Application of metabolomics to measure the Alberta "Foodome"

by

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Abstract

Food is fundamental to life. It is the source of essentially all the chemical and biological components found in our bodies. Given its importance, there is a growing desire among food producers, consumers, nutritionists, and dieticians to have a better understanding of the precise chemical content of foods. Unfortunately, the chemical composition of most foods is not well known. Indeed, standard food composition tables only provide data on a few dozen highly abundant chemicals. However, recent advances in analytical chemistry technologies and in the field of metabolomics now make it possible to identify and quantify thousands of compounds in biological matrices. These developments suggest that it may be possible to use metabolomics to more completely characterize the chemical constituents in food.

The central objectives of my thesis are: 1) to apply modern quantitative metabolomic methodsto identify and quantify the chemical constituents and micronutrients in a select number of Alberta-grown vegetables, fruits, cereals and meats; and 2) to create a fully web accessible database that contains bothexperimentally derived values and literature-derived information on Alberta-grown foods, called the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca).

In working towards Objective #1, a combination of several modern metabolomics techniques, including ICP-MS, DFI-MS/MS, GC-MS, HPLC, and NMR were used to characterize the chemical constituents of nearly 40 different,Alberta-grown food products. Sample preparation, extraction, and separation techniques were developed or optimized to characterize amino acids, fatty acids, trace metals, vitamins, organic acids, phytochemicals, sugars, and lipids. ICP-MS assays generated composition data for up to 54 metal ions. DFI-MS/MS assay yielded data on about 50-110 compounds per food sample, whilethe GC-MS-

based assays generated data for about 30-75 non-volatile compounds, 20-40 volatile compounds, and up to 20 fatty acids for each food sample.NMR assays yielded data on 30-50 compounds per food sample. Detailed literature mining led to the identification of up to 2000 more compounds for certain food products.

By completing this study, I believe I have helped create perhaps the most comprehensive food information resource in the world.Through the AFCDB, Alberta producers have access to some of the most detailed and information-rich data on the food products they produce. This work could lead toa paradigm shift for food-health labeling, making Alberta food products uniquely appealing for health conscious consumers.

Preface

This thesis is an original work by myself, Shima Borzouie, based on an original idea (called the Alberta Food Metabolome Project) and experimental design by my supervisor Dr. David S. Wishart. This research project was led by Dr. David Wishart from the Departments of Biological Sciences and Computing Science at University of Alberta. All experiments and research activities were performed in Dr. Wishart's Lab and The Metabolomics Innovation Centre at the University of Alberta. To complete the work described in this thesis, I was assisted by a number of individuals including Dr. Wishart and members of his laboratory. More specifically, Dr. Wishart supervised my training, coordinated the experimental activities, designed and ovesaw the analytical methods used for this study and played a key role in the writing and editing of this thesis. Dr. Rupasri Mandal, as the TMIC lab manager, trained me in the operation of the equipment and software, helped with the editing of this thesis, performed the Biocrates LC-DI-MS/MS assays, assisted with the NMR assignments and assisted with the GC-MS data acquisition and lipiddata analysis. Dr. Trent Bjorndahl collected all the NMR spectra used or analyzed in this thesis. Dr. Ramnarayan Krishnamurthy developed and tested many of the food extraction methods, trained me in many laboratory techniques, developed and performed the polyphenol assays and performed many of the GC-MS assays described in this thesis. Dr. Zerihun Dame and Dr. Farid Aziat developed and performed the vitamin assays and helped perform many of the other metabolomic assays described in this thesis. The ICP-MS assays were performed by staff members of the Deptartment of Geology at the University of Alberta.Dr. Rosa Vazquez-Fresno helped with the editing of the thesis and with the NMR analysis. Noah Wishart, Elizabeth Wishart, Jenna Poelzer and Jessica Huynh assisted with the food sample acquisition and sample preparations. Tanvir Sajed, Allison Pon and Dr. Anchi Guo designed, programmed

and set up the Alberta Food Metabolome Database and populated the on-line database with the data acquired for the project.

I was responsible for acquiring and collecting all of the food samples, for preparing or supervising the preparation ofmany of the food samples for metabolomic analysis, for delivering the food sample extracts to the TMIC analytical teams, for conducting a number of the HPLC metabolomic assays, for performing GC-MS spectral profiling and NMR spectral profiling, for identifying and testing food analysis or extraction methods from the literature, for consolidating, calculating and checking all of the experimentally measured metabolomic data for the Alberta Food Metabolome Project, for finding, tabulating and annotating all of the literature-derived food composition data for the Alberta Food Composition Database (AFCDB), and for writing this thesis.

Dedication

To my wonderful mother, all that I am, or ever hope to be, I owe to her.

To the innocent soul of my father who is always with me.

To my husband, for his care and support all the time.

Acknowledgement

First and foremost, I would like to express my deep gratitude and sincere thanks to Dr. David S. Wishart, for giving me the opportunity to work in his research group. It is the greatest honour imaginable to study under Dr. Wishart's supervision. I am indebted to him for his invaluable advice, supervision, patience, encouragement, and full support. Without his guidance and support, I would not have been able to succeed in my graduate studies.

It has been a great honour working in the Wishart group with its very diverse group of scientists and students from all kinds of backgrounds and cultures. I would like to acknowledge the past and present members of the Wishart lab for contributing to my experience here at the University of Alberta. This is a very special group of people and I consider its members to be part of my extended family. We were always there for each other and I will always appreciate the encouragement and good will we shared. I am especially thankful to Dr. Ramanarayan Krishnamurthy for his wonderful training, his many ideas, and his invaluable assistance along the way. I am eternally grateful for two very special friends and colleagues, Dr. Fozia Saleem and Dr. Souhaila Bouatra for their generous help. I also want to thank them for all the pleasant times we spent working together. I would also like to express my deepest heartfelt thanks to Dr. Zerihun Dame and Philip Liu. I learned a lot from both of them over the past 3 years and I was constantly amazed by their vast knowledge. Thanks also to Dr. Rupa Mandal, the lab's metabolomics manager, who has been a great source of help and provided wonderful suggestions during my research. Appreciation is extended to Dr. Farid Aziat and Edison Dong, without whom this research would not have been possible. I also wish to acknowledge Ashenafi Abera, Oxana Tarassova, and BeomSoo Han who have offered many opinions and advice about my scientific research and life. Indeed I was so lucky to meet numerous nice people in Wishart lab.

I would like to gratefully acknowledge my generous funding sources, especially Alberta Innovates Bio Solutions and Genome Canada for financial support.

I have no words to express my love and gratitude to my family. Thank you to my best friend and amazing husband, Younes Miar, who has shown tremendous patience and sacrifice in support of my graduate studies. Despite the geographical distance, my family has always been very close to me. I am forever indebted to my mother, Zahra Rahimi for her love, sacrifice, words of wisdom, and prayers during my life, which have shaped me into the person I am today. Thank you to my brothers Sadra Borzouie and Asra Borzouie for being an endless source of love, support, confidence and inspiration in my life.

Last and most important, I am eternally grateful to God for his continuing presence in my life and for everything that I am.

This thesis is only a beginning of my journey…

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List of Terms and Abbreviations

ASE	Accelerated Solvent Extraction
AFCDB	Alberta Food Composition Database
CNF	Canadian Nutrient File
DFI-MS	Direct Flow Injection Mass Spectrometry
FIA	Flow Injection Analysis
GLPC	Gas-liquid Partition Chromatography
GC-MS	Gas Chromatography Mass Spectrometry
HMDB	The Human Metabolome Database
HPLC	High Performance Liquid Chromatography
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
MS	Mass Spectrometry
MRM-MS	Multiple Reaction Monitoring Mass Spectrometry
MRM	Multiple Reaction Monitoring
NINT	National Institute for Nanotechnology
NIST	National Institute of Standards and Technology
NMR	Nuclear Magnetic Resonance
NDL	Nutrient Data Laboratory
PIT	Phenylisothiocyanate
PLE	Pressurized Liquid Extraction
PWE	Pressurized Water Extraction
SWE	Subcritical Water Extraction
SFE	Supercritical Fluid Extraction
TMIC	The Metabolomics Innovation Centre
TOF	Time of Flight
UAE	Ultrasonic Assisted Extraction
USE	Ultrasonication Extraction
UPLC	Ultra Performance Liquid Chromatography
USDA	U.S. Department of Agriculture

Chapter 1.General Introduction

1.1 Introduction

Food is fundamental to life(Jacobs & Tapsell, 2007).It nourishes us, it comforts us and it gives us tremendous pleasure. It is also the source of essentially all the chemical and biological components found in our bodies (i.e. "you are what you eat"). Certainly as producers, consumers and medical professionals become more aware of the good ingredients in foods (polyphenols, phytosterols, vitamins) and the bad ingredients (saturated fats, trans fats), there is a growing desire among both food producers and food consumers to have a better understanding of the precise chemical composition of the foods they produce, prepare or consume. There is also an equally important need for nutritionists and nutritional chemists to know what happens to these food chemicals when they enter our bodies. This is because many food-derived compounds can act as "pseudo-drugs" (e.g. ethanol, caffeine, resveratrol) that can have profound effects on our body, our mind or our state of health. Even if many food-derived compounds are biologically benign, they can still interfere with the read-outs of certain clinical tests or alter the efficacy of prescription drugs (such as grapefruit-derived furans). Unfortunately, despite its clear and overwhelming importance, the chemical composition of most foods is not well known.

The average food item typically contains >10,000 different organic compounds or micronutrients (Wishart et al., 2007). However, standard food composition tables only provide data on ~40-50 highly abundant chemicals or macronutrients (amino acids, lipids, carbohydrates) in foods (Scalbert et al., 2011). They rarely provide much, if any, data on the many of the lower abundance chemicals or more poorly understood compounds such as organic acids, sugar alcohols, esters, aromatics, biogenic amines, phytochemicals, vitamins, trace metals or fatty acids

that are primarily responsible for the flavour, aroma, colour and key health benefits of many raw or partially processed foods. Consequently, it is often very challenging to find answers to such common questions as: What is the compound that gives bacon its distinctive aroma? Why does cilantro taste soapy to certain people? What are the phytochemicals that make vine-ripened tomatoes so flavourful? Why does Australian wine have such a high alcohol content? What are the compounds in grapes that extend the lifespan of rats? The answer to many of these questions can be found through a newly emerging field of science called metabolomics.

Metabolomics is a branch of omics science that focuses on the comprehensive characterization and biological interpretation of small molecule metabolites found in biological samples (Wishart, 2008). It uses techniques such as nuclear magnetic resonance spectroscopy (NMR), liquid chromatography (LC), gas chromatography (GC) and mass spectrometry (MS) to separate, identify and/or quantify large numbers of small molecules (<1500 Daltons) from complex mixtures and matrices. Key to the development of metabolomics has been the creation of software and databases that facilitate this high throughput chemical characterization (Wishart, 2011). When properly performed, metabolomics assays can lead to the detection of >10,000 compounds and the identification or quantification of >1000 compounds in biological samples (Scalbert et al., 2009). Consequently, when metabolomics is used in food science it has the potential to provide "ultra-comprehensive" food composition analysis.

While the applications of conventional analytical chemistry approaches to food composition determination are relatively old, the application of metabolomics to food composition analysis is relatively new. ***My thesis is focused on developing and describing metabolomics techniques that can be used in food analysis***. In particular, my research is aimed at using advanced metabolomics techniques to identify and quantify the chemical constituents of nearly 40

different Alberta-grown foods. The intent of this work is to demonstrate the feasibility of metabolomics in performing ultra-comprehensive food analysis and to show that metabolomics can lead to the identification or quantification of novel macro- and micronutrients that not only affect organoleptic qualities such as flavour, aroma, colour but also those compounds that affect human health (Wishart, 2008).

This introductory chapter is intended to provide an overview of food composition analysis and the application of metabolomics to food analysis. It is organized as follows: The first section discusses the importance of food and diet as it relates to health and disease. The second section provides a brief overview of food composition analysis with particular focus on the history of food analysis techniques. Section 3 describes methods for food sample preparation and extraction as it relates to food composition or nutrient analysis. In section 4, I briefly review the field of food metabolomics and provide an overview of ongoing challenges in food composition analysis, in particular. The chapter concludes with some background on the motivation for my research theme and a description of my research objectives.

1.2 Diet, Disease and Health

The relationship between diet, disease and health is well known. Indeed perhaps the greatest triumphs of nutritional (and even medical) science was the discovery that many chronic illnesses, such as childhood blindness, childhood mental retardation, scurvy, goiter, rickets and pernicious anemia were actually linked to the lack of consumption of certain key vitamins and micronutrients(Chesney, 2001; Pollycove et al., 1956; Sommer et al., 1986). These discoveries led the introduction of mandatory food fortification and the near-elimination of these conditions in most parts of the world by the middle of the 20th century. Prior to the early 1900s, up to 1/3 of

children (and adults – if they lived long enough) were affected by illnesses caused by chronic nutrient deficiencies. More recently, the observation that folate deficits can lead to neural tube defects in newborns and choline deficits can lead to fatty liver disease in adults have led to new recommendations and guidelines for foods containing these essential micronutrients (Raubenheimer et al., 2006; Blencowe et al., 2010). Other kinds of diet-disease connections are becoming much more evident, especially in an era where food is cheap and abundant. For instance, the consumption of excess calories is known to lead to obesity and a greater risk for cardiovascular disease and type II diabetes(Kahn&Hul, 2006; Gaal et al., 2006). Increased intake of sugar (especially high fructose corn syrup) and carbohydrate-rich diets have also been shown to increase the risk of type II diabetes (Janket et al, 2003). Likewise, a high salt diet is known to increase one's risk for stroke and hypertension (Janket at al., 2003; Morgan et al., 1978). Consumption of processed red meat (i.e. smoked or treated with nitrites) is now recognized as a significant cause of cancer (Strazzullo et al., 2009; Cho et al., 2006; Cross et al., 2007).

In some cases the diet-disease link is less clear. For many years, diets rich in cholesterol and fats were believe to increase blood cholesterol levels, leading to atherosclerosis and cardiovascular disease (Kannel & Castelli, 1979). This led to substantial changes in North American and European dietary habits where the consumption of eggs, butter and whole milk were eschewed and the consumption of margarine, skim milk and low-fat foods was encouraged. However this link is now largely discredited(Rice, 2014).

While many diet-disease links are now well known, what is less clear or often more controversial is diet-health or diet-health-protection connections. In the 1980s and 1990s, a large number of epidemiological studies on the cancer protective effects of foods, particularly fruits and vegetables, were conducted. However, many were not able to confirm consistent anti-cancer

associations (Willett, 2010). Indeed, follow up studies that attempted to validate the anti-cancer effects of beta-carotene (found in carrots) and vitamin D actually showed cancer-promoting effects(Peto et al.,1981; Lappe et al., 2007). These early epidemiological studies typically relied on food frequency questionnaires or food diaries as opposed to controlled laboratory feeding studies that use a single compound. Consequently, many of these studies were plagued with problems of recall, small sample size, short sampling periods and selection bias that created spurious associations (Willett, 2010). More recently the methodologies have improved greatly. One of the largest and most complete studies was conducted on 48000 subjects in Europe. This study demonstrated a 4% cancer risk reduction through the augmentation of 200 g per day of fruits and vegetables (Boffetta et al., 2010). A large study in the United States replicated the protective effect of fruit and vegetable consumption on cancer risk(Block et al., 1992).For most types of cancer, individuals with low intake of fruit and vegetable were estimated to havetwice the cancer risk compared with those with high intake. Other studies have largely confirmed these results (Lappe et al., 2007; Boffetta et al., 2010; Cartea et al., 2011; Block et al., 1992; Rao & Rao, 2007; Oberritter et al., 2012).

