	Sample X1	J	0.137	0.126	CaXy21	4.215686275	0.12647059	126.47059
B	9	Blank B	F	0.012					
B	10	Sample X1	F	0.142	0.13	CaGr11	4.411764706	0.13235294	132.35294
B	11	Sample X1	F	0.144	0.132	CaGr11	4.509803922	0.13529412	135.29412
B	12	Sample X1	F	0.142	0.13	CaGr11	4.411764706	0.13235294	132.35294
C	1	Blank B	G	0.017					
C	2	Sample X1	G	0.229	0.212	CaGr12	8.431372549	0.25294118	252.94118
C	3	Sample X1	G	0.231	0.214	CaGr12	8.529411765	0.25588235	255.88235
C	4	Sample X1	G	0.23	0.213	CaGr12	8.480392157	0.25441176	254.41176
C	5	Blank B	H	0.004					

Appendix 6.25 contd.

C	6	Sample X1	H	0.184	0.18	CaGr21	6.862745098	0.20588235	205.88235
C	7	Sample X1	H	0.184	0.18	CaGr21	6.862745098	0.20588235	205.88235
C	8	Sample X1	H	0.184	0.18	CaGr21	6.862745098	0.20588235	205.88235
C	9	Blank B	I	0.001					
C	10	Sample X1	I	0.167	0.166	CaGc11	6.176470588	0.18529412	185.29412
C	11	Sample X1	I	0.169	0.168	CaGc11	6.274509804	0.18823529	188.23529
C	12	Sample X1	I	0.17	0.169	CaGc11	6.323529412	0.18970588	189.70588
D	1	Blank B	J	0.007					
D	2	Sample X1	J	0.16	0.153	CaGc21	5.539215686	0.16617647	166.17647
D	3	Sample X1	J	0.161	0.154	CaGc21	5.588235294	0.16764706	167.64706
D	4	Sample X1	J	0.161	0.154	CaGc21	5.588235294	0.16764706	167.64706
D	5	Blank B	K	0.006					
D	6	Sample X1	K	0.161	0.155	CaGl11	5.637254902	0.16911765	169.11765
D	7	Sample X1	K	0.161	0.155	CaGl11	5.637254902	0.16911765	169.11765
D	8	Sample X1	K	0.162	0.156	CaGl11	5.68627451	0.17058824	170.58824
D	9	Blank B	L	0.005					
D	10	Sample X1	L	0.132	0.127	CaGl21	4.264705882	0.12794118	127.94118
D	11	Sample X1	L	0.131	0.126	CaGl21	4.215686275	0.12647059	126.47059
D	12	Sample X1	L	0.134	0.129	CaGl21	4.362745098	0.13088235	130.88235

Appendix 6.26 RCCDRSM TPC run 26

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µg/GAE/g)
E	1	Blank B	A	0.237					
E	2	Sample X1	A	0.347	0.11	CaSu11	3.43137255	0.10294118	102.9411765
E	3	Sample X1	A	0.349	0.112	CaSu11	3.52941176	0.10588235	105.8823529
E	4	Sample X1	A	0.347	0.11	CaSu11	3.43137255	0.10294118	102.9411765
E	5	Blank B	B	0.081					
E	6	Sample X1	B	0.249	0.168	CaFr11	6.2745098	0.18823529	188.2352941
E	7	Sample X1	B	0.25	0.169	CaFr11	6.32352941	0.18970588	189.7058824
E	8	Sample X1	B	0.253	0.172	CaFr11	6.47058824	0.19411765	194.1176471
E	9	Blank B	C	0.023					
E	10	Sample X1	C	0.339	0.316	CaFr12	13.5294118	0.40588235	405.8823529
E	11	Sample X1	C	0.342	0.319	CaFr12	13.6764706	0.41029412	410.2941176
E	12	Sample X1	C	0.343	0.32	CaFr12	13.7254902	0.41176471	411.7647059
F	1	Blank B	D	0.073					
F	2	Sample X1	D	0.237	0.164	CaFr21	6.07843137	0.18235294	182.3529412
F	3	Sample X1	D	0.235	0.162	CaFr21	5.98039216	0.17941176	179.4117647

Appendix 6.26 contd.

F	4	Sample X1	D	0.238	0.165	CaFr21	6.12745098	0.18382353	183.8235294
D	9	Blank B	L	0.094					
D	10	Sample X1	L	0.195	0.101	CaXy11	2.99019608	0.08970588	89.70588235
D	11	Sample X1	L	0.198	0.104	CaXy11	3.1372549	0.09411765	94.11764706
D	12	Sample X1	L	0.199	0.105	CaXy11	3.18627451	0.09558824	95.58823529
F	5	Blank B	E	0.017					
F	6	Sample X1	E	0.166	0.149	CaXy12	5.34313725	0.16029412	160.2941176
F	7	Sample X1	E	0.167	0.15	CaXy12	5.39215686	0.16176471	161.7647059
F	8	Sample X1	E	0.168	0.151	CaXy12	5.44117647	0.16323529	163.2352941
D	5	Blank B	K	0.099					
D	6	Sample X1	K	0.207	0.108	CaXy21	3.33333333	0.1	100
D	7	Sample X1	K	0.209	0.11	CaXy21	3.43137255	0.10294118	102.9411765
D	8	Sample X1	K	0.207	0.108	CaXy21	3.33333333	0.1	100
F	9	Blank B	F	0.008					
F	10	Sample X1	F	0.294	0.286	CaGr11	12.0588235	0.36176471	361.7647059
F	11	Sample X1	F	0.298	0.29	CaGr11	12.254902	0.36764706	367.6470588
F	12	Sample X1	F	0.292	0.284	CaGr11	11.9607843	0.35882353	358.8235294
G	1	Blank B	G	0.009					
G	2	Sample X1	G	0.288	0.279	CaGr12	11.7156863	0.35147059	351.4705882
G	3	Sample X1	G	0.285	0.276	CaGr12	11.5686275	0.34705882	347.0588235
G	4	Sample X1	G	0.287	0.278	CaGr12	11.6666667	0.35	350
G	5	Blank B	H	0.004					
G	6	Sample X1	H	0.16	0.156	CaGr21	5.68627451	0.17058824	170.5882353
G	7	Sample X1	H	0.162	0.158	CaGr21	5.78431373	0.17352941	173.5294118
G	8	Sample X1	H	0.159	0.155	CaGr21	5.6372549	0.16911765	169.1176471
G	9	Blank B	I	0.009					
G	10	Sample X1	I	0.249	0.24	CaGc11	9.80392157	0.29411765	294.1176471
G	11	Sample X1	I	0.251	0.242	CaGc11	9.90196078	0.29705882	297.0588235
G	12	Sample X1	I	0.248	0.239	CaGc11	9.75490196	0.29264706	292.6470588
H	1	Blank B	J	0.009					
H	2	Sample X1	J	0.206	0.197	CaGc21	7.69607843	0.23088235	230.8823529
H	3	Sample X1	J	0.204	0.195	CaGc21	7.59803922	0.22794118	227.9411765
H	4	Sample X1	J	0.204	0.195	CaGc21	7.59803922	0.22794118	227.9411765
H	5	Blank B	K	0.006					
H	6	Sample X1	K	0.286	0.28	CaGl11	11.7647059	0.35294118	352.9411765
H	7	Sample X1	K	0.287	0.281	CaGl11	11.8137255	0.35441176	354.4117647
H	8	Sample X1	K	0.285	0.279	CaGl11	11.7156863	0.35147059	351.4705882
H	9	Blank B	L	0.004					
H	10	Sample X1	L	0.213	0.209	CaGl21	8.28431373	0.24852941	248.5294118
H	11	Sample X1	L	0.21	0.206	CaGl21	8.1372549	0.24411765	244.1176471
H	12	Sample X1	L	0.212	0.208	CaGl21	8.23529412	0.24705882	247.0588235

Appendix 6.27 RCCDRSM TPC run 27

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.174					
A	2	Sample X1	A	0.315	0.141	CaSu11	4.9509804	0.14852941	148.5294118
A	3	Sample X1	A	0.317	0.143	CaSu11	5.0490196	0.15147059	151.4705882
A	4	Sample X1	A	0.318	0.144	CaSu11	5.0980392	0.15294118	152.9411765
A	5	Blank B	B	0.096					
A	6	Sample X1	B	0.198	0.102	CaFr11	3.0392157	0.09117647	91.17647059
A	7	Sample X1	B	0.2	0.104	CaFr11	3.1372549	0.09411765	94.11764706
A	8	Sample X1	B	0.201	0.105	CaFr11	3.1862745	0.09558824	95.58823529
A	9	Blank B	C	0.114					
A	10	Sample X1	C	0.223	0.109	CaFr12	3.3823529	0.10147059	101.4705882
A	11	Sample X1	C	0.222	0.108	CaFr12	3.3333333	0.1	100
A	12	Sample X1	C	0.221	0.107	CaFr12	3.2843137	0.09852941	98.52941176
B	1	Blank B	D	0.098					
B	2	Sample X1	D	0.199	0.101	CaFr21	2.9901961	0.08970588	89.70588235
B	3	Sample X1	D	0.198	0.1	CaFr21	2.9411765	0.08823529	88.23529412
B	4	Sample X1	D	0.201	0.103	CaFr21	3.0882353	0.09264706	92.64705882
E	1	Blank B	M	0.033					
E	2	Sample X1	M	0.138	0.105	CaXy11	3.1862745	0.09558824	95.58823529
E	3	Sample X1	M	0.133	0.1	CaXy11	2.9411765	0.08823529	88.23529412
E	4	Sample X1	M	0.137	0.104	CaXy11	2.6470588	0.07941176	79.41176471
B	5	Blank B	E	0.051					
B	6	Sample X1	E	0.165	0.114	CaXy12	3.627451	0.10882353	108.8235294
B	7	Sample X1	E	0.166	0.115	CaXy12	3.6764706	0.11029412	110.2941176
B	8	Sample X1	E	0.164	0.113	CaXy12	3.5784314	0.10735294	107.3529412
D	9	Blank B	L	0.012					
D	10	Sample X1	L	0.12	0.108	CaXy21	3.3333333	0.1	100
D	11	Sample X1	L	0.122	0.11	CaXy21	3.4313725	0.10294118	102.9411765
D	12	Sample X1	L	0.12	0.108	CaXy21	3.3333333	0.1	100
B	9	Blank B	F	0.022					
B	10	Sample X1	F	0.167	0.145	CaGr11	5.1470588	0.15441176	154.4117647
B	11	Sample X1	F	0.164	0.142	CaGr11	5	0.15	150
B	12	Sample X1	F	0.164	0.142	CaGr11	5	0.15	150
C	1	Blank B	G	0.013					
C	2	Sample X1	G	0.244	0.231	CaGr12	9.3627451	0.28088235	280.8823529
C	3	Sample X1	G	0.243	0.23	CaGr12	9.3137255	0.27941176	279.4117647
C	4	Sample X1	G	0.243	0.23	CaGr12	9.3137255	0.27941176	279.4117647
C	5	Blank B	H	0.016					

Appendix 6.27 contd.

C	6	Sample X1	H	0.156	0.14	CaGr21	4.9019608	0.14705882	147.0588235
C	7	Sample X1	H	0.157	0.141	CaGr21	4.9509804	0.14852941	148.5294118
C	8	Sample X1	H	0.157	0.141	CaGr21	4.9509804	0.14852941	148.5294118
C	9	Blank B	I	0.085					
C	10	Sample X1	I	0.238	0.153	CaGc11	5.5392157	0.16617647	166.1764706
C	11	Sample X1	I	0.236	0.151	CaGc11	5.4411765	0.16323529	163.2352941
C	12	Sample X1	I	0.235	0.15	CaGc11	5.3921569	0.16176471	161.7647059
D	1	Blank B	J	0.081					
D	2	Sample X1	J	0.184	0.103	CaGc21	3.0882353	0.09264706	92.64705882
D	3	Sample X1	J	0.184	0.103	CaGc21	3.0882353	0.09264706	92.64705882
D	4	Sample X1	J	0.185	0.104	CaGc21	3.1372549	0.09411765	94.11764706
D	5	Blank B	K	0.108					
D	6	Sample X1	K	0.215	0.107	CaGl11	3.2843137	0.09852941	98.52941176
D	7	Sample X1	K	0.213	0.105	CaGl11	3.1862745	0.09558824	95.58823529
D	8	Sample X1	K	0.21	0.102	CaGl11	3.0392157	0.09117647	91.17647059
D	9	Blank B	L	0.064					
D	10	Sample X1	L	0.174	0.11	CaGl21	3.4313725	0.10294118	102.9411765
D	11	Sample X1	L	0.174	0.11	CaGl21	3.4313725	0.10294118	102.9411765
D	12	Sample X1	L	0.176	0.112	CaGl21	3.5294118	0.10588235	105.8823529

Appendix 6.28 RCCDRSM TPC run 28

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	1	Blank B	A	0.192					
E	2	Sample X1	A	0.563	0.371	CaSu11	16.22549	0.4867647	486.76471
E	3	Sample X1	A	0.565	0.374	CaSu11	16.372549	0.4911765	491.17647
E	4	Sample X1	A	0.568	0.376	CaSu11	16.470588	0.4941176	494.11765
E	5	Blank B	B	0.15					
E	6	Sample X1	B	0.835	0.685	CaFr11	31.617647	0.9485294	948.52941
E	7	Sample X1	B	0.838	0.688	CaFr11	31.764706	0.9529412	952.94118
E	8	Sample X1	B	0.837	0.687	CaFr11	31.715686	0.9514706	951.47059
E	9	Blank B	C	0.192					
E	10	Sample X1	C	0.436	0.244	CaFr12	10	0.3	300
E	11	Sample X1	C	0.438	0.246	CaFr12	10.098039	0.3029412	302.94118
E	12	Sample X1	C	0.439	0.247	CaFr12	10.147059	0.3044118	304.41176
F	1	Blank B	D	0.097					
F	2	Sample X1	D	0.199	0.102	CaFr21	3.0392157	0.0911765	91.176471
F	3	Sample X1	D	0.202	0.105	CaFr21	3.1862745	0.0955882	95.588235

Appendix 6.28 contd.

F	4	Sample X1	D	0.205	0.108	CaFr21	3.3333333	0.1	100
E	5	Blank B	N	0.098					
E	6	Sample X1	N	0.208	0.11	CaXy11	3.4313725	0.1029412	102.94118
E	7	Sample X1	N	0.214	0.115	CaXy11	3.6764706	0.1102941	110.29412
E	8	Sample X1	N	0.218	0.119	CaXy11	3.872549	0.1161765	116.17647
F	5	Blank B	E	0.049					
F	6	Sample X1	E	0.19	0.141	CaXy12	4.9509804	0.1485294	148.52941
F	7	Sample X1	E	0.189	0.14	CaXy12	4.9019608	0.1470588	147.05882
F	8	Sample X1	E	0.191	0.142	CaXy12	5	0.15	150
E	1	Blank B	M	0.109					
E	2	Sample X1	M	0.216	0.107	CaXy21	3.2843137	0.0985294	98.529412
E	3	Sample X1	M	0.214	0.105	CaXy21	3.1862745	0.0955882	95.588235
E	4	Sample X1	M	0.218	0.109	CaXy21	3.3823529	0.1014706	101.47059
F	9	Blank B	F	0.023					
F	10	Sample X1	F	0.197	0.174	CaGr11	6.5686275	0.1970588	197.05882
F	11	Sample X1	F	0.199	0.176	CaGr11	6.6666667	0.2	200
F	12	Sample X1	F	0.196	0.173	CaGr11	6.5196078	0.1955882	195.58824
G	1	Blank B	G	0.026					
G	2	Sample X1	G	0.236	0.21	CaGr12	8.3333333	0.25	250
G	3	Sample X1	G	0.238	0.212	CaGr12	8.4313725	0.2529412	252.94118
G	4	Sample X1	G	0.237	0.211	CaGr12	8.3823529	0.2514706	251.47059
G	5	Blank B	H	0.018					
G	6	Sample X1	H	0.124	0.106	CaGr21	3.2352941	0.0970588	97.058824
G	7	Sample X1	H	0.123	0.105	CaGr21	3.1862745	0.0955882	95.588235
G	8	Sample X1	H	0.125	0.107	CaGr21	3.2843137	0.0985294	98.529412
G	9	Blank B	I	0.095					
G	10	Sample X1	I	0.202	0.107	CaGc11	3.2843137	0.0985294	98.529412
G	11	Sample X1	I	0.203	0.108	CaGc11	3.3333333	0.1	100
G	12	Sample X1	I	0.204	0.109	CaGc11	3.3823529	0.1014706	101.47059
H	1	Blank B	J	0.012					
H	2	Sample X1	J	0.17	0.158	CaGc21	5.7843137	0.1735294	173.52941
H	3	Sample X1	J	0.168	0.156	CaGc21	5.6862745	0.1705882	170.58824
H	4	Sample X1	J	0.167	0.155	CaGc21	5.6372549	0.1691176	169.11765
H	5	Blank B	K	0.012					
H	6	Sample X1	K	0.196	0.184	CaGl11	7.0588235	0.2117647	211.76471
H	7	Sample X1	K	0.199	0.187	CaGl11	7.2058824	0.2161765	216.17647
H	8	Sample X1	K	0.195	0.183	CaGl11	7.0098039	0.2102941	210.29412
H	9	Blank B	L	0.023					
H	10	Sample X1	L	0.153	0.13	CaGl21	4.4117647	0.1323529	132.35294
H	11	Sample X1	L	0.153	0.13	CaGl21	4.4117647	0.1323529	132.35294
H	12	Sample X1	L	0.153	0.13	CaGl21	4.4117647	0.1323529	132.35294

Appendix 6.29 RCCDRSM TPC run 29

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
E	1	Blank B	A	0.159					
E	2	Sample X1	A	0.52	0.361	CaSu11	15.7352941	0.23602941	236.02941
E	3	Sample X1	A	0.524	0.365	CaSu11	15.9313725	0.23897059	238.97059
E	4	Sample X1	A	0.522	0.363	CaSu11	15.8333333	0.2375	237.5
E	5	Blank B	B	0.105					
E	6	Sample X1	B	0.963	0.858	CaFr11	40.0980392	0.60147059	601.47059
E	7	Sample X1	B	0.964	0.859	CaFr11	40.1470588	0.60220588	602.20588
E	8	Sample X1	B	0.962	0.857	CaFr11	40.0490196	0.60073529	600.73529
E	9	Blank B	C	0.372					
E	10	Sample X1	C	0.863	0.491	CaFr12	22.1078431	0.33161765	331.61765
E	11	Sample X1	C	0.866	0.494	CaFr12	22.254902	0.33382353	333.82353
E	12	Sample X1	C	0.865	0.493	CaFr12	22.2058824	0.33308824	333.08824
F	1	Blank B	D	0.177					
F	2	Sample X1	D	0.457	0.28	CaFr21	11.7647059	0.17647059	176.47059
F	3	Sample X1	D	0.461	0.284	CaFr21	11.9607843	0.17941176	179.41176
F	4	Sample X1	D	0.46	0.283	CaFr21	11.9117647	0.17867647	178.67647
E	9	Blank B	O	0.1					
E	10	Sample X1	O	0.203	0.103	CaXy11	3.08823529	0.04632353	46.323529
E	11	Sample X1	O	0.205	0.105	CaXy11	3.18627451	0.04779412	47.794118
E	12	Sample X1	O	0.208	0.108	CaXy11	3.33333333	0.05	50
F	5	Blank B	E	0.158					
F	6	Sample X1	E	0.364	0.206	CaXy12	8.1372549	0.12205882	122.05882
F	7	Sample X1	E	0.366	0.208	CaXy12	8.23529412	0.12352941	123.52941
F	8	Sample X1	E	0.362	0.204	CaXy12	8.03921569	0.12058824	120.58824
E	5	Blank B	N	0.098					
E	6	Sample X1	N	0.254	0.156	CaXy21	5.68627451	0.08529412	85.294118
E	7	Sample X1	N	0.257	0.159	CaXy21	5.83333333	0.0875	87.5
E	8	Sample X1	N	0.259	0.161	CaXy21	5.93137255	0.08897059	88.970588
F	9	Blank B	F	0.117					
F	10	Sample X1	F	0.411	0.294	CaGr11	12.4509804	0.18676471	186.76471
F	11	Sample X1	F	0.408	0.291	CaGr11	12.3039216	0.18455882	184.55882
F	12	Sample X1	F	0.41	0.293	CaGr11	12.4019608	0.18602941	186.02941
G	1	Blank B	G	0.092					
G	2	Sample X1	G	0.338	0.246	CaGr12	10.0980392	0.15147059	151.47059
G	3	Sample X1	G	0.341	0.249	CaGr12	10.245098	0.15367647	153.67647
G	4	Sample X1	G	0.339	0.247	CaGr12	10.1470588	0.15220588	152.20588
G	5	Blank B	H	0.129					

Appendix 6.29 contd.

G	6	Sample X1	H	0.271	0.142	CaGr21	5	0.075	75
G	7	Sample X1	H	0.271	0.142	CaGr21	5	0.075	75
G	8	Sample X1	H	0.269	0.14	CaGr21	4.90196078	0.07352941	73.529412
G	9	Blank B	I	0.078					
G	10	Sample X1	I	0.457	0.379	CaGc11	16.6176471	0.24926471	249.26471
G	11	Sample X1	I	0.456	0.378	CaGc11	16.5686275	0.24852941	248.52941
G	12	Sample X1	I	0.455	0.377	CaGc11	16.5196078	0.24779412	247.79412
H	1	Blank B	J	0.103					
H	2	Sample X1	J	0.321	0.218	CaGc21	8.7254902	0.13088235	130.88235
H	3	Sample X1	J	0.321	0.218	CaGc21	8.7254902	0.13088235	130.88235
H	4	Sample X1	J	0.319	0.216	CaGc21	8.62745098	0.12941176	129.41176
H	5	Blank B	K	0.11					
H	6	Sample X1	K	0.323	0.213	CaGl11	8.48039216	0.12720588	127.20588
H	7	Sample X1	K	0.324	0.214	CaGl11	8.52941176	0.12794118	127.94118
H	8	Sample X1	K	0.325	0.215	CaGl11	8.57843137	0.12867647	128.67647
H	9	Blank B	L	0.115					
H	10	Sample X1	L	0.309	0.194	CaGl21	7.54901961	0.11323529	113.23529
H	11	Sample X1	L	0.306	0.191	CaGl21	7.40196078	0.11102941	111.02941
H	12	Sample X1	L	0.308	0.193	CaGl21	7.5	0.1125	112.5

Table 1Appendix 6.30 RCCDRSM TPC run 30

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Code	TPC (mgGAE/l)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.212					
A	2	Sample X1	A	0.443	0.231	CaSu11	9.3627451	0.09362745	93.627451
A	3	Sample X1	A	0.448	0.236	CaSu11	9.60784314	0.09607843	96.0784314
A	4	Sample X1	A	0.451	0.239	CaSu11	9.75490196	0.09754902	97.5490196
A	5	Blank B	B	0.288					
A	6	Sample X1	B	0.958	0.67	CaFr11	30.8823529	0.30882353	308.823529
A	7	Sample X1	B	0.957	0.669	CaFr11	30.8333333	0.30833333	308.333333
A	8	Sample X1	B	0.959	0.671	CaFr11	30.9313725	0.30931373	309.313725
A	9	Blank B	C	0.307					
A	10	Sample X1	C	0.65	0.343	CaFr12	14.8529412	0.14852941	148.529412
A	11	Sample X1	C	0.648	0.341	CaFr12	14.754902	0.14754902	147.54902
A	12	Sample X1	C	0.644	0.337	CaFr12	14.5588235	0.14558824	145.588235
B	1	Blank B	D	0.158					
B	2	Sample X1	D	0.336	0.178	CaFr21	6.76470588	0.06764706	67.6470588
B	3	Sample X1	D	0.334	0.176	CaFr21	6.66666667	0.06666667	66.6666667

Appendix 6.30 contd.

B	4	Sample X1	D	0.328	0.17	CaFr21	6.37254902	0.06372549	63.7254902
F	1	Blank B	P	0.026					
F	2	Sample X1	P	0.14	0.114	CaXy11	3.62745098	0.03627451	36.2745098
F	3	Sample X1	P	0.142	0.116	CaXy11	3.7254902	0.0372549	37.254902
F	4	Sample X1	P	0.141	0.115	CaXy11	3.67647059	0.03676471	36.7647059
B	5	Blank B	E	0.149					
B	6	Sample X1	E	0.327	0.178	CaXy12	6.76470588	0.06764706	67.6470588
B	7	Sample X1	E	0.324	0.175	CaXy12	6.61764706	0.06617647	66.1764706
B	8	Sample X1	E	0.325	0.176	CaXy12	6.66666667	0.06666667	66.6666667
E	9	Blank B	O	0.117					
E	10	Sample X1	O	0.354	0.237	CaXy21	9.65686275	0.09656863	96.5686275
E	11	Sample X1	O	0.356	0.239	CaXy21	9.75490196	0.09754902	97.5490196
E	12	Sample X1	O	0.359	0.243	CaXy21	9.95098039	0.0995098	99.5098039
B	9	Blank B	F	0.119					
B	10	Sample X1	F	0.34	0.221	CaGr11	8.87254902	0.08872549	88.7254902
B	11	Sample X1	F	0.347	0.228	CaGr11	9.21568627	0.09215686	92.1568627
B	12	Sample X1	F	0.343	0.224	CaGr11	9.01960784	0.09019608	90.1960784
C	1	Blank B	G	0.127					
C	2	Sample X1	G	0.489	0.362	CaGr12	15.7843137	0.15784314	157.843137
C	3	Sample X1	G	0.494	0.367	CaGr12	16.0294118	0.16029412	160.294118
C	4	Sample X1	G	0.496	0.369	CaGr12	16.127451	0.16127451	161.27451
C	5	Blank B	H	0.109					
C	6	Sample X1	H	0.229	0.12	CaGr21	3.92156863	0.03921569	39.2156863
C	7	Sample X1	H	0.23	0.121	CaGr21	3.97058824	0.03970588	39.7058824
C	8	Sample X1	H	0.23	0.121	CaGr21	3.97058824	0.03970588	39.7058824
C	9	Blank B	I	0.109					
C	10	Sample X1	I	0.334	0.225	CaGc11	9.06862745	0.09068627	90.6862745
C	11	Sample X1	I	0.339	0.23	CaGc11	9.31372549	0.09313725	93.1372549
C	12	Sample X1	I	0.344	0.235	CaGc11	9.55882353	0.09558824	95.5882353
D	1	Blank B	J	0.106					
D	2	Sample X1	J	0.304	0.198	CaGc21	7.74509804	0.07745098	77.4509804
D	3	Sample X1	J	0.304	0.198	CaGc21	7.74509804	0.07745098	77.4509804
D	4	Sample X1	J	0.306	0.2	CaGc21	7.84313725	0.07843137	78.4313725
D	5	Blank B	K	0.13					
D	6	Sample X1	K	0.297	0.167	CaGl11	6.2254902	0.0622549	62.254902
D	7	Sample X1	K	0.297	0.167	CaGl11	6.2254902	0.0622549	62.254902
D	8	Sample X1	K	0.299	0.169	CaGl11	6.32352941	0.06323529	63.2352941
D	9	Blank B	L	0.117					
D	10	Sample X1	L	0.297	0.18	CaGl21	6.8627451	0.06862745	68.627451
D	11	Sample X1	L	0.3	0.183	CaGl21	7.00980392	0.07009804	70.0980392
D	12	Sample X1	L	0.299	0.182	CaGl21	6.96078431	0.06960784	69.6078431

Appendix 7.1 RCCDRSM TFC run 1.

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TPC (µgQE/g)
A	1	Blank B	A	0.034				
A	2	Sample X1	A	0.122	0.088	CaSu11	6.2890625	62.89063
A	3	Sample X1	A	0.114	0.08	CaSu11	5.6640625	56.64063
A	4	Sample X1	A	0.114	0.08	CaSu11	5.6640625	56.64063
A	5	Blank B	B	0.065				
A	6	Sample X1	B	0.444	0.379	CaFr11	29.0234375	290.2344
A	7	Sample X1	B	0.445	0.38	CaFr11	29.1015625	291.0156
A	8	Sample X1	B	0.446	0.381	CaFr11	29.1796875	291.7969
A	9	Blank B	C	0.059				
A	10	Sample X1	C	0.145	0.086	CaFr12	6.1328125	61.32813
A	11	Sample X1	C	0.144	0.085	CaFr12	6.0546875	60.54688
A	12	Sample X1	C	0.147	0.087	CaFr12	6.2109375	62.10938
B	1	Blank B	D	0.019				
B	2	Sample X1	D	0.103	0.084	CaFr21	5.9765625	59.76563
B	3	Sample X1	D	0.105	0.086	CaFr21	6.1328125	61.32813
B	4	Sample X1	D	0.106	0.087	CaFr21	6.2109375	62.10938
A	1	Blank B	A	0.062				
A	2	Sample X1	A	0.148	0.086	CaXy11	6.1328125	61.32813
A	3	Sample X1	A	0.149	0.087	CaXy11	6.2109375	62.10938
A	4	Sample X1	A	0.149	0.087	CaXy11	6.2109375	62.10938
B	5	Blank B	E	0.02				
B	6	Sample X1	E	0.107	0.087	CaXy12	6.2109375	62.10938
B	7	Sample X1	E	0.101	0.085	CaXy12	6.0546875	60.54688
B	8	Sample X1	E	0.111	0.087	CaXy12	6.2109375	62.10938
A	1	Blank B	A	0.074				
A	2	Sample X1	A	0.171	0.097	CaXy21	6.9921875	69.92188
A	3	Sample X1	A	0.171	0.097	CaXy21	6.9921875	69.92188
A	4	Sample X1	A	0.169	0.095	CaXy21	6.8359375	68.35938
B	9	Blank B	F	0.052				
B	10	Sample X1	F	0.138	0.086	CaGr11	6.1328125	61.32813
B	11	Sample X1	F	0.134	0.082	CaGr11	5.8203125	58.20313
B	12	Sample X1	F	0.132	0.08	CaGr11	5.6640625	56.64063
C	1	Blank B	G	0.075				
C	2	Sample X1	G	0.159	0.084	CaGr12	5.9765625	59.76563
C	3	Sample X1	G	0.159	0.084	CaGr12	5.9765625	59.76563
C	4	Sample X1	G	0.161	0.086	CaGr12	6.1328125	61.32813
C	5	Blank B	H	0.151				

Appendix 7.1 contd.

C	6	Sample X1	H	0.233	0.082	CaGr21	5.8203125	58.20313
C	7	Sample X1	H	0.231	0.08	CaGr21	5.6640625	56.64063
C	8	Sample X1	H	0.234	0.083	CaGr21	5.8984375	58.98438
C	9	Blank B	I	0.08				
C	10	Sample X1	I	0.253	0.173	CaGc11	12.9296875	129.2969
C	11	Sample X1	I	0.25	0.17	CaGc11	12.6953125	126.9531
C	12	Sample X1	I	0.255	0.175	CaGc11	13.0859375	130.8594
D	1	Blank B	J	0.241				
D	2	Sample X1	J	0.337	0.096	CaGc21	6.9140625	69.14063
D	3	Sample X1	J	0.333	0.092	CaGc21	6.6015625	66.01563
D	4	Sample X1	J	0.332	0.091	CaGc21	6.5234375	65.23438
D	5	Blank B	K	0.076				
D	6	Sample X1	K	0.158	0.082	CaGl11	5.8203125	58.20313
D	7	Sample X1	K	0.159	0.083	CaGl11	5.8984375	58.98438
D	8	Sample X1	K	0.157	0.081	CaGl11	5.7421875	57.42188
D	9	Blank B	L	0.057				
D	10	Sample X1	L	0.138	0.081	CaGl21	5.7421875	57.42188
D	11	Sample X1	L	0.142	0.085	CaGl21	6.0546875	60.54688
D	12	Sample X1	L	0.141	0.084	CaGl21	5.9765625	59.76563

Appendix 7.2 RCCDRSM TFC run 2.

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TPC (µgQE/g)
E	1	Blank B	A	0.068				
E	2	Sample X1	A	0.418	0.35	CaSu11	26.7578125	535.1563
E	3	Sample X1	A	0.42	0.352	CaSu11	26.9140625	538.2813
E	4	Sample X1	A	0.419	0.351	CaSu11	26.8359375	536.7188
E	5	Blank B	B	0.079				
E	6	Sample X1	B	0.449	0.37	CaFr11	28.3203125	566.4063
E	7	Sample X1	B	0.445	0.366	CaFr11	28.0078125	560.1563
E	8	Sample X1	B	0.448	0.369	CaFr11	28.2421875	564.8438
E	9	Blank B	C	0.054				
E	10	Sample X1	C	0.135	0.081	CaFr12	5.7421875	114.8438
E	11	Sample X1	C	0.137	0.083	CaFr12	5.8984375	117.9688
E	12	Sample X1	C	0.136	0.082	CaFr12	5.8203125	116.4063
F	1	Blank B	D	0.157				
F	2	Sample X1	D	0.316	0.159	CaFr21	11.8359375	236.7188
F	3	Sample X1	D	0.311	0.154	CaFr21	11.4453125	228.9063

Appendix 7.2 contd.

F	4	Sample X1	D	0.314	0.157	CaFr21	11.6796875	233.5938
A	5	Blank B	B	0.063				
A	6	Sample X1	B	0.144	0.081	CaXy11	5.7421875	114.8438
A	7	Sample X1	B	0.145	0.082	CaXy11	5.8203125	116.4063
A	8	Sample X1	B	0.145	0.082	CaXy11	5.8203125	116.4063
F	5	Blank B	E	0.15				
F	6	Sample X1	E	0.23	0.08	CaXy12	5.6640625	113.2813
F	7	Sample X1	E	0.232	0.082	CaXy12	5.8203125	116.4063
F	8	Sample X1	E	0.233	0.083	CaXy12	5.8984375	117.9688
A	5	Blank B	B	0.052				
A	6	Sample X1	B	0.138	0.086	CaXy21	6.1328125	122.6563
A	7	Sample X1	B	0.136	0.084	CaXy21	5.9765625	119.5313
A	8	Sample X1	B	0.136	0.084	CaXy21	5.9765625	119.5313
F	9	Blank B	F	0.238				
F	10	Sample X1	F	0.385	0.147	CaGr11	10.8984375	217.9688
F	11	Sample X1	F	0.388	0.15	CaGr11	11.1328125	222.6563
F	12	Sample X1	F	0.394	0.156	CaGr11	11.6015625	232.0313
G	1	Blank B	G	0.09				
G	2	Sample X1	G	0.173	0.083	CaGr12	5.8984375	117.9688
G	3	Sample X1	G	0.177	0.087	CaGr12	6.2109375	124.2188
G	4	Sample X1	G	0.176	0.086	CaGr12	6.1328125	122.6563
G	5	Blank B	H	0.106				
G	6	Sample X1	H	0.193	0.087	CaGr21	6.2109375	124.2188
G	7	Sample X1	H	0.195	0.089	CaGr21	6.3671875	127.3438
G	8	Sample X1	H	0.194	0.088	CaGr21	6.2890625	125.7813
G	9	Blank B	I	0.059				
G	10	Sample X1	I	0.185	0.126	CaGc11	9.2578125	185.1563
G	11	Sample X1	I	0.187	0.128	CaGc11	9.4140625	188.2813
G	12	Sample X1	I	0.188	0.129	CaGc11	9.4921875	189.8438
H	1	Blank B	J	0.103				
H	2	Sample X1	J	0.604	0.501	CaGc21	38.5546875	771.0938
H	3	Sample X1	J	0.594	0.491	CaGc21	37.7734375	755.4688
H	4	Sample X1	J	0.602	0.499	CaGc21	38.3984375	767.9688
H	5	Blank B	K	0.1				
H	6	Sample X1	K	0.187	0.087	CaGl11	6.2109375	124.2188
H	7	Sample X1	K	0.185	0.085	CaGl11	6.0546875	121.0938
H	8	Sample X1	K	0.184	0.084	CaGl11	5.9765625	119.5313
H	9	Blank B	L	0.103				
H	10	Sample X1	L	0.186	0.083	CaGl21	5.8984375	117.9688
H	11	Sample X1	L	0.184	0.081	CaGl21	5.7421875	114.8438
H	12	Sample X1	L	0.183	0.08	CaGl21	5.6640625	113.2813

Appendix 7.3 RCCDRSM TFC run 3

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.058				
E	10	Sample X1	A	0.258	0.2	CaSu11	15.039063	225.5859
E	11	Sample X1	A	0.259	0.201	CaSu11	15.117188	226.7578
E	12	Sample X1	A	0.258	0.2	CaSu11	15.039063	225.5859
C	1	Blank B	A	0.079				
C	2	Sample X1	A	0.401	0.322	CaFr11	24.570313	368.5547
C	3	Sample X1	A	0.402	0.323	CaFr11	24.648438	369.7266
C	4	Sample X1	A	0.401	0.322	CaFr11	24.570313	368.5547
C	5	Blank B	B	0.055				
C	6	Sample X1	B	0.351	0.296	CaFr12	22.539063	338.0859
C	7	Sample X1	B	0.352	0.297	CaFr12	22.617188	339.2578
C	8	Sample X1	B	0.353	0.298	CaFr12	22.695313	340.4297
C	9	Blank B	C	0.051				
C	10	Sample X1	C	0.348	0.297	CaFr21	22.617188	339.2578
C	11	Sample X1	C	0.347	0.296	CaFr21	22.539063	338.0859
C	12	Sample X1	C	0.348	0.297	CaFr21	22.617188	339.2578
D	1	Blank B	D	0.053				
D	2	Sample X1	D	0.137	0.084	CaXy11	5.9765625	89.64844
D	3	Sample X1	D	0.134	0.081	CaXy11	5.7421875	86.13281
D	4	Sample X1	D	0.137	0.084	CaXy11	5.9765625	89.64844
D	5	Blank B	E	0.05				
D	6	Sample X1	E	0.132	0.082	CaXy12	5.8203125	87.30469
D	7	Sample X1	E	0.134	0.084	CaXy12	5.9765625	89.64844
D	8	Sample X1	E	0.135	0.085	CaXy12	6.0546875	90.82031
D	9	Blank B	F	0.044				
D	10	Sample X1	F	0.129	0.085	CaXy21	6.0546875	90.82031
D	11	Sample X1	F	0.13	0.086	CaXy21	6.1328125	91.99219
D	12	Sample X1	F	0.128	0.084	CaXy21	5.9765625	89.64844
F	1	Blank B	B	0.054				
F	2	Sample X1	B	0.138	0.084	CaGr11	5.9765625	89.64844
F	3	Sample X1	B	0.14	0.086	CaGr11	6.1328125	91.99219
F	4	Sample X1	B	0.138	0.084	CaGr11	5.9765625	89.64844
F	5	Blank B	C	0.05				
F	6	Sample X1	C	0.135	0.085	CaGr12	6.0546875	90.82031
F	7	Sample X1	C	0.136	0.086	CaGr12	6.1328125	91.99219
F	8	Sample X1	C	0.135	0.085	CaGr12	6.0546875	90.82031
F	9	Blank B	D	0.045				

Appendix 7.3 contd.

F	10	Sample X1	D	0.129	0.084	CaGr21	5.9765625	89.64844
F	11	Sample X1	D	0.13	0.085	CaGr21	6.0546875	90.82031
F	12	Sample X1	D	0.132	0.087	CaGr21	6.2109375	93.16406
G	1	Blank B	E	0.054				
G	2	Sample X1	E	0.686	0.632	CaGc11	48.789063	731.8359
G	3	Sample X1	E	0.686	0.632	CaGc11	48.789063	731.8359
G	4	Sample X1	E	0.687	0.633	CaGc11	48.867188	733.0078
G	5	Blank B	F	0.046				
G	6	Sample X1	F	0.532	0.486	CaGc21	37.382813	560.7422
G	7	Sample X1	F	0.532	0.486	CaGc21	37.382813	560.7422
G	8	Sample X1	F	0.533	0.487	CaGc21	37.460938	561.9141
E	1	Blank B	G	0.532				
E	2	Sample X1	G	0.614	0.082	CaGl11	5.8203125	87.30469
E	3	Sample X1	G	0.615	0.083	CaGl11	5.8984375	88.47656
E	4	Sample X1	G	0.615	0.083	CaGl11	5.8984375	88.47656
E	5	Blank B	H	0.047				
E	6	Sample X1	H	0.132	0.085	CaGl21	6.0546875	90.82031
E	7	Sample X1	H	0.131	0.084	CaGl21	5.9765625	89.64844
E	8	Sample X1	H	0.136	0.089	CaGl21	6.3671875	95.50781

Appendix 7.4 RCCDRSM TFC run 4

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.065				
A	2	Sample X1	A	0.26	0.195	CaSu11	14.64844	219.7266
A	3	Sample X1	A	0.261	0.196	CaSu11	14.72656	220.8984
A	4	Sample X1	A	0.263	0.198	CaSu11	14.88281	223.2422
E	9	Blank B	A	0.09				
E	10	Sample X1	A	0.412	0.322	CaFr11	24.57031	368.5547
E	11	Sample X1	A	0.412	0.322	CaFr11	24.57031	368.5547
E	12	Sample X1	A	0.413	0.323	CaFr11	24.64844	369.7266
F	1	Blank B	B	0.059				
F	2	Sample X1	B	0.354	0.295	CaFr12	22.46094	336.9141
F	3	Sample X1	B	0.352	0.293	CaFr12	22.30469	334.5703
F	4	Sample X1	B	0.356	0.297	CaFr12	22.61719	339.2578
F	5	Blank B	C	0.074				
F	6	Sample X1	C	0.359	0.285	CaFr21	21.67969	325.1953
F	7	Sample X1	C	0.351	0.277	CaFr21	21.05469	315.8203

Appendix 7.4 contd.

F	8	Sample X1	C	0.355	0.281	CaFr21	21.36719	320.5078
F	9	Blank B	D	0.045				
F	10	Sample X1	D	0.13	0.085	CaXy11	6.054688	90.82031
F	11	Sample X1	D	0.13	0.085	CaXy11	6.054688	90.82031
F	12	Sample X1	D	0.129	0.084	CaXy11	5.976563	89.64844
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.138	0.083	CaXy12	5.898438	88.47656
G	3	Sample X1	E	0.141	0.086	CaXy12	6.132813	91.99219
G	4	Sample X1	E	0.139	0.084	CaXy12	5.976563	89.64844
G	5	Blank B	F	0.057				
G	6	Sample X1	F	0.148	0.091	CaXy21	6.523438	97.85156
G	7	Sample X1	F	0.147	0.09	CaXy21	6.445313	96.67969
G	8	Sample X1	F	0.148	0.091	CaXy21	6.523438	97.85156
A	5	Blank B	B	0.056				
A	6	Sample X1	B	0.143	0.087	CaGr11	6.210938	93.16406
A	7	Sample X1	B	0.142	0.086	CaGr11	6.132813	91.99219
A	8	Sample X1	B	0.141	0.085	CaGr11	6.054688	90.82031
A	9	Blank B	C	0.05				
A	10	Sample X1	C	0.135	0.085	CaGr12	6.054688	90.82031
A	11	Sample X1	C	0.132	0.082	CaGr12	5.820313	87.30469
A	12	Sample X1	C	0.131	0.081	CaGr12	5.742188	86.13281
B	1	Blank B	D	0.063				
B	2	Sample X1	D	0.146	0.083	CaGr21	5.898438	88.47656
B	3	Sample X1	D	0.149	0.086	CaGr21	6.132813	91.99219
B	4	Sample X1	D	0.147	0.084	CaGr21	5.976563	89.64844
B	5	Blank B	E	0.054				
B	6	Sample X1	E	0.689	0.635	CaGc11	49.02344	735.3516
B	7	Sample X1	E	0.692	0.638	CaGc11	49.25781	738.8672
B	8	Sample X1	E	0.689	0.635	CaGc11	49.02344	735.3516
B	9	Blank B	F	0.05				
B	10	Sample X1	F	0.537	0.487	CaGc21	37.46094	561.9141
B	11	Sample X1	F	0.539	0.489	CaGc21	37.61719	564.2578
B	12	Sample X1	F	0.534	0.484	CaGc21	37.22656	558.3984
G	9	Blank B	G	0.059				
G	10	Sample X1	G	0.143	0.084	CaGl11	5.976563	89.64844
G	11	Sample X1	G	0.145	0.086	CaGl11	6.132813	91.99219
G	12	Sample X1	G	0.147	0.088	CaGl11	6.289063	94.33594
H	1	Blank B	H	0.061				
H	2	Sample X1	H	0.145	0.084	CaGl21	5.976563	89.64844
H	3	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031
H	4	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031

Appendix 7.5 RCCDRSM TFC run 5

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.058				
E	10	Sample X1	A	0.141	0.083	CaSu11	5.8984375	58.984375
E	11	Sample X1	A	0.145	0.087	CaSu11	6.2109375	62.109375
E	12	Sample X1	A	0.14	0.082	CaSu11	5.8203125	58.203125
C	1	Blank B	A	0.074				
C	2	Sample X1	A	0.25	0.176	CaFr11	13.1640625	131.640625
C	3	Sample X1	A	0.25	0.176	CaFr11	13.1640625	131.640625
C	4	Sample X1	A	0.248	0.174	CaFr11	13.0078125	130.078125
C	5	Blank B	B	0.058				
C	6	Sample X1	B	0.144	0.086	CaFr12	6.1328125	61.328125
C	7	Sample X1	B	0.141	0.083	CaFr12	5.8984375	58.984375
C	8	Sample X1	B	0.142	0.084	CaFr12	5.9765625	59.765625
C	9	Blank B	C	0.052				
C	10	Sample X1	C	0.139	0.087	CaFr21	6.2109375	62.109375
C	11	Sample X1	C	0.136	0.084	CaFr21	5.9765625	59.765625
C	12	Sample X1	C	0.137	0.085	CaFr21	6.0546875	60.546875
D	1	Blank B	D	0.058				
D	2	Sample X1	D	0.144	0.086	CaXy11	6.1328125	61.328125
D	3	Sample X1	D	0.139	0.081	CaXy11	5.7421875	57.421875
D	4	Sample X1	D	0.141	0.083	CaXy11	5.8984375	58.984375
D	5	Blank B	E	0.055				
D	6	Sample X1	E	0.135	0.08	CaXy12	5.6640625	56.640625
D	7	Sample X1	E	0.141	0.086	CaXy12	6.1328125	61.328125
D	8	Sample X1	E	0.136	0.081	CaXy12	5.7421875	57.421875
D	9	Blank B	F	0.05				
D	10	Sample X1	F	0.13	0.08	CaXy21	5.6640625	56.640625
D	11	Sample X1	F	0.13	0.08	CaXy21	5.6640625	56.640625
D	12	Sample X1	F	0.132	0.082	CaXy21	5.8203125	58.203125
F	1	Blank B	B	0.057				
F	2	Sample X1	B	0.137	0.08	CaGr11	5.6640625	56.640625
F	3	Sample X1	B	0.143	0.086	CaGr11	6.1328125	61.328125
F	4	Sample X1	B	0.137	0.08	CaGr11	5.6640625	56.640625
F	5	Blank B	C	0.049				
F	6	Sample X1	C	0.138	0.089	CaGr12	6.3671875	63.671875
F	7	Sample X1	C	0.137	0.088	CaGr12	6.2890625	62.890625
F	8	Sample X1	C	0.131	0.082	CaGr12	5.8203125	58.203125
F	9	Blank B	D	0.042				

Appendix 7.5 contd.

F	10	Sample X1	D	0.125	0.083	CaGr21	5.8984375	58.984375
F	11	Sample X1	D	0.131	0.089	CaGr21	6.3671875	63.671875
F	12	Sample X1	D	0.126	0.084	CaGr21	5.9765625	59.765625
G	1	Blank B	E	0.067				
G	2	Sample X1	E	0.483	0.416	CaGc11	31.9140625	319.140625
G	3	Sample X1	E	0.487	0.42	CaGc11	32.2265625	322.265625
G	4	Sample X1	E	0.486	0.419	CaGc11	32.1484375	321.484375
G	5	Blank B	F	0.048				
G	6	Sample X1	F	0.255	0.207	CaGc21	15.5859375	155.859375
G	7	Sample X1	F	0.254	0.206	CaGc21	15.5078125	155.078125
G	8	Sample X1	F	0.259	0.211	CaGc21	15.8984375	158.984375
E	1	Blank B	G	0.063				
E	2	Sample X1	G	0.15	0.087	CaGl11	6.2109375	62.109375
E	3	Sample X1	G	0.143	0.08	CaGl11	5.6640625	56.640625
E	4	Sample X1	G	0.145	0.082	CaGl11	5.8203125	58.203125
E	5	Blank B	H	0.054				
E	6	Sample X1	H	0.136	0.082	CaGl21	5.8203125	58.203125
E	7	Sample X1	H	0.136	0.082	CaGl21	5.8203125	58.203125
E	8	Sample X1	H	0.138	0.084	CaGl21	5.9765625	59.765625

Appendix 7.6 RCCDRSM TFC run 6

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.061				
E	10	Sample X1	A	0.162	0.101	CaSu11	7.3046875	73.04688
E	11	Sample X1	A	0.161	0.1	CaSu11	7.2265625	72.26563
E	12	Sample X1	A	0.161	0.1	CaSu11	7.2265625	72.26563
C	1	Blank B	A	0.078				
C	2	Sample X1	A	0.319	0.241	CaFr11	18.242188	182.4219
C	3	Sample X1	A	0.318	0.24	CaFr11	18.164063	181.6406
C	4	Sample X1	A	0.318	0.24	CaFr11	18.164063	181.6406
C	5	Blank B	B	0.06				
C	6	Sample X1	B	0.164	0.104	CaFr12	7.5390625	75.39063
C	7	Sample X1	B	0.162	0.102	CaFr12	7.3828125	73.82813
C	8	Sample X1	B	0.167	0.107	CaFr12	7.7734375	77.73438
C	9	Blank B	C	0.054				
C	10	Sample X1	C	0.233	0.179	CaFr21	13.398438	133.9844
C	11	Sample X1	C	0.233	0.179	CaFr21	13.398438	133.9844

Appendix 7.6 contd.

C	12	Sample X1	C	0.231	0.177	CaFr21	13.242188	132.4219
D	1	Blank B	D	0.061				
D	2	Sample X1	D	0.177	0.116	CaXy11	8.4765625	84.76563
D	3	Sample X1	D	0.178	0.117	CaXy11	8.5546875	85.54688
D	4	Sample X1	D	0.178	0.117	CaXy11	8.5546875	85.54688
D	5	Blank B	E	0.057				
D	6	Sample X1	E	0.145	0.088	CaXy12	6.2890625	62.89063
D	7	Sample X1	E	0.144	0.087	CaXy12	6.2109375	62.10938
D	8	Sample X1	E	0.144	0.087	CaXy12	6.2109375	62.10938
D	9	Blank B	F	0.05				
D	10	Sample X1	F	0.152	0.102	CaXy21	7.3828125	73.82813
D	11	Sample X1	F	0.15	0.1	CaXy21	7.2265625	72.26563
D	12	Sample X1	F	0.15	0.1	CaXy21	7.2265625	72.26563
F	1	Blank B	B	0.056				
F	2	Sample X1	B	0.214	0.158	CaGr11	11.757813	117.5781
F	3	Sample X1	B	0.213	0.157	CaGr11	11.679688	116.7969
F	4	Sample X1	B	0.214	0.158	CaGr11	11.757813	117.5781
F	5	Blank B	C	0.046				
F	6	Sample X1	C	0.217	0.171	CaGr12	12.773438	127.7344
F	7	Sample X1	C	0.219	0.173	CaGr12	12.929688	129.2969
F	8	Sample X1	C	0.217	0.171	CaGr12	12.773438	127.7344
F	9	Blank B	D	0.041				
F	10	Sample X1	D	0.167	0.126	CaGr21	9.2578125	92.57813
F	11	Sample X1	D	0.166	0.125	CaGr21	9.1796875	91.79688
F	12	Sample X1	D	0.166	0.125	CaGr21	9.1796875	91.79688
G	1	Blank B	E	0.056				
G	2	Sample X1	E	0.849	0.793	CaGc11	61.367188	613.6719
G	3	Sample X1	E	0.848	0.792	CaGc11	61.289063	612.8906
G	4	Sample X1	E	0.848	0.792	CaGc11	61.289063	612.8906
G	5	Blank B	F	0.045				
G	6	Sample X1	F	0.683	0.638	CaGc21	49.257813	492.5781
G	7	Sample X1	F	0.681	0.636	CaGc21	49.101563	491.0156
G	8	Sample X1	F	0.683	0.638	CaGc21	49.257813	492.5781
E	1	Blank B	G	0.058				
E	2	Sample X1	G	0.452	0.394	CaGl11	30.195313	301.9531
E	3	Sample X1	G	0.458	0.4	CaGl11	30.664063	306.6406
E	4	Sample X1	G	0.458	0.4	CaGl11	30.664063	306.6406
E	5	Blank B	H	0.05				
E	6	Sample X1	H	0.875	0.825	CaGl21	63.867188	638.6719
E	7	Sample X1	H	0.874	0.824	CaGl21	63.789063	637.8906
E	8	Sample X1	H	0.873	0.823	CaGl21	63.710938	637.1094

Appendix 7.7 RCCDRSM TFC run 7

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.33				
A	2	Sample X1	A	0.579	0.249	CaSu11	18.867188	377.34375
A	3	Sample X1	A	0.579	0.249	CaSu11	18.867188	377.34375
A	4	Sample X1	A	0.581	0.251	CaSu11	19.023438	380.46875
A	5	Blank B	B	0.742				
A	6	Sample X1	B	0.975	0.233	CaFr11	17.617188	352.34375
A	7	Sample X1	B	0.976	0.234	CaFr11	17.695313	353.90625
A	8	Sample X1	B	0.973	0.231	CaFr11	17.460938	349.21875
A	9	Blank B	C	0.116				
A	10	Sample X1	C	0.474	0.358	CaFr12	27.382813	547.65625
A	11	Sample X1	C	0.472	0.356	CaFr12	27.226563	544.53125
A	12	Sample X1	C	0.474	0.358	CaFr12	27.382813	547.65625
B	1	Blank B	D	0.513				
B	2	Sample X1	D	0.663	0.15	CaFr21	11.132813	222.65625
B	3	Sample X1	D	0.664	0.151	CaFr21	11.210938	224.21875
B	4	Sample X1	D	0.662	0.149	CaFr21	11.054688	221.09375
A	9	Blank B	C	0.062				
A	10	Sample X1	C	0.144	0.082	CaXy11	5.8203125	116.40625
A	11	Sample X1	C	0.143	0.081	CaXy11	5.7421875	114.84375
A	12	Sample X1	C	0.142	0.08	CaXy11	5.6640625	113.28125
B	5	Blank B	E	0.259				
B	6	Sample X1	E	0.515	0.256	CaXy12	19.414063	388.28125
B	7	Sample X1	E	0.521	0.262	CaXy12	19.882813	397.65625
B	8	Sample X1	E	0.521	0.262	CaXy12	19.882813	397.65625
B	9	Blank B	F	0.052				
B	10	Sample X1	F	0.139	0.087	CaGr11	6.2109375	124.21875
B	11	Sample X1	F	0.135	0.083	CaGr11	5.8984375	117.96875
B	12	Sample X1	F	0.139	0.087	CaGr11	6.2109375	124.21875
C	1	Blank B	G	0.063				
C	2	Sample X1	G	0.148	0.085	CaGr12	6.0546875	121.09375
C	3	Sample X1	G	0.147	0.084	CaGr12	5.9765625	119.53125
C	4	Sample X1	G	0.147	0.084	CaGr12	5.9765625	119.53125
C	5	Blank B	H	0.057				
C	6	Sample X1	H	0.142	0.085	CaGr21	6.0546875	121.09375
C	7	Sample X1	H	0.142	0.085	CaGr21	6.0546875	121.09375
C	8	Sample X1	H	0.141	0.084	CaGr21	5.9765625	119.53125
C	9	Blank B	I	0.063				
C	10	Sample X1	I	0.151	0.088	CaGc11	6.2890625	125.78125

Appendix 7.7 contd.

C	11	Sample X1	I	0.152	0.089	CaGc11	6.3671875	127.34375
C	12	Sample X1	I	0.152	0.089	CaGc11	6.3671875	127.34375
D	1	Blank B	J	0.067				
D	2	Sample X1	J	0.154	0.087	CaGc21	6.2109375	124.21875
D	3	Sample X1	J	0.155	0.088	CaGc21	6.2890625	125.78125
D	4	Sample X1	J	0.155	0.088	CaGc21	6.2890625	125.78125
D	5	Blank B	K	0.092				
D	6	Sample X1	K	0.175	0.083	CaGl11	5.8984375	117.96875
D	7	Sample X1	K	0.181	0.089	CaGl11	6.3671875	127.34375
D	8	Sample X1	K	0.176	0.084	CaGl11	5.9765625	119.53125
D	9	Blank B	L	0.055				
D	10	Sample X1	L	0.143	0.088	CaGl21	6.2890625	125.78125
D	11	Sample X1	L	0.137	0.082	CaGl21	5.8203125	116.40625
D	12	Sample X1	L	0.143	0.088	CaGl21	6.2890625	125.78125

Appendix 7.8 RCCDRSM TFC run 8

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.058				
E	10	Sample X1	A	0.254	0.196	CaSu11	14.726563	220.89844
E	11	Sample X1	A	0.251	0.193	CaSu11	14.492188	217.38281
E	12	Sample X1	A	0.254	0.196	CaSu11	14.726563	220.89844
C	1	Blank B	A	0.079				
C	2	Sample X1	A	0.401	0.322	CaFr11	24.570313	368.55469
C	3	Sample X1	A	0.403	0.324	CaFr11	24.726563	370.89844
C	4	Sample X1	A	0.403	0.324	CaFr11	24.726563	370.89844
C	5	Blank B	B	0.055				
C	6	Sample X1	B	0.345	0.29	CaFr12	22.070313	331.05469
C	7	Sample X1	B	0.346	0.291	CaFr12	22.148438	332.22656
C	8	Sample X1	B	0.346	0.291	CaFr12	22.148438	332.22656
C	9	Blank B	C	0.051				
C	10	Sample X1	C	0.339	0.288	CaFr21	21.914063	328.71094
C	11	Sample X1	C	0.34	0.289	CaFr21	21.992188	329.88281
C	12	Sample X1	C	0.34	0.289	CaFr21	21.992188	329.88281
D	1	Blank B	D	0.053				
D	2	Sample X1	D	0.137	0.084	CaXy11	5.9765625	89.648438
D	3	Sample X1	D	0.134	0.081	CaXy11	5.7421875	86.132813
D	4	Sample X1	D	0.137	0.084	CaXy11	5.9765625	89.648438
D	5	Blank B	E	0.05				

Appendix 7.8 contd.

D	6	Sample X1	E	0.136	0.086	CaXy12	6.1328125	91.992188
D	7	Sample X1	E	0.132	0.082	CaXy12	5.8203125	87.304688
D	8	Sample X1	E	0.132	0.082	CaXy12	5.8203125	87.304688
D	9	Blank B	F	0.044				
D	10	Sample X1	F	0.128	0.084	CaXy21	5.9765625	89.648438
D	11	Sample X1	F	0.124	0.08	CaXy21	5.6640625	84.960938
D	12	Sample X1	F	0.124	0.08	CaXy21	5.6640625	84.960938
F	1	Blank B	B	0.054				
F	2	Sample X1	B	0.137	0.083	CaGr11	5.8984375	88.476563
F	3	Sample X1	B	0.139	0.085	CaGr11	6.0546875	90.820313
F	4	Sample X1	B	0.142	0.088	CaGr11	6.2890625	94.335938
F	5	Blank B	C	0.05				
F	6	Sample X1	C	0.135	0.085	CaGr12	6.0546875	90.820313
F	7	Sample X1	C	0.137	0.087	CaGr12	6.2109375	93.164063
F	8	Sample X1	C	0.137	0.087	CaGr12	6.2109375	93.164063
F	9	Blank B	D	0.045				
F	10	Sample X1	D	0.129	0.084	CaGr21	5.9765625	89.648438
F	11	Sample X1	D	0.13	0.085	CaGr21	6.0546875	90.820313
F	12	Sample X1	D	0.132	0.087	CaGr21	6.2109375	93.164063
G	1	Blank B	E	0.054				
G	2	Sample X1	E	0.696	0.642	CaGc11	49.570313	743.55469
G	3	Sample X1	E	0.698	0.644	CaGc11	49.726563	745.89844
G	4	Sample X1	E	0.696	0.642	CaGc11	49.570313	743.55469
G	5	Blank B	F	0.046				
G	6	Sample X1	F	0.532	0.486	CaGc21	37.382813	560.74219
G	7	Sample X1	F	0.533	0.487	CaGc21	37.460938	561.91406
G	8	Sample X1	F	0.533	0.487	CaGc21	37.460938	561.91406
E	1	Blank B	G	0.062				
E	2	Sample X1	G	0.148	0.086	CaGl11	6.1328125	91.992188
E	3	Sample X1	G	0.143	0.081	CaGl11	5.7421875	86.132813
E	4	Sample X1	G	0.142	0.08	CaGl11	5.6640625	84.960938
E	5	Blank B	H	0.047				
E	6	Sample X1	H	0.136	0.089	CaGl21	6.3671875	95.507813
E	7	Sample X1	H	0.134	0.087	CaGl21	6.2109375	93.164063
E	8	Sample X1	H	0.136	0.089	CaGl21	6.3671875	95.507813

Appendix 7.9 RCCDRSM TFC run 9

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.065				
A	2	Sample X1	A	0.259	0.194	CaSu11	14.57031	218.5547
A	3	Sample X1	A	0.259	0.194	CaSu11	14.57031	218.5547
A	4	Sample X1	A	0.259	0.194	CaSu11	14.57031	218.5547
E	9	Blank B	A	0.09				
E	10	Sample X1	A	0.406	0.316	CaFr11	24.10156	361.5234
E	11	Sample X1	A	0.405	0.315	CaFr11	24.02344	360.3516
E	12	Sample X1	A	0.406	0.316	CaFr11	24.10156	361.5234
F	1	Blank B	B	0.059				
F	2	Sample X1	B	0.347	0.288	CaFr12	21.91406	328.7109
F	3	Sample X1	B	0.348	0.289	CaFr12	21.99219	329.8828
F	4	Sample X1	B	0.348	0.289	CaFr12	21.99219	329.8828
F	5	Blank B	C	0.074				
F	6	Sample X1	C	0.369	0.295	CaFr21	22.46094	336.9141
F	7	Sample X1	C	0.368	0.294	CaFr21	22.38281	335.7422
F	8	Sample X1	C	0.368	0.294	CaFr21	22.38281	335.7422
F	9	Blank B	D	0.045				
F	10	Sample X1	D	0.134	0.089	CaXy11	6.367188	95.50781
F	11	Sample X1	D	0.13	0.085	CaXy11	6.054688	90.82031
F	12	Sample X1	D	0.127	0.082	CaXy11	5.820313	87.30469
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.138	0.083	CaXy12	5.898438	88.47656
G	3	Sample X1	E	0.141	0.086	CaXy12	6.132813	91.99219
G	4	Sample X1	E	0.139	0.084	CaXy12	5.976563	89.64844
G	5	Blank B	F	0.057				
G	6	Sample X1	F	0.139	0.082	CaXy21	5.820313	87.30469
G	7	Sample X1	F	0.138	0.081	CaXy21	5.742188	86.13281
G	8	Sample X1	F	0.139	0.082	CaXy21	5.820313	87.30469
A	5	Blank B	B	0.056				
A	6	Sample X1	B	0.143	0.087	CaGr11	6.210938	93.16406
A	7	Sample X1	B	0.145	0.089	CaGr11	6.367188	95.50781
A	8	Sample X1	B	0.145	0.089	CaGr11	6.367188	95.50781
A	9	Blank B	C	0.05				
A	10	Sample X1	C	0.135	0.085	CaGr12	6.054688	90.82031
A	11	Sample X1	C	0.132	0.082	CaGr12	5.820313	87.30469
A	12	Sample X1	C	0.131	0.081	CaGr12	5.742188	86.13281
B	1	Blank B	D	0.063				

Appendix 7.9 contd.

B	2	Sample X1	D	0.146	0.083	CaGr21	5.898438	88.47656
B	3	Sample X1	D	0.149	0.086	CaGr21	6.132813	91.99219
B	4	Sample X1	D	0.147	0.084	CaGr21	5.976563	89.64844
B	5	Blank B	E	0.054				
B	6	Sample X1	E	0.769	0.715	CaGc11	55.27344	829.1016
B	7	Sample X1	E	0.772	0.718	CaGc11	55.50781	832.6172
B	8	Sample X1	E	0.77	0.716	CaGc11	55.35156	830.2734
B	9	Blank B	F	0.05				
B	10	Sample X1	F	0.517	0.467	CaGc21	35.89844	538.4766
B	11	Sample X1	F	0.519	0.469	CaGc21	36.05469	540.8203
B	12	Sample X1	F	0.51	0.46	CaGc21	35.35156	530.2734
G	9	Blank B	G	0.059				
G	10	Sample X1	G	0.146	0.087	CaGl11	6.210938	93.16406
G	11	Sample X1	G	0.142	0.083	CaGl11	5.898438	88.47656
G	12	Sample X1	G	0.148	0.089	CaGl11	6.367188	95.50781
H	1	Blank B	H	0.061				
H	2	Sample X1	H	0.145	0.084	CaGl21	5.976563	89.64844
H	3	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031
H	4	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031

Appendix 7.10 RCCDRSM TFC run 10

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.055				
C	10	Sample X1	A	0.303	0.248	CaSu11	18.78906	375.7813
C	11	Sample X1	A	0.304	0.249	CaSu11	18.86719	377.3438
C	12	Sample X1	A	0.304	0.249	CaSu11	18.86719	377.3438
A	1	Blank B	A	0.151				
A	2	Sample X1	A	0.609	0.458	CaFr11	35.19531	703.9063
A	3	Sample X1	A	0.605	0.454	CaFr11	34.88281	697.6563
A	4	Sample X1	A	0.605	0.454	CaFr11	34.88281	697.6563
A	5	Blank B	B	0.055				
A	6	Sample X1	B	0.347	0.292	CaFr12	22.22656	444.5313
A	7	Sample X1	B	0.36	0.305	CaFr12	23.24219	464.8438
A	8	Sample X1	B	0.358	0.303	CaFr12	23.08594	461.7188
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.343	0.291	CaFr21	22.14844	442.9688
A	11	Sample X1	C	0.342	0.29	CaFr21	22.07031	441.4063
A	12	Sample X1	C	0.343	0.291	CaFr21	22.14844	442.9688

Appendix 7.10 contd.

B	1	Blank B	D	0.057				
B	2	Sample X1	D	0.182	0.125	CaXy11	9.179688	183.5938
B	3	Sample X1	D	0.184	0.127	CaXy11	9.335938	186.7188
B	4	Sample X1	D	0.184	0.127	CaXy11	9.335938	186.7188
B	5	Blank B	E	0.049				
B	6	Sample X1	E	0.352	0.303	CaXy12	23.08594	461.7188
B	7	Sample X1	E	0.354	0.305	CaXy12	23.24219	464.8438
B	8	Sample X1	E	0.354	0.305	CaXy12	23.24219	464.8438
B	9	Blank B	F	0.044				
B	10	Sample X1	F	0.191	0.147	CaXy21	10.89844	217.9688
B	11	Sample X1	F	0.191	0.147	CaXy21	10.89844	217.9688
B	12	Sample X1	F	0.192	0.148	CaXy21	10.97656	219.5313
D	1	Blank B	B	0.057				
D	2	Sample X1	B	0.237	0.18	CaGr11	13.47656	269.5313
D	3	Sample X1	B	0.239	0.182	CaGr11	13.63281	272.6563
D	4	Sample X1	B	0.239	0.182	CaGr11	13.63281	272.6563
D	5	Blank B	C	0.057				
D	6	Sample X1	C	0.264	0.207	CaGr12	15.58594	311.7188
D	7	Sample X1	C	0.263	0.206	CaGr12	15.50781	310.1563
D	8	Sample X1	C	0.264	0.207	CaGr12	15.58594	311.7188
D	9	Blank B	D	0.06				
D	10	Sample X1	D	0.151	0.091	CaGr21	6.523438	130.4688
D	11	Sample X1	D	0.152	0.092	CaGr21	6.601563	132.0313
D	12	Sample X1	D	0.152	0.092	CaGr21	6.601563	132.0313
E	1	Blank B	E	0.059				
E	2	Sample X1	E	0.791	0.732	CaGc11	56.60156	1132.031
E	3	Sample X1	E	0.79	0.731	CaGc11	56.52344	1130.469
E	4	Sample X1	E	0.791	0.732	CaGc11	56.60156	1132.031
E	5	Blank B	F	0.052				
E	6	Sample X1	F	0.621	0.569	CaGc21	43.86719	877.3438
E	7	Sample X1	F	0.62	0.568	CaGc21	43.78906	875.7813
E	8	Sample X1	F	0.621	0.569	CaGc21	43.86719	877.3438
C	1	Blank B	G	0.066				
C	2	Sample X1	G	0.262	0.196	CaGl11	14.72656	294.5313
C	3	Sample X1	G	0.261	0.195	CaGl11	14.64844	292.9688
C	4	Sample X1	G	0.262	0.196	CaGl11	14.72656	294.5313
C	5	Blank B	H	0.052				
C	6	Sample X1	H	0.179	0.127	CaGl21	9.335938	186.7188
C	7	Sample X1	H	0.177	0.125	CaGl21	9.179688	183.5938
C	8	Sample X1	H	0.179	0.127	CaGl21	9.335938	186.7188

Appendix 7.11 RCCDRSM TFC run 11

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.072				
A	2	Sample X1	A	0.161	0.089	CaSu11	6.3671875	127.34375
A	3	Sample X1	A	0.16	0.088	CaSu11	6.2890625	125.78125
A	4	Sample X1	A	0.16	0.088	CaSu11	6.2890625	125.78125
E	9	Blank B	A	0.077				
E	10	Sample X1	A	0.308	0.231	CaFr11	17.4609375	349.21875
E	11	Sample X1	A	0.308	0.231	CaFr11	17.4609375	349.21875
E	12	Sample X1	A	0.309	0.232	CaFr11	17.5390625	350.78125
F	1	Blank B	B	0.061				
F	2	Sample X1	B	0.145	0.084	CaFr12	5.9765625	119.53125
F	3	Sample X1	B	0.145	0.084	CaFr12	5.9765625	119.53125
F	4	Sample X1	B	0.147	0.086	CaFr12	6.1328125	122.65625
F	5	Blank B	C	0.141				
F	6	Sample X1	C	0.23	0.089	CaFr21	6.3671875	127.34375
F	7	Sample X1	C	0.23	0.089	CaFr21	6.3671875	127.34375
F	8	Sample X1	C	0.226	0.085	CaFr21	6.0546875	121.09375
F	9	Blank B	D	0.07				
F	10	Sample X1	D	0.151	0.081	CaXy11	5.7421875	114.84375
F	11	Sample X1	D	0.152	0.082	CaXy11	5.8203125	116.40625
F	12	Sample X1	D	0.151	0.081	CaXy11	5.7421875	114.84375
G	1	Blank B	E	0.053				
G	2	Sample X1	E	0.138	0.085	CaXy12	6.0546875	121.09375
G	3	Sample X1	E	0.137	0.084	CaXy12	5.9765625	119.53125
G	4	Sample X1	E	0.138	0.085	CaXy12	6.0546875	121.09375
G	5	Blank B	F	0.047				
G	6	Sample X1	F	0.132	0.085	CaXy21	6.0546875	121.09375
G	7	Sample X1	F	0.133	0.086	CaXy21	6.1328125	122.65625
G	8	Sample X1	F	0.132	0.085	CaXy21	6.0546875	121.09375
A	5	Blank B	B	0.064				
A	6	Sample X1	B	0.15	0.086	CaGr11	6.1328125	122.65625
A	7	Sample X1	B	0.151	0.087	CaGr11	6.2109375	124.21875
A	8	Sample X1	B	0.15	0.086	CaGr11	6.1328125	122.65625
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.132	0.08	CaGr12	5.6640625	113.28125
A	11	Sample X1	C	0.132	0.08	CaGr12	5.6640625	113.28125
A	12	Sample X1	C	0.134	0.082	CaGr12	5.8203125	116.40625
B	1	Blank B	D	0.061				
B	2	Sample X1	D	0.146	0.085	CaGr21	6.0546875	121.09375

Appendix 7.11 contd.

B	3	Sample X1	D	0.143	0.082	CaGr21	5.8203125	116.40625
B	4	Sample X1	D	0.143	0.082	CaGr21	5.8203125	116.40625
B	5	Blank B	E	0.062				
B	6	Sample X1	E	0.483	0.421	CaGc11	32.3046875	646.09375
B	7	Sample X1	E	0.482	0.42	CaGc11	32.2265625	644.53125
B	8	Sample X1	E	0.482	0.42	CaGc11	32.2265625	644.53125
B	9	Blank B	F	0.049				
B	10	Sample X1	F	0.276	0.227	CaGc21	17.1484375	342.96875
B	11	Sample X1	F	0.269	0.22	CaGc21	16.6015625	332.03125
B	12	Sample X1	F	0.276	0.227	CaGc21	17.1484375	342.96875
G	9	Blank B	G	0.043				
G	10	Sample X1	G	0.125	0.082	CaGl11	5.8203125	116.40625
G	11	Sample X1	G	0.126	0.083	CaGl11	5.8984375	117.96875
G	12	Sample X1	G	0.126	0.083	CaGl11	5.8984375	117.96875
H	1	Blank B	H	0.178				
H	2	Sample X1	H	0.304	0.126	CaGl21	9.2578125	185.15625
H	3	Sample X1	H	0.305	0.127	CaGl21	9.3359375	186.71875
H	4	Sample X1	H	0.305	0.127	CaGl21	9.3359375	186.71875

Appendix 7.12 RCCDRSM TFC run 12

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.074				
E	2	Sample X1	A	0.156	0.082	CaSu11	5.8203125	116.4063
E	3	Sample X1	A	0.159	0.085	CaSu11	6.0546875	121.0938
E	4	Sample X1	A	0.159	0.085	CaSu11	6.0546875	121.0938
E	5	Blank B	B	0.061				
E	6	Sample X1	B	0.366	0.305	CaFr11	23.242188	464.8438
E	7	Sample X1	B	0.368	0.307	CaFr11	23.398438	467.9688
E	8	Sample X1	B	0.368	0.307	CaFr11	23.398438	467.9688
E	9	Blank B	C	0.073				
E	10	Sample X1	C	0.345	0.272	CaFr12	20.664063	413.2813
E	11	Sample X1	C	0.347	0.274	CaFr12	20.820313	416.4063
E	12	Sample X1	C	0.345	0.272	CaFr12	20.664063	413.2813
F	1	Blank B	D	0.064				
F	2	Sample X1	D	0.153	0.089	CaFr21	6.3671875	127.3438
F	3	Sample X1	D	0.151	0.087	CaFr21	6.2109375	124.2188

Appendix 7.12 contd.

F	4	Sample X1	D	0.151	0.087	CaFr21	6.2109375	124.2188
B	1	Blank B	D	0.072				
B	2	Sample X1	D	0.154	0.082	CaXy11	5.8203125	116.4063
B	3	Sample X1	D	0.153	0.081	CaXy11	5.7421875	114.8438
B	4	Sample X1	D	0.153	0.081	CaXy11	5.7421875	114.8438
F	5	Blank B	E	0.053				
F	6	Sample X1	E	0.137	0.084	CaXy12	5.9765625	119.5313
F	7	Sample X1	E	0.137	0.084	CaXy12	5.9765625	119.5313
F	8	Sample X1	E	0.14	0.087	CaXy12	6.2109375	124.2188
A	9	Blank B	C	0.051				
A	10	Sample X1	C	0.137	0.086	CaXy21	6.1328125	122.6563
A	11	Sample X1	C	0.135	0.084	CaXy21	5.9765625	119.5313
A	12	Sample X1	C	0.137	0.086	CaXy21	6.1328125	122.6563
F	9	Blank B	F	0.044				
F	10	Sample X1	F	0.36	0.316	CaGr11	24.101563	482.0313
F	11	Sample X1	F	0.359	0.315	CaGr11	24.023438	480.4688
F	12	Sample X1	F	0.359	0.315	CaGr11	24.023438	480.4688
G	1	Blank B	G	0.054				
G	2	Sample X1	G	0.164	0.11	CaGr12	8.0078125	160.1563
G	3	Sample X1	G	0.163	0.109	CaGr12	7.9296875	158.5938
G	4	Sample X1	G	0.163	0.109	CaGr12	7.9296875	158.5938
G	5	Blank B	H	0.047				
G	6	Sample X1	H	0.23	0.183	CaGr21	13.710938	274.2188
G	7	Sample X1	H	0.23	0.183	CaGr21	13.710938	274.2188
G	8	Sample X1	H	0.232	0.185	CaGr21	13.867188	277.3438
G	9	Blank B	I	0.043				
G	10	Sample X1	I	0.187	0.144	CaGc11	10.664063	213.2813
G	11	Sample X1	I	0.187	0.144	CaGc11	10.664063	213.2813
G	12	Sample X1	I	0.18	0.137	CaGc11	10.117188	202.3438
H	1	Blank B	J	0.06				
H	2	Sample X1	J	0.142	0.082	CaGc21	5.8203125	116.4063
H	3	Sample X1	J	0.145	0.085	CaGc21	6.0546875	121.0938
H	4	Sample X1	J	0.142	0.082	CaGc21	5.8203125	116.4063
H	5	Blank B	K	0.054				
H	6	Sample X1	K	0.137	0.083	CaGl11	5.8984375	117.9688
H	7	Sample X1	K	0.143	0.089	CaGl11	6.3671875	127.3438
H	8	Sample X1	K	0.143	0.089	CaGl11	6.3671875	127.3438
H	9	Blank B	L	0.045				
H	10	Sample X1	L	0.279	0.234	CaGl21	17.695313	353.9063
H	11	Sample X1	L	0.279	0.234	CaGl21	17.695313	353.9063
H	12	Sample X1	L	0.28	0.235	CaGl21	17.773438	355.4688

Appendix 7.13 RCCDRSM TFC run 13

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.06				
A	2	Sample X1	A	0.558	0.498	CaSu11	38.32031	383.2031
A	3	Sample X1	A	0.559	0.499	CaSu11	38.39844	383.9844
A	4	Sample X1	A	0.559	0.499	CaSu11	38.39844	383.9844
E	9	Blank B	A	0.057				
E	10	Sample X1	A	0.828	0.771	CaFr11	59.64844	596.4844
E	11	Sample X1	A	0.828	0.771	CaFr11	59.64844	596.4844
E	12	Sample X1	A	0.83	0.773	CaFr11	59.80469	598.0469
F	1	Blank B	B	0.06				
F	2	Sample X1	B	0.433	0.373	CaFr12	28.55469	285.5469
F	3	Sample X1	B	0.431	0.371	CaFr12	28.39844	283.9844
F	4	Sample X1	B	0.431	0.371	CaFr12	28.39844	283.9844
F	5	Blank B	C	0.056				
F	6	Sample X1	C	0.487	0.431	CaFr21	33.08594	330.8594
F	7	Sample X1	C	0.491	0.435	CaFr21	33.39844	333.9844
F	8	Sample X1	C	0.491	0.435	CaFr21	33.39844	333.9844
F	9	Blank B	D	0.055				
F	10	Sample X1	D	0.61	0.555	CaXy11	42.77344	427.7344
F	11	Sample X1	D	0.609	0.554	CaXy11	42.69531	426.9531
F	12	Sample X1	D	0.61	0.555	CaXy11	42.77344	427.7344
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.664	0.609	CaXy12	46.99219	469.9219
G	3	Sample X1	E	0.665	0.61	CaXy12	47.07031	470.7031
G	4	Sample X1	E	0.665	0.61	CaXy12	47.07031	470.7031
G	5	Blank B	F	0.056				
G	6	Sample X1	F	0.515	0.459	CaXy21	35.27344	352.7344
G	7	Sample X1	F	0.515	0.459	CaXy21	35.27344	352.7344
G	8	Sample X1	F	0.515	0.459	CaXy21	35.27344	352.7344
A	5	Blank B	B	0.052				
A	6	Sample X1	B	0.919	0.867	CaGr11	67.14844	671.4844
A	7	Sample X1	B	0.92	0.868	CaGr11	67.22656	672.2656
A	8	Sample X1	B	0.919	0.867	CaGr11	67.14844	671.4844
A	9	Blank B	C	0.046				
A	10	Sample X1	C	0.781	0.735	CaGr12	56.83594	568.3594
A	11	Sample X1	C	0.78	0.734	CaGr12	56.75781	567.5781
A	12	Sample X1	C	0.78	0.734	CaGr12	56.75781	567.5781
B	1	Blank B	D	0.054				

Appendix 7.13 contd.