The challenge now is to identify the micro- or macronutrients in fruits and vegetables that are anti-carcinogenic. Many phytochemicals such as glucosinolates, isoflavanoids, stillbenes, carotenoids, indoles, polyphenols, phytosterols, isothiocyanates, dietary fibers, dithiolethiones, limonenes, sulphuraphanes, and allyl sulphur compounds appear to be good candidates(Rosenlund et al., 2011; Kaur & Kapoor, 2001). Likewise other, more ubiquitous compounds such as selenium, vitamin E and vitamin C have been suggested or promoted by various authorities as anti-cancer agents(Rosenlund et al., 2011; Kaur & Kapoor, 2001). Many of these presumptive anti-cancer compounds are known to be good anti-oxidants, which prevent DNA damage (Kaur

&Kapoor, 2001). Others appear to bind to known carcinogens or prevent the formation of carcinogenic compounds (Steinmetz & Potter, 1991). Still others appear to promote the growth of friendly bacteria in the gut that release anti-carcinogenic or anti-inflammatory compounds (Commane et al., 2005). More recently, several studies have shown that some of these phytochemicals have high binding affinities to specific mammalian cell-growth regulators or checkpoint proteins – not unlike some well known anti-cancer drugs(Rajendran et al., 2011). However, no single agent has been shown to be particularly effective on its own. Consequently, it has been argued that there must be a synergistic effect that arises from multiple food compounds acting together (Block et al., 1992).

Another fascinating link between diet and health has been observed with regard to the so-called "French Paradox" and the Mediterranean diet (De Lorgeril et al.; 2002). The French Paradox refers to the observation that the diet in France is particularly rich in high-fat foods (cheese, whole milk, eggs), coffee and red wine, but the incidence of cardiovascular disease in France is very low (Renaud & Lorgeril, 1992). The Mediterranean diet is based on the observation that people living in Mediterranean countries that consume large amounts of red wine, nuts, fish, raw fruits, vegetables and olive oil tend to have low incidences of heart disease and cancer(Wall et al., 2010; La Vecchia, 2007). These observations have led to investigations regarding the components in red wine, coffee, nuts, olive oil, ocean fish and many Mediterranean fruits and vegetables that are protective against heart disease, inflammation, atherosclerosis and cancer(La Vecchia, 2007; Wall et al., 2010). Many of the same health promoting classes of phytochemicals mentioned earlier appear to be abundant in both the French and Mediterranean diets. Another equally important nutrient common to both diets appears to be omega-3 fatty acids (found in

ocean fish and certain vegetable oils) that have been clearly shown to exhibit anti-inflammatory effects (Wall et al., 2010).

The fact that a number of specific food compounds have been identified that either cause or prevent disease is largely due to the implementation of carefully controlled laboratory feeding experiments that have marched in step with the implementation of advanced food analysis techniques. In the next section I will discuss the history of food composition analysis and food chemistry to provide some context to my proposed research goals.

1.3 Food Analysis

Simply stated, food analysis involves the investigation of food properties and their components. More specifically, food analysis employs standard analytical chemistry techniques to assess the composition, nutritional features, quality, authenticity and safety of food products(Elmadfa & Meyer, 2010). It also aims to give chemically specific answers to organoleptic (i.e. sensory) questions regarding food color, texture, flavour, taste and aroma as well as health-related questions regarding micro- and macronutrient content. Food analysis is a very serious business and testing results can have profound implications for national dietary policy, food labeling protocols, food producers/packagers and food consumers. Consequently, food analysis is normally under the purviewof government labs or independent testing labs with strict SOPs (standard operating protocols) that are subject to regular government audits and certifications. The most "sensational" role of food testing laboratories lies in assessing food contamination with exogenous chemicals or toxins such as heavy metals (mercury, arsenic, lead), pesticides or pesticide residue, chemical toxicants (PCBs, drugs) or illegal additives.

For instance, in 1981, food testing revealed that industrial rapeseed oil was being sold as olive oil on Spain's street market leading to the deaths of more than 600 people(De la paz et al., 2001). Diethylene glycol, which is a poisonous solvent with a sweetish taste, was used by some Austrian wine makers to "flavour" their wines until this toxic organic compound was identified by a food testing laboratory in 1985 (De la paz et al., 2001). Food testing is also routinely done to verify the authenticity of food products, especially juices and oils (Reid et al., 2006). Strict rules are in place about juice and oil composition but because it is often easy to generate blended juices or oils using cheaper (or less safe) products that look and taste like the more expensive pure product.

Food analysis is also important from the perspective of nutrition or nutrient labeling. All packaged food companies in North America and Europe are required by law to put nutrition labels that contain an ordered ingredient list on their food packages. Because the practice is so widespread and because nutrition is such a frequently discussed topic, nutrient composition is becoming an increasingly important consideration in food purchases. Studies show that about 65 percent of adult consumers read food labels before making a food purchase decision (Steinmetz & Potter, 1996). As a result, nutrient labeling has become an important marketing tool for packaged food producers to gain market traction. The primary purpose of food labeling is to give consumers sufficient information about the nutritional value of a food product. This not only helps educate consumers, but it also helps them to adopt or adhere to healthy diets. The secondary role of food or nutrient labeling is to ensure the safety of the food product and therefore the health of those consumers that eat that food product (Golan & Kuchler, 2001). An equally compelling role for food labeling is provide fair competition among food manufacturers (Golan & Kuchler, 2001). In

this regard food/nutrient labeling forces food manufacturers to back their advertised nutritional, health or organoleptic claims with hard, factual data.

1.3.1A Short History of Food Analysis

The very first studies of food composition date back to the middle of 19th century when Wilhelm Henneberg, at the Agriculture Research Station in Weende (Germany) developed analytical methods that could measure the content of fat, protein, fibre, carbohydrates, nitrogen and moisture in food (Koivistoinen, 1996). About the same time another well known German chemist, Justus von Liebig (often considered the founder of modern organic chemistry) began classifying foods according to their chemical composition and nitrogen content (Koivistoinen, 1996). By the early 1900's extensive and systematic investigations were being done by another well-known German scientist, Max Rubner, on food quality. Rubner, a physiologist and physician, performed many studies on diet, human nutrition and human energy requirements by measuring the energy values or caloric content of carbohydrates and proteins(McGorrin, 2009).

At the beginning of the twentieth century, so-called "wet chemistry" methods were introduced for food analyses. These methods employed easily accessibly chemicals and equipment to identify or quantify food constituents (McGorrin, 2009). However they often involved relatively labour-intensive and time-consuming procedures including precipitations, evaporations, titrations, distillations, and solvent extractions with a final analytic step being some sort of chemically based colorimetric assessment. Because these methods were so complex and skill-dependent and because the read-outs were relatively qualitative, a push to adopt, faster, more reproducible, more quantitative methods was launched in the 1920s and still continues today. In the following paragraphs, I will provide a brief history of some of the key analytical methods that were developed for detecting and/or separating certain classes of compounds for food analysis.

Vitamin Assays: The Carr-Price colorimetric vitamin A assay was the very first method developed for quantitative vitamin estimation. It was described by Francis Carr and Ernest Price in 1926 to determine vitamin A concentrations in solution with the aid of a colorimetric reagent (Dann, 1938). In this particular protocol, vitamin A could be colorimetrically quantified by its reaction with antimony trichloride which yields an intense blue color (Dann, 1938). Colorimetric assays for food constituents, while popular in the 1920s and 1930s, soon proved to be proved to be particularly difficult for characterizing fruits and vegetables because the food pigments (chlorophyills, carotenes, xanthines, etc.) would interfere with the readout from the colorimetric dye or reagent. Since the 1960s, most vitamin assays have included additional chromatographic steps to eliminate this color interference. Additionally more assays have moved towards vitamin detection via antibodies or mass spectrometry rather than spectrophotometric or colorimetric assays.

Protein Content Measurement: The first estimation of protein content of food was done by Johan Kjeldahl in 1883 (Kirk, 1950). Because proteins contain nitrogen, the Kjeldhal assay was essentially based on determining the nitrogen content of a given substrate(Ranadheera et al., 2010; American Institute for Cancer Research, 2007). In this method, the food itemis processed with hot, concentrated sulfuric acid leading to nitrogen release, which can then be determined by an ammonium ion titration technique(American Institute for Cancer Research, 2007; Ranadheera et al., 2010). The amount of nitrogen can be calculated from the quantity of ammonia ions in the solution. Although, this method cannot discriminate protein from non-protein nitrogen, it persisted as a standard food analysis technique for over 100 years(American Institute for Cancer Research, 2007; Ranadheera et al., 2010). It wasn't until the 1940s, thatJean Baptiste Dumasand colleagues developed a more specific method for quantitative determination of nitrogen to estimate the crude

protein content in foodswhich was done by converting all the forms of nitrogen into gaseous nitrogen oxides by combustion in an oxygen-rich atmosphere, followed by reducing nitrogen oxides to N2 and quantifying the amount of nitrogen by the thermal conductivity (Simonne et al., 1997).

Trace Metal Analysis: Trace metal analysis in food testing is particularly important for identifying or quantifying ions such as iron, selenium and zinc – all of which are essential for life. The earliest methods for metal and mineral identification were based on gravimetric, volumetric and/or colorimetric analyses. Gravimetric analysis of minerals or metals was first introduced in 1830. This is a technique for quantitatively determining the amount of a given ion (in solution) via precipitation through a known chemical reaction (Hey, 1973). An example of gravimetric analysis for the determination of chloride involves the precipitation of silver chloride, which can be done by adding a silver nitrate solution to a chloride ion solution. After precipitation, the silver chloride can be dried and weighed and the amount of chloride in the solution determined. In contrast to gravimetric analysis volumetric analysis, is a method by which the concentration of an analyte is determined by measuring the volume of a solution of known concentration, which is then used to determine the concentration of the analyte of interest. Because of its poor accuracy and large sample size requirements, volumetric methods were not widely adopted for mineral and metal analysis. However volumetric analysis is occasionally used to determine the net oxidation state of an element (Hey, 1973). Colorimetric analysis largely supplanted volumetric and gravimetric methods for the determination of minerals and metals after 1900. This is because it is faster and it typically requires only a fraction of the material that volumetric or gravimetric methods require. However, as with all colorimetric tests, color interference can be problematic (Hey, 1973). Throughout the 1900's other methods for metal and mineral analysis were also developed and

advocated. These include flame photometry, atomic absorption spectrometry, emission spectrography, X-ray fluorescence and a variety of radiochemical methods (Koivistoinen, 1996; Hey, 1973; Houk & Thompson, 1988). With the invention of Inductively Coupled Plasma Mass Spectrometry (ICP-MS) in the 1980s, the field of mineral and trace metal analysis changed quite dramatically. ICP-MS involves ionizing the sample with inductively coupled plasma and then using a mass spectrometer to separate and quantify the metal ions. Because of its sensitivity ICP-MS is able to identify and quantify of wide variety of metal ions at concentrations as low as one part per quadrillion (Houk & Thompson, 1988).

pH testing: The acidity of foods and beverages can profoundly affect their taste and shelf-life. The development of the pH meter (initially called an Acidimeter) was actually motivated by the need for improved food analysis. In particular, the electronic pH meter was designed by Arnold Beckman in 1934 (Figure 1.1) to measure the pH of lemon extracts that were being made into pectin and citric acid. The standard method for measuring the pH of samples at that time was based on colorimetric titration assays or litmus paper. However, litmus paper can be quite sensitive to sulfur dioxide, which is commonly produced by food products (including lemons). At the request of the California Fruit Growers Association (now known as Sunkist) Beckman devised an electrochemical method that used a hydrogen electrode coupled to a vacuum tube amplifier. Beckman's invention worked so well that it led him to launch the Beckman Instruments company (later known as Beckman Coulter Inc.) to sell pH meters worldwide. pH meters are now ubiquitous instruments found in nearly every chemistry, biochemistry and food chemistry lab around the world. pH testing is now routinely done for many foods, beverages and fermented products.

Chromatography: Liquid chromatography is a technique for separating individual components from a liquid mixture based on their differential adsorption or physicochemical interactions as the liquid mixture moves through an immobile or stationary matrix. The development of liquid chromatography was largely motivated by the needs of food chemistry. Indeed, the inventor of chromatography, Mikhail Tswetta Russian-Italian botanist,originally developed the technique in 1901 to separate plant and food pigments (chlorophyll, xanthophyll. carotene) (Ettre, 2003). Since these components have different colors (green, yellow and orange, respectively) the technique was named "chromato"(color) graphy. Chromatography continued to develop as a science through the 1940s and 1950s largely thanks to the work of Archer Martin and Richard Synge (who received the Nobel prize in 1951). They helped establish the principles of partition chromatography, which later led to the development of several chromatographic methods including paper chromatography and gas liquid partition chromatography. Gas-liquid Partition Chromatography (GLPC) or simply gas chromatography (GC) was invented by Martin and Synge in 1941 (Martin and Synge, 1941). Gas chromatography is a technique for separating individual components from a mixture of volatile compounds based on each component's relative boiling point and the relative adsorption or physicochemical interactions as each volatile compound moves past an immobile or stationary matrixGC has played a key role in food analysis with some of the first applications aimed at the separation of volatile fatty acids (James & Martin, 1951). Compared to conventional liquid chromatography, gas chromatography permits shorter run times, better separation, and requires smaller sample sizes. High Pressure Liquid Chromatography (HPLC) is another field of chromatography that has helped revolutionize food analysis. HPLC is a liquid chromatography technique that uses very high pressures and smaller particle sizes to accelerate the separation process while at the same time improving the resolution and

reproducibility of the separation.The first commercial HPLC was manufactured by Waters Corporation (known as ALC100 HPLC) in 1969. HPLC methods permit the separation of compounds by hydrophobicity (reverse phase HPLC), ionic charge (ion exchange HPLC) or molecular weight (size exclusion) based on the type of particles placed in the column. After the analytes have been separated by chromatographic methods they may be detected and quantified through spectrophotometric methods (UV absorption, fluorescence) or through mass spectrometry.

Mass Spectrometry: Mass spectrometry (MS) is a technique for measuring the mass to charge ratio of ions. To perform mass spectrometry, a compound must first be ionized and then accelerated through either a magnetic or electric field (under a strong vacuum) where its speed or rate of curvature can be measured. It was originally developed by Sir Joseph John Thomson in 1919 as a method for measuring the mass of the electron (Griffiths, 1997). However, the concept of mass spectrometry was soon applied to many other areas including the measurement the mass of elemental isotopes and the mass measurement of organic molecules as a means to confirm their identity. The first commercial mass spectrometer was constructed in 1943 by the Consolidated Engineering Corporation. The first application of mass spectrometry to food analysis was performed by Turk et al.(Herschbach, 2001; Spyros & Dais, 2009; Ablett, 1992). They used mass spectrometry to characterize the chemical constituents in apples. By the 1960s mass spectrometry had become a standard analytical tool in many chemical laboratories (Dass, 2007).

Many different kinds of mass spectrometer designs exist, with each having a specific name based on either the ionization technique or the ion separation technology. For instance, time-of-flight (TOF) mass spectrometers measure the time it takes for ions to pass through a long drift tube of a defined distance. Electrospray (ESI) instruments ionize molecules by passing them

through a spraying device under a strong electric field. Inductively coupled mass spectrometers (ICP) ionize atoms using inductively coupled plasma. MALDI or matrix assisted laser desorption ionization instruments ionize molecules by exposing samples to strong laser pulses that co-vaporize the molecule and the matrix that surrounds them. Triple quadrupole (QqQ) mass spectrometers are tandem (or combined) mass spectrometers consisting of two quadrupole electrodes for accelerating ions and one central quadrupole for colliding ions. Each mass spectrometer configuration has its specific strengths and weaknesses with regard to robustness, mass resolution, sensitivity and speed. With respect to food chemistry, mass spectrometry is routinely used to detect, identify and quantify low abundance, easily ionized molecules such as organic acids, amino acids, biogenic amines, flavonoids, pesticides, vitamins, and many aromatic compounds (Careri et al., 2002).

Nuclear Magnetic Resonance Spectroscopy: Nuclear magnetic resonance (NMR) is a spectroscopic technique that measures the absorption of radio waves by certain sensitive nuclei under strong magnetic fields. Different nuclei involved in different chemical bonds or molecular configurations will absorb radiofrequency radiation at different frequencies. These frequencies define the chemical shift of a given atom. Chemical shifts are often called the "mileposts" of NMR spectroscopy and they are often used to identify chemical constituents in molecules and determine the structure or identify of small molecules. Hydrogen atoms are particularly sensitive reporters for the NMR phenomenon. The first functional NMR spectrometer was built in 1946 by Edward Purcell from Harvard University and Felix Bloch from Stanford University(Geva, 2006). They received the Nobel Prize in 1952 for their efforts. NMR is a technique that is particularly well suited to analyzing liquids or characterizing compounds dissolved in liquids. As such NMR

can be used to determine the structure of organic compounds, to track chemical reaction rates over time and to determine the content and purity of a given liquid sample.

NMR was first used in food analysis in 1985, where meat and milk were analyzed (Vogel et al., 1985; Belton et al., 1985). Today NMR is widely used in food analysis applications, especially in food constituent analysis for juices, wines, beers and edible oils. In juice analysis NMR may be used to identify characteristic sugars, alcohols or phenolic compounds for the purposes of contamination analysis or quality control. For edible oil analysis, NMR can be used to measure the extent of conjugation in fatty acids and to assist with oil authentication analysis (Reid et al., 2006). NMR is also an excellent technique for analyzing food moisture content, especially because it is so sensitive to the hydrogen atoms present in water. Pulsed-field gradient NMR can also be used for investigating food microstructure by looking at the differential diffusion of water or other mobile molecules through the food matrix (Ablett, 1992). NMR is now being combined with other kinds of separation and detection technologies such as liquid chromatography (LC) and mass spectrometry (MS) to expand its applications. For instance, LC-NMR and LC-NMR/MS systems are now commercially available to separate complex mixtures into individual components thereby greatly expanding the limits of what can be seen or identified with regard to low molecular weight analytes (Tokunaga & Okamoto, 2010).

1.3.2Food Composition Databases

The first food composition database was published in the late 19th century as a series of tables describing the "Chemical Composition of American Food Materials" (Atwater & Woods, 1896). These authors conducted nearly 2600 analyses for a wide range of foods including common, raw food groups, as well as some processed foods. The compositional categories they used at the time

included ‘refuse’, water, protein, fats, carbohydrates, ash, and ‘fuel value’ (calories).The UK followed suit in 1940 with a book entitled “The Composition of Foods” (McCance & Widdowson, 1940). This book is now in its 6th edition (last published in 2002) and has served as the primary reference for many modern food databases. McCance and Widdowson were alsothe first to use modern analytical chemistry methods to characterize and describe food constituents. More recently, the Dictionary of Food Compoundswas compiled and published(Yannai, 2003). This book, which is nearly 2000 pages long,describes nearly 30,000 compounds found in food including natural food constituents, food additives, food contaminants and nutraceuticals. With the dawn of the internet, most food databases have moved from hard-copy tables and books to web-accessible resources.They have also evolved to become resources used not only by food chemists but also by dieticians, food manufacturers, nutritional scientists and physicians. In many cases food databases play a vital role in characterizing dietary exposures for epidemiological studies of diet–disease relationships. They have also taken on something of a “national” character with different databases being developed by different countries to reflect national differences in food preferences and production.

To date, more than 30 countries have developed national food composition databases including Canada, the USA, the Czech Republic, Denmark, Finland, France, Germany, Greece Iceland, Ireland, Israel, Italy, Lithuania Netherlands, New Zealand, Norway, Poland, Portugal, Serbia, Slovakia, Spain, Sweden, Switzerland, Turkey, and the UK. The USDA (the US Department of Agriculture food database), the DTU (the Danish food database)and the Health Canada food database are among the most widely used food composition databases that are publicly available.

The USDA National Nutrient Database (NND) was developed by the Nutrient Data Laboratory (NDL) and grew from the work of Atwater and Woods work on the "Chemical Composition of American Food Materials" (Atwater & Woods, 1896). The mandate of the NDL is to acquire, evaluate, compile and disseminate data on foods available in the United States (Anon, 2011). As one of the most comprehensive databases in the world, the NND includes data for 7,906 food items (including many processed foods such as frozen foods, prepared foods, sandwiches, etc.) and lists composition data for up to 146 nutrients for some of these foods(Anon, 2011)**.** These nutrients include up to 8 macronutrient values, 7 different sugars, 10 different minerals, 22+ vitamin values, 15-20 amino acids, nearly 30 lipids or fatty acids and 6-10 specialized organic acids, alkaloids or other phytochemicals. All of the NND data can be downloaded or accessed online at http://ndb.nal.usda.gov. As information is updated, new versions of the USDA database are released regularly.

In addition to the USDA's NND, Canada also maintains is own online nutrient database. In particular, Health Canada maintains the Canadian Nutrient File (CNF), an online database (http://webprod3.hc-sc.gc.ca/cnf-fce/index-eng.jsp) that contains nutrient values for many common foods grown or consumed in Canada(Guide, 2010). Much of the data in the CNF was actually derived from the USDA database. The CNF database currently consists of 5807 foods with some food items containing up to 150 nutrient values**.**

The Danish food composition database (DTU) was established in 1983 to systematically monitor Danish foods and to track changes in Danish food constituents. It is one of the most comprehensive European food databases and is freely available online (http://www.foodcomp.dk). The DTU is one of several databases incorporated into the European Food Information

Resourceor EUROFIR (http://www.eurofir.eu). It provides the mean content values of ~100 nutrients for about 1050 foods, beverages, and processed food products.

More recently, specialized food composition databases have started to emerge. One example is Phenol-Explorer (http://phenol-explorer.eu)(Neveu et al., 2010; Rothwell et al., 2012; Rothwell et al., 2013). Phenol-Explorer is particularly notable as it is the first comprehensive web-based database on the polyphenol content in foods. Polyphenols are plant-specific compounds primarily derived from the shikimate/phenylpropanoid and/or the polyketide pathways. They typically have more than one phenolic unit and do not contain any nitrogen-based functions. Polyphenols control many biological functions in plants, including the release and suppression of growth hormones such as auxin, as UV screens to protect against ionizing radiation, herbivore deterrence (sensory properties), the prevention of microbial infections and as signaling molecules in ripening and other growth processes.Polyphenols are also thought to play important roles in human health. Currently Phenol-Explorer has >37,000 data entries collected from 638 scientific articles and contains mean content values for 502 polyphenols in 452 foods and beverages (Neveuet al., 2010). The database is regularly updated and is now in its third release(Rothwel et al., 2013).

While the size and quality of food composition databases has grown considerably over the past decade, it should be clear that these databases only cover a tiny fraction of the known (or expected) chemical constituents in foods. One of the goals of my thesis is to extend the known nutrient and micronutrient data in foods (especially plant foods) by at least an order of magnitude.

1.4. Food Sample Preparation for Chemical Analysis

In the previous section we reviewed some of the analytical methods that have historically been, and currently are, being used to characterize food constituents. While sensitive detection and high-resolution separation tools are essential for proper food analysis, another essential component is proper sample preparation. In particular, high quality analysis of food constituents requires proper storage, handling, preparation and extraction of food products (Figure 1.3). The first step in almost all types of food sample preparation protocols is washing or cleaning. In particular, it is essential to wash, remove and drain irrelevant or extraneous material, especially soil and sand (from fruits, vegetables and fish) or hair/fur (from animal products) after selecting the edible portion of the food item. Rinsing fresh food samples can be done by distilled water to wash out soluble residues and contaminants; however to prevent the leaching of soluble solids, excessive washing should be avoided (Meredith & King, 2002).

The second step in food sample preparation typically involves the storage of samples prior to further analysis. The preferred method, especially for chemical constituent or nutritional analysis, is rapid freezing. Freezing samples in liquid nitrogen allows one to perform "metabolic quenching" which deactivates all enzymes and prevents further metabolite degradation. After this metabolic quenching step, food samples should be stored at -80 °C and should only be removed from the freezer immediately prior to extraction and analysis. Once the preserved metabolites have become frozen, it is relatively safe to store food samples in -80 °C for several years.

Solid food samples such as vegetables, fruits, cereals and meat contain moisture that can contribute to sample heterogeneity. This can confound chemical quantification (Meredith & King, 2002). For most kinds of solid food samples, a drying step is often necessary to remove moisture. Water removal is typically best done by freeze-drying or lyophilisation. Lyophilisation is a

technique for sublimating water from a sample by converting the solid phase (i.e. ice) to a gas phase (water vapour) under a strong vacuum. By avoiding an intermediate dissolution or ice-melting step, lyophilisation prevents any enzymatic degradation of metabolites which could lead to changes in starting metabolite concentrations. Freeze dried samples can be used for extraction at any time; however depending on the objective of the analysis, freshly freeze-dried samples are sometimes better for specific extraction procedures.

After freezing and immediately prior to extraction, food samples such as fruits, vegetables, cereals and grains should be ground and dispersed into a coarse powder.This is done to increase the surface area for optimal solvent penetration and maximal compound recovery. In addition to grinding, other processing methods such as digesting, centrifuging and purging may also be used to facilitate food extraction. All extraction methods are essentially matrix transfer methods. This means they lead to the transfer of chemical compounds from the primary matrix (which is the food tissue or substrate) to a secondary matrix (which is usually a solvent). Sample extraction procedures can vary based on the chemical class or analyte group of interest. The best extraction techniques should allow one to isolate different analytes from different food materials by preserving the chemical integrity of the extracted compounds while at the same time preventing any metabolic transformations (Mendiola et al., 2007). Efficient, effective extraction ensures a reliable downstream analysis. Traditional extraction methods such as wet digestion and solvent extraction can be quite laborious and time consuming resulting in low or variable extraction yields with low selectivity. Many traditional extraction methods use toxic organic solvents (such as chloroform, alcohol or hexanes). These solvents permit the selective isolation of hydrophobic or difficult to solubilize components. However, the long-term use of such solvents can also lead to a number of adverse health effects. Modern extraction methods are now safer, faster, more reliable

and much more effective than the conventional extraction methods. Some of the better extraction methods include: ultrasonic-assisted extraction (UAE), supercritical fluid extraction (SFE), pressurized liquid extraction (PLE), accelerated solvent extraction (ASE), pressurized water extraction (PWE), subcritical water extraction (SWE), ultrasonication extraction (USE) and membrane extraction techniques(Żwir-Ferenc & Biziuk, 2006; Bylda et al., 2014; Buldini et al., 2002).

After extraction it is often necessary to perform a combination of enrichment and/or purification/separation steps. Enrichment is typically used to increase the analyte concentrations above the detection limit at which level that reliable quantitative measurements can be made (Beyer & Biziuk, 2008). Enrichment may include further solvent or two-phase liquid-liquid extractions, volume reduction via drying or evaporation, precipitation or crystallization. The most common approach is through volume reduction via a rotary evaporator or a Speed-Vac concentrator. Occasionally targeted chemical derivatization can used to facilitate enrichment. Enrichment may also be coupled to a clean-up or purification step. The clean-up step is used to remove as many interfering substances as possible to ensure that quantification of the desired analytes is as accurate as possible. The clean-up or purification steps typically involve liquid chromatography (which has already been discussed). Several different types of liquid chromatography can be used depending on the physical properties of the analyte(s) of interest. Hydrophobic compounds are best purified or cleaned-up via reverse phase HPLC methods. Hydrophilic or charged compounds are often separable via ion exchange or HILIC-HPLC methods (Schwalbe-Herrmann et al., 2010). Occasionally some compounds can be purified and isolated through affinity chromatography, which may involve the use of column-bound antibodies.Subsequent characterization and quantification can be done using mass spectrometry,

NMR, UV-absorbance or fluorescence, which is often done in tandem with the chromatographic separation steps.

1.5 Metabolomics

Metabolomics (sometimes called metabonomics) is a newly emerging field of 'omics' research that concerned with the high-throughput characterization, identification, quantification and analysis of small molecules in biological matrices (Wishart, 2008). The collection of small molecule metabolites found in a given cell or organism is called the metabolome. The term "metabolome" was first suggested by Oliver et al. in the late 1990s in a paper which was titled 'Systematic functional analysis of the yeast genome'(Oliver et al., 1998). Metabolomics differs from other "omics' fields in that it is focused on smaller, often neglected, molecules of molecular weights less than 1500 Daltons (Zhang et al., 2010). In contrast, genomics is focused on the study of entire genomes (looking at molecules that are millions of Daltons),transcriptomics, is focused on the study on mRNA (100's of thousands of Daltons), while proteomics is focused on the study of proteins (10's of thousands of Daltons).

Just like genomics, transcriptomics and proteomics, the field of metabolomics has benefited tremendously from advances in analytical technologies for separation and identification. These include significant improvements in mass spectrometry (improved sensitivity and mass resolution), NMR spectroscopy (improved sensitivity with higher field magnets and cryoprobes), and improvements in chromatography (faster separations with HPLC and Ultra-high pressure liquid chromatography or UPLC). A number of these technologies were briefly discussed in section 1.2.1. These technological improvements, along with significant developments in the software and databases needed to identify metabolites from biological mixtures have allowed

metabolomics to grow tremendously over the past 10-15 years. Indeed, the number of papers published in the field has grown from just 1 in 1999 to more than 2500 in 2015 (Figure 1.4). These advances have also led to the development of different "flavours" of metabolomics depending on the application or context. Table 1.1 lists the definitions of the terms commonly used in metabolomic studies. While the popularity of metabolomics has grown tremendously over the past decade, it is now without its challenges or difficulties.

1.5.1 Challenges in Food Metabolomic Studies

When properly performed, metabolomics assays can routinely lead to the detection of >10,000 compounds (or features) and the identification or quantification of >1000 compounds (Scalbert et al., 2009).As a result, when metabolomics is used in food science it has the potential to provide very extensive food composition analysis. However, the application of metabolomics to food composition analysis is relatively new. This is because the chemical diversity of food metabolites is unusually large, and the matrices which contain these metabolites are unusually diverse. In particular, plant-derived foods may consist of several hundred thousand different metabolites (many of which are unknown) spanning dozens of chemical classes such as phytosterols, stilbenes, flavanols, flavanals, isoflavones, terpenes, xanthenes, chlorophylls, complex sugars, complex lipids, waxes, glucosinolates, carotenoids, indoles, isothiocyanates, dithiolethiones, limonenes, sulphuraphanes, and allyl sulphur compounds. Furthermore, food products may consist of raw or cooked material that consists of liquids (oils and beverages), soft, easily extractable material (fruits, vegetables, meats) or hard, cellulosic or fibrous material (seeds, nuts or cooked/dehydrated substrates) that is difficult to extract or handle. This diversity means that one

generally needs more than one analytical platform for metabolic profiling and more than one method for extracting, separating or isolating metabolites.