B	2	Sample X1	D	0.817	0.763	CaGr21	59.02344	590.2344
B	3	Sample X1	D	0.817	0.763	CaGr21	59.02344	590.2344
B	4	Sample X1	D	0.818	0.764	CaGr21	59.10156	591.0156
B	5	Blank B	E	0.047				
B	6	Sample X1	E	0.763	0.716	CaGc11	55.35156	553.5156
B	7	Sample X1	E	0.762	0.715	CaGc11	55.27344	552.7344
B	8	Sample X1	E	0.762	0.715	CaGc11	55.27344	552.7344
B	9	Blank B	F	0.045				
B	10	Sample X1	F	0.47	0.425	CaGc21	32.61719	326.1719
B	11	Sample X1	F	0.47	0.425	CaGc21	32.61719	326.1719
B	12	Sample X1	F	0.469	0.424	CaGc21	32.53906	325.3906
G	9	Blank B	G	0.069				
G	10	Sample X1	G	0.597	0.528	CaGl11	40.66406	406.6406
G	11	Sample X1	G	0.597	0.528	CaGl11	40.66406	406.6406
G	12	Sample X1	G	0.597	0.528	CaGl11	40.66406	406.6406
H	1	Blank B	H	0.062				
H	2	Sample X1	H	0.446	0.384	CaGl21	29.41406	294.1406
H	3	Sample X1	H	0.444	0.382	CaGl21	29.25781	292.5781
H	4	Sample X1	H	0.444	0.382	CaGl21	29.25781	292.5781

Appendix 7.14 RCCDRSM TFC run 14

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.055				
C	10	Sample X1	A	0.155	0.1	CaSu11	7.226563	72.26563
C	11	Sample X1	A	0.156	0.101	CaSu11	7.304688	73.04688
C	12	Sample X1	A	0.155	0.1	CaSu11	7.226563	72.26563
A	1	Blank B	A	0.075				
A	2	Sample X1	A	0.345	0.27	CaFr11	20.50781	205.0781
A	3	Sample X1	A	0.345	0.27	CaFr11	20.50781	205.0781
A	4	Sample X1	A	0.346	0.271	CaFr11	20.58594	205.8594
A	5	Blank B	B	0.057				
A	6	Sample X1	B	0.142	0.085	CaFr12	6.054688	60.54688
A	7	Sample X1	B	0.146	0.089	CaFr12	6.367188	63.67188
A	8	Sample X1	B	0.142	0.085	CaFr12	6.054688	60.54688
A	9	Blank B	C	0.051				
A	10	Sample X1	C	0.181	0.13	CaFr21	9.570313	95.70313
A	11	Sample X1	C	0.185	0.134	CaFr21	9.882813	98.82813

Appendix 7.14 contd.

A	12	Sample X1	C	0.185	0.134	CaFr21	9.882813	98.82813
B	1	Blank B	D	0.048				
B	2	Sample X1	D	0.144	0.096	CaXy11	6.914063	69.14063
B	3	Sample X1	D	0.144	0.096	CaXy11	6.914063	69.14063
B	4	Sample X1	D	0.148	0.1	CaXy11	7.226563	72.26563
B	5	Blank B	E	0.053				
B	6	Sample X1	E	0.141	0.088	CaXy12	6.289063	62.89063
B	7	Sample X1	E	0.139	0.086	CaXy12	6.132813	61.32813
B	8	Sample X1	E	0.139	0.086	CaXy12	6.132813	61.32813
B	9	Blank B	F	0.045				
B	10	Sample X1	F	0.128	0.083	CaXy21	5.898438	58.98438
B	11	Sample X1	F	0.132	0.087	CaXy21	6.210938	62.10938
B	12	Sample X1	F	0.132	0.087	CaXy21	6.210938	62.10938
D	1	Blank B	B	0.072				
D	2	Sample X1	B	0.157	0.085	CaGr11	6.054688	60.54688
D	3	Sample X1	B	0.16	0.088	CaGr11	6.289063	62.89063
D	4	Sample X1	B	0.157	0.085	CaGr11	6.054688	60.54688
D	5	Blank B	C	0.054				
D	6	Sample X1	C	0.138	0.084	CaGr12	5.976563	59.76563
D	7	Sample X1	C	0.138	0.084	CaGr12	5.976563	59.76563
D	8	Sample X1	C	0.135	0.081	CaGr12	5.742188	57.42188
D	9	Blank B	D	0.049				
D	10	Sample X1	D	0.133	0.084	CaGr21	5.976563	59.76563
D	11	Sample X1	D	0.138	0.089	CaGr21	6.367188	63.67188
D	12	Sample X1	D	0.133	0.084	CaGr21	5.976563	59.76563
E	1	Blank B	E	0.057				
E	2	Sample X1	E	0.5	0.443	CaGc11	34.02344	340.2344
E	3	Sample X1	E	0.5	0.443	CaGc11	34.02344	340.2344
E	4	Sample X1	E	0.502	0.445	CaGc11	34.17969	341.7969
E	5	Blank B	F	0.064				
E	6	Sample X1	F	0.457	0.393	CaGc21	30.11719	301.1719
E	7	Sample X1	F	0.453	0.389	CaGc21	29.80469	298.0469
E	8	Sample X1	F	0.453	0.389	CaGc21	29.80469	298.0469
C	1	Blank B	G	0.057				
C	2	Sample X1	G	0.138	0.081	CaGl11	5.742188	57.42188
C	3	Sample X1	G	0.138	0.081	CaGl11	5.742188	57.42188
C	4	Sample X1	G	0.144	0.087	CaGl11	6.210938	62.10938
C	5	Blank B	H	0.051				
C	6	Sample X1	H	0.133	0.082	CaGl21	5.820313	58.20313
C	7	Sample X1	H	0.133	0.082	CaGl21	5.820313	58.20313
C	8	Sample X1	H	0.141	0.09	CaGl21	6.445313	64.45313

Appendix 7.15 RCCDRSM TFC run 15

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
C	9	Blank B	A	0.063				
C	10	Sample X1	A	0.197	0.134	CaSu11	9.8828125	197.65625
C	11	Sample X1	A	0.198	0.135	CaSu11	9.9609375	199.21875
C	12	Sample X1	A	0.197	0.134	CaSu11	9.8828125	197.65625
A	1	Blank B	A	0.071				
A	2	Sample X1	A	0.155	0.084	CaFr11	5.9765625	119.53125
A	3	Sample X1	A	0.154	0.083	CaFr11	5.8984375	117.96875
A	4	Sample X1	A	0.154	0.083	CaFr11	5.8984375	117.96875
A	5	Blank B	B	0.057				
A	6	Sample X1	B	0.143	0.086	CaFr12	6.1328125	122.65625
A	7	Sample X1	B	0.145	0.088	CaFr12	6.2890625	125.78125
A	8	Sample X1	B	0.143	0.086	CaFr12	6.1328125	122.65625
A	9	Blank B	C	0.052				
A	10	Sample X1	C	0.152	0.1	CaFr21	7.2265625	144.53125
A	11	Sample X1	C	0.154	0.102	CaFr21	7.3828125	147.65625
A	12	Sample X1	C	0.152	0.1	CaFr21	7.2265625	144.53125
B	1	Blank B	D	0.05				
B	2	Sample X1	D	0.136	0.086	CaXy11	6.1328125	122.65625
B	3	Sample X1	D	0.136	0.086	CaXy11	6.1328125	122.65625
B	4	Sample X1	D	0.139	0.089	CaXy11	6.3671875	127.34375
B	5	Blank B	E	0.049				
B	6	Sample X1	E	0.133	0.084	CaXy12	5.9765625	119.53125
B	7	Sample X1	E	0.137	0.088	CaXy12	6.2890625	125.78125
B	8	Sample X1	E	0.133	0.084	CaXy12	5.9765625	119.53125
B	9	Blank B	F	0.048				
B	10	Sample X1	F	0.131	0.083	CaXy21	5.8984375	117.96875
B	11	Sample X1	F	0.137	0.089	CaXy21	6.3671875	127.34375
B	12	Sample X1	F	0.131	0.083	CaXy21	5.8984375	117.96875
D	1	Blank B	B	0.059				
D	2	Sample X1	B	0.143	0.084	CaGr11	5.9765625	119.53125
D	3	Sample X1	B	0.145	0.086	CaGr11	6.1328125	122.65625
D	4	Sample X1	B	0.143	0.084	CaGr11	5.9765625	119.53125
D	5	Blank B	C	0.056				
D	6	Sample X1	C	0.137	0.081	CaGr12	5.7421875	114.84375
D	7	Sample X1	C	0.145	0.089	CaGr12	6.3671875	127.34375
D	8	Sample X1	C	0.137	0.081	CaGr12	5.7421875	114.84375
D	9	Blank B	D	0.059				

Appendix 7.15 contd.

D	10	Sample X1	D	0.146	0.087	CaGr21	6.2109375	124.21875
D	11	Sample X1	D	0.145	0.086	CaGr21	6.1328125	122.65625
D	12	Sample X1	D	0.145	0.086	CaGr21	6.1328125	122.65625
E	1	Blank B	E	0.063				
E	2	Sample X1	E	0.599	0.536	CaGc11	41.2890625	825.78125
E	3	Sample X1	E	0.601	0.538	CaGc11	41.4453125	828.90625
E	4	Sample X1	E	0.599	0.536	CaGc11	41.2890625	825.78125
E	5	Blank B	F	0.052				
E	6	Sample X1	F	0.138	0.086	CaGc21	6.1328125	122.65625
E	7	Sample X1	F	0.138	0.086	CaGc21	6.1328125	122.65625
E	8	Sample X1	F	0.139	0.087	CaGc21	6.2109375	124.21875
C	1	Blank B	G	0.089				
C	2	Sample X1	G	0.357	0.268	CaGl11	20.3515625	407.03125
C	3	Sample X1	G	0.358	0.269	CaGl11	20.4296875	408.59375
C	4	Sample X1	G	0.357	0.268	CaGl11	20.3515625	407.03125
C	5	Blank B	H	0.058				
C	6	Sample X1	H	0.235	0.177	CaGl21	13.2421875	264.84375
C	7	Sample X1	H	0.236	0.178	CaGl21	13.3203125	266.40625
C	8	Sample X1	H	0.235	0.177	CaGl21	13.2421875	264.84375

Appendix 7.16 RCCDRSM TFC run 16

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.068				
E	10	Sample X1	A	0.326	0.258	CaSu11	19.57031	391.4063
E	11	Sample X1	A	0.322	0.254	CaSu11	19.25781	385.1563
E	12	Sample X1	A	0.322	0.254	CaSu11	19.25781	385.1563
C	1	Blank B	A	0.076				
C	2	Sample X1	A	0.163	0.087	CaFr11	6.210938	124.2188
C	3	Sample X1	A	0.163	0.087	CaFr11	6.210938	124.2188
C	4	Sample X1	A	0.164	0.088	CaFr11	6.289063	125.7813
C	5	Blank B	B	0.056				
C	6	Sample X1	B	0.145	0.089	CaFr12	6.367188	127.3438
C	7	Sample X1	B	0.14	0.084	CaFr12	5.976563	119.5313
C	8	Sample X1	B	0.14	0.084	CaFr12	5.976563	119.5313
C	9	Blank B	C	0.056				
C	10	Sample X1	C	0.169	0.113	CaFr21	8.242188	164.8438
C	11	Sample X1	C	0.17	0.114	CaFr21	8.320313	166.4063
C	12	Sample X1	C	0.169	0.113	CaFr21	8.242188	164.8438

Appendix 7.16 contd.

D	1	Blank B	D	0.059				
D	2	Sample X1	D	0.148	0.089	CaXy11	6.367188	127.3438
D	3	Sample X1	D	0.143	0.084	CaXy11	5.976563	119.5313
D	4	Sample X1	D	0.148	0.089	CaXy11	6.367188	127.3438
D	5	Blank B	E	0.052				
D	6	Sample X1	E	0.134	0.082	CaXy12	5.820313	116.4063
D	7	Sample X1	E	0.136	0.084	CaXy12	5.976563	119.5313
D	8	Sample X1	E	0.134	0.082	CaXy12	5.820313	116.4063
D	9	Blank B	F	0.057				
D	10	Sample X1	F	0.138	0.081	CaXy21	5.742188	114.8438
D	11	Sample X1	F	0.138	0.081	CaXy21	5.742188	114.8438
D	12	Sample X1	F	0.142	0.085	CaXy21	6.054688	121.0938
F	1	Blank B	B	0.063				
F	2	Sample X1	B	0.152	0.089	CaGr11	6.367188	127.3438
F	3	Sample X1	B	0.143	0.08	CaGr11	5.664063	113.2813
F	4	Sample X1	B	0.143	0.08	CaGr11	5.664063	113.2813
F	5	Blank B	C	0.051				
F	6	Sample X1	C	0.137	0.086	CaGr12	6.132813	122.6563
F	7	Sample X1	C	0.139	0.088	CaGr12	6.289063	125.7813
F	8	Sample X1	C	0.137	0.086	CaGr12	6.132813	122.6563
F	9	Blank B	D	0.055				
F	10	Sample X1	D	0.135	0.08	CaGr21	5.664063	113.2813
F	11	Sample X1	D	0.141	0.086	CaGr21	6.132813	122.6563
F	12	Sample X1	D	0.141	0.086	CaGr21	6.132813	122.6563
G	1	Blank B	E	0.061				
G	2	Sample X1	E	0.509	0.448	CaGc11	34.41406	688.2813
G	3	Sample X1	E	0.511	0.45	CaGc11	34.57031	691.4063
G	4	Sample X1	E	0.509	0.448	CaGc11	34.41406	688.2813
G	5	Blank B	F	0.051				
G	6	Sample X1	F	0.186	0.135	CaGc21	9.960938	199.2188
G	7	Sample X1	F	0.188	0.137	CaGc21	10.11719	202.3438
G	8	Sample X1	F	0.186	0.135	CaGc21	9.960938	199.2188
E	1	Blank B	G	0.058				
E	2	Sample X1	G	0.142	0.084	CaGl11	5.976563	119.5313
E	3	Sample X1	G	0.142	0.084	CaGl11	5.976563	119.5313
E	4	Sample X1	G	0.145	0.087	CaGl11	6.210938	124.2188
E	5	Blank B	H	0.059				
E	6	Sample X1	H	0.274	0.215	CaGl21	16.21094	324.2188
E	7	Sample X1	H	0.276	0.217	CaGl21	16.36719	327.3438
E	8	Sample X1	H	0.274	0.215	CaGl21	16.21094	324.2188

Appendix 7.17 RCCDRSM TFC run 17

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.066				
A	2	Sample X1	A	0.155	0.089	CaSu11	6.3671875	63.67188
A	3	Sample X1	A	0.153	0.087	CaSu11	6.2109375	62.10938
A	4	Sample X1	A	0.153	0.087	CaSu11	6.2109375	62.10938
A	5	Blank B	B	0.059				
A	6	Sample X1	B	0.322	0.263	CaFr11	19.960938	199.6094
A	7	Sample X1	B	0.322	0.263	CaFr11	19.960938	199.6094
A	8	Sample X1	B	0.323	0.264	CaFr11	20.039063	200.3906
A	9	Blank B	C	0.065				
A	10	Sample X1	C	0.149	0.084	CaFr12	5.9765625	59.76563
A	11	Sample X1	C	0.148	0.083	CaFr12	5.8984375	58.98438
A	12	Sample X1	C	0.148	0.083	CaFr12	5.8984375	58.98438
B	1	Blank B	D	0.063				
B	2	Sample X1	D	0.146	0.083	CaFr21	5.8984375	58.98438
B	3	Sample X1	D	0.147	0.084	CaFr21	5.9765625	59.76563
B	4	Sample X1	D	0.147	0.084	CaFr21	5.9765625	59.76563
B	5	Blank B	E	0.058				
B	6	Sample X1	E	0.147	0.089	CaXy11	6.3671875	63.67188
B	7	Sample X1	E	0.145	0.087	CaXy11	6.2109375	62.10938
B	8	Sample X1	E	0.145	0.087	CaXy11	6.2109375	62.10938
B	5	Blank B	E	0.053				
B	6	Sample X1	E	0.14	0.087	CaXy12	6.2109375	62.10938
B	7	Sample X1	E	0.138	0.085	CaXy12	6.0546875	60.54688
B	8	Sample X1	E	0.138	0.085	CaXy12	6.0546875	60.54688
B	1	Blank B	D	0.049				
B	2	Sample X1	D	0.159	0.11	CaXy21	8.0078125	80.07813
B	3	Sample X1	D	0.158	0.109	CaXy21	7.9296875	79.29688
B	4	Sample X1	D	0.158	0.109	CaXy21	7.9296875	79.29688
B	9	Blank B	F	0.079				
B	10	Sample X1	F	0.164	0.085	CaGr11	6.0546875	60.54688
B	11	Sample X1	F	0.16	0.081	CaGr11	5.7421875	57.42188
B	12	Sample X1	F	0.16	0.081	CaGr11	5.7421875	57.42188
C	1	Blank B	G	0.062				
C	2	Sample X1	G	0.147	0.085	CaGr12	6.0546875	60.54688
C	3	Sample X1	G	0.151	0.089	CaGr12	6.3671875	63.67188
C	4	Sample X1	G	0.147	0.085	CaGr12	6.0546875	60.54688
C	5	Blank B	H	0.075				

Appendix 7.17 contd.

C	6	Sample X1	H	0.156	0.081	CaGr21	5.7421875	57.42188
C	7	Sample X1	H	0.16	0.085	CaGr21	6.0546875	60.54688
C	8	Sample X1	H	0.156	0.081	CaGr21	5.7421875	57.42188
C	9	Blank B	I	0.056				
C	10	Sample X1	I	0.146	0.09	CaGc11	6.4453125	64.45313
C	11	Sample X1	I	0.143	0.087	CaGc11	6.2109375	62.10938
C	12	Sample X1	I	0.143	0.087	CaGc11	6.2109375	62.10938
D	1	Blank B	J	0.061				
D	2	Sample X1	J	0.167	0.106	CaGc21	7.6953125	76.95313
D	3	Sample X1	J	0.174	0.113	CaGc21	8.2421875	82.42188
D	4	Sample X1	J	0.167	0.106	CaGc21	7.6953125	76.95313
D	5	Blank B	K	0.09				
D	6	Sample X1	K	0.172	0.082	CaGl11	5.8203125	58.20313
D	7	Sample X1	K	0.173	0.083	CaGl11	5.8984375	58.98438
D	8	Sample X1	K	0.175	0.085	CaGl11	6.0546875	60.54688
D	9	Blank B	L	0.056				
D	10	Sample X1	L	0.139	0.083	CaGl21	5.8984375	58.98438
D	11	Sample X1	L	0.139	0.083	CaGl21	5.8984375	58.98438
D	12	Sample X1	L	0.141	0.085	CaGl21	6.0546875	60.54688

Appendix 7.18 RCCDRSM TFC run 18

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.396				
A	2	Sample X1	A	0.707	0.311	CaSu11	23.710938	948.4375
A	3	Sample X1	A	0.708	0.312	CaSu11	23.789063	951.5625
A	4	Sample X1	A	0.707	0.311	CaSu11	23.710938	948.4375
A	5	Blank B	B	0.217				
A	6	Sample X1	B	0.725	0.508	CaFr11	39.101563	1564.063
A	7	Sample X1	B	0.715	0.498	CaFr11	38.320313	1532.813
A	8	Sample X1	B	0.715	0.498	CaFr11	38.320313	1532.813
A	9	Blank B	C	0.089				
A	10	Sample X1	C	0.362	0.273	CaFr12	20.742188	829.6875
A	11	Sample X1	C	0.364	0.275	CaFr12	20.898438	835.9375
A	12	Sample X1	C	0.362	0.273	CaFr12	20.742188	829.6875
B	1	Blank B	D	0.059				
B	2	Sample X1	D	0.194	0.135	CaFr21	9.9609375	398.4375
B	3	Sample X1	D	0.194	0.135	CaFr21	9.9609375	398.4375
B	4	Sample X1	D	0.196	0.137	CaFr21	10.117188	404.6875

Appendix 7.18 contd.

B	9	Blank B	F	0.04				
B	10	Sample X1	F	0.124	0.084	CaXy11	5.9765625	239.0625
B	11	Sample X1	F	0.124	0.084	CaXy11	5.9765625	239.0625
B	12	Sample X1	F	0.128	0.088	CaXy11	6.2890625	251.5625
B	5	Blank B	E	0.289				
B	6	Sample X1	E	0.627	0.338	CaXy12	25.820313	1032.813
B	7	Sample X1	E	0.626	0.337	CaXy12	25.742188	1029.688
B	8	Sample X1	E	0.626	0.337	CaXy12	25.742188	1029.688
B	5	Blank B	E	0.052				
B	6	Sample X1	E	0.139	0.087	CaXy21	6.2109375	248.4375
B	7	Sample X1	E	0.139	0.087	CaXy21	6.2109375	248.4375
B	8	Sample X1	E	0.141	0.089	CaXy21	6.3671875	254.6875
B	9	Blank B	F	0.052				
B	10	Sample X1	F	0.194	0.142	CaGr11	10.507813	420.3125
B	11	Sample X1	F	0.191	0.139	CaGr11	10.273438	410.9375
B	12	Sample X1	F	0.191	0.139	CaGr11	10.273438	410.9375
C	1	Blank B	G	0.173				
C	2	Sample X1	G	0.282	0.109	CaGr12	7.9296875	317.1875
C	3	Sample X1	G	0.278	0.105	CaGr12	7.6171875	304.6875
C	4	Sample X1	G	0.278	0.105	CaGr12	7.6171875	304.6875
C	5	Blank B	H	0.4				
C	6	Sample X1	H	0.723	0.323	CaGr21	24.648438	985.9375
C	7	Sample X1	H	0.723	0.323	CaGr21	24.648438	985.9375
C	8	Sample X1	H	0.725	0.325	CaGr21	24.804688	992.1875
C	9	Blank B	I	0.241				
C	10	Sample X1	I	0.795	0.554	CaGc11	42.695313	1707.813
C	11	Sample X1	I	0.8	0.559	CaGc11	43.085938	1723.438
C	12	Sample X1	I	0.795	0.554	CaGc11	42.695313	1707.813
D	1	Blank B	J	0.059				
D	2	Sample X1	J	0.431	0.372	CaGc21	28.476563	1139.063
D	3	Sample X1	J	0.427	0.368	CaGc21	28.164063	1126.563
D	4	Sample X1	J	0.431	0.372	CaGc21	28.476563	1139.063
D	5	Blank B	K	0.264				
D	6	Sample X1	K	0.443	0.179	CaGl11	13.398438	535.9375
D	7	Sample X1	K	0.438	0.174	CaGl11	13.007813	520.3125
D	8	Sample X1	K	0.438	0.174	CaGl11	13.007813	520.3125
D	9	Blank B	L	0.079				
D	10	Sample X1	L	0.164	0.085	CaGl21	6.0546875	242.1875
D	11	Sample X1	L	0.161	0.082	CaGl21	5.8203125	232.8125
D	12	Sample X1	L	0.161	0.082	CaGl21	5.8203125	232.8125

Appendix 7.19 RCCDRSM TFC run 19

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.092				
E	2	Sample X1	A	0.18	0.088	CaSu11	6.289063	251.5625
E	3	Sample X1	A	0.178	0.086	CaSu11	6.132813	245.3125
E	4	Sample X1	A	0.178	0.086	CaSu11	6.132813	245.3125
E	5	Blank B	B	0.473				
E	6	Sample X1	B	0.874	0.401	CaFr11	30.74219	1229.688
E	7	Sample X1	B	0.882	0.409	CaFr11	31.36719	1254.688
E	8	Sample X1	B	0.882	0.409	CaFr11	31.36719	1254.688
E	9	Blank B	C	0.161				
E	10	Sample X1	C	0.59	0.429	CaFr12	32.92969	1317.188
E	11	Sample X1	C	0.588	0.427	CaFr12	32.77344	1310.938
E	12	Sample X1	C	0.588	0.427	CaFr12	32.77344	1310.938
F	1	Blank B	D	0.133				
F	2	Sample X1	D	0.221	0.088	CaFr21	6.289063	251.5625
F	3	Sample X1	D	0.222	0.089	CaFr21	6.367188	254.6875
F	4	Sample X1	D	0.221	0.088	CaFr21	6.289063	251.5625
C	1	Blank B	G	0.059				
C	2	Sample X1	G	0.324	0.265	CaXy11	20.11719	804.6875
C	3	Sample X1	G	0.324	0.265	CaXy11	20.11719	804.6875
C	4	Sample X1	G	0.329	0.27	CaXy11	20.50781	820.3125
F	5	Blank B	E	0.205				
F	6	Sample X1	E	0.293	0.088	CaXy12	6.289063	251.5625
F	7	Sample X1	E	0.29	0.085	CaXy12	6.054688	242.1875
F	8	Sample X1	E	0.29	0.085	CaXy12	6.054688	242.1875
B	9	Blank B	F	0.051				
B	10	Sample X1	F	0.135	0.084	CaXy21	5.976563	239.0625
B	11	Sample X1	F	0.135	0.084	CaXy21	5.976563	239.0625
B	12	Sample X1	F	0.139	0.088	CaXy21	6.289063	251.5625
F	9	Blank B	F	0.065				
F	10	Sample X1	F	0.147	0.082	CaGr11	5.820313	232.8125
F	11	Sample X1	F	0.147	0.082	CaGr11	5.820313	232.8125
F	12	Sample X1	F	0.151	0.086	CaGr11	6.132813	245.3125
G	1	Blank B	G	0.058				
G	2	Sample X1	G	0.144	0.086	CaGr12	6.132813	245.3125
G	3	Sample X1	G	0.143	0.085	CaGr12	6.054688	242.1875
G	4	Sample X1	G	0.144	0.086	CaGr12	6.132813	245.3125
G	5	Blank B	H	0.078				
G	6	Sample X1	H	0.166	0.088	CaGr21	6.289063	251.5625

Appendix 7.19 contd.

G	7	Sample X1	H	0.162	0.084	CaGr21	5.976563	239.0625
G	8	Sample X1	H	0.162	0.084	CaGr21	5.976563	239.0625
G	9	Blank B	I	0.17				
G	10	Sample X1	I	0.252	0.082	CaGc11	5.820313	232.8125
G	11	Sample X1	I	0.253	0.083	CaGc11	5.898438	235.9375
G	12	Sample X1	I	0.252	0.082	CaGc11	5.820313	232.8125
H	1	Blank B	J	0.057				
H	2	Sample X1	J	0.145	0.088	CaGc21	6.289063	251.5625
H	3	Sample X1	J	0.143	0.086	CaGc21	6.132813	245.3125
H	4	Sample X1	J	0.143	0.086	CaGc21	6.132813	245.3125
H	5	Blank B	K	0.053				
H	6	Sample X1	K	0.135	0.082	CaGl11	5.820313	232.8125
H	7	Sample X1	K	0.134	0.081	CaGl11	5.742188	229.6875
H	8	Sample X1	K	0.135	0.082	CaGl11	5.820313	232.8125
H	9	Blank B	L	0.178				
H	10	Sample X1	L	0.262	0.084	CaGl21	5.976563	239.0625
H	11	Sample X1	L	0.262	0.084	CaGl21	5.976563	239.0625
H	12	Sample X1	L	0.264	0.086	CaGl21	6.132813	245.3125

Appendix 7.20 RCCDRSM TFC run 20

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.439				
A	2	Sample X1	A	0.928	0.489	CaSu11	37.617188	1504.688
A	3	Sample X1	A	0.928	0.489	CaSu11	37.617188	1504.688
A	4	Sample X1	A	0.929	0.49	CaSu11	37.695313	1507.813
A	5	Blank B	B	0.062				
A	6	Sample X1	B	0.542	0.48	CaFr11	36.914063	1476.563
A	7	Sample X1	B	0.542	0.48	CaFr11	36.914063	1476.563
A	8	Sample X1	B	0.544	0.482	CaFr11	37.070313	1482.813
A	9	Blank B	C	0.049				
A	10	Sample X1	C	0.301	0.252	CaFr12	19.101563	764.0625
A	11	Sample X1	C	0.297	0.248	CaFr12	18.789063	751.5625
A	12	Sample X1	C	0.297	0.248	CaFr12	18.789063	751.5625
B	1	Blank B	D	0.157				
B	2	Sample X1	D	0.24	0.083	CaFr21	5.8984375	235.9375
B	3	Sample X1	D	0.237	0.08	CaFr21	5.6640625	226.5625
B	4	Sample X1	D	0.237	0.08	CaFr21	5.6640625	226.5625

Appendix 7.20 contd.

C	5	Blank B	H	0.053				
C	6	Sample X1	H	0.142	0.089	CaXy11	6.3671875	254.6875
C	7	Sample X1	H	0.138	0.085	CaXy11	6.0546875	242.1875
C	8	Sample X1	H	0.142	0.089	CaXy11	6.3671875	254.6875
B	5	Blank B	E	0.131				
B	6	Sample X1	E	0.421	0.29	CaXy12	22.070313	882.8125
B	7	Sample X1	E	0.415	0.284	CaXy12	21.601563	864.0625
B	8	Sample X1	E	0.415	0.284	CaXy12	21.601563	864.0625
C	1	Blank B	G	0.057				
C	2	Sample X1	G	0.145	0.088	CaXy21	6.2890625	251.5625
C	3	Sample X1	G	0.143	0.086	CaXy21	6.1328125	245.3125
C	4	Sample X1	G	0.145	0.088	CaXy21	6.2890625	251.5625
B	9	Blank B	F	0.167				
B	10	Sample X1	F	0.252	0.085	CaGr11	6.0546875	242.1875
B	11	Sample X1	F	0.255	0.088	CaGr11	6.2890625	251.5625
B	12	Sample X1	F	0.255	0.088	CaGr11	6.2890625	251.5625
C	1	Blank B	G	0.219				
C	2	Sample X1	G	0.322	0.103	CaGr12	7.4609375	298.4375
C	3	Sample X1	G	0.328	0.109	CaGr12	7.9296875	317.1875
C	4	Sample X1	G	0.322	0.103	CaGr12	7.4609375	298.4375
C	5	Blank B	H	0.13				
C	6	Sample X1	H	0.217	0.087	CaGr21	6.2109375	248.4375
C	7	Sample X1	H	0.216	0.086	CaGr21	6.1328125	245.3125
C	8	Sample X1	H	0.216	0.086	CaGr21	6.1328125	245.3125
C	9	Blank B	I	0.125				
C	10	Sample X1	I	0.214	0.089	CaGc11	6.3671875	254.6875
C	11	Sample X1	I	0.213	0.088	CaGc11	6.2890625	251.5625
C	12	Sample X1	I	0.214	0.089	CaGc11	6.3671875	254.6875
D	1	Blank B	J	0.095				
D	2	Sample X1	J	0.179	0.084	CaGc21	5.9765625	239.0625
D	3	Sample X1	J	0.18	0.085	CaGc21	6.0546875	242.1875
D	4	Sample X1	J	0.179	0.084	CaGc21	5.9765625	239.0625
D	5	Blank B	K	0.268				
D	6	Sample X1	K	0.443	0.175	CaGl11	13.085938	523.4375
D	7	Sample X1	K	0.446	0.178	CaGl11	13.320313	532.8125
D	8	Sample X1	K	0.443	0.175	CaGl11	13.085938	523.4375
D	9	Blank B	L	0.062				
D	10	Sample X1	L	0.15	0.088	CaGl21	6.2890625	251.5625
D	11	Sample X1	L	0.147	0.085	CaGl21	6.0546875	242.1875
D	12	Sample X1	L	0.147	0.085	CaGl21	6.0546875	242.1875

Appendix 7.21 RCCDRSM TFC run 21

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
E	9	Blank B	A	0.058				
E	10	Sample X1	A	0.256	0.198	CaSu11	14.88281	223.2422
E	11	Sample X1	A	0.257	0.199	CaSu11	14.96094	224.4141
E	12	Sample X1	A	0.256	0.198	CaSu11	14.88281	223.2422
C	1	Blank B	A	0.079				
C	2	Sample X1	A	0.395	0.316	CaFr11	24.10156	361.5234
C	3	Sample X1	A	0.397	0.318	CaFr11	24.25781	363.8672
C	4	Sample X1	A	0.397	0.318	CaFr11	24.25781	363.8672
C	5	Blank B	B	0.055				
C	6	Sample X1	B	0.333	0.278	CaFr12	21.13281	316.9922
C	7	Sample X1	B	0.331	0.276	CaFr12	20.97656	314.6484
C	8	Sample X1	B	0.331	0.276	CaFr12	20.97656	314.6484
C	9	Blank B	C	0.051				
C	10	Sample X1	C	0.339	0.288	CaFr21	21.91406	328.7109
C	11	Sample X1	C	0.34	0.289	CaFr21	21.99219	329.8828
C	12	Sample X1	C	0.339	0.288	CaFr21	21.91406	328.7109
D	1	Blank B	D	0.053				
D	2	Sample X1	D	0.137	0.084	CaXy11	5.976563	89.64844
D	3	Sample X1	D	0.134	0.081	CaXy11	5.742188	86.13281
D	4	Sample X1	D	0.137	0.084	CaXy11	5.976563	89.64844
D	5	Blank B	E	0.05				
D	6	Sample X1	E	0.136	0.086	CaXy12	6.132813	91.99219
D	7	Sample X1	E	0.132	0.082	CaXy12	5.820313	87.30469
D	8	Sample X1	E	0.132	0.082	CaXy12	5.820313	87.30469
D	9	Blank B	F	0.044				
D	10	Sample X1	F	0.128	0.084	CaXy21	5.976563	89.64844
D	11	Sample X1	F	0.124	0.08	CaXy21	5.664063	84.96094
D	12	Sample X1	F	0.124	0.08	CaXy21	5.664063	84.96094
F	1	Blank B	B	0.054				
F	2	Sample X1	B	0.137	0.083	CaGr11	5.898438	88.47656
F	3	Sample X1	B	0.139	0.085	CaGr11	6.054688	90.82031
F	4	Sample X1	B	0.142	0.088	CaGr11	6.289063	94.33594
F	5	Blank B	C	0.05				
F	6	Sample X1	C	0.13	0.08	CaGr12	5.664063	84.96094
F	7	Sample X1	C	0.137	0.087	CaGr12	6.210938	93.16406
F	8	Sample X1	C	0.137	0.087	CaGr12	6.210938	93.16406
F	9	Blank B	D	0.045				

Appendix 7.21 contd.

F	10	Sample X1	D	0.13	0.085	CaGr21	6.054688	90.82031
F	11	Sample X1	D	0.13	0.085	CaGr21	6.054688	90.82031
F	12	Sample X1	D	0.132	0.087	CaGr21	6.210938	93.16406
G	1	Blank B	E	0.054				
G	2	Sample X1	E	0.681	0.627	CaGc11	48.39844	725.9766
G	3	Sample X1	E	0.68	0.626	CaGc11	48.32031	724.8047
G	4	Sample X1	E	0.681	0.627	CaGc11	48.39844	725.9766
G	5	Blank B	F	0.046				
G	6	Sample X1	F	0.5	0.454	CaGc21	34.88281	523.2422
G	7	Sample X1	F	0.498	0.452	CaGc21	34.72656	520.8984
G	8	Sample X1	F	0.498	0.452	CaGc21	34.72656	520.8984
E	1	Blank B	G	0.062				
E	2	Sample X1	G	0.148	0.086	CaGl11	6.132813	91.99219
E	3	Sample X1	G	0.143	0.081	CaGl11	5.742188	86.13281
E	4	Sample X1	G	0.143	0.081	CaGl11	5.742188	86.13281
E	5	Blank B	H	0.047				
E	6	Sample X1	H	0.136	0.089	CaGl21	6.367188	95.50781
E	7	Sample X1	H	0.134	0.087	CaGl21	6.210938	93.16406
E	8	Sample X1	H	0.136	0.089	CaGl21	6.367188	95.50781

Appendix 7.22 RCCDRSM TFC run 22

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.074				
E	2	Sample X1	A	0.158	0.084	CaSu11	5.976563	298.8281
E	3	Sample X1	A	0.161	0.087	CaSu11	6.210938	310.5469
E	4	Sample X1	A	0.158	0.084	CaSu11	5.976563	298.8281
E	5	Blank B	B	0.06				
E	6	Sample X1	B	0.393	0.333	CaFr11	25.42969	1271.484
E	7	Sample X1	B	0.399	0.339	CaFr11	25.89844	1294.922
E	8	Sample X1	B	0.393	0.333	CaFr11	25.42969	1271.484
E	9	Blank B	C	0.177				
E	10	Sample X1	C	0.275	0.098	CaFr12	7.070313	353.5156
E	11	Sample X1	C	0.272	0.095	CaFr12	6.835938	341.7969
E	12	Sample X1	C	0.272	0.095	CaFr12	6.835938	341.7969
F	1	Blank B	D	0.066				
F	2	Sample X1	D	0.146	0.08	CaFr21	5.664063	283.2031
F	3	Sample X1	D	0.153	0.087	CaFr21	6.210938	310.5469

Appendix 7.22 contd.

F	4	Sample X1	D	0.146	0.08	CaFr21	5.664063	283.2031
C	9	Blank B	I	0.061				
C	10	Sample X1	I	0.142	0.081	CaXy11	5.742188	287.1094
C	11	Sample X1	I	0.143	0.082	CaXy11	5.820313	291.0156
C	12	Sample X1	I	0.142	0.081	CaXy11	5.742188	287.1094
F	5	Blank B	E	0.064				
F	6	Sample X1	E	0.146	0.082	CaXy12	5.820313	291.0156
F	7	Sample X1	E	0.146	0.082	CaXy12	5.820313	291.0156
F	8	Sample X1	E	0.151	0.087	CaXy12	6.210938	310.5469
C	5	Blank B	H	0.052				
C	6	Sample X1	H	0.137	0.085	CaXy21	6.054688	302.7344
C	7	Sample X1	H	0.138	0.086	CaXy21	6.132813	306.6406
C	8	Sample X1	H	0.137	0.085	CaXy21	6.054688	302.7344
F	9	Blank B	F	0.066				
F	10	Sample X1	F	0.155	0.089	CaGr11	6.367188	318.3594
F	11	Sample X1	F	0.153	0.087	CaGr11	6.210938	310.5469
F	12	Sample X1	F	0.153	0.087	CaGr11	6.210938	310.5469
G	1	Blank B	G	0.114				
G	2	Sample X1	G	0.198	0.084	CaGr12	5.976563	298.8281
G	3	Sample X1	G	0.198	0.084	CaGr12	5.976563	298.8281
G	4	Sample X1	G	0.2	0.086	CaGr12	6.132813	306.6406
G	5	Blank B	H	0.07				
G	6	Sample X1	H	0.152	0.082	CaGr21	5.820313	291.0156
G	7	Sample X1	H	0.153	0.083	CaGr21	5.898438	294.9219
G	8	Sample X1	H	0.152	0.082	CaGr21	5.820313	291.0156
G	9	Blank B	I	0.268				
G	10	Sample X1	I	0.453	0.185	CaGc11	13.86719	693.3594
G	11	Sample X1	I	0.451	0.183	CaGc11	13.71094	685.5469
G	12	Sample X1	I	0.453	0.185	CaGc11	13.86719	693.3594
H	1	Blank B	J	0.073				
H	2	Sample X1	J	0.159	0.086	CaGc21	6.132813	306.6406
H	3	Sample X1	J	0.155	0.082	CaGc21	5.820313	291.0156
H	4	Sample X1	J	0.155	0.082	CaGc21	5.820313	291.0156
H	5	Blank B	K	0.238				
H	6	Sample X1	K	0.403	0.165	CaGl11	12.30469	615.2344
H	7	Sample X1	K	0.413	0.175	CaGl11	13.08594	654.2969
H	8	Sample X1	K	0.413	0.175	CaGl11	13.08594	654.2969
H	9	Blank B	L	0.114				
H	10	Sample X1	L	0.199	0.085	CaGl21	6.054688	302.7344
H	11	Sample X1	L	0.202	0.088	CaGl21	6.289063	314.4531
H	12	Sample X1	L	0.202	0.088	CaGl21	6.289063	314.4531

Appendix 7.23 RCCDRSM TFC run 23

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.067				
E	2	Sample X1	A	0.131	0.084	CaSu11	5.976563	89.64844
E	3	Sample X1	A	0.128	0.084	CaSu11	5.976563	89.64844
E	4	Sample X1	A	0.124	0.087	CaSu11	6.210938	93.16406
E	5	Blank B	B	0.075				
E	6	Sample X1	B	0.358	0.283	CaFr11	21.52344	322.8516
E	7	Sample X1	B	0.363	0.288	CaFr11	21.91406	328.7109
E	8	Sample X1	B	0.358	0.283	CaFr11	21.52344	322.8516
E	9	Blank B	C	0.11				
E	10	Sample X1	C	0.192	0.082	CaFr12	5.820313	87.30469
E	11	Sample X1	C	0.198	0.088	CaFr12	6.289063	94.33594
E	12	Sample X1	C	0.198	0.088	CaFr12	6.289063	94.33594
F	1	Blank B	D	0.118				
F	2	Sample X1	D	0.206	0.088	CaFr21	6.289063	94.33594
F	3	Sample X1	D	0.201	0.083	CaFr21	5.898438	88.47656
F	4	Sample X1	D	0.201	0.083	CaFr21	5.898438	88.47656
D	1	Blank B	J	0.058				
D	2	Sample X1	J	0.147	0.089	CaXy11	6.367188	95.50781
D	3	Sample X1	J	0.146	0.088	CaXy11	6.289063	94.33594
D	4	Sample X1	J	0.146	0.088	CaXy11	6.289063	94.33594
F	5	Blank B	E	0.078				
F	6	Sample X1	E	0.165	0.087	CaXy12	6.210938	93.16406
F	7	Sample X1	E	0.167	0.089	CaXy12	6.367188	95.50781
F	8	Sample X1	E	0.165	0.087	CaXy12	6.210938	93.16406
C	9	Blank B	I	0.049				
C	10	Sample X1	I	0.13	0.081	CaXy21	5.742188	86.13281
C	11	Sample X1	I	0.131	0.082	CaXy21	5.820313	87.30469
C	12	Sample X1	I	0.13	0.081	CaXy21	5.742188	86.13281
F	9	Blank B	F	0.08				
F	10	Sample X1	F	0.165	0.085	CaGr11	6.054688	90.82031
F	11	Sample X1	F	0.164	0.084	CaGr11	5.976563	89.64844
F	12	Sample X1	F	0.164	0.084	CaGr11	5.976563	89.64844
G	1	Blank B	G	0.071				
G	2	Sample X1	G	0.156	0.085	CaGr12	6.054688	90.82031
G	3	Sample X1	G	0.158	0.087	CaGr12	6.210938	93.16406
G	4	Sample X1	G	0.156	0.085	CaGr12	6.054688	90.82031

Appendix 7.23 contd.

G	5	Blank B	H	0.048				
G	6	Sample X1	H	0.134	0.086	CaGr21	6.132813	91.99219
G	7	Sample X1	H	0.137	0.089	CaGr21	6.367188	95.50781
G	8	Sample X1	H	0.134	0.086	CaGr21	6.132813	91.99219
G	9	Blank B	I	0.306				
G	10	Sample X1	I	0.461	0.155	CaGc11	11.52344	172.8516
G	11	Sample X1	I	0.461	0.155	CaGc11	11.52344	172.8516
G	12	Sample X1	I	0.463	0.157	CaGc11	11.67969	175.1953
H	1	Blank B	J	0.056				
H	2	Sample X1	J	0.143	0.087	CaGc21	6.210938	93.16406
H	3	Sample X1	J	0.144	0.088	CaGc21	6.289063	94.33594
H	4	Sample X1	J	0.143	0.087	CaGc21	6.210938	93.16406
H	5	Blank B	K	0.072				
H	6	Sample X1	K	0.157	0.085	CaGl11	6.054688	90.82031
H	7	Sample X1	K	0.155	0.083	CaGl11	5.898438	88.47656
H	8	Sample X1	K	0.155	0.083	CaGl11	5.898438	88.47656
H	9	Blank B	L	0.045				
H	10	Sample X1	L	0.129	0.084	CaGl21	5.976563	89.64844
H	11	Sample X1	L	0.134	0.089	CaGl21	6.367188	95.50781
H	12	Sample X1	L	0.129	0.084	CaGl21	5.976563	89.64844

Appendix 7.24 RCCDRSM TFC run 24

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.065				
A	2	Sample X1	A	0.258	0.193	CaSu11	14.49219	217.3828
A	3	Sample X1	A	0.262	0.197	CaSu11	14.80469	222.0703
A	4	Sample X1	A	0.258	0.193	CaSu11	14.49219	217.3828
E	9	Blank B	A	0.09				
E	10	Sample X1	A	0.408	0.318	CaFr11	24.25781	363.8672
E	11	Sample X1	A	0.408	0.318	CaFr11	24.25781	363.8672
E	12	Sample X1	A	0.359	0.319	CaFr11	24.33594	365.0391
F	1	Blank B	B	0.059				
F	2	Sample X1	B	0.335	0.276	CaFr12	20.97656	314.6484
F	3	Sample X1	B	0.336	0.277	CaFr12	21.05469	315.8203
F	4	Sample X1	B	0.335	0.276	CaFr12	20.97656	314.6484
F	5	Blank B	C	0.074				
F	6	Sample X1	C	0.362	0.288	CaFr21	21.91406	328.7109

Appendix 7.24 contd.

F	7	Sample X1	C	0.363	0.289	CaFr21	21.99219	329.8828
F	8	Sample X1	C	0.363	0.289	CaFr21	21.99219	329.8828
F	9	Blank B	D	0.045				
F	10	Sample X1	D	0.134	0.089	CaXy11	6.367188	95.50781
F	11	Sample X1	D	0.13	0.085	CaXy11	6.054688	90.82031
F	12	Sample X1	D	0.127	0.082	CaXy11	5.820313	87.30469
G	1	Blank B	E	0.055				
G	2	Sample X1	E	0.138	0.083	CaXy12	5.898438	88.47656
G	3	Sample X1	E	0.141	0.086	CaXy12	6.132813	91.99219
G	4	Sample X1	E	0.139	0.084	CaXy12	5.976563	89.64844
G	5	Blank B	F	0.057				
G	6	Sample X1	F	0.144	0.087	CaXy21	6.210938	93.16406
G	7	Sample X1	F	0.143	0.086	CaXy21	6.132813	91.99219
G	8	Sample X1	F	0.143	0.086	CaXy21	6.132813	91.99219
A	5	Blank B	B	0.056				
A	6	Sample X1	B	0.143	0.087	CaGr11	6.210938	93.16406
A	7	Sample X1	B	0.145	0.089	CaGr11	6.367188	95.50781
A	8	Sample X1	B	0.145	0.089	CaGr11	6.367188	95.50781
A	9	Blank B	C	0.05				
A	10	Sample X1	C	0.135	0.085	CaGr12	6.054688	90.82031
A	11	Sample X1	C	0.132	0.082	CaGr12	5.820313	87.30469
A	12	Sample X1	C	0.131	0.081	CaGr12	5.742188	86.13281
B	1	Blank B	D	0.063				
B	2	Sample X1	D	0.146	0.083	CaGr21	5.898438	88.47656
B	3	Sample X1	D	0.149	0.086	CaGr21	6.132813	91.99219
B	4	Sample X1	D	0.147	0.084	CaGr21	5.976563	89.64844
B	5	Blank B	E	0.054				
B	6	Sample X1	E	0.769	0.715	CaGc11	55.27344	829.1016
B	7	Sample X1	E	0.772	0.718	CaGc11	55.50781	832.6172
B	8	Sample X1	E	0.77	0.716	CaGc11	55.35156	830.2734
B	9	Blank B	F	0.05				
B	10	Sample X1	F	0.517	0.467	CaGc21	35.89844	538.4766
B	11	Sample X1	F	0.519	0.469	CaGc21	36.05469	540.8203
B	12	Sample X1	F	0.51	0.46	CaGc21	35.35156	530.2734
G	9	Blank B	G	0.059				
G	10	Sample X1	G	0.146	0.087	CaGl11	6.210938	93.16406
G	11	Sample X1	G	0.142	0.083	CaGl11	5.898438	88.47656
G	12	Sample X1	G	0.148	0.089	CaGl11	6.367188	95.50781
H	1	Blank B	H	0.061				
H	2	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031
H	3	Sample X1	H	0.147	0.086	CaGl21	6.132813	91.99219
H	4	Sample X1	H	0.146	0.085	CaGl21	6.054688	90.82031

Appendix 7.25 RCCDRSM TFC run 25

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.13				
A	2	Sample X1	A	0.219	0.089	CaSu11	6.3671875	191.0156
A	3	Sample X1	A	0.212	0.082	CaSu11	5.8203125	174.6094
A	4	Sample X1	A	0.219	0.089	CaSu11	6.3671875	191.0156
A	5	Blank B	B	0.369				
A	6	Sample X1	B	0.458	0.089	CaFr11	6.3671875	191.0156
A	7	Sample X1	B	0.458	0.089	CaFr11	6.3671875	191.0156
A	8	Sample X1	B	0.464	0.095	CaFr11	6.8359375	205.0781
A	9	Blank B	C	0.208				
A	10	Sample X1	C	0.339	0.131	CaFr12	9.6484375	289.4531
A	11	Sample X1	C	0.34	0.132	CaFr12	9.7265625	291.7969
A	12	Sample X1	C	0.339	0.131	CaFr12	9.6484375	289.4531
B	1	Blank B	D	0.077				
B	2	Sample X1	D	0.165	0.088	CaFr21	6.2890625	188.6719
B	3	Sample X1	D	0.164	0.087	CaFr21	6.2109375	186.3281
B	4	Sample X1	D	0.164	0.087	CaFr21	6.2109375	186.3281
D	1	Blank B	J	0.065				
D	2	Sample X1	J	0.231	0.166	CaXy11	12.382813	371.4844
D	3	Sample X1	J	0.231	0.166	CaXy11	12.382813	371.4844
D	4	Sample X1	J	0.23	0.165	CaXy11	12.304688	369.1406
B	5	Blank B	E	0.197				
B	6	Sample X1	E	0.331	0.134	CaXy12	9.8828125	296.4844
B	7	Sample X1	E	0.331	0.134	CaXy12	9.8828125	296.4844
B	8	Sample X1	E	0.335	0.138	CaXy12	10.195313	305.8594
D	5	Blank B	K	0.051				
D	6	Sample X1	K	0.227	0.176	CaXy21	13.164063	394.9219
D	7	Sample X1	K	0.229	0.178	CaXy21	13.320313	399.6094
D	8	Sample X1	K	0.229	0.178	CaXy21	13.320313	399.6094
B	9	Blank B	F	0.059				
B	10	Sample X1	F	0.145	0.086	CaGr11	6.1328125	183.9844
B	11	Sample X1	F	0.145	0.086	CaGr11	6.1328125	183.9844
B	12	Sample X1	F	0.148	0.089	CaGr11	6.3671875	191.0156
C	1	Blank B	G	0.086				
C	2	Sample X1	G	0.17	0.084	CaGr12	5.9765625	179.2969
C	3	Sample X1	G	0.17	0.084	CaGr12	5.9765625	179.2969
C	4	Sample X1	G	0.174	0.088	CaGr12	6.2890625	188.6719
C	5	Blank B	H	0.226				

Appendix 7.25 contd.

C	6	Sample X1	H	0.327	0.101	CaGr21	7.3046875	219.1406
C	7	Sample X1	H	0.328	0.102	CaGr21	7.3828125	221.4844
C	8	Sample X1	H	0.327	0.101	CaGr21	7.3046875	219.1406
C	9	Blank B	I	0.102				
C	10	Sample X1	I	0.651	0.549	CaGc11	42.304688	1269.141
C	11	Sample X1	I	0.651	0.549	CaGc11	42.304688	1269.141
C	12	Sample X1	I	0.652	0.55	CaGc11	42.382813	1271.484
D	1	Blank B	J	0.079				
D	2	Sample X1	J	0.162	0.083	CaGc21	5.8984375	176.9531
D	3	Sample X1	J	0.162	0.083	CaGc21	5.8984375	176.9531
D	4	Sample X1	J	0.166	0.087	CaGc21	6.2109375	186.3281
D	5	Blank B	K	0.088				
D	6	Sample X1	K	0.175	0.087	CaGl11	6.2109375	186.3281
D	7	Sample X1	K	0.17	0.082	CaGl11	5.8203125	174.6094
D	8	Sample X1	K	0.17	0.082	CaGl11	5.8203125	174.6094
D	9	Blank B	L	0.059				
D	10	Sample X1	L	0.143	0.084	CaGl21	5.9765625	179.2969
D	11	Sample X1	L	0.143	0.084	CaGl21	5.9765625	179.2969
D	12	Sample X1	L	0.145	0.086	CaGl21	6.1328125	183.9844

Appendix 7.26 RCCDRSM TFC run 26

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.135				
E	2	Sample X1	A	0.22	0.085	CaSu11	6.0546875	181.6406
E	3	Sample X1	A	0.218	0.083	CaSu11	5.8984375	176.9531
E	4	Sample X1	A	0.218	0.083	CaSu11	5.8984375	176.9531
E	5	Blank B	B	0.066				
E	6	Sample X1	B	0.15	0.084	CaFr11	5.9765625	179.2969
E	7	Sample X1	B	0.155	0.089	CaFr11	6.3671875	191.0156
E	8	Sample X1	B	0.15	0.084	CaFr11	5.9765625	179.2969
E	9	Blank B	C	0.242				
E	10	Sample X1	C	0.399	0.157	CaFr12	11.679688	350.3906
E	11	Sample X1	C	0.395	0.153	CaFr12	11.367188	341.0156
E	12	Sample X1	C	0.399	0.157	CaFr12	11.679688	350.3906
F	1	Blank B	D	0.058				
F	2	Sample X1	D	0.142	0.084	CaFr21	5.9765625	179.2969
F	3	Sample X1	D	0.147	0.089	CaFr21	6.3671875	191.0156

Appendix 7.26 contd.

F	4	Sample X1	D	0.142	0.084	CaFr21	5.9765625	179.2969
D	9	Blank B	L	0.051				
D	10	Sample X1	L	0.136	0.085	CaXy11	6.0546875	181.6406
D	11	Sample X1	L	0.135	0.084	CaXy11	5.9765625	179.2969
D	12	Sample X1	L	0.135	0.084	CaXy11	5.9765625	179.2969
F	5	Blank B	E	0.133				
F	6	Sample X1	E	0.215	0.082	CaXy12	5.8203125	174.6094
F	7	Sample X1	E	0.215	0.082	CaXy12	5.8203125	174.6094
F	8	Sample X1	E	0.219	0.086	CaXy12	6.1328125	183.9844
D	5	Blank B	K	0.051				
D	6	Sample X1	K	0.227	0.176	CaXy21	13.164063	394.9219
D	7	Sample X1	K	0.229	0.178	CaXy21	13.320313	399.6094
D	8	Sample X1	K	0.229	0.178	CaXy21	13.320313	399.6094
F	9	Blank B	F	0.193				
F	10	Sample X1	F	0.311	0.118	CaGr11	8.6328125	258.9844
F	11	Sample X1	F	0.307	0.114	CaGr11	8.3203125	249.6094
F	12	Sample X1	F	0.307	0.114	CaGr11	8.3203125	249.6094
G	1	Blank B	G	0.058				
G	2	Sample X1	G	0.145	0.087	CaGr12	6.2109375	186.3281
G	3	Sample X1	G	0.145	0.087	CaGr12	6.2109375	186.3281
G	4	Sample X1	G	0.143	0.085	CaGr12	6.0546875	181.6406
G	5	Blank B	H	0.097				
G	6	Sample X1	H	0.181	0.084	CaGr21	5.9765625	179.2969
G	7	Sample X1	H	0.181	0.084	CaGr21	5.9765625	179.2969
G	8	Sample X1	H	0.183	0.086	CaGr21	6.1328125	183.9844
G	9	Blank B	I	0.358				
G	10	Sample X1	I	0.576	0.218	CaGc11	16.445313	493.3594
G	11	Sample X1	I	0.582	0.224	CaGc11	16.914063	507.4219
G	12	Sample X1	I	0.582	0.224	CaGc11	16.914063	507.4219
H	1	Blank B	J	0.109				
H	2	Sample X1	J	0.198	0.089	CaGc21	6.3671875	191.0156
H	3	Sample X1	J	0.195	0.086	CaGc21	6.1328125	183.9844
H	4	Sample X1	J	0.195	0.086	CaGc21	6.1328125	183.9844
H	5	Blank B	K	0.172				
H	6	Sample X1	K	0.259	0.087	CaGl11	6.2109375	186.3281
H	7	Sample X1	K	0.261	0.089	CaGl11	6.3671875	191.0156
H	8	Sample X1	K	0.261	0.089	CaGl11	6.3671875	191.0156
H	9	Blank B	L	0.097				
H	10	Sample X1	L	0.18	0.083	CaGl21	5.8984375	176.9531
H	11	Sample X1	L	0.182	0.085	CaGl21	6.0546875	181.6406
H	12	Sample X1	L	0.18	0.083	CaGl21	5.8984375	176.9531

Appendix 7.27 RCCDRSM TFC run 27

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.134				
A	2	Sample X1	A	0.218	0.084	CaSu11	5.9765625	179.2969
A	3	Sample X1	A	0.22	0.086	CaSu11	6.1328125	183.9844
A	4	Sample X1	A	0.218	0.084	CaSu11	5.9765625	179.2969
A	5	Blank B	B	0.152				
A	6	Sample X1	B	0.241	0.089	CaFr11	6.3671875	191.0156
A	7	Sample X1	B	0.241	0.089	CaFr11	6.3671875	191.0156
A	8	Sample X1	B	0.238	0.086	CaFr11	6.1328125	183.9844
A	9	Blank B	C	0.445				
A	10	Sample X1	C	0.822	0.377	CaFr12	28.867188	866.0156
A	11	Sample X1	C	0.818	0.373	CaFr12	28.554688	856.6406
A	12	Sample X1	C	0.822	0.377	CaFr12	28.867188	866.0156
B	1	Blank B	D	0.089				
B	2	Sample X1	D	0.178	0.089	CaFr21	6.3671875	191.0156
B	3	Sample X1	D	0.175	0.086	CaFr21	6.1328125	183.9844
B	4	Sample X1	D	0.175	0.086	CaFr21	6.1328125	183.9844
E	1	Blank B	M	0.061				
E	2	Sample X1	M	0.147	0.086	CaXy11	6.1328125	183.9844
E	3	Sample X1	M	0.145	0.084	CaXy11	5.9765625	179.2969
E	4	Sample X1	M	0.145	0.084	CaXy11	5.9765625	179.2969
B	5	Blank B	E	0.323				
B	6	Sample X1	E	0.58	0.257	CaXy12	19.492188	584.7656
B	7	Sample X1	E	0.582	0.259	CaXy12	19.648438	589.4531
B	8	Sample X1	E	0.58	0.257	CaXy12	19.492188	584.7656
D	9	Blank B	L	0.056				
D	10	Sample X1	L	0.138	0.082	CaXy21	5.8203125	174.6094
D	11	Sample X1	L	0.138	0.082	CaXy21	5.8203125	174.6094
D	12	Sample X1	L	0.137	0.081	CaXy21	5.7421875	172.2656
B	9	Blank B	F	0.135				
B	10	Sample X1	F	0.218	0.083	CaGr11	5.8984375	176.9531
B	11	Sample X1	F	0.218	0.083	CaGr11	5.8984375	176.9531
B	12	Sample X1	F	0.221	0.086	CaGr11	6.1328125	183.9844
C	1	Blank B	G	0.266				
C	2	Sample X1	G	0.461	0.195	CaGr12	14.648438	439.4531
C	3	Sample X1	G	0.461	0.195	CaGr12	14.648438	439.4531
C	4	Sample X1	G	0.467	0.201	CaGr12	15.117188	453.5156
C	5	Blank B	H	0.067				

Appendix 7.27 contd.

C	6	Sample X1	H	0.15	0.083	CaGr21	5.8984375	176.9531
C	7	Sample X1	H	0.153	0.086	CaGr21	6.1328125	183.9844
C	8	Sample X1	H	0.15	0.083	CaGr21	5.8984375	176.9531
C	9	Blank B	I	0.074				
C	10	Sample X1	I	0.156	0.082	CaGc11	5.8203125	174.6094
C	11	Sample X1	I	0.158	0.084	CaGc11	5.9765625	179.2969
C	12	Sample X1	I	0.156	0.082	CaGc11	5.8203125	174.6094
D	1	Blank B	J	0.109				
D	2	Sample X1	J	0.195	0.086	CaGc21	6.1328125	183.9844
D	3	Sample X1	J	0.198	0.089	CaGc21	6.3671875	191.0156
D	4	Sample X1	J	0.195	0.086	CaGc21	6.1328125	183.9844
D	5	Blank B	K	0.117				
D	6	Sample X1	K	0.198	0.081	CaGl11	5.7421875	172.2656
D	7	Sample X1	K	0.204	0.087	CaGl11	6.2109375	186.3281
D	8	Sample X1	K	0.198	0.081	CaGl11	5.7421875	172.2656
D	9	Blank B	L	0.063				
D	10	Sample X1	L	0.147	0.084	CaGl21	5.9765625	179.2969
D	11	Sample X1	L	0.151	0.088	CaGl21	6.2890625	188.6719
D	12	Sample X1	L	0.147	0.084	CaGl21	5.9765625	179.2969

Appendix 7.28 RCCDRSM TFC run 28

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
E	1	Blank B	A	0.203				
E	2	Sample X1	A	0.312	0.109	CaSu11	7.9296875	237.8906
E	3	Sample X1	A	0.309	0.106	CaSu11	7.6953125	230.8594
E	4	Sample X1	A	0.309	0.106	CaSu11	7.6953125	230.8594
E	5	Blank B	B	0.07				
E	6	Sample X1	B	0.31	0.24	CaFr11	18.164063	544.9219
E	7	Sample X1	B	0.31	0.24	CaFr11	18.164063	544.9219
E	8	Sample X1	B	0.311	0.241	CaFr11	18.242188	547.2656
E	9	Blank B	C	0.231				
E	10	Sample X1	C	0.37	0.139	CaFr12	10.273438	308.2031
E	11	Sample X1	C	0.374	0.143	CaFr12	10.585938	317.5781
E	12	Sample X1	C	0.37	0.139	CaFr12	10.273438	308.2031
F	1	Blank B	D	0.066				
F	2	Sample X1	D	0.152	0.086	CaFr21	6.1328125	183.9844

Appendix 7.28 contd.

F	3	Sample X1	D	0.152	0.086	CaFr21	6.1328125	183.9844
F	4	Sample X1	D	0.153	0.087	CaFr21	6.2109375	186.3281
E	5	Blank B	N	0.054				
E	6	Sample X1	N	0.138	0.084	CaXy11	5.9765625	179.2969
E	7	Sample X1	N	0.137	0.083	CaXy11	5.8984375	176.9531
E	8	Sample X1	N	0.138	0.084	CaXy11	5.9765625	179.2969
F	5	Blank B	E	0.135				
F	6	Sample X1	E	0.219	0.084	CaXy12	5.9765625	179.2969
F	7	Sample X1	E	0.224	0.089	CaXy12	6.3671875	191.0156
F	8	Sample X1	E	0.219	0.084	CaXy12	5.9765625	179.2969
E	1	Blank B	M	0.059				
E	2	Sample X1	M	0.141	0.082	CaXy21	5.8203125	174.6094
E	3	Sample X1	M	0.141	0.082	CaXy21	5.8203125	174.6094
E	4	Sample X1	M	0.14	0.081	CaXy21	5.7421875	172.2656
F	9	Blank B	F	0.046				
F	10	Sample X1	F	0.134	0.088	CaGr11	6.2890625	188.6719
F	11	Sample X1	F	0.132	0.086	CaGr11	6.1328125	183.9844
F	12	Sample X1	F	0.134	0.088	CaGr11	6.2890625	188.6719
G	1	Blank B	G	0.066				
G	2	Sample X1	G	0.148	0.082	CaGr12	5.8203125	174.6094
G	3	Sample X1	G	0.152	0.086	CaGr12	6.1328125	183.9844
G	4	Sample X1	G	0.148	0.082	CaGr12	5.8203125	174.6094
G	5	Blank B	H	0.107				
G	6	Sample X1	H	0.195	0.088	CaGr21	6.2890625	188.6719
G	7	Sample X1	H	0.196	0.089	CaGr21	6.3671875	191.0156
G	8	Sample X1	H	0.195	0.088	CaGr21	6.2890625	188.6719
G	9	Blank B	I	0.086				
G	10	Sample X1	I	0.17	0.084	CaGc11	5.9765625	179.2969
G	11	Sample X1	I	0.171	0.085	CaGc11	6.0546875	181.6406
G	12	Sample X1	I	0.17	0.084	CaGc11	5.9765625	179.2969
H	1	Blank B	J	0.106				
H	2	Sample X1	J	0.194	0.088	CaGc21	6.2890625	188.6719
H	3	Sample X1	J	0.192	0.086	CaGc21	6.1328125	183.9844
H	4	Sample X1	J	0.192	0.086	CaGc21	6.1328125	183.9844
H	5	Blank B	K	0.248				
H	6	Sample X1	K	0.422	0.174	CaGl11	13.007813	390.2344
H	7	Sample X1	K	0.422	0.174	CaGl11	13.007813	390.2344
H	8	Sample X1	K	0.425	0.177	CaGl11	13.242188	397.2656
H	9	Blank B	L	0.077				
H	10	Sample X1	L	0.088	0.087	CaGl21	6.2109375	186.3281
H	11	Sample X1	L	0.075	0.083	CaGl21	5.8984375	176.9531
H	12	Sample X1	L	0.094	0.087	CaGl21	6.2109375	186.3281

Appendix 7.29 RCCDRSM TFC run 29

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.088				
A	2	Sample X1	A	0.205	0.117	CaSu11	8.5546875	128.3203
A	3	Sample X1	A	0.207	0.119	CaSu11	8.7109375	130.6641
A	4	Sample X1	A	0.205	0.117	CaSu11	8.5546875	128.3203
A	5	Blank B	B	0.11				
A	6	Sample X1	B	0.226	0.116	CaFr11	8.4765625	127.1484
A	7	Sample X1	B	0.222	0.113	CaFr11	8.2421875	123.6328
A	8	Sample X1	B	0.226	0.116	CaFr11	8.4765625	127.1484
A	9	Blank B	C	0.081				
A	10	Sample X1	C	0.199	0.118	CaFr12	8.6328125	129.4922
A	11	Sample X1	C	0.2	0.119	CaFr12	8.7109375	130.6641
A	12	Sample X1	C	0.2	0.119	CaFr12	8.7109375	130.6641
B	1	Blank B	D	0.157				
B	2	Sample X1	D	0.242	0.085	CaFr21	6.0546875	90.82031
B	3	Sample X1	D	0.242	0.085	CaFr21	6.0546875	90.82031
B	4	Sample X1	D	0.241	0.084	CaFr21	5.9765625	89.64844
E	9	Blank B	O	0.046				
E	10	Sample X1	O	0.136	0.09	CaXy11	6.4453125	96.67969
E	11	Sample X1	O	0.136	0.09	CaXy11	6.4453125	96.67969
E	12	Sample X1	O	0.137	0.091	CaXy11	6.5234375	97.85156
B	5	Blank B	E	0.171				
B	6	Sample X1	E	0.257	0.086	CaXy12	6.1328125	91.99219
B	7	Sample X1	E	0.255	0.084	CaXy12	5.9765625	89.64844
B	8	Sample X1	E	0.255	0.084	CaXy12	5.9765625	89.64844
E	5	Blank B	N	0.053				
E	6	Sample X1	N	0.221	0.168	CaXy21	12.539063	188.0859
E	7	Sample X1	N	0.222	0.169	CaXy21	12.617188	189.2578
E	8	Sample X1	N	0.222	0.169	CaXy21	12.617188	189.2578
B	9	Blank B	F	0.254				
B	10	Sample X1	F	0.417	0.163	CaGr11	12.148438	182.2266
B	11	Sample X1	F	0.417	0.163	CaGr11	12.148438	182.2266
B	12	Sample X1	F	0.419	0.165	CaGr11	12.304688	184.5703
C	1	Blank B	G	0.15				
C	2	Sample X1	G	0.238	0.088	CaGr12	6.2890625	94.33594
C	3	Sample X1	G	0.238	0.088	CaGr12	6.2890625	94.33594
C	4	Sample X1	G	0.235	0.085	CaGr12	6.0546875	90.82031
C	5	Blank B	H	0.071				

Appendix 7.29 contd.

C	6	Sample X1	H	0.155	0.084	CaGr21	5.9765625	89.64844
C	7	Sample X1	H	0.157	0.086	CaGr21	6.1328125	91.99219
C	8	Sample X1	H	0.157	0.086	CaGr21	6.1328125	91.99219
C	9	Blank B	I	0.123				
C	10	Sample X1	I	0.204	0.081	CaGc11	5.7421875	86.13281
C	11	Sample X1	I	0.204	0.081	CaGc11	5.7421875	86.13281
C	12	Sample X1	I	0.209	0.086	CaGc11	6.1328125	91.99219
D	1	Blank B	J	0.085				
D	2	Sample X1	J	0.17	0.085	CaGc21	6.0546875	90.82031
D	3	Sample X1	J	0.17	0.085	CaGc21	6.0546875	90.82031
D	4	Sample X1	J	0.173	0.088	CaGc21	6.2890625	94.33594
D	5	Blank B	K	0.17				
D	6	Sample X1	K	0.257	0.087	CaGl11	6.2109375	93.16406
D	7	Sample X1	K	0.259	0.089	CaGl11	6.3671875	95.50781
D	8	Sample X1	K	0.257	0.087	CaGl11	6.2109375	93.16406
D	9	Blank B	L	0.132				
D	10	Sample X1	L	0.218	0.086	CaGl21	6.1328125	91.99219
D	11	Sample X1	L	0.218	0.086	CaGl21	6.1328125	91.99219
D	12	Sample X1	L	0.217	0.085	CaGl21	6.0546875	90.82031

Appendix 7.30 RCCDRSM TFC run 30

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/ml)	TFC (µgQE/g)
A	1	Blank B	A	0.061				
A	2	Sample X1	A	0.142	0.081	CaSu11	5.7421875	57.42188
A	3	Sample X1	A	0.142	0.081	CaSu11	5.7421875	57.42188
A	4	Sample X1	A	0.145	0.084	CaSu11	5.9765625	59.76563
A	5	Blank B	B	0.06				
A	6	Sample X1	B	0.389	0.329	CaFr11	25.117188	251.1719
A	7	Sample X1	B	0.389	0.329	CaFr11	25.117188	251.1719
A	8	Sample X1	B	0.394	0.334	CaFr11	25.507813	255.0781
A	9	Blank B	C	0.168				
A	10	Sample X1	C	0.253	0.085	CaFr12	6.0546875	60.54688
A	11	Sample X1	C	0.253	0.085	CaFr12	6.0546875	60.54688
A	12	Sample X1	C	0.252	0.084	CaFr12	5.9765625	59.76563
B	1	Blank B	D	0.165				
B	2	Sample X1	D	0.246	0.081	CaFr21	5.7421875	57.42188
B	3	Sample X1	D	0.246	0.081	CaFr21	5.7421875	57.42188

Appendix 7.30 contd.

B	4	Sample X1	D	0.246	0.081	CaFr21	5.7421875	57.42188
F	1	Blank B	P	0.061				
F	2	Sample X1	P	0.147	0.086	CaXy11	6.1328125	61.32813
F	3	Sample X1	P	0.147	0.086	CaXy11	6.1328125	61.32813
F	4	Sample X1	P	0.146	0.085	CaXy11	6.0546875	60.54688
B	5	Blank B	E	0.086				
B	6	Sample X1	E	0.173	0.087	CaXy12	6.2109375	62.10938
B	7	Sample X1	E	0.172	0.086	CaXy12	6.1328125	61.32813
B	8	Sample X1	E	0.174	0.088	CaXy12	6.2890625	61.32813
E	9	Blank B	O	0.051				
E	10	Sample X1	O	0.377	0.326	CaXy21	24.882813	248.8281
E	11	Sample X1	O	0.377	0.326	CaXy21	24.882813	248.8281
E	12	Sample X1	O	0.375	0.324	CaXy21	24.726563	247.2656
B	9	Blank B	F	0.063				
B	10	Sample X1	F	0.145	0.082	CaGr11	5.8203125	58.20313
B	11	Sample X1	F	0.145	0.082	CaGr11	5.8203125	58.20313
B	12	Sample X1	F	0.151	0.088	CaGr11	6.2890625	62.89063
C	1	Blank B	G	0.122				
C	2	Sample X1	G	0.206	0.084	CaGr12	5.9765625	59.76563
C	3	Sample X1	G	0.211	0.089	CaGr12	6.3671875	63.67188
C	4	Sample X1	G	0.206	0.084	CaGr12	5.9765625	59.76563
C	5	Blank B	H	0.105				
C	6	Sample X1	H	0.186	0.081	CaGr21	5.7421875	57.42188
C	7	Sample X1	H	0.186	0.081	CaGr21	5.7421875	57.42188
C	8	Sample X1	H	0.187	0.082	CaGr21	5.8203125	58.20313
C	9	Blank B	I	0.264				
C	10	Sample X1	I	0.345	0.081	CaGc11	5.7421875	57.42188
C	11	Sample X1	I	0.344	0.08	CaGc11	5.6640625	56.64063
C	12	Sample X1	I	0.344	0.08	CaGc11	5.6640625	56.64063
D	1	Blank B	J	0.118				
D	2	Sample X1	J	0.214	0.096	CaGc21	6.9140625	69.14063
D	3	Sample X1	J	0.214	0.096	CaGc21	6.9140625	69.14063
D	4	Sample X1	J	0.224	0.106	CaGc21	7.6953125	76.95313
D	5	Blank B	K	0.356				
D	6	Sample X1	K	0.577	0.221	CaGl11	16.679688	166.7969
D	7	Sample X1	K	0.57	0.214	CaGl11	16.132813	161.3281
D	8	Sample X1	K	0.576	0.22	CaGl11	16.601563	166.0156
D	9	Blank B	L	0.096				
D	10	Sample X1	L	0.183	0.087	CaGl21	6.2109375	62.10938
D	11	Sample X1	L	0.192	0.096	CaGl21	6.9140625	69.14063
D	12	Sample X1	L	0.183	0.087	CaGl21	6.2109375	62.10938

Appendix 8.1 RCCDRSM CUPRAC run 1

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.11				
A	2	Sample X1	A	0.201	0.091	CaSu11	0.310562	3.1056202
A	3	Sample X1	A	0.201	0.091	CaSu11	0.310562	3.1056202
A	4	Sample X1	A	0.202	0.092	CaSu11	0.3129845	3.129845
A	5	Blank B	B	0.092				
A	6	Sample X1	B	0.186	0.096	CaFr11	0.3226744	3.2267442
A	7	Sample X1	B	0.184	0.092	CaFr11	0.3129845	3.129845
A	8	Sample X1	B	0.188	0.096	CaFr11	0.3226744	3.2267442
A	9	Blank B	C	0.064				
A	10	Sample X1	C	0.158	0.094	CaFr12	0.3178295	3.1782946
A	11	Sample X1	C	0.157	0.093	CaFr12	0.315407	3.1540698
A	12	Sample X1	C	0.158	0.094	CaFr12	0.3178295	3.1782946
B	1	Blank B	D	0.14				
B	2	Sample X1	D	0.23	0.09	CaFr21	0.3081395	3.0813953
B	3	Sample X1	D	0.231	0.091	CaFr21	0.310562	3.1056202
B	4	Sample X1	D	0.231	0.091	CaFr21	0.310562	3.1056202
A	1	Blank B	A	0.118				
A	2	Sample X1	A	0.212	0.094	CaXy11	0.3178295	3.1782946
A	3	Sample X1	A	0.215	0.097	CaXy11	0.3250969	3.250969
A	4	Sample X1	A	0.212	0.094	CaXy11	0.3178295	3.1782946
B	5	Blank B	E	0.061				
B	6	Sample X1	E	0.16	0.099	CaXy12	0.3299419	3.2994186
B	7	Sample X1	E	0.16	0.099	CaXy12	0.3299419	3.2994186
B	8	Sample X1	E	0.157	0.096	CaXy12	0.3226744	3.2267442
A	1	Blank B	A	0.128				
A	2	Sample X1	A	0.219	0.091	CaXy21	0.310562	3.1056202
A	3	Sample X1	A	0.219	0.091	CaXy21	0.310562	3.1056202
A	4	Sample X1	A	0.219	0.091	CaXy21	0.310562	3.1056202
B	9	Blank B	F	0.097				
B	10	Sample X1	F	0.193	0.096	CaGr11	0.3226744	3.2267442
B	11	Sample X1	F	0.191	0.094	CaGr11	0.3178295	3.1782946
B	12	Sample X1	F	0.191	0.094	CaGr11	0.3178295	3.1782946
C	1	Blank B	G	0.104				
C	2	Sample X1	G	0.2	0.096	CaGr12	0.3226744	3.2267442
C	3	Sample X1	G	0.198	0.094	CaGr12	0.3178295	3.1782946
C	4	Sample X1	G	0.198	0.094	CaGr12	0.3178295	3.1782946
C	5	Blank B	H	0.079				

Appendix 8.1 contd.