Certainly with the establishment of national metabolomics core facilities, such as The Metabolomics Innovation Centre (TMIC) at the University of Alberta, the issue of instrument diversity or platform availability is much less of a challenge today than it was 10 years ago. However, three issues continue to challenge food metabolomics: 1) sample selection; 2) sample extraction and 3) compound identification and/or quantification.

Sample selection has always been a challenge in food analysis, with the biggest issue being how to find a representative sample. There are several factors that can affect food composition including, but not limited to sampling site (tissue), variety or species, growing season, geographic origin, presence of pathogens, diet (in the case of animals) or fertilizer and irrigation (in the case of plants)(Pietola & Salo, 2000; Sharma & Rao, 2013; Balint et al., 2001; Hattori & Chino, 2001; Hopkins & Elsen, 1959). Ideally the best route to deal with variation is to sample broadly and to obtain a sufficient number of biological replicates to ensure that most of this variation is captured. In this regard, the high throughput nature of metabolomics is ideal for performing large numbers of replicate analyses and for gathering the necessary statistics. Equally important is to capture as much "meta-data" as possible about all of the variables mentioned above.

With regard to sample extraction or separation, there continue to be a number of challenges in metabolomics-based food analysis. As a high throughput "omics" science, most metabolomics protocols are designed for rapidly preparing clean, relatively uniform and somewhat simple matrices or extracts. Optimized, roboticized protocols are being developed for food sample extraction and many of the newer extraction techniques mentioned above are

amenable to automation. However, most laboratories do not have access to robotic systems and many labs do not have the equipment or infrastructure funds to support some of the newer (more expensive) extraction techniques. Consequently most labs depend on manual methods, which can lead to somewhat variable results in overall recovery and consistency. Another issue with sample extraction lies in the fact that there are so many food types. This means there are a large number of food-specific or even species-specific extraction protocols. Unfortunately many of these have not been fully validated for metabolomics studies. This makes protocol selection and subsequent data comparison difficult. Often the best (and only) way of validating an extraction or isolation protocol is to see if a good portion of the measured metabolites match previously reported identities or values.

The most significant challenge in food metabolomics, and in fact all of metabolomics, is compound identification/quantification. As noted before, plant-derived foods may consist of several hundred thousand different metabolites (many of which are unknown) spanning dozens of chemical classes. Identifying which peaks (NMR or MS) correspond to which metabolites requires very extensive databases of compound structures, masses (m/z values) and MS, MS/MS or NMR spectra. While the number of known structures and metabolites (compiled through literature searches) is certainly increasing, the number of reference MS or NMR spectra is not growing at the same rate. Some of the most comprehensive reference MS spectra for food constituents and food contaminants can be found in the National Institute of Standards and Technology (NIST) EI-MS database. These spectra are ideal for EI-MS analyses that are commonly performed for GC-MS studies. However because metabolomics often uses LC-MS or NMR to complement GC-MS information, a continuing challenge is to obtain appropriate referential ESI-MS/MS or NMR spectra. Therefore significant efforts and costs must be incurred

by anyone wishing to do food metabolomics to collect/purchase or synthesize the large number of metabolite standards needed to obtain the needed reference spectra. These standards are not only needed for identification (via direct spectral comparison) but also for quantification. Certainly a number of metabolomics laboratories are working to prepare, acquire or consolidate these standards, but this effort will likely take many years and cost millions of dollars.

1.6Motivation and Research Objectives

Food metabolomics clearly has its challenges but it also has the potential to significantly improve our understanding of food products in terms of quality, taste, utility, health and safety. Because of its potential and promise, I have chosen explore the field of food metabolomics. Broadly speaking, my thesis project is targeted at developing and refining metabolomics techniques that can be used in food analysis. In particular, my research is aimed at using advanced metabolomics techniques to identify and quantify the chemical constituents of nearly 40 different Alberta-grown foods. The intent of this work is to demonstrate the feasibility of metabolomics in performing ultra-comprehensive food analysis and to show that metabolomics can lead to the identification or quantification of novel macro- and micronutrients that not only affect organoleptic qualities such as flavour, aroma, colour but also those compounds that affect human health. Overall, the specific objectives of my thesis are: 1) to apply modern quantitative metabolomic methods to identify and quantify the chemical constituents and micronutrients in a select number of Alberta-grown vegetables, fruits and cereals; and 2) to create a fully web accessible database that contains both experimentally derived values and literature-derived information on Alberta-grown foods, called the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca). The AFCDB will not only

cover chemical composition data but alsophysico-chemical effects, presumptive health effects, chemistry and biochemistry of each identified food compound.

The first objective has been broken down into several phases. Phase one involved collecting food samples from local Alberta food or farmer's markets (primarily based in Edmonton).A total of 32 common Alberta vegetables and fruits were collected including Swiss chard, green bean, yellow bean, sunburst squash, Green/ red/ orange/ yellow bell pepper, red beet root, spinach, onion, lettuce, cauliflower, parsnip, garlic, turnip, white cabbage, Japanese pumpkin, carrot, eggplant, dill, broccoli, Italian sweet red pepper, Persian cucumber, yellow/ green zucchini, russet potato, tomato, Nanking cherry, Saskatoon berry, raspberry and crab apple as well as samples for 4 of Alberta's cereal crops including, oats, rye, wheat and barley. Finally, 4 kinds of Alberta meats were collected including beef, chicken, venison and bison (due to time and space constraints, the meat analyses will not appear in this thesis).

The second step involved performing metabolite extractions from all of the above listed food samples. A number of different protocols were used, including many that were borrowed from previous studies as well as a number of others that I designed or optimized. Several protocols were chemical-class specific (hydrophobic metabolites, hydrophilic metabolites, metals, etc.) The extracted mixtures were then analyzed using, LC-MS, GC-MS, NMR, ICP-MS and HPLC-UV or HPLC-FD to separate, identify and quantify as many food metabolites or constituents as possible. Most sample preparation protocols and metabolomic data analyses were conducted at The Metabolomic Innovation Centre (TMIC) at the University of Alberta. Additional analyses were conducted at the National Institute for Nanotechnology (NINT-NRC), and in the Department of Chemistry at the University of Alberta. Metabolite identification and quantification depended on comparing the experimental spectral data to a number of different reference spectral

libraries (the NIST library, the HMDB library) using several different software packages (Chenomx, AMDIS). Finally, wherever possible, the identified metabolites and corresponding concentration values were compared to literature values to ensure that the assays were yielding reasonable results. Once validated, the metabolites and their corresponding concentrations were added to the Alberta Food Composition Database (AFCDB) – which corresponds to Objective #2 of my thesis project.

The interface design and back-end structure of the AFCDB was developed in cooperation with a number of bioinformaticians and computing staff members in Dr. Wishart's laboratory. Much of the AFCDB was built using existing components from another literature-derived database, maintained in the Wishart lab, called FooDB. Data that was experimentally measured in the first phase was combined with literature-derived data on flavour, aroma, chemistry and health benefit claims for a number of these metabolites and micronutrients. Each chemical entry in the AFCDB contains more than 100 data fields covering detailed compositional, biochemical and physiological information. Users can view the content of the AFCDB from the "FoodView" (listing foods by their chemical composition) or the "ChemView" (listing chemicals by their food sources). A number of the food items we analyzed also have an on-line "Food Factsheet" describing, in plain language, the health benefits of the most important or novel micronutrients we identified. While many other food composition databases are available, as far as we are aware the AFCDB (along with FooDB) provides some of the most detailed information on food products, their micronutrient composition, and the features that give foods their flavour and their health promoting qualities of any database in the world. Indeed, many food compounds in the AFCDB were identified, quantified and reported for the very first time.

In the following chapters I will describe, in detail, the analyses I performed and the results I generated for this thesis project. Chapter 2 will describe the application of multi-platform metabolomics methods for the characterization of the chemical composition of 32 different fruits and vegetables. Chapter 3 will describe the application of multi-platform metabolomics methods for characterization of the chemical composition of 4 different whole grain cereals. Finally, Chapter 4 will provide some concluding remarks and comments on possible future directions.

Table 1.1 Terms and terminology used in metabolite studies.

Term	Definition
Metabolites	Bio-active small molecules which involves in general metabolic reactions and that are required for the maintenance, growth and normal function of a cell (Schripsema, 2010).
Metabolome	Collection of all metabolites or chemicals that present in a cell, organ or organism (Wishart, 2008).
Metabolomics	Characterization, identification and quantification of small molecule metabolites using advanced technologies (Wishart, 2008).
Metabonomics	Quantitative measurement of the dynamic multiparametric metabolic response of living systems to pathophysiological stimuli or genetic manipulation (Nicholson et al., 1999).
Metabolic profiling	Quantitative analysis of group of metabolites in a selected biochemical pathway or belong to a certain class of compounds (Schripsema, 2010).
Metabolic fingerprinting	Global, high throughput, unbiased analysis to provide sample classification based on metabolite patterns (Ellis et al., 2007).
Metabolic footprinting	Analysis of extracellular metabolites secreted or excreted by an organism (Ellis et al., 2007).

Figure 1.1A picture of original model of pH meter constructed in 1934 by Arnold Beckman. Picture courtesy of Beckman Coulter, Inc.

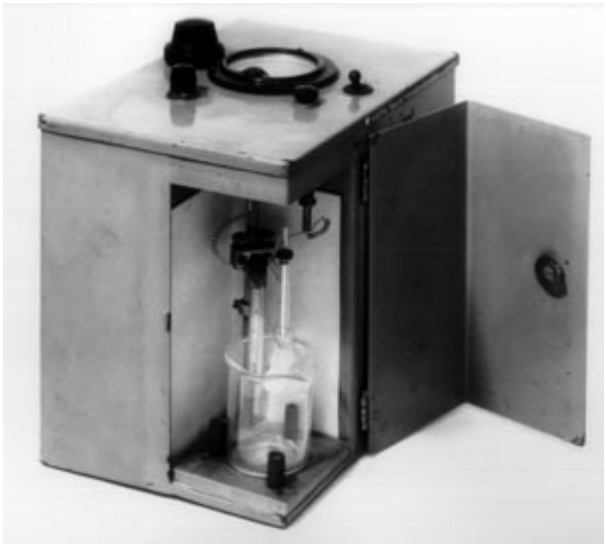


Figure 1.2A typical workflow for food analysis.

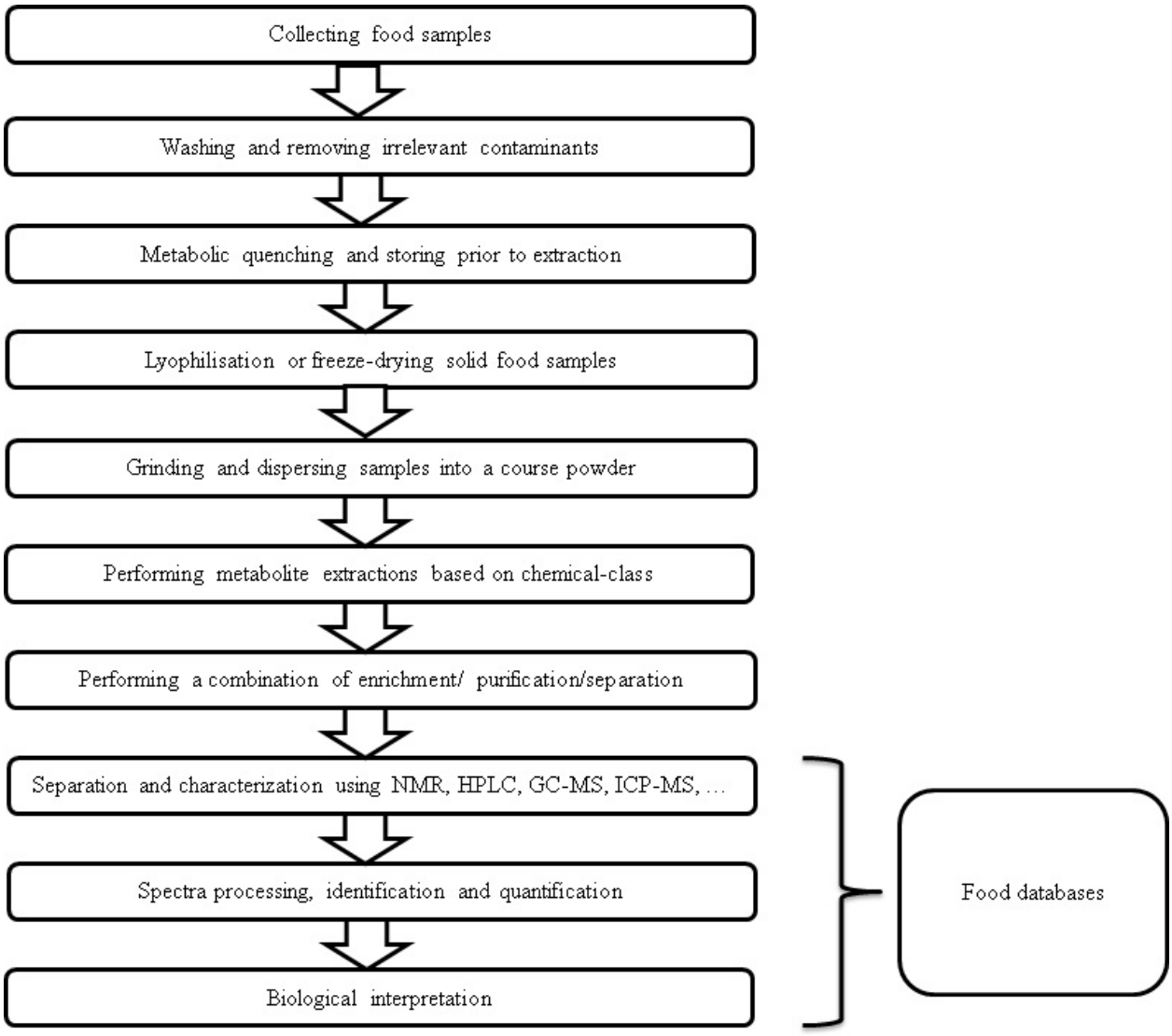
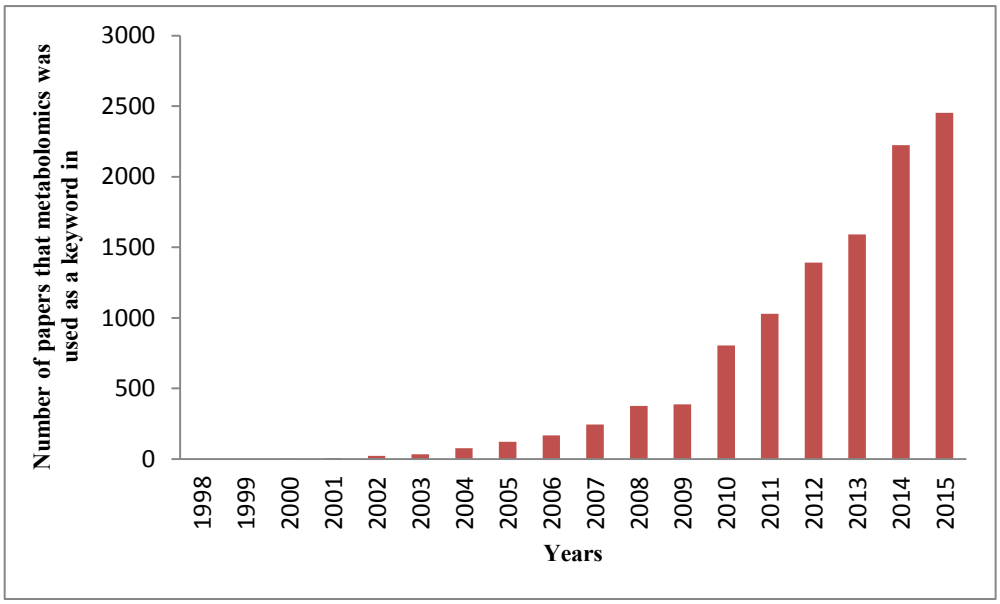


Figure 1.3 Number of publications in the research field of metabolomics from 1998 to 2015.