C	6	Sample X1	H	0.174	0.095	CaGr21	0.3202519	3.2025194
C	7	Sample X1	H	0.172	0.093	CaGr21	0.315407	3.1540698
C	8	Sample X1	H	0.172	0.093	CaGr21	0.315407	3.1540698
C	9	Blank B	I	0.094				
C	10	Sample X1	I	0.189	0.095	CaGc11	0.3202519	3.2025194
C	11	Sample X1	I	0.187	0.093	CaGc11	0.315407	3.1540698
C	12	Sample X1	I	0.187	0.093	CaGc11	0.315407	3.1540698
D	1	Blank B	J	0.087				
D	2	Sample X1	J	0.178	0.091	CaGc21	0.310562	3.1056202
D	3	Sample X1	J	0.178	0.091	CaGc21	0.310562	3.1056202
D	4	Sample X1	J	0.179	0.092	CaGc21	0.3129845	3.129845
D	5	Blank B	K	0.087				
D	6	Sample X1	K	0.182	0.095	CaGl11	0.3202519	3.2025194
D	7	Sample X1	K	0.179	0.092	CaGl11	0.3129845	3.129845
D	8	Sample X1	K	0.179	0.092	CaGl11	0.3129845	3.129845
D	9	Blank B	L	0.086				
D	10	Sample X1	L	0.183	0.097	CaGl21	0.3250969	3.250969
D	11	Sample X1	L	0.178	0.092	CaGl21	0.3129845	3.129845
D	12	Sample X1	L	0.178	0.092	CaGl21	0.3129845	3.129845

Appendix 8.2 RCCDRSM CURAC run 2

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.097				
E	2	Sample X1	A	0.191	0.094	CaSu11	0.3178295	6.356589
E	3	Sample X1	A	0.191	0.094	CaSu11	0.3178295	6.356589
E	4	Sample X1	A	0.19	0.093	CaSu11	0.315407	6.30814
E	5	Blank B	B	0.108				
E	6	Sample X1	B	0.203	0.094	CaFr11	0.3178295	6.356589
E	7	Sample X1	B	0.202	0.093	CaFr11	0.315407	6.30814
E	8	Sample X1	B	0.203	0.094	CaFr11	0.3178295	6.356589
E	9	Blank B	C	0.172				
E	10	Sample X1	C	0.263	0.091	CaFr12	0.310562	6.21124
E	11	Sample X1	C	0.263	0.091	CaFr12	0.310562	6.21124
E	12	Sample X1	C	0.264	0.092	CaFr12	0.3129845	6.25969
F	1	Blank B	D	0.125				
F	2	Sample X1	D	0.216	0.091	CaFr21	0.310562	6.21124
F	3	Sample X1	D	0.215	0.09	CaFr21	0.3081395	6.162791

Appendix 8.2 contd.

F	4	Sample X1	D	0.215	0.09	CaFr21	0.3081395	6.162791
A	5	Blank B	B	0.101				
A	6	Sample X1	B	0.193	0.092	CaXy11	0.3129845	6.25969
A	7	Sample X1	B	0.192	0.091	CaXy11	0.310562	6.21124
A	8	Sample X1	B	0.192	0.091	CaXy11	0.310562	6.21124
F	5	Blank B	E	0.065				
F	6	Sample X1	E	0.16	0.095	CaXy12	0.3202519	6.405039
F	7	Sample X1	E	0.16	0.095	CaXy12	0.3202519	6.405039
F	8	Sample X1	E	0.158	0.093	CaXy12	0.315407	6.30814
A	5	Blank B	B	0.101				
A	6	Sample X1	B	0.194	0.093	CaXy21	0.315407	6.30814
A	7	Sample X1	B	0.192	0.091	CaXy21	0.310562	6.21124
A	8	Sample X1	B	0.192	0.091	CaXy21	0.310562	6.21124
F	9	Blank B	F	0.128				
F	10	Sample X1	F	0.211	0.093	CaGr11	0.315407	6.30814
F	11	Sample X1	F	0.21	0.092	CaGr11	0.3129845	6.25969
F	12	Sample X1	F	0.21	0.092	CaGr11	0.3129845	6.25969
G	1	Blank B	G	0.114				
G	2	Sample X1	G	0.207	0.093	CaGr12	0.315407	6.30814
G	3	Sample X1	G	0.207	0.093	CaGr12	0.315407	6.30814
G	4	Sample X1	G	0.211	0.097	CaGr12	0.3250969	6.501938
G	5	Blank B	H	0.133				
G	6	Sample X1	H	0.224	0.091	CaGr21	0.310562	6.21124
G	7	Sample X1	H	0.225	0.092	CaGr21	0.3129845	6.25969
G	8	Sample X1	H	0.224	0.091	CaGr21	0.310562	6.21124
G	9	Blank B	I	0.097				
G	10	Sample X1	I	0.191	0.094	CaGc11	0.3178295	6.356589
G	11	Sample X1	I	0.191	0.094	CaGc11	0.3178295	6.356589
G	12	Sample X1	I	0.19	0.093	CaGc11	0.315407	6.30814
H	1	Blank B	J	0.106				
H	2	Sample X1	J	0.198	0.092	CaGc21	0.3129845	6.25969
H	3	Sample X1	J	0.198	0.092	CaGc21	0.3129845	6.25969
H	4	Sample X1	J	0.199	0.093	CaGc21	0.315407	6.30814
H	5	Blank B	K	0.126				
H	6	Sample X1	K	0.224	0.098	CaGl11	0.3275194	6.550388
H	7	Sample X1	K	0.225	0.099	CaGl11	0.3299419	6.598837
H	8	Sample X1	K	0.224	0.098	CaGl11	0.3275194	6.550388
H	9	Blank B	L	0.12				
H	10	Sample X1	L	0.213	0.093	CaGl21	0.315407	6.30814
H	11	Sample X1	L	0.214	0.094	CaGl21	0.3178295	6.356589
H	12	Sample X1	L	0.213	0.093	CaGl21	0.315407	6.30814

Appendix 8.3 RCCDRSM CUPRAC run 3

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.122				
D	2	Sample X1	J	0.213	0.091	CaSu11	0.31056202	4.65843023
D	3	Sample X1	J	0.215	0.093	CaSu11	0.31540698	4.73110465
D	4	Sample X1	J	0.215	0.093	CaSu11	0.31540698	4.73110465
A	1	Blank B	A	0.136				
A	2	Sample X1	A	0.232	0.096	CaFr11	0.32267442	4.84011628
A	3	Sample X1	A	0.233	0.097	CaFr11	0.3250969	4.87645349
A	4	Sample X1	A	0.233	0.097	CaFr11	0.3250969	4.87645349
A	5	Blank B	B	0.103				
A	6	Sample X1	B	0.201	0.098	CaFr12	0.32751938	4.9127907
A	7	Sample X1	B	0.199	0.096	CaFr12	0.32267442	4.84011628
A	8	Sample X1	B	0.201	0.098	CaFr12	0.32751938	4.9127907
A	9	Blank B	C	0.117				
A	10	Sample X1	C	0.21	0.093	CaFr21	0.31540698	4.73110465
A	11	Sample X1	C	0.21	0.093	CaFr21	0.31540698	4.73110465
A	12	Sample X1	C	0.212	0.095	CaFr21	0.32025194	4.80377907
B	1	Blank B	D	0.093				
B	2	Sample X1	D	0.187	0.094	CaXy11	0.31782946	4.76744186
B	3	Sample X1	D	0.187	0.094	CaXy11	0.31782946	4.76744186
B	4	Sample X1	D	0.19	0.097	CaXy11	0.3250969	4.87645349
B	5	Blank B	E	0.106				
B	6	Sample X1	E	0.196	0.09	CaXy12	0.30813953	4.62209302
B	7	Sample X1	E	0.197	0.091	CaXy12	0.31056202	4.65843023
B	8	Sample X1	E	0.197	0.091	CaXy12	0.31056202	4.65843023
B	9	Blank B	F	0.099				
B	10	Sample X1	F	0.195	0.096	CaXy21	0.32267442	4.84011628
B	11	Sample X1	F	0.195	0.096	CaXy21	0.32267442	4.84011628
B	12	Sample X1	F	0.197	0.098	CaXy21	0.32751938	4.9127907
C	1	Blank B	G	0.095				
C	2	Sample X1	G	0.12	0.095	CaGr11	0.32025194	4.80377907
C	3	Sample X1	G	0.111	0.096	CaGr11	0.32267442	4.84011628
C	4	Sample X1	G	0.12	0.095	CaGr11	0.32025194	4.80377907
C	5	Blank B	H	0.103				
C	6	Sample X1	H	0.103	0.09	CaGr12	0.30813953	4.62209302
C	7	Sample X1	H	0.103	0.09	CaGr12	0.30813953	4.62209302
C	8	Sample X1	H	0.105	0.092	CaGr12	0.3129845	4.69476744
C	9	Blank B	I	0.08				
C	10	Sample X1	I	0.172	0.092	CaGr21	0.3129845	4.69476744

Appendix 8.3 contd.

C	11	Sample X1	I	0.171	0.091	CaGr21	0.31056202	4.65843023
C	12	Sample X1	I	0.171	0.091	CaGr21	0.31056202	4.65843023
D	5	Blank B	K	0.084				
D	6	Sample X1	K	0.178	0.094	CaGc11	0.31782946	4.76744186
D	7	Sample X1	K	0.178	0.094	CaGc11	0.31782946	4.76744186
D	8	Sample X1	K	0.177	0.093	CaGc11	0.31540698	4.73110465
D	9	Blank B	L	0.065				
D	10	Sample X1	L	0.161	0.096	CaGc21	0.32267442	4.84011628
D	11	Sample X1	L	0.161	0.096	CaGc21	0.32267442	4.84011628
D	12	Sample X1	L	0.159	0.094	CaGc21	0.31782946	4.76744186
E	1	Blank B	M	0.091				
E	2	Sample X1	M	0.184	0.093	CaGl11	0.31540698	4.73110465
E	3	Sample X1	M	0.184	0.093	CaGl11	0.31540698	4.73110465
E	4	Sample X1	M	0.185	0.094	CaGl11	0.31782946	4.76744186
E	5	Blank B	N	0.09				
E	6	Sample X1	N	0.18	0.09	CaGl21	0.30813953	4.62209302
E	7	Sample X1	N	0.18	0.09	CaGl21	0.30813953	4.62209302
E	8	Sample X1	N	0.18	0.09	CaGl21	0.30813953	4.62209302

Appendix 8.4 RCCDRSM CUPRAC run 4

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.108				
D	2	Sample X1	J	0.204	0.096	CaSu11	0.32267442	4.84011628
D	3	Sample X1	J	0.206	0.098	CaSu11	0.32751938	4.9127907
D	4	Sample X1	J	0.204	0.096	CaSu11	0.32267442	4.84011628
A	1	Blank B	A	0.133				
A	2	Sample X1	A	0.227	0.094	CaFr11	0.31782946	4.76744186
A	3	Sample X1	A	0.226	0.093	CaFr11	0.31540698	4.73110465
A	4	Sample X1	A	0.226	0.093	CaFr11	0.31540698	4.73110465
A	5	Blank B	B	0.091				
A	6	Sample X1	B	0.182	0.091	CaFr12	0.31056202	4.65843023
A	7	Sample X1	B	0.183	0.092	CaFr12	0.3129845	4.69476744
A	8	Sample X1	B	0.183	0.092	CaFr12	0.3129845	4.69476744
A	9	Blank B	C	0.102				
A	10	Sample X1	C	0.194	0.092	CaFr21	0.3129845	4.69476744
A	11	Sample X1	C	0.193	0.091	CaFr21	0.31056202	4.65843023
A	12	Sample X1	C	0.193	0.091	CaFr21	0.31056202	4.65843023
B	1	Blank B	D	0.072				

Appendix 8.4 contd.

B	2	Sample X1	D	0.166	0.094	CaXy11	0.31782946	4.76744186
B	3	Sample X1	D	0.165	0.093	CaXy11	0.31540698	4.73110465
B	4	Sample X1	D	0.166	0.094	CaXy11	0.31782946	4.76744186
B	5	Blank B	E	0.085				
B	6	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.87645349
B	7	Sample X1	E	0.181	0.096	CaXy12	0.32267442	4.84011628
B	8	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.87645349
B	9	Blank B	F	0.071				
B	10	Sample X1	F	0.164	0.093	CaXy21	0.31540698	4.73110465
B	11	Sample X1	F	0.162	0.091	CaXy21	0.31056202	4.65843023
B	12	Sample X1	F	0.164	0.093	CaXy21	0.31540698	4.73110465
C	1	Blank B	G	0.064				
C	2	Sample X1	G	0.162	0.098	CaGr11	0.32751938	4.9127907
C	3	Sample X1	G	0.162	0.098	CaGr11	0.32751938	4.9127907
C	4	Sample X1	G	0.161	0.096	CaGr11	0.32267442	4.84011628
C	5	Blank B	H	0.086				
C	6	Sample X1	H	0.182	0.096	CaGr12	0.32267442	4.84011628
C	7	Sample X1	H	0.183	0.097	CaGr12	0.3250969	4.87645349
C	8	Sample X1	H	0.182	0.096	CaGr12	0.32267442	4.84011628
C	9	Blank B	I	0.074				
C	10	Sample X1	I	0.165	0.091	CaGr21	0.31056202	4.65843023
C	11	Sample X1	I	0.165	0.091	CaGr21	0.31056202	4.65843023
C	12	Sample X1	I	0.166	0.092	CaGr21	0.3129845	4.69476744
D	5	Blank B	K	0.063				
D	6	Sample X1	K	0.167	0.104	CaGc11	0.34205426	5.13081395
D	7	Sample X1	K	0.166	0.103	CaGc11	0.33963178	5.09447674
D	8	Sample X1	K	0.166	0.103	CaGc11	0.33963178	5.09447674
D	9	Blank B	L	0.08				
D	10	Sample X1	L	0.176	0.096	CaGc21	0.32267442	4.84011628
D	11	Sample X1	L	0.177	0.097	CaGc21	0.3250969	4.87645349
D	12	Sample X1	L	0.176	0.096	CaGc21	0.32267442	4.84011628
E	1	Blank B	M	0.095				
E	2	Sample X1	M	0.192	0.097	CaGl11	0.3250969	4.87645349
E	3	Sample X1	M	0.19	0.095	CaGl11	0.32025194	4.80377907
E	4	Sample X1	M	0.192	0.097	CaGl11	0.3250969	4.87645349
E	5	Blank B	N	0.082				
E	6	Sample X1	N	0.173	0.091	CaGl21	0.31056202	4.65843023
E	7	Sample X1	N	0.172	0.09	CaGl21	0.30813953	4.62209302
E	8	Sample X1	N	0.173	0.091	CaGl21	0.31056202	4.65843023

Appendix 8.5 RCCDRSM CUPRAC run 5

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.091				
D	2	Sample X1	J	0.189	0.098	CaSu11	0.32751938	3.2751938
D	3	Sample X1	J	0.189	0.098	CaSu11	0.32751938	3.2751938
D	4	Sample X1	J	0.189	0.098	CaSu11	0.32751938	3.2751938
A	1	Blank B	A	0.111				
A	2	Sample X1	A	0.234	0.123	CaFr11	0.3880814	3.88081395
A	3	Sample X1	A	0.232	0.121	CaFr11	0.38323643	3.83236434
A	4	Sample X1	A	0.232	0.121	CaFr11	0.38323643	3.83236434
A	5	Blank B	B	0.087				
A	6	Sample X1	B	0.182	0.095	CaFr12	0.32025194	3.20251938
A	7	Sample X1	B	0.182	0.095	CaFr12	0.32025194	3.20251938
A	8	Sample X1	B	0.18	0.093	CaFr12	0.31540698	3.15406977
A	9	Blank B	C	0.082				
A	10	Sample X1	C	0.177	0.095	CaFr21	0.32025194	3.20251938
A	11	Sample X1	C	0.174	0.093	CaFr21	0.31540698	3.15406977
A	12	Sample X1	C	0.174	0.093	CaFr21	0.31540698	3.15406977
B	1	Blank B	D	0.07				
B	2	Sample X1	D	0.165	0.095	CaXy11	0.32025194	3.20251938
B	3	Sample X1	D	0.164	0.094	CaXy11	0.31782946	3.17829457
B	4	Sample X1	D	0.164	0.094	CaXy11	0.31782946	3.17829457
B	5	Blank B	E	0.095				
B	6	Sample X1	E	0.186	0.091	CaXy12	0.31056202	3.10562016
B	7	Sample X1	E	0.185	0.09	CaXy12	0.30813953	3.08139535
B	8	Sample X1	E	0.186	0.091	CaXy12	0.31056202	3.10562016
B	9	Blank B	F	0.07				
B	10	Sample X1	F	0.16	0.09	CaXy21	0.30813953	3.08139535
B	11	Sample X1	F	0.162	0.092	CaXy21	0.3129845	3.12984496
B	12	Sample X1	F	0.162	0.092	CaXy21	0.3129845	3.12984496
C	1	Blank B	G	0.073				
C	2	Sample X1	G	0.171	0.098	CaGr11	0.32751938	3.2751938
C	3	Sample X1	G	0.168	0.095	CaGr11	0.32025194	3.20251938
C	4	Sample X1	G	0.168	0.095	CaGr11	0.32025194	3.20251938
C	5	Blank B	H	0.088				
C	6	Sample X1	H	0.182	0.094	CaGr12	0.31782946	3.17829457
C	7	Sample X1	H	0.18	0.092	CaGr12	0.3129845	3.12984496
C	8	Sample X1	H	0.18	0.092	CaGr12	0.3129845	3.12984496
C	9	Blank B	I	0.07				

Appendix 8.5 contd.

C	10	Sample X1	I	0.163	0.093	CaGr21	0.31540698	3.15406977
C	11	Sample X1	I	0.164	0.094	CaGr21	0.31782946	3.17829457
C	12	Sample X1	I	0.163	0.093	CaGr21	0.31540698	3.15406977
D	5	Blank B	K	0.075				
D	6	Sample X1	K	0.165	0.09	CaGc11	0.30813953	3.08139535
D	7	Sample X1	K	0.165	0.09	CaGc11	0.30813953	3.08139535
D	8	Sample X1	K	0.167	0.092	CaGc11	0.3129845	3.12984496
D	9	Blank B	L	0.073				
D	10	Sample X1	L	0.165	0.092	CaGc21	0.3129845	3.12984496
D	11	Sample X1	L	0.166	0.093	CaGc21	0.31540698	3.15406977
D	12	Sample X1	L	0.166	0.093	CaGc21	0.31540698	3.15406977
E	1	Blank B	M	0.091				
E	2	Sample X1	M	0.183	0.092	CaGl11	0.3129845	3.12984496
E	3	Sample X1	M	0.183	0.092	CaGl11	0.3129845	3.12984496
E	4	Sample X1	M	0.192	0.091	CaGl11	0.31056202	3.10562016
E	5	Blank B	N	0.08				
E	6	Sample X1	N	0.175	0.095	CaGl21	0.32025194	3.20251938
E	7	Sample X1	N	0.173	0.093	CaGl21	0.31540698	3.15406977
E	8	Sample X1	N	0.173	0.093	CaGl21	0.31540698	3.15406977

Appendix 8.6 RCCDRSM CUPRAC run 6

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.096				
D	2	Sample X1	J	0.186	0.093	CaSu11	0.315406977	3.154069767
D	3	Sample X1	J	0.186	0.093	CaSu11	0.315406977	3.154069767
D	4	Sample X1	J	0.186	0.093	CaSu11	0.315406977	3.154069767
A	1	Blank B	A	0.163				
A	2	Sample X1	A	0.256	0.093	CaFr11	0.315406977	3.468992248
A	3	Sample X1	A	0.254	0.091	CaFr11	0.310562016	3.105620155
A	4	Sample X1	A	0.254	0.091	CaFr11	0.310562016	3.105620155
A	5	Blank B	B	0.098				
A	6	Sample X1	B	0.191	0.093	CaFr12	0.315406977	3.154069767
A	7	Sample X1	B	0.193	0.095	CaFr12	0.320251938	3.20251938
A	8	Sample X1	B	0.191	0.093	CaFr12	0.315406977	3.154069767
A	9	Blank B	C	0.091				
A	10	Sample X1	C	0.198	0.107	CaFr21	0.349321705	3.493217054
A	11	Sample X1	C	0.197	0.106	CaFr21	0.346899225	3.468992248

Appendix 8.6 contd.

A	12	Sample X1	C	0.197	0.106	CaFr21	0.346899225	3.468992248
B	1	Blank B	D	0.078				
B	2	Sample X1	D	0.174	0.096	CaXy11	0.322674419	3.226744186
B	3	Sample X1	D	0.177	0.099	CaXy11	0.32994186	3.299418605
B	4	Sample X1	D	0.174	0.096	CaXy11	0.322674419	3.226744186
B	5	Blank B	E	0.097				
B	6	Sample X1	E	0.194	0.097	CaXy12	0.325096899	3.250968992
B	7	Sample X1	E	0.195	0.098	CaXy12	0.32751938	3.275193798
B	8	Sample X1	E	0.194	0.097	CaXy12	0.325096899	3.250968992
B	9	Blank B	F	0.071				
B	10	Sample X1	F	0.201	0.13	CaXy21	0.40503876	4.050387597
B	11	Sample X1	F	0.199	0.128	CaXy21	0.400193798	4.001937984
B	12	Sample X1	F	0.201	0.13	CaXy21	0.40503876	4.050387597
C	1	Blank B	G	0.076				
C	2	Sample X1	G	0.23	0.154	CaGr11	0.463178295	4.631782946
C	3	Sample X1	G	0.232	0.156	CaGr11	0.468023256	4.680232558
C	4	Sample X1	G	0.23	0.154	CaGr11	0.463178295	4.631782946
C	5	Blank B	H	0.072				
C	6	Sample X1	H	0.23	0.158	CaGr12	0.472868217	4.728682171
C	7	Sample X1	H	0.232	0.16	CaGr12	0.477713178	4.777131783
C	8	Sample X1	H	0.232	0.16	CaGr12	0.477713178	4.777131783
C	9	Blank B	I	0.062				
C	10	Sample X1	I	0.156	0.094	CaGr21	0.317829457	3.178294574
C	11	Sample X1	I	0.153	0.091	CaGr21	0.310562016	3.105620155
C	12	Sample X1	I	0.156	0.094	CaGr21	0.317829457	3.178294574
D	5	Blank B	K	0.067				
D	6	Sample X1	K	0.189	0.122	CaGc11	0.385658915	3.856589147
D	7	Sample X1	K	0.189	0.122	CaGc11	0.385658915	3.856589147
D	8	Sample X1	K	0.189	0.122	CaGc11	0.385658915	3.856589147
D	9	Blank B	L	0.058				
D	10	Sample X1	L	0.164	0.106	CaGc21	0.346899225	3.468992248
D	11	Sample X1	L	0.164	0.106	CaGc21	0.346899225	3.468992248
D	12	Sample X1	L	0.164	0.106	CaGc21	0.346899225	3.468992248
E	1	Blank B	M	0.072				
E	2	Sample X1	M	0.22	0.128	CaGl11	0.400193798	4.001937984
E	3	Sample X1	M	0.22	0.128	CaGl11	0.400193798	4.001937984
E	4	Sample X1	M	0.22	0.128	CaGl11	0.400193798	4.001937984
E	5	Blank B	N	0.067				
E	6	Sample X1	N	0.16	0.093	CaGl21	0.315406977	3.154069767
E	7	Sample X1	N	0.16	0.093	CaGl21	0.315406977	3.154069767
E	8	Sample X1	N	0.16	0.093	CaGl21	0.315406977	3.154069767

Appendix 8.7 RCCDRSM CUPRAC run 7

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.103				
A	2	Sample X1	A	0.199	0.096	CaSu11	0.3226744	6.453488
A	3	Sample X1	A	0.2	0.097	CaSu11	0.3250969	6.501938
A	4	Sample X1	A	0.199	0.096	CaSu11	0.3226744	6.453488
A	5	Blank B	B	0.123				
A	6	Sample X1	B	0.216	0.093	CaFr11	0.315407	6.30814
A	7	Sample X1	B	0.216	0.093	CaFr11	0.315407	6.30814
A	8	Sample X1	B	0.216	0.093	CaFr11	0.315407	6.30814
A	9	Blank B	C	0.137				
A	10	Sample X1	C	0.231	0.094	CaFr12	0.3178295	6.356589
A	11	Sample X1	C	0.232	0.095	CaFr12	0.3202519	6.405039
A	12	Sample X1	C	0.232	0.095	CaFr12	0.3202519	6.405039
B	1	Blank B	D	0.117				
B	2	Sample X1	D	0.209	0.092	CaFr21	0.3129845	6.25969
B	3	Sample X1	D	0.209	0.092	CaFr21	0.3129845	6.25969
B	4	Sample X1	D	0.209	0.092	CaFr21	0.3129845	6.25969
A	9	Blank B	C	0.141				
A	10	Sample X1	C	0.235	0.094	CaXy11	0.3178295	6.356589
A	11	Sample X1	C	0.236	0.095	CaXy11	0.3202519	6.405039
A	12	Sample X1	C	0.236	0.095	CaXy11	0.3202519	6.405039
B	5	Blank B	E	0.124				
B	6	Sample X1	E	0.216	0.092	CaXy12	0.3129845	6.25969
B	7	Sample X1	E	0.216	0.092	CaXy12	0.3129845	6.25969
B	8	Sample X1	E	0.217	0.093	CaXy12	0.315407	6.30814
B	9	Blank B	F	0.114				
B	10	Sample X1	F	0.205	0.091	CaGr11	0.310562	6.21124
B	11	Sample X1	F	0.204	0.09	CaGr11	0.3081395	6.162791
B	12	Sample X1	F	0.204	0.09	CaGr11	0.3081395	6.162791
C	1	Blank B	G	0.11				
C	2	Sample X1	G	0.202	0.092	CaGr12	0.3129845	6.25969
C	3	Sample X1	G	0.2	0.09	CaGr12	0.3081395	6.162791
C	4	Sample X1	G	0.202	0.092	CaGr12	0.3129845	6.25969
C	5	Blank B	H	0.083				
C	6	Sample X1	H	0.176	0.093	CaGr21	0.315407	6.30814
C	7	Sample X1	H	0.177	0.094	CaGr21	0.3178295	6.356589
C	8	Sample X1	H	0.176	0.093	CaGr21	0.315407	6.30814
C	9	Blank B	I	0.103				

Appendix 8.7 contd.

C	10	Sample X1	I	0.2	0.097	CaGc11	0.3250969	6.501938
C	11	Sample X1	I	0.195	0.092	CaGc11	0.3129845	6.25969
C	12	Sample X1	I	0.195	0.092	CaGc11	0.3129845	6.25969
D	1	Blank B	J	0.107				
D	2	Sample X1	J	0.204	0.097	CaGc21	0.3250969	6.501938
D	3	Sample X1	J	0.204	0.097	CaGc21	0.3250969	6.501938
D	4	Sample X1	J	0.206	0.099	CaGc21	0.3299419	6.598837
D	5	Blank B	K	0.111				
D	6	Sample X1	K	0.203	0.092	CaGl11	0.3129845	6.25969
D	7	Sample X1	K	0.203	0.092	CaGl11	0.3129845	6.25969
D	8	Sample X1	K	0.203	0.092	CaGl11	0.3129845	6.25969
D	9	Blank B	L	0.088				
D	10	Sample X1	L	0.178	0.09	CaGl21	0.3081395	6.162791
D	11	Sample X1	L	0.179	0.091	CaGl21	0.310562	6.21124
D	12	Sample X1	L	0.178	0.09	CaGl21	0.3081395	6.162791

Appendix 8.8 RCCDRSM CUPRAC run 8

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.122				
D	2	Sample X1	J	0.212	0.09	CaSu11	0.30813953	4.622093
D	3	Sample X1	J	0.212	0.09	CaSu11	0.30813953	4.622093
D	4	Sample X1	J	0.215	0.093	CaSu11	0.31540698	4.731105
A	1	Blank B	A	0.136				
A	2	Sample X1	A	0.232	0.096	CaFr11	0.32267442	4.840116
A	3	Sample X1	A	0.233	0.097	CaFr11	0.3250969	4.876453
A	4	Sample X1	A	0.233	0.097	CaFr11	0.3250969	4.876453
A	5	Blank B	B	0.103				
A	6	Sample X1	B	0.195	0.092	CaFr12	0.3129845	4.694767
A	7	Sample X1	B	0.195	0.092	CaFr12	0.3129845	4.694767
A	8	Sample X1	B	0.195	0.092	CaFr12	0.3129845	4.694767
A	9	Blank B	C	0.117				
A	10	Sample X1	C	0.21	0.093	CaFr21	0.31540698	4.731105
A	11	Sample X1	C	0.21	0.093	CaFr21	0.31540698	4.731105
A	12	Sample X1	C	0.212	0.095	CaFr21	0.32025194	4.803779
B	1	Blank B	D	0.093				
B	2	Sample X1	D	0.187	0.094	CaXy11	0.31782946	4.767442
B	3	Sample X1	D	0.187	0.094	CaXy11	0.31782946	4.767442
B	4	Sample X1	D	0.19	0.097	CaXy11	0.3250969	4.876453

Appendix 8.8 contd.

B	5	Blank B	E	0.106				
B	6	Sample X1	E	0.202	0.096	CaXy12	0.32267442	4.840116
B	7	Sample X1	E	0.203	0.097	CaXy12	0.3250969	4.876453
B	8	Sample X1	E	0.203	0.097	CaXy12	0.3250969	4.876453
B	9	Blank B	F	0.099				
B	10	Sample X1	F	0.195	0.096	CaXy21	0.32267442	4.840116
B	11	Sample X1	F	0.197	0.098	CaXy21	0.32751938	4.912791
B	12	Sample X1	F	0.197	0.098	CaXy21	0.32751938	4.912791
C	1	Blank B	G	0.095				
C	2	Sample X1	G	0.19	0.095	CaGr11	0.32025194	4.803779
C	3	Sample X1	G	0.191	0.096	CaGr11	0.32267442	4.840116
C	4	Sample X1	G	0.19	0.095	CaGr11	0.32025194	4.803779
C	5	Blank B	H	0.103				
C	6	Sample X1	H	0.193	0.09	CaGr12	0.30813953	4.622093
C	7	Sample X1	H	0.193	0.09	CaGr12	0.30813953	4.622093
C	8	Sample X1	H	0.195	0.092	CaGr12	0.3129845	4.694767
C	9	Blank B	I	0.08				
C	10	Sample X1	I	0.172	0.092	CaGr21	0.3129845	4.694767
C	11	Sample X1	I	0.171	0.091	CaGr21	0.31056202	4.65843
C	12	Sample X1	I	0.171	0.091	CaGr21	0.31056202	4.65843
D	5	Blank B	K	0.084				
D	6	Sample X1	K	0.176	0.092	CaGc11	0.3129845	4.694767
D	7	Sample X1	K	0.176	0.092	CaGc11	0.3129845	4.694767
D	8	Sample X1	K	0.176	0.092	CaGc11	0.3129845	4.694767
D	9	Blank B	L	0.065				
D	10	Sample X1	L	0.159	0.094	CaGc21	0.31782946	4.767442
D	11	Sample X1	L	0.161	0.096	CaGc21	0.32267442	4.840116
D	12	Sample X1	L	0.159	0.094	CaGc21	0.31782946	4.767442
E	1	Blank B	M	0.091				
E	2	Sample X1	M	0.119	0.092	CaGl11	0.3129845	4.694767
E	3	Sample X1	M	0.104	0.091	CaGl11	0.31056202	4.65843
E	4	Sample X1	M	0.105	0.091	CaGl11	0.31056202	4.65843
E	5	Blank B	N	0.09				
E	6	Sample X1	N	0.184	0.094	CaGl21	0.31782946	4.767442
E	7	Sample X1	N	0.18	0.09	CaGl21	0.30813953	4.622093
E	8	Sample X1	N	0.18	0.09	CaGl21	0.30813953	4.622093

Appendix 8.9 RCCDRSM CUPRAC run 9

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.108				
D	2	Sample X1	J	0.204	0.096	CaSu11	0.3226744	4.840116
D	3	Sample X1	J	0.206	0.098	CaSu11	0.3275194	4.912791
D	4	Sample X1	J	0.204	0.096	CaSu11	0.3226744	4.840116
A	1	Blank B	A	0.133				
A	2	Sample X1	A	0.227	0.094	CaFr11	0.3178295	4.767442
A	3	Sample X1	A	0.226	0.093	CaFr11	0.315407	4.731105
A	4	Sample X1	A	0.226	0.093	CaFr11	0.315407	4.731105
A	5	Blank B	B	0.091				
A	6	Sample X1	B	0.182	0.091	CaFr12	0.310562	4.65843
A	7	Sample X1	B	0.183	0.092	CaFr12	0.3129845	4.694767
A	8	Sample X1	B	0.183	0.092	CaFr12	0.3129845	4.694767
A	9	Blank B	C	0.102				
A	10	Sample X1	C	0.192	0.09	CaFr21	0.3081395	4.622093
A	11	Sample X1	C	0.194	0.092	CaFr21	0.3129845	4.694767
A	12	Sample X1	C	0.194	0.092	CaFr21	0.3129845	4.694767
B	1	Blank B	D	0.072				
B	2	Sample X1	D	0.169	0.094	CaXy11	0.3178295	4.767442
B	3	Sample X1	D	0.168	0.093	CaXy11	0.315407	4.731105
B	4	Sample X1	D	0.169	0.094	CaXy11	0.3178295	4.767442
B	5	Blank B	E	0.085				
B	6	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.876453
B	7	Sample X1	E	0.181	0.096	CaXy12	0.3226744	4.840116
B	8	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.876453
B	9	Blank B	F	0.071				
B	10	Sample X1	F	0.164	0.093	CaXy21	0.315407	4.731105
B	11	Sample X1	F	0.162	0.091	CaXy21	0.310562	4.65843
B	12	Sample X1	F	0.164	0.093	CaXy21	0.315407	4.731105
C	1	Blank B	G	0.064				
C	2	Sample X1	G	0.167	0.103	CaGr11	0.3396318	5.094477
C	3	Sample X1	G	0.167	0.103	CaGr11	0.3396318	5.094477
C	4	Sample X1	G	0.17	0.106	CaGr11	0.3468992	5.203488
C	5	Blank B	H	0.086				
C	6	Sample X1	H	0.182	0.096	CaGr12	0.3226744	4.840116
C	7	Sample X1	H	0.183	0.097	CaGr12	0.3250969	4.876453
C	8	Sample X1	H	0.182	0.096	CaGr12	0.3226744	4.840116
C	9	Blank B	I	0.074				
C	10	Sample X1	I	0.171	0.097	CaGr21	0.3250969	4.876453

Appendix 8.9 contd.

C	11	Sample X1	I	0.169	0.095	CaGr21	0.3202519	4.803779
C	12	Sample X1	I	0.169	0.095	CaGr21	0.3202519	4.803779
D	5	Blank B	K	0.063				
D	6	Sample X1	K	0.168	0.104	CaGc11	0.3420543	5.130814
D	7	Sample X1	K	0.167	0.103	CaGc11	0.3396318	5.094477
D	8	Sample X1	K	0.167	0.103	CaGc11	0.3396318	5.094477
D	9	Blank B	L	0.08				
D	10	Sample X1	L	0.176	0.096	CaGc21	0.3226744	4.840116
D	11	Sample X1	L	0.177	0.097	CaGc21	0.3250969	4.876453
D	12	Sample X1	L	0.176	0.096	CaGc21	0.3226744	4.840116
E	1	Blank B	M	0.095				
E	2	Sample X1	M	0.192	0.097	CaGl11	0.3250969	4.876453
E	3	Sample X1	M	0.192	0.097	CaGl11	0.3250969	4.876453
E	4	Sample X1	M	0.194	0.099	CaGl11	0.3299419	4.949128
E	5	Blank B	N	0.082				
E	6	Sample X1	N	0.174	0.092	CaGl21	0.3129845	4.694767
E	7	Sample X1	N	0.173	0.091	CaGl21	0.310562	4.65843
E	8	Sample X1	N	0.173	0.091	CaGl21	0.310562	4.65843

Appendix 8.10 RCCDRSM CUPRAC run 10

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.098				
D	2	Sample X1	J	0.192	0.094	CaSu11	0.3178295	6.356589
D	3	Sample X1	J	0.19	0.092	CaSu11	0.3129845	6.25969
D	4	Sample X1	J	0.19	0.092	CaSu11	0.3129845	6.25969
A	1	Blank B	A	0.126				
A	2	Sample X1	A	0.318	0.192	CaFr11	0.5552326	11.10465
A	3	Sample X1	A	0.318	0.192	CaFr11	0.5552326	11.10465
A	4	Sample X1	A	0.318	0.192	CaFr11	0.5552326	11.10465
A	5	Blank B	B	0.113				
A	6	Sample X1	B	0.243	0.13	CaFr12	0.4050388	8.100775
A	7	Sample X1	B	0.241	0.128	CaFr12	0.4001938	8.003876
A	8	Sample X1	B	0.243	0.13	CaFr12	0.4050388	8.100775
A	9	Blank B	C	0.11				
A	10	Sample X1	C	0.221	0.111	CaFr21	0.3590116	7.180233
A	11	Sample X1	C	0.225	0.115	CaFr21	0.3687016	7.374031
A	12	Sample X1	C	0.221	0.111	CaFr21	0.3590116	7.180233
B	1	Blank B	D	0.074				

Appendix 8.10 contd.

B	2	Sample X1	D	0.212	0.138	CaXy11	0.4244186	8.488372
B	3	Sample X1	D	0.208	0.134	CaXy11	0.4147287	8.294574
B	4	Sample X1	D	0.208	0.134	CaXy11	0.4147287	8.294574
B	5	Blank B	E	0.08				
B	6	Sample X1	E	0.191	0.111	CaXy12	0.3590116	7.180233
B	7	Sample X1	E	0.191	0.111	CaXy12	0.3590116	7.180233
B	8	Sample X1	E	0.191	0.111	CaXy12	0.3590116	7.180233
B	9	Blank B	F	0.064				
B	10	Sample X1	F	0.212	0.148	CaXy21	0.4486434	8.972868
B	11	Sample X1	F	0.214	0.15	CaXy21	0.4534884	9.069767
B	12	Sample X1	F	0.212	0.148	CaXy21	0.4486434	8.972868
C	1	Blank B	G	0.087				
C	2	Sample X1	G	0.246	0.159	CaGr11	0.4752907	9.505814
C	3	Sample X1	G	0.246	0.159	CaGr11	0.4752907	9.505814
C	4	Sample X1	G	0.246	0.159	CaGr11	0.4752907	9.505814
C	5	Blank B	H	0.086				
C	6	Sample X1	H	0.243	0.137	CaGr12	0.4219961	8.439922
C	7	Sample X1	H	0.241	0.135	CaGr12	0.4171512	8.343023
C	8	Sample X1	H	0.241	0.135	CaGr12	0.4171512	8.343023
C	9	Blank B	I	0.061				
C	10	Sample X1	I	0.206	0.145	CaGr21	0.441376	8.827519
C	11	Sample X1	I	0.207	0.146	CaGr21	0.4437984	8.875969
C	12	Sample X1	I	0.207	0.146	CaGr21	0.4437984	8.875969
D	5	Blank B	K	0.076				
D	6	Sample X1	K	0.16	0.084	CaGc11	0.2936047	5.872093
D	7	Sample X1	K	0.16	0.084	CaGc11	0.2936047	5.872093
D	8	Sample X1	K	0.159	0.083	CaGc11	0.2911822	5.823643
D	9	Blank B	L	0.066				
D	10	Sample X1	L	0.174	0.108	CaGc21	0.3517442	7.034884
D	11	Sample X1	L	0.174	0.108	CaGc21	0.3517442	7.034884
D	12	Sample X1	L	0.174	0.108	CaGc21	0.3517442	7.034884
F	1	Blank B	M	0.075				
E	2	Sample X1	M	0.166	0.091	CaGl11	0.310562	6.21124
E	3	Sample X1	M	0.165	0.09	CaGl11	0.3081395	6.162791
E	4	Sample X1	M	0.165	0.09	CaGl11	0.3081395	6.162791
E	5	Blank B	N	0.066				
E	6	Sample X1	N	0.172	0.106	CaGl21	0.3468992	6.937984
E	7	Sample X1	N	0.174	0.108	CaGl21	0.3517442	7.034884
E	8	Sample X1	N	0.172	0.106	CaGl21	0.3468992	6.937984

Appendix 8.11 RCCDRSM CUPRAC run 11

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.093				
D	2	Sample X1	J	0.185	0.092	CaSu11	0.312984496	6.25969
D	3	Sample X1	J	0.186	0.093	CaSu11	0.315406977	6.30814
D	4	Sample X1	J	0.186	0.093	CaSu11	0.315406977	6.30814
A	1	Blank B	A	0.095				
A	2	Sample X1	A	0.202	0.107	CaFr11	0.349321705	6.986434
A	3	Sample X1	A	0.201	0.106	CaFr11	0.346899225	6.937984
A	4	Sample X1	A	0.201	0.106	CaFr11	0.346899225	6.937984
A	5	Blank B	B	0.093				
A	6	Sample X1	B	0.188	0.095	CaFr12	0.320251938	6.405039
A	7	Sample X1	B	0.189	0.096	CaFr12	0.322674419	6.453488
A	8	Sample X1	B	0.188	0.095	CaFr12	0.320251938	6.405039
A	9	Blank B	C	0.083				
A	10	Sample X1	C	0.175	0.092	CaFr21	0.312984496	6.25969
A	11	Sample X1	C	0.174	0.091	CaFr21	0.310562016	6.21124
A	12	Sample X1	C	0.174	0.091	CaFr21	0.310562016	6.550388
B	1	Blank B	D	0.052				
B	2	Sample X1	D	0.103	0.095	CaXy11	0.320251938	6.405039
B	3	Sample X1	D	0.108	0.095	CaXy11	0.320251938	6.405039
B	4	Sample X1	D	0.1	0.094	CaXy11	0.317829457	6.356589
B	5	Blank B	E	0.071				
B	6	Sample X1	E	0.164	0.093	CaXy12	0.315406977	6.30814
B	7	Sample X1	E	0.163	0.092	CaXy12	0.312984496	6.25969
B	8	Sample X1	E	0.163	0.092	CaXy12	0.312984496	6.25969
B	9	Blank B	F	0.067				
B	10	Sample X1	F	0.161	0.094	CaXy21	0.317829457	6.356589
B	11	Sample X1	F	0.16	0.093	CaXy21	0.315406977	6.30814
B	12	Sample X1	F	0.16	0.093	CaXy21	0.315406977	6.30814
C	1	Blank B	G	0.059				
C	2	Sample X1	G	0.153	0.094	CaGr11	0.317829457	6.356589
C	3	Sample X1	G	0.152	0.093	CaGr11	0.315406977	6.30814
C	4	Sample X1	G	0.153	0.094	CaGr11	0.317829457	6.356589
C	5	Blank B	H	0.203				
C	6	Sample X1	H	0.3	0.097	CaGr12	0.325096899	6.501938
C	7	Sample X1	H	0.3	0.097	CaGr12	0.325096899	6.501938
C	8	Sample X1	H	0.301	0.098	CaGr12	0.32751938	6.550388
C	9	Blank B	I	0.073				

Appendix 8.11 contd.

C	10	Sample X1	I	0.166	0.093	CaGr21	0.315406977	6.30814
C	11	Sample X1	I	0.166	0.093	CaGr21	0.315406977	6.30814
C	12	Sample X1	I	0.164	0.091	CaGr21	0.310562016	6.21124
D	5	Blank B	K	0.073				
D	6	Sample X1	K	0.165	0.092	CaGc11	0.312984496	6.25969
D	7	Sample X1	K	0.165	0.092	CaGc11	0.312984496	6.25969
D	8	Sample X1	K	0.165	0.092	CaGc11	0.312984496	6.25969
D	9	Blank B	L	0.071				
D	10	Sample X1	L	0.164	0.093	CaGc21	0.315406977	6.30814
D	11	Sample X1	L	0.163	0.092	CaGc21	0.312984496	6.25969
D	12	Sample X1	L	0.163	0.092	CaGc21	0.312984496	6.25969
E	1	Blank B	M	0.082				
E	2	Sample X1	M	0.174	0.092	CaGl11	0.312984496	6.25969
E	3	Sample X1	M	0.174	0.092	CaGl11	0.312984496	6.25969
E	4	Sample X1	M	0.176	0.094	CaGl11	0.317829457	6.356589
E	5	Blank B	N	0.078				
E	6	Sample X1	N	0.173	0.095	CaGl21	0.320251938	6.405039
E	7	Sample X1	N	0.173	0.095	CaGl21	0.320251938	6.405039
E	8	Sample X1	N	0.177	0.099	CaGl21	0.32994186	6.598837

Appendix 8.12 RCCDRSM CUPRAC run 12

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.129				
E	2	Sample X1	A	0.222	0.093	CaSu11	0.31540698	6.30813953
E	3	Sample X1	A	0.223	0.094	CaSu11	0.31782946	6.35658915
E	4	Sample X1	A	0.222	0.093	CaSu11	0.31540698	6.30813953
E	5	Blank B	B	0.174				
E	6	Sample X1	B	0.273	0.099	CaFr11	0.32994186	6.59883721
E	7	Sample X1	B	0.271	0.097	CaFr11	0.3250969	6.50193798
E	8	Sample X1	B	0.271	0.097	CaFr11	0.3250969	6.50193798
E	9	Blank B	C	0.186				
E	10	Sample X1	C	0.28	0.094	CaFr12	0.31782946	6.35658915
E	11	Sample X1	C	0.276	0.09	CaFr12	0.30813953	6.1627907
E	12	Sample X1	C	0.28	0.094	CaFr12	0.31782946	6.35658915
F	1	Blank B	D	0.154				
F	2	Sample X1	D	0.246	0.092	CaFr21	0.3129845	6.25968992
F	3	Sample X1	D	0.246	0.092	CaFr21	0.3129845	6.25968992

Appendix 8.12 contd.

F	4	Sample X1	D	0.245	0.091	CaFr21	0.31056202	6.21124031
B	1	Blank B	D	0.109				
B	2	Sample X1	D	0.2	0.091	CaXy11	0.31056202	6.21124031
B	3	Sample X1	D	0.199	0.09	CaXy11	0.30813953	6.1627907
B	4	Sample X1	D	0.199	0.09	CaXy11	0.30813953	6.1627907
F	5	Blank B	E	0.146				
F	6	Sample X1	E	0.237	0.091	CaXy12	0.31056202	6.21124031
F	7	Sample X1	E	0.237	0.091	CaXy12	0.31056202	6.21124031
F	8	Sample X1	E	0.237	0.091	CaXy12	0.31056202	6.21124031
A	9	Blank B	C	0.091				
A	10	Sample X1	C	0.242	0.151	CaXy21	0.45591085	9.11821705
A	11	Sample X1	C	0.245	0.154	CaXy21	0.46317829	9.26356589
A	12	Sample X1	C	0.242	0.151	CaXy21	0.45591085	9.11821705
F	9	Blank B	F	0.119				
F	10	Sample X1	F	0.213	0.094	CaGr11	0.31782946	6.35658915
F	11	Sample X1	F	0.21	0.091	CaGr11	0.31056202	6.21124031
F	12	Sample X1	F	0.213	0.094	CaGr11	0.31782946	6.35658915
G	1	Blank B	G	0.14				
G	2	Sample X1	G	0.23	0.09	CaGr12	0.30813953	6.1627907
G	3	Sample X1	G	0.231	0.091	CaGr12	0.31056202	6.21124031
G	4	Sample X1	G	0.23	0.09	CaGr12	0.30813953	6.1627907
G	5	Blank B	H	0.141				
G	6	Sample X1	H	0.233	0.092	CaGr21	0.3129845	6.25968992
G	7	Sample X1	H	0.234	0.093	CaGr21	0.31540698	6.30813953
G	8	Sample X1	H	0.233	0.092	CaGr21	0.3129845	6.25968992
G	9	Blank B	I	0.122				
G	10	Sample X1	I	0.218	0.096	CaGc11	0.32267442	6.45348837
G	11	Sample X1	I	0.218	0.096	CaGc11	0.32267442	6.45348837
G	12	Sample X1	I	0.219	0.097	CaGc11	0.3250969	6.50193798
H	1	Blank B	J	0.153				
H	2	Sample X1	J	0.143	0.09	CaGc21	0.30813953	6.1627907
H	3	Sample X1	J	0.145	0.092	CaGc21	0.3129845	6.25968992
H	4	Sample X1	J	0.145	0.092	CaGc21	0.3129845	6.25968992
H	5	Blank B	K	0.152				
H	6	Sample X1	K	0.146	0.094	CaGl11	0.31782946	6.35658915
H	7	Sample X1	K	0.145	0.093	CaGl11	0.31540698	6.30813953
H	8	Sample X1	K	0.145	0.093	CaGl11	0.31540698	6.30813953
H	9	Blank B	L	0.131				
H	10	Sample X1	L	0.223	0.092	CaGl21	0.3129845	6.25968992
H	11	Sample X1	L	0.223	0.092	CaGl21	0.3129845	6.25968992
H	12	Sample X1	L	0.222	0.091	CaGl21	0.31056202	6.21124031

Appendix 8.13 RCCDRSM CUPRAC run 13

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.091				
D	2	Sample X1	J	0.227	0.136	CaSu11	0.4195736	4.195736
D	3	Sample X1	J	0.229	0.138	CaSu11	0.4244186	4.244186
D	4	Sample X1	J	0.227	0.136	CaSu11	0.4195736	4.195736
A	1	Blank B	A	0.126				
A	2	Sample X1	A	0.357	0.231	CaFr11	0.6497093	6.497093
A	3	Sample X1	A	0.357	0.231	CaFr11	0.6497093	6.497093
A	4	Sample X1	A	0.357	0.231	CaFr11	0.6497093	6.497093
A	5	Blank B	B	0.082				
A	6	Sample X1	B	0.224	0.136	CaFr12	0.4195736	4.195736
A	7	Sample X1	B	0.201	0.136	CaFr12	0.4195736	4.195736
A	8	Sample X1	B	0.228	0.136	CaFr12	0.4195736	4.195736
A	9	Blank B	C	0.095				
A	10	Sample X1	C	0.344	0.249	CaFr21	0.693314	6.93314
A	11	Sample X1	C	0.342	0.247	CaFr21	0.688469	6.88469
A	12	Sample X1	C	0.342	0.247	CaFr21	0.688469	6.88469
B	1	Blank B	D	0.073				
B	2	Sample X1	D	0.278	0.205	CaXy11	0.5867248	5.867248
B	3	Sample X1	D	0.28	0.207	CaXy11	0.5915698	5.915698
B	4	Sample X1	D	0.28	0.207	CaXy11	0.5915698	5.915698
B	5	Blank B	E	0.079				
B	6	Sample X1	E	0.275	0.196	CaXy12	0.5649225	5.649225
B	7	Sample X1	E	0.276	0.197	CaXy12	0.567345	5.67345
B	8	Sample X1	E	0.276	0.197	CaXy12	0.567345	5.67345
B	9	Blank B	F	0.076				
B	10	Sample X1	F	0.26	0.184	CaXy21	0.5358527	5.358527
B	11	Sample X1	F	0.262	0.186	CaXy21	0.5406977	5.406977
B	12	Sample X1	F	0.26	0.184	CaXy21	0.5358527	5.358527
C	1	Blank B	G	0.085				
C	2	Sample X1	G	0.321	0.236	CaGr11	0.6618217	6.618217
C	3	Sample X1	G	0.321	0.236	CaGr11	0.6618217	6.618217
C	4	Sample X1	G	0.316	0.231	CaGr11	0.6497093	6.497093
C	5	Blank B	H	0.096				
C	6	Sample X1	H	0.353	0.257	CaGr12	0.7126938	7.126938
C	7	Sample X1	H	0.351	0.254	CaGr12	0.7054264	7.054264
C	8	Sample X1	H	0.351	0.254	CaGr12	0.7054264	7.054264
C	9	Blank B	I	0.069				

Appendix 8.13 contd.

C	10	Sample X1	I	0.366	0.297	CaGr21	0.809593	8.09593
C	11	Sample X1	I	0.366	0.297	CaGr21	0.809593	8.09593
C	12	Sample X1	I	0.366	0.297	CaGr21	0.809593	8.09593
D	5	Blank B	K	0.078				
D	6	Sample X1	K	0.23	0.152	CaGc11	0.4583333	4.583333
D	7	Sample X1	K	0.231	0.153	CaGc11	0.4607558	4.607558
D	8	Sample X1	K	0.231	0.153	CaGc11	0.4607558	4.607558
D	9	Blank B	L	0.074				
D	10	Sample X1	L	0.2	0.126	CaGc21	0.3953488	3.953488
D	11	Sample X1	L	0.199	0.125	CaGc21	0.3929264	3.929264
D	12	Sample X1	L	0.199	0.125	CaGc21	0.3929264	3.929264
E	1	Blank B	M	0.081				
E	2	Sample X1	M	0.317	0.236	CaGl11	0.6618217	6.618217
E	3	Sample X1	M	0.312	0.231	CaGl11	0.6497093	6.497093
E	4	Sample X1	M	0.312	0.231	CaGl11	0.6497093	6.497093
E	5	Blank B	N	0.069				
E	6	Sample X1	N	0.273	0.204	CaGl21	0.5843023	5.843023
E	7	Sample X1	N	0.277	0.208	CaGl21	0.5939922	5.939922
E	8	Sample X1	N	0.273	0.204	CaGl21	0.5843023	5.843023

Appendix 8.14 RCCDRSM CUPRAC

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.09				
D	2	Sample X1	J	0.183	0.093	CaSu11	0.315407	3.15407
D	3	Sample X1	J	0.182	0.092	CaSu11	0.3129845	3.129845
D	4	Sample X1	J	0.182	0.092	CaSu11	0.3129845	3.129845
A	1	Blank B	A	0.089				
A	2	Sample X1	A	0.198	0.109	CaFr11	0.3541667	3.541667
A	3	Sample X1	A	0.199	0.11	CaFr11	0.3565891	3.565891
A	4	Sample X1	A	0.198	0.109	CaFr11	0.3541667	3.541667
A	5	Blank B	B	0.085				
A	6	Sample X1	B	0.181	0.096	CaFr12	0.3226744	3.226744
A	7	Sample X1	B	0.181	0.096	CaFr12	0.3226744	3.226744
A	8	Sample X1	B	0.18	0.095	CaFr12	0.3202519	3.202519
A	9	Blank B	C	0.097				
A	10	Sample X1	C	0.191	0.094	CaFr21	0.3178295	3.178295

Appendix 8.14 contd.

A	11	Sample X1	C	0.189	0.092	CaFr21	0.3129845	3.129845
A	12	Sample X1	C	0.189	0.092	CaFr21	0.3129845	3.129845
B	1	Blank B	D	0.074				
B	2	Sample X1	D	0.167	0.093	CaXy11	0.315407	3.15407
B	3	Sample X1	D	0.168	0.094	CaXy11	0.3178295	3.178295
B	4	Sample X1	D	0.167	0.093	CaXy11	0.315407	3.15407
B	5	Blank B	E	0.081				
B	6	Sample X1	E	0.173	0.092	CaXy12	0.3129845	3.129845
B	7	Sample X1	E	0.174	0.093	CaXy12	0.315407	3.15407
B	8	Sample X1	E	0.173	0.092	CaXy12	0.3129845	3.129845
B	9	Blank B	F	0.078				
B	10	Sample X1	F	0.17	0.092	CaXy21	0.3129845	3.129845
B	11	Sample X1	F	0.17	0.092	CaXy21	0.3129845	3.129845
B	12	Sample X1	F	0.17	0.092	CaXy21	0.3129845	3.129845
C	1	Blank B	G	0.08				
C	2	Sample X1	G	0.175	0.095	CaGr11	0.3202519	3.202519
C	3	Sample X1	G	0.174	0.094	CaGr11	0.3178295	3.178295
C	4	Sample X1	G	0.174	0.094	CaGr11	0.3178295	3.178295
C	5	Blank B	H	0.08				
C	6	Sample X1	H	0.174	0.094	CaGr12	0.3178295	3.178295
C	7	Sample X1	H	0.173	0.093	CaGr12	0.315407	3.15407
C	8	Sample X1	H	0.173	0.093	CaGr12	0.315407	3.15407
C	9	Blank B	I	0.065				
C	10	Sample X1	I	0.162	0.097	CaGr21	0.3250969	3.250969
C	11	Sample X1	I	0.164	0.099	CaGr21	0.3299419	3.299419
C	12	Sample X1	I	0.162	0.097	CaGr21	0.3250969	3.250969
D	5	Blank B	K	0.08				
D	6	Sample X1	K	0.171	0.091	CaGc11	0.310562	3.10562
D	7	Sample X1	K	0.171	0.091	CaGc11	0.310562	3.10562
D	8	Sample X1	K	0.171	0.091	CaGc11	0.310562	3.10562
D	9	Blank B	L	0.066				
D	10	Sample X1	L	0.163	0.097	CaGc21	0.3250969	3.250969
D	11	Sample X1	L	0.163	0.097	CaGc21	0.3250969	3.250969
D	12	Sample X1	L	0.163	0.097	CaGc21	0.3250969	3.250969
E	1	Blank B	M	0.086				
E	2	Sample X1	M	0.181	0.095	CaGl11	0.3202519	3.202519
E	3	Sample X1	M	0.179	0.093	CaGl11	0.315407	3.15407
E	4	Sample X1	M	0.179	0.093	CaGl11	0.315407	3.15407
E	5	Blank B	N	0.07				
E	6	Sample X1	N	0.163	0.093	CaGl21	0.315407	3.15407
E	7	Sample X1	N	0.162	0.092	CaGl21	0.3129845	3.129845
E	8	Sample X1	N	0.162	0.092	CaGl21	0.3129845	3.129845

Appendix 8.15 RCCDRSM CUPRAC run 15

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.096				
D	2	Sample X1	J	0.194	0.098	CaSu11	0.32751938	6.550387597
D	3	Sample X1	J	0.193	0.097	CaSu11	0.325096899	6.501937984
D	4	Sample X1	J	0.194	0.098	CaSu11	0.32751938	6.550387597
A	1	Blank B	A	0.1				
A	2	Sample X1	A	0.194	0.094	CaFr11	0.317829457	6.356589147
A	3	Sample X1	A	0.193	0.093	CaFr11	0.315406977	6.308139535
A	4	Sample X1	A	0.194	0.094	CaFr11	0.317829457	6.356589147
A	5	Blank B	B	0.088				
A	6	Sample X1	B	0.18	0.092	CaFr12	0.312984496	6.259689922
A	7	Sample X1	B	0.18	0.092	CaFr12	0.312984496	6.259689922
A	8	Sample X1	B	0.179	0.091	CaFr12	0.310562016	6.21124031
A	9	Blank B	C	0.094				
A	10	Sample X1	C	0.187	0.093	CaFr21	0.315406977	6.308139535
A	11	Sample X1	C	0.187	0.093	CaFr21	0.315406977	6.308139535
A	12	Sample X1	C	0.186	0.092	CaFr21	0.312984496	6.259689922
B	1	Blank B	D	0.073				
B	2	Sample X1	D	0.165	0.092	CaXy11	0.312984496	6.259689922
B	3	Sample X1	D	0.165	0.092	CaXy11	0.312984496	6.259689922
B	4	Sample X1	D	0.166	0.093	CaXy11	0.315406977	6.308139535
B	5	Blank B	E	0.083				
B	6	Sample X1	E	0.175	0.092	CaXy12	0.312984496	6.259689922
B	7	Sample X1	E	0.175	0.092	CaXy12	0.312984496	6.259689922
B	8	Sample X1	E	0.175	0.092	CaXy12	0.312984496	6.259689922
B	9	Blank B	F	0.064				
B	10	Sample X1	F	0.156	0.092	CaXy21	0.312984496	6.259689922
B	11	Sample X1	F	0.156	0.092	CaXy21	0.312984496	6.259689922
B	12	Sample X1	F	0.154	0.09	CaXy21	0.308139535	6.162790698
C	1	Blank B	G	0.079				
C	2	Sample X1	G	0.171	0.094	CaGr11	0.317829457	6.356589147
C	3	Sample X1	G	0.171	0.094	CaGr11	0.317829457	6.356589147
C	4	Sample X1	G	0.172	0.095	CaGr11	0.320251938	6.40503876
C	5	Blank B	H	0.088				
C	6	Sample X1	H	0.18	0.092	CaGr12	0.312984496	6.259689922
C	7	Sample X1	H	0.178	0.09	CaGr12	0.308139535	6.162790698
C	8	Sample X1	H	0.18	0.092	CaGr12	0.312984496	6.259689922
C	9	Blank B	I	0.08				

Appendix 8.15 contd.

C	10	Sample X1	I	0.173	0.093	CaGr21	0.315406977	6.308139535
C	11	Sample X1	I	0.172	0.092	CaGr21	0.312984496	6.259689922
C	12	Sample X1	I	0.172	0.092	CaGr21	0.312984496	6.259689922
D	5	Blank B	K	0.084				
D	6	Sample X1	K	0.182	0.098	CaGc11	0.32751938	6.550387597
D	7	Sample X1	K	0.182	0.098	CaGc11	0.32751938	6.550387597
D	8	Sample X1	K	0.181	0.097	CaGc11	0.325096899	6.501937984
D	9	Blank B	L	0.081				
D	10	Sample X1	L	0.175	0.094	CaGc21	0.317829457	6.356589147
D	11	Sample X1	L	0.174	0.093	CaGc21	0.315406977	6.308139535
D	12	Sample X1	L	0.174	0.093	CaGc21	0.315406977	6.308139535
E	1	Blank B	M	0.095				
E	2	Sample X1	M	0.186	0.091	CaGl11	0.310562016	6.21124031
E	3	Sample X1	M	0.186	0.091	CaGl11	0.310562016	6.21124031
E	4	Sample X1	M	0.185	0.09	CaGl11	0.308139535	6.162790698
E	5	Blank B	N	0.1				
E	6	Sample X1	N	0.192	0.091	CaGl21	0.310562016	6.21124031
E	7	Sample X1	N	0.193	0.092	CaGl21	0.312984496	6.259689922
E	8	Sample X1	N	0.192	0.091	CaGl21	0.310562016	6.21124031

Appendix 8.16 RCCDRSM CUPRAC run16

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.112				
D	2	Sample X1	J	0.203	0.091	CaSu11	0.310562016	6.21124031
D	3	Sample X1	J	0.203	0.091	CaSu11	0.310562016	6.21124031
D	4	Sample X1	J	0.205	0.093	CaSu11	0.315406977	6.308139535
A	1	Blank B	A	0.137				
A	2	Sample X1	A	0.217	0.09	CaFr11	0.308139535	6.162790698
A	3	Sample X1	A	0.217	0.09	CaFr11	0.308139535	6.162790698
A	4	Sample X1	A	0.217	0.09	CaFr11	0.308139535	6.162790698
A	5	Blank B	B	0.1				
A	6	Sample X1	B	0.194	0.094	CaFr12	0.317829457	6.356589147
A	7	Sample X1	B	0.196	0.096	CaFr12	0.322674419	6.453488372
A	8	Sample X1	B	0.196	0.096	CaFr12	0.322674419	6.453488372
A	9	Blank B	C	0.117				
A	10	Sample X1	C	0.212	0.095	CaFr21	0.320251938	6.40503876
A	11	Sample X1	C	0.212	0.095	CaFr21	0.320251938	6.40503876

Appendix 8.16 contd.

A	12	Sample X1	C	0.212	0.095	CaFr21	0.320251938	6.40503876
B	1	Blank B	D	0.076				
B	2	Sample X1	D	0.171	0.095	CaXy11	0.320251938	6.40503876
B	3	Sample X1	D	0.171	0.095	CaXy11	0.320251938	6.40503876
B	4	Sample X1	D	0.172	0.096	CaXy11	0.322674419	6.453488372
B	5	Blank B	E	0.107				
B	6	Sample X1	E	0.2	0.093	CaXy12	0.315406977	6.308139535
B	7	Sample X1	E	0.201	0.094	CaXy12	0.317829457	6.356589147
B	8	Sample X1	E	0.201	0.094	CaXy12	0.317829457	6.356589147
B	9	Blank B	F	0.079				
B	10	Sample X1	F	0.174	0.095	CaXy21	0.320251938	6.40503876
B	11	Sample X1	F	0.172	0.093	CaXy21	0.315406977	6.308139535
B	12	Sample X1	F	0.173	0.094	CaXy21	0.317829457	6.356589147
C	1	Blank B	G	0.087				
C	2	Sample X1	G	0.179	0.092	CaGr11	0.312984496	6.259689922
C	3	Sample X1	G	0.178	0.091	CaGr11	0.310562016	6.21124031
C	4	Sample X1	G	0.179	0.092	CaGr11	0.312984496	6.259689922
C	5	Blank B	H	0.088				
C	6	Sample X1	H	0.183	0.095	CaGr12	0.320251938	6.40503876
C	7	Sample X1	H	0.183	0.095	CaGr12	0.320251938	6.40503876
C	8	Sample X1	H	0.182	0.094	CaGr12	0.317829457	6.356589147
C	9	Blank B	I	0.065				
C	10	Sample X1	I	0.162	0.097	CaGr21	0.325096899	6.501937984
C	11	Sample X1	I	0.16	0.095	CaGr21	0.320251938	6.40503876
C	12	Sample X1	I	0.161	0.096	CaGr21	0.322674419	6.453488372
D	5	Blank B	K	0.077				
D	6	Sample X1	K	0.17	0.093	CaGc11	0.315406977	6.308139535
D	7	Sample X1	K	0.171	0.094	CaGc11	0.317829457	6.356589147
D	8	Sample X1	K	0.171	0.094	CaGc11	0.317829457	6.356589147
D	9	Blank B	L	0.054				
D	10	Sample X1	L	0.151	0.097	CaGc21	0.325096899	6.501937984
D	11	Sample X1	L	0.151	0.097	CaGc21	0.325096899	6.501937984
D	12	Sample X1	L	0.151	0.097	CaGc21	0.325096899	6.501937984
E	1	Blank B	M	0.052				
E	2	Sample X1	M	0.157	0.105	CaGl11	0.344476744	6.889534884
E	3	Sample X1	M	0.157	0.105	CaGl11	0.344476744	6.889534884
E	4	Sample X1	M	0.159	0.107	CaGl11	0.349321705	6.986434109
E	5	Blank B	N	0.053				
E	6	Sample X1	N	0.121	0.096	CaGl21	0.322674419	6.453488372
E	7	Sample X1	N	0.103	0.095	CaGl21	0.320251938	6.40503876
E	8	Sample X1	N	0.107	0.095	CaGl21	0.320251938	6.40503876

Appendix 8.17 RCCDRSM CUPRAC run 17

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.107				
A	2	Sample X1	A	0.205	0.098	CaSu11	0.3275194	3.275194
A	3	Sample X1	A	0.203	0.096	CaSu11	0.3226744	3.226744
A	4	Sample X1	A	0.203	0.096	CaSu11	0.3226744	3.226744
A	5	Blank B	B	0.103				
A	6	Sample X1	B	0.237	0.134	CaFr11	0.4147287	4.147287
A	7	Sample X1	B	0.24	0.137	CaFr11	0.4219961	4.219961
A	8	Sample X1	B	0.24	0.137	CaFr11	0.4219961	4.219961
A	9	Blank B	C	0.134				
A	10	Sample X1	C	0.224	0.09	CaFr12	0.3081395	3.081395
A	11	Sample X1	C	0.225	0.091	CaFr12	0.310562	3.10562
A	12	Sample X1	C	0.224	0.09	CaFr12	0.3081395	3.081395
B	1	Blank B	D	0.184				
B	2	Sample X1	D	0.177	0.093	CaFr21	0.315407	3.15407
B	3	Sample X1	D	0.176	0.092	CaFr21	0.3129845	3.129845
B	4	Sample X1	D	0.176	0.092	CaFr21	0.3129845	3.129845
B	5	Blank B	E	0.097				
B	6	Sample X1	E	0.194	0.097	CaXy11	0.3250969	3.250969
B	7	Sample X1	E	0.191	0.094	CaXy11	0.3178295	3.178295
B	8	Sample X1	E	0.191	0.094	CaXy11	0.3178295	3.178295
B	5	Blank B	E	0.112				
B	6	Sample X1	E	0.203	0.091	CaXy12	0.310562	3.10562
B	7	Sample X1	E	0.202	0.09	CaXy12	0.3081395	3.081395
B	8	Sample X1	E	0.203	0.091	CaXy12	0.310562	3.10562
B	1	Blank B	D	0.104				
B	2	Sample X1	D	0.194	0.09	CaXy21	0.3081395	3.081395
B	3	Sample X1	D	0.194	0.09	CaXy21	0.3081395	3.081395
B	4	Sample X1	D	0.196	0.092	CaXy21	0.3129845	3.129845
B	9	Blank B	F	0.083				
B	10	Sample X1	F	0.178	0.095	CaGr11	0.3202519	3.202519
B	11	Sample X1	F	0.178	0.095	CaGr11	0.3202519	3.202519
B	12	Sample X1	F	0.177	0.094	CaGr11	0.3178295	3.178295
C	1	Blank B	G	0.116				
C	2	Sample X1	G	0.208	0.092	CaGr12	0.3129845	3.129845
C	3	Sample X1	G	0.208	0.092	CaGr12	0.3129845	3.129845
C	4	Sample X1	G	0.208	0.092	CaGr12	0.3129845	3.129845
C	5	Blank B	H	0.095				

Appendix 8.17 contd.

C	6	Sample X1	H	0.19	0.095	CaGr21	0.3202519	3.202519
C	7	Sample X1	H	0.187	0.092	CaGr21	0.3129845	3.129845
C	8	Sample X1	H	0.187	0.092	CaGr21	0.3129845	3.129845
C	9	Blank B	I	0.078				
C	10	Sample X1	I	0.174	0.096	CaGc11	0.3226744	3.226744
C	11	Sample X1	I	0.174	0.096	CaGc11	0.3226744	3.226744
C	12	Sample X1	I	0.172	0.094	CaGc11	0.3178295	3.178295
D	1	Blank B	J	0.122				
D	2	Sample X1	J	0.212	0.09	CaGc21	0.3081395	3.081395
D	3	Sample X1	J	0.212	0.09	CaGc21	0.3081395	3.081395
D	4	Sample X1	J	0.213	0.091	CaGc21	0.310562	3.10562
D	5	Blank B	K	0.122				
D	6	Sample X1	K	0.214	0.092	CaGl11	0.3129845	3.129845
D	7	Sample X1	K	0.214	0.092	CaGl11	0.3129845	3.129845
D	8	Sample X1	K	0.212	0.09	CaGl11	0.3081395	3.081395
D	9	Blank B	L	0.099				
D	10	Sample X1	L	0.189	0.09	CaGl21	0.3081395	3.081395
D	11	Sample X1	L	0.19	0.091	CaGl21	0.310562	3.10562
D	12	Sample X1	L	0.189	0.09	CaGl21	0.3081395	3.081395

Appendix 8.18 RCCDRSM CUPRAC run 18

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.113				
E	2	Sample X1	A	0.204	0.091	CaSu11	0.31056202	12.42248
E	3	Sample X1	A	0.203	0.09	CaSu11	0.30813953	12.32558
E	4	Sample X1	A	0.204	0.091	CaSu11	0.31056202	12.42248
E	5	Blank B	B	0.117				
E	6	Sample X1	B	0.207	0.09	CaFr11	0.30813953	12.32558
E	7	Sample X1	B	0.207	0.09	CaFr11	0.30813953	12.32558
E	8	Sample X1	B	0.208	0.091	CaFr11	0.31056202	12.42248
E	9	Blank B	C	0.147				
E	10	Sample X1	C	24	0.093	CaFr12	0.31540698	12.61628
E	11	Sample X1	C	0.239	0.092	CaFr12	0.3129845	12.51938
E	12	Sample X1	C	0.241	0.094	CaFr12	0.31782946	12.71318
F	1	Blank B	D	0.183				
F	2	Sample X1	D	0.28	0.097	CaFr21	0.3250969	13.00388
F	3	Sample X1	D	0.28	0.097	CaFr21	0.3250969	13.00388

Appendix 8.18 contd.

F	4	Sample X1	D	0.278	0.096	CaFr21	0.32267442	12.90698
B	9	Blank B	F	0.108				
B	10	Sample X1	F	0.198	0.09	CaXy11	0.30813953	12.32558
B	11	Sample X1	F	0.199	0.091	CaXy11	0.31056202	12.42248
B	12	Sample X1	F	0.198	0.09	CaXy11	0.30813953	12.32558
F	5	Blank B	E	0.118				
F	6	Sample X1	E	0.209	0.091	CaXy12	0.31056202	12.42248
F	7	Sample X1	E	0.209	0.091	CaXy12	0.31056202	12.42248
F	8	Sample X1	E	0.209	0.091	CaXy12	0.31056202	12.42248
B	5	Blank B	E	0.087				
B	6	Sample X1	E	0.184	0.097	CaXy21	0.3250969	13.00388
B	7	Sample X1	E	0.184	0.097	CaXy21	0.3250969	13.00388
B	8	Sample X1	E	0.186	0.099	CaXy21	0.32994186	13.19767
F	9	Blank B	F	0.098				
F	10	Sample X1	F	0.19	0.092	CaGr11	0.3129845	12.51938
F	11	Sample X1	F	0.19	0.092	CaGr11	0.3129845	12.51938
F	12	Sample X1	F	0.188	0.09	CaGr11	0.30813953	12.32558
G	1	Blank B	G	0.107				
G	2	Sample X1	G	0.197	0.09	CaGr12	0.30813953	12.32558
G	3	Sample X1	G	0.197	0.09	CaGr12	0.30813953	12.32558
G	4	Sample X1	G	0.198	0.091	CaGr12	0.31056202	12.42248
G	5	Blank B	H	0.121				
G	6	Sample X1	H	0.212	0.091	CaGr21	0.31056202	12.42248
G	7	Sample X1	H	0.212	0.091	CaGr21	0.31056202	12.42248
G	8	Sample X1	H	0.213	0.093	CaGr21	0.31540698	12.61628
G	9	Blank B	I	0.078				
G	10	Sample X1	I	0.171	0.093	CaGc11	0.31540698	12.61628
G	11	Sample X1	I	0.17	0.092	CaGc11	0.3129845	12.51938
G	12	Sample X1	I	0.169	0.091	CaGc11	0.31056202	12.42248
H	1	Blank B	J	0.099				
	2	Sample X1	J	0.189	0.09	CaGc21	0.30813953	12.32558
H	3	Sample X1	J	0.189	0.09	CaGc21	0.30813953	12.32558
H	4	Sample X1	J	0.19	0.091	CaGc21	0.31056202	12.42248
H	5	Blank B	K	0.13				
H	6	Sample X1	K	0.221	0.091	CaGl11	0.31056202	12.42248
H	7	Sample X1	K	0.221	0.091	CaGl11	0.31056202	12.42248
H	8	Sample X1	K	0.222	0.092	CaGl11	0.3129845	12.51938
H	9	Blank B	L	0.097				
H	10	Sample X1	L	0.187	0.09	CaGl21	0.30813953	12.32558
H	11	Sample X1	L	0.187	0.09	CaGl21	0.30813953	12.32558
H	12	Sample X1	L	0.187	0.09	CaGl21	0.30813953	12.32558

Appendix 8.19 RCCDRSM CUPRAC run 19

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.105				
A	2	Sample X1	A	0.196	0.091	CaSu11	0.310562	12.42248
A	3	Sample X1	A	0.195	0.09	CaSu11	0.3081395	12.32558
A	4	Sample X1	A	0.196	0.091	CaSu11	0.310562	12.42248
A	5	Blank B	B	0.1				
A	6	Sample X1	B	0.19	0.09	CaFr11	0.3081395	12.32558
A	7	Sample X1	B	0.19	0.09	CaFr11	0.3081395	12.32558
A	8	Sample X1	B	0.19	0.09	CaFr11	0.3081395	12.32558
A	9	Blank B	C	0.106				
A	10	Sample X1	C	0.196	0.09	CaFr12	0.3081395	12.32558
A	11	Sample X1	C	0.196	0.09	CaFr12	0.3081395	12.32558
A	12	Sample X1	C	0.196	0.09	CaFr12	0.3081395	12.32558
B	1	Blank B	D	0.111				
B	2	Sample X1	D	0.202	0.091	CaFr21	0.310562	12.42248
B	3	Sample X1	D	0.202	0.091	CaFr21	0.310562	12.42248
B	4	Sample X1	D	0.202	0.091	CaFr21	0.310562	12.42248
C	1	Blank B	G	0.098				
C	2	Sample X1	G	0.19	0.092	CaXy11	0.3129845	12.51938
C	3	Sample X1	G	0.188	0.09	CaXy11	0.3081395	12.32558
C	4	Sample X1	G	0.188	0.09	CaXy11	0.3081395	12.32558
B	5	Blank B	E	0.101				
B	6	Sample X1	E	0.191	0.09	CaXy12	0.3081395	12.32558
B	7	Sample X1	E	0.191	0.09	CaXy12	0.3081395	12.32558
B	8	Sample X1	E	0.191	0.09	CaXy12	0.3081395	12.32558
B	9	Blank B	F	0.085				
B	10	Sample X1	F	0.175	0.09	CaXy21	0.3081395	12.32558
B	11	Sample X1	F	0.177	0.092	CaXy21	0.3129845	12.51938
B	12	Sample X1	F	0.176	0.091	CaXy21	0.310562	12.42248
B	9	Blank B	F	0.08				
B	10	Sample X1	F	0.172	0.092	CaGr11	0.3129845	12.51938
B	11	Sample X1	F	0.17	0.09	CaGr11	0.3081395	12.32558
B	12	Sample X1	F	0.172	0.092	CaGr11	0.3129845	12.51938
C	1	Blank B	G	0.092				
C	2	Sample X1	G	0.185	0.093	CaGr12	0.315407	12.61628
C	3	Sample X1	G	0.184	0.092	CaGr12	0.3129845	12.51938
C	4	Sample X1	G	0.184	0.092	CaGr12	0.3129845	12.51938
C	5	Blank B	H	0.109				

Appendix 8.19 contd.

C	6	Sample X1	H	0.199	0.09	CaGr21	0.3081395	12.32558
C	7	Sample X1	H	0.199	0.09	CaGr21	0.3081395	12.32558
C	8	Sample X1	H	0.199	0.09	CaGr21	0.3081395	12.32558
C	9	Blank B	I	0.089				
C	10	Sample X1	I	0.179	0.09	CaGc11	0.3081395	12.32558
C	11	Sample X1	I	0.179	0.09	CaGc11	0.3081395	12.32558
C	12	Sample X1	I	0.179	0.09	CaGc11	0.3081395	12.32558
D	1	Blank B	J	0.109				
D	2	Sample X1	J	0.2	0.091	CaGc21	0.310562	12.42248
D	3	Sample X1	J	0.199	0.09	CaGc21	0.3081395	12.32558
D	4	Sample X1	J	0.199	0.09	CaGc21	0.3081395	12.32558
D	5	Blank B	K	0.094				
D	6	Sample X1	K	0.184	0.09	CaGl11	0.3081395	12.32558
D	7	Sample X1	K	0.184	0.09	CaGl11	0.3081395	12.32558
D	8	Sample X1	K	0.184	0.09	CaGl11	0.3081395	12.32558
D	9	Blank B	L	0.075				
D	10	Sample X1	L	0.165	0.092	CaGl21	0.3129845	12.51938
D	11	Sample X1	L	0.165	0.092	CaGl21	0.3129845	12.51938
D	12	Sample X1	L	0.165	0.092	CaGl21	0.3129845	12.51938

Appendix 8.20 RCCDRSM CUPRAC run 20

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.113				
E	2	Sample X1	A	0.207	0.094	CaSu11	0.3178295	12.71318
E	3	Sample X1	A	0.207	0.094	CaSu11	0.3178295	12.71318
E	4	Sample X1	A	0.206	0.093	CaSu11	0.315407	12.61628
E	5	Blank B	B	0.103				
E	6	Sample X1	B	0.194	0.091	CaFr11	0.310562	12.42248
E	7	Sample X1	B	0.193	0.09	CaFr11	0.3081395	12.32558
E	8	Sample X1	B	0.193	0.09	CaFr11	0.3081395	12.32558
E	9	Blank B	C	0.108				
E	10	Sample X1	C	0.2	0.092	CaFr12	0.3129845	12.51938
E	11	Sample X1	C	0.2	0.092	CaFr12	0.3129845	12.51938
E	12	Sample X1	C	0.2	0.092	CaFr12	0.3129845	12.51938
F	1	Blank B	D	0.096				
F	2	Sample X1	D	0.186	0.09	CaFr21	0.3081395	12.32558

Appendix 8.20 contd.

F	3	Sample X1	D	0.188	0.092	CaFr21	0.3129845	12.51938
F	4	Sample X1	D	0.188	0.092	CaFr21	0.3129845	12.51938
C	5	Blank B	H	0.128				
C	6	Sample X1	H	0.219	0.091	CaXy11	0.310562	12.42248
C	7	Sample X1	H	0.22	0.092	CaXy11	0.3129845	12.51938
C	8	Sample X1	H	0.219	0.091	CaXy11	0.310562	12.42248
F	5	Blank B	E	0.092				
F	6	Sample X1	E	0.184	0.092	CaXy12	0.3129845	12.51938
F	7	Sample X1	E	0.184	0.092	CaXy12	0.3129845	12.51938
F	8	Sample X1	E	0.186	0.094	CaXy12	0.3178295	12.71318
C	1	Blank B	G	0.113				
C	2	Sample X1	G	0.203	0.09	CaXy21	0.3081395	15.40698
C	3	Sample X1	G	0.203	0.09	CaXy21	0.3081395	12.32558
C	4	Sample X1	G	0.203	0.09	CaXy21	0.3081395	12.32558
F	9	Blank B	F	0.093				
F	10	Sample X1	F	0.185	0.092	CaGr11	0.3129845	12.51938
F	11	Sample X1	F	0.184	0.091	CaGr11	0.310562	12.42248
F	12	Sample X1	F	0.185	0.092	CaGr11	0.3129845	12.51938
G	1	Blank B	G	0.097				
G	2	Sample X1	G	0.187	0.09	CaGr12	0.3081395	12.32558
G	3	Sample X1	G	0.188	0.091	CaGr12	0.310562	12.42248
G	4	Sample X1	G	0.187	0.09	CaGr12	0.3081395	12.32558
G	5	Blank B	H	0.092				
G	6	Sample X1	H	0.183	0.091	CaGr21	0.310562	12.42248
G	7	Sample X1	H	0.183	0.091	CaGr21	0.310562	12.42248
G	8	Sample X1	H	0.183	0.091	CaGr21	0.310562	12.42248
G	9	Blank B	I	0.103				
G	10	Sample X1	I	0.193	0.09	CaGc11	0.3081395	12.32558
G	11	Sample X1	I	0.193	0.09	CaGc11	0.3081395	12.32558
G	12	Sample X1	I	0.194	0.091	CaGc11	0.310562	12.42248
H	1	Blank B	J	0.101				
H	2	Sample X1	J	0.192	0.091	CaGc21	0.310562	12.42248
H	3	Sample X1	J	0.193	0.092	CaGc21	0.3129845	12.51938
H	4	Sample X1	J	0.193	0.092	CaGc21	0.3129845	12.51938
H	5	Blank B	K	0.104				
H	6	Sample X1	K	0.195	0.091	CaGl11	0.310562	12.42248
H	7	Sample X1	K	0.194	0.09	CaGl11	0.3081395	12.32558
H	8	Sample X1	K	0.195	0.091	CaGl11	0.310562	12.42248
H	9	Blank B	L	0.084				
H	10	Sample X1	L	0.178	0.094	CaGl21	0.3178295	12.71318
H	11	Sample X1	L	0.177	0.093	CaGl21	0.315407	12.61628
H	12	Sample X1	L	0.177	0.093	CaGl21	0.315407	12.61628

Appendix 8.21 RCCDRSM CUPRAC run 21

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample Code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.122				
D	2	Sample X1	J	0.213	0.091	CaSu11	0.310562016	4.658430233
D	3	Sample X1	J	0.215	0.093	CaSu11	0.315406977	4.731104651
D	4	Sample X1	J	0.215	0.093	CaSu11	0.315406977	4.731104651
A	1	Blank B	A	0.136				
A	2	Sample X1	A	0.232	0.096	CaFr11	0.322674419	4.840116279
A	3	Sample X1	A	0.233	0.097	CaFr11	0.325096899	4.876453488
A	4	Sample X1	A	0.233	0.097	CaFr11	0.325096899	4.876453488
A	5	Blank B	B	0.103				
A	6	Sample X1	B	0.201	0.098	CaFr12	0.32751938	4.912790698
A	7	Sample X1	B	0.199	0.096	CaFr12	0.322674419	4.840116279
A	8	Sample X1	B	0.199	0.096	CaFr12	0.322674419	4.840116279
A	9	Blank B	C	0.117				
A	10	Sample X1	C	0.21	0.093	CaFr21	0.315406977	4.731104651
A	11	Sample X1	C	0.21	0.093	CaFr21	0.315406977	4.731104651
A	12	Sample X1	C	0.212	0.095	CaFr21	0.320251938	4.80377907
B	1	Blank B	D	0.093				
B	2	Sample X1	D	0.187	0.094	CaXy11	0.317829457	4.76744186
B	3	Sample X1	D	0.187	0.094	CaXy11	0.317829457	4.76744186
B	4	Sample X1	D	0.19	0.097	CaXy11	0.325096899	4.876453488
B	5	Blank B	E	0.106				
B	6	Sample X1	E	0.201	0.096	CaXy12	0.322674419	4.840116279
B	7	Sample X1	E	0.202	0.097	CaXy12	0.325096899	4.876453488
B	8	Sample X1	E	0.202	0.097	CaXy12	0.325096899	4.876453488
B	9	Blank B	F	0.099				
B	10	Sample X1	F	0.195	0.096	CaXy21	0.322674419	4.840116279
B	11	Sample X1	F	0.197	0.098	CaXy21	0.32751938	4.912790698
B	12	Sample X1	F	.197.	0.098	CaXy21	0.32751938	4.912790698
C	1	Blank B	G	0.095				
C	2	Sample X1	G	0.19	0.095	CaGr11	0.320251938	4.80377907
C	3	Sample X1	G	0.191	0.096	CaGr11	0.322674419	4.840116279
C	4	Sample X1	G	0.19	0.095	CaGr11	0.320251938	4.80377907
C	5	Blank B	H	0.103				
C	6	Sample X1	H	0.194	0.091	CaGr12	0.310562016	4.658430233
C	7	Sample X1	H	0.194	0.091	CaGr12	0.310562016	4.658430233
C	8	Sample X1	H	0.195	0.092	CaGr12	0.312984496	4.694767442
C	9	Blank B	I	0.08				

Appendix 8.21 contd.

C	10	Sample X1	I	0.172	0.092	CaGr21	0.312984496	4.694767442
C	11	Sample X1	I	0.171	0.091	CaGr21	0.310562016	4.658430233
C	12	Sample X1	I	0.171	0.091	CaGr21	0.310562016	4.658430233
D	5	Blank B	K	0.084				
D	6	Sample X1	K	0.182	0.098	CaGc11	0.32751938	4.912790698
D	7	Sample X1	K	0.178	0.094	CaGc11	0.317829457	4.76744186
D	8	Sample X1	K	0.178	0.094	CaGc11	0.317829457	4.76744186
D	9	Blank B	L	0.065				
D	10	Sample X1	L	0.158	0.093	CaGc21	0.315406977	4.731104651
D	11	Sample X1	L	0.159	0.094	CaGc21	0.317829457	4.76744186
D	12	Sample X1	L	0.159	0.094	CaGc21	0.317829457	4.76744186
E	1	Blank B	M	0.091				
E	2	Sample X1	M	0.183	0.092	CaGl11	0.312984496	4.694767442
E	3	Sample X1	M	0.182	0.091	CaGl11	0.310562016	4.658430233
E	4	Sample X1	M	0.182	0.091	CaGl11	0.310562016	4.658430233
E	5	Blank B	N	0.09				
E	6	Sample X1	N	0.181	0.091	CaGl21	0.310562016	4.658430233
E	7	Sample X1	N	0.18	0.09	CaGl21	0.308139535	4.622093023
E	8	Sample X1	N	0.18	0.09	CaGl21	0.308139535	4.622093023

Appendix 8.22 RCCDRSM CUPRAC run 22

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.1				
A	2	Sample X1	A	0.194	0.094	CaSu11	0.3178295	15.891473
A	3	Sample X1	A	0.192	0.092	CaSu11	0.3129845	15.649225
A	4	Sample X1	A	0.194	0.094	CaSu11	0.3178295	15.891473
A	5	Blank B	B	0.129				
A	6	Sample X1	B	0.31	0.181	CaFr11	0.5285853	26.429264
A	7	Sample X1	B	0.309	0.18	CaFr11	0.5261628	26.30814
A	8	Sample X1	B	0.309	0.18	CaFr11	0.5261628	26.30814
A	9	Blank B	C	0.135				
A	10	Sample X1	C	0.225	0.09	CaFr12	0.3081395	15.406977
A	11	Sample X1	C	0.225	0.09	CaFr12	0.3081395	15.406977
A	12	Sample X1	C	0.227	0.092	CaFr12	0.3129845	15.649225
B	1	Blank B	D	0.14				
B	2	Sample X1	D	0.232	0.092	CaFr21	0.3129845	15.649225
B	3	Sample X1	D	0.232	0.092	CaFr21	0.3129845	15.649225

Appendix 8.22 contd.

B	4	Sample X1	D	0.232	0.092	CaFr21	0.3129845	15.649225
C	9	Blank B	I	0.08				
C	10	Sample X1	I	0.173	0.093	CaXy11	0.315407	15.770349
C	11	Sample X1	I	0.173	0.093	CaXy11	0.315407	15.770349
C	12	Sample X1	I	0.177	0.097	CaXy11	0.3250969	16.254845
B	5	Blank B	E	0.117				
B	6	Sample X1	E	0.211	0.094	CaXy12	0.3178295	15.891473
B	7	Sample X1	E	0.209	0.092	CaXy12	0.3129845	15.649225
B	8	Sample X1	E	0.209	0.092	CaXy12	0.3129845	15.649225
C	5	Blank B	H	0.102				
C	6	Sample X1	H	0.2	0.098	CaXy21	0.3275194	16.375969
C	7	Sample X1	H	0.201	0.099	CaXy21	0.3299419	16.497093
C	8	Sample X1	H	0.2	0.098	CaXy21	0.3275194	16.375969
B	9	Blank B	F	0.106				
B	10	Sample X1	F	0.199	0.093	CaGr11	0.315407	15.770349
B	11	Sample X1	F	0.199	0.093	CaGr11	0.315407	15.770349
B	12	Sample X1	F	0.2	0.094	CaGr11	0.3178295	15.891473
C	1	Blank B	G	0.102				
C	2	Sample X1	G	0.196	0.094	CaGr12	0.3178295	15.891473
C	3	Sample X1	G	0.195	0.093	CaGr12	0.315407	15.770349
C	4	Sample X1	G	0.195	0.093	CaGr12	0.315407	15.770349
C	5	Blank B	H	0.101				
C	6	Sample X1	H	0.198	0.097	CaGr21	0.3250969	16.254845
C	7	Sample X1	H	0.198	0.097	CaGr21	0.3250969	16.254845
C	8	Sample X1	H	0.2	0.099	CaGr21	0.3299419	16.497093
C	9	Blank B	I	0.133				
C	10	Sample X1	I	0.224	0.091	CaGc11	0.310562	15.528101
C	11	Sample X1	I	0.225	0.092	CaGc11	0.3129845	15.649225
C	12	Sample X1	I	0.225	0.092	CaGc11	0.3129845	15.649225
D	1	Blank B	J	0.122				
D	2	Sample X1	J	0.213	0.091	CaGc21	0.310562	15.528101
D	3	Sample X1	J	0.213	0.091	CaGc21	0.310562	15.528101
D	4	Sample X1	J	0.212	0.09	CaGc21	0.3081395	15.406977
D	5	Blank B	K	0.099				
D	6	Sample X1	K	0.189	0.09	CaGl11	0.3081395	15.406977
D	7	Sample X1	K	0.19	0.091	CaGl11	0.310562	15.528101
D	8	Sample X1	K	0.189	0.09	CaGl11	0.3081395	15.406977
D	9	Blank B	L	0.111				
D	10	Sample X1	L	0.201	0.09	CaGl21	0.3081395	15.406977
D	11	Sample X1	L	0.202	0.091	CaGl21	0.310562	15.528101
D	12	Sample X1	L	0.201	0.09	CaGl21	0.3081395	15.406977

Appendix 8.23 RCCDRSM CUPRAC run 23

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.126				
E	2	Sample X1	A	0.224	0.098	CaSu11	0.3275194	4.912791
E	3	Sample X1	A	0.224	0.098	CaSu11	0.3275194	4.912791
E	4	Sample X1	A	0.218	0.092	CaSu11	0.3129845	4.694767
E	5	Blank B	B	0.158				
E	6	Sample X1	B	0.338	0.18	CaFr11	0.5261628	7.892442
E	7	Sample X1	B	0.338	0.18	CaFr11	0.5261628	7.892442
E	8	Sample X1	B	0.339	0.181	CaFr11	0.5285853	7.928779
E	9	Blank B	C	0.176				
E	10	Sample X1	C	0.268	0.092	CaFr12	0.3129845	4.694767
E	11	Sample X1	C	0.267	0.091	CaFr12	0.310562	4.65843
E	12	Sample X1	C	0.268	0.092	CaFr12	0.3129845	4.694767
F	1	Blank B	D	0.149				
F	2	Sample X1	D	0.252	0.103	CaFr21	0.3396318	5.094477
F	3	Sample X1	D	0.251	0.102	CaFr21	0.3372093	5.05814
F	4	Sample X1	D	0.251	0.102	CaFr21	0.3372093	5.05814
D	1	Blank B	J	0.098				
D	2	Sample X1	J	0.191	0.093	CaXy11	0.315407	4.731105
D	3	Sample X1	J	0.19	0.092	CaXy11	0.3129845	4.694767
D	4	Sample X1	J	0.19	0.092	CaXy11	0.3129845	4.694767
F	5	Blank B	E	0.104				
F	6	Sample X1	E	0.196	0.092	CaXy12	0.3129845	4.694767
F	7	Sample X1	E	0.199	0.095	CaXy12	0.3202519	4.803779
F	8	Sample X1	E	0.199	0.095	CaXy12	0.3202519	4.803779
C	9	Blank B	I	0.089				
C	10	Sample X1	I	0.184	0.095	CaXy21	0.3202519	4.803779
C	11	Sample X1	I	0.184	0.095	CaXy21	0.3202519	4.803779
C	12	Sample X1	I	0.181	0.092	CaXy21	0.3129845	4.694767
F	9	Blank B	F	0.096				
F	10	Sample X1	F	0.194	0.098	CaGr11	0.3275194	4.912791
F	11	Sample X1	F	0.194	0.098	CaGr11	0.3275194	4.912791
F	12	Sample X1	F	0.191	0.095	CaGr11	0.3202519	4.803779
G	1	Blank B	G	0.103				
G	2	Sample X1	G	0.234	0.131	CaGr12	0.4074612	6.111919
G	3	Sample X1	G	0.236	0.133	CaGr12	0.4123062	6.184593
G	4	Sample X1	G	0.234	0.131	CaGr12	0.4074612	6.111919
G	5	Blank B	H	0.086				

Appendix 8.23 contd.

G	6	Sample X1	H	0.178	0.092	CaGr21	0.3129845	4.694767
G	7	Sample X1	H	0.178	0.092	CaGr21	0.3129845	4.694767
G	8	Sample X1	H	0.179	0.093	CaGr21	0.315407	4.731105
G	9	Blank B	I	0.1				
G	10	Sample X1	I	0.21	0.11	CaGc11	0.3565891	5.348837
G	11	Sample X1	I	0.21	0.11	CaGc11	0.3565891	5.348837
G	12	Sample X1	I	0.211	0.111	CaGc11	0.3590116	5.385174
H	1	Blank B	J	0.092				
H	2	Sample X1	J	0.187	0.095	CaGc21	0.3202519	4.803779
H	3	Sample X1	J	0.19	0.098	CaGc21	0.3275194	4.912791
H	4	Sample X1	J	0.187	0.095	CaGc21	0.3202519	4.803779
H	5	Blank B	K	0.093				
H	6	Sample X1	K	0.199	0.106	CaGl11	0.3468992	5.203488
H	7	Sample X1	K	0.199	0.106	CaGl11	0.3468992	5.203488
H	8	Sample X1	K	0.201	0.108	CaGl11	0.3517442	5.276163
H	9	Blank B	L	0.101				
H	10	Sample X1	L	0.194	0.093	CaGl21	0.315407	4.731105
H	11	Sample X1	L	0.194	0.093	CaGl21	0.315407	4.731105
H	12	Sample X1	L	0.196	0.095	CaGl21	0.3202519	4.803779

Appendix 8.24 RCCDRSM CUPRAC run 24

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
D	1	Blank B	J	0.108				
D	2	Sample X1	J	0.206	0.096	CaSu11	0.3226744	4.840116
D	3	Sample X1	J	0.208	0.098	CaSu11	0.3275194	4.912791
D	4	Sample X1	J	0.206	0.096	CaSu11	0.3226744	4.840116
A	1	Blank B	A	0.133				
A	2	Sample X1	A	0.207	0.094	CaFr11	0.3178295	4.767442
A	3	Sample X1	A	0.206	0.093	CaFr11	0.315407	4.731105
A	4	Sample X1	A	0.206	0.093	CaFr11	0.315407	4.731105
A	5	Blank B	B	0.091				
A	6	Sample X1	B	0.187	0.096	CaFr12	0.3226744	4.840116
A	7	Sample X1	B	0.186	0.095	CaFr12	0.3202519	4.803779
A	8	Sample X1	B	0.186	0.095	CaFr12	0.3202519	4.803779
A	9	Blank B	C	0.102				
A	10	Sample X1	C	0.199	0.097	CaFr21	0.3250969	4.876453
A	11	Sample X1	C	0.194	0.092	CaFr21	0.3129845	4.694767

Appendix 8.24 contd.

A	12	Sample X1	C	0.194	0.092	CaFr21	0.3129845	4.694767
B	1	Blank B	D	0.072				
B	2	Sample X1	D	0.167	0.095	CaXy11	0.3202519	4.803779
B	3	Sample X1	D	0.167	0.095	CaXy11	0.3202519	4.803779
B	4	Sample X1	D	0.169	0.097	CaXy11	0.3250969	4.876453
B	5	Blank B	E	0.085				
B	6	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.876453
B	7	Sample X1	E	0.181	0.096	CaXy12	0.3226744	4.840116
B	8	Sample X1	E	0.182	0.097	CaXy12	0.3250969	4.876453
B	9	Blank B	F	0.071				
B	10	Sample X1	F	0.164	0.093	CaXy21	0.315407	4.731105
B	11	Sample X1	F	0.162	0.091	CaXy21	0.310562	4.65843
B	12	Sample X1	F	0.164	0.093	CaXy21	0.315407	4.731105
C	1	Blank B	G	0.064				
C	2	Sample X1	G	0.167	0.103	CaGr11	0.3396318	5.094477
C	3	Sample X1	G	0.17	0.106	CaGr11	0.3468992	5.203488
C	4	Sample X1	G	0.17	0.106	CaGr11	0.3468992	5.203488
C	5	Blank B	H	0.086				
C	6	Sample X1	H	0.179	0.093	CaGr12	0.315407	4.731105
C	7	Sample X1	H	0.182	0.096	CaGr12	0.3226744	4.840116
C	8	Sample X1	H	0.182	0.096	CaGr12	0.3226744	4.840116
C	9	Blank B	I	0.074				
C	10	Sample X1	I	0.165	0.091	CaGr21	0.310562	4.65843
C	11	Sample X1	I	0.165	0.091	CaGr21	0.310562	4.65843
C	12	Sample X1	I	0.166	0.092	CaGr21	0.3129845	4.694767
D	5	Blank B	K	0.063				
D	6	Sample X1	K	0.167	0.104	CaGc11	0.3420543	5.130814
D	7	Sample X1	K	0.166	0.103	CaGc11	0.3396318	5.094477
D	8	Sample X1	K	0.166	0.103	CaGc11	0.3396318	5.094477
D	9	Blank B	L	0.08				
D	10	Sample X1	L	0.175	0.095	CaGc21	0.3202519	4.803779
D	11	Sample X1	L	0.176	0.096	CaGc21	0.3226744	4.840116
D	12	Sample X1	L	0.176	0.096	CaGc21	0.3226744	4.840116
E	1	Blank B	M	0.095				
E	2	Sample X1	M	0.192	0.097	CaGl11	0.3250969	4.876453
E	3	Sample X1	M	0.19	0.095	CaGl11	0.3202519	4.803779
E	4	Sample X1	M	0.19	0.095	CaGl11	0.3202519	4.803779
E	5	Blank B	N	0.082				
E	6	Sample X1	N	0.184	0.092	CaGl21	0.3129845	4.694767
E	7	Sample X1	N	0.187	0.095	CaGl21	0.3202519	4.803779
E	8	Sample X1	N	0.187	0.095	CaGl21	0.3202519	4.803779

Appendix 8.25 RCCDRSM CUPRAC run 25

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.114				
A	2	Sample X1	A	0.208	0.094	CaSu11	0.3178295	9.534884
A	3	Sample X1	A	0.206	0.092	CaSu11	0.3129845	9.389535
A	4	Sample X1	A	0.206	0.092	CaSu11	0.3129845	9.389535
A	5	Blank B	B	0.127				
A	6	Sample X1	B	0.22	0.093	CaFr11	0.315407	9.462209
A	7	Sample X1	B	0.221	0.094	CaFr11	0.3178295	9.534884
A	8	Sample X1	B	0.221	0.094	CaFr11	0.3178295	9.534884
A	9	Blank B	C	0.123				
A	10	Sample X1	C	0.214	0.091	CaFr12	0.310562	9.31686
A	11	Sample X1	C	0.215	0.092	CaFr12	0.3129845	9.389535
A	12	Sample X1	C	0.215	0.092	CaFr12	0.3129845	9.389535
B	1	Blank B	D	0.11				
B	2	Sample X1	D	0.205	0.095	CaFr21	0.3202519	9.607558
B	3	Sample X1	D	0.205	0.095	CaFr21	0.3202519	9.607558
B	4	Sample X1	D	0.202	0.092	CaFr21	0.3129845	9.389535
D	5	Blank B	K	0.11				
D	6	Sample X1	K	0.091	0.092	CaXy11	0.3129845	9.389535
D	7	Sample X1	K	0.101	0.094	CaXy11	0.3178295	9.534884
D	8	Sample X1	K	0.102	0.092	CaXy11	0.3129845	9.389535
B	5	Blank B	E	0.097				
B	6	Sample X1	E	0.189	0.092	CaXy12	0.3129845	9.389535
B	7	Sample X1	E	0.191	0.094	CaXy12	0.3178295	9.534884
B	8	Sample X1	E	0.189	0.092	CaXy12	0.3129845	9.389535
D	1	Blank B	J	0.107				
D	2	Sample X1	J	0.198	0.091	CaXy21	0.310562	9.31686
D	3	Sample X1	J	0.199	0.092	CaXy21	0.3129845	9.389535
D	4	Sample X1	J	0.198	0.091	CaXy21	0.310562	9.31686
B	9	Blank B	F	0.094				
B	10	Sample X1	F	0.186	0.092	CaGr11	0.3129845	9.389535
B	11	Sample X1	F	0.187	0.093	CaGr11	0.315407	9.462209
B	12	Sample X1	F	0.186	0.092	CaGr11	0.3129845	9.389535
C	1	Blank B	G	0.102				
C	2	Sample X1	G	0.193	0.091	CaGr12	0.310562	9.31686
C	3	Sample X1	G	0.194	0.092	CaGr12	0.3129845	9.389535
C	4	Sample X1	G	0.193	0.091	CaGr12	0.310562	9.31686
C	5	Blank B	H	0.101				

Appendix 8.25 contd.

C	6	Sample X1	H	0.192	0.091	CaGr21	0.310562	9.31686
C	7	Sample X1	H	0.191	0.09	CaGr21	0.3081395	9.244186
C	8	Sample X1	H	0.192	0.091	CaGr21	0.310562	9.31686
C	9	Blank B	I	0.099				
C	10	Sample X1	I	0.19	0.091	CaGc11	0.310562	9.31686
C	11	Sample X1	I	0.19	0.091	CaGc11	0.310562	9.31686
C	12	Sample X1	I	0.189	0.09	CaGc11	0.3081395	9.244186
D	1	Blank B	J	0.092				
D	2	Sample X1	J	0.182	0.09	CaGc21	0.3081395	9.244186
D	3	Sample X1	J	0.184	0.092	CaGc21	0.3129845	9.389535
D	4	Sample X1	J	0.184	0.092	CaGc21	0.3129845	9.389535
D	5	Blank B	K	0.099				
D	6	Sample X1	K	0.192	0.093	CaGl11	0.315407	9.462209
D	7	Sample X1	K	0.192	0.093	CaGl11	0.315407	9.462209
D	8	Sample X1	K	0.196	0.097	CaGl11	0.3250969	9.752907
D	9	Blank B	L	0.097				
D	10	Sample X1	L	0.192	0.095	CaGl21	0.3202519	9.607558
D	11	Sample X1	L	0.196	0.099	CaGl21	0.3299419	9.898256
D	12	Sample X1	L	0.192	0.095	CaGl21	0.3202519	9.607558

Appendix 8.26 RCCDRSM CUPRAC run 26

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.203				
E	2	Sample X1	A	0.293	0.09	CaSu11	0.308139535	9.244186
E	3	Sample X1	A	0.294	0.091	CaSu11	0.310562016	9.31686
E	4	Sample X1	A	0.294	0.091	CaSu11	0.310562016	9.31686
E	5	Blank B	B	0.128				
E	6	Sample X1	B	0.219	0.091	CaFr11	0.310562016	9.31686
E	7	Sample X1	B	0.219	0.091	CaFr11	0.310562016	9.31686
E	8	Sample X1	B	0.22	0.092	CaFr11	0.312984496	9.389535
E	9	Blank B	C	0.137				
E	10	Sample X1	C	0.228	0.091	CaFr12	0.310562016	9.31686
E	11	Sample X1	C	0.228	0.091	CaFr12	0.310562016	9.31686
E	12	Sample X1	C	0.229	0.092	CaFr12	0.312984496	9.389535
F	1	Blank B	D	0.146				
F	2	Sample X1	D	0.238	0.092	CaFr21	0.312984496	9.389535
F	3	Sample X1	D	0.238	0.092	CaFr21	0.312984496	9.389535

Appendix 8.26 contd.

F	4	Sample X1	D	0.24	0.094	CaFr21	0.317829457	9.534884
D	9	Blank B	L	0.107				
D	10	Sample X1	L	0.197	0.09	CaXy11	0.308139535	9.244186
D	11	Sample X1	L	0.197	0.09	CaXy11	0.308139535	9.244186
D	12	Sample X1	L	0.197	0.09	CaXy11	0.308139535	9.244186
F	5	Blank B	E	0.095				
F	6	Sample X1	E	0.188	0.093	CaXy12	0.315406977	9.462209
F	7	Sample X1	E	0.187	0.092	CaXy12	0.312984496	9.389535
F	8	Sample X1	E	0.187	0.092	CaXy12	0.312984496	9.389535
D	5	Blank B	K	0.103				
D	6	Sample X1	K	0.193	0.09	CaXy21	0.308139535	9.244186
D	7	Sample X1	K	0.193	0.09	CaXy21	0.308139535	9.244186
D	8	Sample X1	K	0.193	0.09	CaXy21	0.308139535	9.244186
F	9	Blank B	F	0.088				
F	10	Sample X1	F	0.183	0.095	CaGr11	0.320251938	9.607558
F	11	Sample X1	F	0.185	0.097	CaGr11	0.325096899	9.752907
F	12	Sample X1	F	0.183	0.095	CaGr11	0.320251938	9.607558
G	1	Blank B	G	0.097				
G	2	Sample X1	G	0.189	0.092	CaGr12	0.312984496	9.389535
G	3	Sample X1	G	0.187	0.09	CaGr12	0.308139535	9.244186
G	4	Sample X1	G	0.187	0.09	CaGr12	0.308139535	9.244186
G	5	Blank B	H	0.105				
G	6	Sample X1	H	0.199	0.094	CaGr21	0.317829457	9.534884
G	7	Sample X1	H	0.197	0.092	CaGr21	0.312984496	9.389535
G	8	Sample X1	H	0.199	0.094	CaGr21	0.317829457	9.534884
G	9	Blank B	I	0.086				
G	10	Sample X1	I	0.184	0.098	CaGc11	0.32751938	9.825581
G	11	Sample X1	I	0.185	0.099	CaGc11	0.32994186	9.898256
G	12	Sample X1	I	0.184	0.098	CaGc11	0.32751938	9.825581
H	1	Blank B	J	0.104				
H	2	Sample X1	J	0.199	0.095	CaGc21	0.320251938	9.607558
H	3	Sample X1	J	0.197	0.093	CaGc21	0.315406977	9.462209
H	4	Sample X1	J	0.197	0.093	CaGc21	0.315406977	9.462209
H	5	Blank B	K	0.113				
H	6	Sample X1	K	0.208	0.095	CaGl11	0.320251938	9.607558
H	7	Sample X1	K	0.208	0.095	CaGl11	0.320251938	9.607558
H	8	Sample X1	K	0.207	0.094	CaGl11	0.317829457	9.534884
H	9	Blank B	L	0.123				
H	10	Sample X1	L	0.213	0.09	CaGl21	0.308139535	9.244186
H	11	Sample X1	L	0.213	0.09	CaGl21	0.308139535	9.244186
H	12	Sample X1	L	0.213	0.09	CaGl21	0.308139535	9.244186

Appendix 8.27 RCCDRSM CUPRAC run 27

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.389				
A	2	Sample X1	A	0.481	0.092	CaSu11	0.312984496	9.389535
A	3	Sample X1	A	0.481	0.092	CaSu11	0.312984496	9.389535
A	4	Sample X1	A	0.48	0.091	CaSu11	0.310562016	9.31686
A	5	Blank B	B	0.118				
A	6	Sample X1	B	0.211	0.093	CaFr11	0.315406977	9.462209
A	7	Sample X1	B	0.208	0.09	CaFr11	0.308139535	9.244186
A	8	Sample X1	B	0.211	0.093	CaFr11	0.315406977	9.462209
A	9	Blank B	C	0.172				
A	10	Sample X1	C	0.268	0.096	CaFr12	0.322674419	9.680233
A	11	Sample X1	C	0.267	0.095	CaFr12	0.320251938	9.607558
A	12	Sample X1	C	0.267	0.095	CaFr12	0.320251938	9.607558
B	1	Blank B	D	0.477				
B	2	Sample X1	D	0.573	0.096	CaFr21	0.322674419	9.680233
B	3	Sample X1	D	0.573	0.096	CaFr21	0.322674419	9.680233
B	4	Sample X1	D	0.574	0.097	CaFr21	0.325096899	9.752907
E	1	Blank B	M	0.124				
E	2	Sample X1	M	0.221	0.097	CaXy11	0.325096899	9.752907
E	3	Sample X1	M	0.221	0.097	CaXy11	0.325096899	9.752907
E	4	Sample X1	M	0.218	0.093	CaXy11	0.315406977	9.462209
B	5	Blank B	E	0.11				
B	6	Sample X1	E	0.206	0.096	CaXy12	0.322674419	9.680233
B	7	Sample X1	E	0.206	0.096	CaXy12	0.322674419	9.680233
B	8	Sample X1	E	0.207	0.097	CaXy12	0.325096899	9.752907
D	9	Blank B	L	0.08				
D	10	Sample X1	L	0.179	0.099	CaXy21	0.32994186	9.898256
D	11	Sample X1	L	0.176	0.096	CaXy21	0.322674419	9.680233
D	12	Sample X1	L	0.179	0.099	CaXy21	0.32994186	9.898256
B	9	Blank B	F	0.121				
B	10	Sample X1	F	0.212	0.091	CaGr11	0.310562016	9.31686
B	11	Sample X1	F	0.215	0.094	CaGr11	0.317829457	9.534884
B	12	Sample X1	F	0.212	0.091	CaGr11	0.310562016	9.31686
C	1	Blank B	G	0.129				
C	2	Sample X1	G	0.222	0.093	CaGr12	0.315406977	9.462209
C	3	Sample X1	G	0.219	0.091	CaGr12	0.310562016	9.31686
C	4	Sample X1	G	0.222	0.093	CaGr12	0.315406977	9.462209
C	5	Blank B	H	0.093				
C	6	Sample X1	H	0.186	0.093	CaGr21	0.315406977	9.462209

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C	7	Sample X1	H	0.186	0.093	CaGr21	0.315406977	9.462209
C	8	Sample X1	H	0.187	0.094	CaGr21	0.317829457	9.534884
C	9	Blank B	I	0.103				
C	10	Sample X1	I	0.195	0.092	CaGc11	0.312984496	9.389535
C	11	Sample X1	I	0.195	0.092	CaGc11	0.312984496	9.389535
C	12	Sample X1	I	0.194	0.091	CaGc11	0.310562016	9.31686
D	1	Blank B	J	0.113				
D	2	Sample X1	J	0.203	0.09	CaGc21	0.308139535	9.244186
D	3	Sample X1	J	0.203	0.09	CaGc21	0.308139535	9.244186
D	4	Sample X1	J	0.203	0.09	CaGc21	0.308139535	9.244186
D	5	Blank B	K	0.129				
D	6	Sample X1	K	0.225	0.096	CaGl11	0.322674419	9.680233
D	7	Sample X1	K	0.226	0.097	CaGl11	0.325096899	9.752907
D	8	Sample X1	K	0.225	0.096	CaGl11	0.322674419	9.680233
D	9	Blank B	L	0.108				
D	10	Sample X1	L	0.199	0.091	CaGl21	0.310562016	9.31686
D	11	Sample X1	L	0.199	0.091	CaGl21	0.310562016	9.31686
D	12	Sample X1	L	0.199	0.091	CaGl21	0.310562016	9.31686

Appendix 8.28 RCCDRSM CUPRAC run 28

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.126				
E	2	Sample X1	A	0.229	0.103	CaSu11	0.33963178	10.18895
E	3	Sample X1	A	0.231	0.105	CaSu11	0.34447674	10.3343
E	4	Sample X1	A	0.231	0.105	CaSu11	0.34447674	10.3343
E	5	Blank B	B	0.144				
E	6	Sample X1	B	0.324	0.18	CaFr11	0.52616279	15.78488
E	7	Sample X1	B	0.326	0.182	CaFr11	0.53100775	15.93023
E	8	Sample X1	B	0.324	0.18	CaFr11	0.52616279	15.78488
E	9	Blank B	C	0.135				
E	10	Sample X1	C	0.227	0.092	CaFr12	0.3129845	9.389535
E	11	Sample X1	C	0.225	0.09	CaFr12	0.30813953	9.244186
E	12	Sample X1	C	0.225	0.09	CaFr12	0.30813953	9.244186
F	1	Blank B	D	0.12				
F	2	Sample X1	D	0.21	0.09	CaFr21	0.30813953	9.244186
F	3	Sample X1	D	0.212	0.092	CaFr21	0.3129845	9.389535
F	4	Sample X1	D	0.212	0.092	CaFr21	0.3129845	9.389535
E	5	Blank B	N	0.105				

Appendix 8.28 contd.

E	6	Sample X1	N	0.196	0.091	CaXy11	0.31056202	9.31686
E	7	Sample X1	N	0.195	0.09	CaXy11	0.30813953	9.244186
E	8	Sample X1	N	0.195	0.09	CaXy11	0.30813953	9.244186
F	5	Blank B	E	0.114				
F	6	Sample X1	E	0.207	0.093	CaXy12	0.31540698	9.462209
F	7	Sample X1	E	0.208	0.094	CaXy12	0.31782946	9.534884
F	8	Sample X1	E	0.207	0.093	CaXy12	0.31540698	9.462209
E	1	Blank B	M	0.099				
E	2	Sample X1	M	0.189	0.09	CaXy21	0.30813953	9.244186
E	3	Sample X1	M	0.19	0.091	CaXy21	0.31056202	9.31686
E	4	Sample X1	M	0.189	0.09	CaXy21	0.30813953	9.244186
F	9	Blank B	F	0.099				
F	10	Sample X1	F	0.196	0.097	CaGr11	0.3250969	9.752907
F	11	Sample X1	F	0.193	0.093	CaGr11	0.31540698	9.462209
F	12	Sample X1	F	0.196	0.097	CaGr11	0.3250969	9.752907
G	1	Blank B	G	0.089				
G	2	Sample X1	G	0.183	0.094	CaGr12	0.31782946	9.534884
G	3	Sample X1	G	0.182	0.093	CaGr12	0.31540698	9.462209
G	4	Sample X1	G	0.182	0.093	CaGr12	0.31540698	9.462209
G	5	Blank B	H	0.106				
G	6	Sample X1	H	0.198	0.092	CaGr21	0.3129845	9.389535
G	7	Sample X1	H	0.197	0.091	CaGr21	0.31056202	9.31686
G	8	Sample X1	H	0.198	0.092	CaGr21	0.3129845	9.389535
G	9	Blank B	I	0.104				
G	10	Sample X1	I	0.196	0.092	CaGc11	0.3129845	9.389535
G	11	Sample X1	I	0.197	0.093	CaGc11	0.31540698	9.462209
G	12	Sample X1	I	0.197	0.093	CaGc11	0.31540698	9.462209
H	1	Blank B	J	0.337				
H	2	Sample X1	J	0.429	0.092	CaGc21	0.3129845	9.389535
H	3	Sample X1	J	0.429	0.092	CaGc21	0.3129845	9.389535
H	4	Sample X1	J	0.428	0.091	CaGc21	0.31056202	9.31686
H	5	Blank B	K	0.251				
H	6	Sample X1	K	0.345	0.094	CaGl11	0.31782946	9.534884
H	7	Sample X1	K	0.345	0.094	CaGl11	0.31782946	9.534884
H	8	Sample X1	K	0.342	0.091	CaGl11	0.31056202	9.31686
H	9	Blank B	L	0.11				
H	10	Sample X1	L	0.209	0.099	CaGl21	0.32994186	9.898256
H	11	Sample X1	L	0.208	0.098	CaGl21	0.32751938	9.825581
H	12	Sample X1	L	0.209	0.099	CaGl21	0.32994186	9.898256

Appendix 8.29 RCCDRSM CUPRAC run 29

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/ml)	CUPRAC (µMTE/g)
A	1	Blank B	A	0.136				
A	2	Sample X1	A	0.119	0.09	CaSu11	0.3081395	4.622093
A	3	Sample X1	A	0.127	0.09	CaSu11	0.3081395	4.622093
A	4	Sample X1	A	0.135	0.09	CaSu11	0.3081395	4.622093
A	5	Blank B	B	0.126				
A	6	Sample X1	B	0.269	0.143	CaFr11	0.436531	6.5479651
A	7	Sample X1	B	0.262	0.143	CaFr11	0.436531	6.5479651
A	8	Sample X1	B	0.277	0.143	CaFr11	0.436531	6.5479651
A	9	Blank B	C	0.092				
A	10	Sample X1	C	0.162	0.097	CaFr12	0.3250969	4.8764535
A	11	Sample X1	C	0.126	0.094	CaFr12	0.3178295	4.7674419
A	12	Sample X1	C	0.12	0.097	CaFr12	0.3250969	4.8764535
B	1	Blank B	D	0.088				
B	2	Sample X1	D	0.121	0.093	CaFr21	0.315407	4.7311047
B	3	Sample X1	D	0.121	0.093	CaFr21	0.315407	4.7311047
B	4	Sample X1	D	0.115	0.092	CaFr21	0.3129845	4.6947674
E	9	Blank B	O	0.106				
E	10	Sample X1	O	0.121	0.092	CaXy11	0.3129845	4.6947674
E	11	Sample X1	O	0.135	0.092	CaXy11	0.3129845	4.6947674
E	12	Sample X1	O	0.141	0.093	CaXy11	0.315407	4.7311047
B	5	Blank B	E	0.105				
B	6	Sample X1	E	0.157	0.092	CaXy12	0.3129845	4.6947674
B	7	Sample X1	E	0.115	0.091	CaXy12	0.310562	4.6584302
B	8	Sample X1	E	0.134	0.092	CaXy12	0.3129845	4.6947674
E	5	Blank B	N	0.137				
E	6	Sample X1	N	0.132	0.095	CaXy21	0.3202519	4.8037791
E	7	Sample X1	N	0.133	0.094	CaXy21	0.3178295	4.7674419
E	8	Sample X1	N	0.151	0.094	CaXy21	0.3178295	4.7674419
B	9	Blank B	F	0.085				
B	10	Sample X1	F	0.141	0.095	CaGr11	0.3202519	4.8037791
B	11	Sample X1	F	0.137	0.095	CaGr11	0.3202519	4.8037791
B	12	Sample X1	F	0.135	0.094	CaGr11	0.3178295	4.7674419
C	1	Blank B	G	0.095				
C	2	Sample X1	G	0.195	0.091	CaGr12	0.310562	4.6584302
C	3	Sample X1	G	0.164	0.09	CaGr12	0.3081395	4.622093
C	4	Sample X1	G	0.144	0.09	CaGr12	0.3081395	4.622093
C	5	Blank B	H	0.231				
C	6	Sample X1	H	0.135	0.091	CaGr21	0.310562	4.6584302

C	7	Sample X1	H	0.16	0.091	CaGr21	0.310562	4.6584302
C	8	Sample X1	H	0.222	0.09	CaGr21	0.3081395	4.622093
C	9	Blank B	I	0.078				
C	10	Sample X1	I	0.205	0.15	CaGc11	0.4534884	6.8023256
C	11	Sample X1	I	0.213	0.15	CaGc11	0.4534884	6.8023256
C	12	Sample X1	I	0.266	0.151	CaGc11	0.4559109	6.8386628
D	1	Blank B	J	0.104				
D	2	Sample X1	J	0.188	0.095	CaGc21	0.3202519	4.8037791
D	3	Sample X1	J	0.148	0.094	CaGc21	0.3178295	4.7674419
D	4	Sample X1	J	0.155	0.095	CaGc21	0.3202519	4.8037791
D	5	Blank B	K	0.104				
D	6	Sample X1	K	0.159	0.095	CaGl11	0.3202519	4.8037791
D	7	Sample X1	K	0.128	0.094	CaGl11	0.3178295	4.7674419
D	8	Sample X1	K	0.142	0.095	CaGl11	0.3202519	4.8037791
D	9	Blank B	L	0.095				
D	10	Sample X1	L	0.125	0.093	CaGl21	0.315407	4.7311047
D	11	Sample X1	L	0.115	0.092	CaGl21	0.3129845	4.6947674
D	12	Sample X1	L	0.131	0.093	CaGl21	0.315407	4.7311047

Appendix 8.30 RCCDRSM CUPRAC run 30

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (µMTE/mL)	CUPRAC (µMTE/g)
E	1	Blank B	A	0.148				
E	2	Sample X1	A	0.242	0.094	CaSu11	0.3178295	3.1782946
E	3	Sample X1	A	0.24	0.092	CaSu11	0.3129845	3.129845
E	4	Sample X1	A	0.24	0.092	CaSu11	0.3129845	3.129845
E	5	Blank B	B	0.147				
E	6	Sample X1	B	0.202	0.155	CaFr11	0.4656008	4.6560078
E	7	Sample X1	B	0.202	0.155	CaFr11	0.4656008	4.6560078
E	8	Sample X1	B	0.201	0.154	CaFr11	0.4631783	4.6317829
E	9	Blank B	C	0.116				
E	10	Sample X1	C	0.208	0.092	CaFr12	0.3129845	3.129845
E	11	Sample X1	C	0.208	0.092	CaFr12	0.3129845	3.129845
E	12	Sample X1	C	0.209	0.093	CaFr12	0.315407	3.1540698
F	1	Blank B	D	0.107				
F	2	Sample X1	D	0.2	0.093	CaFr21	0.315407	3.1540698
F	3	Sample X1	D	0.199	0.091	CaFr21	0.310562	3.1056202
F	4	Sample X1	D	0.2	0.093	CaFr21	0.315407	3.1540698
F	1	Blank B	P	0.111				
F	2	Sample X1	P	0.202	0.091	CaXy11	0.310562	3.1056202

Appendix 8.30 contd.

F	3	Sample X1	P	0.202	0.092	CaXy11	0.3129845	3.129845
F	4	Sample X1	P	0.201	0.091	CaXy11	0.310562	3.1540698
F	5	Blank B	E	0.111				
F	6	Sample X1	E	0.204	0.093	CaXy12	0.315407	3.1540698
F	7	Sample X1	E	0.204	0.093	CaXy12	0.315407	3.1540698
F	8	Sample X1	E	0.203	0.092	CaXy12	0.3129845	3.129845
E	9	Blank B	O	0.066				
E	10	Sample X1	O	0.162	0.096	CaXy21	0.3226744	3.2267442
E	11	Sample X1	O	0.164	0.098	CaXy21	0.3275194	3.2751938
E	12	Sample X1	O	0.162	0.096	CaXy21	0.3226744	3.2267442
F	9	Blank B	F	0.212				
F	10	Sample X1	F	0.304	0.092	CaGr11	0.3129845	3.129845
F	11	Sample X1	F	0.306	0.094	CaGr11	0.3178295	3.1782946
F	12	Sample X1	F	0.304	0.092	CaGr11	0.3129845	3.129845
G	1	Blank B	G	0.083				
G	2	Sample X1	G	0.286	0.203	CaGr12	0.5818798	5.8187984
G	3	Sample X1	G	0.286	0.203	CaGr12	0.5818798	5.8187984
G	4	Sample X1	G	0.289	0.206	CaGr12	0.5891473	5.8914729
G	5	Blank B	H	0.073				
G	6	Sample X1	H	0.171	0.098	CaGr21	0.3275194	3.2751938
G	7	Sample X1	H	0.171	0.098	CaGr21	0.3275194	3.2751938
G	8	Sample X1	H	0.172	0.099	CaGr21	0.3299419	3.2994186
G	9	Blank B	I	0.283				
G	10	Sample X1	I	0.374	0.091	CaGc11	0.310562	3.1056202
G	11	Sample X1	I	0.374	0.091	CaGc11	0.310562	3.1056202
G	12	Sample X1	I	0.376	0.093	CaGc11	0.315407	3.1540698
H	1	Blank B	J	0.115				
H	2	Sample X1	J	0.205	0.09	CaGc21	0.3081395	3.0813953
H	3	Sample X1	J	0.206	0.091	CaGc21	0.310562	3.1056202
H	4	Sample X1	J	0.205	0.09	CaGc21	0.3081395	3.0813953
H	5	Blank B	K	0.1				
H	6	Sample X1	K	0.194	0.094	CaGl11	0.3178295	3.1782946
H	7	Sample X1	K	0.194	0.094	CaGl11	0.3178295	3.1782946
H	8	Sample X1	K	0.193	0.093	CaGl11	0.315407	3.1540698
H	9	Blank B	L	0.153				
H	10	Sample X1	L	0.251	0.098	CaGl21	0.3275194	3.2751938
H	11	Sample X1	L	0.25	0.097	CaGl21	0.3250969	3.250969
H	12	Sample X1	L	0.25	0.097	CaGl21	0.3250969	3.250969

Appendix 9.1 RCCDRSM FRAP run 1

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.094					
A	2	Sample X1	A	0.317	0.223	CaSu11	172.8461538	0.172846154	1.728461538
A	3	Sample X1	A	0.316	0.222	CaSu11	172.0769231	0.172076923	1.720769231
A	4	Sample X1	A	0.319	0.225	CaSu11	174.3846154	0.174384615	1.743846154
A	5	Blank B	B	0.041					
A	6	Sample X1	B	0.458	0.417	CaFr11	322.0769231	0.322076923	3.220769231
A	7	Sample X1	B	0.456	0.415	CaFr11	320.5384615	0.320538462	3.205384615
A	8	Sample X1	B	0.457	0.416	CaFr11	321.3076923	0.321307692	3.213076923
A	9	Blank B	C	0.673					
A	10	Sample X1	C	0.769	0.096	CaFr12	75.15384615	0.075153846	0.751538462
A	11	Sample X1	C	0.769	0.096	CaFr12	75.15384615	0.075153846	0.751538462
A	12	Sample X1	C	0.768	0.095	CaFr12	74.38461538	0.074384615	0.743846154
B	1	Blank B	D	0.733					
B	2	Sample X1	D	0.844	0.111	CaFr21	86.69230769	0.086692308	0.866923077
B	3	Sample X1	D	0.843	0.11	CaFr21	85.92307692	0.085923077	0.859230769
B	4	Sample X1	D	0.843	0.11	CaFr21	85.92307692	0.085923077	0.859230769
A	1	Blank B	A	0.658					
A	2	Sample X1	A	0.885	0.227	CaXy11	175.9230769	0.175923077	1.759230769
A	3	Sample X1	A	0.884	0.226	CaXy11	175.1538462	0.175153846	1.751538462
A	4	Sample X1	A	0.884	0.226	CaXy11	175.1538462	0.175153846	1.751538462
B	5	Blank B	E	0.601					
B	6	Sample X1	E	0.711	0.11	CaXy12	85.92307692	0.085923077	0.859230769
B	7	Sample X1	E	0.711	0.11	CaXy12	85.92307692	0.085923077	0.859230769
B	8	Sample X1	E	0.711	0.11	CaXy12	85.92307692	0.085923077	0.859230769
A	1	Blank B	A	0.691					
A	2	Sample X1	A	0.849	0.158	CaXy21	122.8461538	0.122846154	1.228461538
A	3	Sample X1	A	0.849	0.158	CaXy21	122.8461538	0.122846154	1.228461538
A	4	Sample X1	A	0.849	0.158	CaXy21	122.8461538	0.122846154	1.228461538
B	9	Blank B	F	0.683					
B	10	Sample X1	F	0.776	0.093	CaGr11	72.84615385	0.072846154	0.728461538
B	11	Sample X1	F	0.776	0.093	CaGr11	72.84615385	0.072846154	0.728461538
B	12	Sample X1	F	0.777	0.094	CaGr11	73.61538462	0.073615385	0.736153846
C	1	Blank B	G	0.703					
C	2	Sample X1	G	0.794	0.091	CaGr12	71.30769231	0.071307692	0.713076923
C	3	Sample X1	G	0.796	0.093	CaGr12	72.84615385	0.072846154	0.728461538
C	4	Sample X1	G	0.795	0.092	CaGr12	72.07692308	0.072076923	0.720769231
C	5	Blank B	H	0.556					

Appendix 9.1 contd.

C	6	Sample X1	H	0.647	0.091	CaGr21	71.30769231	0.071307692	0.713076923
C	7	Sample X1	H	0.648	0.092	CaGr21	72.07692308	0.072076923	0.720769231
C	8	Sample X1	H	0.648	0.092	CaGr21	72.07692308	0.072076923	0.720769231
C	9	Blank B	I	0.534					
C	10	Sample X1	I	0.627	0.093	CaGc11	72.84615385	0.072846154	0.728461538
C	11	Sample X1	I	0.63	0.096	CaGc11	75.15384615	0.075153846	0.751538462
C	12	Sample X1	I	0.627	0.093	CaGc11	72.84615385	0.072846154	0.728461538
D	1	Blank B	J	0.603					
D	2	Sample X1	J	0.696	0.093	CaGc21	72.84615385	0.072846154	0.728461538
D	3	Sample X1	J	0.695	0.092	CaGc21	72.07692308	0.072076923	0.720769231
D	4	Sample X1	J	0.694	0.091	CaGc21	71.30769231	0.071307692	0.713076923
D	5	Blank B	K	0.527					
D	6	Sample X1	K	0.62	0.093	CaGl11	72.84615385	0.072846154	0.728461538
D	7	Sample X1	K	0.617	0.09	CaGl11	70.53846154	0.070538462	0.705384615
D	8	Sample X1	K	0.62	0.093	CaGl11	72.84615385	0.072846154	0.728461538
D	9	Blank B	L	0.539					
D	10	Sample X1	L	0.651	0.112	CaGl21	87.46153846	0.087461538	0.874615385
D	11	Sample X1	L	0.652	0.113	CaGl21	88.23076923	0.088230769	0.882307692
D	12	Sample X1	L	0.652	0.113	CaGl21	88.23076923	0.088230769	0.882307692

Appendix 9.2 RCCDRSM FRAP run 2

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.849					
E	2	Sample X1	A	0.976	0.127	CaSu11	99	0.099	0.99
E	3	Sample X1	A	0.976	0.127	CaSu11	99	0.099	0.99
E	4	Sample X1	A	0.974	0.125	CaSu11	97.461538	0.0974615	0.974615
E	5	Blank B	B	0.89					
E	6	Sample X1	B	0.936	0.046	CaFr11	36.692308	0.0366923	0.366923
E	7	Sample X1	B	0.938	0.048	CaFr11	38.230769	0.0382308	0.382308
E	8	Sample X1	B	0.938	0.048	CaFr11	38.230769	0.0382308	0.382308
E	9	Blank B	C	0.698					
E	10	Sample X1	C	0.793	0.095	CaFr12	74.384615	0.0743846	0.743846
E	11	Sample X1	C	0.792	0.094	CaFr12	73.615385	0.0736154	0.736154
E	12	Sample X1	C	0.792	0.094	CaFr12	73.615385	0.0736154	0.736154
F	1	Blank B	D	0.73					
F	2	Sample X1	D	0.82	0.09	CaFr21	70.538462	0.0705385	0.705385
F	3	Sample X1	D	0.82	0.09	CaFr21	70.538462	0.0705385	0.705385

Appendix 9.2 contd.

F	4	Sample X1	D	0.82	0.09	CaFr21	70.538462	0.0705385	0.705385
A	5	Blank B	B	0.598					
A	6	Sample X1	B	0.778	0.18	CaXy11	139.76923	0.1397692	1.397692
A	7	Sample X1	B	0.777	0.179	CaXy11	139	0.139	1.39
A	8	Sample X1	B	0.777	0.179	CaXy11	139	0.139	1.39
F	5	Blank B	E	0.678					
F	6	Sample X1	E	0.769	0.091	CaXy12	71.307692	0.0713077	0.713077
F	7	Sample X1	E	0.771	0.093	CaXy12	72.846154	0.0728462	0.728462
F	8	Sample X1	E	0.769	0.091	CaXy12	71.307692	0.0713077	0.713077
A	5	Blank B	B	0.652					
A	6	Sample X1	B	0.773	0.121	CaXy21	94.384615	0.0943846	0.943846
A	7	Sample X1	B	0.776	0.124	CaXy21	96.692308	0.0966923	0.966923
A	8	Sample X1	B	0.773	0.121	CaXy21	94.384615	0.0943846	0.943846
F	9	Blank B	F	0.554					
F	10	Sample X1	F	0.65	0.096	CaGr11	75.153846	0.0751538	0.751538
F	11	Sample X1	F	0.65	0.096	CaGr11	75.153846	0.0751538	0.751538
F	12	Sample X1	F	0.65	0.096	CaGr11	75.153846	0.0751538	0.751538
G	1	Blank B	G	0.595					
G	2	Sample X1	G	0.86	0.265	CaGr12	205.15385	0.2051538	2.051538
G	3	Sample X1	G	0.862	0.267	CaGr12	206.69231	0.2066923	2.066923
G	4	Sample X1	G	0.861	0.266	CaGr12	205.92308	0.2059231	2.059231
G	5	Blank B	H	0.592					
G	6	Sample X1	H	0.744	0.152	CaGr21	118.23077	0.1182308	1.182308
G	7	Sample X1	H	0.743	0.151	CaGr21	117.46154	0.1174615	1.174615
G	8	Sample X1	H	0.742	0.15	CaGr21	116.69231	0.1166923	1.166923
G	9	Blank B	I	0.513					
G	10	Sample X1	I	0.609	0.096	CaGc11	75.153846	0.0751538	0.751538
G	11	Sample X1	I	0.609	0.096	CaGc11	75.153846	0.0751538	0.751538
G	12	Sample X1	I	0.608	0.095	CaGc11	74.384615	0.0743846	0.743846
H	1	Blank B	J	0.568					
H	2	Sample X1	J	0.658	0.09	CaGc21	70.538462	0.0705385	0.705385
H	3	Sample X1	J	0.658	0.09	CaGc21	70.538462	0.0705385	0.705385
H	4	Sample X1	J	0.659	0.091	CaGc21	71.307692	0.0713077	0.713077
H	5	Blank B	K	0.633					
H	6	Sample X1	K	0.723	0.09	CaGl11	70.538462	0.0705385	0.705385
H	7	Sample X1	K	0.724	0.091	CaGl11	71.307692	0.0713077	0.713077
H	8	Sample X1	K	0.724	0.091	CaGl11	71.307692	0.0713077	0.713077
H	9	Blank B	L	0.525					
H	10	Sample X1	L	0.645	0.12	CaGl21	93.615385	0.0936154	0.936154
H	11	Sample X1	L	0.647	0.122	CaGl21	95.153846	0.0951538	0.951538
H	12	Sample X1	L	0.645	0.12	CaGl21	93.615385	0.0936154	0.936154

Appendix 9.3 RCCDRSM FRAP run 3

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.525					
D	2	Sample X1	J	0.615	0.09	CaSu11	70.53846154	0.070538462	1.058077
D	3	Sample X1	J	0.615	0.09	CaSu11	70.53846154	0.070538462	1.058077
D	4	Sample X1	J	0.616	0.091	CaSu11	71.30769231	0.071307692	1.069615
A	1	Blank B	A	0.623					
A	2	Sample X1	A	0.717	0.094	CaFr11	73.61538462	0.073615385	1.104231
A	3	Sample X1	A	0.718	0.095	CaFr11	74.38461538	0.074384615	1.115769
A	4	Sample X1	A	0.717	0.094	CaFr11	73.61538462	0.073615385	1.104231
A	5	Blank B	B	0.696					
A	6	Sample X1	B	0.787	0.091	CaFr12	71.30769231	0.071307692	1.069615
A	7	Sample X1	B	0.786	0.09	CaFr12	70.53846154	0.070538462	1.058077
A	8	Sample X1	B	0.787	0.091	CaFr12	71.30769231	0.071307692	1.069615
A	9	Blank B	C	0.64					
A	10	Sample X1	C	0.735	0.095	CaFr21	74.38461538	0.074384615	1.115769
A	11	Sample X1	C	0.733	0.093	CaFr21	72.84615385	0.072846154	1.092692
A	12	Sample X1	C	0.735	0.095	CaFr21	74.38461538	0.074384615	1.115769
B	1	Blank B	D	0.542					
B	2	Sample X1	D	0.638	0.096	CaXy11	75.15384615	0.075153846	1.127308
B	3	Sample X1	D	0.637	0.095	CaXy11	74.38461538	0.074384615	1.115769
B	4	Sample X1	D	0.637	0.095	CaXy11	74.38461538	0.074384615	1.115769
B	5	Blank B	E	0.532					
B	6	Sample X1	E	0.624	0.092	CaXy12	72.07692308	0.072076923	1.081154
B	7	Sample X1	E	0.624	0.092	CaXy12	72.07692308	0.072076923	1.081154
B	8	Sample X1	E	0.623	0.091	CaXy12	71.30769231	0.071307692	1.069615
B	9	Blank B	F	0.56					
B	10	Sample X1	F	0.657	0.097	CaXy21	75.92307692	0.075923077	1.138846
B	11	Sample X1	F	0.658	0.098	CaXy21	76.69230769	0.076692308	1.150385
B	12	Sample X1	F	0.658	0.098	CaXy21	76.69230769	0.076692308	1.150385
C	1	Blank B	G	0.615					
C	2	Sample X1	G	0.71	0.095	CaGr11	74.38461538	0.074384615	1.115769
C	3	Sample X1	G	0.711	0.096	CaGr11	75.15384615	0.075153846	1.127308
C	4	Sample X1	G	0.709	0.094	CaGr11	73.61538462	0.073615385	1.104231
C	5	Blank B	H	0.583					
C	6	Sample X1	H	0.673	0.09	CaGr12	70.53846154	0.070538462	1.058077
C	7	Sample X1	H	0.674	0.091	CaGr12	71.30769231	0.071307692	1.069615
C	8	Sample X1	H	0.674	0.091	CaGr12	71.30769231	0.071307692	1.069615
C	9	Blank B	I	0.571					

Appendix 9.3 contd.

C	10	Sample X1	I	0.662	0.091	CaGr21	71.30769231	0.071307692	1.069615
C	11	Sample X1	I	0.662	0.091	CaGr21	71.30769231	0.071307692	1.069615
C	12	Sample X1	I	0.661	0.09	CaGr21	70.53846154	0.070538462	1.058077
D	5	Blank B	K	0.333					
D	6	Sample X1	K	0.429	0.096	CaGc11	75.15384615	0.075153846	1.127308
D	7	Sample X1	K	0.431	0.098	CaGc11	76.69230769	0.076692308	1.150385
D	8	Sample X1	K	0.429	0.096	CaGc11	75.15384615	0.075153846	1.127308
D	9	Blank B	L	0.375					
D	10	Sample X1	L	0.467	0.092	CaGc21	72.07692308	0.072076923	1.081154
D	11	Sample X1	L	0.468	0.093	CaGc21	72.84615385	0.072846154	1.092692
D	12	Sample X1	L	0.468	0.093	CaGc21	72.84615385	0.072846154	1.092692
E	1	Blank B	M	0.495					
E	2	Sample X1	M	0.59	0.095	CaGl11	74.38461538	0.074384615	1.115769
E	3	Sample X1	M	0.59	0.095	CaGl11	74.38461538	0.074384615	1.115769
E	4	Sample X1	M	0.592	0.097	CaGl11	75.92307692	0.075923077	1.138846
E	5	Blank B	N	0.479					
E	6	Sample X1	N	0.575	0.096	CaGl21	75.15384615	0.075153846	1.127308
E	7	Sample X1	N	0.575	0.096	CaGl21	75.15384615	0.075153846	1.127308
E	8	Sample X1	N	0.574	0.095	CaGl21	74.38461538	0.074384615	1.115769

Appendix 9.4 RCCDRSM FRAP run 4

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.583					
D	2	Sample X1	J	0.676	0.093	CaSu11	72.8461538	0.07284615	1.09269231
D	3	Sample X1	J	0.676	0.093	CaSu11	72.8461538	0.07284615	1.09269231
D	4	Sample X1	J	0.677	0.094	CaSu11	73.6153846	0.07361538	1.10423077
A	1	Blank B	A	0.611					
A	2	Sample X1	A	0.705	0.094	CaFr11	73.6153846	0.07361538	1.10423077
A	3	Sample X1	A	0.707	0.096	CaFr11	75.1538462	0.07515385	1.12730769
A	4	Sample X1	A	0.705	0.094	CaFr11	73.6153846	0.07361538	1.10423077
A	5	Blank B	B	0.627					
A	6	Sample X1	B	0.719	0.092	CaFr12	72.0769231	0.07207692	1.08115385
A	7	Sample X1	B	0.723	0.096	CaFr12	75.1538462	0.07515385	1.12730769
A	8	Sample X1	B	0.719	0.092	CaFr12	72.0769231	0.07207692	1.08115385
A	9	Blank B	C	0.672					
A	10	Sample X1	C	0.762	0.09	CaFr21	70.5384615	0.07053846	1.05807692
A	11	Sample X1	C	0.762	0.09	CaFr21	70.5384615	0.07053846	1.05807692

Appendix 9.4 contd.

A	12	Sample X1	C	0.763	0.091	CaFr21	71.3076923	0.07130769	1.06961538
B	1	Blank B	D	0.512					
B	2	Sample X1	D	0.603	0.091	CaXy11	71.3076923	0.07130769	1.06961538
B	3	Sample X1	D	0.602	0.09	CaXy11	70.5384615	0.07053846	1.05807692
B	4	Sample X1	D	0.603	0.091	CaXy11	71.3076923	0.07130769	1.06961538
B	5	Blank B	E	0.533					
B	6	Sample X1	E	0.623	0.09	CaXy12	70.5384615	0.07053846	1.05807692
B	7	Sample X1	E	0.624	0.091	CaXy12	71.3076923	0.07130769	1.06961538
B	8	Sample X1	E	0.624	0.091	CaXy12	71.3076923	0.07130769	1.06961538
B	9	Blank B	F	0.567					
B	10	Sample X1	F	0.658	0.091	CaXy21	71.3076923	0.07130769	1.06961538
B	11	Sample X1	F	0.659	0.092	CaXy21	72.0769231	0.07207692	1.08115385
B	12	Sample X1	F	0.659	0.092	CaXy21	72.0769231	0.07207692	1.08115385
C	1	Blank B	G	0.582					
C	2	Sample X1	G	0.676	0.094	CaGr11	73.6153846	0.07361538	1.10423077
C	3	Sample X1	G	0.673	0.091	CaGr11	71.3076923	0.07130769	1.06961538
C	4	Sample X1	G	0.674	0.092	CaGr11	72.0769231	0.07207692	1.08115385
C	5	Blank B	H	0.547					
C	6	Sample X1	H	0.715	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	7	Sample X1	H	0.638	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	8	Sample X1	H	0.639	0.092	CaGr12	72.0769231	0.07207692	1.08115385
C	9	Blank B	I	0.519					
C	10	Sample X1	I	0.611	0.092	CaGr21	72.0769231	0.07207692	1.08115385
C	11	Sample X1	I	0.612	0.093	CaGr21	72.8461538	0.07284615	1.09269231
C	12	Sample X1	I	0.612	0.093	CaGr21	72.8461538	0.07284615	1.09269231
D	5	Blank B	K	0.298					
D	6	Sample X1	K	0.389	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	7	Sample X1	K	0.389	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	8	Sample X1	K	0.389	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	9	Blank B	L	0.313					
D	10	Sample X1	L	0.403	0.09	CaGc21	70.5384615	0.07053846	1.05807692
D	11	Sample X1	L	0.403	0.09	CaGc21	70.5384615	0.07053846	1.05807692
D	12	Sample X1	L	0.403	0.09	CaGc21	70.5384615	0.07053846	1.05807692
E	1	Blank B	M	0.467					
E	2	Sample X1	M	0.558	0.091	CaGl11	71.3076923	0.07130769	1.06961538
E	3	Sample X1	M	0.558	0.091	CaGl11	71.3076923	0.07130769	1.06961538
E	4	Sample X1	M	0.557	0.09	CaGl11	70.5384615	0.07053846	1.05807692
E	5	Blank B	N	0.472					
E	6	Sample X1	N	0.563	0.091	CaGl21	71.3076923	0.07130769	1.06961538
E	7	Sample X1	N	0.562	0.09	CaGl21	70.5384615	0.07053846	1.05807692
E	8	Sample X1	N	0.562	0.09	CaGl21	70.5384615	0.07053846	1.05807692

Appendix 9.5 RCCDRSM FRAP run 5

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.211					
D	2	Sample X1	J	0.308	0.097	CaSu11	75.9230769	0.075923077	0.759230769
D	3	Sample X1	J	0.306	0.095	CaSu11	74.3846154	0.074384615	0.743846154
D	4	Sample X1	J	0.308	0.097	CaSu11	75.9230769	0.075923077	0.759230769
A	1	Blank B	A	0.496					
A	2	Sample X1	A	0.627	0.131	CaFr11	102.076923	0.102076923	1.020769231
A	3	Sample X1	A	0.633	0.137	CaFr11	106.692308	0.106692308	1.066923077
A	4	Sample X1	A	0.627	0.131	CaFr11	102.076923	0.102076923	1.020769231
A	5	Blank B	B	0.417					
A	6	Sample X1	B	0.519	0.102	CaFr12	79.7692308	0.079769231	0.797692308
A	7	Sample X1	B	0.523	0.106	CaFr12	82.8461538	0.082846154	0.828461538
A	8	Sample X1	B	0.52	0.103	CaFr12	80.5384615	0.080538462	0.805384615
A	9	Blank B	C	0.454					
A	10	Sample X1	C	0.546	0.092	CaFr21	72.0769231	0.072076923	0.720769231
A	11	Sample X1	C	0.548	0.094	CaFr21	73.6153846	0.073615385	0.736153846
A	12	Sample X1	C	0.551	0.097	CaFr21	75.9230769	0.075923077	0.759230769
B	1	Blank B	D	0.363					
B	2	Sample X1	D	0.456	0.093	CaXy11	72.8461538	0.072846154	0.728461538
B	3	Sample X1	D	0.459	0.096	CaXy11	75.1538462	0.075153846	0.751538462
B	4	Sample X1	D	0.46	0.097	CaXy11	75.9230769	0.075923077	0.759230769
B	5	Blank B	E	0.317					
B	6	Sample X1	E	0.414	0.097	CaXy12	75.9230769	0.075923077	0.759230769
B	7	Sample X1	E	0.411	0.094	CaXy12	73.6153846	0.073615385	0.736153846
B	8	Sample X1	E	0.415	0.098	CaXy12	76.6923077	0.076692308	0.766923077
B	9	Blank B	F	0.286					
B	10	Sample X1	F	0.379	0.093	CaXy21	72.8461538	0.072846154	0.728461538
B	11	Sample X1	F	0.382	0.096	CaXy21	75.1538462	0.075153846	0.751538462
B	12	Sample X1	F	0.378	0.092	CaXy21	72.0769231	0.072076923	0.720769231
C	1	Blank B	G	0.237					
C	2	Sample X1	G	0.329	0.092	CaGr11	72.0769231	0.072076923	0.720769231
C	3	Sample X1	G	0.331	0.094	CaGr11	73.6153846	0.073615385	0.736153846
C	4	Sample X1	G	0.329	0.092	CaGr11	72.0769231	0.072076923	0.720769231
C	5	Blank B	H	0.261					
C	6	Sample X1	H	0.355	0.094	CaGr12	73.6153846	0.073615385	0.736153846
C	7	Sample X1	H	0.355	0.094	CaGr12	73.6153846	0.073615385	0.736153846
C	8	Sample X1	H	0.359	0.098	CaGr12	76.6923077	0.076692308	0.766923077
C	9	Blank B	I	0.224					

Appendix 9.5 contd.

C	10	Sample X1	I	0.317	0.093	CaGr21	72.8461538	0.072846154	0.728461538
C	11	Sample X1	I	0.315	0.091	CaGr21	71.3076923	0.071307692	0.713076923
C	12	Sample X1	I	0.318	0.094	CaGr21	73.6153846	0.073615385	0.736153846
D	5	Blank B	K	0.246					
D	6	Sample X1	K	0.337	0.091	CaGc11	71.3076923	0.071307692	0.713076923
D	7	Sample X1	K	0.338	0.092	CaGc11	72.0769231	0.072076923	0.720769231
D	8	Sample X1	K	0.337	0.091	CaGc11	71.3076923	0.071307692	0.713076923
D	9	Blank B	L	0.164					
D	10	Sample X1	L	0.255	0.091	CaGc21	71.3076923	0.071307692	0.713076923
D	11	Sample X1	L	0.255	0.091	CaGc21	71.3076923	0.071307692	0.713076923
D	12	Sample X1	L	0.254	0.09	CaGc21	70.5384615	0.070538462	0.705384615
E	1	Blank B	M	0.191					
E	2	Sample X1	M	0.284	0.093	CaGl11	72.8461538	0.072846154	0.728461538
E	3	Sample X1	M	0.286	0.095	CaGl11	74.3846154	0.074384615	0.743846154
E	4	Sample X1	M	0.287	0.096	CaGl11	75.1538462	0.075153846	0.751538462
E	5	Blank B	N	0.102					
E	6	Sample X1	N	0.197	0.095	CaGl21	74.3846154	0.074384615	0.743846154
E	7	Sample X1	N	0.198	0.096	CaGl21	75.1538462	0.075153846	0.751538462
E	8	Sample X1	N	0.201	0.099	CaGl21	77.4615385	0.077461538	0.774615385

Appendix 9.6 RCCDRSM FRAP run 6

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.583					
D	2	Sample X1	J	0.677	0.094	CaSu11	73.615385	0.0736154	0.7361538
D	3	Sample X1	J	0.678	0.095	CaSu11	74.384615	0.0743846	0.7438462
D	4	Sample X1	J	0.679	0.096	CaSu11	75.153846	0.0751538	0.7515385
A	1	Blank B	A	0.654					
A	2	Sample X1	A	0.747	0.093	CaFr11	72.846154	0.0728462	0.7284615
A	3	Sample X1	A	0.748	0.094	CaFr11	73.615385	0.0736154	0.7361538
A	4	Sample X1	A	0.748	0.094	CaFr11	73.615385	0.0736154	0.7361538
A	5	Blank B	B	0.65					
A	6	Sample X1	B	0.868	0.218	CaFr12	169	0.169	1.69
A	7	Sample X1	B	0.87	0.22	CaFr12	170.53846	0.1705385	1.7053846
A	8	Sample X1	B	0.87	0.22	CaFr12	170.53846	0.1705385	1.7053846
A	9	Blank B	C	0.056					
A	10	Sample X1	C	0.198	0.142	CaFr21	110.53846	0.1105385	1.1053846
A	11	Sample X1	C	0.203	0.147	CaFr21	114.38462	0.1143846	1.1438462

Appendix 9.6 contd.

A	12	Sample X1	C	0.198	0.142	CaFr21	110.53846	0.1105385	1.1053846
B	1	Blank B	D	0.493					
B	2	Sample X1	D	0.642	0.149	CaXy11	115.92308	0.1159231	1.1592308
B	3	Sample X1	D	0.643	0.15	CaXy11	116.69231	0.1166923	1.1669231
B	4	Sample X1	D	0.643	0.15	CaXy11	116.69231	0.1166923	1.1669231
B	5	Blank B	E	0.407					
B	6	Sample X1	E	0.538	0.131	CaXy12	102.07692	0.1020769	1.0207692
B	7	Sample X1	E	0.539	0.132	CaXy12	102.84615	0.1028462	1.0284615
B	8	Sample X1	E	0.538	0.131	CaXy12	102.07692	0.1020769	1.0207692
B	9	Blank B	F	0.421					
B	10	Sample X1	F	0.699	0.278	CaXy21	215.15385	0.2151538	2.1515385
B	11	Sample X1	F	0.697	0.276	CaXy21	213.61538	0.2136154	2.1361538
B	12	Sample X1	F	0.697	0.276	CaXy21	213.61538	0.2136154	2.1361538
C	1	Blank B	G	0.309					
C	2	Sample X1	G	0.408	0.099	CaGr11	77.461538	0.0774615	0.7746154
C	3	Sample X1	G	0.407	0.098	CaGr11	76.692308	0.0766923	0.7669231
C	4	Sample X1	G	0.407	0.098	CaGr11	76.692308	0.0766923	0.7669231
C	5	Blank B	H	0.338					
C	6	Sample X1	H	0.625	0.287	CaGr12	222.07692	0.2220769	2.2207692
C	7	Sample X1	H	0.628	0.29	CaGr12	224.38462	0.2243846	2.2438462
C	8	Sample X1	H	0.628	0.29	CaGr12	224.38462	0.2243846	2.2438462
C	9	Blank B	I	0.353					
C	10	Sample X1	I	0.447	0.094	CaGr21	73.615385	0.0736154	0.7361538
C	11	Sample X1	I	0.449	0.096	CaGr21	75.153846	0.0751538	0.7515385
C	12	Sample X1	I	0.447	0.094	CaGr21	73.615385	0.0736154	0.7361538
D	5	Blank B	K	0.468					
D	6	Sample X1	K	0.559	0.091	CaGc11	71.307692	0.0713077	0.7130769
D	7	Sample X1	K	0.559	0.091	CaGc11	71.307692	0.0713077	0.7130769
D	8	Sample X1	K	0.559	0.091	CaGc11	71.307692	0.0713077	0.7130769
D	9	Blank B	L	0.475					
D	10	Sample X1	L	0.566	0.091	CaGc21	71.307692	0.0713077	0.7130769
D	11	Sample X1	L	0.566	0.091	CaGc21	71.307692	0.0713077	0.7130769
D	12	Sample X1	L	0.565	0.09	CaGc21	70.538462	0.0705385	0.7053846
E	1	Blank B	M	0.511					
E	2	Sample X1	M	0.606	0.095	CaGl11	74.384615	0.0743846	0.7438462
E	3	Sample X1	M	0.605	0.094	CaGl11	73.615385	0.0736154	0.7361538
E	4	Sample X1	M	0.606	0.095	CaGl11	74.384615	0.0743846	0.7438462
E	5	Blank B	N	0.501					
E	6	Sample X1	N	0.597	0.096	CaGl21	75.153846	0.0751538	0.7515385
E	7	Sample X1	N	0.595	0.094	CaGl21	73.615385	0.0736154	0.7361538
E	8	Sample X1	N	0.595	0.094	CaGl21	73.615385	0.0736154	0.7361538

Appendix 9.7 RCCDRSM FRAP run 7

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.423					
A	2	Sample X1	A	0.924	0.501	CaSu11	386.692308	0.38669231	7.7338462
A	3	Sample X1	A	0.929	0.506	CaSu11	390.538462	0.39053846	7.8107692
A	4	Sample X1	A	0.929	0.506	CaSu11	390.538462	0.39053846	7.8107692
A	5	Blank B	B	0.868					
A	6	Sample X1	B	0.984	0.116	CaFr11	90.5384615	0.09053846	1.8107692
A	7	Sample X1	B	0.987	0.119	CaFr11	92.8461538	0.09284615	1.8569231
A	8	Sample X1	B	0.984	0.116	CaFr11	90.5384615	0.09053846	1.8107692
A	9	Blank B	C	0.849					
A	10	Sample X1	C	0.948	0.099	CaFr12	77.4615385	0.07746154	1.5492308
A	11	Sample X1	C	0.946	0.097	CaFr12	75.9230769	0.07592308	1.5184615
A	12	Sample X1	C	0.948	0.099	CaFr12	77.4615385	0.07746154	1.5492308
B	1	Blank B	D	0.869					
B	2	Sample X1	D	0.963	0.094	CaFr21	73.6153846	0.07361538	1.4723077
B	3	Sample X1	D	0.963	0.094	CaFr21	73.6153846	0.07361538	1.4723077
B	4	Sample X1	D	0.962	0.093	CaFr21	72.8461538	0.07284615	1.4569231
A	9	Blank B	C	0.867					
A	10	Sample X1	C	0.958	0.091	CaXy11	71.3076923	0.07130769	1.4261538
A	11	Sample X1	C	0.958	0.091	CaXy11	71.3076923	0.07130769	1.4261538
A	12	Sample X1	C	0.957	0.09	CaXy11	70.5384615	0.07053846	1.4107692
B	5	Blank B	E	0.851					
B	6	Sample X1	E	0.945	0.094	CaXy12	73.6153846	0.07361538	1.4723077
B	7	Sample X1	E	0.948	0.097	CaXy12	75.9230769	0.07592308	1.5184615
B	8	Sample X1	E	0.945	0.094	CaXy12	73.6153846	0.07361538	1.4723077
B	9	Blank B	F	0.724					
B	10	Sample X1	F	0.819	0.095	CaGr11	74.3846154	0.07438462	1.4876923
B	11	Sample X1	F	0.815	0.091	CaGr11	71.3076923	0.07130769	1.4261538
B	12	Sample X1	F	0.815	0.091	CaGr11	71.3076923	0.07130769	1.4261538
C	1	Blank B	G	0.788					
C	2	Sample X1	G	0.884	0.096	CaGr12	75.1538462	0.07515385	1.5030769
C	3	Sample X1	G	0.886	0.098	CaGr12	76.6923077	0.07669231	1.5338462
C	4	Sample X1	G	0.885	0.097	CaGr12	75.9230769	0.07592308	1.5184615
C	5	Blank B	H	0.721					
C	6	Sample X1	H	0.815	0.094	CaGr21	73.6153846	0.07361538	1.4723077
C	7	Sample X1	H	0.815	0.094	CaGr21	73.6153846	0.07361538	1.4723077
C	8	Sample X1	H	0.815	0.094	CaGr21	73.6153846	0.07361538	1.4723077

Appendix 9.7 contd.