Chapter 2.The Application of Multi-platform Metabolomics Methods for the Characterization of the Chemical Composition of Common GardenFruits and Vegetables

2.1 Introduction

The average fruit or vegetable is estimated to contain >20,000 different chemical compounds or micronutrients (www.foodb.ca). However, standard food composition tables only provide data on a few dozen highly abundant chemicals or macronutrients (amino acids, lipids, carbohydrates) for most fruits or vegetables. Very little data is publicly available on the many lower abundance chemicals or more poorly understood compounds that are primarily responsible for the flavour, aroma, colour and key health benefits of many fruits and vegetables. Given the growing interest among food producers, consumers, nutritionists, and dieticians on the micronutrient content of many foods (including fruits and vegetables), there is a clear unmet need for the development of more comprehensive food composition information and more in-depth food characterization techniques. Over the past two decades, a number of efforts have been made to remedy this situation(Cevallos-Cevallosa et al., 2009; Herrero et al., 2011). Some of these include the development of improved analytical technologies and specially targeted assays aimed at characterizing certain classes of compounds such as polyphenols, phytosterols or terpenoids(Hamm et al., 2003; Strauss et al., 1987; Lagarda et al., 2006; Motilva et al., 2013; Naczka & Shahidi, 2004; Moreaua et al., 2002). These targeted or class-specific phytochemical techniques have enabled the routine identification of perhaps 20-30 more chemicals in fruits and vegetables(Lakoa et al., 2007; Prior & Guohua, 2000).More recently, advances in the field of metabolomics, have made it possible to identify and quantify not just hundreds, but thousands of compounds in biological matrices. These developments suggest that it may be possible to use

metabolomics to more completely characterize the chemical constituents of foods, especially fruits and vegetables.

Metabolomics is a branch of omics science that focuses on the comprehensive characterization and biological interpretation of small molecule metabolites found in biological samples(Wishart,2008). It uses techniques such as nuclear magnetic resonance spectroscopy (NMR), liquid chromatography (LC), gas chromatography (GC) and mass spectrometry (MS) to separate, identify and/or quantify large numbers of small molecules from complex mixtures and matrices. Key to the development of metabolomics has been the creation of software and databases that facilitate this high throughput chemical characterization. When properly performed, untargeted metabolomics assays can lead to the detection of >10,000 features and the identification or quantification of >1000 compounds in biological samples (Fiehn & Spranger, 2003). Consequently, when metabolomics is used in food science it has the potential to provide "ultra-comprehensive" food composition analysis (Wishart, 2008).

However, despite its promise and the many potential advantages of metabolomics over existing food composition analysis techniques, the application of metabolomics to food analysis (especially with regard to fruits and vegetables) is not particularly widespread. A review of PubMed and Google Scholar indicates that fewer than two-dozen papers on fruit and vegetable characterization have been published with the word "metabolomics" in the title. Furthermore, almost all published papers describing the application of metabolomics towards fruit and vegetable characterization have been restricted to a single metabolomics platform such as MS or NMR (Bunzel & Ralph, 2006; Daferera et al., 2000)or a single type of fruit or vegetable (Aaby et al., 2007; Tikunov et al., 2005).

In an effort to more fully explore the strengths and limitations of metabolomics in food composition analysis we decided to conduct a comprehensive, multi-platform quantitative metabolomic study on a large number of common garden fruits and vegetables. More specifically, we chose to analyze a total of 28 different common garden-grown vegetables and 4 common garden-grown fruits (Table 2.1) using a combination of NMR spectroscopy, GC-MS, LC-MS, ICP-MS (Inductive Coupled Plasma Mass Spectrometry), lipidomics and several targeted HPLC-based assays. In addition to these experimental metabolomic techniques, we also conducted a comprehensive literature review (covering approximately 800 papers) of published food composition data for each these 32 fruits and vegetables. This literature review was done to both validate the experimental results and to extend the overall chemical coverage for these fruits and vegetables.

In conducting such a comprehensive metabolomics assessment we wanted to: 1) gain a more complete picture of the chemical composition of many common fruits and vegetables; 2) assess the utility of different metabolomics platforms for fruit and vegetable composition analysis; 3) determine the maximum degree of chemical coverage attainable by multiple, quantitative metabolomic methods; 4) compare the coverage obtained by metabolomics methods with other food analysis techniques and 5) extend our experimental analyses using literature mining and make all of the data available through a public, web-accessible database called the Alberta Food Composition Database (AFCDB: http://afcdb.ca). In undertaking this study and in describing the results, it is particularly important to emphasize that this is both a feasibility study (for metabolomics) and survey study on food composition, which attempts answer the question "approximately how much of chemical X is typically in plant Y". It was not designed to look at variables such as location, farming practice, soil, temperature, sunlight, moisture, harvesting or

storage conditions on compound concentrations. Such a study would obviously require significantly more resources and would be addressing fundamentally different questions.

Overall, we found this multi-platform metabolomics approach to be remarkably effective. On average, each fruit or vegetable analyzed by our multi-metabolomic pipeline had more than 200 different compounds experimentally identified, validated and quantified. This included ~40 compounds by NMR spectroscopy, ~80 compounds by LC-MS methods, ~50 compounds by ICP-MS methods, ~150 compounds via lipidomics assaysand GC-MS methods and another ~40 compounds via more specialized or hybrid assays. Literature derived data, combined with very conservative estimates of the "minimal plant metabolome" (the set of metabolites required by plants to sustain a plant cell) led to the identification of another ~10,000 metabolites (primarily lipids) for each fruit and vegetable. Additional details regarding the materials, methods, results and interpretation of these data are given below. All of the information compiled from this study, as well as additional literature-derived information regarding the known concentration ranges, organoleptic qualities and potential health effects (as indicated by peer-reviewed literature) of many of the identified compounds is freely available through the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca).

2.2 Materials and Methods

2.2.1 Materials

This study was designed as a broad survey of the chemical/metabolite composition of 28common, garden-grown vegetables and 4 common, garden-grown fruits from the Edmonton region in the province of Alberta, Canada. At 54^{o}N latitude, the Edmonton region has a humidcontinental climate with relatively low precipitation. It falls into the USDA plant hardiness zone 4a. This

means that the fruits and vegetables typically grown in this region tend to be relatively cold-hardy. While the diversity of vegetablesgrown in this zone is quite broad, the diversity of fruits tends to be relatively small (tomatoes, some grapes, apples, a few varieties of hardy cherries, Saskatoon berries, raspberries, strawberries and crab apples). A complete list of the fruits and vegetables collected and evaluated in this study is shown in Table 2.1. All vegetable and fruit samples were purchased from local farmers markets in the city of Edmonton and kept refrigerated ($4^{o}C$) for 1-2 days until further processing. All samples were produced locally and grown organically in the Edmonton region.According to the producers,the foods were free of synthetic pesticides, chemical fertilizers, and dyes. In all cases the fruit and vegetable samples were harvested 1-2 days prior to acquisition. Prior to any preparation, samples were washed thoroughly with cold tap water to remove dirt and sand, then, rinsed with ddH_2O (Milli-Q system, Millipore Corp) three times and finally dried by a gentle stream of air. All inedible, spoiled or damaged parts were removed. Fresh samples were immediately snap-frozen in liquid nitrogen for 5 minutes and stored in plastic Falcon tubes at -80°C until platform-specific extraction.

2.2.2 Extraction of Trace Minerals from Vegetables and Fruits

All metabolomic studies were conducted at The Metabolomic Innovation Centre (TMIC) at the University of Alberta.The HNO_3 and H_2O_2 were of suprapure quality (Fisher Scientific, Ontario). Extraction of trace minerals was conducted according to the method of Jabeen et al. (2014) with some minor modifications.Briefly, previously frozen samples were lyophilized for 48 hours. The lyophilized samples were then powdered in an agate mortar using liquid nitrogen. A total of 10 mg of each sample was placed in a 50 ml Falcon tube and extracted with 600 µl of hydrogen peroxide followed by 5 minutes of vortexing and a further 10 minutes of sonication at 234 watts in

an ultrasonic water bath (Branson Ultrasonic bath, Model 2210; Ultrasonics Corporation, Danbury, CT)to improve extractability. The mixture was then subjected to acid digestion by adding 2 ml of 8 M HNO_3,held in a boiling waterbath for 10 minutes and then centrifuging the sample in a Beckman GPKRcentrifugeat 3000 rpm for 10 minutes. Prior to conducting the Inductively Coupled Plasma Mass Spectrometry (ICP-MS) analysis, the supernatant was taken and filtered through Whatman (grade 2) filter paperto remove debris.The remaining filtrate was dried and used for ICP-MS based elemental analysis. A detailed description of the ICP-MS analysis method is givenin section 2.2.7.

2.2.3Extraction of Polar Metabolites from Fruits and Vegetables

Our extraction method was based on the protocoldescribed by Wu et al. (2008) for polar metabolite extraction of biological tissues,with some minor modifications.Two biological replicates or independent samples,which were grown in the same farmwere used for each sample.A total of 100 mg of each freeze-dried sample was ground with 3 ml of isopropanolina mortar and pestleto obtain a homogeneousslurrybefore adding the extraction solvent. The extraction solvent consisted of 4 ml of cold HPLC grade methanol and 0.85 ml of cold HPLC grade H_2O. The solvent was added to the tissue,which was then placed in a 40 mlglass tube, vortexed for 3 minutes and subsequently sonicated using a bath sonicator (Branson Model 2210 ultrasonic bath; Ultrasonics Corporation, Danbury, CT) at 234 watts,in an ice bath sonicatorfor ~7 minutes. After the sonication step, 4 ml of chloroform and 4.4 ml of HPLC grade water(Fisher Scientific, Fair Lawn, NJ) were added to the sample and the mixture was vortexed for 1 minute, after which 2.5 ml of 0.88% KCl was added to the vial. The emulsion was placed on a cell shaker for an hourat 50 rpm (Lab-Line Shaker, Model #4626, VWR Ontario, Canada) to wash out all the

water-soluble and lipid soluble metabolites. The sample was then left on ice for 10 min before centrifuging in a Beckman Coulter centrifuge equipped with GH3.7 swinging bucket rotor for 30 minutes at 3000 rpm and 4 °C. The upper layer wasused for analysis by both LC-MS/MS and nuclear magnetic resonance spectroscopy (NMR)(see section 2.2.8 and 2.2.9) while the lower layer was used for non-polar metabolite analysis (see section 2.2.10).

2.2.4 Extraction of Lipids and Non-polar Metabolites from Fruits and Vegetables

As noted earlier, extraction of polar metabolites by isopropanol, methanol, water and chloroform resulted in two layers, an aqueous (polar) layer and a nonpolar chloroform layer. The chloroform layer on the bottom was collected and placed in another tube and stored at -20 °C to await further lipid analysis. For the lipid analysis, the total lipid extract was concentrated via evaporation under a stream of nitrogen. The total lipid extract was then fractionated using silica Sep-Pak cartridges (3ml containing 500mg of the separation matrix, Supelco, St. Louis, MO, USA) based on the method of Hamilton and Comai(1984) with some modifications. Briefly 10 ml of chloroform was applied to Sep-Pak cartridge to rinse any residual lipid before transferring the total lipid extract to the column. A total of 10 ml of chloroform (100%) was added to elute the neutral lipids from the column. After the first solvent was drained, 15 ml of acetone: methanol (9:1 v/v) was added to elute the glycolipids (GL). Subsequently, by adding 15 ml of 100% methanol the phospholipids (PL) were eluted. All three fractions were evaporated under a stream of nitrogen and dissolved in chloroform:methanol (2:1). Neutral lipids were fractionated into four classes including: cholesterol esters (CE), triglycerides (TG), free fatty acids (FF) and hydrocarbons using the method described by Christie(2003). Hydrocarbons were eluted first by adding 3 ml of hexane to the cartridge and then cholesterol esters were washed out by adding 6 ml of a hexane:diethyl

ethersolution (99:1). Subsequently, 5 ml of hexane:diethylether solution (95:5) was used to elute the triglycerides, followed by the addition of 5 ml of hexane:diethyl ether solution (92:8) to elute all free fatty acids. After the elutions were complete, all the fractions were evaporated under nitrogen and the dried lipids were dissolved in a small amount of chloroform. The identification and quantification of the lipids and other non-polar molecules is described in section 2.2.10.

2.2.5 Polyphenol Extraction of Fruits and Vegetables

An extraction procedure based on that of Gorinstein et al.(2007), with some modifications, was used to extract and deglycosylate the polyphenols from our fruit and vegetable samples.Specifically, a lyophilized tissue sample was first powdered with a pestle and mortar using liquid nitrogen. A total of 100 mg of the powdered sample was placed in a 5 ml Falcon tube and homogenized in 2 ml of a 1.5 M hydrochloric acid solution. The sample was vortexed for 5 min and shaken thoroughly on a Lab-Linetabletop shaker, for 30 min at 300 rpm. After adding 500 µl of 70% methanol, the extract was incubated in a boiling water bath for 40 min with vortexing at regular intervals (once every 10 min). The aqueous extract was centrifuged at 1300 rpm for 20 min in a Beckman GPKR centrifuge (equipped with a GH3.7 rotor)at room temperature and the supernatant recovered. The remaining material was subjected to a second and third extraction using a stronger solvent. Specifically, the residue was extracted twice using 2 ml of 70% methanol containing 1.5 M HCl, followed by adding 1 ml of 70%methanol. The sample was then incubated at 80 ºC in a water bath for 30 min, and vortexed at regular intervals (once every 10 min).The extract was centrifuged at 3000 rpm for 20 minutesin a Beckman GPKR centrifuge. The combined supernatant of all three extracts was filtered through Whatman filter

paper (grade 2) and purged under a nitrogen stream. The (aglycone) polyphenol extracts were collected and analyzed via HPLC using 2 biological replicates each as described in section 2.2.11.

2.2.6 Vitamin Extraction of Fruits and Vegetables

To perform comprehensive vitamin analysis on our fruit and vegetable samples, we used a modified procedure first described by Santosa et al. (2012) to extract both water and fat-soluble vitamins.Extractions were performed on two biological replicates for each fruit or vegetable sample. Specifically 0.5 g of each dry-powdered sample was spiked with 40 μL of an internal vitamin standard solution (isotopically labeled fat-soluble vitamins A, E and K1) and then treated with 16 mL of 10 mM ammonium acetate/methanol (50:50, v/v) containing 0.1% butylated hydroxytoluene, in a 50 ml Falcon tube. The samples were then shaken for 15 min at 450 rpm (Lab-Line tabletop shaker) and placed in an ice bath and sonicated (Branson Model 2210 ultrasonic bath) for 15 min. The samples were then centrifuged at 4000 rpm for 15 min (Beckman GPKR centrifuge). The bottom layer containing fat-soluble vitamins was collected for further analysis. The aqueous supernatant on top layer, which containedthe water-soluble vitamins, was collected in a new microfuge tube that was then placed in a Speed-Vac centrifuge for 15 min and evaporated to dryness. The supernatant was dissolved in 500 μL methanol and 500 μL HPLC water and applied to Supelclean LC-C18filtercartridges (500 mg) prior to analysis by LC-MS.