C	9	Blank B	I	0.874					
C	10	Sample X1	I	0.971	0.097	CaGc11	75.9230769	0.07592308	1.5184615
C	11	Sample X1	I	0.971	0.097	CaGc11	75.9230769	0.07592308	1.5184615
C	12	Sample X1	I	0.973	0.099	CaGc11	77.4615385	0.07746154	1.5492308
D	1	Blank B	J	0.851					
D	2	Sample X1	J	0.945	0.094	CaGc21	73.6153846	0.07361538	1.4723077
D	3	Sample X1	J	0.946	0.095	CaGc21	74.3846154	0.07438462	1.4876923
D	4	Sample X1	J	0.945	0.094	CaGc21	73.6153846	0.07361538	1.4723077
D	5	Blank B	K	0.737					
D	6	Sample X1	K	0.91	0.173	CaGl11	134.384615	0.13438462	2.6876923
D	7	Sample X1	K	0.909	0.172	CaGl11	133.615385	0.13361538	2.6723077
D	8	Sample X1	K	0.909	0.172	CaGl11	133.615385	0.13361538	2.6723077
D	9	Blank B	L	0.702					
D	10	Sample X1	L	0.793	0.091	CaGl21	71.3076923	0.07130769	1.4261538
D	11	Sample X1	L	0.794	0.092	CaGl21	72.0769231	0.07207692	1.4415385
D	12	Sample X1	L	0.794	0.092	CaGl21	72.0769231	0.07207692	1.4415385

Appendix 9.8 RCCDRSM FRAP run 8

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.625					
D	2	Sample X1	J	0.721	0.096	CaSu11	75.1538462	0.07515385	1.12730769
D	3	Sample X1	J	0.721	0.096	CaSu11	75.1538462	0.07515385	1.12730769
D	4	Sample X1	J	0.723	0.098	CaSu11	76.6923077	0.07669231	1.15038462
A	1	Blank B	A	0.781					
A	2	Sample X1	A	0.876	0.095	CaFr11	74.3846154	0.07438462	1.11576923
A	3	Sample X1	A	0.876	0.095	CaFr11	74.3846154	0.07438462	1.11576923
A	4	Sample X1	A	0.875	0.094	CaFr11	73.6153846	0.07361538	1.10423077
A	5	Blank B	B	0.796					
A	6	Sample X1	B	0.887	0.091	CaFr12	71.3076923	0.07130769	1.06961538
A	7	Sample X1	B	0.887	0.091	CaFr12	71.3076923	0.07130769	1.06961538
A	8	Sample X1	B	0.886	0.09	CaFr12	70.5384615	0.07053846	1.05807692
A	9	Blank B	C	0.74					
A	10	Sample X1	C	0.832	0.092	CaFr21	72.0769231	0.07207692	1.08115385
A	11	Sample X1	C	0.833	0.093	CaFr21	72.8461538	0.07284615	1.09269231
A	12	Sample X1	C	0.83	0.09	CaFr21	70.5384615	0.07053846	1.05807692
B	1	Blank B	D	0.742					

Appendix 9.8 contd.

B	2	Sample X1	D	0.838	0.096	CaXy11	75.1538462	0.07515385	1.12730769
B	3	Sample X1	D	0.837	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	4	Sample X1	D	0.971	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	5	Blank B	E	0.732					
B	6	Sample X1	E	0.829	0.097	CaXy12	75.9230769	0.07592308	1.13884615
B	7	Sample X1	E	0.828	0.096	CaXy12	75.1538462	0.07515385	1.12730769
B	8	Sample X1	E	0.828	0.096	CaXy12	75.1538462	0.07515385	1.12730769
B	9	Blank B	F	0.66					
B	10	Sample X1	F	0.75	0.09	CaXy21	70.5384615	0.07053846	1.05807692
B	11	Sample X1	F	0.75	0.09	CaXy21	70.5384615	0.07053846	1.05807692
B	12	Sample X1	F	0.752	0.092	CaXy21	72.0769231	0.07207692	1.08115385
C	1	Blank B	G	0.615					
C	2	Sample X1	G	0.706	0.091	CaGr11	71.3076923	0.07130769	1.06961538
C	3	Sample X1	G	0.706	0.091	CaGr11	71.3076923	0.07130769	1.06961538
C	4	Sample X1	G	0.707	0.092	CaGr11	72.0769231	0.07207692	1.08115385
C	5	Blank B	H	0.583					
C	6	Sample X1	H	0.673	0.09	CaGr12	70.5384615	0.07053846	1.05807692
C	7	Sample X1	H	0.674	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	8	Sample X1	H	0.674	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	9	Blank B	I	0.571					
C	10	Sample X1	I	0.661	0.09	CaGr21	70.5384615	0.07053846	1.05807692
C	11	Sample X1	I	0.661	0.09	CaGr21	70.5384615	0.07053846	1.05807692
C	12	Sample X1	I	0.662	0.091	CaGr21	71.3076923	0.07130769	1.06961538
D	5	Blank B	K	0.533					
D	6	Sample X1	K	0.623	0.09	CaGc11	70.5384615	0.07053846	1.05807692
D	7	Sample X1	K	0.623	0.09	CaGc11	70.5384615	0.07053846	1.05807692
D	8	Sample X1	K	0.624	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	9	Blank B	L	0.475					
D	10	Sample X1	L	0.573	0.098	CaGc21	76.6923077	0.07669231	1.15038462
D	11	Sample X1	L	0.573	0.098	CaGc21	76.6923077	0.07669231	1.15038462
D	12	Sample X1	L	0.571	0.096	CaGc21	75.1538462	0.07515385	1.12730769
E	1	Blank B	M	0.495					
E	2	Sample X1	M	0.592	0.097	CaGl11	75.9230769	0.07592308	1.13884615
E	3	Sample X1	M	0.59	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	4	Sample X1	M	0.59	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	5	Blank B	N	0.479					
E	6	Sample X1	N	0.575	0.096	CaGl21	75.1538462	0.07515385	1.12730769
E	7	Sample X1	N	0.575	0.096	CaGl21	75.1538462	0.07515385	1.12730769
E	8	Sample X1	N	0.574	0.095	CaGl21	74.3846154	0.07438462	1.11576923

Appendix 9.9 RCCDRSM FRAP run 9

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.575					
D	2	Sample X1	J	0.682	0.107	CaSu11	83.6153846	0.08361538	1.2542308
D	3	Sample X1	J	0.681	0.106	CaSu11	82.8461538	0.08284615	1.2426923
D	4	Sample X1	J	0.681	0.106	CaSu11	82.8461538	0.08284615	1.2426923
A	1	Blank B	A	0.731					
A	2	Sample X1	A	0.835	0.104	CaFr11	81.3076923	0.08130769	1.2196154
A	3	Sample X1	A	0.835	0.104	CaFr11	81.3076923	0.08130769	1.2196154
A	4	Sample X1	A	0.834	0.103	CaFr11	80.5384615	0.08053846	1.2080769
A	5	Blank B	B	0.708					
A	6	Sample X1	B	0.8	0.092	CaFr12	72.0769231	0.07207692	1.0811538
A	7	Sample X1	B	0.827	0.096	CaFr12	75.1538462	0.07515385	1.1273077
A	8	Sample X1	B	0.823	0.092	CaFr12	72.0769231	0.07207692	1.0811538
A	9	Blank B	C	0.742					
A	10	Sample X1	C	0.832	0.09	CaFr21	70.5384615	0.07053846	1.0580769
A	11	Sample X1	C	0.832	0.09	CaFr21	70.5384615	0.07053846	1.0580769
A	12	Sample X1	C	0.833	0.091	CaFr21	71.3076923	0.07130769	1.0696154
B	1	Blank B	D	0.687					
B	2	Sample X1	D	0.78	0.093	CaXy11	72.8461538	0.07284615	1.0926923
B	3	Sample X1	D	0.782	0.095	CaXy11	74.3846154	0.07438462	1.1157692
B	4	Sample X1	D	0.78	0.093	CaXy11	72.8461538	0.07284615	1.0926923
B	5	Blank B	E	0.651					
B	6	Sample X1	E	0.743	0.092	CaXy12	72.0769231	0.07207692	1.0811538
B	7	Sample X1	E	0.743	0.092	CaXy12	72.0769231	0.07207692	1.0811538
B	8	Sample X1	E	0.748	0.097	CaXy12	75.9230769	0.07592308	1.1388462
B	9	Blank B	F	0.615					
B	10	Sample X1	F	0.706	0.091	CaXy21	71.3076923	0.07130769	1.0696154
B	11	Sample X1	F	0.705	0.09	CaXy21	70.5384615	0.07053846	1.0580769
B	12	Sample X1	F	0.705	0.09	CaXy21	70.5384615	0.07053846	1.0580769
C	1	Blank B	G	0.552					
C	2	Sample X1	G	0.642	0.09	CaGr11	70.5384615	0.07053846	1.0580769
C	3	Sample X1	G	0.643	0.091	CaGr11	71.3076923	0.07130769	1.0696154
C	4	Sample X1	G	0.644	0.092	CaGr11	72.0769231	0.07207692	1.0811538
C	5	Blank B	H	0.513					
C	6	Sample X1	H	0.604	0.091	CaGr12	71.3076923	0.07130769	1.0696154
C	7	Sample X1	H	0.603	0.09	CaGr12	70.5384615	0.07053846	1.0580769
C	8	Sample X1	H	0.603	0.09	CaGr12	70.5384615	0.07053846	1.0580769
C	9	Blank B	I	0.571					

Appendix 9.9 contd.

C	10	Sample X1	I	0.67	0.099	CaGr21	77.4615385	0.07746154	1.1619231
C	11	Sample X1	I	0.668	0.097	CaGr21	75.9230769	0.07592308	1.1388462
C	12	Sample X1	I	0.67	0.099	CaGr21	77.4615385	0.07746154	1.1619231
D	5	Blank B	K	0.456					
D	6	Sample X1	K	0.547	0.091	CaGc11	71.3076923	0.07130769	1.0696154
D	7	Sample X1	K	0.548	0.092	CaGc11	72.0769231	0.07207692	1.0811538
D	8	Sample X1	K	0.546	0.09	CaGc11	70.5384615	0.07053846	1.0580769
D	9	Blank B	L	0.427					
D	10	Sample X1	L	0.524	0.097	CaGc21	75.9230769	0.07592308	1.1388462
D	11	Sample X1	L	0.524	0.097	CaGc21	75.9230769	0.07592308	1.1388462
D	12	Sample X1	L	0.522	0.095	CaGc21	74.3846154	0.07438462	1.1157692
E	1	Blank B	M	0.415					
E	2	Sample X1	M	0.509	0.094	CaGl11	73.6153846	0.07361538	1.1042308
E	3	Sample X1	M	0.51	0.095	CaGl11	74.3846154	0.07438462	1.1157692
E	4	Sample X1	M	0.51	0.095	CaGl11	74.3846154	0.07438462	1.1157692
E	5	Blank B	N	0.428					
E	6	Sample X1	N	0.525	0.097	CaGl21	75.9230769	0.07592308	1.1388462
E	7	Sample X1	N	0.525	0.097	CaGl21	75.9230769	0.07592308	1.1388462
E	8	Sample X1	N	0.527	0.099	CaGl21	77.4615385	0.07746154	1.1619231

Appendix 9.10 RCCDRSM FRAP run 10

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.558					
D	2	Sample X1	J	0.664	0.106	CaSu11	82.84615385	0.082846154	1.65692308
D	3	Sample X1	J	0.664	0.106	CaSu11	82.84615385	0.082846154	1.65692308
D	4	Sample X1	J	0.662	0.104	CaSu11	81.30769231	0.081307692	1.62615385
A	1	Blank B	A	0.569					
A	2	Sample X1	A	0.919	0.35	CaFr11	270.5384615	0.270538462	5.41076923
A	3	Sample X1	A	0.917	0.348	CaFr11	269	0.269	5.38
A	4	Sample X1	A	0.919	0.35	CaFr11	270.5384615	0.270538462	5.41076923
A	5	Blank B	B	0.591					
A	6	Sample X1	B	0.766	0.175	CaFr12	135.9230769	0.135923077	2.71846154
A	7	Sample X1	B	0.766	0.175	CaFr12	135.9230769	0.135923077	2.71846154
A	8	Sample X1	B	0.767	0.176	CaFr12	136.6923077	0.136692308	2.73384615
A	9	Blank B	C	0.592					
A	10	Sample X1	C	0.784	0.192	CaFr21	149	0.149	2.98
A	11	Sample X1	C	0.782	0.19	CaFr21	147.4615385	0.147461538	2.94923077

Appendix 9.10 contd.

A	12	Sample X1	C	0.782	0.19	CaFr21	147.4615385	0.147461538	2.94923077
B	1	Blank B	D	0.592					
B	2	Sample X1	D	0.686	0.094	CaXy11	73.61538462	0.073615385	1.47230769
B	3	Sample X1	D	0.687	0.095	CaXy11	74.38461538	0.074384615	1.48769231
B	4	Sample X1	D	0.687	0.095	CaXy11	74.38461538	0.074384615	1.48769231
B	5	Blank B	E	0.586					
B	6	Sample X1	E	0.677	0.091	CaXy12	71.30769231	0.071307692	1.42615385
B	7	Sample X1	E	0.677	0.091	CaXy12	71.30769231	0.071307692	1.42615385
B	8	Sample X1	E	0.677	0.091	CaXy12	71.30769231	0.071307692	1.42615385
B	9	Blank B	F	0.578					
B	10	Sample X1	F	0.698	0.12	CaXy21	93.61538462	0.093615385	1.87230769
B	11	Sample X1	F	0.698	0.12	CaXy21	93.61538462	0.093615385	1.87230769
B	12	Sample X1	F	0.699	0.121	CaXy21	94.38461538	0.094384615	1.88769231
C	1	Blank B	G	0.551					
C	2	Sample X1	G	0.649	0.098	CaGr11	76.69230769	0.076692308	1.53384615
C	3	Sample X1	G	0.649	0.098	CaGr11	76.69230769	0.076692308	1.53384615
C	4	Sample X1	G	0.65	0.099	CaGr11	77.46153846	0.077461538	1.54923077
C	5	Blank B	H	0.508					
C	6	Sample X1	H	0.832	0.324	CaGr12	250.5384615	0.250538462	5.01076923
C	7	Sample X1	H	0.834	0.326	CaGr12	252.0769231	0.252076923	5.04153846
C	8	Sample X1	H	0.834	0.326	CaGr12	252.0769231	0.252076923	5.04153846
C	9	Blank B	I	0.566					
C	10	Sample X1	I	0.667	0.101	CaGr21	79	0.079	1.58
C	11	Sample X1	I	0.667	0.101	CaGr21	79	0.079	1.58
C	12	Sample X1	I	0.668	0.102	CaGr21	79.76923077	0.079769231	1.59538462
D	5	Blank B	K	0.562					
D	6	Sample X1	K	0.658	0.096	CaGc11	75.15384615	0.075153846	1.50307692
D	7	Sample X1	K	0.66	0.098	CaGc11	76.69230769	0.076692308	1.53384615
D	8	Sample X1	K	0.658	0.096	CaGc11	75.15384615	0.075153846	1.50307692
D	9	Blank B	L	0.468					
D	10	Sample X1	L	0.574	0.106	CaGc21	82.84615385	0.082846154	1.65692308
D	11	Sample X1	L	0.572	0.104	CaGc21	81.30769231	0.081307692	1.62615385
D	12	Sample X1	L	0.574	0.106	CaGc21	82.84615385	0.082846154	1.65692308
E	1	Blank B	M	0.428					
E	2	Sample X1	M	0.537	0.109	CaGl11	85.15384615	0.085153846	1.70307692
E	3	Sample X1	M	0.536	0.108	CaGl11	84.38461538	0.084384615	1.68769231
E	4	Sample X1	M	0.536	0.108	CaGl11	84.38461538	0.084384615	1.68769231
E	5	Blank B	N	0.437					
E	6	Sample X1	N	0.53	0.093	CaGl21	72.84615385	0.072846154	1.45692308
E	7	Sample X1	N	0.533	0.096	CaGl21	75.15384615	0.075153846	1.50307692
E	8	Sample X1	N	0.53	0.093	CaGl21	72.84615385	0.072846154	1.45692308

Appendix 9.11 RCCDRSM FRAP run 11

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.29					
D	2	Sample X1	J	0.92	0.63	CaSu11	485.9230769	0.485923077	9.718461538
D	3	Sample X1	J	0.924	0.634	CaSu11	489	0.489	9.78
D	4	Sample X1	J	0.924	0.634	CaSu11	489	0.489	9.78
A	1	Blank B	A	0.303					
A	2	Sample X1	A	0.954	0.651	CaFr11	502.0769231	0.502076923	10.04153846
A	3	Sample X1	A	0.953	0.65	CaFr11	501.3076923	0.501307692	10.02615385
A	4	Sample X1	A	0.953	0.65	CaFr11	501.3076923	0.501307692	10.02615385
A	5	Blank B	B	0.328					
A	6	Sample X1	B	0.993	0.665	CaFr12	512.8461538	0.512846154	10.25692308
A	7	Sample X1	B	0.993	0.665	CaFr12	512.8461538	0.512846154	10.25692308
A	8	Sample X1	B	0.995	0.667	CaFr12	514.3846154	0.514384615	10.28769231
A	9	Blank B	C	0.217					
A	10	Sample X1	C	0.917	0.7	CaFr21	539.7692308	0.539769231	10.79538462
A	11	Sample X1	C	0.915	0.698	CaFr21	538.2307692	0.538230769	10.76461538
A	12	Sample X1	C	0.917	0.7	CaFr21	539.7692308	0.539769231	10.79538462
B	1	Blank B	D	0.026					
B	2	Sample X1	D	0.759	0.733	CaXy11	565.1538462	0.565153846	11.30307692
B	3	Sample X1	D	0.76	0.734	CaXy11	565.9230769	0.565923077	11.31846154
B	4	Sample X1	D	0.762	0.736	CaXy11	567.4615385	0.567461538	11.34923077
B	5	Blank B	E	0.027					
B	6	Sample X1	E	0.677	0.65	CaXy12	501.3076923	0.501307692	10.02615385
B	7	Sample X1	E	0.675	0.648	CaXy12	499.7692308	0.499769231	9.995384615
B	8	Sample X1	E	0.677	0.65	CaXy12	501.3076923	0.501307692	10.02615385
B	9	Blank B	F	0.073					
B	10	Sample X1	F	0.691	0.618	CaXy21	476.6923077	0.476692308	9.533846154
B	11	Sample X1	F	0.687	0.614	CaXy21	473.6153846	0.473615385	9.472307692
B	12	Sample X1	F	0.691	0.618	CaXy21	476.6923077	0.476692308	9.533846154
C	1	Blank B	G	0.064					
C	2	Sample X1	G	0.668	0.604	CaGr11	465.9230769	0.465923077	9.318461538
C	3	Sample X1	G	0.664	0.6	CaGr11	462.8461538	0.462846154	9.256923077
C	4	Sample X1	G	0.664	0.6	CaGr11	462.8461538	0.462846154	9.256923077
C	5	Blank B	H	0.098					
C	6	Sample X1	H	0.644	0.546	CaGr12	421.3076923	0.421307692	8.426153846
C	7	Sample X1	H	0.646	0.548	CaGr12	422.8461538	0.422846154	8.456923077
C	8	Sample X1	H	0.644	0.546	CaGr12	421.3076923	0.421307692	8.426153846
C	9	Blank B	I	0.042					

Appendix 9.11 contd.

C	10	Sample X1	I	0.729	0.687	CaGr21	529.7692308	0.529769231	10.59538462
C	11	Sample X1	I	0.731	0.689	CaGr21	531.3076923	0.531307692	10.62615385
C	12	Sample X1	I	0.729	0.687	CaGr21	529.7692308	0.529769231	10.59538462
D	5	Blank B	K	0.072					
D	6	Sample X1	K	0.593	0.521	CaGc11	402.0769231	0.402076923	8.041538462
D	7	Sample X1	K	0.594	0.522	CaGc11	402.8461538	0.402846154	8.056923077
D	8	Sample X1	K	0.593	0.521	CaGc11	402.0769231	0.402076923	8.041538462
D	9	Blank B	L	0.074					
D	10	Sample X1	L	0.256	0.182	CaGc21	141.3076923	0.141307692	2.826153846
D	11	Sample X1	L	0.257	0.183	CaGc21	142.0769231	0.142076923	2.841538462
D	12	Sample X1	L	0.256	0.182	CaGc21	141.3076923	0.141307692	2.826153846
E	1	Blank B	M	0.059					
E	2	Sample X1	M	0.15	0.091	CaGl11	71.30769231	0.071307692	1.426153846
E	3	Sample X1	M	0.155	0.096	CaGl11	75.15384615	0.075153846	1.503076923
E	4	Sample X1	M	0.15	0.091	CaGl11	71.30769231	0.071307692	1.426153846
E	5	Blank B	N	0.047					
E	6	Sample X1	N	0.14	0.093	CaGl21	72.84615385	0.072846154	1.456923077
E	7	Sample X1	N	0.138	0.091	CaGl21	71.30769231	0.071307692	1.426153846
E	8	Sample X1	N	0.14	0.093	CaGl21	72.84615385	0.072846154	1.456923077

Appendix 9.12 RCCDRSM FRAP run 12

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
	1	Blank B	A	0.039					
E	2	Sample X1	A	0.133	0.094	CaSu11	73.615385	0.0736154	1.47230769
E	3	Sample X1	A	0.133	0.094	CaSu11	73.615385	0.0736154	1.47230769
E	4	Sample X1	A	0.132	0.093	CaSu11	72.846154	0.0728462	1.45692308
E	5	Blank B	B	0.058					
E	6	Sample X1	B	0.442	0.384	CaFr11	296.69231	0.2966923	5.93384615
E	7	Sample X1	B	0.443	0.385	CaFr11	297.46154	0.2974615	5.94923077
E	8	Sample X1	B	0.442	0.384	CaFr11	296.69231	0.2966923	5.94923077
E	9	Blank B	C	0.025					
E	10	Sample X1	C	0.152	0.127	CaFr12	99	0.099	1.98
E	11	Sample X1	C	0.154	0.129	CaFr12	100.53846	0.1005385	2.01076923
E	12	Sample X1	C	0.152	0.127	CaFr12	99	0.099	1.98
F	1	Blank B	D	0.874					
F	2	Sample X1	D	0.986	0.112	CaFr21	87.461538	0.0874615	1.74923077
F	3	Sample X1	D	0.986	0.112	CaFr21	87.461538	0.0874615	1.74923077

Appendix 9.12 contd.

F	4	Sample X1	D	0.988	0.114	CaFr21	89	0.089	1.78
B	1	Blank B	D	0.024					
B	2	Sample X1	D	0.118	0.094	CaXy11	73.615385	0.0736154	1.47230769
B	3	Sample X1	D	0.121	0.097	CaXy11	75.923077	0.0759231	1.51846154
B	4	Sample X1	D	0.12	0.096	CaXy11	75.153846	0.0751538	1.50307692
F	5	Blank B	E	0.017					
F	6	Sample X1	E	0.11	0.093	CaXy12	72.846154	0.0728462	1.45692308
F	7	Sample X1	E	0.111	0.094	CaXy12	73.615385	0.0736154	1.47230769
F	8	Sample X1	E	0.11	0.093	CaXy12	72.846154	0.0728462	1.45692308
A	9	Blank B	C	0.027					
A	10	Sample X1	C	0.12	0.093	CaXy21	72.846154	0.0728462	1.45692308
A	11	Sample X1	C	0.122	0.095	CaXy21	74.384615	0.0743846	1.48769231
A	12	Sample X1	C	0.122	0.095	CaXy21	74.384615	0.0743846	1.48769231
F	9	Blank B	F	0.078					
F	10	Sample X1	F	0.173	0.095	CaGr11	74.384615	0.0743846	1.48769231
F	11	Sample X1	F	0.174	0.096	CaGr11	75.153846	0.0751538	1.50307692
F	12	Sample X1	F	0.173	0.095	CaGr11	74.384615	0.0743846	1.48769231
G	1	Blank B	G	0.053					
G	2	Sample X1	G	0.147	0.094	CaGr12	73.615385	0.0736154	1.47230769
G	3	Sample X1	G	0.147	0.094	CaGr12	73.615385	0.0736154	1.47230769
G	4	Sample X1	G	0.147	0.094	CaGr12	73.615385	0.0736154	1.47230769
G	5	Blank B	H	0.128					
G	6	Sample X1	H	0.334	0.206	CaGr21	159.76923	0.1597692	3.19538462
G	7	Sample X1	H	0.334	0.206	CaGr21	159.76923	0.1597692	3.19538462
G	8	Sample X1	H	0.335	0.207	CaGr21	160.53846	0.1605385	3.21076923
G	9	Blank B	I	0.385					
G	10	Sample X1	I	0.48	0.095	CaGc11	74.384615	0.0743846	1.48769231
G	11	Sample X1	I	0.477	0.092	CaGc11	72.076923	0.0720769	1.44153846
G	12	Sample X1	I	0.477	0.092	CaGc11	72.076923	0.0720769	1.44153846
H	1	Blank B	J	0.315					
H	2	Sample X1	J	0.413	0.098	CaGc21	76.692308	0.0766923	1.53384615
H	3	Sample X1	J	0.414	0.099	CaGc21	77.461538	0.0774615	1.54923077
H	4	Sample X1	J	0.413	0.098	CaGc21	76.692308	0.0766923	1.53384615
H	5	Blank B	K	0.57					
H	6	Sample X1	K	0.664	0.094	CaGl11	73.615385	0.0736154	1.47230769
H	7	Sample X1	K	0.666	0.096	CaGl11	75.153846	0.0751538	1.50307692
H	8	Sample X1	K	0.664	0.094	CaGl11	73.615385	0.0736154	1.47230769
H	9	Blank B	L	0.512					
H	10	Sample X1	L	0.608	0.096	CaGl21	75.153846	0.0751538	1.50307692
H	11	Sample X1	L	0.607	0.095	CaGl21	74.384615	0.0743846	1.48769231
H	12	Sample X1	L	0.608	0.096	CaGl21	75.153846	0.0751538	1.50307692

Appendix 9.13 RCCDRSM FRAP run 13

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.575					
D	2	Sample X1	J	0.808	0.233	CaSu11	180.538462	0.18053846	1.805384615
D	3	Sample X1	J	0.809	0.234	CaSu11	181.307692	0.18130769	1.813076923
D	4	Sample X1	J	0.808	0.233	CaSu11	180.538462	0.18053846	1.805384615
A	1	Blank B	A	0.491					
A	2	Sample X1	A	0.972	0.481	CaFr11	371.307692	0.37130769	3.713076923
A	3	Sample X1	A	0.975	0.484	CaFr11	373.615385	0.37361538	3.736153846
A	4	Sample X1	A	0.977	0.486	CaFr11	375.153846	0.37515385	3.751538462
A	5	Blank B	B	0.489					
A	6	Sample X1	B	0.65	0.161	CaFr12	125.153846	0.12515385	1.251538462
A	7	Sample X1	B	0.652	0.163	CaFr12	126.692308	0.12669231	1.266923077
A	8	Sample X1	B	0.652	0.163	CaFr12	126.692308	0.12669231	1.266923077
A	9	Blank B	C	0.449					
A	10	Sample X1	C	0.723	0.274	CaFr21	212.076923	0.21207692	2.120769231
A	11	Sample X1	C	0.724	0.275	CaFr21	212.846154	0.21284615	2.128461538
A	12	Sample X1	C	0.725	0.276	CaFr21	213.615385	0.21361538	2.136153846
B	1	Blank B	D	0.677					
B	2	Sample X1	D	0.858	0.181	CaXy11	140.538462	0.14053846	1.405384615
B	3	Sample X1	D	0.864	0.187	CaXy11	145.153846	0.14515385	1.451538462
B	4	Sample X1	D	0.862	0.185	CaXy11	143.615385	0.14361538	1.436153846
B	5	Blank B	E	0.691					
B	6	Sample X1	E	0.859	0.168	CaXy12	130.538462	0.13053846	1.305384615
B	7	Sample X1	E	0.861	0.17	CaXy12	132.076923	0.13207692	1.320769231
B	8	Sample X1	E	0.861	0.17	CaXy12	132.076923	0.13207692	1.320769231
B	9	Blank B	F	0.624					
B	10	Sample X1	F	0.927	0.303	CaXy21	234.384615	0.23438462	2.343846154
B	11	Sample X1	F	0.926	0.302	CaXy21	233.615385	0.23361538	2.336153846
B	12	Sample X1	F	0.926	0.302	CaXy21	233.615385	0.23361538	2.336153846
C	1	Blank B	G	0.625					
C	2	Sample X1	G	0.941	0.316	CaGr11	244.384615	0.24438462	2.443846154
C	3	Sample X1	G	0.939	0.314	CaGr11	242.846154	0.24284615	2.428461538
C	4	Sample X1	G	0.937	0.312	CaGr11	241.307692	0.24130769	2.413076923
C	5	Blank B	H	0.62					
C	6	Sample X1	H	0.872	0.252	CaGr12	195.153846	0.19515385	1.951538462
C	7	Sample X1	H	0.872	0.252	CaGr12	195.153846	0.19515385	1.951538462
C	8	Sample X1	H	0.873	0.253	CaGr12	195.923077	0.19592308	1.959230769
C	9	Blank B	I	0.543					

Appendix 9.13 contd.

C	10	Sample X1	I	0.819	0.303	CaGr21	234.384615	0.23438462	2.343846154
C	11	Sample X1	I	0.848	0.304	CaGr21	235.153846	0.23515385	2.351538462
C	12	Sample X1	I	0.871	0.303	CaGr21	234.384615	0.23438462	2.343846154
D	5	Blank B	K	0.564					
D	6	Sample X1	K	0.656	0.092	CaGc11	72.0769231	0.07207692	0.720769231
D	7	Sample X1	K	0.658	0.094	CaGc11	73.6153846	0.07361538	0.736153846
D	8	Sample X1	K	0.659	0.095	CaGc11	74.3846154	0.07438462	0.743846154
D	9	Blank B	L	0.463					
D	10	Sample X1	L	0.625	0.162	CaGc21	125.923077	0.12592308	1.259230769
D	11	Sample X1	L	0.623	0.16	CaGc21	124.384615	0.12438462	1.243846154
D	12	Sample X1	L	0.623	0.16	CaGc21	124.384615	0.12438462	1.243846154
E	1	Blank B	M	0.509					
E	2	Sample X1	M	0.771	0.262	CaGl11	202.846154	0.20284615	2.028461538
E	3	Sample X1	M	0.771	0.262	CaGl11	202.846154	0.20284615	2.028461538
E	4	Sample X1	M	0.771	0.262	CaGl11	202.846154	0.20284615	2.028461538
E	5	Blank B	N	0.458					
E	6	Sample X1	N	0.599	0.141	CaGl21	109.769231	0.10976923	1.097692308
E	7	Sample X1	N	0.599	0.141	CaGl21	109.769231	0.10976923	1.097692308
E	8	Sample X1	N	0.6	0.142	CaGl21	110.538462	0.11053846	1.105384615

Appendix 9.14 RCCDRSM FRAP run 14

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.659					
D	2	Sample X1	J	0.624	0.095	CaSu11	74.3846154	0.07438462	0.74384615
D	3	Sample X1	J	0.644	0.095	CaSu11	74.3846154	0.07438462	0.74384615
D	4	Sample X1	J	0.627	0.092	CaSu11	72.0769231	0.07207692	0.72076923
A	1	Blank B	A	0.724					
A	2	Sample X1	A	0.854	0.13	CaFr11	101.307692	0.10130769	1.01307692
A	3	Sample X1	A	0.853	0.129	CaFr11	100.538462	0.10053846	1.00538462
A	4	Sample X1	A	0.854	0.13	CaFr11	101.307692	0.10130769	1.01307692
A	5	Blank B	B	0.717					
A	6	Sample X1	B	0.811	0.094	CaFr12	73.6153846	0.07361538	0.73615385
A	7	Sample X1	B	0.811	0.094	CaFr12	73.6153846	0.07361538	0.73615385
A	8	Sample X1	B	0.813	0.096	CaFr12	75.1538462	0.07515385	0.75153846
A	9	Blank B	C	0.793					
A	10	Sample X1	C	f28+e27	0.113	CaFr21	88.2307692	0.08823077	0.88230769
A	11	Sample X1	C	0.908	0.115	CaFr21	89.7692308	0.08976923	0.89769231
A	12	Sample X1	C	0.908	0.115	CaFr21	89.7692308	0.08976923	0.89769231

B	1	Blank B	D	0.779					
B	2	Sample X1	D	0.875	0.096	CaXy11	75.1538462	0.07515385	0.75153846
B	3	Sample X1	D	0.875	0.096	CaXy11	75.1538462	0.07515385	0.75153846
B	4	Sample X1	D	0.875	0.096	CaXy11	75.1538462	0.07515385	0.75153846
B	5	Blank B	E	0.727					
B	6	Sample X1	E	0.819	0.092	CaXy12	72.0769231	0.07207692	0.72076923
B	7	Sample X1	E	0.819	0.092	CaXy12	72.0769231	0.07207692	0.72076923
B	8	Sample X1	E	0.818	0.091	CaXy12	71.3076923	0.07130769	0.71307692
B	9	Blank B	F	0.679					
B	10	Sample X1	F	0.894	0.215	CaXy21	166.692308	0.16669231	1.66692308
B	11	Sample X1	F	0.894	0.215	CaXy21	166.692308	0.16669231	1.66692308
B	12	Sample X1	F	0.896	0.217	CaXy21	168.230769	0.16823077	1.68230769
C	1	Blank B	G	0.683					
C	2	Sample X1	G	0.779	0.096	CaGr11	75.1538462	0.07515385	0.75153846
C	3	Sample X1	G	0.777	0.094	CaGr11	73.6153846	0.07361538	0.73615385
C	4	Sample X1	G	0.777	0.094	CaGr11	73.6153846	0.07361538	0.73615385
C	5	Blank B	H	0.64					
C	6	Sample X1	H	0.733	0.093	CaGr12	72.8461538	0.07284615	0.72846154
C	7	Sample X1	H	0.731	0.091	CaGr12	71.3076923	0.07130769	0.71307692
C	8	Sample X1	H	0.733	0.093	CaGr12	72.8461538	0.07284615	0.72846154
C	9	Blank B	I	0.576					
C	10	Sample X1	I	0.667	0.091	CaGr21	71.3076923	0.07130769	0.71307692
C	11	Sample X1	I	0.668	0.092	CaGr21	72.0769231	0.07207692	0.72076923
C	12	Sample X1	I	0.668	0.092	CaGr21	72.0769231	0.07207692	0.72076923
D	5	Blank B	K	0.572					
D	6	Sample X1	K	0.664	0.092	CaGc11	72.0769231	0.07207692	0.72076923
D	7	Sample X1	K	0.664	0.092	CaGc11	72.0769231	0.07207692	0.72076923
D	8	Sample X1	K	0.663	0.091	CaGc11	71.3076923	0.07130769	0.71307692
D	9	Blank B	L	0.638					
D	10	Sample X1	L	0.729	0.091	CaGc21	71.3076923	0.07130769	0.71307692
D	11	Sample X1	L	0.729	0.091	CaGc21	71.3076923	0.07130769	0.71307692
D	12	Sample X1	L	0.729	0.091	CaGc21	71.3076923	0.07130769	0.71307692
E	1	Blank B	M	0.521					
E	2	Sample X1	M	0.62	0.099	CaGl11	77.4615385	0.07746154	0.77461538
E	3	Sample X1	M	0.619	0.098	CaGl11	76.6923077	0.07669231	0.76692308
E	4	Sample X1	M	0.618	0.097	CaGl11	75.9230769	0.07592308	0.75923077
E	5	Blank B	N	0.557					
E	6	Sample X1	N	0.648	0.091	CaGl21	71.3076923	0.07130769	0.71307692
E	7	Sample X1	N	0.648	0.091	CaGl21	71.3076923	0.07130769	0.71307692
E	8	Sample X1	N	0.648	0.091	CaGl21	71.3076923	0.07130769	0.71307692

Appendix 9.15 RCCDRSM FRAP run 15

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.554					
D	2	Sample X1	J	0.651	0.097	CaSu11	75.923077	0.0759231	1.518461538
D	3	Sample X1	J	0.65	0.096	CaSu11	75.153846	0.0751538	1.503076923
D	4	Sample X1	J	0.65	0.096	CaSu11	75.153846	0.0751538	1.503076923
A	1	Blank B	A	0.665					
A	2	Sample X1	A	0.763	0.098	CaFr11	76.692308	0.0766923	1.533846154
A	3	Sample X1	A	0.761	0.096	CaFr11	75.153846	0.0751538	1.503076923
A	4	Sample X1	A	0.761	0.096	CaFr11	75.153846	0.0751538	1.503076923
A	5	Blank B	B	0.644					
A	6	Sample X1	B	0.738	0.094	CaFr12	73.615385	0.0736154	1.472307692
A	7	Sample X1	B	0.739	0.095	CaFr12	74.384615	0.0743846	1.487692308
A	8	Sample X1	B	0.738	0.094	CaFr12	73.615385	0.0736154	1.472307692
A	9	Blank B	C	0.637					
A	10	Sample X1	C	0.731	0.094	CaFr21	73.615385	0.0736154	1.472307692
A	11	Sample X1	C	0.731	0.094	CaFr21	73.615385	0.0736154	1.472307692
A	12	Sample X1	C	0.734	0.097	CaFr21	75.923077	0.0759231	1.518461538
B	1	Blank B	D	0.568					
B	2	Sample X1	D	0.666	0.098	CaXy11	76.692308	0.0766923	1.533846154
B	3	Sample X1	D	0.664	0.096	CaXy11	75.153846	0.0751538	1.503076923
B	4	Sample X1	D	0.664	0.096	CaXy11	75.153846	0.0751538	1.503076923
B	5	Blank B	E	0.52					
B	6	Sample X1	E	0.612	0.092	CaXy12	72.076923	0.0720769	1.441538462
B	7	Sample X1	E	0.613	0.093	CaXy12	72.846154	0.0728462	1.456923077
B	8	Sample X1	E	0.612	0.092	CaXy12	72.076923	0.0720769	1.441538462
B	9	Blank B	F	0.507					
B	10	Sample X1	F	0.602	0.095	CaXy21	74.384615	0.0743846	1.487692308
B	11	Sample X1	F	0.602	0.095	CaXy21	74.384615	0.0743846	1.487692308
B	12	Sample X1	F	0.6	0.093	CaXy21	72.846154	0.0728462	1.456923077
C	1	Blank B	G	0.573					
C	2	Sample X1	G	0.665	0.092	CaGr11	72.076923	0.0720769	1.441538462
C	3	Sample X1	G	0.665	0.092	CaGr11	72.076923	0.0720769	1.441538462
C	4	Sample X1	G	0.666	0.093	CaGr11	72.846154	0.0728462	1.456923077
C	5	Blank B	H	0.549					
C	6	Sample X1	H	0.647	0.098	CaGr12	76.692308	0.0766923	1.533846154
C	7	Sample X1	H	0.647	0.098	CaGr12	76.692308	0.0766923	1.533846154
C	8	Sample X1	H	0.648	0.099	CaGr12	77.461538	0.0774615	1.549230769
C	9	Blank B	I	0.484					

Appendix 9.15 contd.

C	10	Sample X1	I	0.581	0.097	CaGr21	75.923077	0.0759231	1.518461538
C	11	Sample X1	I	0.583	0.099	CaGr21	77.461538	0.0774615	1.549230769
C	12	Sample X1	I	0.581	0.097	CaGr21	75.923077	0.0759231	1.518461538
D	5	Blank B	K	0.503					
D	6	Sample X1	K	0.602	0.099	CaGc11	77.461538	0.0774615	1.549230769
D	7	Sample X1	K	0.601	0.098	CaGc11	76.692308	0.0766923	1.533846154
D	8	Sample X1	K	0.601	0.098	CaGc11	76.692308	0.0766923	1.533846154
D	9	Blank B	L	0.46					
D	10	Sample X1	L	0.554	0.094	CaGc21	73.615385	0.0736154	1.472307692
D	11	Sample X1	L	0.554	0.094	CaGc21	73.615385	0.0736154	1.472307692
D	12	Sample X1	L	0.556	0.096	CaGc21	75.153846	0.0751538	1.503076923
E	1	Blank B	M	0.453					
E	2	Sample X1	M	0.546	0.093	CaGl11	72.846154	0.0728462	1.456923077
E	3	Sample X1	M	0.547	0.094	CaGl11	73.615385	0.0736154	1.472307692
E	4	Sample X1	M	0.546	0.093	CaGl11	72.846154	0.0728462	1.456923077
E	5	Blank B	N	0.429					
E	6	Sample X1	N	0.527	0.098	CaGl21	76.692308	0.0766923	1.533846154
E	7	Sample X1	N	0.524	0.095	CaGl21	74.384615	0.0743846	1.487692308
E	8	Sample X1	N	0.527	0.098	CaGl21	76.692308	0.0766923	1.533846154

Appendix 9.16 RCCDRSM FRAP run 16

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.633					
D	2	Sample X1	J	0.731	0.098	CaSu11	76.6923077	0.07669231	1.533846154
D	3	Sample X1	J	0.729	0.096	CaSu11	75.1538462	0.07515385	1.503076923
D	4	Sample X1	J	0.731	0.098	CaSu11	76.6923077	0.07669231	1.533846154
A	1	Blank B	A	0.895					
A	2	Sample X1	A	0.989	0.094	CaFr11	73.6153846	0.07361538	1.472307692
A	3	Sample X1	A	0.99	0.095	CaFr11	74.3846154	0.07438462	1.487692308
A	4	Sample X1	A	0.989	0.094	CaFr11	73.6153846	0.07361538	1.472307692
A	5	Blank B	B	0.795					
A	6	Sample X1	B	0.888	0.093	CaFr12	72.8461538	0.07284615	1.456923077
A	7	Sample X1	B	0.886	0.091	CaFr12	71.3076923	0.07130769	1.426153846
A	8	Sample X1	B	0.886	0.091	CaFr12	71.3076923	0.07130769	1.426153846
A	9	Blank B	C	0.752					
A	10	Sample X1	C	0.845	0.093	CaFr21	72.8461538	0.07284615	1.456923077
A	11	Sample X1	C	0.846	0.094	CaFr21	73.6153846	0.07361538	1.472307692

Appendix 9.16 contd.

A	12	Sample X1	C	0.845	0.093	CaFr21	72.8461538	0.07284615	1.456923077
B	1	Blank B	D	0.697					
B	2	Sample X1	D	0.79	0.093	CaXy11	72.8461538	0.07284615	1.456923077
B	3	Sample X1	D	0.792	0.095	CaXy11	74.3846154	0.07438462	1.487692308
B	4	Sample X1	D	0.79	0.093	CaXy11	72.8461538	0.07284615	1.456923077
B	5	Blank B	E	0.67					
B	6	Sample X1	E	0.763	0.093	CaXy12	72.8461538	0.07284615	1.456923077
B	7	Sample X1	E	0.763	0.093	CaXy12	72.8461538	0.07284615	1.456923077
B	8	Sample X1	E	0.765	0.095	CaXy12	74.3846154	0.07438462	1.487692308
B	9	Blank B	F	0.609					
B	10	Sample X1	F	0.713	0.104	CaXy21	81.3076923	0.08130769	1.626153846
B	11	Sample X1	F	0.715	0.106	CaXy21	82.8461538	0.08284615	1.656923077
B	12	Sample X1	F	0.715	0.106	CaXy21	82.8461538	0.08284615	1.656923077
C	1	Blank B	G	0.628					
C	2	Sample X1	G	0.719	0.091	CaGr11	71.3076923	0.07130769	1.426153846
C	3	Sample X1	G	0.72	0.092	CaGr11	72.0769231	0.07207692	1.441538462
C	4	Sample X1	G	0.718	0.09	CaGr11	70.5384615	0.07053846	1.410769231
C	5	Blank B	H	0.572					
C	6	Sample X1	H	0.664	0.092	CaGr12	72.0769231	0.07207692	1.441538462
C	7	Sample X1	H	0.667	0.095	CaGr12	74.3846154	0.07438462	1.487692308
C	8	Sample X1	H	0.664	0.092	CaGr12	72.0769231	0.07207692	1.441538462
C	9	Blank B	I	0.519					
C	10	Sample X1	I	0.615	0.096	CaGr21	75.1538462	0.07515385	1.503076923
C	11	Sample X1	I	0.614	0.095	CaGr21	74.3846154	0.07438462	1.487692308
C	12	Sample X1	I	0.614	0.095	CaGr21	74.3846154	0.07438462	1.487692308
D	5	Blank B	K	0.529					
D	6	Sample X1	K	0.628	0.099	CaGc11	77.4615385	0.07746154	1.549230769
D	7	Sample X1	K	0.626	0.097	CaGc11	75.9230769	0.07592308	1.518461538
D	8	Sample X1	K	0.626	0.097	CaGc11	75.9230769	0.07592308	1.518461538
D	9	Blank B	L	0.462					
D	10	Sample X1	L	0.556	0.094	CaGc21	73.6153846	0.07361538	1.472307692
D	11	Sample X1	L	0.555	0.093	CaGc21	72.8461538	0.07284615	1.456923077
D	12	Sample X1	L	0.555	0.093	CaGc21	72.8461538	0.07284615	1.456923077
E	1	Blank B	M	0.493					
E	2	Sample X1	M	0.586	0.093	CaGl11	72.8461538	0.07284615	1.456923077
E	3	Sample X1	M	0.585	0.092	CaGl11	72.0769231	0.07207692	1.441538462
E	4	Sample X1	M	0.585	0.092	CaGl11	72.0769231	0.07207692	1.441538462
E	5	Blank B	N	0.483					
E	6	Sample X1	N	0.578	0.095	CaGl21	74.3846154	0.07438462	1.487692308
E	7	Sample X1	N	0.577	0.094	CaGl21	73.6153846	0.07361538	1.472307692
E	8	Sample X1	N	0.578	0.095	CaGl21	74.3846154	0.07438462	1.487692308

Appendix 9.17 RCCDRSM FRAP run 17

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.302					
A	2	Sample X1	A	0.398	0.096	CaSu11	75.1538462	0.07515385	0.75153846
A	3	Sample X1	A	0.399	0.097	CaSu11	75.9230769	0.07592308	0.75923077
A	4	Sample X1	A	0.398	0.096	CaSu11	75.1538462	0.07515385	0.75153846
A	5	Blank B	B	0.178					
A	6	Sample X1	B	0.461	0.283	CaFr11	219	0.219	2.19
A	7	Sample X1	B	0.46	0.282	CaFr11	218.230769	0.21823077	2.18230769
A	8	Sample X1	B	0.46	0.282	CaFr11	218.230769	0.21823077	2.18230769
A	9	Blank B	C	0.126					
A	10	Sample X1	C	0.219	0.093	CaFr12	72.8461538	0.07284615	0.72846154
A	11	Sample X1	C	0.222	0.096	CaFr12	75.1538462	0.07515385	0.75153846
A	12	Sample X1	C	0.222	0.096	CaFr12	75.1538462	0.07515385	0.75153846
B	1	Blank B	D	0.117					
B	2	Sample X1	D	0.213	0.096	CaFr21	75.1538462	0.07515385	0.75153846
B	3	Sample X1	D	0.21	0.093	CaFr21	72.8461538	0.07284615	0.72846154
B	4	Sample X1	D	0.21	0.093	CaFr21	72.8461538	0.07284615	0.72846154
B	5	Blank B	E	0.168					
B	6	Sample X1	E	0.261	0.093	CaXy11	72.8461538	0.07284615	0.72846154
B	7	Sample X1	E	0.261	0.093	CaXy11	72.8461538	0.07284615	0.72846154
B	8	Sample X1	E	0.26	0.092	CaXy11	72.0769231	0.07207692	0.72846154
B	5	Blank B	E	0.155					
B	6	Sample X1	E	0.247	0.092	CaXy12	72.0769231	0.07207692	0.72076923
B	7	Sample X1	E	0.247	0.092	CaXy12	72.0769231	0.07207692	0.72076923
B	8	Sample X1	E	0.248	0.093	CaXy12	72.8461538	0.07284615	0.72846154
B	1	Blank B	D	0.198					
B	2	Sample X1	D	0.292	0.094	CaXy21	73.6153846	0.07361538	0.73615385
B	3	Sample X1	D	0.292	0.094	CaXy21	73.6153846	0.07361538	0.73615385
B	4	Sample X1	D	0.293	0.095	CaXy21	74.3846154	0.07438462	0.74384615
B	9	Blank B	F	0.613					
B	10	Sample X1	F	0.709	0.096	CaGr11	75.1538462	0.07515385	0.75153846
B	11	Sample X1	F	0.71	0.097	CaGr11	75.9230769	0.07592308	0.75923077
B	12	Sample X1	F	0.709	0.096	CaGr11	75.1538462	0.07515385	0.75153846
C	1	Blank B	G	0.678					
C	2	Sample X1	G	0.771	0.093	CaGr12	72.8461538	0.07284615	0.72846154
C	3	Sample X1	G	0.772	0.094	CaGr12	73.6153846	0.07361538	0.73615385
C	4	Sample X1	G	0.772	0.094	CaGr12	73.6153846	0.07361538	0.73615385
C	5	Blank B	H	0.615					
C	6	Sample X1	H	0.709	0.094	CaGr21	73.6153846	0.07361538	0.73615385

Appendix 9.17 contd.

C	7	Sample X1	H	0.71	0.095	CaGr21	74.3846154	0.07438462	0.74384615
C	8	Sample X1	H	0.712	0.097	CaGr21	75.9230769	0.07592308	0.75923077
C	9	Blank B	I	0.629					
C	10	Sample X1	I	0.722	0.093	CaGc11	72.8461538	0.07284615	0.72846154
C	11	Sample X1	I	0.722	0.093	CaGc11	72.8461538	0.07284615	0.72846154
C	12	Sample X1	I	0.721	0.092	CaGc11	72.0769231	0.07207692	0.72076923
D	1	Blank B	J	0.683					
D	2	Sample X1	J	0.777	0.094	CaGc21	73.6153846	0.07361538	0.73615385
D	3	Sample X1	J	0.777	0.094	CaGc21	73.6153846	0.07361538	0.73615385
D	4	Sample X1	J	0.779	0.096	CaGc21	75.1538462	0.07515385	0.75153846
D	5	Blank B	K	0.688					
D	6	Sample X1	K	0.783	0.095	CaGl11	74.3846154	0.07438462	0.74384615
D	7	Sample X1	K	0.786	0.098	CaGl11	76.6923077	0.07669231	0.76692308
D	8	Sample X1	K	0.783	0.095	CaGl11	74.3846154	0.07438462	0.74384615
D	9	Blank B	L	0.605					
D	10	Sample X1	L	0.701	0.096	CaGl21	75.1538462	0.07515385	0.75153846
D	11	Sample X1	L	0.699	0.094	CaGl21	73.6153846	0.07361538	0.73615385
D	12	Sample X1	L	0.701	0.096	CaGl21	75.1538462	0.07515385	0.75153846

Appendix 9.18 RCCDRSM FRAP run 18

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.032					
E	2	Sample X1	A	0.218	0.186	CaSu11	144.384615	0.14438462	2.88769231
E	3	Sample X1	A	0.214	0.182	CaSu11	141.307692	0.14130769	2.82615385
E	4	Sample X1	A	0.215	0.183	CaSu11	142.076923	0.14207692	2.84153846
E	5	Blank B	B	0.069					
E	6	Sample X1	B	0.176	0.107	CaFr11	83.6153846	0.08361538	1.67230769
E	7	Sample X1	B	0.172	0.103	CaFr11	80.5384615	0.08053846	1.61076923
E	8	Sample X1	B	0.174	0.105	CaFr11	82.0769231	0.08207692	1.64153846
E	9	Blank B	C	0.087					
E	10	Sample X1	C	0.185	0.098	CaFr12	76.6923077	0.07669231	1.53384615
E	11	Sample X1	C	0.186	0.099	CaFr12	77.4615385	0.07746154	1.54923077
E	12	Sample X1	C	0.186	0.099	CaFr12	77.4615385	0.07746154	1.54923077
F	1	Blank B	D	0.276					
F	2	Sample X1	D	0.369	0.093	CaFr21	72.8461538	0.07284615	1.45692308
F	3	Sample X1	D	0.369	0.093	CaFr21	72.8461538	0.07284615	1.45692308
F	4	Sample X1	D	0.37	0.094	CaFr21	73.6153846	0.07361538	1.47230769

Appendix 9.18 contd.

B	9	Blank B	F	0.608					
B	10	Sample X1	F	0.706	0.098	CaXy11	76.6923077	0.07669231	1.53384615
B	11	Sample X1	F	0.706	0.098	CaXy11	76.6923077	0.07669231	1.53384615
B	12	Sample X1	F	0.704	0.096	CaXy11	75.1538462	0.07515385	1.50307692
F	5	Blank B	E	0.13					
F	6	Sample X1	E	0.224	0.094	CaXy12	73.6153846	0.07361538	1.47230769
F	7	Sample X1	E	0.226	0.096	CaXy12	75.1538462	0.07515385	1.50307692
F	8	Sample X1	E	0.226	0.096	CaXy12	75.1538462	0.07515385	1.50307692
B	5	Blank B	E	0.59					
B	6	Sample X1	E	0.688	0.098	CaXy21	76.6923077	0.07669231	1.53384615
B	7	Sample X1	E	0.685	0.095	CaXy21	74.3846154	0.07438462	1.48769231
B	8	Sample X1	E	0.688	0.098	CaXy21	76.6923077	0.07669231	1.53384615
F	9	Blank B	F	0.11					
F	10	Sample X1	F	0.205	0.095	CaGr11	74.3846154	0.07438462	1.48769231
F	11	Sample X1	F	0.204	0.094	CaGr11	73.6153846	0.07361538	1.47230769
F	12	Sample X1	F	0.204	0.094	CaGr11	73.6153846	0.07361538	1.47230769
G	1	Blank B	G	0.265					
G	2	Sample X1	G	0.357	0.092	CaGr12	72.0769231	0.07207692	1.44153846
G	3	Sample X1	G	0.356	0.091	CaGr12	71.3076923	0.07130769	1.42615385
G	4	Sample X1	G	0.356	0.091	CaGr12	71.3076923	0.07130769	1.42615385
G	5	Blank B	H	0.293					
G	6	Sample X1	H	0.386	0.093	CaGr21	72.8461538	0.07284615	1.45692308
G	7	Sample X1	H	0.39	0.097	CaGr21	75.9230769	0.07592308	1.51846154
G	8	Sample X1	H	0.388	0.095	CaGr21	74.3846154	0.07438462	1.48769231
G	9	Blank B	I	0.291					
G	10	Sample X1	I	0.384	0.093	CaGc11	72.8461538	0.07284615	1.45692308
G	11	Sample X1	I	0.387	0.096	CaGc11	75.1538462	0.07515385	1.50307692
G	12	Sample X1	I	0.388	0.097	CaGc11	75.9230769	0.07592308	1.51846154
H	1	Blank B	J	0.291					
H	2	Sample X1	J	0.388	0.097	CaGc21	75.9230769	0.07592308	1.51846154
H	3	Sample X1	J	0.39	0.099	CaGc21	77.4615385	0.07746154	1.54923077
H	4	Sample X1	J	0.389	0.098	CaGc21	76.6923077	0.07669231	1.53384615
H	5	Blank B	K	0.493					
H	6	Sample X1	K	0.589	0.096	CaGl11	75.1538462	0.07515385	1.50307692
H	7	Sample X1	K	0.589	0.096	CaGl11	75.1538462	0.07515385	1.50307692
H	8	Sample X1	K	0.587	0.094	CaGl11	73.6153846	0.07361538	1.47230769
H	9	Blank B	L	0.42					
H	10	Sample X1	L	0.512	0.092	CaGl21	72.0769231	0.07207692	1.44153846
H	11	Sample X1	L	0.517	0.097	CaGl21	75.9230769	0.07592308	1.51846154
H	12	Sample X1	L	0.517	0.097	CaGl21	75.9230769	0.07592308	1.51846154

Appendix 9.19 RCCDRSM FRAP run 19

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.295					
A	2	Sample X1	A	0.39	0.095	CaSu11	74.3846154	0.07438462	2.975384615
A	3	Sample X1	A	0.39	0.095	CaSu11	74.3846154	0.07438462	2.975384615
A	4	Sample X1	A	0.389	0.094	CaSu11	73.6153846	0.07361538	2.944615385
A	5	Blank B	B	0.146					
A	6	Sample X1	B	0.245	0.099	CaFr11	77.4615385	0.07746154	3.098461538
A	7	Sample X1	B	0.245	0.099	CaFr11	77.4615385	0.07746154	3.098461538
A	8	Sample X1	B	0.245	0.099	CaFr11	77.4615385	0.07746154	3.098461538
A	9	Blank B	C	0.18					
A	10	Sample X1	C	0.274	0.094	CaFr12	73.6153846	0.07361538	2.944615385
A	11	Sample X1	C	0.274	0.094	CaFr12	73.6153846	0.07361538	2.944615385
A	12	Sample X1	C	0.273	0.093	CaFr12	72.8461538	0.07284615	2.913846154
B	1	Blank B	D	0.16					
B	2	Sample X1	D	0.255	0.095	CaFr21	74.3846154	0.07438462	2.975384615
B	3	Sample X1	D	0.255	0.095	CaFr21	74.3846154	0.07438462	2.975384615
B	4	Sample X1	D	0.253	0.093	CaFr21	72.8461538	0.07284615	2.913846154
C	1	Blank B	G	0.322					
C	2	Sample X1	G	0.414	0.092	CaXy11	72.0769231	0.07207692	2.883076923
C	3	Sample X1	G	0.414	0.092	CaXy11	72.0769231	0.07207692	2.883076923
C	4	Sample X1	G	0.413	0.091	CaXy11	71.3076923	0.07130769	2.852307692
B	5	Blank B	E	0.383					
B	6	Sample X1	E	0.474	0.091	CaXy12	71.3076923	0.07130769	2.852307692
B	7	Sample X1	E	0.474	0.091	CaXy12	71.3076923	0.07130769	2.852307692
B	8	Sample X1	E	0.475	0.092	CaXy12	72.0769231	0.07207692	2.883076923
B	9	Blank B	F	0.423					
B	10	Sample X1	F	0.63	0.207	CaXy21	160.538462	0.16053846	6.421538462
B	11	Sample X1	F	0.63	0.207	CaXy21	160.538462	0.16053846	6.421538462
B	12	Sample X1	F	0.63	0.207	CaXy21	160.538462	0.16053846	6.421538462
B	9	Blank B	F	0.413					
B	10	Sample X1	F	0.503	0.09	CaGr11	70.5384615	0.07053846	2.821538462
B	11	Sample X1	F	0.503	0.09	CaGr11	70.5384615	0.07053846	2.821538462
B	12	Sample X1	F	0.504	0.091	CaGr11	71.3076923	0.07130769	2.852307692
C	1	Blank B	G	0.419					
C	2	Sample X1	G	0.51	0.091	CaGr12	71.3076923	0.07130769	2.852307692
C	3	Sample X1	G	0.51	0.091	CaGr12	71.3076923	0.07130769	2.852307692
C	4	Sample X1	G	0.51	0.091	CaGr12	71.3076923	0.07130769	2.852307692
C	5	Blank B	H	0.434					

Appendix 9.19 contd.

C	6	Sample X1	H	0.526	0.092	CaGr21	72.0769231	0.07207692	2.883076923
C	7	Sample X1	H	0.529	0.095	CaGr21	74.3846154	0.07438462	2.975384615
C	8	Sample X1	H	0.526	0.092	CaGr21	72.0769231	0.07207692	2.883076923
C	9	Blank B	I	0.481					
C	10	Sample X1	I	0.575	0.094	CaGc11	73.6153846	0.07361538	2.944615385
C	11	Sample X1	I	0.577	0.096	CaGc11	75.1538462	0.07515385	3.006153846
C	12	Sample X1	I	0.575	0.094	CaGc11	73.6153846	0.07361538	2.944615385
D	1	Blank B	J	0.476					
D	2	Sample X1	J	0.567	0.091	CaGc21	71.3076923	0.07130769	2.852307692
D	3	Sample X1	J	0.567	0.091	CaGc21	71.3076923	0.07130769	2.852307692
D	4	Sample X1	J	0.568	0.092	CaGc21	72.0769231	0.07207692	2.883076923
D	5	Blank B	K	0.415					
D	6	Sample X1	K	0.506	0.091	CaGl11	71.3076923	0.07130769	2.852307692
D	7	Sample X1	K	0.505	0.09	CaGl11	70.5384615	0.07053846	2.821538462
D	8	Sample X1	K	0.505	0.09	CaGl11	70.5384615	0.07053846	2.821538462
D	9	Blank B	L	0.407					
D	10	Sample X1	L	0.498	0.091	CaGl21	71.3076923	0.07130769	2.852307692
D	11	Sample X1	L	0.498	0.091	CaGl21	71.3076923	0.07130769	2.852307692
D	12	Sample X1	L	0.498	0.091	CaGl21	71.3076923	0.07130769	2.852307692

Appendix 9.20 RCCDRSM FRAP run 20

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.116					
E	2	Sample X1	A	0.322	0.206	CaSu11	159.769231	0.15976923	6.39076923
E	3	Sample X1	A	0.321	0.205	CaSu11	159	0.159	6.36
E	4	Sample X1	A	0.322	0.206	CaSu11	159.769231	0.15976923	6.39076923
E	5	Blank B	B	0.129					
E	6	Sample X1	B	0.22	0.091	CaFr11	71.3076923	0.07130769	2.85230769
E	7	Sample X1	B	0.222	0.093	CaFr11	72.8461538	0.07284615	2.91384615
E	8	Sample X1	B	0.22	0.091	CaFr11	71.3076923	0.07130769	2.85230769
E	9	Blank B	C	0.123					
E	10	Sample X1	C	0.22	0.097	CaFr12	75.9230769	0.07592308	3.03692308
E	11	Sample X1	C	0.219	0.096	CaFr12	75.1538462	0.07515385	3.00615385
E	12	Sample X1	C	0.219	0.096	CaFr12	75.1538462	0.07515385	3.00615385
F	1	Blank B	D	0.161					
F	2	Sample X1	D	0.257	0.096	CaFr21	75.1538462	0.07515385	3.00615385
F	3	Sample X1	D	0.255	0.094	CaFr21	73.6153846	0.07361538	2.94461538

Appendix 9.20 contd.

F	4	Sample X1	D	0.255	0.094	CaFr21	73.6153846	0.07361538	2.94461538
C	5	Blank B	H	0.101					
C	6	Sample X1	H	0.194	0.093	CaXy11	72.8461538	0.07284615	2.91384615
C	7	Sample X1	H	0.192	0.091	CaXy11	71.3076923	0.07130769	2.85230769
C	8	Sample X1	H	0.192	0.091	CaXy11	71.3076923	0.07130769	2.85230769
F	5	Blank B	E	0.096					
F	6	Sample X1	E	0.312	0.216	CaXy12	167.461538	0.16746154	6.69846154
F	7	Sample X1	E	0.312	0.216	CaXy12	167.461538	0.16746154	6.69846154
F	8	Sample X1	E	0.31	0.214	CaXy12	165.923077	0.16592308	6.63692308
C	1	Blank B	G	0.072					
C	2	Sample X1	G	0.168	0.096	CaXy21	75.1538462	0.07515385	3.00615385
C	3	Sample X1	G	0.167	0.095	CaXy21	74.3846154	0.07438462	2.97538462
C	4	Sample X1	G	0.167	0.095	CaXy21	74.3846154	0.07438462	2.97538462
F	9	Blank B	F	0.081					
F	10	Sample X1	F	0.175	0.096	CaGr11	75.1538462	0.07515385	3.00615385
F	11	Sample X1	F	0.179	0.098	CaGr11	76.6923077	0.07669231	3.06769231
F	12	Sample X1	F	0.177	0.096	CaGr11	75.1538462	0.07515385	3.00615385
G	1	Blank B	G	0.097					
G	2	Sample X1	G	0.194	0.097	CaGr12	75.9230769	0.07592308	3.03692308
G	3	Sample X1	G	0.194	0.097	CaGr12	75.9230769	0.07592308	3.03692308
G	4	Sample X1	G	0.194	0.097	CaGr12	75.9230769	0.07592308	3.03692308
G	5	Blank B	H	0.211					
G	6	Sample X1	H	0.981	0.77	CaGr21	593.615385	0.59361538	23.7446154
G	7	Sample X1	H	0.981	0.77	CaGr21	593.615385	0.59361538	23.7446154
G	8	Sample X1	H	0.979	0.768	CaGr21	592.076923	0.59207692	23.6830769
G	9	Blank B	I	0.091					
G	10	Sample X1	I	0.183	0.093	CaGc11	72.8461538	0.07284615	2.91384615
G	11	Sample X1	I	0.185	0.094	CaGc11	73.6153846	0.07361538	2.94461538
G	12	Sample X1	I	0.184	0.093	CaGc11	72.8461538	0.07284615	2.91384615
H	1	Blank B	J	0.13					
H	2	Sample X1	J	0.224	0.094	CaGc21	73.6153846	0.07361538	2.94461538
H	3	Sample X1	J	0.223	0.093	CaGc21	72.8461538	0.07284615	2.91384615
H	4	Sample X1	J	0.223	0.093	CaGc21	72.8461538	0.07284615	2.91384615
H	5	Blank B	K	0.384					
H	6	Sample X1	K	0.477	0.093	CaGl11	72.8461538	0.07284615	2.91384615
H	7	Sample X1	K	0.479	0.095	CaGl11	74.3846154	0.07438462	2.97538462
H	8	Sample X1	K	0.479	0.095	CaGl11	74.3846154	0.07438462	2.97538462
H	9	Blank B	L	0.326					
H	10	Sample X1	L	0.425	0.099	CaGl21	77.4615385	0.07746154	3.09846154
H	11	Sample X1	L	0.425	0.099	CaGl21	77.4615385	0.07746154	3.09846154
H	12	Sample X1	L	0.421	0.095	CaGl21	74.3846154	0.07438462	2.97538462

Appendix 9.21 RCCDRSM FRAP run 21

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.625					
D	2	Sample X1	J	0.721	0.096	CaSu11	75.1538462	0.07515385	1.12730769
D	3	Sample X1	J	0.721	0.096	CaSu11	75.1538462	0.07515385	1.12730769
D	4	Sample X1	J	0.723	0.098	CaSu11	76.6923077	0.07669231	1.15038462
A	1	Blank B	A	0.781					
A	2	Sample X1	A	0.875	0.094	CaFr11	73.6153846	0.07361538	1.10423077
A	3	Sample X1	A	0.876	0.095	CaFr11	74.3846154	0.07438462	1.11576923
A	4	Sample X1	A	0.875	0.094	CaFr11	73.6153846	0.07361538	1.10423077
A	5	Blank B	B	0.696					
A	6	Sample X1	B	0.792	0.096	CaFr12	75.1538462	0.07515385	1.12730769
A	7	Sample X1	B	0.792	0.096	CaFr12	75.1538462	0.07515385	1.12730769
A	8	Sample X1	B	0.791	0.095	CaFr12	74.3846154	0.07438462	1.11576923
A	9	Blank B	C	0.67					
A	10	Sample X1	C	0.762	0.092	CaFr21	72.0769231	0.07207692	1.08115385
A	11	Sample X1	C	0.763	0.093	CaFr21	72.8461538	0.07284615	1.09269231
A	12	Sample X1	C	0.762	0.092	CaFr21	72.0769231	0.07207692	1.08115385
B	1	Blank B	D	0.642					
B	2	Sample X1	D	0.738	0.096	CaXy11	75.1538462	0.07515385	1.12730769
B	3	Sample X1	D	0.737	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	4	Sample X1	D	0.737	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	5	Blank B	E	0.637					
B	6	Sample X1	E	0.734	0.097	CaXy12	75.9230769	0.07592308	1.13884615
B	7	Sample X1	E	0.733	0.096	CaXy12	75.1538462	0.07515385	1.12730769
B	8	Sample X1	E	0.733	0.096	CaXy12	75.1538462	0.07515385	1.12730769
B	9	Blank B	F	0.66					
B	10	Sample X1	F	0.757	0.097	CaXy21	75.9230769	0.07592308	1.13884615
B	11	Sample X1	F	0.757	0.097	CaXy21	75.9230769	0.07592308	1.13884615
B	12	Sample X1	F	0.755	0.095	CaXy21	74.3846154	0.07438462	1.11576923
C	1	Blank B	G	0.615					
C	2	Sample X1	G	0.706	0.091	CaGr11	71.3076923	0.07130769	1.06961538
C	3	Sample X1	G	0.707	0.092	CaGr11	72.0769231	0.07207692	1.08115385
C	4	Sample X1	G	0.707	0.092	CaGr11	72.0769231	0.07207692	1.08115385
C	5	Blank B	H	0.583					
C	6	Sample X1	H	0.673	0.09	CaGr12	70.5384615	0.07053846	1.05807692
C	7	Sample X1	H	0.674	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	8	Sample X1	H	0.674	0.091	CaGr12	71.3076923	0.07130769	1.06961538
C	9	Blank B	I	0.571					

Appendix 9.21 contd.

C	10	Sample X1	I	0.661	0.09	CaGr21	70.5384615	0.07053846	1.05807692
C	11	Sample X1	I	0.662	0.091	CaGr21	71.3076923	0.07130769	1.06961538
C	12	Sample X1	I	0.662	0.091	CaGr21	71.3076923	0.07130769	1.06961538
D	5	Blank B	K	0.533					
D	6	Sample X1	K	0.624	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	7	Sample X1	K	0.624	0.091	CaGc11	71.3076923	0.07130769	1.06961538
D	8	Sample X1	K	0.625	0.092	CaGc11	72.0769231	0.07207692	1.08115385
D	9	Blank B	L	0.475					
D	10	Sample X1	L	0.573	0.098	CaGc21	76.6923077	0.07669231	1.15038462
D	11	Sample X1	L	0.573	0.098	CaGc21	76.6923077	0.07669231	1.15038462
D	12	Sample X1	L	0.571	0.096	CaGc21	75.1538462	0.07515385	1.12730769
E	1	Blank B	M	0.495					
E	2	Sample X1	M	0.592	0.097	CaGl11	75.9230769	0.07592308	1.13884615
E	3	Sample X1	M	0.59	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	4	Sample X1	M	0.59	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	5	Blank B	N	0.479					
E	6	Sample X1	N	0.575	0.096	CaGl21	75.1538462	0.07515385	1.12730769
E	7	Sample X1	N	0.574	0.095	CaGl21	74.3846154	0.07438462	1.11576923
E	8	Sample X1	N	0.575	0.096	CaGl21	75.1538462	0.07515385	1.12730769

Appendix 9.22 RCCDRSM FRAP run 22

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.451					
A	2	Sample X1	A	0.977	0.526	CaSu11	405.9230769	0.405923077	20.29615385
A	3	Sample X1	A	0.977	0.526	CaSu11	405.9230769	0.405923077	20.29615385
A	4	Sample X1	A	0.978	0.527	CaSu11	406.6923077	0.406692308	20.33461538
A	5	Blank B	B	0.248					
A	6	Sample X1	B	0.573	0.325	CaFr11	251.3076923	0.251307692	12.56538462
A	7	Sample X1	B	0.575	0.327	CaFr11	252.8461538	0.252846154	12.64230769
A	8	Sample X1	B	0.573	0.325	CaFr11	251.3076923	0.251307692	12.56538462
A	9	Blank B	C	0.263					
A	10	Sample X1	C	0.358	0.095	CaFr12	74.38461538	0.074384615	3.719230769
A	11	Sample X1	C	0.36	0.097	CaFr12	75.92307692	0.075923077	3.796153846
A	12	Sample X1	C	0.358	0.095	CaFr12	74.38461538	0.074384615	3.719230769
B	1	Blank B	D	0.233					
B	2	Sample X1	D	0.329	0.096	CaFr21	75.15384615	0.075153846	3.757692308
B	3	Sample X1	D	0.33	0.097	CaFr21	75.92307692	0.075923077	3.796153846

Appendix 9.22 contd.

B	4	Sample X1	D	0.33	0.097	CaFr21	75.92307692	0.075923077	3.796153846
C	9	Blank B	I	0.596					
C	10	Sample X1	I	0.689	0.093	CaXy11	72.84615385	0.072846154	3.642307692
C	11	Sample X1	I	0.691	0.095	CaXy11	74.38461538	0.074384615	3.719230769
C	12	Sample X1	I	0.691	0.095	CaXy11	74.38461538	0.074384615	3.719230769
B	5	Blank B	E	0.591					
B	6	Sample X1	E	0.683	0.092	CaXy12	72.07692308	0.072076923	3.603846154
B	7	Sample X1	E	0.684	0.093	CaXy12	72.84615385	0.072846154	3.642307692
B	8	Sample X1	E	0.685	0.094	CaXy12	73.61538462	0.073615385	3.680769231
C	5	Blank B	H	0.579					
C	6	Sample X1	H	0.698	0.119	CaXy21	92.84615385	0.092846154	4.642307692
C	7	Sample X1	H	0.696	0.117	CaXy21	91.30769231	0.091307692	4.565384615
C	8	Sample X1	H	0.698	0.119	CaXy21	92.84615385	0.092846154	4.642307692
B	9	Blank B	F	0.413					
B	10	Sample X1	F	0.511	0.098	CaGr11	76.69230769	0.076692308	3.834615385
B	11	Sample X1	F	0.509	0.096	CaGr11	75.15384615	0.075153846	3.757692308
B	12	Sample X1	F	0.509	0.096	CaGr11	75.15384615	0.075153846	3.757692308
C	1	Blank B	G	0.454					
C	2	Sample X1	G	0.553	0.099	CaGr12	77.46153846	0.077461538	3.873076923
C	3	Sample X1	G	0.553	0.099	CaGr12	77.46153846	0.077461538	3.873076923
C	4	Sample X1	G	0.552	0.098	CaGr12	76.69230769	0.076692308	3.834615385
C	5	Blank B	H	0.417					
C	6	Sample X1	H	0.836	0.419	CaGr21	323.6153846	0.323615385	16.18076923
C	7	Sample X1	H	0.837	0.42	CaGr21	324.3846154	0.324384615	16.21923077
C	8	Sample X1	H	0.837	0.42	CaGr21	324.3846154	0.324384615	16.21923077
C	9	Blank B	I	0.571					
C	10	Sample X1	I	0.85	0.279	CaGc11	215.9230769	0.215923077	10.79615385
C	11	Sample X1	I	0.85	0.279	CaGc11	215.9230769	0.215923077	10.79615385
C	12	Sample X1	I	0.85	0.279	CaGc11	215.9230769	0.215923077	10.79615385
D	1	Blank B	J	0.521					
D	2	Sample X1	J	0.702	0.181	CaGc21	140.5384615	0.140538462	7.026923077
D	3	Sample X1	J	0.705	0.184	CaGc21	142.8461538	0.142846154	7.142307692
D	4	Sample X1	J	0.702	0.181	CaGc21	140.5384615	0.140538462	7.026923077
D	5	Blank B	K	0.409					
D	6	Sample X1	K	0.678	0.269	CaGl11	208.2307692	0.208230769	10.41153846
D	7	Sample X1	K	0.674	0.265	CaGl11	205.1538462	0.205153846	10.25769231
D	8	Sample X1	K	0.674	0.265	CaGl11	205.1538462	0.205153846	10.25769231
D	9	Blank B	L	0.406					
D	10	Sample X1	L	0.769	0.363	CaGl21	280.5384615	0.280538462	14.02692308
D	11	Sample X1	L	0.766	0.36	CaGl21	278.2307692	0.278230769	13.91153846
D	12	Sample X1	L	0.766	0.36	CaGl21	278.2307692	0.278230769	13.91153846

Appendix 9.23 RCCDRSM FRAP run 23

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.554					
E	2	Sample X1	A	0.646	0.092	CaSu11	72.07692308	0.072076923	1.081154
E	3	Sample X1	A	0.647	0.093	CaSu11	72.84615385	0.072846154	1.092692
E	4	Sample X1	A	0.647	0.093	CaSu11	72.84615385	0.072846154	1.092692
E	5	Blank B	B	0.513					
E	6	Sample X1	B	0.993	0.48	CaFr11	370.5384615	0.370538462	5.558077
E	7	Sample X1	B	0.993	0.48	CaFr11	370.5384615	0.370538462	5.558077
E	8	Sample X1	B	0.993	0.48	CaFr11	370.5384615	0.370538462	5.558077
E	9	Blank B	C	0.539					
E	10	Sample X1	C	0.633	0.091	CaFr12	71.30769231	0.071307692	1.069615
E	11	Sample X1	C	0.636	0.091	CaFr12	71.30769231	0.071307692	1.069615
E	12	Sample X1	C	0.632	0.092	CaFr12	72.07692308	0.072076923	1.081154
F	1	Blank B	D	0.518					
F	2	Sample X1	D	0.616	0.098	CaFr21	76.69230769	0.076692308	1.150385
F	3	Sample X1	D	0.616	0.098	CaFr21	76.69230769	0.076692308	1.150385
F	4	Sample X1	D	0.614	0.096	CaFr21	75.15384615	0.075153846	1.127308
D	1	Blank B	J	0.567					
D	2	Sample X1	J	0.681	0.114	CaXy11	89	0.089	1.335
D	3	Sample X1	J	0.679	0.112	CaXy11	87.46153846	0.087461538	1.311923
D	4	Sample X1	J	0.679	0.112	CaXy11	87.46153846	0.087461538	1.311923
F	5	Blank B	E	0.564					
F	6	Sample X1	E	0.658	0.094	CaXy12	73.61538462	0.073615385	1.104231
F	7	Sample X1	E	0.661	0.097	CaXy12	75.92307692	0.075923077	1.138846
F	8	Sample X1	E	0.658	0.094	CaXy12	73.61538462	0.073615385	1.104231
C	9	Blank B	I	0.558					
C	10	Sample X1	I	0.656	0.098	CaXy21	76.69230769	0.076692308	1.150385
C	11	Sample X1	I	0.655	0.097	CaXy21	75.92307692	0.075923077	1.138846
C	12	Sample X1	I	0.655	0.097	CaXy21	75.92307692	0.075923077	1.138846
F	9	Blank B	F	0.591					
F	10	Sample X1	F	0.685	0.094	CaGr11	73.61538462	0.073615385	1.104231
F	11	Sample X1	F	0.686	0.095	CaGr11	74.38461538	0.074384615	1.115769
F	12	Sample X1	F	0.686	0.095	CaGr11	74.38461538	0.074384615	1.115769
G	1	Blank B	G	0.578					
G	2	Sample X1	G	0.671	0.093	CaGr12	72.84615385	0.072846154	1.092692
G	3	Sample X1	G	0.671	0.093	CaGr12	72.84615385	0.072846154	1.092692
G	4	Sample X1	G	0.67	0.092	CaGr12	72.07692308	0.072076923	1.081154
G	5	Blank B	H	0.607					

Appendix 9.23 contd.

G	6	Sample X1	H	0.702	0.095	CaGr21	74.38461538	0.074384615	1.115769
G	7	Sample X1	H	0.703	0.096	CaGr21	75.15384615	0.075153846	1.127308
G	8	Sample X1	H	0.703	0.096	CaGr21	75.15384615	0.075153846	1.127308
G	9	Blank B	I	0.675					
G	10	Sample X1	I	0.768	0.093	CaGc11	72.84615385	0.072846154	1.092692
G	11	Sample X1	I	0.767	0.092	CaGc11	72.07692308	0.072076923	1.081154
G	12	Sample X1	I	0.768	0.093	CaGc11	72.84615385	0.072846154	1.092692
H	1	Blank B	J	0.51					
H	2	Sample X1	J	0.605	0.095	CaGc21	74.38461538	0.074384615	1.115769
H	3	Sample X1	J	0.603	0.093	CaGc21	72.84615385	0.072846154	1.092692
H	4	Sample X1	J	0.603	0.093	CaGc21	72.84615385	0.072846154	1.092692
H	5	Blank B	K	0.489					
H	6	Sample X1	K	0.581	0.092	CaGl11	72.07692308	0.072076923	1.081154
H	7	Sample X1	K	0.58	0.091	CaGl11	71.30769231	0.071307692	1.069615
H	8	Sample X1	K	0.58	0.091	CaGl11	71.30769231	0.071307692	1.069615
H	9	Blank B	L	0.446					
H	10	Sample X1	L	0.57	0.124	CaGl21	96.69230769	0.096692308	1.450385
H	11	Sample X1	L	0.568	0.122	CaGl21	95.15384615	0.095153846	1.427308
H	12	Sample X1	L	0.571	0.125	CaGl21	97.46153846	0.097461538	1.461923

Appendix 9.24 RCCDRSM FRAP run 24

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
D	1	Blank B	J	0.283					
D	2	Sample X1	J	0.374	0.091	CaSu11	71.3076923	0.07130769	1.06961538
D	3	Sample X1	J	0.375	0.092	CaSu11	72.0769231	0.07207692	1.08115385
D	4	Sample X1	J	0.375	0.092	CaSu11	72.0769231	0.07207692	1.08115385
A	1	Blank B	A	0.051					
A	2	Sample X1	A	0.449	0.398	CaFr11	307.461538	0.30746154	4.61192308
A	3	Sample X1	A	0.451	0.4	CaFr11	309	0.309	4.635
A	4	Sample X1	A	0.451	0.4	CaFr11	309	0.309	4.635
A	5	Blank B	B	0.038					
A	6	Sample X1	B	0.13	0.092	CaFr12	72.0769231	0.07207692	1.08115385
A	7	Sample X1	B	0.134	0.096	CaFr12	75.1538462	0.07515385	1.12730769
A	8	Sample X1	B	0.13	0.092	CaFr12	72.0769231	0.07207692	1.08115385
A	9	Blank B	C	0.071					
A	10	Sample X1	C	0.161	0.09	CaFr21	70.5384615	0.07053846	1.05807692
A	11	Sample X1	C	0.161	0.09	CaFr21	70.5384615	0.07053846	1.05807692

Appendix 9.24 RCCDRSM FRAP run 24

A	12	Sample X1	C	0.162	0.091	CaFr21	71.3076923	0.07130769	1.06961538
B	1	Blank B	D	0.091					
B	2	Sample X1	D	0.186	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	3	Sample X1	D	0.186	0.095	CaXy11	74.3846154	0.07438462	1.11576923
B	4	Sample X1	D	0.187	0.096	CaXy11	75.1538462	0.07515385	1.12730769
B	5	Blank B	E	0.086					
B	6	Sample X1	E	0.178	0.092	CaXy12	72.0769231	0.07207692	1.08115385
B	7	Sample X1	E	0.178	0.092	CaXy12	72.0769231	0.07207692	1.08115385
B	8	Sample X1	E	0.18	0.094	CaXy12	73.6153846	0.07361538	1.10423077
B	9	Blank B	F	0.019					
B	10	Sample X1	F	0.112	0.093	CaXy21	72.8461538	0.07284615	1.09269231
B	11	Sample X1	F	0.114	0.095	CaXy21	74.3846154	0.07438462	1.11576923
B	12	Sample X1	F	0.114	0.095	CaXy21	74.3846154	0.07438462	1.11576923
C	1	Blank B	G	0.011					
C	2	Sample X1	G	0.108	0.097	CaGr11	75.9230769	0.07592308	1.13884615
C	3	Sample X1	G	0.11	0.099	CaGr11	77.4615385	0.07746154	1.16192308
C	4	Sample X1	G	0.11	0.099	CaGr11	77.4615385	0.07746154	1.16192308
C	5	Blank B	H	0.028					
C	6	Sample X1	H	0.124	0.096	CaGr12	75.1538462	0.07515385	1.12730769
C	7	Sample X1	H	0.122	0.094	CaGr12	73.6153846	0.07361538	1.10423077
C	8	Sample X1	H	0.122	0.094	CaGr12	73.6153846	0.07361538	1.10423077
C	9	Blank B	I	0.012					
C	10	Sample X1	I	0.104	0.092	CaGr21	72.0769231	0.07207692	1.08115385
C	11	Sample X1	I	0.105	0.093	CaGr21	72.8461538	0.07284615	1.09269231
C	12	Sample X1	I	0.105	0.093	CaGr21	72.8461538	0.07284615	1.09269231
D	5	Blank B	K	0.017					
D	6	Sample X1	K	0.116	0.099	CaGc11	77.4615385	0.07746154	1.16192308
D	7	Sample X1	K	0.116	0.099	CaGc11	77.4615385	0.07746154	1.16192308
D	8	Sample X1	K	0.116	0.099	CaGc11	77.4615385	0.07746154	1.16192308
D	9	Blank B	L	0.014					
D	10	Sample X1	L	0.111	0.097	CaGc21	75.9230769	0.07592308	1.13884615
D	11	Sample X1	L	0.111	0.097	CaGc21	75.9230769	0.07592308	1.13884615
D	12	Sample X1	L	0.109	0.095	CaGc21	74.3846154	0.07438462	1.11576923
E	1	Blank B	M	0.019					
E	2	Sample X1	M	0.113	0.094	CaGl11	73.6153846	0.07361538	1.10423077
E	3	Sample X1	M	0.114	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	4	Sample X1	M	0.114	0.095	CaGl11	74.3846154	0.07438462	1.11576923
E	5	Blank B	N	0.016					
E	6	Sample X1	N	0.113	0.097	CaGl21	75.9230769	0.07592308	1.13884615
E	7	Sample X1	N	0.111	0.095	CaGl21	74.3846154	0.07438462	1.11576923
E	8	Sample X1	N	0.113	0.097	CaGl21	75.9230769	0.07592308	1.13884615

Appendix 9.25 RCCDRSM FRAP run 25

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.558					
A	2	Sample X1	A	0.744	0.186	CaSu11	144.384615	0.14438462	4.331538462
A	3	Sample X1	A	0.742	0.184	CaSu11	142.846154	0.14284615	4.285384615
A	4	Sample X1	A	0.744	0.186	CaSu11	144.384615	0.14438462	4.331538462
A	5	Blank B	B	0.264					
A	6	Sample X1	B	0.834	0.57	CaFr11	439.769231	0.43976923	13.19307692
A	7	Sample X1	B	0.834	0.57	CaFr11	439.769231	0.43976923	13.19307692
A	8	Sample X1	B	0.836	0.572	CaFr11	441.307692	0.44130769	13.23923077
A	9	Blank B	C	0.282					
A	10	Sample X1	C	0.383	0.101	CaFr12	79	0.079	2.37
A	11	Sample X1	C	0.385	0.103	CaFr12	80.5384615	0.08053846	2.416153846
A	12	Sample X1	C	0.383	0.101	CaFr12	79	0.079	2.37
B	1	Blank B	D	0.248					
B	2	Sample X1	D	0.344	0.096	CaFr21	75.1538462	0.07515385	2.254615385
B	3	Sample X1	D	0.344	0.096	CaFr21	75.1538462	0.07515385	2.254615385
B	4	Sample X1	D	0.345	0.097	CaFr21	75.9230769	0.07592308	2.277692308
D	5	Blank B	K	0.263					
D	6	Sample X1	K	0.358	0.095	CaXy11	74.3846154	0.07438462	2.231538462
D	7	Sample X1	K	0.356	0.093	CaXy11	72.8461538	0.07284615	2.185384615
D	8	Sample X1	K	0.358	0.095	CaXy11	74.3846154	0.07438462	2.231538462
B	5	Blank B	E	0.227					
B	6	Sample X1	E	0.578	0.351	CaXy12	271.307692	0.27130769	8.139230769
B	7	Sample X1	E	0.579	0.352	CaXy12	272.076923	0.27207692	8.162307692
B	8	Sample X1	E	0.577	0.35	CaXy12	270.538462	0.27053846	8.116153846
D	1	Blank B	J	0.248					
D	2	Sample X1	J	0.345	0.097	CaXy21	75.9230769	0.07592308	2.277692308
D	3	Sample X1	J	0.344	0.096	CaXy21	75.1538462	0.07515385	2.254615385
D	4	Sample X1	J	0.345	0.097	CaXy21	75.9230769	0.07592308	2.277692308
B	9	Blank B	F	0.279					
B	10	Sample X1	F	0.373	0.094	CaGr11	73.6153846	0.07361538	2.208461538
B	11	Sample X1	F	0.373	0.094	CaGr11	73.6153846	0.07361538	2.208461538
B	12	Sample X1	F	0.37	0.091	CaGr11	71.3076923	0.07130769	2.139230769
C	1	Blank B	G	0.245					
C	2	Sample X1	G	0.41	0.165	CaGr12	128.230769	0.12823077	3.846923077
C	3	Sample X1	G	0.407	0.162	CaGr12	125.923077	0.12592308	3.777692308
C	4	Sample X1	G	0.41	0.165	CaGr12	128.230769	0.12823077	3.846923077
C	5	Blank B	H	0.209					

Appendix 9.25 contd.

C	6	Sample X1	H	0.303	0.094	CaGr21	73.6153846	0.07361538	2.208461538
C	7	Sample X1	H	0.303	0.094	CaGr21	73.6153846	0.07361538	2.208461538
C	8	Sample X1	H	0.303	0.094	CaGr21	73.6153846	0.07361538	2.208461538
C	9	Blank B	I	0.264					
C	10	Sample X1	I	0.355	0.091	CaGc11	71.3076923	0.07130769	2.139230769
C	11	Sample X1	I	0.355	0.091	CaGc11	71.3076923	0.07130769	2.139230769
C	12	Sample X1	I	0.356	0.092	CaGc11	72.0769231	0.07207692	2.162307692
D	1	Blank B	J	0.256					
D	2	Sample X1	J	0.348	0.092	CaGc21	72.0769231	0.07207692	2.162307692
D	3	Sample X1	J	0.348	0.092	CaGc21	72.0769231	0.07207692	2.162307692
D	4	Sample X1	J	0.348	0.092	CaGc21	72.0769231	0.07207692	2.162307692
D	5	Blank B	K	0.233					
D	6	Sample X1	K	0.367	0.134	CaGl11	104.384615	0.10438462	3.131538462
D	7	Sample X1	K	0.366	0.133	CaGl11	103.615385	0.10361538	3.108461538
D	8	Sample X1	K	0.367	0.134	CaGl11	104.384615	0.10438462	3.131538462
D	9	Blank B	L	0.231					
D	10	Sample X1	L	0.327	0.096	CaGl21	75.1538462	0.07515385	2.254615385
D	11	Sample X1	L	0.329	0.098	CaGl21	76.6923077	0.07669231	2.300769231
D	12	Sample X1	L	0.328	0.097	CaGl21	75.9230769	0.07592308	2.277692308

Appendix 9.26 RCCDRSM FRAP run 26

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.665					
E	2	Sample X1	A	0.756	0.091	CaSu11	71.3076923	0.07130769	2.13923077
E	3	Sample X1	A	0.756	0.091	CaSu11	71.3076923	0.07130769	2.13923077
E	4	Sample X1	A	0.756	0.091	CaSu11	71.3076923	0.07130769	2.13923077
E	5	Blank B	B	0.585					
E	6	Sample X1	B	0.677	0.092	CaFr11	72.0769231	0.07207692	2.16230769
E	7	Sample X1	B	0.678	0.093	CaFr11	72.8461538	0.07284615	2.18538462
E	8	Sample X1	B	0.677	0.092	CaFr11	72.0769231	0.07207692	2.16230769
E	9	Blank B	C	0.512					
E	10	Sample X1	C	0.604	0.092	CaFr12	72.0769231	0.07207692	2.16230769
E	11	Sample X1	C	0.604	0.092	CaFr12	72.0769231	0.07207692	2.16230769
E	12	Sample X1	C	0.605	0.093	CaFr12	72.8461538	0.07284615	2.18538462
F	1	Blank B	D	0.565					
F	2	Sample X1	D	0.663	0.098	CaFr21	76.6923077	0.07669231	2.30076923
F	3	Sample X1	D	0.663	0.098	CaFr21	76.6923077	0.07669231	2.30076923

Appendix 9.26 RCCDRSM FRAP run 26

F	4	Sample X1	D	0.662	0.097	CaFr21	75.9230769	0.07592308	2.27769231
D	9	Blank B	L	0.555					
D	10	Sample X1	L	0.646	0.091	CaXy11	71.3076923	0.07130769	2.13923077
D	11	Sample X1	L	0.647	0.092	CaXy11	72.0769231	0.07207692	2.16230769
D	12	Sample X1	L	0.646	0.091	CaXy11	71.3076923	0.07130769	2.13923077
F	5	Blank B	E	0.556					
F	6	Sample X1	E	0.659	0.103	CaXy12	80.5384615	0.08053846	2.41615385
F	7	Sample X1	E	0.648	0.102	CaXy12	79.7692308	0.07976923	2.39307692
F	8	Sample X1	E	0.639	0.103	CaXy12	80.5384615	0.08053846	2.41615385
D	5	Blank B	K	0.534					
D	6	Sample X1	K	0.63	0.096	CaXy21	75.1538462	0.07515385	2.25461538
D	7	Sample X1	K	0.628	0.094	CaXy21	73.6153846	0.07361538	2.20846154
D	8	Sample X1	K	0.63	0.096	CaXy21	75.1538462	0.07515385	2.25461538
F	9	Blank B	F	0.543					
F	10	Sample X1	F	0.638	0.095	CaGr11	74.3846154	0.07438462	2.23153846
F	11	Sample X1	F	0.638	0.095	CaGr11	74.3846154	0.07438462	2.23153846
F	12	Sample X1	F	0.637	0.094	CaGr11	73.6153846	0.07361538	2.20846154
G	1	Blank B	G	0.553					
G	2	Sample X1	G	0.644	0.091	CaGr12	71.3076923	0.07130769	2.13923077
G	3	Sample X1	G	0.644	0.091	CaGr12	71.3076923	0.07130769	2.13923077
G	4	Sample X1	G	0.644	0.091	CaGr12	71.3076923	0.07130769	2.13923077
G	5	Blank B	H	0.508					
G	6	Sample X1	H	0.607	0.099	CaGr21	77.4615385	0.07746154	2.32384615
G	7	Sample X1	H	0.607	0.099	CaGr21	77.4615385	0.07746154	2.32384615
G	8	Sample X1	H	0.606	0.098	CaGr21	76.6923077	0.07669231	2.30076923
G	9	Blank B	I	0.515					
G	10	Sample X1	I	0.612	0.097	CaGc11	75.9230769	0.07592308	2.27769231
G	11	Sample X1	I	0.612	0.097	CaGc11	75.9230769	0.07592308	2.27769231
G	12	Sample X1	I	0.612	0.097	CaGc11	75.9230769	0.07592308	2.27769231
H	1	Blank B	J	0.558					
H	2	Sample X1	J	0.655	0.097	CaGc21	75.9230769	0.07592308	2.27769231
H	3	Sample X1	J	0.653	0.095	CaGc21	74.3846154	0.07438462	2.23153846
H	4	Sample X1	J	0.655	0.097	CaGc21	75.9230769	0.07592308	2.27769231
H	5	Blank B	K	0.516					
H	6	Sample X1	K	0.612	0.096	CaGl11	75.1538462	0.07515385	2.25461538
H	7	Sample X1	K	0.615	0.099	CaGl11	77.4615385	0.07746154	2.32384615
H	8	Sample X1	K	0.615	0.099	CaGl11	77.4615385	0.07746154	2.32384615
H	9	Blank B	L	0.57					
H	10	Sample X1	L	0.666	0.096	CaGl21	75.1538462	0.07515385	2.25461538
H	11	Sample X1	L	0.666	0.096	CaGl21	75.1538462	0.07515385	2.25461538
H	12	Sample X1	L	0.664	0.094	CaGl21	73.6153846	0.07361538	2.20846154

Appendix 9.27 RCCDRSM FRAP run 27

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.551					
A	2	Sample X1	A	0.644	0.093	CaSu11	72.84615385	0.072846154	2.18538462
A	3	Sample X1	A	0.643	0.092	CaSu11	72.07692308	0.072076923	2.16230769
A	4	Sample X1	A	0.644	0.093	CaSu11	72.84615385	0.072846154	2.18538462
A	5	Blank B	B	0.486					
A	6	Sample X1	B	0.578	0.092	CaFr11	72.07692308	0.072076923	2.16230769
A	7	Sample X1	B	0.578	0.092	CaFr11	72.07692308	0.072076923	2.16230769
A	8	Sample X1	B	0.579	0.093	CaFr11	72.84615385	0.072846154	2.18538462
A	9	Blank B	C	0.515					
A	10	Sample X1	C	0.608	0.093	CaFr12	72.84615385	0.072846154	2.18538462
A	11	Sample X1	C	0.609	0.094	CaFr12	73.61538462	0.073615385	2.20846154
A	12	Sample X1	C	0.608	0.093	CaFr12	72.84615385	0.072846154	2.18538462
B	1	Blank B	D	0.515					
B	2	Sample X1	D	0.61	0.095	CaFr21	74.38461538	0.074384615	2.23153846
B	3	Sample X1	D	0.609	0.094	CaFr21	73.61538462	0.073615385	2.20846154
B	4	Sample X1	D	0.609	0.094	CaFr21	73.61538462	0.073615385	2.20846154
E	1	Blank B	M	0.491					
E	2	Sample X1	M	0.585	0.094	CaXy11	73.61538462	0.073615385	2.20846154
E	3	Sample X1	M	0.585	0.094	CaXy11	73.61538462	0.073615385	2.20846154
E	4	Sample X1	M	0.584	0.093	CaXy11	72.84615385	0.072846154	2.18538462
B	5	Blank B	E	0.429					
B	6	Sample X1	E	0.553	0.124	CaXy12	96.69230769	0.096692308	2.90076923
B	7	Sample X1	E	0.549	0.12	CaXy12	93.61538462	0.093615385	2.80846154
B	8	Sample X1	E	0.549	0.12	CaXy12	93.61538462	0.093615385	2.80846154
D	9	Blank B	L	0.475					
D	10	Sample X1	L	0.568	0.093	CaXy21	72.84615385	0.072846154	2.18538462
D	11	Sample X1	L	0.568	0.093	CaXy21	72.84615385	0.072846154	2.18538462
D	12	Sample X1	L	0.569	0.094	CaXy21	73.61538462	0.073615385	2.20846154
B	9	Blank B	F	0.63					
B	10	Sample X1	F	0.724	0.094	CaGr11	73.61538462	0.073615385	2.20846154
B	11	Sample X1	F	0.724	0.094	CaGr11	73.61538462	0.073615385	2.20846154
B	12	Sample X1	F	0.723	0.093	CaGr11	72.84615385	0.072846154	2.18538462
C	1	Blank B	G	0.626					
C	2	Sample X1	G	0.719	0.093	CaGr12	72.84615385	0.072846154	2.18538462
C	3	Sample X1	G	0.719	0.093	CaGr12	72.84615385	0.072846154	2.18538462
C	4	Sample X1	G	0.719	0.093	CaGr12	72.84615385	0.072846154	2.18538462
C	5	Blank B	H	0.604					

Appendix 9.27 contd.

C	6	Sample X1	H	0.696	0.092	CaGr21	72.07692308	0.072076923	2.16230769
C	7	Sample X1	H	0.696	0.092	CaGr21	72.07692308	0.072076923	2.16230769
C	8	Sample X1	H	0.696	0.092	CaGr21	72.07692308	0.072076923	2.16230769
C	9	Blank B	I	0.569					
C	10	Sample X1	I	0.663	0.094	CaGc11	73.61538462	0.073615385	2.20846154
C	11	Sample X1	I	0.663	0.094	CaGc11	73.61538462	0.073615385	2.20846154
C	12	Sample X1	I	0.665	0.096	CaGc11	75.15384615	0.075153846	2.25461538
D	1	Blank B	J	0.387					
D	2	Sample X1	J	0.487	0.1	CaGc21	78.23076923	0.078230769	2.34692308
D	3	Sample X1	J	0.485	0.098	CaGc21	76.69230769	0.076692308	2.30076923
D	4	Sample X1	J	0.487	0.1	CaGc21	78.23076923	0.078230769	2.34692308
D	5	Blank B	K	0.349					
D	6	Sample X1	K	0.441	0.092	CaGl11	72.07692308	0.072076923	2.16230769
D	7	Sample X1	K	0.441	0.092	CaGl11	72.07692308	0.072076923	2.16230769
D	8	Sample X1	K	0.441	0.092	CaGl11	72.07692308	0.072076923	2.16230769
D	9	Blank B	L	0.321					
D	10	Sample X1	L	0.436	0.115	CaGl21	89.76923077	0.089769231	2.69307692
D	11	Sample X1	L	0.436	0.115	CaGl21	89.76923077	0.089769231	2.69307692
D	12	Sample X1	L	0.436	0.115	CaGl21	89.76923077	0.089769231	2.69307692

Appendix 9.28 RCCDRSM FRAP run 28

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.539					
E	2	Sample X1	A	0.634	0.095	CaSu11	74.3846154	0.07438462	2.231538462
E	3	Sample X1	A	0.636	0.097	CaSu11	75.9230769	0.07592308	2.277692308
E	4	Sample X1	A	0.634	0.095	CaSu11	74.3846154	0.07438462	2.231538462
E	5	Blank B	B	0.505					
E	6	Sample X1	B	0.799	0.294	CaFr11	227.461538	0.22746154	6.823846154
E	7	Sample X1	B	0.8	0.295	CaFr11	228.230769	0.22823077	6.846923077
E	8	Sample X1	B	0.799	0.294	CaFr11	227.461538	0.22746154	6.823846154
E	9	Blank B	C	0.574					
E	10	Sample X1	C	0.67	0.096	CaFr12	75.1538462	0.07515385	2.254615385
E	11	Sample X1	C	0.671	0.097	CaFr12	75.9230769	0.07592308	2.277692308
E	12	Sample X1	C	0.67	0.096	CaFr12	75.1538462	0.07515385	2.254615385
F	1	Blank B	D	0.589					
F	2	Sample X1	D	0.684	0.095	CaFr21	74.3846154	0.07438462	2.231538462

Appendix 9.28 contd.

F	3	Sample X1	D	0.685	0.096	CaFr21	75.1538462	0.07515385	2.254615385
F	4	Sample X1	D	0.685	0.096	CaFr21	75.1538462	0.07515385	2.254615385
E	5	Blank B	N	0.557					
E	6	Sample X1	N	0.647	0.09	CaXy11	70.5384615	0.07053846	2.116153846
E	7	Sample X1	N	0.648	0.091	CaXy11	71.3076923	0.07130769	2.139230769
E	8	Sample X1	N	0.648	0.091	CaXy11	71.3076923	0.07130769	2.139230769
F	5	Blank B	E	0.563					
F	6	Sample X1	E	0.655	0.092	CaXy12	72.0769231	0.07207692	2.162307692
F	7	Sample X1	E	0.656	0.093	CaXy12	72.8461538	0.07284615	2.185384615
F	8	Sample X1	E	0.656	0.093	CaXy12	72.8461538	0.07284615	2.185384615
E	1	Blank B	M	0.519					
E	2	Sample X1	M	0.61	0.091	CaXy21	71.3076923	0.07130769	2.139230769
E	3	Sample X1	M	0.611	0.092	CaXy21	72.0769231	0.07207692	2.162307692
E	4	Sample X1	M	0.61	0.091	CaXy21	71.3076923	0.07130769	2.139230769
F	9	Blank B	F	0.533					
F	10	Sample X1	F	0.624	0.091	CaGr11	71.3076923	0.07130769	2.139230769
F	11	Sample X1	F	0.626	0.093	CaGr11	72.8461538	0.07284615	2.185384615
F	12	Sample X1	F	0.624	0.091	CaGr11	71.3076923	0.07130769	2.139230769
G	1	Blank B	G	0.505					
G	2	Sample X1	G	0.6	0.095	CaGr12	74.3846154	0.07438462	2.231538462
G	3	Sample X1	G	0.599	0.094	CaGr12	73.6153846	0.07361538	2.208461538
G	4	Sample X1	G	0.6	0.095	CaGr12	74.3846154	0.07438462	2.231538462
G	5	Blank B	H	0.55					
G	6	Sample X1	H	0.648	0.098	CaGr21	76.6923077	0.07669231	2.300769231
G	7	Sample X1	H	0.649	0.099	CaGr21	77.4615385	0.07746154	2.323846154
G	8	Sample X1	H	0.648	0.098	CaGr21	76.6923077	0.07669231	2.300769231
G	9	Blank B	I	0.539					
G	10	Sample X1	I	0.632	0.093	CaGc11	72.8461538	0.07284615	2.185384615
G	11	Sample X1	I	0.631	0.092	CaGc11	72.0769231	0.07207692	2.162307692
G	12	Sample X1	I	0.632	0.093	CaGc11	72.8461538	0.07284615	2.185384615
H	1	Blank B	J	0.529					
H	2	Sample X1	J	0.624	0.095	CaGc21	74.3846154	0.07438462	2.231538462
H	3	Sample X1	J	0.624	0.095	CaGc21	74.3846154	0.07438462	2.231538462
H	4	Sample X1	J	0.622	0.093	CaGc21	72.8461538	0.07284615	2.185384615
H	5	Blank B	K	0.575					
H	6	Sample X1	K	0.667	0.092	CaGl11	72.0769231	0.07207692	2.162307692
H	7	Sample X1	K	0.667	0.092	CaGl11	72.0769231	0.07207692	2.162307692
H	8	Sample X1	K	0.667	0.092	CaGl11	72.0769231	0.07207692	2.162307692
H	9	Blank B	L	0.518					
H	10	Sample X1	L	0.613	0.095	CaGl21	74.3846154	0.07438462	2.231538462
H	11	Sample X1	L	0.613	0.095	CaGl21	74.3846154	0.07438462	2.231538462
H	12	Sample X1	L	0.612	0.094	CaGl21	73.6153846	0.07438462	2.231538462

Appendix 9.29 RCCDRSM FRAP run 29

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.464					
A	2	Sample X1	A	0.575	0.106	CaSu11	82.8461538	0.08284615	1.242692308
A	3	Sample X1	A	0.57	0.106	CaSu11	82.8461538	0.08284615	1.242692308
A	4	Sample X1	A	0.562	0.103	CaSu11	80.5384615	0.08053846	1.208076923
A	5	Blank B	B	0.264					
A	6	Sample X1	B	0.674	0.427	CaFr11	329.769231	0.32976923	4.946538462
A	7	Sample X1	B	0.691	0.427	CaFr11	329.769231	0.32976923	4.946538462
A	8	Sample X1	B	0.708	0.427	CaFr11	329.769231	0.32976923	4.946538462
A	9	Blank B	C	0.291					
A	10	Sample X1	C	0.54	0.097	CaFr12	75.9230769	0.07592308	1.138846154
A	11	Sample X1	C	0.535	0.097	CaFr12	75.9230769	0.07592308	1.138846154
A	12	Sample X1	C	0.57	0.094	CaFr12	73.6153846	0.07361538	1.104230769
B	1	Blank B	D	0.232					
B	2	Sample X1	D	0.542	0.097	CaFr21	75.9230769	0.07592308	1.138846154
B	3	Sample X1	D	0.599	0.097	CaFr21	75.9230769	0.07592308	1.138846154
B	4	Sample X1	D	0.612	0.098	CaFr21	76.6923077	0.07669231	1.150384615
E	9	Blank B	O	0.549					
E	10	Sample X1	O	0.504	0.095	CaXy11	74.3846154	0.07438462	1.115769231
E	11	Sample X1	O	0.54	0.095	CaXy11	74.3846154	0.07438462	1.115769231
E	12	Sample X1	O	0.56	0.094	CaXy11	73.6153846	0.07361538	1.104230769
B	5	Blank B	E	0.596					
B	6	Sample X1	E	0.572	0.095	CaXy12	74.3846154	0.07438462	1.115769231
B	7	Sample X1	E	0.521	0.095	CaXy12	74.3846154	0.07438462	1.115769231
B	8	Sample X1	E	0.53	0.096	CaXy12	75.1538462	0.07515385	1.127307692
E	5	Blank B	N	0.579					
E	6	Sample X1	N	0.543	0.096	CaXy21	75.1538462	0.07515385	1.127307692
E	7	Sample X1	N	0.517	0.096	CaXy21	75.1538462	0.07515385	1.127307692
E	8	Sample X1	N	0.536	0.094	CaXy21	73.6153846	0.07361538	1.104230769
B	9	Blank B	F	0.037					
B	10	Sample X1	F	0.575	0.096	CaGr11	75.1538462	0.07515385	1.127307692
B	11	Sample X1	F	0.556	0.098	CaGr11	76.6923077	0.07669231	1.150384615
B	12	Sample X1	F	0.579	0.098	CaGr11	76.6923077	0.07669231	1.150384615
C	1	Blank B	G	0.017					
C	2	Sample X1	G	0.452	0.435	CaGr12	335.923077	0.33592308	5.038846154
C	3	Sample X1	G	0.441	0.434	CaGr12	335.153846	0.33515385	5.027307692
C	4	Sample X1	G	0.462	0.435	CaGr12	335.923077	0.33592308	5.038846154
C	5	Blank B	H	0.012					

Appendix 9.29 contd.

C	6	Sample X1	H	0.547	0.095	CaGr21	74.3846154	0.07438462	1.115769231
C	7	Sample X1	H	0.535	0.093	CaGr21	72.8461538	0.07284615	1.092692308
C	8	Sample X1	H	0.559	0.095	CaGr21	74.3846154	0.07438462	1.115769231
C	9	Blank B	I	0.409					
C	10	Sample X1	I	0.474	0.092	CaGc11	72.0769231	0.07207692	1.081153846
C	11	Sample X1	I	0.481	0.092	CaGc11	72.0769231	0.07207692	1.081153846
C	12	Sample X1	I	0.468	0.094	CaGc11	73.6153846	0.07361538	1.104230769
D	1	Blank B	J	0.401					
D	2	Sample X1	J	0.53	0.129	CaGc21	100.538462	0.10053846	1.508076923
D	3	Sample X1	J	0.514	0.129	CaGc21	100.538462	0.10053846	1.508076923
D	4	Sample X1	J	0.532	0.131	CaGc21	102.076923	0.10207692	1.531153846
D	5	Blank B	K	0.195					
D	6	Sample X1	K	0.555	0.097	CaGl11	75.9230769	0.07592308	1.138846154
D	7	Sample X1	K	0.565	0.096	CaGl11	75.1538462	0.07515385	1.127307692
D	8	Sample X1	K	0.603	0.096	CaGl11	75.1538462	0.07515385	1.127307692
D	9	Blank B	L	0.193					
D	10	Sample X1	L	0.568	0.355	CaGl21	274.384615	0.27438462	4.115769231
D	11	Sample X1	L	0.531	0.355	CaGl21	274.384615	0.27438462	4.115769231
D	12	Sample X1	L	0.54	0.35	CaGl21	270.538462	0.27053846	4.058076923

Appendix 9.30 RCCDRSM FRAP run 30

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample Code	FRAP (µMTE/l)	FRAP (µMTE/ml)	FRAP (µMTE/g)
E	1	Blank B	A	0.525					
E	2	Sample X1	A	0.745	0.22	CaSu11	170.538462	0.17053846	1.70538462
E	3	Sample X1	A	0.74	0.215	CaSu11	166.692308	0.16669231	1.66692308
E	4	Sample X1	A	0.745	0.22	CaSu11	170.538462	0.17053846	1.70538462
E	5	Blank B	B	0.408					
E	6	Sample X1	B	0.581	0.173	CaFr11	134.384615	0.13438462	1.34384615
E	7	Sample X1	B	0.583	0.175	CaFr11	135.923077	0.13592308	1.35923077
E	8	Sample X1	B	0.581	0.173	CaFr11	134.384615	0.13438462	1.34384615
E	9	Blank B	C	0.451					
E	10	Sample X1	C	0.544	0.093	CaFr12	72.8461538	0.07284615	0.72846154
E	11	Sample X1	C	0.542	0.091	CaFr12	71.3076923	0.07130769	0.71307692
E	12	Sample X1	C	0.544	0.093	CaFr12	72.8461538	0.07284615	0.12141026
F	1	Blank B	D	0.456					
F	2	Sample X1	D	0.547	0.091	CaFr12	71.3076923	0.07130769	0.71307692
F	3	Sample X1	D	0.546	0.09	CaFr12	70.5384615	0.07053846	0.70538462

Appendix 9.30 contd.

F	4	Sample X1	D	0.547	0.091	CaFr12	71.3076923	0.07130769	0.71307692
F	1	Blank B	P	0.418					
F	2	Sample X1	P	0.552	0.134	CaFr21	104.384615	0.10438462	1.04384615
F	3	Sample X1	P	0.552	0.134	CaFr21	104.384615	0.10438462	1.04384615
F	4	Sample X1	P	0.553	0.135	CaFr21	105.153846	0.10515385	1.05153846
F	5	Blank B	E	0.438					
F	6	Sample X1	E	0.655	0.217	CaXy11	168.230769	0.16823077	1.68230769
F	7	Sample X1	E	0.653	0.215	CaXy11	166.692308	0.16669231	1.66692308
F	8	Sample X1	E	0.655	0.217	CaXy11	168.230769	0.16823077	1.68230769
E	9	Blank B	O	0.453					
E	10	Sample X1	O	0.551	0.098	CaXy12	76.6923077	0.07669231	0.76692308
E	11	Sample X1	O	0.548	0.095	CaXy12	74.3846154	0.07438462	0.74384615
E	12	Sample X1	O	0.551	0.098	CaXy12	76.6923077	0.07669231	0.76692308
F	9	Blank B	F	0.508					
F	10	Sample X1	F	0.607	0.099	CaXy21	77.4615385	0.07746154	0.77461538
F	11	Sample X1	F	0.607	0.099	CaXy21	77.4615385	0.07746154	0.77461538
F	12	Sample X1	F	0.602	0.094	CaXy21	73.6153846	0.07361538	0.73615385
G	1	Blank B	G	0.592					
G	2	Sample X1	G	0.685	0.093	CaGr11	72.8461538	0.07284615	0.72846154
G	3	Sample X1	G	0.684	0.092	CaGr11	72.0769231	0.07207692	0.72076923
G	4	Sample X1	G	0.684	0.092	CaGr11	72.0769231	0.07207692	0.72076923
G	5	Blank B	H	0.539					
G	6	Sample X1	H	0.827	0.288	CaGr21	222.846154	0.22284615	2.22846154
G	7	Sample X1	H	0.827	0.288	CaGr21	222.846154	0.22284615	2.22846154
G	8	Sample X1	H	0.829	0.29	CaGr21	224.384615	0.22438462	2.24384615
G	9	Blank B	I	0.215					
G	10	Sample X1	I	0.875	0.66	CaGc11	509	0.509	5.09
G	11	Sample X1	I	0.872	0.657	CaGc11	506.692308	0.50669231	5.06692308
G	12	Sample X1	I	0.875	0.66	CaGc11	509	0.509	5.09
H	1	Blank B	J	0.26					
H	2	Sample X1	J	0.517	0.257	CaGc21	199	0.199	1.99
H	3	Sample X1	J	0.52	0.26	CaGc21	201.307692	0.20130769	2.01307692
H	4	Sample X1	J	0.52	0.26	CaGc21	201.307692	0.20130769	2.01307692
H	5	Blank B	K	0.334					
H	6	Sample X1	K	0.428	0.094	CaGl11	73.6153846	0.07361538	0.73615385
H	7	Sample X1	K	0.428	0.094	CaGl11	73.6153846	0.07361538	0.73615385
H	8	Sample X1	K	0.427	0.093	CaGl11	72.8461538	0.07284615	0.72846154
H	9	Blank B	L	0.357					
H	10	Sample X1	L	0.737	0.38	CaGl21	293.615385	0.29361538	2.93615385
H	11	Sample X1	L	0.738	0.381	CaGl21	294.384615	0.29438462	2.94384615
H	12	Sample X1	L	0.737	0.38	CaGl21	293.615385	0.29361538	2.93615385

Appendix 10.1 RCCDRSM DPPH run 1

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.061					
A	2	Control C1	A	1.094	1.033				
A	3	Control C1	A	1.085	1.024	0.986333			
A	4	Control C1	A	0.963	0.902				
A	5	Sample X1	A	0.791	0.723	CaSu11	26.69821	10.9177849	109.1778
A	6	Sample X1	A	0.784	0.723	CaSu11	26.69821	10.9177849	109.1778
A	7	Sample X1	A	0.783	0.722	CaSu11	26.79959	10.915655	109.1565
A	8	Blank B	B	0.051					
A	9	Control C1	B	1.024	0.973				
A	10	Control C1	B	0.98	0.929	0.953333			
A	11	Control C1	B	1.009	0.958				
A	12	Sample X1	B	0.27	0.219	CaFr11	77.02797	9.84430245	98.44302
B	1	Sample X1	B	0.265	0.214	CaFr11	77.55245	9.83365282	98.33653
B	2	Sample X1	B	0.27	0.219	CaFr11	77.02797	9.84430245	98.44302
B	3	Blank B	C	0.059					
B	4	Control C1	C	1.235	1.176				
B	5	Control C1	C	1.357	1.299	1.241			
B	6	Control C1	C	1.307	1.248				
B	7	Sample X1	C	0.937	0.878	CaFr12	29.2506	11.2479233	112.4792
B	8	Sample X1	C	0.938	0.879	CaFr12	29.17002	11.2500532	112.5005
B	9	Sample X1	C	0.936	0.878	CaFr12	29.2506	11.2479233	112.4792
B	10	Blank B	D	0.048					
B	11	Control C1	D	1.619	1.571				
B	12	Control C1	D	1.774	1.726	1.644667			
C	1	Control C1	D	1.685	1.637				
C	2	Sample X1	D	0.859	0.811	CaFr21	50.6891	11.1052183	111.0522
C	3	Sample X1	D	0.859	0.811	CaFr21	50.6891	11.1052183	111.0522
C	4	Sample X1	D	0.858	0.81	CaFr21	50.7499	11.1030884	111.0309
A	1	Blank B	A	0.043					
A	2	Control C1	A	0.751	0.708				
A	3	Control C1	A	0.932	0.889	0.846			
A	4	Control C1	A	0.984	0.941				
A	5	Sample X1	A	0.554	0.546	CaXy11	35.46099	10.5407881	105.4079
A	6	Sample X1	A	0.61	0.547	CaXy11	35.34279	10.542918	105.4292
A	7	Sample X1	A	0.604	0.546	CaXy11	35.46099	10.5407881	105.4079
C	5	Blank B	E	0.051					
C	6	Control C1	E	1.399	1.348				

Appendix 10.1 contd.

C	7	Control C1	E	1.225	1.174	1.2			
C	8	Control C1	E	1.129	1.078				
C	9	Sample X1	E	0.244	0.193	CaXy12	83.91667	9.78892439	97.88924
C	10	Sample X1	E	0.246	0.195	CaXy12	83.75	9.79318424	97.93184
C	11	Sample X1	E	0.247	0.196	CaXy12	83.66667	9.79531416	97.95314
A	1	Blank B	A	0.044					
A	2	Control C1	A	0.885	0.841				
A	3	Control C1	A	1.019	0.975	0.923333			
A	4	Control C1	A	0.998	0.954				
A	5	Sample X1	A	0.357	0.31	CaXy21	66.42599	10.0381257	100.3813
A	6	Sample X1	A	0.367	0.31	CaXy21	66.42599	10.0381257	100.3813
A	7	Sample X1	A	0.332	0.304	CaXy21	67.07581	10.0253461	100.2535
C	12	Blank B	F	0.048					
D	1	Control C1	F	1.3	1.252				
D	2	Control C1	F	1.227	1.179	1.218333			
D	3	Control C1	F	1.272	1.224				
D	4	Sample X1	F	0.77	0.722	CaGr11	40.73871	10.915655	109.1565
D	5	Sample X1	F	0.77	0.722	CaGr11	40.73871	10.915655	109.1565
D	6	Sample X1	F	0.771	0.723	CaGr11	40.65663	10.9177849	109.1778
D	7	Blank B	G	0.061					
D	8	Control C1	G	1.336	1.275				
D	9	Control C1	G	1.134	1.073	1.229333			
D	10	Control C1	G	1.401	1.34				
D	11	Sample X1	G	0.279	0.218	CaGr12	82.26681	9.84217252	98.42173
D	12	Sample X1	G	0.276	0.215	CaGr12	82.51085	9.83578275	98.35783
E	1	Sample X1	G	0.273	0.212	CaGr12	82.75488	9.82939297	98.29393
E	2	Blank B	H	0.054					
E	3	Control C1	H	1.168	1.115				
E	4	Control C1	H	1.057	1.003	1.043667			
E	5	Control C1	H	1.067	1.013				
E	6	Sample X1	H	0.772	0.718	CaGr21	31.20409	10.9071353	109.0714
E	7	Sample X1	H	0.764	0.711	CaGr21	31.8748	10.8922258	108.9223
E	8	Sample X1	H	0.768	0.714	CaGr21	31.58735	10.8986155	108.9862
E	9	Blank B	I	0.051					
E	10	Control C1	I	2.064	2.013				
E	11	Control C1	I	1.38	1.329	1.576			
E	12	Control C1	I	1.437	1.386				
F	1	Sample X1	I	0.291	0.24	CaGc11	84.77157	9.88903088	98.89031
F	2	Sample X1	I	0.294	0.243	CaGc11	84.58122	9.89542066	98.95421
F	3	Sample X1	I	0.296	0.245	CaGc11	84.45431	9.89968051	98.99681
F	4	Blank B	J	0.056					
F	5	Control C1	J	1.255	1.2				

Appendix 10.1 contd.

F	6	Control C1	J	1.115	1.06	1.101667			
F	7	Control C1	J	1.101	1.045				
F	8	Sample X1	J	0.561	0.505	CaGc21	54.16036	10.4534611	104.5346
F	9	Sample X1	J	0.558	0.502	CaGc21	54.43268	10.4470714	104.4707
F	10	Sample X1	J	0.558	0.502	CaGc21	54.43268	10.4470714	104.4707
F	11	Blank B	K	0.059					
F	12	Control C1	K	1.513	1.454				
G	1	Control C1	K	1.281	1.222	1.246333			
G	2	Control C1	K	1.121	1.063				
G	3	Sample X1	K	0.797	0.738	CaGl11	40.78631	10.9497338	109.4973
G	4	Sample X1	K	0.795	0.736	CaGl11	40.94678	10.9454739	109.4547
G	5	Sample X1	K	0.793	0.734	CaGl11	41.10725	10.9412141	109.4121
G	6	Blank B	L	0.058					
G	7	Control C1	L	1.341	1.282				
G	8	Control C1	L	1.212	1.153	1.245333			
G	9	Control C1	L	1.359	1.301				
G	10	Sample X1	L	0.884	0.826	CaGl21	33.67238	11.1371672	111.3717
G	11	Sample X1	L	0.901	0.843	CaGl21	32.30728	11.1733759	111.7338
G	12	Sample X1	L	0.911	0.853	CaGl21	31.50428	11.1946752	111.9468

Appendix 10.2 RCCDRSM DPPH run 2

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.067					
A	2	Control C1	A	1.199	1.132				
A	3	Control C1	A	1.173	1.105	1.115667			
A	4	Control C1	A	1.178	1.11				
A	5	Sample X1	A	0.176	0.109	CaSu11	90.23006	9.61001065	192.2002
A	6	Sample X1	A	0.172	0.105	CaSu11	90.58859	9.60149095	192.0298
A	7	Sample X1	A	0.175	0.108	CaSu11	90.31969	9.60788072	192.1576
A	8	Blank B	B	0.051					
A	9	Control C1	B	1.51	1.459				
A	10	Control C1	B	1.421	1.37	1.4			
A	11	Control C1	B	1.422	1.371				
A	12	Sample X1	B	0.161	0.11	CaFr11	92.14286	9.61214058	192.2428
B	1	Sample X1	B	0.165	0.114	CaFr11	91.85714	9.62066028	192.4132
B	2	Sample X1	B	0.164	0.113	CaFr11	91.92857	9.61853035	192.3706
B	3	Blank B	C	0.058					

Appendix 10.2 contd.

B	4	Control C1	C	1.291	1.232				
B	5	Control C1	C	1.407	1.349	1.323			
B	6	Control C1	C	1.446	1.388				
B	7	Sample X1	C	0.195	0.137	CaFr12	89.64475	9.66964856	193.393
B	8	Sample X1	C	0.195	0.137	CaFr12	89.64475	9.66964856	193.393
B	9	Sample X1	C	0.196	0.138	CaFr12	89.56916	9.67177849	193.4356
B	10	Blank B	D	0.057					
B	11	Control C1	D	1.335	1.279				
B	12	Control C1	D	1.241	1.184	1.244667			
C	1	Control C1	D	1.327	1.271				
C	2	Sample X1	D	0.935	0.878	CaFr21	29.45903	11.2479233	224.9585
C	3	Sample X1	D	0.942	0.885	CaFr21	28.89663	11.2628328	225.2567
C	4	Sample X1	D	0.933	0.876	CaFr21	29.61971	11.2436635	224.8733
A	8	Blank B	B	0.041					
A	9	Control C1	B	1.058	1.017				
A	10	Control C1	B	1.199	1.158	1.121333			
A	11	Control C1	B	1.23	1.189				
A	12	Sample X1	B	0.949	0.908	CaXy11	19.02497	11.3118211	226.2364
B	1	Sample X1	B	0.949	0.908	CaXy11	19.02497	11.3118211	226.2364
B	2	Sample X1	B	0.949	0.908	CaXy11	19.02497	11.3118211	226.2364
C	5	Blank B	E	0.047					
C	6	Control C1	E	1.191	1.143				
C	7	Control C1	E	1.214	1.166	1.183			
C	8	Control C1	E	1.287	1.24				
C	9	Sample X1	E	0.176	0.129	CaXy12	89.09552	9.65260916	193.0522
C	10	Sample X1	E	0.172	0.125	CaXy12	89.43364	9.64408946	192.8818
C	11	Sample X1	E	0.176	0.129	CaXy12	89.09552	9.65260916	193.0522
A	8	Blank B	B	0.04					
A	9	Control C1	B	1.208	1.168				
A	10	Control C1	B	1.192	1.152	1.123333			
A	11	Control C1	B	1.089	1.05				
A	12	Sample X1	B	0.555	0.565	CaXy21	49.70326	10.5812567	211.6251
B	1	Sample X1	B	0.608	0.568	CaXy21	49.4362	10.5876464	211.7529
B	2	Sample X1	B	0.652	0.562	CaXy21	49.97033	10.5748669	211.4973
C	12	Blank B	F	0.05					
D	1	Control C1	F	1.283	1.233				
D	2	Control C1	F	1.363	1.314	1.246333			
D	3	Control C1	F	1.242	1.192				
D	4	Sample X1	F	0.157	0.107	CaGr11	91.41482	9.6057508	192.115
D	5	Sample X1	F	0.152	0.102	CaGr11	91.81599	9.59510117	191.902
D	6	Sample X1	F	0.153	0.103	CaGr11	91.73576	9.5972311	191.9446
D	7	Blank B	G	0.05					

Appendix 10.2 contd.

D	8	Control C1	G	1.221	1.17				
D	9	Control C1	G	1.157	1.107	1.182667			
D	10	Control C1	G	1.321	1.271				
D	11	Sample X1	G	1.038	0.988	CaGr12	16.45998	11.4822151	229.6443
D	12	Sample X1	G	1.036	0.986	CaGr12	16.62909	11.4779553	229.5591
E	1	Sample X1	G	1.037	0.987	CaGr12	16.54453	11.4800852	229.6017
E	2	Blank B	H	0.062					
E	3	Control C1	H	1.285	1.223				
E	4	Control C1	H	1.25	1.188	1.187333			
E	5	Control C1	H	1.213	1.151				
E	6	Sample X1	H	0.916	0.854	CaGr21	28.07412	11.1968051	223.9361
E	7	Sample X1	H	0.913	0.851	CaGr21	28.32678	11.1904153	223.8083
E	8	Sample X1	H	0.915	0.853	CaGr21	28.15834	11.1946752	223.8935
E	9	Blank B	I	0.046					
E	10	Control C1	I	1.197	1.152				
E	11	Control C1	I	1.178	1.132	1.188667			
E	12	Control C1	I	1.328	1.282				
F	1	Sample X1	I	0.804	0.758	CaGc11	36.23107	10.9923323	219.8466
F	2	Sample X1	I	0.806	0.76	CaGc11	36.06282	10.9965921	219.9318
F	3	Sample X1	I	0.801	0.755	CaGc11	36.48345	10.9859425	219.7188
F	4	Blank B	J	0.052					
F	5	Control C1	J	1.227	1.175				
F	6	Control C1	J	1.243	1.191	1.216667			
F	7	Control C1	J	1.336	1.284				
F	8	Sample X1	J	0.272	0.22	CaGc21	81.91781	9.84643237	196.9286
F	9	Sample X1	J	0.271	0.219	CaGc21	82	9.84430245	196.886
F	10	Sample X1	J	0.273	0.221	CaGc21	81.83562	9.8485623	196.9712
F	11	Blank B	K	0.06					
F	12	Control C1	K	1.301	1.241				
G	1	Control C1	K	1.25	1.19	1.25			
G	2	Control C1	K	1.378	1.319				
G	3	Sample X1	K	0.968	0.908	CaGl11	27.36	11.3118211	226.2364
G	4	Sample X1	K	0.966	0.906	CaGl11	27.52	11.3075612	226.1512
G	5	Sample X1	K	0.963	0.903	CaGl11	27.76	11.3011715	226.0234
G	6	Blank B	L	0.053					
G	7	Control C1	L	1.16	1.107				
G	8	Control C1	L	1.329	1.276	1.198			
G	9	Control C1	L	1.265	1.211				
G	10	Sample X1	L	0.88	0.827	CaGl21	30.96828	11.1527157	223.0543
G	11	Sample X1	L	0.883	0.83	CaGl21	30.71786	11.1456869	222.9137
G	12	Sample X1	L	0.88	0.827	CaGl21	30.96828	11.1392971	222.7859

Appendix 10.3 RCCDRSM DPPH run 3

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/ml)	DPPH (µMTE/g)
D	9	Blank B	J	0.067					
D	2	Control C1	J	1.117	1.033				
D	3	Control C1	J	1.108	1.024	0.986333			
D	4	Control C1	J	0.986	0.902				
D	10	Sample X1	J	0.287	0.22	CaSu11	77.6951673	9.84643237	147.6965
D	11	Sample X1	J	0.285	0.218	CaSu11	77.8979385	9.84217252	147.6326
D	12	Sample X1	J	0.287	0.22	CaSu11	77.6951673	9.84643237	147.6965
A	1	Blank B	A	0.084					
A	2	Control C1	A	1.024	0.94				
A	3	Control C1	A	0.98	0.896	0.920333			
A	4	Control C1	A	1.009	0.925				
A	5	Sample X1	A	0.224	0.154	CaFr11	83.2669323	9.70585729	145.5879
A	6	Sample X1	A	0.228	0.154	CaFr11	83.2669323	9.70585729	145.5879
A	7	Sample X1	A	0.242	0.158	CaFr11	82.8323071	9.714377	145.7157
B	1	Blank B	B	0.091					
B	2	Control C1	B	1.235	1.144				
B	3	Control C1	B	1.357	1.266	1.208667			
B	4	Control C1	B	1.307	1.216				
B	5	Sample X1	B	0.223	0.132	CaFr12	89.0788748	9.65899894	144.885
B	6	Sample X1	B	0.225	0.134	CaFr12	88.9134032	9.66325879	144.9489
B	7	Sample X1	B	0.223	0.132	CaFr12	89.0788748	9.65899894	144.885
C	1	Blank B	C	0.043					
C	2	Control C1	C	1.619	1.576				
C	3	Control C1	C	1.774	1.731	1.679333			
C	4	Control C1	C	1.685	1.731				
C	5	Sample X1	C	0.264	0.221	CaFr21	86.8400159	9.8485623	147.7284
C	6	Sample X1	C	0.258	0.225	CaFr21	86.6018261	9.857082	147.8562
C	7	Sample X1	C	0.274	0.221	CaFr21	86.8400159	9.8485623	147.7284
F	9	Blank B	D	0.081					
F	6	Control C1	E	1.399	1.358				
F	7	Control C1	E	1.225	1.184	1.21			
F	8	Control C1	E	1.129	1.088				
F	10	Sample X1	D	0.282	0.201	CaXy11	83.3884298	9.80596379	147.0895
F	11	Sample X1	D	0.282	0.201	CaXy11	83.3884298	9.80596379	147.0895
F	12	Sample X1	D	0.285	0.204	CaXy11	83.1404959	9.81235357	147.1853
G	1	Blank B	E	0.041					
G	6	Control C1	E	1.399	1.358				

Appendix 10.3 contd.

G	7	Control C1	E	1.225	1.184	1.21			
G	8	Control C1	E	1.129	1.088				
G	2	Sample X1	E	0.149	0.108	CaXy12	91.0743802	9.60788072	144.1182
G	3	Sample X1	E	0.146	0.105	CaXy12	91.322314	9.60149095	144.0224
G	4	Sample X1	E	0.143	0.102	CaXy12	91.5702479	9.59510117	143.9265
H	5	Blank B	F	0.011					
G	6	Control C1	E	1.399	1.358				
G	7	Control C1	E	1.225	1.184	1.21			
G	8	Control C1	E	1.129	1.088				
H	6	Sample X1	F	0.215	0.204	CaXy21	83.1404959	9.81235357	147.1853
H	7	Sample X1	F	0.211	0.2	CaXy21	83.4710744	9.80383387	147.0575
H	8	Sample X1	F	0.215	0.204	CaXy21	83.1404959	9.81235357	147.1853
A	9	Blank B	G	0.096					
A	1	Control C1	G	1.3	1.204				
A	2	Control C1	G	1.227	1.131	1.170333			
A	3	Control C1	G	1.272	1.176				
A	10	Sample X1	G	0.288	0.192	CaGr11	83.5944175	9.78679446	146.8019
A	11	Sample X1	G	0.287	0.191	CaGr11	83.6798633	9.78466454	146.77
A	12	Sample X1	G	0.282	0.186	CaGr11	84.107092	9.77401491	146.6102
B	1	Blank B	H	0.073					
B	8	Control C1	H	1.336	1.263				
B	9	Control C1	H	1.134	1.061	1.217333			
B	10	Control C1	H	1.401	1.328				
B	2	Sample X1	H	0.229	0.156	CaGr12	87.1851041	9.71011715	145.6518
B	3	Sample X1	H	0.208	0.135	CaGr12	88.9101862	9.66538871	144.9808
B	4	Sample X1	H	0.218	0.145	CaGr12	88.0887185	9.68668797	145.3003
C	5	Blank B	I	0.043					
C	3	Control C1	I	1.168	1.125				
C	4	Control C1	I	1.057	1.014	1.054333			
C	5	Control C1	I	1.067	1.024				
C	6	Sample X1	I	0.166	0.123	CaGr21	87.1851041	9.63982961	144.5974
C	7	Sample X1	I	0.168	0.125	CaGr21	88.9101862	9.64408946	144.6613
C	8	Sample X1	I	0.172	0.129	CaGr21	88.0887185	9.65260916	144.7891
G	1	Blank B	A	1.896					
G	2	Control C1	A	2.064	2.013				
G	3	Control C1	A	1.38	1.329	1.576			
G	4	Control C1	A	1.437	1.386				
G	5	Sample X1	A	2.16	0.164	CaGc11	89.5939086	9.72715655	145.9073
G	6	Sample X1	A	2.157	0.161	CaGc11	89.784264	9.72076677	145.8115
G	7	Sample X1	A	2.16	0.164	CaGc11	89.5939086	9.72715655	145.9073
H	8	Blank B	M	0.867					
H	9	Control C1	M	1.255	1.2				

Appendix 10.3 contd.

H	10	Control C1	M	1.115	1.06	1.101667			
H	11	Control C1	M	1.101	1.045				
H	12	Sample X1	M	0.967	0.1	CaGc21	90.9228442	9.59084132	143.8626
H	1	Sample X1	M	0.967	0.1	CaGc21	90.9228442	9.59084132	143.8626
H	2	Sample X1	M	0.967	0.1	CaGc21	90.9228442	9.59084132	143.8626
E	5	Blank B	K	0.08					
E	12	Control C1	K	1.513	1.454				
E	1	Control C1	K	1.281	1.222	1.246333			
E	2	Control C1	K	1.121	1.063				
E	6	Sample X1	K	0.87	0.82	CaGl11	34.2070072	11.1243876	166.8658
E	7	Sample X1	K	0.925	0.83	CaGl11	33.4046537	11.1456869	167.1853
E	8	Sample X1	K	0.925	0.83	CaGl11	33.4046537	11.1456869	167.1853
F	9	Blank B	L	0.839					
F	7	Control C1	L	1.341	1.282				
F	8	Control C1	L	1.212	1.153	1.245333			
F	9	Control C1	L	1.359	1.301				
F	10	Sample X1	L	0.884	0.145	CaGl21	88.356531	9.68668797	145.3003
F	11	Sample X1	L	0.872	0.133	CaGl21	89.3201285	9.66112886	144.9169
F	12	Sample X1	L	0.865	0.126	CaGl21	89.882227	9.64621938	144.6933

Appendix 10.7 RCCDRSM DPPH run 7

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.048						
A	2	Control C1	A	1.12	1.072					
A	3	Control C1	A	1.12	1.072	1.078667				
A	4	Control C1	A	1.14	1.092					
A	5	Sample X1	A	0.954	0.906	CaSu11	16.00742	11.307561	0.0113076	0.113076
A	6	Sample X1	A	0.957	0.909	CaSu11	15.7293	11.313951	0.011314	0.11314
A	7	Sample X1	A	0.954	0.906	CaSu11	16.00742	11.307561	0.0113076	0.113076
A	8	Blank B	B	0.039						
A	9	Control C1	B	1.144	1.105					
A	10	Control C1	B	1.143	1.104	1.105333				
A	11	Control C1	B	1.146	1.107					
A	12	Sample X1	B	0.929	0.89	CaFr11	19.4813	11.273482	0.0112735	0.112735
B	1	Sample X1	B	0.929	0.89	CaFr11	19.4813	11.273482	0.0112735	0.112735
B	2	Sample X1	B	0.923	0.884	CaFr11	20.02413	11.260703	0.0112607	0.112607
B	3	Blank B	C	0.069						

Appendix 10.7 contd.

B	4	Control C1	C	1.133	1.064					
B	5	Control C1	C	1.133	1.064	1.064667				
B	6	Control C1	C	1.135	1.066					
B	7	Sample X1	C	0.979	0.91	CaFr12	14.52724	11.316081	0.0113161	0.113161
B	8	Sample X1	C	0.978	0.909	CaFr12	14.62116	11.313951	0.011314	0.11314
B	9	Sample X1	C	0.978	0.909	CaFr12	14.62116	11.313951	0.011314	0.11314
B	10	Blank B	D	0.043						
B	11	Control C1	D	1.005	0.962					
B	12	Control C1	D	1.005	0.962	0.962667				
C	1	Control C1	D	1.007	0.964					
C	2	Sample X1	D	0.681	0.638	CaFr21	33.72576	10.736741	0.0107367	0.107367
C	3	Sample X1	D	0.68	0.637	CaFr21	33.82964	10.734611	0.0107346	0.107346
C	4	Sample X1	D	0.682	0.639	CaFr21	33.62188	10.738871	0.0107389	0.107389
B	3	Blank B	C	0.777						
B	4	Control C1	C	0.915	0.138					
B	5	Control C1	C	0.911	0.134	0.136667				
B	6	Control C1	C	0.915	0.138					
B	7	Sample X1	C	0.815	0.038	CaXy11	72.19512	9.4587859	0.0094588	0.094588
B	8	Sample X1	C	0.816	0.039	CaXy11	71.46341	9.4609159	0.0094609	0.094609
B	9	Sample X1	C	0.816	0.039	CaXy11	71.46341	9.4609159	0.0094609	0.094609
C	5	Blank B	E	0.177						
C	6	Control C1	E	0.954	0.777					
C	7	Control C1	E	0.954	0.777	0.776				
C	8	Control C1	E	0.951	0.774					
C	9	Sample X1	E	0.867	0.69	CaXy12	11.08247	10.847497	0.0108475	0.108475
C	10	Sample X1	E	0.866	0.689	CaXy12	11.21134	10.845367	0.0108454	0.108454
C	11	Sample X1	E	0.866	0.689	CaXy12	11.21134	10.845367	0.0108454	0.108454
C	12	Blank B	F	0.041						
D	1	Control C1	F	1.028	0.987					
D	2	Control C1	F	1.027	0.986	0.986667				
D	3	Control C1	F	1.028	0.987					
D	4	Sample X1	F	0.793	0.752	CaGr11	23.78378	10.979553	0.0109796	0.109796
D	5	Sample X1	F	0.792	0.751	CaGr11	23.88514	10.977423	0.0109774	0.109774
D	6	Sample X1	F	0.793	0.752	CaGr11	23.78378	10.979553	0.0109796	0.109796
D	7	Blank B	G	0.038						
D	8	Control C1	G	1.115	1.077					
D	9	Control C1	G	1.115	1.077	1.077				
D	10	Control C1	G	1.115	1.077					
D	11	Sample X1	G	0.985	0.947	CaGr21	12.07057	11.394888	0.0113949	0.113949
D	12	Sample X1	G	0.985	0.947	CaGr21	12.07057	11.394888	0.0113949	0.113949
E	1	Sample X1	G	0.988	0.95	CaGr21	11.79201	11.401278	0.0114013	0.114013
E	2	Blank B	H	0.047						

Appendix 10.7 contd.

E	3	Control C1	H	0.945	0.898					
E	4	Control C1	H	0.941	0.894	0.896667				
E	5	Control C1	H	0.945	0.898					
E	6	Sample X1	H	0.906	0.856	CaGr21	4.535316	11.201065	0.0112011	0.112011
E	7	Sample X1	H	0.906	0.859	CaGr21	4.200743	11.207455	0.0112075	0.112075
E	8	Sample X1	H	0.903	0.856	CaGr21	4.535316	11.201065	0.0112011	0.112011
E	9	Blank B	I	0.086						
E	10	Control C1	I	1.193	1.107					
E	11	Control C1	I	1.194	1.108	1.107667				
E	12	Control C1	I	1.194	1.108					
F	1	Sample X1	I	0.622	0.536	CaGc11	51.60999	10.519489	0.0105195	0.105195
F	2	Sample X1	I	0.624	0.538	CaGc11	51.42943	10.523749	0.0105237	0.105237
F	3	Sample X1	I	0.624	0.538	CaGc11	51.42943	10.523749	0.0105237	0.105237
F	4	Blank B	J	0.067						
F	5	Control C1	J	1.087	1.02					
F	6	Control C1	J	1.083	1.016	0.863				
F	7	Control C1	J	1.085	1.018					
F	8	Sample X1	J	0.62	0.553	CaGc21	35.92121	10.555698	0.0105557	0.105557
F	9	Sample X1	J	0.62	0.553	CaGc21	35.92121	10.555698	0.0105557	0.105557
F	10	Sample X1	J	0.618	0.551	CaGc21	36.15295	10.551438	0.0105514	0.105514
F	11	Blank B	K	0.035						
F	12	Control C1	K	1.053	1.018					
G	1	Control C1	K	1.058	1.023	1.02				
G	2	Control C1	K	1.054	1.019					
G	3	Sample X1	K	0.69	0.655	CaGl11	35.78431	10.77295	0.0107729	0.107729
G	4	Sample X1	K	0.69	0.655	CaGl11	35.78431	10.77295	0.0107729	0.107729
G	5	Sample X1	K	0.689	0.654	CaGl11	35.88235	10.77082	0.0107708	0.107708
G	6	Blank B	L	0.056						
G	7	Control C1	L	0.892	0.836					
G	8	Control C1	L	0.894	0.838	0.837333				
G	9	Control C1	L	0.894	0.838					
G	10	Sample X1	L	0.862	0.806	CaGl21	3.742038	11.094569	0.0110946	0.110946
G	11	Sample X1	L	0.861	0.805	CaGl21	3.861465	11.092439	0.0110924	0.110924
G	12	Sample X1	L	0.861	0.805	CaGl21	3.861465	11.092439	0.0110924	0.110924

Appendix 10.12 RCCDRSM DPPH run 12

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.062						
A	2	Control C1	A	0.924	0.862					
A	3	Control C1	A	0.924	0.862	0.862				
A	4	Control C1	A	0.924	0.862					
A	5	Sample X1	A	0.493	0.431	CaSu11	50	10.295847	0.0102958	0.205917
A	6	Sample X1	A	0.496	0.434	CaSu11	49.65197	10.302236	0.0103022	0.206045
A	7	Sample X1	A	0.496	0.434	CaSu11	49.65197	10.302236	0.0103022	0.206045
A	8	Blank B	B	0.047						
A	9	Control C1	B	0.934	0.887					
A	10	Control C1	B	0.938	0.891	0.889667				
A	11	Control C1	B	0.938	0.891					
A	12	Sample X1	B	0.313	0.266	CaFr11	70.10116	9.9444089	0.0099444	0.198888
B	1	Sample X1	B	0.312	0.265	CaFr11	70.21356	9.942279	0.0099423	0.198846
B	2	Sample X1	B	0.313	0.266	CaFr11	70.10116	9.9444089	0.0099444	0.198888
B	3	Blank B	C	0.059						
B	4	Control C1	C	0.664	0.605					
B	5	Control C1	C	0.666	0.607	0.605667				
B	6	Control C1	C	0.664	0.605					
B	7	Sample X1	C	0.581	0.522	CaFr12	13.81398	10.48967	0.0104897	0.209793
B	8	Sample X1	C	0.581	0.522	CaFr12	13.81398	10.48967	0.0104897	0.209793
B	9	Sample X1	C	0.583	0.524	CaFr12	13.48376	10.49393	0.0104939	0.209879
B	10	Blank B	D	0.067						
B	11	Control C1	D	0.762	0.695					
B	12	Control C1	D	0.764	0.697	0.696333				
C	1	Control C1	D	0.764	0.697					
C	2	Sample X1	D	0.614	0.547	CaFr21	21.44567	10.542918	0.0105429	0.210858
C	3	Sample X1	D	0.613	0.546	CaFr21	21.58928	10.540788	0.0105408	0.210816
C	4	Sample X1	D	0.614	0.547	CaFr21	21.44567	10.542918	0.0105429	0.210858
B	10	Blank B	D	0.838						
B	11	Control C1	D	1.034	0.196					
B	12	Control C1	D	1.034	0.196	0.197333				
C	1	Control C1	D	1.038	0.2					
C	2	Sample X1	D	0.938	0.1	CaXy11	49.32432	9.5908413	0.0095908	0.191817
C	3	Sample X1	D	0.938	0.1	CaXy11	49.32432	9.5908413	0.0095908	0.191817
C	4	Sample X1	D	0.938	0.1	CaXy11	49.32432	9.5908413	0.0095908	0.191817
C	5	Blank B	E	0.05						
C	6	Control C1	E	1.055	1.005					

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C	7	Control C1	E	1.056	1.006	1.005667				
C	8	Control C1	E	1.056	1.006					
C	9	Sample X1	E	0.822	0.772	CaXy12	23.235	11.022151	0.0110222	0.220443
C	10	Sample X1	E	0.821	0.771	CaXy12	23.33444	11.020021	0.01102	0.2204
C	11	Sample X1	E	0.822	0.772	CaXy12	23.235	11.022151	0.0110222	0.220443
B	3	Blank B	C	0.051						
B	4	Control C1	C	0.948	0.897					
B	5	Control C1	C	0.947	0.896	0.896333				
B	6	Control C1	C	0.947	0.896					
B	7	Sample X1	C	0.625	0.574	CaXy21	35.96132	10.600426	0.0106004	0.212009
B	8	Sample X1	C	0.625	0.574	CaXy21	35.96132	10.600426	0.0106004	0.212009
B	9	Sample X1	C	0.625	0.574	CaXy21	35.96132	10.600426	0.0106004	0.212009
C	12	Blank B	F	0.048						
D	1	Control C1	F	1.084	1.036					
D	2	Control C1	F	1.083	1.035	1.036333				
D	3	Control C1	F	1.086	1.038					
D	4	Sample X1	F	0.542	0.494	CaGr11	52.33194	10.430032	0.01043	0.208601
D	5	Sample X1	F	0.541	0.493	CaGr11	52.42843	10.427902	0.0104279	0.208558
D	6	Sample X1	F	0.543	0.495	CaGr11	52.23545	10.432162	0.0104322	0.208643
D	7	Blank B	G	0.049						
D	8	Control C1	G	0.775	0.726					
D	9	Control C1	G	0.775	0.726	0.485				
D	10	Control C1	G	0.778	0.003					
D	11	Sample X1	G	0.183	0.134	CaGr12	72.37113	9.7045989	0.0097046	0.194092
D	12	Sample X1	G	0.184	0.135	CaGr12	72.16495	9.6653887	0.0096654	0.193308
E	1	Sample X1	G	0.183	0.134	CaGr12	72.37113	9.6632588	0.0096633	0.193265
E	2	Blank B	H	0.054						
E	3	Control C1	H	0.962	0.908					
E	4	Control C1	H	0.961	0.907	0.909				
E	5	Control C1	H	0.966	0.912					
E	6	Sample X1	H	0.675	0.621	CaGr21	31.68317	10.700532	0.0107005	0.214011
E	7	Sample X1	H	0.678	0.624	CaGr21	31.35314	10.706922	0.0107069	0.214138
E	8	Sample X1	H	0.675	0.621	CaGr21	31.68317	10.700532	0.0107005	0.214011
E	9	Blank B	I	0.053						
E	10	Control C1	I	0.995	0.942					
E	11	Control C1	I	0.992	0.939	0.94				
E	12	Control C1	I	0.992	0.939					
F	1	Sample X1	I	0.854	0.801	CaGc11	14.78723	11.083919	0.0110839	0.221678
F	2	Sample X1	I	0.859	0.806	CaGc11	14.25532	11.094569	0.0110946	0.221891
F	3	Sample X1	I	0.859	0.806	CaGc11	14.25532	11.094569	0.0110946	0.221891
F	4	Blank B	J	0.051						
F	5	Control C1	J	0.594	0.543					

Appendix 10.12 contd.

F	6	Control C1	J	0.596	0.545	0.544667				
F	7	Control C1	J	0.597	0.546					
F	8	Sample X1	J	0.102	0.051	CaGc21	90.63647	9.486475	0.0094865	0.189729
F	9	Sample X1	J	0.099	0.048	CaGc21	91.18727	9.4800852	0.0094801	0.189602
F	10	Sample X1	J	0.101	0.05	CaGc21	90.82007	9.484345	0.0094843	0.189687
F	11	Blank B	K	0.046						
F	12	Control C1	K	1.068	1.022					
G	1	Control C1	K	1.069	1.023	1.022333				
G	2	Control C1	K	1.068	1.022					
G	3	Sample X1	K	0.708	0.662	CaGl11	35.24617	10.787859	0.0107879	0.215757
G	4	Sample X1	K	0.709	0.663	CaGl11	35.14835	10.789989	0.01079	0.2158
G	5	Sample X1	K	0.708	0.662	CaGl11	35.24617	10.787859	0.0107879	0.215757
G	6	Blank B	L	0.045						
G	7	Control C1	L	0.84	0.795					
G	8	Control C1	L	0.839	0.794	0.794333				
G	9	Control C1	L	0.839	0.794					
G	10	Sample X1	L	0.745	0.7	CaGl21	11.87579	10.868797	0.0108688	0.217376
G	11	Sample X1	L	0.745	0.7	CaGl21	11.87579	10.868797	0.0108688	0.217376
G	12	Sample X1	L	0.746	0.701	CaGl21	11.7499	10.870927	0.0108709	0.217419

Appendix 10.17 RCCDRSM DPPH run 17

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.05						
A	2	Control C1	A	1.554	1.504					
A	3	Control C1	A	1.554	1.504	1.505667				
A	4	Control C1	A	1.559	1.509					
A	5	Sample X1	A	1.161	1.111	CaSu11	26.21209	11.744196	0.0117442	0.117442
A	6	Sample X1	A	1.167	1.117	CaSu11	25.81359	11.756976	0.011757	0.11757
A	7	Sample X1	A	1.161	1.111	CaSu11	26.21209	11.744196	0.0117442	0.117442
A	8	Blank B	B	0.038						
A	9	Control C1	B	1.218	1.18					
A	10	Control C1	B	1.217	1.179	1.179667				
A	11	Control C1	B	1.218	1.18					
A	12	Sample X1	B	0.415	0.377	CaFr11	68.04182	10.180831	0.0101808	0.101808
B	1	Sample X1	B	0.415	0.377	CaFr11	68.04182	10.180831	0.0101808	0.101808
B	2	Sample X1	B	0.412	0.374	CaFr11	68.29613	10.174441	0.0101744	0.101744
B	3	Blank B	C	0.063						

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B	4	Control C1	C	0.965	0.902					
B	5	Control C1	C	0.964	0.901	0.901				
B	6	Control C1	C	0.963	0.9					
B	7	Sample X1	C	0.389	0.326	CaFr12	63.81798	10.072204	0.0100722	0.100722
B	8	Sample X1	C	0.387	0.324	CaFr12	64.03996	10.067945	0.0100679	0.100679
B	9	Sample X1	C	0.389	0.326	CaFr12	63.81798	10.072204	0.0100722	0.100722
B	10	Blank B	D	0.042						
B	11	Control C1	D	1.386	1.344					
B	12	Control C1	D	1.436	1.394	1.347				
C	1	Control C1	D	1.345	1.303					
C	2	Sample X1	D	1.04	0.998	CaFr21	25.90943	11.503514	0.0115035	0.115035
C	3	Sample X1	D	1.018	0.976	CaFr21	27.54269	11.456656	0.0114567	0.114567
C	4	Sample X1	D	1.063	1.021	CaFr21	24.20193	11.552503	0.0115525	0.115525
C	5	Blank B	E	0.685						
C	6	Control C1	E	0.992	0.307					
C	7	Control C1	E	0.992	0.307	0.308				
C	8	Control C1	E	0.995	0.31					
C	9	Sample X1	E	0.876	0.191	CaXy11	37.98701	9.7846645	0.0097847	0.097847
C	10	Sample X1	E	0.878	0.193	CaXy11	37.33766	9.7889244	0.0097889	0.097889
C	11	Sample X1	E	0.876	0.191	CaXy11	37.98701	9.7846645	0.0097847	0.097847
C	5	Blank B	E	0.027						
C	6	Control C1	E	1.419	1.392					
C	7	Control C1	E	1.416	1.389	1.391				
C	8	Control C1	E	1.419	1.392					
C	9	Sample X1	E	1.229	1.202	CaXy12	13.58735	11.938019	0.011938	0.11938
C	10	Sample X1	E	1.226	1.199	CaXy12	13.80302	11.931629	0.0119316	0.119316
C	11	Sample X1	E	1.226	1.199	CaXy12	13.80302	11.931629	0.0119316	0.119316
B	10	Blank B	D	0.039						
B	11	Control C1	D	0.974	0.935					
B	12	Control C1	D	0.972	0.933	0.934333				
C	1	Control C1	D	0.974	0.935					
C	2	Sample X1	D	0.585	0.546	CaXy21	41.56261	10.540788	0.0105408	0.105408
C	3	Sample X1	D	0.589	0.55	CaXy21	41.1345	10.549308	0.0105493	0.105493
C	4	Sample X1	D	0.585	0.546	CaXy21	41.56261	10.540788	0.0105408	0.105408
C	12	Blank B	F	0.046						
D	1	Control C1	F	1.386	1.34					
D	2	Control C1	F	1.386	1.34	1.340333				
D	3	Control C1	F	1.387	1.341					
D	4	Sample X1	F	0.987	0.941	CaGr11	29.79358	11.382109	0.0113821	113.8211
D	5	Sample X1	F	0.981	0.935	CaGr11	30.24123	11.369329	0.0113693	113.6933
D	6	Sample X1	F	0.981	0.935	CaGr11	30.24123	11.369329	0.0113693	113.6933
D	7	Blank B	G	0.046						

Appendix 10.17 contd.