Fat-soluble vitamins were collected from the bottom layer and re-extracted 3 times using6 mL of ethyl acetate and 6 ml of 0.1% butylated hydroxytoluene. Each time the samples were shaken for 15 min at 450 rpm and placed in an ultrasonic bath (Branson Model 2210) for 15 min, followed by centrifugation(Beckman-GPKR Centrifuge; Beckman Coulter)for 15 min at 3000 rpm. The supernatant containing all fat-soluble vitamins were combined and dried under nitrogen

in a Speed-Vac. When dry, the samples were resuspended in 500 µL ethyl acetate for HPLC-UV analysis.

2.2.7 Trace Element Analysis Using ICP-MS

For our ICP-MS analyses a total of 32 different samples consisting of 28 different vegetables and 4 different fruits were analyzed using 2 biological replicates. All 64 samples were analyzed for 64 elementsincluding Li, B, Na, Mg, Al, P, K, Ca, Ti, V, Cr, Fe, Mn, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Rb, Sr, Y, Zr, Nb, Mo, Ru, Cd, Sn, Sb, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Gd, Dy, Er, Tm, Yb, Lu, Hf, Ta, W, Os, Au, Pb, Th, Ag, Be, Ho, Ir, Pd, Pt, Re, Si, Tb, Te, Tl, and U. The ICP-MS analysis was carried out using a Perkin Elmer Sciex Elan 6000 quadrupole ICP-MS operating in a dual detector mode with an ICP RF power of 1300 W. Blank subtraction was applied after internal standard correction with Bi, Sc and In being used as internal standards. Quantification of all elements was done by four point calibration curves (0, 0.25, 0.50 and 1.00 ppm for Na, Ca, Mg, Fe, K, P, and 0, 0.005, 0.010, and 0.020 ppm for other remaining elements). The flow rate was approximately 1 ml/min with 35 sweeps per reading using one reading per replicate with three replicates being measured. Dwell times were 150 ms for Se, 10 ms for Na, Al, K, Cu, Zn, Sr, and 20 ms for all other elements. The integration times were 5250 ms for Se, 350 ms for Na, Al, K, Cu, Zn, Sr and 700 ms for all other elements. The relative standard deviation for As, Ni, Pb, and Zn was between 5 and 10%.The accuracy of the ICP-MS analytical protocol was periodically evaluated via the analysis of certified reference standard materials (whole rock powders) BE-N and DR-N available from the SARM laboratory at the CRPG (Centre de Recherches Petrographiques et Geologiques).

2.2.8Compound Identification and Quantification by NMR

For our NMR analyses a total of 32 different samples consisting of 28 different vegetables and 4 different fruits were analyzed using 2 biological replicate.To prepare the NMR samples, the extractgenerated using the protocol described in section 2.2.3 was lyophilized, yielding about 50 mgof dried material. The powder was placed in a 1.5 ml Eppendorf tube and then dissolved in 470 µL of HPLC-grade water followed by the addition of 70 µL of D_2O and 60 µL of a standard NMR buffer solution (11.667 mM of disodium-2,2 dimethyl 2-silapentane-5-sulphonate, 730 mM imidazole, and 0.47% NaN_3 in H_2O). The sample was then transferred into a standard thin-walled 5 mm cylindrical glass NMR tube(Wilmad, Buena, NJ, USA) for spectral analysis. All ^{1}H-NMR spectral data were obtained on a 500 MHz Inova (Varian Inc., Palo Alto, CA) NMR spectrometer equipped with a 5 mm pulsed field gradient Varian cold-probe. One-dimensional ^{1}H-NMR spectra were acquired at 25°C using the first transient of the tnnoesy-presaturation pulse sequence which yields a high degree of quantitative accuracy (Saude et al., 2006). Spectra were collected with 256 transients, an acquisition time of 4 seconds, and a recycle delay of 1 second. Prior to spectral analysis, all FIDs were zero-filled to 64,000 data points and line broadened by 0.5 Hz. The methyl singlet produced by a known quantity of DSS was used as an internal standard for chemical shift referencing (set to 0 ppm) and for quantification. All ^{1}H-NMR spectra were processed and analyzed using the Chenomx NMR Suite Professional software package version 7.7 (Chenomx Inc., Edmonton, AB), as previously described.

2.2.9LC MS/MS Compound Identification and Quantification

For our LC-MS/MS analyses a total of 32 different samples consisting of 28 different vegetables and 4 different fruits were analyzed using 2 biological replicates. A commercially available kit

(the Absolute*IDQ* kit - Biocrates Life Sciences AG, Austria) was used in combination with an ABI 4000 Q-Trap (Applied Biosystems/MDS Sciex) mass spectrometer to detect and quantify up to 186 metabolites including amino acids, acylcarnitines, biogenic amines, and glycerophospholipids. This kit-based method involves derivatization and extraction of metabolites from the sample of interest, along with selective mass-spectrometric detection and quantification via multiple reaction monitoring (MRM). Isotopically-labeled internal standards are integrated into the kit plate filter to facilitate metabolite quantification. The exact details of the method have been described elsewhere(Mandal et al., 2012; Bouatraet al., 2013; Psychogios et al., 2011). The kit was originally designed for plasma and serum samples, but cross validation of the fruit and vegetable extracts measured by the Biocrates kit with other techniques such as NMR and GC-MS showed excellent agreement, which gave us the confidence to use the kit for these plant extract samples.

The BioCrates kit plate consists of 96 wells withthe first 14 wellsbeingused for quality control or internal standardization and the remaining 82 wells being set aside for sample analysis. Ten microliters of each extract (prepared in Section 2.2.3)was loaded onto the kit's filter paper substrate and dried under nitrogen. Subsequently, 20 µL of a 5% phenylisothiocyanate solution was added for derivatization and after 20 min incubation the filter spots were dried using a nitrogen evaporator. Extraction of the metabolites was then achieved using methanol containing 5 mM ammonium acetate. The extracts were analyzed using an ABI 4000 Q-Trap (Applied Biosystems/MDS Sciex) mass spectrometer equipped with a solvent delivery system. A standard flow injection protocol consisting of two 20 µL injections (one for the positive and one for the negative ion detection mode) was applied for all measurements. MRM detection was used for quantification. The MetIDQ software was used to control the entire assay workflow, from sample

registration to automated calculation of metabolite concentrations to the export of data into other data analysis programs.

2.2.10 GC-MS Analysis of Fruit and Vegetable Extracts

Using the lipid fractions extracted as described in section 2.2.4, a GC-MS analysis was performed to identify and quantify the constituent lipid metabolites. For these GC-MS analyses a total of 32 different samples consisting of 28 different vegetables and 4 different fruits were analyzed using 2 biological replicates. Fatty acid methyl esters (FAMEs) from all of the lipid fractions (glycolipids [GL], phospholipids [PL], cholesterol esters [CE], triglycerides [TG] and free fatty acids [FF]) were prepared using the method described by Christie (2003). Briefly, 1 ml of 2% H_2SO_4 in methanol was added to each fraction. All the fractions were incubated at 86° C for 1 hr followed by cooling on ice for 5 min and adding 0.5 ml of 0.5% sodium chloride solution.The caps were replaced with aluminum foil, which was perforated with small holes to relaese pressure during the incubation period.Subsequently, 2 ml of hexane was added to each vial followed by vortexing for 5 minutes. The supernatant was then taken and recovered. An additional 1 ml of hexane was added to increase the solubility of metabolites in the matrix and vortexed for a minute. The upper organic layers were transferred to a 2 mL vial and the solvent evaporated under a stream of nitrogen gas and reconstituted in 100 µL of hexane. All GC-MS data was collected on an Agilent Technologies 7890A gas chromatograph–5975N mass spectrometer (GC-MS)using an HP-88 (100 m × 0.250 mm × 0.2 µm) capillary column (Agilent Technologies Inc., Palo Alto, CA). The oven temperature was 70 °C(1 min), which was raised to 76 °Cat 1 °C/min and then increasedto 250 °C at a rate of 6.1 °C/min. The flow rate was set to 11.6 cm/s (helium). The split ratio, the quadrupole temperature, and the detector temperature were set at 10:1, 185 and 250 °C, respectively. Confirmation of each fatty acid was performed by comparing EI-MS spectra and

retention times to laboratory standards (Sigma-Aldrich, St Louis, MO, USA). Quantification of the lipids and fatty acids was achieved using defined fatty acid methyl ester standards (FAMEs).

2.2.11HPLC Analysis of Polyphenols

For our polyphenol analyses a total of 32 different samples consisting of 28 different vegetables and 4 different fruits were analyzed using 2 biological replicates. HPLC analysesof our polyphenol extracts (see section 2.2.5) wereperformed on an Agilent 1100 HPLC system equipped with an Agilent G1315B diode array detector (with a scanning wavelength between 190 and 500 nm), using a Phenomenex 00G-4336 E0 (SYNERGI 4u POLAR-RP 80A 250 x 4.6mm) reversed-phase column,an automatic injector and a column oven. The temperature was maintained at 30º C, with an injection volume of 15 µl and the flow rate of 1 ml/min. The HPLC mobile phases were 0.05% sodium phosphate buffer (w/v),pH 2.5 as solvent A and methanol (100%) as solvent B. The column was equilibrated with the solvents for 30 min prior to each run. The elutiongradient was linear and started at a flow rate of 1 ml/min going from 0% to 95% methanol (buffer A) over a period of80 min and stayed at 95% for an extra 10 min with stable flow rate of 1 ml/min. The full gradient mixing and elution protocol is given in Table 2.2. The total elution time was 90 min.This protocol allowed us to identify and quantify a total of 19 different deglycosylated polyphenols including, gallic acid, catechin, chlorogenic acid, caffeic acid, vanillic acid, syringic acid, coumaric acid, benzoic acid, ferulic acid, sinapic acid, rutin, resveratrol, myricetin, quercetin, luteolin, kaempferol, isorhamnetin, apigenin and 3, 4-dihydroxybenzoic acid.Quantitation was carried out using seven-point calibration curves for each standard, covering a concentration range of 0.01–1 mg/mL. Each calibration curve was obtained by plotting peak areas vs the concentration of the standard.The absolute concentrations of 19 polyphenols were determined using the

regression equation obtained from the calibration curves. Each polyphenol concentration for every fruit/vegetable was measured on 2 biological replicates.

2.2.12Vitamin analysis using HPLC-UV

For the vitamin analyses, a total of 32 samples, consisting of 28 vegetables and 4 fruits were analyzed using 2 biological replicates. An Agilent 1100 HPLC system equipped with an Agilent G1315B diode array detector (with a scanning wavelength between 190 and 500 nm), a reversed-phase HPLC column Kinetex C18, and an automatic injector were used for the analysis and quantitation of all vitamins in the fruit and vegetable samples extracted in section 2.2.6. The mobile phase consisted of 20 mM ammonium formate in water, with 0.1% formic acid (Solvent A) and 100% methanol (Solvent B). The sample injection volume was 10 µl. The oven temperature was programmed at 40°C and the flow-rate was set at 0.5 mL/min.

For the water soluble vitamins, a gradient profile was used for elution which started with 95% solvent A, which was decreased linearly to 85% over 3 min and was then followed by a linear decrease to 40% solvent A over 3 min. The profile was completed by a further linear gradient to 95% solvent A in the next 2 min interval and kept at 95% for the last 2 min. The total run time was 10 min. For fat-soluble vitamins, the gradient profile started at 70% solvent B and linearly increased to 100% over 2 min and was kept at 100% for the next 5 minutes. The gradient was set back to 70% for 5 min and kept at that state for another 3 min. The total run time was 10 min.

2.2.13Literature Analysis, Text Mining and Compound Annotation

A literature search on PubMed and Google Scholar was conducted using different combinations of each of the fruit and vegetable names (including Latin names and synonyms) along with the words “metabolomics”, “metabolome”, “metabonomics”, “chemical analysis”, “food analysis”, “food composition”, “chemical composition”, “nutrientcomposition”, “nutritional composition”, “food analysis”, “metabolite profile”, “NMR”, “GC-MS”, “MS/MS”, “polyphenol”, and “phytochemical”. This search yielding about 800 articles related to the chemical composition of these fruits and vegetables.The results of this literature search are summarized in Table 2.3. Additional literature searches were performed for fruit and vegetableconstituents (and concentrations) by scanning through the Dictionary of Food Compounds(Yanna, 2012), The Composition of Foods (McCance, 2002)and other textbooks(Pennington & Spungen, 2010). These were supplemented by additional data retrieval from various online National food composition tables (the USDA NND [National Nutrient Database], the DTU [Danish Food Composition Database], and the Health Canada food composition tables) as well as FooDB (Wishart, 2015),the HMDB(Wishart et al., 2013), MetaboLights(Haug et al., 2013), Phenol-Explorer(Neveu et al., 2010; Rothwell et al., 2012; Rothwell et al., 2013), Dr. Duke's Phytochemical database(Duke, 2000)and KNApSAcK(Nakamura et al., 2013). All compound identifications, concentrations and references were compiled, compared and their names “normalized” to match HMDB, CAS and PubChem identifiers. Themanually derived compound data was further annotated using an in-house program called DataWrangler which automatically generates names, synonyms, descriptions, structures, chemical taxonomies, physical property data, organoleptic features, as well as health benefits, biological effects, pathways, targets, transporters, and bioavailability. The data extracted by DataWrangler (especially with regard to descriptions and health/biological

effects) was manually checked and then entered into the Alberta Food Composition Database (AFCDB: http://afcdb.ca).

2.3 Results and Discussion

This study usedquantitative, multi-platform metabolomics techniques to perform comprehensive characterization of 32 common, garden-grown fruits and vegetables. The content of minerals, lipids, amino acids, polyphenols, vitamins, sugars and other miscellaneous metabolites were determined for all samples using sixdifferent quantitative assays or analytical platforms (Table 2.4). Compound identification was confirmed using authentic reference standards and standardized reference spectra. Quantitative analysis was performed using external standardscoupled with carefully constructed calibration curves for each standard. In conducting this study we wished to: 1) gain a more complete picture of the chemical composition of many common fruits and vegetables; 2) assess the utility of different metabolomics platforms for food composition analysis; 3) determine the maximum degree of chemical coverage attainable by multiple, quantitative metabolomic methods; 4) compare the coverage obtained by metabolomics methods with other food analysis techniques and other published values and 5) extend our experimental analysis through literature mining and make all of the data available through a public, web-accessible database called the Alberta Food Composition Database (AFCDB: http://afcdb.ca). The results concerning each of these objectives are outlined below:

2.3.1 Platform and Assay Comparison

The six different metabolomics platforms or compound class-specific assays used in this study were: 1) ICP-MS; 2) NMR; 3) DFI/LC-MS/MS; 4) GC-MS (fatty acids/lipids); 5) polyphenolic assays; and 6) vitamin assays.ICP-MS identified and quantified an average of 43 (range = 35-53)

compounds (metals); NMR spectroscopy was able to identify and quantify an average of 32 (range = 26-38) compounds; DFI/LC-MS/MS identified and quantified and average of 73 (range = 50-103) metabolites; GC-MS based lipidomics detected and quantified an average of 54 (range = 4-165) compounds; the vitamin assays identified and quantified an average of 6 (range = 3-8) vitamins and the polyphenol assays identified and quantified and average of 13 (range = 9-17) compounds. The Venn diagram in Figure 2.1 summarizes these results. Overall, it is clear that there is relatively little overlap between the different platforms or methods. It is also evident that the DFI/LC-MS/MS approach provided the largest average number of metabolites, while the specialized assays (vitamins and polyphenols) provided the fewest. A more detailed description of what was found for each platform or method is given below.

2.3.1.1 – ICP-MS Results

Inductively coupled plasma mass spectrometry (ICP-MS) is considered to be the gold standard for ultra-sensitive trace element analysis(Benkhedda et al., 2000; Kohlmeyer et al., 2003). Our ICP-MS assaysprovided quantitative results for nearly 60 trace mineralsas shown in Table 2.5. Measured concentrations for all detected trace elements for all the fruits and vegetables we studied are also reported in the AFCDB website. The fruit/vegetable that was most fully characterized by ICP-MS was spinach which had 53 metal ions identified and quantified. The fruit/vegetable that yielded the lowest number of ICP-MS-identifiable trace elements was bell pepper (for all 3 varietals: yellow, red and orange), which had just 35metal ions identified and quantified. The lowest concentration we found was 3.19ng/100 grams fresh weight, for niobium (Nb) in raspberry.The highest concentration we found was 936.4 mg/100 grams fresh weight (FW) for potassium in spinach. Across all plant species, the most abundant ions were potassium

(131.43 to 936.4 mg/100 g FW),phosphorous (11.8 to 147 mg/100 g FW), calcium (4.19 to 169.7mg/100 g FW), magnesium (4.6 to 78.7 mg/100 g FW), and sodium (0.3 to 110.11 mg/100 g FW), respectively.Spinach, dill, broccoli, Swiss chard, and garlic are generally the best sources of minerals. According to our data, among the selected fruits and vegetables, spinach and broccoli are the best sources of potassium, phosphate, calcium, sodium, magnesium, and iron. Swiss chard, broccoli, and, garlic are the best sources of boron and dill is the best source of calcium.These results align with data from most nutritional textbooks and on-line nutrient databases (USDA, the Danish Food Composition Databank). As can be seen in Table 2.5, only 6-7 elemental ions dominate while the other ions are present only at trace amounts.Also our experimental results demonstrate the presence of substantial levels of aluminum in almost all vegetable and fruit samples. Aluminum is releasedwhen soil pH is low and Alberta is known to have somewhat acidic soils (Penney et al. 1997).

To the best of our knowledge, this is the largest multi-elemental study on fruits and vegetables ever conducted using ICP-MS.Comparing the results we obtained with those previously reported in the literature for the same (or similar) food items and the same trace elements (Table 2.5) shows very good agreement.However it is also important to remember that a number of factors may influence content of minerals and trace elements including the local environment, level of fertilization, irrigation, soil mineral content, ground or rainwater mineral content and plant cultivar(Hopkins & Elsen, 1959; Hattori & Chino, 2001; Sharma & Rao, 2013; Pietola, 2000; Balint et al., 2001).As can be seen in Table 2.5, many of the minerals we identified and quantified are being reported forthe very first time in this study.

2.3.1.2 – NMR Results

NMR was used to determine the content of a wide range of water-soluble sugars, alcohols, amino acids, organic acids and various phytochemicals for our fruit and vegetable samples. Our NMR assays provided quantitative results for an average of 36 high-concentration (>1μM), water-soluble compounds as shown in Table 2.6. Measured concentrations for all detected compounds for all the fruits and vegetables we studied are also providedat the AFCDB website, along with the literature-derived values and their associated citations. Typically about 70% of the total peak area in any given fruit/vegetable ^{1}H NMR spectrum could be assigned. This suggests that potentially another 15-25compounds could be identified if reference NMR spectra existed for these "unknown" compounds. The fruit/vegetable that was most fully characterized by NMR was eggplant which had 38 compounds identified and quantified. The fruit/vegetable that yielded the lowest number of NMR-identifiable metabolites was red beetroot which had just 26 compounds identified and quantified. The lowest concentration we found by NMR was 0.7mg/100 grams fresh weight for betaine inJapanese pumpkin. The highest concentration we found by NMR was 3.1 g/100 grams fresh weight for fructose in orange bell pepper. Across all plant species, the most frequently detected compounds were glucose, fructose, leucine, isoleucine, tyrosine, glutamine, serine, alanine, and phenylalanine. Our results demonstrate that fruits and vegetables are great sources of essential amino acids including phenylalanine, valine, threonine, tryptophan, methionine, leucine, isoleucine, lysine, and histidine (as shown in Table 2.6).Note that all amino acid values reported for this NMR study represent the concentrations of free amino acids. Protein hydrolysis was not performed, so the total amino acid content reported for this kind of analysis will differ slightly from those provided by many national food tables. However, inspection of Table 2.6 shows that the agreement with literature-reported values (which likely didn't

includeprotein hydrolysis in the quantitation process) is actually quite good.These results align with data from other nutritional nutrient databases. Unlike the situation with ICP-MS, the results from our NMR study showed a much narrower range of concentrations (varying by 3 orders of magnitude) compared toICP-MS, which exhibited variations of 6 orders of magnitude because NMR spectroscopy is an inherently less sensitive technique than mass spectrometry.This reflects the differing sensitivity of the measuring systems (ICP-MS is very sensitive compared to NMR) as well as the tendency of NMR to identify many more essential metabolite/nutrients.

We believe this is the largest and most comprehensive food composition study on fruits and vegetables ever conducted using NMR spectroscopy. Comparing the results we obtained with those previously reported in the literature for the same (or similar) food items show generally good agreement andthe percentage of agreement was 86% using ± 50% threshold. About 50% of our values couldn't be found in previously published quantified data.However, it is also important to remember that these values can be influenced by a number of factors including the local environment, level of fertilization, irrigation, and plant cultivar (Hopkins & Elsen, 1959; Hattori & Chino, 2001; Sharma & Rao, 2013; Pietola, 2000; Balint et al., 2001).It is also important to remember that the use of different analytical or extraction methods, as well as different technologies from different periods in history will also lead to systematic differences. Therefore we would, and should not, expect a perfect match between our NMR results and those in the literature that were measured using other (somewhat dated) technologies (Asseen in Table 2.14).

2.3.1.3 – Direct flow injection/LC-MS/MS Results

Direct flow injection and LC-MS/MS via the Biocrates kit was used to determine the content of biogenic amines, amino acids, fatty acids and lipids for our fruit and vegetable samples. These

DFI/LC-MS/MS assays provided quantitative results for an average of 73 compounds as shown in Table 2.7. Measured values for all the fruits and vegetables are also reported in the AFCDB website, along with the literature-derived values and their associated citations. Since there was no protein hydrolyzing, all the reported amino acid values do not include protein hydrolysates.The fruit/vegetable that was most fully characterized by LC-MS/MS was yellow bell pepper which had 103 compounds identified and quantified. The fruit/vegetable that yielded the lowest number of DFI/LC-MS/MS-identifiable metabolites was Nanking cherry, which had just 50compounds identified and quantified. The lowest concentration we found by DFI/LC-MS/MS was 0.35 μg/100 grams fresh weight for hexadecadienyl-l-carnitine, in cucumber. The highest concentration we found by DFI/LC-MS/MS was 436.5 mg/100 grams fresh weight for glutamic acid in garlic. Note that all amino acid values reported here represent the concentrations of free amino acids. As shown in Table 2.7, the total amino acid content reported for this kind of LC-MS/MS analysis and literature values are based on not performing protein anlysis. Across all plant species, the most frequently detected compounds were aspartic acid, glutamic acid, alanine, glucose, fructose, phenylalanine, glutamine, asparagine, and isoleucine. Based on Table 2.7, four amino acids: glutamic acid, glutamine, serine, and alanine, were the most abundant compounds among all the fruit and vegetable samples.Also the largest numbers of detectable compounds werefound in yellow bell pepper, yellow zucchini, garlic, cucumber, and orange bell pepperwith a total number of 103, 94, 89, 89, and 89 compounds respectively.According to our data, garlic was a good source of 5 amino acids including leucine, lysine, isoleucine, proline, and glutamine.Beans were good sources of 4 amino acids including asparatic acid, glutamic acid, and glutamine. Most sweet peppers were good sources of asparatic acid and glutamic acid. These results are all in good agreement with data from other on-line nutrient databases. In particular,the percentage of

compounds measured by DFI-LC-MS/MS that showed good (defined as ± 50% with literature/database values) agreement was 71.2%. However for about 70% of values we couldn't find any refreneces to compare our data with previous studies.

This is the first food composition study on fruits and vegetables ever conducted using the Biocrates AbsoluteIDQ kit. Comparisons with identical metabolites measured by us using NMR,GC-MS as well as comparisons with data reported in the literature indicate that the values reported by the AbsoluteIDQ kit are generally very consistent, correct and accurate (see Table 2.14). Comparing the results we obtained via this kit with other previous studies proved to be difficult for some metabolites as essentially no other studies provided data on phospholipids, biogenic amines or acyl carnitines. Comparisons to reported amino acid content values also proved to be difficult, as our analysis focused on the quantification of free amino acids, as opposed to total amino acids (obtained via protein hydrolysis combined with free amino acids). For the compounds that could be compared (largely amino acids and biogenic amines) we provide literature-derived values in Table 2.7.

2.3.1.4 – Polyphenolic Analysis Results

High performance liquid chromatography coupled with UV detection was used in the separation, characterization, and quantification of phenolic compounds for our fruit and vegetable samples. Measured concentrations for all detected polyphenols for various common garden fruits and vegetables are reported in Table 2.8 as well as in the AFCDB website. The website also provides the literature-derived values and their associated citations. These results align with data from other previously published studies. Our experimental results show a moderate agreemenet (75%)between the phenolic compounds we measuredcompared to previously published studies by

considering ± 50% of threshold value. Persian cucumber and Italian red pepper had the greatest diversity of polyphenols with17 polyphenols identified and quantified. The fruit/vegetable that yielded the lowest number of polyphenols detectable by HPLC was white cabbage,which had 9 compounds identified and quantified. The lowest concentration we found was 0.24μg/100 grams fresh weight for benzoic acid in Romaine lettuce. The highest concentration we found was 30.6 mg/100 grams fresh weight for syringic acid in red Swiss chard. Across all plant species, the most common polyphenolic compounds were galli acidvanillic acid, quercetin, and sinapic acid. Also across our selected 32 fruits and vegetables and 19 polyphenols, broccoli, parsnip, Swiss chard, and spinach had the highest quantities of phenolic compounds.According to our data, Swiss chard is the best source of syringic acid and ferulic acid, parsnip is a good source of gallic acid, coumaric acid and ferulic acid, dill is the best source of quercetin and isorhamnetin, and Italian sweet red pepper is the best source of benzoic acid and sinapic acid.

There have been numerous laboratory studies on food phenolic compounds over the past few decades. Many of these are summarized and tabulatedin the Phenol-Explorer database(Neveuet al., 2010; Rothwell et al., 2012; Rothwell et al., 2013)**.** The latest version of Phenol-Explorer(Phenol-Explorer 3.0) contains polyphenol content data on>100 foods, covering 161 different polyphenols. Much of the data described in Phenol-Explorer was derived from similarkinds of targeted HPLC-UV techniques that we used for this study(Campus, 1999; Huang et al., 2007; Pyo et al., 2004). However, Phenol-Explorer is by no means complete. As shown in Table 2.8, ourwork revealed a number of polyphenols in the fruits and vegetables studied here that have not been previously reported either in Phenol-Explorer, in the literature or in any other public food database. Certainly many more polyphenols likely exist in the fruits and vegetables

that we studied. However, the lack of authentic reference standardsprevented us from fully identifying and quantifying them.

2.3.1.5 – GC-MS Lipidomics Results

In this study, the lipid and fatty acid composition of various vegetables and fruits were examined using a combination of lipid extraction, solid phase separation and GC-FAMES. A technique known as Combinatorial Lipid Reconstruction (CLR) (Psychogios et al, 2011) was used to computationally regenerate precise lipid structures and to approximate the lipid concentration ranges (in mole percent).The results for the fatty acid composition for each of 5 different lipid classes are presented in Table 2.9. The 5 lipid classes include glycolipids (GL), phospholipids (PL), choleteryl esters (CE), triglycerides (CL) and free fatty acids. A total of 27 different types of fatty acids were selected andmeasured for these 5 lipid classes. Two Fatty acids were not found (or not at detectable levels) in any fruit of vergetable, these included C12 and C13. Also our Lipidomics approachshowed that thetotal number of free fatty acids in vegetables and fruitswas varied in the range between 2 and 12(an average of 7 free fatty acids).The fewest number of free fatty acids was observed in potato with only 2 and the largest numbers were found in broccoli with 12 free fatty acids.Unfortunately, insufficient data was collected to obtain fully quantitative information about some of these lipid classes (with the possible exception of the cholesteryl esters). Nevertheless, these data demonstrate that fruits and vegetables contain a diverse collection of fatty acids and lipids with carbon chain lengths greater than 14 and that these exist as both free fatty acids as well as in glycolipids, neutral lipids, phospholipids and cholesterol esters (Table 2.9). As can be seen from our data, cucumber, potato, turnip, and onion were the richest in palmitic acid (C16:0). Cauliflower and sunburst squash were the richest in Linolenic acid

(C18:3).Eggplant and crab apple were the richest in stearic acid (C18:0). Fruits and vegetables appear to be good sources of myristic acid (C14:0), palmitic acid (C16:0), linolenic acid (18:2), heptadecanoic acid (17:0), and α-Linolenic acid (C18:2), as seen in Table 2.9. Combinatorial lipid reconstruction was used to further analyze the triglycerides (which contain more than one fatty acid chain) to determine their identities and concentrations (Tables 2.10 and 2.11). CLR is able to estimate the most probable and the upper limit concentrations for each reconstructed lipid by using the fractional abundance of each fatty acid chain and the total value of a given lipid class. Using direct measurements for fatty acid compositions along with their associated lipid groups as well as CLR data for triglycerides, we identified and quantified (or semi-quantified) 1716triacylglycerol compositions(an average of 54) in 32 vegetables and fruits (Table 2.11). Based on the CLR estimates, the highest concentration was 65.2 M for TG (C16:0/C16:0/C16:0) and the lowest estimated concentration was 583 nM for TG(C22:0/22:0/22:0).

Comparing the results we obtained for our lipid analysisto what was available in the literaturerevealed thatthere were published few studies on fruits or vegetablesthat have been particularly successful in quantifying the fatty acid or lipid compositions.Furthermore, only a few food databases such as the USDA Food Tables and the Danish Food Composition Databank report fatty acid content(Amaral et al., 2003; Jeong & Lachance, 2001; San & Yildirim, 2010). Previously published literature has mainly focused on the total fatty acid composition of fruits and vegetables, without distinguishing lipid classes(Kris-Etherton et al., 2000; Simopoulos, 1999). To our knowledge, these lipid results are a new contribution to the literature.