D	8	Control C1	G	1.635	1.589					
D	9	Control C1	G	1.635	1.589	1.589667				
D	10	Control C1	G	1.637	1.591					
D	11	Sample X1	G	0.275	0.229	CaGr12	85.59446	9.8656017	0.0098656	0.098656
D	12	Sample X1	G	0.275	0.229	CaGr12	85.59446	9.8656017	0.0098656	0.098656
E	1	Sample X1	G	0.274	0.228	CaGr12	85.65737	9.8634718	0.0098635	0.098635
E	2	Blank B	H	0.041						
E	3	Control C1	H	1.752	1.711					
E	4	Control C1	H	1.756	1.715	1.713667				
E	5	Control C1	H	1.756	1.715					
E	6	Sample X1	H	0.973	0.932	CaGr21	45.61369	11.370205	0.0113702	0.113702
E	7	Sample X1	H	0.975	0.935	CaGr21	45.43863	11.376598	0.0113766	0.113766
E	8	Sample X1	H	0.973	0.932	CaGr21	45.61369	11.362939	0.0113629	0.113629
E	9	Blank B	I	0.026						
E	10	Control C1	I	1.258	1.232					
E	11	Control C1	I	1.257	1.231	1.231667				
E	12	Control C1	I	1.258	1.232					
F	1	Sample X1	I	0.856	0.83	CaGc11	32.61164	11.145687	0.0111457	0.111457
F	2	Sample X1	I	0.856	0.83	CaGc11	32.61164	11.145687	0.0111457	0.111457
F	3	Sample X1	I	0.854	0.828	CaGc11	32.77402	11.141427	0.0111414	0.111414
F	4	Blank B	J	0.049						
F	5	Control C1	J	1.465	1.416					
F	6	Control C1	J	1.463	1.414	1.415333				
F	7	Control C1	J	1.465	1.416					
F	8	Sample X1	J	0.166	0.117	CaGc21	91.7334	9.6270501	0.0096271	0.096271
F	9	Sample X1	J	0.164	0.115	CaGc21	91.87471	9.6227902	0.0096228	0.096228
F	10	Sample X1	J	0.166	0.117	CaGc21	91.7334	9.6270501	0.0096271	0.096271
F	11	Blank B	K	0.04						
F	12	Control C1	K	1.347	1.307					
G	1	Control C1	K	1.349	1.309	1.307667				
G	2	Control C1	K	1.347	1.307					
G	3	Sample X1	K	1.137	1.097	CaGl11	16.11012	11.714377	0.0117144	0.117144
G	4	Sample X1	K	1.139	1.099	CaGl11	15.95718	11.718637	0.0117186	0.117186
G	5	Sample X1	K	1.139	1.099	CaGl11	15.95718	11.718637	0.0117186	0.117186
G	6	Blank B	L	0.051						
G	7	Control C1	L	1.256	1.205					
G	8	Control C1	L	1.253	1.202	1.203				
G	9	Control C1	L	1.253	1.202					
G	10	Sample X1	L	0.895	0.844	CaGl21	29.84206	11.175506	0.0111755	0.111755
G	11	Sample X1	L	0.892	0.841	CaGl21	30.09144	11.169116	0.0111691	0.111691
G	12	Sample X1	L	0.895	0.844	CaGl21	29.84206	11.175506	0.0111755	0.111755

Appendix 10.18 RCCDRSM DPPH run 18

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.05						
A	2	Control C1	A	1.418	1.368					
A	3	Control C1	A	1.419	1.369	1.368333				
A	4	Control C1	A	1.418	1.368					
A	5	Sample X1	A	1.306	1.256	CaSu11	8.209501	12.053035	0.012053	0.482121
A	6	Sample X1	A	1.306	1.256	CaSu11	8.209501	12.053035	0.012053	0.482121
A	7	Sample X1	A	1.303	1.253	CaSu11	8.428745	12.046645	0.0120466	0.481866
A	8	Blank B	B	0.033						
A	9	Control C1	B	1.513	1.48					
A	10	Control C1	B	1.514	1.481	1.480667				
A	11	Control C1	B	1.514	1.481					
A	12	Sample X1	B	1.322	1.289	CaFr11	12.94462	12.123323	0.0121233	0.484933
B	1	Sample X1	B	1.321	1.288	CaFr11	13.01216	12.121193	0.0121212	0.484848
B	2	Sample X1	B	1.321	1.288	CaFr11	13.01216	12.121193	0.0121212	0.484848
B	3	Blank B	C	0.059						
B	4	Control C1	C	1.499	1.44					
B	5	Control C1	C	1.499	1.44	1.439667				
B	6	Control C1	C	1.498	1.439					
B	7	Sample X1	C	1.475	1.416	CaFr12	1.643899	12.393823	0.0123938	0.495753
B	8	Sample X1	C	1.478	1.419	CaFr12	1.435517	12.400213	0.0124002	0.496009
B	9	Sample X1	C	1.478	1.419	CaFr12	1.435517	12.400213	0.0124002	0.496009
B	10	Blank B	D	0.041						
B	11	Control C1	D	1.441	1.4					
B	12	Control C1	D	1.447	1.406	1.404				
C	1	Control C1	D	1.447	1.406					
C	2	Sample X1	D	1.426	1.385	CaFr21	1.353276	14.46975	0.0144698	0.57879
C	3	Sample X1	D	1.424	1.383	CaFr21	1.495726	12.323536	0.0123235	0.492941
C	4	Sample X1	D	1.426	1.385	CaFr21	1.353276	12.327796	0.0123278	0.493112
C	12	Blank B	F	0.62						
D	1	Control C1	F	0.736	0.116					
D	2	Control C1	F	0.733	0.113	0.115				
D	3	Control C1	F	0.736	0.116					
D	4	Sample X1	F	0.673	0.053	CaXy11	53.91304	9.4907348	0.0094907	0.379629
D	5	Sample X1	F	0.675	0.055	CaXy11	52.17391	9.4949947	0.009495	0.3798
D	6	Sample X1	F	0.673	0.053	CaXy11	53.91304	9.4907348	0.0094907	0.379629
C	5	Blank B	E	0.078						
C	6	Control C1	E	1.607	1.529					

Appendix 10.18 contd.

C	7	Control C1	E	1.606	1.528	1.528333				
C	8	Control C1	E	1.606	1.528					
C	9	Sample X1	E	1.586	1.508	CaXy12	1.330425	12.589776	0.0125898	0.503591
C	10	Sample X1	E	1.586	1.508	CaXy12	1.330425	12.589776	0.0125898	0.503591
C	11	Sample X1	E	1.585	1.507	CaXy12	1.395856	12.587646	0.0125876	0.503506
C	5	Blank B	E	0.035						
C	6	Control C1	E	0.795	0.76					
C	7	Control C1	E	0.792	0.757	0.759				
C	8	Control C1	E	0.795	0.76					
C	9	Sample X1	E	0.738	0.703	CaXy21	7.378129	10.875186	0.0108752	0.435007
C	10	Sample X1	E	0.739	0.703	CaXy21	7.378129	10.875186	0.0108752	0.435007
C	11	Sample X1	E	0.738	0.703	CaXy21	7.378129	10.875186	0.0108752	0.435007
C	12	Blank B	F	0.054						
D	1	Control C1	F	1.701	1.647					
D	2	Control C1	F	1.701	1.647	1.648667				
D	3	Control C1	F	1.706	1.652					
D	4	Sample X1	F	1.36	1.306	CaGr11	20.78447	12.896486	0.0128965	0.515859
D	5	Sample X1	F	1.367	1.313	CaGr11	20.35989	12.174441	0.0121744	0.486978
D	6	Sample X1	F	1.36	1.306	CaGr11	20.78447	12.159531	0.0121595	0.486381
D	7	Blank B	G	0.053						
D	8	Control C1	G	1.638	1.585					
D	9	Control C1	G	1.639	1.586	15.85333				
D	10	Control C1	G	1.638	1.585					
D	11	Sample X1	G	1.423	1.37	CaGr12 CaGr21	91.35828	12.295847	0.0122958	0.491834
D	12	Sample X1	G	1.428	1.37	CaGr12 CaGr21	91.35828	12.295847	0.0122958	0.491834
E	1	Sample X1	G	1.423	1.37	CaGr12 CaGr21	91.35828	12.295847	0.0122958	0.491834
E	2	Blank B	H	0.05						
E	3	Control C1	H	1.749	1.699					
E	4	Control C1	H	1.747	1.697	1.698333				
E	5	Control C1	H	1.749	1.699					
E	6	Sample X1	H	1.275	1.225	CaGr21	27.87046	11.987007	0.011987	0.47948
E	7	Sample X1	H	1.272	1.222	CaGr21	28.04711	11.980618	0.0119806	0.479225
E	8	Sample X1	H	1.275	1.225	CaGr21	27.87046	68.739854	0.0687399	2.749594
E	9	Blank B	I	0.064						
E	10	Control C1	I	1.308	1.244					
E	11	Control C1	I	1.305	1.241	1.243				
E	12	Control C1	I	1.308	1.244					
F	1	Sample X1	I	0.917	0.853	CaGc11	31.3757	11.194675	0.0111947	0.447787

Appendix 10.18 contd.

F	2	Sample X1	I	0.916	0.852	CaGc11	31.45615	11.192545	0.0111925	0.447702
F	3	Sample X1	I	0.916	0.852	CaGc11	31.45615	11.192545	0.0111925	0.447702
F	4	Blank B	J	0.061						
F	5	Control C1	J	1.798	1.737					
F	6	Control C1	J	1.799	1.738	1.737333	F			
F	7	Control C1	J	1.798	1.737					
F	8	Sample X1	J	1.237	1.176	CaGc21	32.31005	11.882641	0.0118826	0.475306
F	9	Sample X1	J	1.236	1.175	CaGc21	32.36761	11.880511	0.0118805	0.47522
F	10	Sample X1	J	1.236	1.175	CaGc21	32.36761	11.880511	0.0118805	0.047522
F	11	Blank B	K	0.042						
F	12	Control C1	K	1.268	1.226					
G	1	Control C1	K	1.266	1.224	1.225333				
G	2	Control C1	K	1.268	1.226					
G	3	Sample X1	K	1.053	1.011	CaGl11	17.49184	11.531203	0.0115312	0.461248
G	4	Sample X1	K	1.058	1.016	CaGl11	17.08379	11.541853	0.0115419	0.461674
G	5	Sample X1	K	1.053	1.011	CaGl11	17.49184	11.531203	0.0115312	0.461248
G	6	Blank B	L	0.125						
G	7	Control C1	L	0.808	0.683					
G	8	Control C1	L	0.806	0.681	0.681667				
G	9	Control C1	L	0.806	0.681					
G	10	Sample X1	L	0.798	0.673	CaGl21	1.271394	10.811289	0.0108113	0.432452
G	11	Sample X1	L	0.795	0.67	CaGl21	1.711491	10.804899	0.0108049	0.432196
G	12	Sample X1	L	0.795	0.67	CaGl21	1.711491	10.804899	0.0108049	0.432196

Appendix 10.19 RCCDRSM DPPH run 19

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.05						
A	2	Control C1	A	1.235	1.185					
A	3	Control C1	A	1.239	1.189	1.187333				
A	4	Control C1	A	1.238	1.188					
A	5	Sample X1	A	0.556	0.506	CaSu11	57.38349	10.455591	0.0104556	0.418224
A	6	Sample X1	A	0.556	0.506	CaSu11	57.38349	10.455591	0.0104556	0.418224
A	7	Sample X1	A	0.557	0.507	CaSu11	57.29927	10.457721	0.0104577	0.418309
A	8	Blank B	B	0.045						
A	9	Control C1	B	1.831	1.786					
A	10	Control C1	B	1.839	1.794	1.788667				
A	11	Control C1	B	1.831	1.786					

Appendix 10.19 contd.

A	12	Sample X1	B	1.424	1.379	CaFr11	22.90347	12.315016	0.012315	0.492601
B	1	Sample X1	B	1.422	1.377	CaFr11	23.01528	12.310756	0.0123108	0.49243
B	2	Sample X1	B	1.422	1.377	CaFr11	23.01528	12.310756	0.0123108	0.49243
B	3	Blank B	C	0.054						
B	4	Control C1	C	1.704	1.65					
B	5	Control C1	C	1.701	1.647	1.649				
B	6	Control C1	C	1.704	1.65					
B	7	Sample X1	C	1.294	1.24	CaFr12	24.80291	12.018956	0.012019	0.480758
B	8	Sample X1	C	1.294	1.24	CaFr12	24.80291	12.018956	0.012019	0.480758
B	9	Sample X1	C	1.29	1.236	CaFr12	25.04548	12.010437	0.0120104	0.480417
B	10	Blank B	D	0.038						
B	11	Control C1	D	1.682	1.644					
B	12	Control C1	D	1.682	1.644	1.644333				
C	1	Control C1	D	1.683	1.645					
C	2	Sample X1	D	1.525	1.487	CaFr21	9.568214	12.545048	0.012545	0.501802
C	3	Sample X1	D	1.521	1.483	CaFr21	9.811474	12.536528	0.0125365	0.501461
C	4	Sample X1	D	1.525	1.487	CaFr21	9.568214	12.545048	0.012545	0.501802
D	7	Blank B	G	0.786						
D	8	Control C1	G	0.855	0.069					
D	9	Control C1	G	0.855	0.069	0.07				
D	10	Control C1	G	0.858	0.072					
D	11	Sample X1	G	0.842	0.056	CaXy11	20	9.4971246	0.0094971	0.379885
D	12	Sample X1	G	0.842	0.056	CaXy11	20	9.4971246	0.0094971	0.379885
E	1	Sample X1	G	0.844	0.058	CaXy11	17.14286	9.5013845	0.0095014	0.380055
C	5	Blank B	E	0.043						
C	6	Control C1	E	1.619	1.576					
C	7	Control C1	E	1.619	1.576	1.575667				
C	8	Control C1	E	1.618	1.575					
C	9	Sample X1	E	1.474	1.431	CaXy12	9.181299	12.425772	0.0124258	0.497031
C	10	Sample X1	E	1.474	1.431	CaXy12	9.181299	12.425772	0.0124258	0.497031
C	11	Sample X1	E	1.475	1.432	CaXy12	9.117834	12.427902	0.0124279	0.497116
C	12	Blank B	F	0.044						
D	1	Control C1	F	1.128	1.084					
D	2	Control C1	F	1.128	1.084	1.084				
D	3	Control C1	F	1.128	1.084					
D	4	Sample X1	F	0.965	0.921	CaXy21	15.0369	11.33951	0.0113395	0.45358
D	5	Sample X1	F	0.967	0.923	CaXy21	14.8524	11.34377	0.0113438	0.453751
D	6	Sample X1	F	0.967	0.923	CaXy21	14.8524	11.34377	0.0113438	0.453751
C	12	Blank B	F	0.04						
D	1	Control C1	F	1.259	1.219					
D	2	Control C1	F	1.256	1.216	1.217				

Appendix 10.19 contd.

D	3	Control C1	F	1.256	1.216					
D	4	Sample X1	F	1.119	1.079	CaGr11	11.33936	11.676038	0.011676	0.467042
D	5	Sample X1	F	1.117	1.077	CaGr11	11.5037	11.671778	0.0116718	0.466871
D	6	Sample X1	F	1.119	1.079	CaGr11	11.33936	11.676038	0.011676	0.467042
D	7	Blank B	G	0.04						
D	8	Control C1	G	1.444	1.404					
D	9	Control C1	G	1.444	1.404	1.404667				
D	10	Control C1	G	1.446	1.406					
D	11	Sample X1	G	1.407	1.367	CaGr12	2.681538	12.289457	0.0122895	0.491578
D	12	Sample X1	G	1.407	1.367	CaGr12	2.681538	12.289457	0.0122895	0.491578
E	1	Sample X1	G	1.408	1.368	CaGr12	2.610346	12.291587	0.0122916	0.491663
E	2	Blank B	H	0.042						
E	3	Control C1	H	1.579	1.537					
E	4	Control C1	H	1.576	1.534	1.535				
E	5	Control C1	H	1.576	1.534					
E	6	Sample X1	H	1.352	1.31	CaGr21	14.65798	12.168051	0.0121681	0.486722
E	7	Sample X1	H	1.352	1.31	CaGr21	14.65798	12.168051	0.0121681	0.486722
E	8	Sample X1	H	1.354	1.312	CaGr21	14.52769	12.172311	0.0121723	0.486722
E	9	Blank B	I	0.047						
E	10	Control C1	I	2.105	2.058					
E	11	Control C1	I	2.103	2.056	2.057333				
E	12	Control C1	I	2.105	2.058					
F	1	Sample X1	I	0.999	0.952	CaGc11	53.72651	11.405538	0.0114055	0.456222
F	2	Sample X1	I	0.952	0.905	CaGc11	56.01102	11.305431	0.0113054	0.452217
F	3	Sample X1	I	0.954	0.907	CaGc11	55.9138	11.309691	0.0113097	0.452388
F	4	Blank B	J	0.051						
F	5	Control C1	J	1.668	1.617					
F	6	Control C1	J	1.668	1.617	1.616667				
F	7	Control C1	J	1.667	1.616					
F	8	Sample X1	J	1.345	1.294	CaGc21	19.95876	12.133972	0.012134	0.485359
F	9	Sample X1	J	1.344	1.293	CaGc21	20.02062	12.131842	0.0121318	0.485274
F	10	Sample X1	J	1.345	1.294	CaGc21	19.95876	12.133972	0.012134	0.485359
F	11	Blank B	K	0.048						
F	12	Control C1	K	2.069	2.021					
G	1	Control C1	K	2.069	2.021	2.019				
G	2	Control C1	K	2.063	2.015					
G	3	Sample X1	K	1.574	1.526	CaGl11	24.41803	12.628115	0.0126281	0.505125
G	4	Sample X1	K	1.577	1.529	CaGl11	24.26944	12.634505	0.0126345	0.50538
G	5	Sample X1	K	1.574	1.526	CaGl11	24.41803	12.628115	0.0126281	0.505125
G	6	Blank B	L	0.054						
G	7	Control C1	L	1.536	1.482					
G	8	Control C1	L	1.536	1.482	1.483				

Appendix 10.19 contd.

G	9	Control C1	L	1.539	1.485					
G	10	Sample X1	L	1.495	1.441	CaGl21	2.832097	12.447071	0.0124471	0.497883
G	11	Sample X1	L	1.492	1.438	CaGl21	3.03439	12.440682	0.0124407	0.497627
G	12	Sample X1	L	1.495	1.441	CaGl21	2.832097	12.447071	0.0124471	0.497883

Appendix 10.20 RCCDRSM DPPH run 20

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.046						
A	2	Control C1	A	1.384	1.338					
A	3	Control C1	A	1.384	1.338	1.338333				
A	4	Control C1	A	1.385	1.339					
A	5	Sample X1	A	0.372	0.326	CaSu11	75.64134	10.072204	0.0100722	0.402888
A	6	Sample X1	A	0.372	0.326	CaSu11	75.64134	10.072204	0.0100722	0.402888
A	7	Sample X1	A	0.375	0.329	CaSu11	75.41719	10.078594	0.0100786	0.403144
A	8	Blank B	B	0.047						
A	9	Control C1	B	1.586	1.539					
A	10	Control C1	B	1.585	1.538	1.538				
A	11	Control C1	B	1.584	1.537					
A	12	Sample X1	B	0.677	0.63	CaFr11	59.03771	10.719702	0.0107197	0.428788
B	1	Sample X1	B	0.673	0.626	CaFr11	59.29779	10.711182	0.0107112	0.428447
B	2	Sample X1	B	0.678	0.631	CaFr11	58.97269	10.721832	0.0107218	0.428873
B	3	Blank B	C	0.041						
B	4	Control C1	C	1.552	1.511					
B	5	Control C1	C	1.551	1.51	1.510333				
B	6	Control C1	C	1.551	1.51					
B	7	Sample X1	C	0.423	0.382	CaFr12	74.70757	10.19148	0.0101915	0.407659
B	8	Sample X1	C	0.424	0.383	CaFr12	74.64136	10.19361	0.0101936	0.407744
B	9	Sample X1	C	0.424	0.383	CaFr12	74.64136	10.19361	0.0101936	0.407744
B	10	Blank B	D	0.044						
B	11	Control C1	D	1.386	1.342					
B	12	Control C1	D	1.388	1.344	1.343333				
C	1	Control C1	D	1.388	1.344					
C	2	Sample X1	D	0.427	0.383	CaFr21	71.48883	10.19361	0.0101936	0.407744
C	3	Sample X1	D	0.425	0.381	CaFr21	71.63772	10.18935	0.0101894	0.407574
C	4	Sample X1	D	0.426	0.382	CaFr21	71.56328	10.19148	0.0101915	0.407659
E	2	Blank B	H	0.064						
E	3	Control C1	H	0.936	0.872					

Appendix 10.20 contd.

E	4	Control C1	H	0.936	0.872	0.873				
E	5	Control C1	H	0.939	0.875					
E	6	Sample X1	H	0.848	0.784	CaXy11	10.19473	11.04771	0.0110477	0.441908
E	7	Sample X1	H	0.846	0.782	CaXy11	10.42383	11.04345	0.0110435	0.441738
E	8	Sample X1	H	0.846	0.782	CaXy11	10.42383	11.04345	0.0110435	0.441738
C	5	Blank B	E	0.054						
C	6	Control C1	E	1.715	1.661					
C	7	Control C1	E	1.712	1.658	1.66				
C	8	Control C1	E	1.715	1.661					
C	9	Sample X1	E	0.627	0.573	CaXy12	65.48193	10.598296	0.0105983	0.423932
C	10	Sample X1	E	0.627	0.573	CaXy12	65.48193	10.598296	0.0105983	0.423932
C	11	Sample X1	E	0.623	0.569	CaXy12	65.72289	10.589776	0.0105898	0.423591
D	7	Blank B	G	0.039						
D	8	Control C1	G	1.044	1.005					
D	9	Control C1	G	1.046	1.007	1.005333				
D	10	Control C1	G	1.043	1.004					
D	11	Sample X1	G	0.726	0.687	CaXy21	31.66446	10.841108	0.0108411	0.433644
D	12	Sample X1	G	0.726	0.687	CaXy21	31.66446	10.841108	0.0108411	0.433644
E	1	Sample X1	G	0.728	0.689	CaXy21	31.46552	10.845367	0.0108454	0.433815
C	12	Blank B	F	0.052						
D	1	Control C1	F	1.613	1.561					
D	2	Control C1	F	1.614	1.562	1.561667				
D	3	Control C1	F	1.614	1.562					
D	4	Sample X1	F	0.758	0.706	CaGr11	54.79189	10.881576	0.0108816	0.435263
D	5	Sample X1	F	0.757	0.705	CaGr11	54.85592	10.879446	0.0108794	0.435178
D	6	Sample X1	F	0.757	0.705	CaGr11	54.85592	10.879446	0.0108794	0.435178
D	7	Blank B	G	0.048						
D	8	Control C1	G	2.122	2.074					
D	9	Control C1	G	2.121	2.073	2.073333				
D	10	Control C1	G	2.121	2.073					
D	11	Sample X1	G	0.544	0.496	CaGr12	76.07717	10.434292	0.0104343	0.417372
D	12	Sample X1	G	0.542	0.494	CaGr12	76.17363	10.430032	0.01043	0.417201
E	1	Sample X1	G	0.544	0.496	CaGr12	76.07717	10.434292	0.0104343	0.417372
E	2	Blank B	H	0.057						
E	3	Control C1	H	1.545	1.488					
E	4	Control C1	H	1.546	1.489	1.488667				
E	5	Control C1	H	1.546	1.489					
E	6	Sample X1	H	0.253	0.196	CaGr21	86.83386	9.7953142	0.0097953	0.391813
E	7	Sample X1	H	0.253	0.196	CaGr21	86.83386	9.7953142	0.0097953	0.391813
E	8	Sample X1	H	0.252	0.195	CaGr21	86.90103	9.7931842	0.0097932	0.391727
E	9	Blank B	I	0.058						
E	10	Control C1	I	1.635	1.577					

Appendix 10.20 contd.

E	11	Control C1	I	1.638	1.58	1.578				
E	12	Control C1	I	1.635	1.577					
F	1	Sample X1	I	0.315	0.257	CaGc11	83.71356	9.9252396	0.0099252	0.39701
F	2	Sample X1	I	0.315	0.257	CaGc11	83.71356	9.9252396	0.0099252	0.39701
F	3	Sample X1	I	0.319	0.261	CaGc11	83.46008	9.9337593	0.0099338	0.39735
F	4	Blank B	J	0.058						
F	5	Control C1	J	1.256	1.198					
F	6	Control C1	J	1.254	1.196	1.196667				
F	7	Control C1	J	1.254	1.196					
F	8	Sample X1	J	0.963	0.905	CaGc21	24.37326	11.305431	0.0113054	0.452217
F	9	Sample X1	J	0.962	0.904	CaGc21	24.37326	11.303301	0.0113033	0.452132
F	10	Sample X1	J	0.961	0.903	CaGc21	24.54039	11.301171	0.0113012	0.452047
F	11	Blank B	K	0.063						
F	12	Control C1	K	1.456	1.393					
G	1	Control C1	K	1.459	1.396	1.394				
G	2	Control C1	K	1.456	1.393					
G	3	Sample X1	K	0.617	0.554	CaGl11	60.25825	10.557827	0.0105578	0.422313
G	4	Sample X1	K	0.617	0.554	CaGl11	60.25825	10.557827	0.0105578	0.422313
G	5	Sample X1	K	0.615	0.552	CaGl11	60.40172	10.553568	0.0105536	0.422143
G	6	Blank B	L	0.059						
G	7	Control C1	L	1.289	1.23					
G	8	Control C1	L	1.288	1.229	1.229				
G	9	Control C1	L	1.287	1.228					
G	10	Sample X1	L	0.349	0.29	CaGl21	76.40358	9.9955272	0.0099955	0.399821
G	11	Sample X1	L	0.344	0.285	CaGl21	76.81041	9.9848775	0.0099849	0.399395
G	12	Sample X1	L	0.345	0.286	CaGl21	76.72905	9.9870075	0.009987	0.39948

Appendix 10.22 RCCDRSM DPPH run 22

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.044						
A	2	Control C1	A	0.832	0.788					
A	3	Control C1	A	0.835	0.791	0.789				
A	4	Control C1	A	0.832	0.788					
A	5	Sample X1	A	0.619	0.575	CaSu11	27.12294	10.602556	0.0106026	0.530128
A	6	Sample X1	A	0.616	0.572	CaSu11	27.50317	10.596166	0.0105962	0.529808
A	7	Sample X1	A	0.616	0.572	CaSu11	27.50317	10.596166	0.0105962	0.529808
A	8	Blank B	B	0.046						

Appendix 10.22 contd.

A	9	Control C1	B	0.889	0.843					
A	10	Control C1	B	0.886	0.84	0.842				
A	11	Control C1	B	0.889	0.843					
A	12	Sample X1	B	0.186	0.14	CaFr11	83.37292	9.6760383	0.009676	0.483802
B	1	Sample X1	B	0.187	0.141	CaFr11	83.25416	9.6781683	0.0096782	0.483908
B	2	Sample X1	B	0.186	0.14	CaFr11	83.37292	9.6760383	0.009676	0.483802
B	3	Blank B	C	0.477						
B	4	Control C1	C	1.076	0.599					
B	5	Control C1	C	1.074	0.597	0.598333				
B	6	Control C1	C	1.076	0.599					
B	7	Sample X1	C	0.634	0.157	CaFr12	73.76045	9.7122471	0.0097122	0.485612
B	8	Sample X1	C	0.637	0.16	CaFr12	73.25905	9.7186368	0.0097186	0.485932
B	9	Sample X1	C	0.634	0.157	CaFr12	73.76045	9.7122471	0.0097122	0.485612
B	10	Blank B	D	0.065						
B	11	Control C1	D	0.817	0.752					
B	12	Control C1	D	0.817	0.752	0.752667				
C	1	Control C1	D	0.819	0.754					
C	2	Sample X1	D	0.815	0.75	CaFr21	0.354296	10.975293	0.0109753	0.548765
C	3	Sample X1	D	0.815	0.75	CaFr21	0.354296	10.975293	0.0109753	0.548765
C	4	Sample X1	D	0.812	0.747	CaFr21	0.752879	10.968903	0.0109689	0.548445
A	1	Blank B	A	0.04						
A	2	Control C1	A	0.904	0.864					
A	3	Control C1	A	0.901	0.861	0.863333				
A	4	Control C1	A	0.905	0.865					
A	5	Sample X1	A	0.884	0.844	CaXy11	2.239382	11.175506	0.0111755	0.558775
A	6	Sample X1	A	0.883	0.843	CaXy11	2.355212	11.173376	0.0111734	0.558669
A	7	Sample X1	A	0.883	0.843	CaXy11	2.355212	11.173376	0.0111734	0.446935
C	5	Blank B	E	0.027						
C	6	Control C1	E	0.928	0.901					
C	7	Control C1	E	0.928	0.901	0.900667				
C	8	Control C1	E	0.927	0.9					
C	9	Sample X1	E	0.873	0.846	CaXy12	6.069578	11.179766	0.0111798	0.558988
C	10	Sample X1	E	0.873	0.846	CaXy12	6.069578	11.179766	0.0111798	0.558988
C	11	Sample X1	E	0.874	0.847	CaXy12	5.958549	11.181896	0.0111819	0.559095
E	2	Blank B	H	0.04						
E	3	Control C1	H	0.954	0.914					
E	4	Control C1	H	0.951	0.911	0.912333				
E	5	Control C1	H	0.952	0.912					
E	6	Sample X1	H	0.861	0.821	CaXy21	10.01096	11.126518	0.0111265	0.556326
E	7	Sample X1	H	0.863	0.823	CaXy21	9.791743	11.130777	0.0111308	0.556539
E	8	Sample X1	H	0.861	0.821	CaXy21	10.01096	11.126518	0.0111265	0.556326
C	12	Blank B	F	0.045						

D	1	Control C1	F	0.846	0.801					
D	2	Control C1	F	0.845	0.8	0.800667				
D	3	Control C1	F	0.846	0.801					
D	4	Sample X1	F	0.756	0.711	CaGr11	11.199	10.892226	0.0108922	0.435689
D	5	Sample X1	F	0.756	0.711	CaGr11	11.199	10.892226	0.0108922	0.544611
D	6	Sample X1	F	0.757	0.712	CaGr11	11.0741	10.894356	0.0108944	0.544718
D	7	Blank B	G	0.049						
D	8	Control C1	G	0.985	0.936					
D	9	Control C1	G	0.982	0.933	0.933667				
D	10	Control C1	G	0.981	0.932					
D	11	Sample X1	G	0.701	0.652	CaGr12	30.1678	10.76656	0.0107666	0.538328
D	12	Sample X1	G	0.704	0.655	CaGr12	29.84648	10.77295	0.0107729	0.538647
E	1	Sample X1	G	0.706	0.657	CaGr12	29.63227	10.77721	0.0107772	0.53886
E	2	Blank B	H	0.045						
E	3	Control C1	H	0.983	0.938					
E	4	Control C1	H	0.982	0.937	0.938667				
E	5	Control C1	H	0.986	0.941					
E	6	Sample X1	H	0.845	0.8	CaGr21	14.77273	11.081789	0.0110818	0.554089
E	7	Sample X1	H	0.844	0.799	CaGr21	14.87926	11.079659	0.0110797	0.553983
E	8	Sample X1	H	0.847	0.802	CaGr21	14.55966	11.086049	0.011086	0.554302
E	9	Blank B	I	0.051						
E	10	Control C1	I	1.016	0.965					
E	11	Control C1	I	1.017	0.966	0.963667				
E	12	Control C1	I	1.011	0.96					
F	1	Sample X1	I	0.952	0.901	CaGc11	6.50294	11.296912	0.0112969	0.564846
F	2	Sample X1	I	0.952	0.901	CaGc11	6.50294	11.296912	0.0112969	0.564846
F	3	Sample X1	I	0.952	0.901	CaGc11	6.50294	11.296912	0.0112969	0.564846
F	4	Blank B	J	0.052						
F	5	Control C1	J	0.826	0.774					
F	6	Control C1	J	0.823	0.771	0.773				
F	7	Control C1	J	0.826	0.774					
F	8	Sample X1	J	0.627	0.575	CaGc21	25.61449	11.026411	0.0110264	0.551321
F	9	Sample X1	J	0.625	0.573	CaGc21	25.87322	10.598296	0.0105983	0.529915
F	10	Sample X1	J	0.625	0.573	CaGc21	25.87322	10.598296	0.0105983	0.529915
F	11	Blank B	K	0.046						
F	12	Control C1	K	0.754	0.708					
G	1	Control C1	K	0.754	0.708	0.708333				
G	2	Control C1	K	0.755	0.709					
G	3	Sample X1	K	0.701	0.655	CaGl11	7.529412	10.77295	0.0107729	0.538647
G	4	Sample X1	K	0.705	0.659	CaGl11	6.964706	10.78147	0.0107815	0.539073
G	5	Sample X1	K	0.705	0.659	CaGl11	6.964706	10.78147	0.0107815	0.539073

Appendix 10.22 contd.

G	6	Blank B	L	0.058						
G	7	Control C1	L	0.843	0.785					
G	8	Control C1	L	0.845	0.787	0.785667				
G	9	Control C1	L	0.843	0.785					
G	10	Sample X1	L	0.737	0.679	CaGl21	13.57658	10.824068	0.0108241	0.541203
G	11	Sample X1	L	0.732	0.674	CaGl21	14.21298	10.813419	0.0108134	0.540671
G	12	Sample X1	L	0.737	0.679	CaGl21	13.57658	10.824068	0.0108241	0.541203

Appendix 10.23 RCCDRSM DPPH run 23

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.056						
A	2	Control C1	A	0.604	0.548					
A	3	Control C1	A	0.607	0.551	0.55				
A	4	Control C1	A	0.607	0.551					
A	5	Sample X1	A	0.462	0.406	CaSu11	26.18182	10.242599	0.0102426	0.153639
A	6	Sample X1	A	0.462	0.406	CaSu11	26.18182	10.242599	0.0102426	0.153639
A	7	Sample X1	A	0.465	0.409	CaSu11	25.63636	10.248988	0.010249	0.153735
A	8	Blank B	B	0.041						
A	9	Control C1	B	0.751	0.71					
A	10	Control C1	B	0.751	0.71	0.712667				
A	11	Control C1	B	0.759	0.718					
A	12	Sample X1	B	0.201	0.16	CaFr11	77.54911	9.7186368	0.0097186	0.14578
B	1	Sample X1	B	0.208	0.167	CaFr11	76.56688	9.7335463	0.0097335	0.146003
B	2	Sample X1	B	0.208	0.167	CaFr11	76.56688	9.7335463	0.0097335	0.146003
B	3	Blank B	C	0.091						
B	4	Control C1	C	0.761	0.67					
B	5	Control C1	C	0.763	0.672	0.671				
B	6	Control C1	C	0.762	0.671					
B	7	Sample X1	C	0.625	0.534	CaFr12	20.41729	10.515229	0.0105152	0.157728
B	8	Sample X1	C	0.625	0.534	CaFr12	20.41729	10.515229	0.0105152	0.157728
B	9	Sample X1	C	0.623	0.532	CaFr12	20.71535	10.510969	0.010511	0.157665
B	10	Blank B	D	0.045						
B	11	Control C1	D	0.902	0.857					
B	12	Control C1	D	0.906	0.861	0.858333				
C	1	Control C1	D	0.902	0.857					
C	2	Sample X1	D	0.672	0.627	CaFr21	26.95146	10.713312	0.0107133	0.1607
C	3	Sample X1	D	0.672	0.627	CaFr21	26.95146	10.713312	0.0107133	0.1607
C	4	Sample X1	D	0.676	0.631	CaFr21	26.48544	10.721832	0.0107218	0.160827

Appendix 10.23 contd.

A	8	Blank B	B	0.034						
A	9	Control C1	B	0.821	0.787					
A	10	Control C1	B	0.824	0.79	0.789				
A	11	Control C1	B	0.824	0.79					
A	12	Sample X1	B	0.664	0.63	CaXy11	20.15209	10.719702	0.0107197	0.160796
B	1	Sample X1	B	0.663	0.629	CaXy11	20.27883	10.717572	0.0107176	0.160764
B	2	Sample X1	B	0.664	0.63	CaXy11	20.15209	10.719702	0.0107197	0.160796
C	5	Blank B	E	0.052						
C	6	Control C1	E	0.712	0.66					
C	7	Control C1	E	0.712	0.66	0.66				
C	8	Control C1	E	0.712	0.66					
C	9	Sample X1	E	0.657	0.605	CaXy12	8.333333	10.666454	0.0106665	0.159997
C	10	Sample X1	E	0.653	0.601	CaXy12	8.939394	10.657934	0.0106579	0.159869
C	11	Sample X1	E	0.657	0.605	CaXy12	8.333333	10.666454	0.0106665	0.159997
A	1	Blank B	A	0.059						
A	2	Control C1	A	1.297	1.238					
A	3	Control C1	A	1.298	1.239	1.238667				
A	4	Control C1	A	1.298	1.239					
A	5	Sample X1	A	0.408	0.349	CaXy21	71.82454	10.121193	0.0101212	0.151818
A	6	Sample X1	A	0.409	0.35	CaXy21	71.74381	10.123323	0.0101233	0.15185
A	7	Sample X1	A	0.408	0.349	CaXy21	71.82454	10.121193	0.0101212	0.151818
C	12	Blank B	F	0.035						
D	1	Control C1	F	0.865	0.83					
D	2	Control C1	F	0.865	0.83	0.830333				
D	3	Control C1	F	0.866	0.831					
D	4	Sample X1	F	0.655	0.62	CaGr11	25.33119	10.698403	0.0106984	0.160476
D	5	Sample X1	F	0.655	0.62	CaGr11	25.33119	10.698403	0.0106984	0.160476
D	6	Sample X1	F	0.651	0.616	CaGr11	25.81293	10.689883	0.0106899	0.160348
D	7	Blank B	G	0.044						
D	8	Control C1	G	0.863	0.819					
D	9	Control C1	G	0.862	0.818	0.818333				
D	10	Control C1	G	0.862	0.818					
D	11	Sample X1	G	0.219	0.175	CaGr12	78.61507	9.7505857	0.0097506	0.146259
D	12	Sample X1	G	0.215	0.171	CaGr12	79.10387	9.742066	0.0097421	0.146131
E	1	Sample X1	G	0.215	0.171	CaGr12	79.10387	9.742066	0.0097421	0.146131
E	2	Blank B	H	0.04						
E	3	Control C1	H	0.805	0.765					
E	4	Control C1	H	0.805	0.765	0.763667				
E	5	Control C1	H	0.801	0.761					
E	6	Sample X1	H	0.539	0.499	CaGr21	34.65735	10.440682	0.0104407	0.15661
E	7	Sample X1	H	0.539	0.499	CaGr21	34.65735	10.440682	0.0104407	0.15661
E	8	Sample X1	H	0.537	0.497	CaGr21	34.91925	10.436422	0.0104364	0.156546

Appendix 10.23 contd.

E	9	Blank B	I	0.034						
E	10	Control C1	I	0.803	0.769					
E	11	Control C1	I	0.804	0.77	0.769333				
E	12	Control C1	I	0.803	0.769					
F	1	Sample X1	I	0.578	0.544	CaGc11	29.28943	10.536528	0.0105365	0.158048
F	2	Sample X1	I	0.578	0.544	CaGc11	29.28943	10.536528	0.0105365	0.158048
F	3	Sample X1	I	0.579	0.545	CaGc11	29.15945	10.538658	0.0105387	0.15808
F	4	Blank B	J	0.053						
F	5	Control C1	J	0.905	0.852					
F	6	Control C1	J	0.905	0.852	0.852333				
F	7	Control C1	J	0.906	0.853					
F	8	Sample X1	J	0.208	0.155	CaGc21	81.81463	9.7079872	0.009708	0.14562
F	9	Sample X1	J	0.208	0.155	CaGc21	81.81463	9.7079872	0.009708	0.14562
F	10	Sample X1	J	0.209	0.156	CaGc21	81.6973	9.7101171	0.0097101	0.145652
F	11	Blank B	K	0.036						
F	12	Control C1	K	0.899	0.863					
G	1	Control C1	K	0.899	0.863	0.861667				
G	2	Control C1	K	0.895	0.859					
G	3	Sample X1	K	0.678	0.642	CaGl11	25.49323	10.745261	0.0107453	0.161179
G	4	Sample X1	K	0.672	0.636	CaGl11	26.18956	10.732481	0.0107325	0.160987
G	5	Sample X1	K	0.678	0.642	CaGl11	25.49323	10.745261	0.0107453	0.161179
G	6	Blank B	L	0.035						
G	7	Control C1	L	0.936	0.901					
G	8	Control C1	L	0.938	0.903	0.902333				
G	9	Control C1	L	0.938	0.903					
G	10	Sample X1	L	0.724	0.689	CaGl21	23.64241	10.845367	0.0108454	0.162681
G	11	Sample X1	L	0.725	0.69	CaGl21	23.53158	10.847497	0.0108475	0.162712
G	12	Sample X1	L	0.724	0.689	CaGl21	23.64241	10.845367	0.0108454	0.162681

Appendix 10.25 RCCDRSM DPPH run 25

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.062						
A	2	Control C1	A	0.625	0.563					
A	3	Control C1	A	0.627	0.565	0.563667				
A	4	Control C1	A	0.625	0.563					
A	5	Sample X1	A	0.526	0.464	CaSu11	17.68185	10.366134	0.0103661	0.310984
A	6	Sample X1	A	0.529	0.467	CaSu11	17.14962	10.372524	0.0103725	0.311176

Appendix 10.25 contd.

A	7	Sample X1	A	0.528	0.466	CaSu11	17.32703	10.370394	0.0103704	0.311112
A	8	Blank B	B	0.034						
A	9	Control C1	B	0.874	0.84					
A	10	Control C1	B	0.873	0.839	0.849333				
A	11	Control C1	B	0.873	0.869					
A	12	Sample X1	B	0.192	0.158	CaFr11	81.39717	9.714377	0.0097144	0.291431
B	1	Sample X1	B	0.193	0.159	CaFr11	81.27943	9.7165069	0.0097165	0.291495
B	2	Sample X1	B	0.192	0.158	CaFr11	81.39717	9.714377	0.0097144	0.291431
B	3	Blank B	C	0.046						
B	4	Control C1	C	0.705	0.659					
B	5	Control C1	C	0.703	0.657	0.658				
B	6	Control C1	C	0.704	0.658					
B	7	Sample X1	C	0.558	0.512	CaFr12	22.18845	10.468371	0.0104684	0.314051
B	8	Sample X1	C	0.558	0.512	CaFr12	22.18845	10.468371	0.0104684	0.314051
B	9	Sample X1	C	0.553	0.507	CaFr12	22.94833	10.457721	0.0104577	0.313732
B	10	Blank B	D	0.05						
B	11	Control C1	D	0.827	0.777					
B	12	Control C1	D	0.826	0.776	0.776667				
C	1	Control C1	D	0.827	0.777					
C	2	Sample X1	D	0.596	0.546	CaFr21	29.69957	10.540788	0.0105408	0.316224
C	3	Sample X1	D	0.597	0.547	CaFr21	29.57082	10.542918	0.0105429	0.316288
C	4	Sample X1	D	0.597	0.547	CaFr21	29.57082	10.542918	0.0105429	0.316288
B	3	Blank B	C	0.04						
B	4	Control C1	C	0.796	0.756					
B	5	Control C1	C	0.797	0.757	0.755667				
B	6	Control C1	C	0.794	0.754					
B	7	Sample X1	C	0.653	0.613	CaXy11	18.87958	10.683493	0.0106835	0.320505
B	8	Sample X1	C	0.657	0.617	CaXy11	18.35024	10.692013	0.010692	0.32076
B	9	Sample X1	C	0.653	0.613	CaXy11	18.87958	10.683493	0.0106835	0.320505
C	5	Blank B	E	0.049						
C	6	Control C1	E	0.758	0.709					
C	7	Control C1	E	0.758	0.709	0.709333				
C	8	Control C1	E	0.759	0.71					
C	9	Sample X1	E	0.718	0.669	CaXy12	5.68609	10.802769	0.0108028	0.324083
C	10	Sample X1	E	0.715	0.666	CaXy12	6.109023	10.796379	0.0107964	0.323891
C	11	Sample X1	E	0.718	0.669	CaXy12	5.68609	10.802769	0.0108028	0.324083
A	8	Blank B	B	0.041						
A	9	Control C1	B	1.129	1.088					
A	10	Control C1	B	1.129	1.088	1.087667				
A	11	Control C1	B	1.128	1.087					
A	12	Sample X1	B	0.763	0.722	CaXy21	33.61937	10.915655	0.0109157	0.32747
B	1	Sample X1	B	0.763	0.722	CaXy21	33.61937	10.915655	0.0109157	0.32747

Appendix 10.25 contd.

B	2	Sample X1	B	0.763	0.722	CaXy21	33.61937	10.915655	0.0109157	0.32747
C	12	Blank B	F	0.051						
D	1	Control C1	F	0.748	0.697					
D	2	Control C1	F	0.749	0.698	0.697667				
D	3	Control C1	F	0.749	0.698					
D	4	Sample X1	F	0.661	0.61	CaGr11	12.5657	10.677103	0.0106771	0.320313
D	5	Sample X1	F	0.661	0.61	CaGr11	12.5657	10.677103	0.0106771	0.320313
D	6	Sample X1	F	0.662	0.611	CaGr11	12.42236	10.679233	0.0106792	0.320377
D	7	Blank B	G	0.044						
D	8	Control C1	G	0.858	0.814					
D	9	Control C1	G	0.857	0.813	0.811333				
D	10	Control C1	G	0.851	0.807					
D	11	Sample X1	G	0.654	0.61	CaGr12	24.81512	10.818956	0.010819	0.324569
D	12	Sample X1	G	0.652	0.608	CaGr12	25.06163	10.672843	0.0106728	0.320185
E	1	Sample X1	G	0.654	0.61	CaGr12	24.81512	10.677103	0.0106771	0.320313
E	2	Blank B	H	0.049						
E	3	Control C1	H	0.91	0.861					
E	4	Control C1	H	0.919	0.87	0.864				
E	5	Control C1	H	0.91	0.861					
E	6	Sample X1	H	0.694	0.645	CaGr21	25.34722	10.751651	0.0107517	0.32255
E	7	Sample X1	H	0.696	0.647	CaGr21	25.11574	10.755911	0.0107559	0.322677
E	8	Sample X1	H	0.694	0.645	CaGr21	25.34722	10.751651	0.0107517	0.32255
E	9	Blank B	I	0.031						
E	10	Control C1	I	0.689	0.658					
E	11	Control C1	I	0.681	0.65	0.652667				
E	12	Control C1	I	0.681	0.65					
F	1	Sample X1	I	0.552	0.521	CaGc11	20.17365	10.48754	0.0104875	0.314626
F	2	Sample X1	I	0.552	0.521	CaGc11	20.17365	10.48754	0.0104875	0.314626
F	3	Sample X1	I	0.552	0.521	CaGc11	20.17365	10.48754	0.0104875	0.314626
F	4	Blank B	J	0.051						
F	5	Control C1	J	0.885	0.834					
F	6	Control C1	J	0.883	0.832	0.833333				
F	7	Control C1	J	0.885	0.834					
F	8	Sample X1	J	0.498	0.447	CaGc21	46.36	10.329925	0.0103299	0.309898
F	9	Sample X1	J	0.498	0.447	CaGc21	46.36	10.329925	0.0103299	0.309898
F	10	Sample X1	J	0.496	0.445	CaGc21	46.6	10.325666	0.0103257	0.30977
F	11	Blank B	K	0.037						
F	12	Control C1	K	0.967	0.93					
G	1	Control C1	K	0.966	0.929	0.929333				
G	2	Control C1	K	0.966	0.929					
G	3	Sample X1	K	0.754	0.717	CaGl11	22.84792	10.905005	0.010905	0.32715
G	4	Sample X1	K	0.758	0.721	CaGl11	22.4175	10.913525	0.0109135	0.327406

Appendix 10.25 contd.

G	5	Sample X1	K	0.758	0.721	CaGl11	22.4175	10.913525	0.0109135	0.327406
G	6	Blank B	L	0.103						
G	7	Control C1	L	0.755	0.652					
G	8	Control C1	L	0.755	0.652	0.651667				
G	9	Control C1	L	0.754	0.651					
G	10	Sample X1	L	0.643	0.54	CaGl21	17.13555	10.528009	0.010528	0.31584
G	11	Sample X1	L	0.648	0.545	CaGl21	16.36829	10.538658	0.0105387	0.31616
G	12	Sample X1	L	0.648	0.545	CaGl21	16.36829	10.538658	0.0105387	0.31616

Appendix 10.26 RCCDRSM DPPH run 26

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/ml)	DPPH (µMTE/g)
A	1	Blank B	A	0.05						
A	2	Control C1	A	0.716	0.666					
A	3	Control C1	A	0.717	0.667	0.666333				
A	4	Control C1	A	0.716	0.666					
A	5	Sample X1	A	0.374	0.324	CaSu11	51.37569	10.067945	0.0100679	0.302038
A	6	Sample X1	A	0.377	0.327	CaSu11	50.92546	10.074334	0.0100743	0.30223
A	7	Sample X1	A	0.377	0.327	CaSu11	50.92546	10.074334	0.0100743	0.30223
A	8	Blank B	B	0.04						
A	9	Control C1	B	0.674	0.634					
A	10	Control C1	B	0.674	0.634	0.634333				
A	11	Control C1	B	0.675	0.635					
A	12	Sample X1	B	0.393	0.353	CaFr11	44.35102	10.129712	0.0101297	0.303891
B	1	Sample X1	B	0.394	0.354	CaFr11	44.19338	10.131842	0.0101318	0.303955
B	2	Sample X1	B	0.394	0.354	CaFr11	44.19338	10.131842	0.0101318	0.303955
B	3	Blank B	C	0.043						
B	4	Control C1	C	0.901	0.858					
B	5	Control C1	C	0.901	0.858	0.858				
B	6	Control C1	C	0.901	0.858					
B	7	Sample X1	C	0.768	0.725	CaFr12	15.50117	10.922045	0.010922	0.327661
B	8	Sample X1	C	0.768	0.725	CaFr12	15.50117	10.922045	0.010922	0.327661
B	9	Sample X1	C	0.768	0.725	CaFr12	15.50117	10.922045	0.010922	0.327661
B	10	Blank B	D	0.044						
B	11	Control C1	D	0.968	0.924					
B	12	Control C1	D	0.967	0.923	0.923667				
C	1	Control C1	D	0.968	0.924					
C	2	Sample X1	D	0.592	0.548	CaFr2	40.67124	10.545048	0.010545	0.316351

Appendix 10.26 contd.

C	3	Sample X1	D	0.592	0.548	CaFr21	40.67124	10.545048	0.010545	0.316351
C	4	Sample X1	D	0.592	0.548	CaFr21	40.67124	10.545048	0.010545	0.316351
B	10	Blank B	D	0.052						
B	11	Control C1	D	0.826	0.774					
B	12	Control C1	D	0.827	0.775	0.774				
C	1	Control C1	D	0.825	0.773					
C	2	Sample X1	D	0.238	0.186	CaXy11	75.96899	9.7740149	0.009774	0.29322
C	3	Sample X1	D	0.238	0.186	CaXy11	75.96899	9.7740149	0.009774	0.29322
C	4	Sample X1	D	0.239	0.187	CaXy11	75.83979	9.7761448	0.0097761	0.293284
C	5	Blank B	E	0.048						
C	6	Control C1	E	0.479	0.431					
C	7	Control C1	E	0.475	0.427	0.429333				
C	8	Control C1	E	0.478	0.43					
C	9	Sample X1	E	0.385	0.337	CaXy12	21.50621	10.095634	0.0100956	0.302869
C	10	Sample X1	E	0.382	0.334	CaXy12	22.20497	10.089244	0.0100892	0.302677
C	11	Sample X1	E	0.382	0.334	CaXy12	22.20497	10.089244	0.0100892	0.302677
B	3	Blank B	C	0.048						
B	4	Control C1	C	0.814	0.766					
B	5	Control C1	C	0.814	0.766	0.766667				
B	6	Control C1	C	0.816	0.768					
B	7	Sample X1	C	0.633	0.585	CaXy21	23.69565	10.623855	0.0106239	0.318716
B	8	Sample X1	C	0.638	0.59	CaXy21	23.04348	10.634505	0.0106345	0.319035
B	9	Sample X1	C	0.633	0.585	CaXy21	23.69565	10.623855	0.0106239	0.318716
C	12	Blank B	F	0.046						
D	1	Control C1	F	0.726	0.68					
D	2	Control C1	F	0.726	0.68	0.679667				
D	3	Control C1	F	0.725	0.679					
D	4	Sample X1	F	0.561	0.515	CaGr11	24.22756	10.47476	0.0104748	0.314243
D	5	Sample X1	F	0.565	0.519	CaGr11	23.63904	10.48328	0.0104833	0.314498
D	6	Sample X1	F	0.561	0.515	CaGr11	24.22756	10.47476	0.0104748	0.314243
D	7	Blank B	G	0.04						
D	8	Control C1	G	0.837	0.797					
D	9	Control C1	G	0.838	0.798	0.798				
D	10	Control C1	G	0.839	0.799					
D	11	Sample X1	G	0.512	0.472	CaGr12	40.85213	10.383174	0.0103832	0.311495
D	12	Sample X1	G	0.514	0.474	CaGr12	40.6015	10.387433	0.0103874	0.311623
E	1	Sample X1	G	0.514	0.474	CaGr12	40.6015	10.387433	0.0103874	0.311623
E	2	Blank B	H	0.043						
E	3	Control C1	H	0.668	0.625					
E	4	Control C1	H	0.662	0.619	0.621				
E	5	Control C1	H	0.662	0.619					
E	6	Sample X1	H	0.574	0.531	CaGr21	14.49275	10.508839	0.0105088	0.315265

Appendix 10.26 contd.

E	7	Sample X1	H	0.574	0.531	CaGr21	14.49275	10.508839	0.0105088	0.315265
E	8	Sample X1	H	0.574	0.531	CaGr21	14.49275	10.508839	0.0105088	0.315265
E	9	Blank B	I	0.037						
E	10	Control C1	I	0.731	0.694					
E	11	Control C1	I	0.736	0.699	0.695667				
E	12	Control C1	I	0.731	0.694					
F	1	Sample X1	I	0.552	0.515	CaGc11	25.97029	10.47476	0.0104748	0.314243
F	2	Sample X1	I	0.553	0.516	CaGc11	25.82655	10.47689	0.0104769	0.314307
F	3	Sample X1	I	0.552	0.515	CaGc11	25.97029	10.47476	0.0104748	0.314243
F	4	Blank B	J	0.047						
F	5	Control C1	J	0.835	0.788					
F	6	Control C1	J	0.835	0.788	0.788333				
F	7	Control C1	J	0.836	0.789					
F	8	Sample X1	J	0.261	0.214	CaGc21	72.85412	9.8336528	0.0098337	0.29501
F	9	Sample X1	J	0.261	0.214	CaGc21	72.85412	9.8336528	0.0098337	0.29501
F	10	Sample X1	J	0.261	0.214	CaGc21	72.85412	9.8336528	0.0098337	0.29501
F	11	Blank B	K	0.046						
F	12	Control C1	K	0.786	0.74					
G	1	Control C1	K	0.782	0.736	0.738667				
G	2	Control C1	K	0.786	0.74					
G	3	Sample X1	K	0.656	0.61	CaGl11	17.41877	10.677103	0.0106771	0.320313
G	4	Sample X1	K	0.656	0.61	CaGl11	17.41877	10.677103	0.0106771	0.320313
G	5	Sample X1	K	0.658	0.612	CaGl11	17.14801	10.681363	0.0106771	0.320313
G	6	Blank B	L	0.048						
G	7	Control C1	L	0.785	0.737					
G	8	Control C1	L	0.785	0.737	0.737333				
G	9	Control C1	L	0.786	0.738					
G	10	Sample X1	L	0.726	0.678	CaGl21	8.047016	10.821938	0.0108219	0.324658
G	11	Sample X1	L	0.727	0.679	CaGl21	7.911392	10.824068	0.0108241	0.324722
G	12	Sample X1	L	0.727	0.679	CaGl21	7.911392	10.824068	0.0108241	0.324722

Appendix 10.27 RCCDRSM DPPH run 27

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH µMTE/g)
A	1	Blank B	A	0.044					
A	2	Control C1	A	0.483	0.439				
A	3	Control C1	A	0.482	0.438	0.438333			
A	4	Control C1	A	0.482	0.438				

Appendix 10.27 contd.

A	5	Sample X1	A	0.456	0.412	CaSu11	6.007605	10.255378	307.6613
A	6	Sample X1	A	0.456	0.412	CaSu11	6.007605	10.255378	307.6613
A	7	Sample X1	A	0.457	0.413	CaSu11	5.779468	10.257508	307.7252
A	8	Blank B	B	0.054					
A	9	Control C1	B	0.953	0.899				
A	10	Control C1	B	0.953	0.899	0.900667			
A	11	Control C1	B	0.958	0.904				
A	12	Sample X1	B	0.848	0.794	CaFr11	11.84308	11.06901	332.0703
B	1	Sample X1	B	0.841	0.787	CaFr11	12.62028	11.0541	331.623
B	2	Sample X1	B	0.841	0.787	CaFr11	12.62028	11.0541	331.623
B	3	Blank B	C	0.054					
B	4	Control C1	C	1.025	0.971				
B	5	Control C1	C	1.027	0.973	0.972333			
B	6	Control C1	C	1.027	0.973				
B	7	Sample X1	C	0.998	0.944	CaFr12	2.913953	11.388498	341.655
B	8	Sample X1	C	0.998	0.944	CaFr12	2.913953	11.388498	341.655
B	9	Sample X1	C	0.991	0.937	CaFr12	3.63387	11.373589	341.2077
B	10	Blank B	D	0.044					
B	11	Control C1	D	1.143	1.099				
B	12	Control C1	D	1.148	1.104	1.100667			
C	1	Control C1	D	1.143	1.099				
C	2	Sample X1	D	0.828	0.784	CaFr21	28.77044	11.04771	331.4313
C	3	Sample X1	D	0.822	0.778	CaFr21	29.31557	11.034931	331.0479
C	4	Sample X1	D	0.822	0.778	CaFr21	29.31557	11.034931	331.0479
C	5	Blank B	E	0.054					
C	6	Control C1	E	1.041	0.987				
C	7	Control C1	E	1.041	0.987	0.987333			
C	8	Control C1	E	1.042	0.988				
C	9	Sample X1	E	0.968	0.914	CaXy11	7.427414	11.324601	339.738
C	10	Sample X1	E	0.964	0.91	CaXy11	7.832546	11.316081	339.4824
C	11	Sample X1	E	0.964	0.91	CaXy11	7.832546	11.316081	339.4824
C	5	Blank B	E	0.035					
C	6	Control C1	E	0.782	0.747				
C	7	Control C1	E	0.784	0.749	0.748333			
C	8	Control C1	E	0.784	0.749				
C	9	Sample X1	E	0.734	0.699	CaXy12	6.592428	10.866667	326
C	10	Sample X1	E	0.733	0.698	CaXy12	6.726058	10.864537	325.9361
C	11	Sample X1	E	0.733	0.698	CaXy12	6.726058	10.864537	325.9361
B	10	Blank B	D	0.042					
B	11	Control C1	D	0.814	0.772				
B	12	Control C1	D	0.811	0.769	0.77			
C	1	Control C1	D	0.814	0.772				

Appendix 10.27 contd.

C	2	Sample X1	D	0.802	0.76	CaXy21	1.298701	10.996592	329.8978
C	3	Sample X1	D	0.804	0.762	CaXy21	1.038961	11.000852	330.0256
C	4	Sample X1	D	0.804	0.762	CaXy21	1.038961	11.000852	330.0256
C	12	Blank B	F	0.048					
D	1	Control C1	F	0.734	0.686				
D	2	Control C1	F	0.734	0.686	0.686333			
D	3	Control C1	F	0.735	0.687				
D	4	Sample X1	F	0.671	0.623	CaGr11	9.22778	10.704792	321.1438
D	5	Sample X1	F	0.672	0.624	CaGr11	9.082079	10.706922	321.2077
D	6	Sample X1	F	0.673	0.625	CaGr11	8.936377	10.709052	321.2716
D	7	Blank B	G	0.055					
D	8	Control C1	G	0.884	0.829				
D	9	Control C1	G	0.885	0.83	0.83			
D	10	Control C1	G	0.886	0.831				
D	11	Sample X1	G	0.591	0.536	CaGr12	35.42169	10.519489	315.5847
D	12	Sample X1	G	0.597	0.542	CaGr12	34.6988	10.532268	315.9681
E	1	Sample X1	G	0.591	0.536	CaGr12	35.42169	10.519489	315.5847
E	2	Blank B	H	0.05					
E	3	Control C1	H	0.815	0.765				
E	4	Control C1	H	0.815	0.765	0.765667			
E	5	Control C1	H	0.817	0.767				
E	6	Sample X1	H	0.692	0.642	CaGr21	16.1515	10.745261	322.3578
E	7	Sample X1	H	0.698	0.648	CaGr21	15.36787	10.75804	322.7412
E	8	Sample X1	H	0.692	0.642	CaGr21	16.1515	10.745261	322.3578
E	9	Blank B	I	0.045					
E	10	Control C1	I	0.847	0.802				
E	11	Control C1	I	0.848	0.803	0.802667			
E	12	Control C1	I	0.848	0.803				
F	1	Sample X1	I	0.745	0.7	CaGc11	12.7907	10.868797	326.0639
F	2	Sample X1	I	0.745	0.7	CaGc11	12.7907	10.868797	326.0639
F	3	Sample X1	I	0.742	0.697	CaGc11	13.16445	10.862407	325.8722
F	4	Blank B	J	0.052					
F	5	Control C1	J	0.468	0.416				
F	6	Control C1	J	0.468	0.416	0.416333			
F	7	Control C1	J	0.469	0.417				
F	8	Sample X1	J	0.318	0.266	CaGc21	36.10889	9.9444089	298.3323
F	9	Sample X1	J	0.316	0.264	CaGc21	36.58927	9.9401491	298.2045
F	10	Sample X1	J	0.316	0.264	CaGc21	36.58927	9.9401491	298.2045
F	11	Blank B	K	0.044					
F	12	Control C1	K	0.896	0.852				
G	1	Control C1	K	0.894	0.85	0.851333			
G	2	Control C1	K	0.896	0.852				

Appendix 10.27 contd.

G	3	Sample X1	K	0.587	0.543	CaGl11	36.2177	10.534398	316.0319
G	4	Sample X1	K	0.582	0.538	CaGl11	36.80501	10.523749	315.7125
G	5	Sample X1	K	0.582	0.538	CaGl11	36.80501	10.523749	315.7125
G	6	Blank B	L	0.046					
G	7	Control C1	L	0.847	0.801				
G	8	Control C1	L	0.848	0.802	0.801333			
G	9	Control C1	L	0.847	0.801				
G	10	Sample X1	L	0.782	0.736	CaGl21	8.153078	10.945474	328.3642
G	11	Sample X1	L	0.782	0.736	CaGl21	8.153078	10.945474	328.3642
G	12	Sample X1	L	0.781	0.735	CaGl21	8.27787	10.943344	328.3003

Appendix 10.28 RCCDRSM DPPH run 28

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/g)
A	1	Blank B	A	0.097					
A	2	Control C1	A	0.596	0.499				
A	3	Control C1	A	0.595	0.498	0.498667			
A	4	Control C1	A	0.596	0.499				
A	5	Sample X1	A	0.472	0.375	CaSu11	24.79947	10.176571	305.2971
A	6	Sample X1	A	0.477	0.38	CaSu11	23.79679	10.18722	305.6166
A	7	Sample X1	A	0.472	0.375	CaSu11	24.79947	10.176571	305.2971
A	8	Blank B	B	0.046					
A	9	Control C1	B	0.693	0.647				
A	10	Control C1	B	0.693	0.647	0.646667			
A	11	Control C1	B	0.692	0.646				
A	12	Sample X1	B	0.226	0.18	CaFr11	72.16495	9.7612354	292.8371
B	1	Sample X1	B	0.226	0.18	CaFr11	72.16495	9.7612354	292.8371
B	2	Sample X1	B	0.228	0.182	CaFr11	71.85567	9.7654952	292.9649
B	3	Blank B	C	0.06					
B	4	Control C1	C	0.737	0.677				
B	5	Control C1	C	0.739	0.679	0.678333			
B	6	Control C1	C	0.739	0.679				
B	7	Sample X1	C	0.616	0.556	CaFr12	18.0344	10.562087	316.8626
B	8	Sample X1	C	0.618	0.558	CaFr12	17.73956	10.566347	316.9904
B	9	Sample X1	C	0.616	0.556	CaFr12	18.0344	10.562087	316.8626
B	10	Blank B	D	0.099					
B	11	Control C1	D	0.741	0.642				
B	12	Control C1	D	0.741	0.642	0.642			

Appendix 10.28 contd.

C	1	Control C1	D	0.741	0.642				
C	2	Sample X1	D	0.488	0.389	CaFr21	39.4081	10.20639	306.1917
C	3	Sample X1	D	0.484	0.385	CaFr21	40.03115	10.19787	305.9361
C	4	Sample X1	D	0.484	0.385	CaFr21	40.03115	10.19787	305.9361
C	12	Blank B	F	0.042					
D	1	Control C1	F	0.814	0.772				
D	2	Control C1	F	0.813	0.771	0.771667			
D	3	Control C1	F	0.814	0.772				
D	4	Sample X1	F	0.213	0.171	CaXy11	77.84017	9.742066	292.262
D	5	Sample X1	F	0.215	0.173	CaXy11	77.58099	9.7463259	292.3898
D	6	Sample X1	F	0.213	0.171	CaXy11	77.84017	9.742066	292.262
C	5	Blank B	E	0.053					
C	6	Control C1	E	0.687	0.634				
C	7	Control C1	E	0.687	0.634	0.633333			
C	8	Control C1	E	0.685	0.632				
C	9	Sample X1	E	0.545	0.492	CaXy12	22.31579	10.425772	312.7732
C	10	Sample X1	E	0.542	0.489	CaXy12	22.78947	10.419382	312.5815
C	11	Sample X1	E	0.542	0.489	CaXy12	22.78947	10.419382	312.5815
C	5	Blank B	E	0.055					
C	6	Control C1	E	0.823	0.768				
C	7	Control C1	E	0.822	0.767	0.767333			
C	8	Control C1	E	0.822	0.767				
C	9	Sample X1	E	0.813	0.758	CaXy21	1.216334	10.992332	329.77
C	10	Sample X1	E	0.815	0.76	CaXy21	0.955691	10.996592	329.8978
C	11	Sample X1	E	0.813	0.758	CaXy21	1.216334	10.992332	329.77
C	12	Blank B	F	0.359					
D	1	Control C1	F	0.825	0.466				
D	2	Control C1	F	0.825	0.466	0.466667			
D	3	Control C1	F	0.827	0.468				
D	4	Sample X1	F	0.647	0.288	CaGr11	38.28571	9.9912673	299.738
D	5	Sample X1	F	0.647	0.288	CaGr11	38.28571	9.9912673	299.738
D	6	Sample X1	F	0.646	0.287	CaGr11	38.5	9.9891374	299.6741
D	7	Blank B	G	0.059					
D	8	Control C1	G	0.693	0.634				
D	9	Control C1	G	0.696	0.637	0.635			
D	10	Control C1	G	0.693	0.634				
D	11	Sample X1	G	0.509	0.45	CaGr12	29.13386	10.336315	310.0895
D	12	Sample X1	G	0.508	0.449	CaGr12	29.29134	10.334185	310.0256
E	1	Sample X1	G	0.509	0.45	CaGr12	29.13386	10.336315	310.0895
E	2	Blank B	H	0.046					
E	3	Control C1	H	0.632	0.586				
E	4	Control C1	H	0.637	0.591	0.589333			

Appendix 10.28 contd.

E	5	Control C1	H	0.637	0.591				
E	6	Sample X1	H	0.326	0.28	CaGr21	52.48869	9.9742279	299.2268
E	7	Sample X1	H	0.326	0.28	CaGr21	52.48869	9.9742279	299.2268
E	8	Sample X1	H	0.326	0.28	CaGr21	52.48869	9.9742279	299.2268
E	9	Blank B	I	0.043					
E	10	Control C1	I	0.732	0.689				
E	11	Control C1	I	0.738	0.695	0.693			
E	12	Control C1	I	0.738	0.695				
F	1	Sample X1	I	0.242	0.199	CaGc11	71.28427	9.8017039	294.0511
F	2	Sample X1	I	0.244	0.201	CaGc11	70.99567	9.8059638	294.1789
F	3	Sample X1	I	0.244	0.201	CaGc11	70.99567	9.8059638	294.1789
F	4	Blank B	J	0.054					
F	5	Control C1	J	0.544	0.49				
F	6	Control C1	J	0.547	0.493	0.491			
F	7	Control C1	J	0.544	0.49				
F	8	Sample X1	J	0.278	0.224	CaGc21	54.37882	9.8549521	295.6486
F	9	Sample X1	J	0.279	0.225	CaGc21	54.17515	9.857082	295.7125
F	10	Sample X1	J	0.278	0.224	CaGc21	54.37882	9.8549521	295.6486
F	11	Blank B	K	0.049					
F	12	Control C1	K	0.596	0.547				
G	1	Control C1	K	0.595	0.546	0.546667			
G	2	Control C1	K	0.596	0.547				
G	3	Sample X1	K	0.473	0.424	CaGl11	22.43902	10.280937	308.4281
G	4	Sample X1	K	0.471	0.422	CaGl11	22.80488	10.276677	308.3003
G	5	Sample X1	K	0.471	0.422	CaGl11	22.80488	10.276677	308.3003
G	6	Blank B	L	0.062					
G	7	Control C1	L	0.675	0.613				
G	8	Control C1	L	0.676	0.614	0.613333			
G	9	Control C1	L	0.675	0.613				
G	10	Sample X1	L	0.548	0.486	CaGl21	20.76087	10.412993	312.3898
G	11	Sample X1	L	0.548	0.486	CaGl21	20.76087	10.412993	312.3898
G	12	Sample X1	L	0.547	0.485	CaGl21	20.92391	10.410863	312.3259

Appendix 10.29 RCCDRSM DPPH run 29

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/g)
A	1	Blank B	A	0.055					
A	2	Control C1	A	0.777	0.722				
A	3	Control C1	A	0.778	0.723	0.722667			
A	4	Control C1	A	0.778	0.723				
A	5	Sample X1	A	0.647	0.592	CaSu11	18.08118	10.638765	319.1629
A	6	Sample X1	A	0.643	0.588	CaSu11	18.63469	10.630245	318.9073
A	7	Sample X1	A	0.647	0.592	CaSu11	18.08118	10.638765	319.1629
A	8	Blank B	B	0.048					
A	9	Control C1	B	0.831	0.783				
A	10	Control C1	B	0.831	0.783	0.784667			
A	11	Control C1	B	0.836	0.788				
A	12	Sample X1	B	0.245	0.197	CaFr11	74.8938	9.7974441	146.9617
B	1	Sample X1	B	0.249	0.201	CaFr11	74.38403	9.8059638	147.0895
B	2	Sample X1	B	0.249	0.201	CaFr11	74.38403	9.8059638	147.0895
B	3	Blank B	C	0.049					
B	4	Control C1	C	0.784	0.735				
B	5	Control C1	C	0.786	0.737	0.735667			
B	6	Control C1	C	0.784	0.735				
B	7	Sample X1	C	0.635	0.586	CaFr12	20.34436	10.625985	159.3898
B	8	Sample X1	C	0.639	0.59	CaFr12	19.80063	10.634505	159.5176
B	9	Sample X1	C	0.635	0.586	CaFr12	20.34436	10.625985	159.3898
B	10	Blank B	D	0.048					
B	11	Control C1	D	0.774	0.726				
B	12	Control C1	D	0.772	0.724	0.725333			
C	1	Control C1	D	0.774	0.726				
C	2	Sample X1	D	0.473	0.425	CaFr21	41.40625	10.283067	154.246
C	3	Sample X1	D	0.472	0.424	CaFr21	41.54412	10.280937	154.2141
C	4	Sample X1	D	0.472	0.424	CaFr21	41.54412	10.280937	154.2141
D	7	Blank B	G	0.04					
D	8	Control C1	G	1.188	1.148				
D	9	Control C1	G	1.183	1.143	1.146333			
D	10	Control C1	G	1.188	1.148				
D	11	Sample X1	G	0.897	0.857	CaXy11	25.2399	11.203195	168.0479
D	12	Sample X1	G	0.894	0.854	CaXy11	25.5016	11.196805	167.9521
E	1	Sample X1	G	0.894	0.854	CaXy11	25.5016	11.196805	167.9521
C	5	Blank B	E	0.15					
C	6	Control C1	E	1.017	0.867				
C	7	Control C1	E	1.019	0.869	0.868			

Appendix 10.29 contd.

C	8	Control C1	E	1.018	0.868				
C	9	Sample X1	E	0.594	0.444	CaXy12	48.84793	10.323536	154.853
C	10	Sample X1	E	0.594	0.444	CaXy12	48.84793	10.323536	154.853
C	11	Sample X1	E	0.595	0.445	CaXy12	48.73272	10.325666	154.885
C	12	Blank B	F	0.049					
D	1	Control C1	F	0.875	0.826				
D	2	Control C1	F	0.875	0.826	0.825333			
D	3	Control C1	F	0.873	0.824				
D	4	Sample X1	F	0.779	0.73	CaXy21	11.55089	10.932694	163.9904
D	5	Sample X1	F	0.778	0.729	CaXy21	11.67205	10.930564	163.9585
D	6	Sample X1	F	0.779	0.73	CaXy21	11.55089	10.932694	163.9904
C	12	Blank B	F	0.042					
D	1	Control C1	F	0.908	0.866				
D	2	Control C1	F	0.905	0.863	0.864333			
D	3	Control C1	F	0.906	0.864				
D	4	Sample X1	F	0.564	0.522	CaGr11	39.60663	10.48967	157.345
D	5	Sample X1	F	0.554	0.512	CaGr11	40.76359	10.468371	157.0256
D	6	Sample X1	F	0.571	0.529	CaGr11	38.79676	10.504579	157.5687
D	7	Blank B	G	0.028					
D	8	Control C1	G	0.705	0.677				
D	9	Control C1	G	0.708	0.68	0.678			
D	10	Control C1	G	0.705	0.677				
D	11	Sample X1	G	0.225	0.197	CaGr12	70.94395	9.7974441	146.9617
D	12	Sample X1	G	0.221	0.193	CaGr12	71.53392	9.7889244	146.8339
E	1	Sample X1	G	0.225	0.197	CaGr12	70.94395	9.7974441	146.9617
E	2	Blank B	H	0.047					
E	3	Control C1	H	0.793	0.746				
E	4	Control C1	H	0.793	0.746	0.745333			
E	5	Control C1	H	0.791	0.744				
E	6	Sample X1	H	0.549	0.502	CaGr21	32.64758	10.447071	156.7061
	7	Sample X1	H	0.548	0.501	CaGr21	32.78175	10.444941	156.6741
E	8	Sample X1	H	0.548	0.501	CaGr21	32.78175	10.444941	156.6741
E	9	Blank B	I	0.058					
E	10	Control C1	I	0.762	0.704				
E	11	Control C1	I	0.761	0.703	0.703667			
E	12	Control C1	I	0.762	0.704				
F	1	Sample X1	I	0.443	0.385	CaGc11	45.28659	10.19787	152.9681
F	2	Sample X1	I	0.447	0.389	CaGc11	44.71814	10.20639	153.0958
F	3	Sample X1	I	0.443	0.385	CaGc11	45.28659	10.19787	152.9681
F	4	Blank B	J	0.065					
F	5	Control C1	J	0.486	0.421				
F	6	Control C1	J	0.486	0.421	0.421667			

Appendix 10.29 contd.

F	7	Control C1	J	0.488	0.423				
F	8	Sample X1	J	0.228	0.163	CaGc21	61.34387	9.7250266	145.8754
F	9	Sample X1	J	0.227	0.162	CaGc21	61.58103	9.7228967	145.8435
F	10	Sample X1	J	0.228	0.163	CaGc21	61.34387	9.7250266	145.8754
F	11	Blank B	K	0.044					
F	12	Control C1	K	0.733	0.689				
G	1	Control C1	K	0.733	0.689	0.688333			
G	2	Control C1	K	0.731	0.687				
G	3	Sample X1	K	0.609	0.565	CaGl11	17.91768	10.581257	158.7188
G	4	Sample X1	K	0.608	0.564	CaGl11	18.06295	10.579127	158.6869
G	5	Sample X1	K	0.608	0.564	CaGl11	18.06295	10.579127	158.6869
G	6	Blank B	L	0.062					
G	7	Control C1	L	0.893	0.831				
G	8	Control C1	L	0.896	0.834	0.832667			
G	9	Control C1	L	0.895	0.833				
G	10	Sample X1	L	0.565	0.503	CaGl21	39.59167	10.449201	156.738
G	11	Sample X1	L	0.564	0.502	CaGl21	39.71177	10.447071	156.7061
G	12	Sample X1	L	0.564	0.502	CaGl21	39.71177	10.447071	156.7061

Appendix 10.30 RCCDRSM DPPH run 30

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample Code	% Inhibition	DPPH (µMTE/l)	DPPH (µMTE/g)
A	1	Blank B	A	0.045					
A	2	Control C1	A	0.789	0.744				
A	3	Control C1	A	0.781	0.736	0.738667			
A	4	Control C1	A	0.781	0.736				
A	5	Sample X1	A	0.516	0.471	CaSu11	36.23646	10.381044	103.8104
A	6	Sample X1	A	0.515	0.47	CaSu11	36.37184	10.378914	103.7891
A	7	Sample X1	A	0.516	0.471	CaSu11	36.23646	10.381044	103.8104
A	8	Blank B	B	0.058					
A	9	Control C1	B	0.766	0.708				
A	10	Control C1	B	0.767	0.709	0.708667			
A	11	Control C1	B	0.767	0.709				
A	12	Sample X1	B	0.187	0.129	CaFr11	81.7968	9.6526092	96.52609
B	1	Sample X1	B	0.187	0.129	CaFr11	81.7968	9.6526092	96.52609
B	2	Sample X1	B	0.182	0.124	CaFr11	82.50235	9.6419595	96.4196
B	3	Blank B	C	0.063					
B	4	Control C1	C	0.866	0.803				

Appendix 10.30 contd.

B	5	Control C1	C	0.868	0.805	0.803667			
B	6	Control C1	C	0.866	0.803				
B	7	Sample X1	C	0.368	0.305	CaFr12	62.04894	10.027476	100.2748
B	8	Sample X1	C	0.368	0.305	CaFr12	62.04894	10.027476	100.2748
B	9	Sample X1	C	0.367	0.304	CaFr12	62.17337	10.025346	100.2535
B	10	Blank B	D	0.16					
B	11	Control C1	D	0.538	0.378				
B	12	Control C1	D	0.535	0.375	0.377			
C	1	Control C1	D	0.538	0.378				
C	2	Sample X1	D	0.429	0.269	CaFr21	28.64721	9.9507987	99.50799
C	3	Sample X1	D	0.425	0.265	CaFr21	29.70822	9.942279	99.42279
C	4	Sample X1	D	0.428	0.268	CaFr21	28.91247	9.9486688	99.48669
C	5	Blank B	E	0.051					
C	6	Control C1	E	0.665	0.614				
C	7	Control C1	E	0.665	0.614	0.614			
C	8	Control C1	E	0.665	0.614				
C	9	Sample X1	E	0.638	0.587	CaXy12	4.397394	10.628115	106.2812
C	10	Sample X1	E	0.635	0.584	CaXy12	4.885993	10.621725	106.2173
C	11	Sample X1	E	0.638	0.587	CaXy12	4.397394	10.628115	106.2812
C	12	Blank B	F	0.061					
D	1	Control C1	F	0.857	0.796				
D	2	Control C1	F	0.858	0.797	0.796			
D	3	Control C1	F	0.856	0.795				
D	4	Sample X1	F	0.433	0.372	CaGr11	53.26633	10.170181	101.7018
D	5	Sample X1	F	0.433	0.372	CaGr11	53.26633	10.170181	101.7018
D	6	Sample X1	F	0.432	0.371	CaGr11	53.39196	10.168051	101.6805
D	7	Blank B	G	0.044					
D	8	Control C1	G	0.868	0.824				
D	9	Control C1	G	0.863	0.819	0.822333			
D	10	Control C1	G	0.868	0.824				
D	11	Sample X1	G	0.229	0.185	CaGr12	77.50304	9.771885	97.71885
D	12	Sample X1	G	0.228	0.184	CaGr12	77.62465	9.7697551	97.69755
E	1	Sample X1	G	0.229	0.185	CaGr12	77.50304	9.771885	97.71885
E	2	Blank B	H	0.048					
E	3	Control C1	H	0.626	0.578				
E	4	Control C1	H	0.627	0.579	0.578667			
E	5	Control C1	H	0.627	0.579				
E	6	Sample X1	H	0.437	0.389	CaGr21	32.7765	10.20639	102.0639
E	7	Sample X1	H	0.434	0.386	CaGr21	33.29493	10.2	102
E	8	Sample X1	H	0.434	0.386	CaGr21	33.29493	10.2	102
E	9	Blank B	I	0.039					
E	10	Control C1	I	0.847	0.808				

Appendix 10.30 contd.

E	11	Control C1	I	0.847	0.808	0.807333			
E	12	Control C1	I	0.845	0.806				
F	1	Sample X1	I	0.215	0.176	CaGc11	78.19983	9.7527157	97.52716
F	2	Sample X1	I	0.215	0.176	CaGc11	78.19983	9.7527157	97.52716
F	3	Sample X1	I	0.214	0.175	CaGc11	78.3237	9.7505857	97.50586
F	4	Blank B	J	0.205					
F	5	Control C1	J	0.768	0.563				
F	6	Control C1	J	0.768	0.563	0.563333			
F	7	Control C1	J	0.769	0.564				
F	8	Sample X1	J	0.324	0.119	CaGc21	78.87574	9.6313099	96.3131
F	9	Sample X1	J	0.328	0.123	CaGc21	78.16568	9.6398296	96.3983
F	10	Sample X1	J	0.324	0.119	CaGc21	78.87574	9.6313099	96.3131
F	11	Blank B	K	0.048					
F	12	Control C1	K	0.991	0.943				
G	1	Control C1	K	0.991	0.943	0.943667			
G	2	Control C1	K	0.993	0.945				
G	3	Sample X1	K	0.526	0.478	CaGl11	49.34652	10.395953	103.9595
G	4	Sample X1	K	0.523	0.475	CaGl11	49.66443	10.389563	103.8956
G	5	Sample X1	K	0.523	0.475	CaGl11	49.66443	10.389563	103.8956
G	6	Blank B	L	0.054					
G	7	Control C1	L	0.761	0.707				
G	8	Control C1	L	0.765	0.711	0.709667			
G	9	Control C1	L	0.765	0.711				
G	10	Sample X1	L	0.474	0.42	CaGl21	40.81729	10.272417	102.7242
G	11	Sample X1	L	0.475	0.421	CaGl21	40.67637	10.274547	102.7455
G	12	Sample X1	L	0.474	0.42	CaGl21	40.81729	10.272417	102.7242

Appendix 11.1 Optimized experiment TPC

Row	Col	Content	Group	Raw Data (765)	Blank corrected based on Raw Data (765)	Sample code	TPC (mgGAE/L)	TPC (mgGAE/g)	TPC (µgGAE/g)
A	1	Blank B	A	0.093					
A	2	Sample X1	A	0.485	0.392	CaSu11	17.25490196	0.8627451	862.7451
A	3	Sample X1	A	0.483	0.39	CaSu11	17.15686275	0.8578431	857.84314
A	4	Sample X1	A	0.484	0.391	CaSu11	17.20588235	0.8602941	860.29412
A	1	Blank B	A	0.094					
A	2	Sample X1	A	0.487	0.393	CaSu11	17.30392157	0.8651961	865.19608
A	3	Sample X1	A	0.488	0.394	CaSu11	17.35294118	0.8676471	867.64706
A	4	Sample X1	A	0.482	0.388	CaSu11	17.05882353	0.8529412	852.94118

Appendix 11.1 contd.

A	1	Blank B	A	0.093					
A	2	Sample X1	A	0.482	0.389	CaSu11	17.10784314	0.8553922	855.39216
A	3	Sample X1	A	0.483	0.39	CaSu11	17.15686275	0.8578431	857.84314
A	4	Sample X1	A	0.484	0.391	CaSu11	17.20588235	0.8602941	860.29412
A	5	Blank B	B	0.018					
A	6	Sample X1	B	0.585	0.567	CaFr11	25.83333333	1.2916667	1291.6667
A	7	Sample X1	B	0.586	0.568	CaFr11	25.88235294	1.2941176	1294.1176
A	8	Sample X1	B	0.585	0.567	CaFr11	25.83333333	1.2916667	1291.6667
A	5	Blank B	B	0.019					
A	6	Sample X1	B	0.588	0.569	CaFr11	25.93137255	1.2965686	1296.5686
A	7	Sample X1	B	0.586	0.567	CaFr11	25.83333333	1.2916667	1291.6667
A	8	Sample X1	B	0.589	0.57	CaFr11	25.98039216	1.2990196	1299.0196
A	5	Blank B	B	0.019					
A	6	Sample X1	B	0.584	0.565	CaFr11	25.73529412	1.2867647	1286.7647
A	7	Sample X1	B	0.583	0.564	CaFr11	25.68627451	1.2843137	1284.3137
A	8	Sample X1	B	0.582	0.563	CaFr11	25.6372549	1.2818627	1281.8627
A	9	Blank B	C	0.013					
A	10	Sample X1	C	0.362	0.349	CaFr12	15.14705882	0.7573529	757.35294
A	11	Sample X1	C	0.367	0.354	CaFr12	15.39215686	0.7696078	769.60784
A	12	Sample X1	C	0.363	0.35	CaFr12	15.19607843	0.7598039	759.80392
A	9	Blank B	C	0.012					
A	10	Sample X1	C	0.359	0.347	CaFr12	15.04901961	0.752451	752.45098
A	11	Sample X1	C	0.352	0.34	CaFr12	14.70588235	0.7352941	735.29412
A	12	Sample X1	C	0.354	0.342	CaFr12	14.80392157	0.7401961	740.19608
A	9	Blank B	C	0.013					
A	10	Sample X1	C	0.356	0.343	CaFr12	14.85294118	0.7426471	742.64706
A	11	Sample X1	C	0.357	0.344	CaFr12	14.90196078	0.745098	745.09804
A	12	Sample X1	C	0.353	0.34	CaFr12	14.70588235	0.7352941	735.29412
B	1	Blank B	D	0.132					
B	2	Sample X1	D	0.293	0.161	CaFr21	5.931372549	0.2965686	296.56863
B	3	Sample X1	D	0.299	0.167	CaFr21	6.225490196	0.3112745	311.27451
B	4	Sample X1	D	0.296	0.164	CaFr21	6.078431373	0.3039216	303.92157
B	1	Blank B	D	0.141					
B	2	Sample X1	D	0.292	0.151	CaFr21	5.441176471	0.2720588	272.05882
B	3	Sample X1	D	0.295	0.154	CaFr21	5.588235294	0.2794118	279.41176
B	4	Sample X1	D	0.292	0.151	CaFr21	5.441176471	0.2720588	272.05882
B	9	Blank B	F	0.147					
B	10	Sample X1	F	0.294	0.147	CaFr21	5.245098039	0.2622549	262.2549
B	11	Sample X1	F	0.293	0.146	CaFr21	5.196078431	0.2598039	259.80392
B	12	Sample X1	F	0.298	0.151	CaFr21	5.441176471	0.2720588	272.05882
B	5	Blank B	E	0.054					
B	6	Sample X1	E	0.246	0.192	CaXy1	7.450980392	0.372549	372.54902

Appendix 11.1 contd.

B	7	Sample X1	E	0.247	0.193	CaXy11	7.5	0.375	375
B	8	Sample X1	E	0.242	0.188	CaXy11	7.254901961	0.3627451	362.7451
B	5	Blank B	E	0.052					
B	6	Sample X1	E	0.242	0.19	CaXy11	7.352941176	0.3676471	367.64706
B	7	Sample X1	E	0.247	0.195	CaXy11	7.598039216	0.379902	379.90196
B	8	Sample X1	E	0.243	0.191	CaXy11	7.401960784	0.370098	370.09804
B	5	Blank B	E	0.059					
B	6	Sample X1	E	0.243	0.184	CaXy11	7.058823529	0.3529412	352.94118
B	7	Sample X1	E	0.241	0.182	CaXy11	6.960784314	0.3480392	348.03922
B	8	Sample X1	E	0.245	0.186	CaXy11	7.156862745	0.3578431	357.84314
B	9	Blank B	F	0.092					
B	10	Sample X1	F	0.371	0.279	CaXy12	11.71568627	0.5857843	585.78431
B	11	Sample X1	F	0.374	0.282	CaXy12	11.8627451	0.5931373	593.13725
B	12	Sample X1	F	0.379	0.287	CaXy12	12.10784314	0.6053922	605.39216
B	9	Blank B	F	0.097					
B	10	Sample X1	F	0.371	0.274	CaXy12	11.47058824	0.5735294	573.52941
B	11	Sample X1	F	0.373	0.276	CaXy12	11.56862745	0.5784314	578.43137
B	12	Sample X1	F	0.378	0.281	CaXy12	11.81372549	0.5906863	590.68627
B	9	Blank B	F	0.093					
B	10	Sample X1	F	0.372	0.279	CaXy12	11.71568627	0.5857843	585.78431
B	11	Sample X1	F	0.374	0.281	CaXy12	11.81372549	0.5906863	590.68627
B	12	Sample X1	F	0.376	0.283	CaXy12	11.91176471	0.5955882	595.58824
C	1	Blank B	G	0.042					
C	2	Sample X1	G	0.202	0.16	CaXy21	5.882352941	0.2941176	294.11765
C	3	Sample X1	G	0.204	0.162	CaXy21	5.980392157	0.2990196	299.01961
C	4	Sample X1	G	0.203	0.161	CaXy21	5.931372549	0.2965686	296.56863
C	1	Blank B	G	0.046					
C	2	Sample X1	G	0.203	0.157	CaXy21	5.735294118	0.2867647	286.76471
C	3	Sample X1	G	0.204	0.158	CaXy21	5.784313725	0.2892157	289.21569
C	4	Sample X1	G	0.202	0.156	CaXy21	5.68627451	0.2843137	284.31373
C	1	Blank B	G	0.049					
C	2	Sample X1	G	0.208	0.159	CaXy21	5.833333333	0.2916667	291.66667
C	3	Sample X1	G	0.202	0.153	CaXy21	5.539215686	0.2769608	276.96078
C	4	Sample X1	G	0.207	0.158	CaXy21	5.784313725	0.2892157	289.21569
C	5	Blank B	H	0.079					
C	6	Sample X1	H	0.333	0.254	CaGr11	10.49019608	0.5245098	524.5098
C	7	Sample X1	H	0.332	0.253	CaGr11	10.44117647	0.5220588	522.05882
C	8	Sample X1	H	0.338	0.259	CaGr11	10.73529412	0.5367647	536.76471
C	5	Blank B	H	0.077					
C	6	Sample X1	H	0.334	0.257	CaGr11	10.6372549	0.5318627	531.86275
C	7	Sample X1	H	0.336	0.259	CaGr11	10.73529412	0.5367647	536.76471
C	8	Sample X1	H	0.332	0.255	CaGr11	10.53921569	0.5269608	526.96078

Appendix 11.1 contd.

C	5	Blank B	H	0.078					
C	6	Sample X1	H	0.347	0.269	CaGr11	11.2254902	0.5612745	561.27451
C	7	Sample X1	H	0.349	0.271	CaGr11	11.32352941	0.5661765	566.17647
C	8	Sample X1	H	0.343	0.265	CaGr11	11.02941176	0.5514706	551.47059
C	9	Blank B	I	0.055					
C	10	Sample X1	I	0.403	0.348	CaGr12	15.09803922	0.754902	754.90196
C	11	Sample X1	I	0.409	0.354	CaGr12	15.39215686	0.7696078	769.60784
C	12	Sample X1	I	0.404	0.349	CaGr12	15.14705882	0.7573529	757.35294
C	9	Blank B	I	0.058					
C	10	Sample X1	I	0.402	0.344	CaGr12	14.90196078	0.745098	745.09804
C	11	Sample X1	I	0.406	0.348	CaGr12	15.09803922	0.754902	754.90196
C	12	Sample X1	I	0.407	0.349	CaGr12	15.14705882	0.7573529	757.35294
C	9	Blank B	I	0.056					
C	10	Sample X1	I	0.401	0.345	CaGr12	14.95098039	0.747549	747.54902
C	11	Sample X1	I	0.404	0.348	CaGr12	15.09803922	0.754902	754.90196
C	12	Sample X1	I	0.402	0.346	CaGr12	15	0.75	750
D	1	Blank B	J	0.096					
D	2	Sample X1	J	0.296	0.2	CaGr21	7.843137255	0.3921569	392.15686
D	3	Sample X1	J	0.299	0.203	CaGr21	7.990196078	0.3995098	399.5098
D	4	Sample X1	J	0.288	0.192	CaGr21	7.450980392	0.372549	372.54902
D	1	Blank B	J	0.093					
D	2	Sample X1	J	0.299	0.206	CaGr21	8.137254902	0.4068627	406.86275
D	3	Sample X1	J	0.295	0.202	CaGr21	7.941176471	0.3970588	397.05882
D	4	Sample X1	J	0.296	0.203	CaGr21	7.990196078	0.3995098	399.5098
D	1	Blank B	J	0.095					
D	2	Sample X1	J	0.298	0.203	CaGr21	7.990196078	0.3995098	399.5098
D	3	Sample X1	J	0.297	0.202	CaGr21	7.941176471	0.3970588	397.05882
D	4	Sample X1	J	0.299	0.204	CaGr21	8.039215686	0.4019608	401.96078
D	5	Blank B	K	0.122					
D	6	Sample X1	K	0.353	0.231	CaGc11	9.362745098	0.4681373	468.13725
D	7	Sample X1	K	0.352	0.23	CaGc11	9.31372549	0.4656863	465.68627
D	8	Sample X1	K	0.354	0.232	CaGc11	9.411764706	0.4705882	470.58824
D	5	Blank B	K	0.117					
D	6	Sample X1	K	0.356	0.239	CaGc11	9.754901961	0.4877451	487.7451
D	7	Sample X1	K	0.352	0.235	CaGc11	9.558823529	0.4779412	477.94118
D	8	Sample X1	K	0.351	0.234	CaGc11	9.509803922	0.4754902	475.4902
D	5	Blank B	K	0.119					
D	6	Sample X1	K	0.351	0.232	CaGc11	9.411764706	0.4705882	470.58824
D	7	Sample X1	K	0.351	0.232	CaGc11	9.411764706	0.4705882	470.58824
D	8	Sample X1	K	0.359	0.24	CaGc11	9.803921569	0.4901961	490.19608
D	9	Blank B	L	0.142					
D	10	Sample X1	L	0.385	0.243	CaGc21	9.950980392	0.497549	497.54902

Appendix 11.1 contd.

D	11	Sample X1	L	0.389	0.247	CaGc21	10.14705882	0.5073529	507.35294
D	12	Sample X1	L	0.381	0.239	CaGc21	9.754901961	0.4877451	487.7451
D	9	Blank B	L	0.136					
D	10	Sample X1	L	0.383	0.247	CaGc21	10.14705882	0.5073529	507.35294
D	11	Sample X1	L	0.385	0.249	CaGc21	10.24509804	0.5122549	512.2549
D	12	Sample X1	L	0.381	0.245	CaGc21	10.04901961	0.502451	502.45098
D	9	Blank B	L	0.137					
D	10	Sample X1	L	0.381	0.244	CaGc21	10	0.5	500
D	11	Sample X1	L	0.385	0.248	CaGc21	10.19607843	0.5098039	509.80392
D	12	Sample X1	L	0.381	0.244	CaGc21	10	0.5	500
E	1	Blank B	M	0.212					
E	2	Sample X1	M	0.524	0.312	CaGl11	13.33333333	0.6666667	666.66667
E	3	Sample X1	M	0.526	0.314	CaGl11	13.43137255	0.6715686	671.56863
E	4	Sample X1	M	0.525	0.313	CaGl11	13.38235294	0.6691176	669.11765
E	1	Blank B	M	0.216					
E	2	Sample X1	M	0.522	0.306	CaGl11	13.03921569	0.6519608	651.96078
E	3	Sample X1	M	0.525	0.309	CaGl11	13.18627451	0.6593137	659.31373
E	4	Sample X1	M	0.525	0.309	CaGl11	13.18627451	0.6593137	659.31373
E	1	Blank B	M	0.217					
E	2	Sample X1	M	0.525	0.308	CaGl11	13.1372549	0.6568627	656.86275
E	3	Sample X1	M	0.522	0.305	CaGl11	12.99019608	0.6495098	649.5098
E	4	Sample X1	M	0.525	0.308	CaGl11	13.1372549	0.6568627	656.86275
E	5	Blank B	N	0.114					
E	6	Sample X1	N	0.437	0.323	CaGl21	13.87254902	0.6936275	693.62745
E	7	Sample X1	N	0.437	0.323	CaGl21	13.87254902	0.6936275	693.62745
E	8	Sample X1	N	0.431	0.317	CaGl21	13.57843137	0.6789216	678.92157
E	5	Blank B	N	0.114					
E	6	Sample X1	N	0.432	0.318	CaGl21	13.62745098	0.6813725	681.37255
E	7	Sample X1	N	0.434	0.32	CaGl21	13.7254902	0.6862745	686.27451
E	8	Sample X1	N	0.438	0.324	CaGl21	13.92156863	0.6960784	696.07843
E	5	Blank B	N	0.113					
E	6	Sample X1	N	0.439	0.326	CaGl21	14.01960784	0.7009804	700.98039
E	7	Sample X1	N	0.431	0.318	CaGl21	13.62745098	0.6813725	681.37255
E	8	Sample X1	N	0.432	0.319	CaGl21	13.67647059	0.6838235	683.82353
E	9	Blank B	O	0.157					
E	10	Sample X1	O	0.252	0.095	WE	2.696078431	0.1348039	134.80392
E	11	Sample X1	O	0.259	0.102	WE	3.039215686	0.1519608	151.96078
E	12	Sample X1	O	0.254	0.097	WE	2.794117647	0.1397059	139.70588
E	9	Blank B	O	0.153					
E	10	Sample X1	O	0.256	0.103	WE	3.088235294	0.1544118	154.41176
E	11	Sample X1	O	0.257	0.104	WE	3.137254902	0.1568627	156.86275
E	12	Sample X1	O	0.251	0.098	WE	2.843137255	0.1421569	142.15686

Appendix 11.1 contd.

E	9	Blank B	O	0.157					
E	10	Sample X1	O	0.253	0.096	WE	2.745098039	0.1372549	137.2549
E	11	Sample X1	O	0.254	0.097	WE	2.794117647	0.1397059	139.70588
E	12	Sample X1	O	0.255	0.098	WE	2.843137255	0.1421569	142.15686

Appendix 11.2 Optimized experiment TFC

Row	Col	Content	Group	Raw Data (415)	Blank corrected based on Raw Data (415)	Sample code	TFC (µgQE/mL)	TFC (µgQE/g)
A	1	Blank B	A	0.482				
A	2	Sample X1	A	0.792	0.31	CaSu11	23.632813	1181.641
A	3	Sample X1	A	0.794	0.312	CaSu11	23.789063	1189.453
A	4	Sample X1	A	0.794	0.312	CaSu11	23.789063	1189.453
A	1	Blank B	A	0.489				
A	2	Sample X1	A	0.792	0.303	CaSu11	23.085938	1154.297
A	3	Sample X1	A	0.794	0.305	CaSu11	23.242188	1162.109
A	4	Sample X1	A	0.794	0.305	CaSu11	23.242188	1162.109
A	1	Blank B	A	0.484				
A	2	Sample X1	A	0.794	0.31	CaSu11	23.632813	1181.641
A	3	Sample X1	A	0.794	0.31	CaSu11	23.632813	1181.641
A	4	Sample X1	A	0.794	0.31	CaSu11	23.632813	1181.641
A	5	Blank B	B	0.064				
A	6	Sample X1	B	0.681	0.617	CaFr11	47.617188	2380.859
A	7	Sample X1	B	0.684	0.62	CaFr11	47.851563	2392.578
A	8	Sample X1	B	0.687	0.623	CaFr11	48.085938	2404.297
A	5	Blank B	B	0.059				
A	6	Sample X1	B	0.684	0.625	CaFr11	48.242188	2412.109
A	7	Sample X1	B	0.689	0.63	CaFr11	48.632813	2431.641
A	8	Sample X1	B	0.689	0.63	CaFr11	48.632813	2431.641
A	5	Blank B	B	0.071				
A	6	Sample X1	B	0.689	0.618	CaFr11	47.695313	2384.766
A	7	Sample X1	B	0.685	0.614	CaFr11	47.382813	2369.141
A	8	Sample X1	B	0.688	0.617	CaFr11	47.617188	2380.859
A	9	Blank B	C	0.228				
A	10	Sample X1	C	0.604	0.376	CaFr12	28.789063	1439.453
A	11	Sample X1	C	0.608	0.38	CaFr12	29.101563	1455.078
A	12	Sample X1	C	0.607	0.379	CaFr12	29.023438	1451.172
A	9	Blank B	C	0.228				
A	10	Sample X1	C	0.601	0.373	CaFr12	28.554688	1427.734
A	11	Sample X1	C	0.609	0.381	CaFr12	29.179688	1458.984

Appendix 11.2 contd.

A	12	Sample X1	C	0.605	0.377	CaFr12	28.867188	1443.359
A	9	Blank B	C	0.226				
A	10	Sample X1	C	0.601	0.375	CaFr12	28.710938	1435.547
A	11	Sample X1	C	0.608	0.382	CaFr12	29.257813	1462.891
A	12	Sample X1	C	0.602	0.376	CaFr12	28.789063	1439.453
B	1	Blank B	D	0.112				
B	2	Sample X1	D	0.237	0.125	CaFr21	9.1796875	458.9844
B	3	Sample X1	D	0.231	0.119	CaFr21	8.7109375	435.5469
B	4	Sample X1	D	0.234	0.122	CaFr21	8.9453125	447.2656
B	1	Blank B	D	0.114				
B	2	Sample X1	D	0.232	0.118	CaFr21	8.6328125	431.6406
B	3	Sample X1	D	0.234	0.12	CaFr21	8.7890625	439.4531
B	4	Sample X1	D	0.238	0.12	CaFr21	8.7890625	439.4531
B	1	Blank B	D	0.116				
B	2	Sample X1	D	0.236	0.12	CaFr21	8.7890625	439.4531
B	3	Sample X1	D	0.235	0.119	CaFr21	8.7109375	435.5469
B	4	Sample X1	D	0.239	0.123	CaFr21	9.0234375	451.1719
B	5	Blank B	E	0.011				
B	6	Sample X1	E	0.177	0.166	CaXy11	12.382813	619.1406
B	7	Sample X1	E	0.179	0.168	CaXy11	12.539063	626.9531
B	8	Sample X1	E	0.178	0.167	CaXy11	12.460938	623.0469
B	5	Blank B	E	0.01				
B	6	Sample X1	E	0.179	0.169	CaXy11	12.617188	630.8594
B	7	Sample X1	E	0.176	0.166	CaXy11	12.382813	619.1406
B	8	Sample X1	E	0.177	0.167	CaXy11	12.460938	623.0469
B	5	Blank B	E	0.014				
B	6	Sample X1	E	0.174	0.16	CaXy11	11.914063	595.7031
B	7	Sample X1	E	0.178	0.164	CaXy11	12.226563	611.3281
B	8	Sample X1	E	0.179	0.165	CaXy11	12.304688	615.2344
B	9	Blank B	F	0.114				
B	10	Sample X1	F	0.573	0.459	CaXy12	35.273438	1763.672
B	11	Sample X1	F	0.574	0.46	CaXy12	35.351563	1767.578
B	12	Sample X1	F	0.577	0.463	CaXy12	35.585938	1779.297
B	9	Blank B	F	0.111				
B	10	Sample X1	F	0.571	0.46	CaXy12	35.351563	1767.578
B	11	Sample X1	F	0.577	0.466	CaXy12	35.820313	1791.016
B	12	Sample X1	F	0.577	0.466	CaXy12	35.820313	1791.016
B	9	Blank B	F	0.113				
B	10	Sample X1	F	0.576	0.463	CaXy12	35.585938	1779.297
B	11	Sample X1	F	0.577	0.464	CaXy12	35.664063	1783.203
B	12	Sample X1	F	0.574	0.461	CaXy12	35.429688	1771.484
C	1	Blank B	G	0.019				

Appendix 11.2 contd.

C	2	Sample X1	G	0.173	0.154	CaXy21	11.445313	572.2656
C	3	Sample X1	G	0.174	0.155	CaXy21	11.523438	576.1719
C	4	Sample X1	G	0.172	0.153	CaXy21	11.367188	568.3594
C	1	Blank B	G	0.011				
C	2	Sample X1	G	0.177	0.166	CaXy21	12.382813	619.1406
C	3	Sample X1	G	0.172	0.161	CaXy21	11.992188	599.6094
C	4	Sample X1	G	0.172	0.161	CaXy21	11.992188	599.6094
C	1	Blank B	G	0.019				
C	2	Sample X1	G	0.171	0.152	CaXy21	11.289063	564.4531
C	3	Sample X1	G	0.178	0.159	CaXy21	11.835938	591.7969
C	4	Sample X1	G	0.173	0.154	CaXy21	11.445313	572.2656
C	5	Blank B	H	0.011				
C	6	Sample X1	H	0.184	0.173	CaGr11	12.929688	646.4844
C	7	Sample X1	H	0.186	0.175	CaGr11	13.085938	654.2969
C	8	Sample X1	H	0.189	0.178	CaGr11	13.320313	666.0156
C	5	Blank B	H	0.018				
C	6	Sample X1	H	0.183	0.165	CaGr11	12.304688	615.2344
C	7	Sample X1	H	0.184	0.166	CaGr11	12.382813	619.1406
C	8	Sample X1	H	0.181	0.163	CaGr11	12.148438	607.4219
C	5	Blank B	H	0.016				
C	6	Sample X1	H	0.181	0.165	CaGr11	12.304688	615.2344
C	7	Sample X1	H	0.188	0.172	CaGr11	12.851563	642.5781
C	8	Sample X1	H	0.186	0.17	CaGr11	12.695313	634.7656
C	9	Blank B	I	0.013				
C	10	Sample X1	I	0.246	0.233	CaGr12	17.617188	880.8594
C	11	Sample X1	I	0.249	0.236	CaGr12	17.851563	892.5781
C	12	Sample X1	I	0.241	0.228	CaGr12	17.226563	861.3281
C	9	Blank B	I	0.017				
C	10	Sample X1	I	0.244	0.227	CaGr12	17.148438	857.4219
C	11	Sample X1	I	0.248	0.231	CaGr12	17.460938	873.0469
C	12	Sample X1	I	0.245	0.228	CaGr12	17.226563	861.3281
C	9	Blank B	I	0.016				
C	10	Sample X1	I	0.243	0.227	CaGr12	17.148438	857.4219
C	11	Sample X1	I	0.248	0.232	CaGr12	17.539063	876.9531
C	12	Sample X1	I	0.245	0.229	CaGr12	17.304688	865.2344
D	1	Blank B	J	0.017				
D	2	Sample X1	J	0.187	0.17	CaGr21	12.695313	634.7656
D	3	Sample X1	J	0.181	0.164	CaGr21	12.226563	611.3281
D	4	Sample X1	J	0.189	0.172	CaGr21	12.851563	642.5781
D	1	Blank B	J	0.016				
D	2	Sample X1	J	0.184	0.168	CaGr21	12.539063	626.9531
D	3	Sample X1	J	0.187	0.171	CaGr21	12.773438	638.6719

Appendix 11.2 contd.

D	4	Sample X1	J	0.184	0.168	CaGr21	12.539063	626.9531
D	1	Blank B	J	0.013				
D	2	Sample X1	J	0.185	0.172	CaGr21	12.851563	642.5781
D	3	Sample X1	J	0.182	0.169	CaGr21	12.617188	630.8594
D	4	Sample X1	J	0.184	0.171	CaGr21	12.773438	638.6719
D	5	Blank B	K	0.314				
D	6	Sample X1	K	0.662	0.348	CaGc11	26.601563	1330.078
D	7	Sample X1	K	0.666	0.352	CaGc11	26.914063	1345.703
D	8	Sample X1	K	0.665	0.351	CaGc11	26.835938	1341.797
D	5	Blank B	K	0.311				
D	6	Sample X1	K	0.661	0.35	CaGc11	26.757813	1337.891
D	7	Sample X1	K	0.668	0.357	CaGc11	27.304688	1365.234
D	8	Sample X1	K	0.669	0.358	CaGc11	27.382813	1369.141
D	5	Blank B	K	0.311				
D	6	Sample X1	K	0.669	0.358	CaGc11	27.382813	1369.141
D	7	Sample X1	K	0.668	0.357	CaGc11	27.304688	1365.234
D	8	Sample X1	K	0.668	0.357	CaGc11	27.304688	1365.234
D	9	Blank B	L	0.212				
D	10	Sample X1	L	0.563	0.351	CaGc21	26.835938	1341.797
D	11	Sample X1	L	0.565	0.353	CaGc21	26.992188	1349.609
D	12	Sample X1	L	0.564	0.352	CaGc21	26.914063	1345.703
D	9	Blank B	L	0.215				
D	10	Sample X1	L	0.562	0.347	CaGc21	26.523438	1326.172
D	11	Sample X1	L	0.563	0.348	CaGc21	26.601563	1330.078
D	12	Sample X1	L	0.566	0.351	CaGc21	26.835938	1341.797
D	9	Blank B	L	0.215				
D	10	Sample X1	L	0.569	0.354	CaGc21	27.070313	1353.516
D	11	Sample X1	L	0.565	0.35	CaGc21	26.757813	1337.891
D	12	Sample X1	L	0.567	0.352	CaGc21	26.914063	1345.703
E	1	Blank B	M	0.117				
E	2	Sample X1	M	0.456	0.339	CaGl11	25.898438	1294.922
E	3	Sample X1	M	0.457	0.34	CaGl11	25.976563	1298.828
E	4	Sample X1	M	0.459	0.342	CaGl11	26.132813	1306.641
E	1	Blank B	M	0.118				
E	2	Sample X1	M	0.452	0.334	CaGl11	25.507813	1275.391
E	3	Sample X1	M	0.457	0.339	CaGl11	25.898438	1294.922
E	4	Sample X1	M	0.458	0.34	CaGl11	25.976563	1298.828
E	1	Blank B	M	0.119				
E	2	Sample X1	M	0.455	0.336	CaGl11	25.664063	1283.203
E	3	Sample X1	M	0.455	0.336	CaGl11	25.664063	1283.203
E	4	Sample X1	M	0.458	0.339	CaGl11	25.898438	1294.922
E	5	Blank B	N	0.116				

Appendix 11.2 contd.

E	6	Sample X1	N	0.388	0.272	CaGl21	20.664063	1033.203
E	7	Sample X1	N	0.385	0.269	CaGl21	20.429688	1021.484
E	8	Sample X1	N	0.383	0.267	CaGl21	20.273438	1013.672
E	5	Blank B	N	0.115				
E	6	Sample X1	N	0.385	0.27	CaGl21	20.507813	1025.391
E	7	Sample X1	N	0.388	0.273	CaGl21	20.742188	1037.109
E	8	Sample X1	N	0.388	0.273	CaGl21	20.742188	1037.109
E	5	Blank B	N	0.116				
E	6	Sample X1	N	0.387	0.271	CaGl21	20.585938	1029.297
E	7	Sample X1	N	0.383	0.267	CaGl21	20.273438	1013.672
E	8	Sample X1	N	0.384	0.268	CaGl21	20.351563	1017.578
E	9	Blank B	O	0.037				
E	10	Sample X1	O	0.199	0.162	WE	12.070313	603.5156
E	11	Sample X1	O	0.193	0.156	WE	11.601563	580.0781
E	12	Sample X1	O	0.196	0.159	WE	11.835938	591.7969
E	9	Blank B	O	0.037				
E	10	Sample X1	O	0.199	0.162	WE	12.070313	603.5156
E	11	Sample X1	O	0.192	0.155	WE	11.523438	576.1719
E	12	Sample X1	O	0.198	0.161	WE	11.992188	599.6094
E	9	Blank B	O	0.037				
E	10	Sample X1	O	0.194	0.157	WE	11.679688	583.9844
E	11	Sample X1	O	0.195	0.158	WE	11.757813	587.8906
E	12	Sample X1	O	0.193	0.156	WE	11.601563	580.0781

Appendix 11.3 optimized experiment CUPRAC

Row	Col	Content	Group	Raw Data (450)	Blank corrected based on Raw Data (450)	Sample code	CUPRAC (mMTE/mL)	CUPRAC (mMTE/g)
A	1	Blank B	A	0.018				
A	2	Sample X1	A	0.188	0.17	CaSu11	0.50193798	25.096899
A	3	Sample X1	A	0.189	0.171	CaSu11	0.50436047	25.218023
A	4	Sample X1	A	0.181	0.163	CaSu11	0.48498062	24.249031
A	1	Blank B	A	0.018				
A	2	Sample X1	A	0.184	0.166	CaSu11	0.49224806	24.612403
A	3	Sample X1	A	0.185	0.167	CaSu11	0.49467054	24.733527
A	4	Sample X1	A	0.182	0.164	CaSu11	0.4874031	24.370155
A	1	Blank B	A	0.018				
A	2	Sample X1	A	0.181	0.163	CaSu11	0.48498062	24.249031
A	3	Sample X1	A	0.185	0.167	CaSu11	0.49467054	24.733527
A	4	Sample X1	A	0.189	0.171	CaSu11	0.50436047	25.218023

Appendix 11.3 contd.

A	5	Blank B	B	0.114				
A	6	Sample X1	B	0.398	0.284	CaFr11	0.77810078	38.905039
A	7	Sample X1	B	0.393	0.279	CaFr11	0.76598837	38.299419
A	8	Sample X1	B	0.399	0.285	CaFr11	0.78052326	39.026163
A	5	Blank B	B	0.115				
A	6	Sample X1	B	0.393	0.278	CaFr11	0.76356589	38.178295
A	7	Sample X1	B	0.398	0.283	CaFr11	0.77567829	38.783915
A	8	Sample X1	B	0.392	0.277	CaFr11	0.76114341	38.057171
A	5	Blank B	B	0.118				
A	6	Sample X1	B	0.397	0.279	CaFr11	0.76598837	38.299419
A	7	Sample X1	B	0.398	0.28	CaFr11	0.76841085	38.420543
A	8	Sample X1	B	0.392	0.274	CaFr11	0.75387597	37.693798
A	9	Blank B	C	0.015				
A	10	Sample X1	C	0.193	0.178	CaFr12	0.52131783	26.065891
A	11	Sample X1	C	0.199	0.184	CaFr12	0.53585271	26.792636
A	12	Sample X1	C	0.196	0.181	CaFr12	0.52858527	26.429264
A	9	Blank B	C	0.016				
A	10	Sample X1	C	0.195	0.179	CaFr12	0.52374031	26.187016
A	11	Sample X1	C	0.196	0.18	CaFr12	0.52616279	26.30814
A	12	Sample X1	C	0.191	0.175	CaFr12	0.51405039	25.702519
A	9	Blank B	C	0.017				
A	10	Sample X1	C	0.194	0.177	CaFr12	0.51889535	25.944767
A	11	Sample X1	C	0.198	0.181	CaFr12	0.52858527	26.429264
A	12	Sample X1	C	0.198	0.181	CaFr12	0.52858527	26.429264
B	1	Blank B	D	0.016				
B	2	Sample X1	D	0.182	0.166	CaFr21	0.49224806	24.612403
B	3	Sample X1	D	0.186	0.17	CaFr21	0.50193798	25.096899
B	4	Sample X1	D	0.185	0.169	CaFr21	0.4995155	24.975775
B	1	Blank B	D	0.012				
B	2	Sample X1	D	0.183	0.171	CaFr21	0.50436047	25.218023
B	3	Sample X1	D	0.185	0.173	CaFr21	0.50920543	25.460271
B	4	Sample X1	D	0.182	0.17	CaFr21	0.50193798	25.096899
B	1	Blank B	D	0.014				
B	2	Sample X1	D	0.187	0.173	CaFr21	0.50920543	25.460271
B	3	Sample X1	D	0.186	0.172	CaFr21	0.50678295	25.339147
B	4	Sample X1	D	0.188	0.174	CaFr21	0.51162791	25.581395
B	5	Blank B	E	0.056				
B	6	Sample X1	E	0.228	0.172	CaXy11	0.50678295	25.339147
B	7	Sample X1	E	0.222	0.166	CaXy11	0.49224806	24.612403
B	8	Sample X1	E	0.229	0.173	CaXy11	0.50920543	25.460271
B	5	Blank B	E	0.061				
B	6	Sample X1	E	0.222	0.161	CaXy11	0.48013566	24.006783

Appendix 11.3 contd.

B	7	Sample X1	E	0.225	0.164	CaXy11	0.4874031	24.370155
B	8	Sample X1	E	0.226	0.165	CaXy11	0.48982558	24.491279
B	5	Blank B	E	0.061				
B	6	Sample X1	E	0.226	0.165	CaXy11	0.48982558	24.491279
B	7	Sample X1	E	0.227	0.166	CaXy11	0.49224806	24.612403
B	8	Sample X1	E	0.225	0.164	CaXy11	0.4874031	24.370155
B	9	Blank B	F	0.111				
B	10	Sample X1	F	0.317	0.206	CaXy12	0.58914729	29.457364
B	11	Sample X1	F	0.314	0.203	CaXy12	0.58187984	29.093992
B	12	Sample X1	F	0.312	0.201	CaXy12	0.57703488	28.851744
B	9	Blank B	F	0.113				
B	10	Sample X1	F	0.318	0.205	CaXy12	0.58672481	29.33624
B	11	Sample X1	F	0.319	0.206	CaXy12	0.58914729	29.457364
B	12	Sample X1	F	0.314	0.201	CaXy12	0.57703488	28.851744
B	9	Blank B	F	0.119				
B	10	Sample X1	F	0.314	0.195	CaXy12	0.5625	28.125
B	11	Sample X1	F	0.314	0.195	CaXy12	0.5625	28.125
B	12	Sample X1	F	0.317	0.198	CaXy12	0.56976744	28.488372
C	1	Blank B	G	0.214				
C	2	Sample X1	G	0.424	0.21	CaXy21	0.59883721	29.94186
C	3	Sample X1	G	0.426	0.212	CaXy21	0.60368217	30.184109
C	4	Sample X1	G	0.426	0.212	CaXy21	0.60368217	30.184109
C	1	Blank B	G	0.216				
C	2	Sample X1	G	0.421	0.205	CaXy21	0.58672481	29.33624
C	3	Sample X1	G	0.423	0.207	CaXy21	0.59156977	29.578488
C	4	Sample X1	G	0.423	0.207	CaXy21	0.59156977	29.578488
C	1	Blank B	G	0.121				
C	2	Sample X1	G	0.321	0.2	CaXy21	0.5746124	28.73062
C	3	Sample X1	G	0.324	0.203	CaXy21	0.58187984	29.093992
C	4	Sample X1	G	0.321	0.2	CaXy21	0.5746124	28.73062
C	5	Blank B	H	0.122				
C	6	Sample X1	H	0.349	0.227	CaGr11	0.64001938	32.000969
C	7	Sample X1	H	0.346	0.224	CaGr11	0.63275194	31.637597
C	8	Sample X1	H	0.345	0.223	CaGr11	0.63032946	31.516473
C	5	Blank B	H	0.119				
C	6	Sample X1	H	0.349	0.23	CaGr11	0.64728682	32.364341
C	7	Sample X1	H	0.349	0.23	CaGr11	0.64728682	32.364341
C	8	Sample X1	H	0.348	0.229	CaGr11	0.64486434	32.243217
C	5	Blank B	H	0.114				
C	6	Sample X1	H	0.349	0.235	CaGr11	0.65939922	32.969961
C	7	Sample X1	H	0.349	0.235	CaGr11	0.65939922	32.969961
C	8	Sample X1	H	0.348	0.234	CaGr11	0.65697674	32.848837

Appendix 11.3 contd.

C	9	Blank B	I	0.118				
C	10	Sample X1	I	0.328	0.21	CaGr12	0.59883721	29.94186
C	11	Sample X1	I	0.328	0.21	CaGr12	0.59883721	29.94186
C	12	Sample X1	I	0.329	0.211	CaGr12	0.60125969	30.062984
C	9	Blank B	I	0.117				
C	10	Sample X1	I	0.324	0.207	CaGr12	0.59156977	29.578488
C	11	Sample X1	I	0.325	0.208	CaGr12	0.59399225	29.699612
C	12	Sample X1	I	0.323	0.206	CaGr12	0.58914729	29.457364
C	9	Blank B	I	0.115				
C	10	Sample X1	I	0.328	0.213	CaGr12	0.60610465	30.305233
C	11	Sample X1	I	0.322	0.207	CaGr12	0.59156977	29.578488
C	12	Sample X1	I	0.329	0.214	CaGr12	0.60852713	30.426357
D	1	Blank B	J	0.218				
D	2	Sample X1	J	0.429	0.211	CaGr21	0.60125969	30.062984
D	3	Sample X1	J	0.426	0.208	CaGr21	0.59399225	29.699612
D	4	Sample X1	J	0.428	0.21	CaGr21	0.59883721	29.94186
D	1	Blank B	J	0.216				
D	2	Sample X1	J	0.428	0.212	CaGr21	0.60368217	30.184109
D	3	Sample X1	J	0.429	0.213	CaGr21	0.60610465	30.305233
D	4	Sample X1	J	0.429	0.213	CaGr21	0.60610465	30.305233
D	1	Blank B	J	0.218				
D	2	Sample X1	J	0.425	0.207	CaGr21	0.59156977	29.578488
D	3	Sample X1	J	0.428	0.21	CaGr21	0.59883721	29.94186
D	4	Sample X1	J	0.421	0.203	CaGr21	0.58187984	29.093992
D	5	Blank B	K	0.018				
D	6	Sample X1	K	0.165	0.147	CaGc11	0.44622093	22.311047
D	7	Sample X1	K	0.167	0.149	CaGc11	0.45106589	22.553295
D	8	Sample X1	K	0.167	0.149	CaGc11	0.45106589	22.553295
D	5	Blank B	K	0.012				
D	6	Sample X1	K	0.166	0.154	CaGc11	0.46317829	23.158915
D	7	Sample X1	K	0.161	0.149	CaGc11	0.45106589	22.553295
D	8	Sample X1	K	0.169	0.157	CaGc11	0.47044574	23.522287
D	5	Blank B	K	0.013				
D	6	Sample X1	K	0.163	0.15	CaGc11	0.45348837	22.674419
D	7	Sample X1	K	0.164	0.151	CaGc11	0.45591085	22.795543
D	8	Sample X1	K	0.169	0.156	CaGc11	0.46802326	23.401163
D	9	Blank B	L	0.087				
D	10	Sample X1	L	0.249	0.162	CaGc21	0.48255814	24.127907
D	11	Sample X1	L	0.248	0.161	CaGc21	0.48013566	24.006783
D	12	Sample X1	L	0.248	0.161	CaGc21	0.48013566	24.006783
D	9	Blank B	L	0.091				
D	10	Sample X1	L	0.245	0.154	CaGc21	0.46317829	23.158915

Appendix 11.3 contd.

D	11	Sample X1	L	0.245	0.154	CaGc21	0.46317829	23.158915
D	12	Sample X1	L	0.246	0.155	CaGc21	0.46560078	23.280039
D	9	Blank B	L	0.084				
D	10	Sample X1	L	0.248	0.164	CaGc21	0.4874031	24.370155
D	11	Sample X1	L	0.249	0.165	CaGc21	0.48982558	24.491279
D	12	Sample X1	L	0.246	0.162	CaGc21	0.48255814	24.127907
E	1	Blank B	M	0.115				
E	2	Sample X1	M	0.287	0.172	CaGl11	0.50678295	25.339147
E	3	Sample X1	M	0.287	0.172	CaGl11	0.50678295	25.339147
E	4	Sample X1	M	0.288	0.173	CaGl11	0.50920543	25.460271
E	1	Blank B	M	0.111				
E	2	Sample X1	M	0.282	0.171	CaGl11	0.50436047	25.218023
E	3	Sample X1	M	0.286	0.175	CaGl11	0.51405039	25.702519
E	4	Sample X1	M	0.284	0.173	CaGl11	0.50920543	25.460271
E	1	Blank B	M	0.113				
E	2	Sample X1	M	0.285	0.172	CaGl11	0.50678295	25.339147
E	3	Sample X1	M	0.284	0.171	CaGl11	0.50436047	25.218023
E	4	Sample X1	M	0.287	0.174	CaGl11	0.51162791	25.581395
E	5	Blank B	N	0.208				
E	6	Sample X1	N	0.379	0.171	CaGl21	0.50436047	25.218023
E	7	Sample X1	N	0.379	0.171	CaGl21	0.50436047	25.218023
E	8	Sample X1	N	0.372	0.164	CaGl21	0.4874031	24.370155
E	5	Blank B	N	0.201				
E	6	Sample X1	N	0.379	0.178	CaGl21	0.52131783	26.065891
E	7	Sample X1	N	0.374	0.173	CaGl21	0.50920543	25.460271
E	8	Sample X1	N	0.376	0.175	CaGl21	0.51405039	25.702519
E	5	Blank B	N	0.201				
E	6	Sample X1	N	0.379	0.178	CaGl21	0.52131783	26.065891
E	7	Sample X1	N	0.378	0.177	CaGl21	0.51889535	25.944767
E	8	Sample X1	N	0.376	0.175	CaGl21	0.51405039	25.702519
E	9	Blank B	O	0.015				
E	10	Sample X1	O	0.166	0.151	WE	0.45591085	22.795543
E	11	Sample X1	O	0.164	0.149	WE	0.45106589	22.553295
E	12	Sample X1	O	0.166	0.151	WE	0.45591085	22.795543
E	9	Blank B	O	0.012				
E	10	Sample X1	O	0.169	0.157	WE	0.47044574	23.522287
E	11	Sample X1	O	0.167	0.155	WE	0.46560078	23.280039
E	12	Sample X1	O	0.166	0.154	WE	0.46317829	23.158915
E	9	Blank B	O	0.017				
E	10	Sample X1	O	0.164	0.147	WE	0.44622093	22.311047
E	11	Sample X1	O	0.161	0.144	WE	0.43895349	21.947674
E	12	Sample X1	O	0.169	0.152	WE	0.45833333	22.916667

Appendix 11.4. Optimized experiment FRAP

Row	Col	Content	Group	Raw Data (593)	Blank corrected based on Raw Data (593)	Sample code	FRAP (µMTE/L)	FRAP (µMTE/ml)	FRAP (µMTE/g)
A	1	Blank B	A	0.186					
A	2	Sample X1	A	0.919	0.733	CaSu11	565.153846	0.56515385	28.25769
A	3	Sample X1	A	0.911	0.725	CaSu11	559	0.559	27.95
A	4	Sample X1	A	0.911	0.725	CaSu11	559	0.559	27.95
A	1	Blank B	A	0.185					
A	2	Sample X1	A	0.911	0.726	CaSu11	559.769231	0.55976923	27.98846
A	3	Sample X1	A	0.917	0.732	CaSu11	564.384615	0.56438462	28.21923
A	4	Sample X1	A	0.915	0.73	CaSu11	562.846154	0.56284615	28.14231
A	1	Blank B	A	0.183					
A	2	Sample X1	A	0.919	0.736	CaSu11	567.461538	0.56746154	28.37308
A	3	Sample X1	A	0.919	0.736	CaSu11	567.461538	0.56746154	28.37308
A	4	Sample X1	A	0.916	0.733	CaSu11	565.153846	0.56515385	28.25769
A	5	Blank B	B	0.069					
A	6	Sample X1	B	0.752	0.683	CaFr11	526.692308	0.52669231	26.33462
A	7	Sample X1	B	0.755	0.686	CaFr11	529	0.529	26.45
A	8	Sample X1	B	0.757	0.688	CaFr11	530.538462	0.53053846	26.52692
A	5	Blank B	B	0.067					
A	6	Sample X1	B	0.758	0.691	CaFr11	532.846154	0.53284615	26.64231
A	7	Sample X1	B	0.754	0.687	CaFr11	529.769231	0.52976923	26.48846
A	8	Sample X1	B	0.752	0.685	CaFr11	528.230769	0.52823077	26.41154
A	5	Blank B	B	0.065					
A	6	Sample X1	B	0.757	0.692	CaFr11	533.615385	0.53361538	26.68077
A	7	Sample X1	B	0.754	0.689	CaFr11	531.307692	0.53130769	26.56538
A	8	Sample X1	B	0.753	0.688	CaFr11	530.538462	0.53053846	26.52692
A	9	Blank B	C	0.339					
A	10	Sample X1	C	0.782	0.443	CaFr12	342.076923	0.34207692	17.10385
A	11	Sample X1	C	0.789	0.45	CaFr12	347.461538	0.34746154	17.37308
A	12	Sample X1	C	0.787	0.448	CaFr12	345.923077	0.34592308	17.29615
A	9	Blank B	C	0.334					
A	10	Sample X1	C	0.782	0.448	CaFr12	345.923077	0.34592308	17.29615
A	11	Sample X1	C	0.788	0.454	CaFr12	350.538462	0.35053846	17.52692
A	12	Sample X1	C	0.782	0.448	CaFr12	345.923077	0.34592308	17.29615
A	9	Blank B	C	0.336					
A	10	Sample X1	C	0.782	0.446	CaFr12	344.384615	0.34438462	17.21923
A	11	Sample X1	C	0.787	0.451	CaFr12	348.230769	0.34823077	17.41154
A	12	Sample X1	C	0.783	0.447	CaFr12	345.153846	0.34515385	17.25769
B	1	Blank B	D	0.389					

Appendix 11.4 contd.

B	2	Sample X1	D	0.866	0.477	CaFr21	368.230769	0.36823077	18.41154
B	3	Sample X1	D	0.865	0.476	CaFr21	367.461538	0.36746154	18.37308
B	4	Sample X1	D	0.869	0.48	CaFr21	370.538462	0.37053846	18.52692
B	1	Blank B	D	0.388					
B	2	Sample X1	D	0.864	0.476	CaFr21	367.461538	0.36746154	18.37308
B	3	Sample X1	D	0.865	0.477	CaFr21	368.230769	0.36823077	18.41154
B	4	Sample X1	D	0.864	0.476	CaFr21	367.461538	0.36746154	18.37308
B	1	Blank B	D	0.388					
B	2	Sample X1	D	0.869	0.481	CaFr21	371.307692	0.37130769	18.56538
B	3	Sample X1	D	0.868	0.48	CaFr21	370.538462	0.37053846	18.52692
B	4	Sample X1	D	0.867	0.479	CaFr21	369.769231	0.36976923	18.48846
B	5	Blank B	E	0.168					
B	6	Sample X1	E	0.661	0.493	CaXy11	380.538462	0.38053846	19.02692
B	7	Sample X1	E	0.667	0.499	CaXy11	385.153846	0.38515385	19.25769
B	8	Sample X1	E	0.669	0.501	CaXy11	386.692308	0.38669231	19.33462
B	5	Blank B	E	0.168					
B	6	Sample X1	E	0.669	0.501	CaXy11	386.692308	0.38669231	19.33462
B	7	Sample X1	E	0.663	0.495	CaXy11	382.076923	0.38207692	19.10385
B	8	Sample X1	E	0.662	0.494	CaXy11	381.307692	0.38130769	19.06538
B	5	Blank B	E	0.166					
B	6	Sample X1	E	0.663	0.497	CaXy11	383.615385	0.38361538	19.18077
B	7	Sample X1	E	0.662	0.496	CaXy11	382.846154	0.38284615	19.14231
B	8	Sample X1	E	0.669	0.503	CaXy11	388.230769	0.38823077	19.41154
B	9	Blank B	F	0.267					
B	10	Sample X1	F	0.738	0.471	CaXy12	363.615385	0.36361538	18.18077
B	11	Sample X1	F	0.739	0.472	CaXy12	364.384615	0.36438462	18.21923
B	12	Sample X1	F	0.738	0.471	CaXy12	363.615385	0.36361538	18.18077
B	9	Blank B	F	0.268					
B	10	Sample X1	F	0.738	0.47	CaXy12	362.846154	0.36284615	18.14231
B	11	Sample X1	F	0.736	0.468	CaXy12	361.307692	0.36130769	18.06538
B	12	Sample X1	F	0.736	0.468	CaXy12	361.307692	0.36130769	18.06538
B	9	Blank B	F	0.268					
B	10	Sample X1	F	0.736	0.468	CaXy12	361.307692	0.36130769	18.06538
B	11	Sample X1	F	0.739	0.471	CaXy12	363.615385	0.36361538	18.18077
B	12	Sample X1	F	0.737	0.469	CaXy12	362.076923	0.36207692	18.10385
C	1	Blank B	G	0.218					
C	2	Sample X1	G	0.635	0.417	CaXy21	322.076923	0.32207692	16.10385
C	3	Sample X1	G	0.636	0.418	CaXy21	322.846154	0.32284615	16.14231
C	4	Sample X1	G	0.635	0.417	CaXy21	322.076923	0.32207692	16.10385
C	1	Blank B	G	0.217					
C	2	Sample X1	G	0.631	0.414	CaXy21	319.769231	0.31976923	15.98846
C	3	Sample X1	G	0.637	0.42	CaXy21	324.384615	0.32438462	16.21923

Appendix 11.4 contd.

C	4	Sample X1	G	0.639	0.422	CaXy21	325.923077	0.32592308	16.29615
C	1	Blank B	G	0.214					
C	2	Sample X1	G	0.634	0.42	CaXy21	324.384615	0.32438462	16.21923
C	3	Sample X1	G	0.637	0.423	CaXy21	326.692308	0.32669231	16.33462
C	4	Sample X1	G	0.636	0.422	CaXy21	325.923077	0.32592308	16.29615
C	5	Blank B	H	0.274					
C	6	Sample X1	H	0.713	0.439	CaGr11	339	0.339	16.95
C	7	Sample X1	H	0.712	0.438	CaGr11	338.230769	0.33823077	16.91154
C	8	Sample X1	H	0.718	0.444	CaGr11	342.846154	0.34284615	17.14231
C	5	Blank B	H	0.273					
C	6	Sample X1	H	0.716	0.443	CaGr12	342.076923	0.34207692	17.10385
C	7	Sample X1	H	0.712	0.439	CaGr12	339	0.339	16.95
C	8	Sample X1	H	0.713	0.44	CaGr12	339.769231	0.33976923	16.98846
C	5	Blank B	H	0.272					
C	6	Sample X1	H	0.714	0.442	CaGr12	341.307692	0.34130769	17.06538
C	7	Sample X1	H	0.717	0.445	CaGr12	343.615385	0.34361538	17.18077
C	8	Sample X1	H	0.713	0.441	CaGr12	340.538462	0.34053846	17.02692
C	9	Blank B	I	0.163					
C	10	Sample X1	I	0.648	0.485	CaGr12	374.384615	0.37438462	18.71923
C	11	Sample X1	I	0.649	0.486	CaGr12	375.153846	0.37515385	18.75769
C	12	Sample X1	I	0.647	0.484	CaGr12	373.615385	0.37361538	18.68077
C	9	Blank B	I	0.166					
C	10	Sample X1	I	0.645	0.479	CaGr12	369.769231	0.36976923	18.48846
C	11	Sample X1	I	0.642	0.476	CaGr12	367.461538	0.36746154	18.37308
C	12	Sample X1	I	0.648	0.482	CaGr12	372.076923	0.37207692	18.60385
C	9	Blank B	I	0.169					
C	10	Sample X1	I	0.645	0.476	CaGr12	367.461538	0.36746154	18.37308
C	11	Sample X1	I	0.642	0.473	CaGr12	365.153846	0.36515385	18.25769
C	12	Sample X1	I	0.646	0.477	CaGr12	368.230769	0.36823077	18.41154
D	1	Blank B	J	0.054					
D	2	Sample X1	J	0.737	0.683	CaGr21	526.692308	0.52669231	26.33462
D	3	Sample X1	J	0.731	0.677	CaGr21	522.076923	0.52207692	26.10385
D	4	Sample X1	J	0.739	0.685	CaGr21	528.230769	0.52823077	26.41154
D	1	Blank B	J	0.055					
D	2	Sample X1	J	0.733	0.678	CaGr21	522.846154	0.52284615	26.14231
D	3	Sample X1	J	0.736	0.681	CaGr21	525.153846	0.52515385	26.25769
D	4	Sample X1	J	0.731	0.676	CaGr21	521.307692	0.52130769	26.06538
D	1	Blank B	J	0.057					
D	2	Sample X1	J	0.735	0.678	CaGr21	522.846154	0.52284615	26.14231
D	3	Sample X1	J	0.739	0.682	CaGr21	525.923077	0.52592308	26.29615
D	4	Sample X1	J	0.735	0.678	CaGr21	522.846154	0.52284615	26.14231
D	5	Blank B	K	0.087					

Appendix 11.4 contd.

D	6	Sample X1	K	0.538	0.451	CaGc11	348.230769	0.34823077	17.41154
D	7	Sample X1	K	0.534	0.447	CaGc11	345.153846	0.34515385	17.25769
D	8	Sample X1	K	0.536	0.449	CaGc11	346.692308	0.34669231	17.33462
D	5	Blank B	K	0.084					
D	6	Sample X1	K	0.532	0.448	CaGc11	345.923077	0.34592308	17.29615
D	7	Sample X1	K	0.532	0.448	CaGc11	345.923077	0.34592308	17.29615
D	8	Sample X1	K	0.537	0.453	CaGc11	349.769231	0.34976923	17.48846
D	5	Blank B	K	0.094					
D	6	Sample X1	K	0.532	0.438	CaGc11	338.230769	0.33823077	16.91154
D	7	Sample X1	K	0.533	0.439	CaGc11	339	0.339	16.95
D	8	Sample X1	K	0.532	0.438	CaGc11	338.230769	0.33823077	16.91154
D	9	Blank B	L	0.293					
D	10	Sample X1	L	0.486	0.193	CaGc21	149.769231	0.14976923	7.488462
D	11	Sample X1	L	0.482	0.189	CaGc21	146.692308	0.14669231	7.334615
D	12	Sample X1	L	0.488	0.195	CaGc21	151.307692	0.15130769	7.565385
D	9	Blank B	L	0.292					
D	10	Sample X1	L	0.489	0.197	CaGc21	152.846154	0.15284615	7.642308
D	11	Sample X1	L	0.486	0.194	CaGc21	150.538462	0.15053846	7.526923
D	12	Sample X1	L	0.487	0.195	CaGc21	151.307692	0.15130769	7.565385
D	9	Blank B	L	0.288					
D	10	Sample X1	L	0.486	0.198	CaGc21	153.615385	0.15361538	7.680769
D	11	Sample X1	L	0.489	0.201	CaGc21	155.923077	0.15592308	7.796154
D	12	Sample X1	L	0.487	0.199	CaGc21	154.384615	0.15438462	7.719231
E	1	Blank B	M	0.301					
E	2	Sample X1	M	0.524	0.223	CaGl11	172.846154	0.17284615	8.642308
E	3	Sample X1	M	0.524	0.223	CaGl11	172.846154	0.17284615	8.642308
E	4	Sample X1	M	0.528	0.227	CaGl11	175.923077	0.17592308	8.796154
E	1	Blank B	M	0.307					
E	2	Sample X1	M	0.523	0.216	CaGl11	167.461538	0.16746154	8.373077
E	3	Sample X1	M	0.529	0.222	CaGl11	172.076923	0.17207692	8.603846
E	4	Sample X1	M	0.529	0.222	CaGl11	172.076923	0.17207692	8.603846
E	1	Blank B	M	0.306					
E	2	Sample X1	M	0.523	0.217	CaGl11	168.230769	0.16823077	8.411538
E	3	Sample X1	M	0.529	0.223	CaGl11	172.846154	0.17284615	8.642308
E	4	Sample X1	M	0.527	0.221	CaGl11	171.307692	0.17130769	8.565385
E	5	Blank B	N	0.184					
E	6	Sample X1	N	0.488	0.304	CaGl21	235.153846	0.23515385	11.75769
E	7	Sample X1	N	0.489	0.305	CaGl21	235.923077	0.23592308	11.79615
E	8	Sample X1	N	0.481	0.297	CaGl21	229.769231	0.22976923	11.48846
E	5	Blank B	N	0.186					
E	6	Sample X1	N	0.482	0.296	CaGl21	229	0.229	11.45
E	7	Sample X1	N	0.481	0.295	CaGl21	228.230769	0.22823077	11.41154

Appendix 11.4 contd.

E	8	Sample X1	N	0.489	0.303	CaGl21	234.384615	0.23438462	11.71923
E	5	Blank B	N	0.189					
E	6	Sample X1	N	0.487	0.298	CaGl21	230.538462	0.23053846	11.52692
E	7	Sample X1	N	0.487	0.298	CaGl21	230.538462	0.23053846	11.52692
E	8	Sample X1	N	0.489	0.3	CaGl21	232.076923	0.23207692	11.60385
E	9	Blank B	O	0.163					
E	10	Sample X1	O	0.478	0.315	WE	243.615385	0.24361538	12.18077
E	11	Sample X1	O	0.476	0.313	WE	242.076923	0.24207692	12.10385
E	12	Sample X1	O	0.477	0.314	WE	242.846154	0.24284615	12.14231
E	9	Blank B	O	0.165					
E	10	Sample X1	O	0.472	0.307	WE	237.461538	0.23746154	11.87308
E	11	Sample X1	O	0.475	0.31	WE	239.769231	0.23976923	11.98846
E	12	Sample X1	O	0.472	0.307	WE	237.461538	0.23746154	11.87308
E	9	Blank B	O	0.161					
E	10	Sample X1	O	0.473	0.312	WE	241.307692	0.24130769	12.06538
E	11	Sample X1	O	0.479	0.318	WE	245.923077	0.24592308	12.29615
E	12	Sample X1	O	0.474	0.313	WE	242.076923	0.24207692	12.10385

Appendix 11.5 Optimized experiment DPPH

Row	Col	Content	Group	Raw Data (517)	Blank corrected based on Raw Data (517)	Sample code	% Inhibition	DPPH (µMTE/L)	DPPH (µMTE/g)
A	1	Blank B	A	0.106					
A	2	Control C1	A	0.868	0.762				
A	3	Control C1	A	1.072	0.966	0.929			
A	4	Control C1	A	1.165	1.059				
A	5	Sample X1	A	0.365	0.259	CaSu11	72.12056	9.929499	496.475
A	6	Sample X1	A	0.363	0.257	CaSu11	72.33584	9.92524	496.262
A	7	Sample X1	A	0.364	0.258	CaSu11	72.2282	9.92737	496.3685
A	5	Sample X1	A	0.365	0.259	CaSu11	72.12056	9.929499	496.475
A	6	Sample X1	A	0.363	0.257	CaSu11	72.33584	9.92524	496.262
A	7	Sample X1	A	0.365	0.259	CaSu11	72.12056	9.929499	496.475
A	5	Sample X1	A	0.361	0.255	CaSu11	72.55113	9.92098	496.049
A	6	Sample X1	A	0.364	0.258	CaSu11	72.2282	9.92737	496.3685
A	7	Sample X1	A	0.365	0.259	CaSu11	72.12056	9.929499	496.475
A	8	Blank B	B	0.152					
A	9	Control C1	B	0.942	0.79				
A	10	Control C1	B	1.106	0.954	0.874667			
A	11	Control C1	B	1.032	0.88				

Appendix 11.5 contd.

A	12	Sample X1	B	0.381	0.229	CaFr11	73.8186	9.865602	493.2801
B	1	Sample X1	B	0.382	0.23	CaFr11	73.70427	9.867732	493.3866
B	2	Sample X1	B	0.386	0.234	CaFr11	73.24695	9.876251	493.8126
A	12	Sample X1	B	0.386	0.234	CaFr11	73.24695	9.876251	493.8126
B	1	Sample X1	B	0.386	0.234	CaFr11	73.24695	9.876251	493.8126
B	2	Sample X1	B	0.383	0.231	CaFr11	73.58994	9.869862	493.4931
A	12	Sample X1	B	0.381	0.229	CaFr11	73.8186	9.865602	493.2801
B	1	Sample X1	B	0.383	0.231	CaFr11	73.58994	9.869862	493.4931
B	2	Sample X1	B	0.382	0.23	CaFr11	73.70427	9.867732	493.3866
B	3	Blank B	C	0.251					
B	4	Control C1	C	0.949	0.698				
B	5	Control C1	C	0.932	0.681	0.721			
B	6	Control C1	C	1.035	0.784				
B	7	Sample X1	C	0.365	0.114	CaFr12	84.18863	9.62066	481.033
B	8	Sample X1	C	0.364	0.113	CaFr12	84.32732	9.61853	480.9265
B	9	Sample X1	C	0.363	0.112	CaFr12	84.46602	9.6164	480.82
B	7	Sample X1	C	0.367	0.116	CaFr12	83.91123	9.62492	481.246
B	8	Sample X1	C	0.361	0.11	CaFr12	84.74341	9.612141	480.607
B	9	Sample X1	C	0.364	0.113	CaFr12	84.32732	9.61853	480.9265
B	7	Sample X1	C	0.368	0.117	CaFr12	83.77254	9.62705	481.3525
B	8	Sample X1	C	0.369	0.118	CaFr12	83.63384	9.62918	481.459
B	9	Sample X1	C	0.364	0.113	CaFr12	84.32732	9.61853	480.9265
B	10	Blank B	D	0.153					
B	11	Control C1	D	0.888	0.735				
B	12	Control C1	D	1.202	1.049	0.903			
C	1	Control C1	D	1.078	0.925				
C	2	Sample X1	D	0.295	0.142	CaFr21	84.27464	9.680298	484.0149
C	3	Sample X1	D	0.299	0.146	CaFr21	83.83167	9.688818	484.4409
C	4	Sample X1	D	0.299	0.146	CaFr21	83.83167	9.688818	484.4409
C	2	Sample X1	D	0.293	0.14	CaFr21	84.49612	9.676038	483.8019
C	3	Sample X1	D	0.293	0.14	CaFr21	84.49612	9.676038	483.8019
C	4	Sample X1	D	0.291	0.138	CaFr21	84.71761	9.671778	483.5889
C	2	Sample X1	D	0.297	0.144	CaFr21	84.05316	9.684558	484.2279
C	3	Sample X1	D	0.298	0.145	CaFr21	83.94241	9.686688	484.3344
C	4	Sample X1	D	0.291	0.138	CaFr21	84.71761	9.671778	483.5889
C	5	Blank B	E	0.054					
C	6	Control C1	E	0.824	0.77				
C	7	Control C1	E	0.826	0.772	0.770333			
C	8	Control C1	E	0.823	0.769				
C	9	Sample X1	E	0.322	0.268	CaXy11	65.20987	9.948669	497.4334
C	10	Sample X1	E	0.326	0.272	CaXy11	64.69061	9.957188	497.8594
C	11	Sample X1	E	0.325	0.271	CaXy11	64.82042	9.955059	497.7529

Appendix 11.5 contd.

C	9	Sample X1	E	0.329	0.275	CaXy11	64.30117	9.963578	498.1789
C	10	Sample X1	E	0.327	0.273	CaXy11	64.5608	9.959318	497.9659
C	11	Sample X1	E	0.324	0.27	CaXy11	64.95024	9.952929	497.6464
C	9	Sample X1	E	0.325	0.271	CaXy11	64.82042	9.955059	497.7529
C	10	Sample X1	E	0.325	0.271	CaXy11	64.82042	9.955059	497.7529
C	11	Sample X1	E	0.325	0.271	CaXy11	64.82042	9.955059	497.7529
C	12	Blank B	F	0.105					
D	1	Control C1	F	0.874	0.769				
D	2	Control C1	F	0.823	0.718	0.739667			
D	3	Control C1	F	0.837	0.732				
D	4	Sample X1	F	0.128	0.023	CaXy12	96.89049	9.426837	471.3419
D	5	Sample X1	F	0.129	0.024	CaXy12	96.7553	9.428967	471.4483
D	6	Sample X1	F	0.125	0.02	CaXy12	97.29608	9.420447	471.0224
D	4	Sample X1	F	0.124	0.019	CaXy12	97.43128	9.418317	470.9159
D	5	Sample X1	F	0.124	0.019	CaXy12	97.43128	9.418317	470.9159
D	6	Sample X1	F	0.124	0.019	CaXy12	97.43128	9.418317	470.9159
D	4	Sample X1	F	0.121	0.016	CaXy12	97.83686	9.411928	470.5964
D	5	Sample X1	F	0.121	0.016	CaXy12	97.83686	9.411928	470.5964
D	6	Sample X1	F	0.121	0.016	CaXy12	97.83686	9.411928	470.5964
D	7	Blank B	G	0.249					
D	8	Control C1	G	0.893	0.644				
D	9	Control C1	G	0.94	0.691	0.686333			
D	10	Control C1	G	0.973	0.724				
D	11	Sample X1	G	0.497	0.248	CaXy21	63.86595	9.90607	495.3035
D	12	Sample X1	G	0.495	0.246	CaXy21	64.15736	9.90181	495.0905
E	1	Sample X1	G	0.495	0.246	CaXy21	64.15736	9.90181	495.0905
D	11	Sample X1	G	0.492	0.243	CaXy21	64.59446	9.895421	494.771
D	12	Sample X1	G	0.492	0.243	CaXy21	64.59446	9.895421	494.771
E	1	Sample X1	G	0.498	0.249	CaXy21	63.72025	9.9082	495.41
D	11	Sample X1	G	0.496	0.247	CaXy21	64.01166	9.90394	495.197
D	12	Sample X1	G	0.496	0.247	CaXy21	64.01166	9.90394	495.197
E	1	Sample X1	G	0.492	0.243	CaXy21	64.59446	9.895421	494.771
E	2	Blank B	H	0.151					
E	3	Control C1	H	1.156	1.005				
E	4	Control C1	H	1.329	1.178	1.108			
E	5	Control C1	H	1.292	1.141				
E	6	Sample X1	H	0.331	0.18	CaGr11	83.75451	9.761235	488.0618
E	7	Sample X1	H	0.335	0.184	CaGr11	83.3935	9.769755	488.4878
E	8	Sample X1	H	0.331	0.18	CaGr11	83.75451	9.761235	488.0618
E	6	Sample X1	H	0.33	0.179	CaGr11	83.84477	9.759105	487.9553
E	7	Sample X1	H	0.337	0.186	CaGr11	83.75451	9.774015	488.7007
E	8	Sample X1	H	0.336	0.185	CaGr11	83.30325	9.771885	488.5942

Appendix 11.5 contd.

E	6	Sample X1	H	0.333	0.182	CaGr11	83.57401	9.765495	488.2748
E	7	Sample X1	H	0.334	0.183	CaGr11	83.48375	9.767625	488.3813
E	8	Sample X1	H	0.338	0.187	CaGr11	83.12274	9.776145	488.8072
A	1	Blank B	A	0.164					
A	2	Control C1	A	0.952	0.788				
A	3	Control C1	A	0.952	0.788	0.79			
A	4	Control C1	A	0.958	0.794				
A	5	Sample X1	A	0.243	0.079	CaGr12	90	9.546113	477.3056
A	6	Sample X1	A	0.246	0.082	CaGr12	89.62025	9.552503	477.6251
A	7	Sample X1	A	0.249	0.085	CaGr12	89.24051	9.558892	477.9446
A	5	Sample X1	A	0.244	0.08	CaGr12	89.87342	9.548243	477.4121
A	6	Sample X1	A	0.244	0.08	CaGr12	89.87342	9.548243	477.4121
A	7	Sample X1	A	0.245	0.081	CaGr12	89.74684	9.550373	477.5186
A	5	Sample X1	A	0.242	0.078	CaGr12	90.12658	9.543983	477.1991
A	6	Sample X1	A	0.249	0.085	CaGr12	89.24051	9.558892	477.9446
A	7	Sample X1	A	0.246	0.082	CaGr12	89.62025	9.552503	477.6251
A	8	Blank B	B	0.133					
A	9	Control C1	B	1.262	1.129				
A	10	Control C1	B	1.373	1.24	1.265667			
A	11	Control C1	B	1.561	1.428				
A	12	Sample X1	B	0.379	0.246	CaGr21	80.5636	9.90181	495.0905
B	1	Sample X1	B	0.374	0.241	CaGr21	80.95865	9.891161	494.558
B	2	Sample X1	B	0.372	0.239	CaGr21	81.11667	9.886901	494.345
A	12	Sample X1	B	0.371	0.238	CaGr21	81.19568	9.884771	494.2386
B	1	Sample X1	B	0.376	0.243	CaGr21	80.80063	9.895421	494.771
B	2	Sample X1	B	0.374	0.241	CaGr21	80.95865	9.891161	494.558
A	12	Sample X1	B	0.377	0.244	CaGr21	80.72162	9.897551	494.8775
B	1	Sample X1	B	0.373	0.24	CaGr21	81.03766	9.889031	494.4515
B	2	Sample X1	B	0.373	0.24	CaGr21	81.03766	9.889031	494.4515
B	3	Blank B	C	0.249					
B	4	Control C1	C	0.995	0.746				
B	5	Control C1	C	0.994	0.745	0.744			
B	6	Control C1	C	0.99	0.741				
B	7	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	8	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	9	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	7	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	8	Sample X1	C	0.355	0.106	CaGc11	85.75269	9.603621	480.181
B	9	Sample X1	C	0.354	0.105	CaGc11	85.8871	9.601491	480.0745
B	7	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	8	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616
B	9	Sample X1	C	0.352	0.103	CaGc11	86.15591	9.597231	479.8616

Appendix 11.5 contd.

B	10	Blank B	D	0.147					
B	11	Control C1	D	1.314	1.167				
B	12	Control C1	D	1.351	1.204	1.180333			
C	1	Control C1	D	1.317	1.17				
C	2	Sample X1	D	0.262	0.115	CaGc21	90.25699	9.62279	481.1395
C	3	Sample X1	D	0.269	0.122	CaGc21	89.66394	9.6377	481.885
C	4	Sample X1	D	0.263	0.116	CaGc21	90.17227	9.62492	481.246
C	2	Sample X1	D	0.261	0.114	CaGc21	90.34171	9.62066	481.033
C	3	Sample X1	D	0.266	0.119	CaGc21	89.9181	9.63131	481.5655
C	4	Sample X1	D	0.266	0.119	CaGc21	89.9181	9.63131	481.5655
C	2	Sample X1	D	0.267	0.12	CaGc21	89.83338	9.63344	481.672
C	3	Sample X1	D	0.262	0.115	CaGc21	90.25699	9.62279	481.1395
C	4	Sample X1	D	0.264	0.117	CaGc21	90.08755	9.62705	481.3525
C	5	Blank B	E	0.261					
C	6	Control C1	E	1.198	0.937				
C	7	Control C1	E	1.329	1.068	0.984667			
C	8	Control C1	E	1.21	0.949				
C	9	Sample X1	E	0.909	0.648	CaGl11	34.19093	10.75804	537.902
C	10	Sample X1	E	0.902	0.641	CaGl11	34.90183	10.74313	537.1565
C	11	Sample X1	E	0.903	0.642	CaGl11	34.80027	10.74526	537.263
C	9	Sample X1	E	0.901	0.64	CaGl11	35.00339	10.741	537.0501
C	10	Sample X1	E	0.904	0.643	CaGl11	34.69871	10.74739	537.3695
C	11	Sample X1	E	0.903	0.642	CaGl11	34.80027	10.74526	537.263
C	9	Sample X1	E	0.902	0.641	CaGl11	34.90183	10.74313	537.1565
C	10	Sample X1	E	0.904	0.643	CaGl11	34.69871	10.74739	537.3695
C	11	Sample X1	E	0.902	0.641	CaGl11	34.90183	10.74313	537.1565
C	12	Blank B	F	0.354					
D	1	Control C1	F	1.256	0.902				
D	2	Control C1	F	1.217	0.863	0.900333			
D	3	Control C1	F	1.29	0.936				
D	4	Sample X1	F	0.475	0.121	CaGl21	86.56053	9.63557	481.7785
D	5	Sample X1	F	0.478	0.124	CaGl21	86.22732	9.64196	482.098
D	6	Sample X1	F	0.473	0.119	CaGl21	86.78267	9.63131	481.5655
D	4	Sample X1	F	0.475	0.122	CaGl21	86.44946	9.6377	481.885
D	5	Sample X1	F	0.476	0.122	CaGl21	86.44946	9.6377	481.885
D	6	Sample X1	F	0.476	0.122	CaGl21	86.44946	9.6377	481.885
D	4	Sample X1	F	0.479	0.125	CaGl21	86.11625	9.644089	482.2045
D	5	Sample X1	F	0.471	0.117	CaGl21	87.00481	9.62705	481.3525
D	6	Sample X1	F	0.477	0.123	CaGl21	86.33839	9.63983	481.9915
D	7	Blank B	G	0.141					
D	8	Control C1	G	1.305	1.164				
D	9	Control C1	G	1.476	1.335	1.238667			

Appendix 11.5 contd.

D	10	Control C1	G	1.358	1.217				
D	11	Sample X1	G	1.238	1.097	WE	11.43703	11.71438	585.7188
D	12	Sample X1	G	1.232	1.091	WE	11.92142	11.7016	585.0799
E	1	Sample X1	G	1.235	1.094	WE	11.67922	11.70799	585.3994
D	11	Sample X1	G	1.236	1.095	WE	11.59849	11.71012	585.5059
D	12	Sample X1	G	1.23	1.089	WE	12.08288	11.69734	584.8669
E	1	Sample X1	G	1.234	1.093	WE	11.75996	11.70586	585.2929
D	11	Sample X1	G	1.237	1.096	WE	11.51776	11.71225	585.6124
D	12	Sample X1	G	1.233	1.092	WE	11.84069	11.70373	585.1864
E	1	Sample X1	G	1.239	1.098	WE	11.3563	11.71651	585.8253