2.3.1.6 – Vitamin Assay Results

High pressure liquid chromatography (HPLC) with UV detection was used to determine the vitamin content of all the fruits and vegetables in this study. Our vitamin assays provided

quantitative results for 7 water-soluble vitamins and4 fat-soluble vitamins, as shown in Table 2.13. All the vitamin data have also been deposited into the AFCDB website, along with the literature-derived values and their associated citations. Vitamin A was not measured here due to expreminetal difiilulties uing HPLC-UV assay. The HPLC-MS is our recommended method to measure vitamin A. Also vitamins with concentration lower than 1 mg/100g FW couldn't be detected using this assay. The fruit/vegetable that had the highest number of detectable vitamins by this assay was broccoli, which had 8 vitamins identified and quantified. Turnip, which had 4detectable vitamins,was the most "vitamin-poor" fruit or vegetable. As shown in Table 2.13, the highest concentration for any vitamin was77.9 mg/100 grams fresh weight for vitamin C in green bell peppers. The lowest concentration was 0.26 µg/100 grams fresh weight, observed for Vitamin B7 (biotin) in crab apples. Across all plant species, broccoli, Swiss chard, spinach, and berries have the highest amount of total vitamins. Across our selectedfruits and vegetables, the most abundant vitamins were vitamin C(up to 77.9 mg/100g FW),vitamin E (up to to 2.6 mg/100g FW) and the least abundant vitamins were vitamin D(as low as 0.006mg/100g FW), vitamin B7(as low as 0.0003 mg/100g FW), and vitamin B1(as low as 0.18 mg/100g FW). According to our data, the best sources of vitamin C aresweet bell peppers, whilethe best source of vitamin B1 isparsnip. The best source for vitamin B12 is wax bean, for vitamin B5 it isbroccoli, for vitamin B7 it is zucchini, vitamin B9isbroccoli and vitamin B2is garlic. The best source of vitamin Eisgreen bell pepper, and vitamin K is spinach.

To the best of our knowledge, this is the most extensive vitamin characterizationforgarden-grown fruits and vegetables ever published. Obviously vitamin assays are routinely conducted by national food agencies (Canada, the USDA, Australia, the European Union) but the methods, sample preparation and other experimental details are rarely provided. With regard topublished

studies on vitamin content, most typically report just one or two vitamins over a range of fruits and vegetables(Rickman et al., 2007; Franke et al., 2004). However, there is at least one studythat reported thedetermination of 9 vitamins in a total of 12 different fresh-cut vegetables and fruits using LC–MS/MS and LC–DAD (Santosa et al., 2012). Relative to most other food constituents, vitamin content values are probably the most extensively covered and reported. Comparisons with the vitamin content we measured and those values reported in various national food tables and other literature-derived sources are summarized in Table 2.13. It is not unexpected to see differing vitamin concentrations due to various biotic and abiotic factors (Pietola & Salo, 2000; Sharma & Rao, 2013; Balint et al., 2001; Hattori & Chino, 2001; Hopkins & Elsen, 1959).

2.3.2 Assessing the Extent of Compound Coverage

In this study, we used six different analytical platforms or compound-specific methods: NMR, DFI/LC-MS/MS, ICP-MS, GC-MS-based lipidomics, an HPLC-based polyphenol assay, and an HPLC-based vitamin assay to comprehensively characterize the chemical constituents of 32 common, garden-grown fruits and vegetables. Using all six platforms and methods, 6,985metabolite measurements were made over 32 different fruits or vegetables – or an average of 218 metabolites per fruit or vegetable. Altogether at totalof 339chemically distinct metabolites were identified and quantifiedfrom all plant food samples in this study. Based on the spectral libraries (NMR and GC-MS) and the available reference standards (for DFI/LC-MS, ICP-MS, vitamins and polyphenols), we estimate that our 6 platforms had the capability of identifying a total of ~2000 unique compounds. This suggests that we were able to detect about 20% (387/2000) of all potentially measurable compounds in our fruits and vegetables. Given that many

of the compounds we were attempting to detect are more commonly found in mammalian species or are known to be in very low abundance, this result is not unexpected.

Onion had the lowest level of coverage with 207 compounds, while dill had the highest level of compound coverage with a total of 387 compounds identified and quantified. Based on an extensive review of the literature, these numbers represent the largest number of fruit/vegetable compounds ever identified and quantified in a single study. As seen in the Venn diagram (Fig. 2.1), some methods provide completely unique data (ICP-MS, in particular), while other methods such as NMR, DFI/LC-MS/MS and the vitamin/polyphenol assays exhibit some modest overlap. The most effective approach for generating completely novel or never-before reported data was ICP-MS (with an average of 88% of the metabolites having no prior literature value), followed by the DFI/LC-MS/MS method (with an average of 80% of the metabolites having no prior literature values) and the polyphenol assay (with an average of 60% of the metabolites having no prior literature values). The assay that provided the least amount of novel or never-before-seen data was the vitamin assay, with an average of just 15% of the vitamins having no prior literature value.

2.3.3 Compound Coverage: Literature Comparison

As noted in section 2.3.2, Tables 2.5-2.13 provide comparisons between our experimentally measured values and those reported in the literature. The exact literature sourcesandassociated referencesare provided on the AFCDB web site (there is insufficient space to provide this information in the attached tables). In many cases, only a single literature value was found.However, when 3 or more values were obtainable, an average and a standard deviation are provided.

Table 2.5 provides a comparison of the extent of metal ion or trace element coverage for different food composition databases and previously reported studies relative to the data reported

here. As can be seen from this table, modern food composition tables typically report values for 8-10 of the most abundant or nutritionally important minerals for most fruits and vegetables, such as potassium, calcium, phosphate, magnesium, iron and zinc. In our literature review we identified ~25 studies that provided modest or reasonably extensive trace metal analysis on fruit and vegetable samples using atomic absorption spectroscopy, flame ionization spectroscopy, and ICP-MS. The atomic absorption studies would typically report ~10 metals, while the flame ionization methods would typically report 5 trace elements, while the ICP-MS studies typically reported between 9 to 14 trace elements (Radwan & Salama, 2006;Turkdogan et al., 2003;Tinggi et al., 1997; Chen et al., 2007; Ekholm et al., 2007).Many of these did not report absolute concentrations but rather simply reported trace minerals detection. Overall, most of these trace element studies of fruits and vegetables achieved only relatively modest trace element coverage with an average of 13 minerals reported for 10-15 different fruits or vegetables. The most complete metal ion study we could find was that reported by Mayer (1997). They studied 42 fruits/vegetables and achieved an average coverage of 7trace elements (Mayer, 1997). Our study achieved an average coverage of 43 trace element values for 32 different fruits and vegetables.

To date there have only been a few NMR studies on fruits and vegetables that resulted in both the quantitation and identification of specific compounds in fruits (or fruit juices) and vegetables(Zanatta et al., 2005; Bunzel & Ralph, 2006; Dachtler et al., 2001). On the other hand, there are quite a few NMR studies that report compound characterization (Aman et al., 2005; Bunzel & Ralph, 2006).One of the most complete NMR studies we wound was a report by Gal et al (2003). They identified and quantified a total of 29 compounds in tomato fruitsby NMR analysis of tomato juice and extract. Based on these data, our study appears to be one of the

largest NMR studies ever conducted on fruit/vegetable samples. We achieved an average coverage of 34 NMR values for 32 different fruits and vegetables.

LC-MS/MS has generally been the preferred method for identifying (and occasionally quantifying) plant metabolites. In our literature survey we found ~10 studies that used this technique or variations thereof for various fruit or vegetable samples. Out of these studies, however, only a small number (3) used multiple or single reaction monitoring to determine absolute concentrations. In terms of compound identification for fruits and vegetables, the most extensive LC-MS study we found was one performed by Kuhnle et al. (2007) who used an ABI 4000 QTRAP mass spectrometeron a total of 58 fruits and vegetables and succeeded in identifying 12 compounds across all samples (Kuhnle et al., 2007). Anothernotable LC-MS study reported the phytoestrogen content of ~100 fruits and vegetables(Kuhnle et al. 2009). These researchers identified and quantified a total of 11 different phytoestrogens across all plant species(Kuhnle et al., 2009). In comparison, our study achieved an average coverage of 70 compounds for 32 different fruits and vegetables. Our LC-MS study also demonstrated that it is possible to determine the concentration of water-soluble compounds in food samples using DFI/LC-MS/MS via the Biocrates AbsolutIDQ™ p180 kit. However, some caution is warranted. In particular there were a number of mammalian-specific compounds (sphingomyelins, creatinine, carnosine) which had to be manually excluded after the initial analysis. This is because the kit would occasionally misidentify these compounds in the plant matrix (likely due to the existence of as-yet unidentified plant compounds with identical molecular weights (to sphingomyelins or creatinine) and similar retention times. It is worth noting that Biocrates AbsolutIDQ™ kits have been applied to various biological sample types for metabolic analysis butas far as we are aware, this is the first study of vegetable and fruit extracts using the BiocratesIDQ system. The principle

advantages of this method are its ease of use, its level of quantification and its high level of reproducibility(Gustavsson et al., 2007a). It is also routinely able to detect/quantify more compounds than GC–MS and NMR (Saleem et al., 2012).

Table 2.8 provides a comparison of the extent of our polyphenol coverage compared to previously reported studies. Note that there are hundreds of polyphenol studies that report the identification of polyphenolic compounds (typically via LC-MS/MS) but there are relatively few studies that report both identification and absolute quantification. Indeed, as can be seen from Table 2.8, most previous polyphenol studies achieved very limited polyphenol coverage of 2-6 polyphenols for the targeted fruits and vegetables. Based on data from PhenolExplorer (Neveu et al., 2010) as well as our own literature surveys, the most common methods for polyphenol determination are: 1) LC-MS/MS, 2) NMR, 3) flow injection methods and 4) HPLC-based methods – such as the one we used here.One of the more comprehensive studies we found was a report by Campus (1999) who reported the identification ofup to 6 major polyphenols for 4 vegetables and fruits using a HPLC system and photodiode array detector. Other published studies include one that determinedthe concentration and identifiecation of 3 polyphenols for 12 culturally specific vegetables (Huang et al., 2007) and another that studied 12 phenolic compounds for Swiss chard, using reversed-phase HPLC with a coulometric array detection system (Pyo et al., 2004). Our study achieved an average coverage of 13 polyphenol values for 32 different fruits and vegetables. As shown in Table 2.8, our results revealed some polyphenols that have not been previously reported in other food databases.

Tables2.9-2.12 provide a detailed list offatty acidand lipid coverage for the fruits and vegetables analyzed in this study. Most modern food composition tables typically report values for 10-15 fatty acids for fruits and vegetables, with the most abundant being myristic acid (14:0),

palmitic acid (16:0), linolenic acid (18:2).Literature surveys of previously published lipid or fatty acid analyses of fruits and vegetables show only marginally better coverage with an average of 8 lipids or fatty acids reported for 10-15 different fruits or vegetables. Some of the most impressive published studies regarding lipids/fatty acids in fruits and vegetables include those of Speer and Kölling-Speer(2006) who identified 16 fatty acids in green coffeebean and a study by Cakir(2004) who identified 15 fatty acidsin two local fruits using GC-MS. As can be seen in Tables 2.9-2.12, our study achieved an average coverage of 27 fatty acidsfor each of the 5 major classes of lipids.

Table 2.13presents a comparison of vitamin results we obtained via HPLC/UV with those previously published values. As can be seen from the table, previous studies and food composition tables achieved relatively good coverage. Based on our literature surveys, the most common methods for vitamin determination are; 1) LC-MS/MS, 2) NMR and 3) HPLC-based methods – such as the one we used here. The most extensive vitamin studies we could find for multiple fruits and/or vegetables were those reported in 2012(Santosa et al., 2012). This study used LC–MS/MS and LC–DAD to analyze fresh-cut green leafy vegetables. They identified and quantified a total of 9 vitamins for 12 samples. Another notable study used liquid chromatography coupled with fluorimetric detection to analyze 5fruits and vegetables (Ndaw et al., 2000) leading to the identification and quantification of3vitamins for each food item. Vitamin data reported in national food tables is generally more extensive than what is reported in most published scientific studies. However, in many cases, the methods are not reported and the measurements do not cover many common, garden-grown fruits and vegetables. Compared to existing studies, our study yielded comparable or greatercoverage than most national food tables or databases with an average of 6vitamins for 32 different fruits and vegetables.Notably, thequantitative determination of

severalvitamins was performed the first time forseveral fruits and vegetables including the Saskatoon berry, crabapple, sunburst squash,andthe Nanking cherry.

2.3.4 Literature Survey and Alberta Food Composition Database

Our literature survey, which covered approximately 800 different journal articles, textbooks and online databases, identified a total of 62,040metabolites and an average of 2,216 unique compoundsspanning all of the 32 common, garden-grown fruits and vegetables selected for our study. The fruit/vegetable with the most literature reported metabolites was potatowith 2,599compounds identified. The fruit/vegetable with the fewest number ofliterature reported metabolites was Nanking cherrywith 1,909compounds identified. In addition to this literature survey we also used literature data to infer the existence of 28,628 lipids covering 12 lipid classes which are known to be in every crop plant (Table 2.12). If these lipids are included in our literature total, we would have identified at total of 923,081 metabolites for an average of 28,846 compounds for each fruit/vegetable. Whether one uses the average of 2,216 (non-lipid molecules) or 28,846 (lipid and non-lipid molecules), the vast majority of the "identified" metabolites reported for these fruits and vegetables are "inferred" meaning that they are derived from metabolic reconstructions of related, previouslysequenced food or crop plants (Zhang at al., 2005). These inferred metabolites represent the minimum subset of metabolites that a plant or a plant cell must have to sustain itself. Metabolic reconstructions do not take into account the metabolic specializationthat different plant tissues (leaves vs. fruits vs. roots) must have or the metabolic differences that may evolve over a plant's lifetime. They also do not fully account for many secondary plant metabolites (which are poorly modeled in metabolic reconstructions). So while metabolic reconstructions provide a useful framework for the approximate or expected size and diversity of a plant metabolome, they are more theoretical than practical. For comparison

purposes, a more useful total is the number of literature-derived metabolites that have been both identified and quantified. In this regard, our literature survey identified and average of 201 metabolites (that were identified and quantified) for each of the 32 common, garden-grown fruits and vegetables.This compares to an average of 258 metabolites for our experimental work reported here. The fruit/vegetable with the most literature identified+quantified metabolites wasdill with 378 compounds. The fruit/vegetable with the least reported identified+quantified metabolites was onionwith 198compounds. The total number of non-repetetive metabolites that were both identified and quantified from our literature survey was 2721. In contrast, the number of non-repetetive metabolites determined from our experimental analysis was 28,967 (including 28,628 inferred lipids).

All of the data collected from this study, including both the experimental and literature-derived data has been placed into the Alberta Food Composition Database (AFCDB). The AFCDB(http://afcdb.ca)is a freely available, easily queried and web-enabled database that allows users to view the contents of the AFCDB from either a "FoodView" (listing foods by their chemical composition) or a "ChemView" (listing chemicals by their food sources) (Figure 2.2). The AFCDB is fully searchable and a tabular view is generated by clicking on the browse button allowing users to casually scroll through the database by food source, compound names, nutrients, or food contents. Each food entry in the AFDCB provides the scientific name, description, classification, and chemical composition information (Figure 2.3).The AFCDB is capable of performing searches on the structure, concentration range, average concentration, and reference types. Many of the entries are hyperlinked to other food composition databases such as Phenol-Explorer, Dr. Duke's database, KNApSAcK, the USDA Food Tables, the Danish Food Composition Databank and other useful resources. The download button also provides links to

collected data on food constituents, health effects, synonyms, chemistry and biology information. Overall, the AFCDB database contains nutritional information for nearly 40 Alberta-grown foods and more than 17,000 content values.

2.4 Conclusion

In this study we have used a variety of quantitative metabolomics approaches tocomprehensivelycharacterize the chemical composition of 32 common garden-grown fruits and vegetables. We useda total of 5 different platforms including GC-MS, ICP-MS, DFI/LC-MS/MS, NMR, and HPLC/UV to measure a range of metabolites including trace elements, polyphenols, vitamins, amino acids, acylcarnitines, lipids, fatty acids, organic acids, biogenic amines, sugars, alcohols and a variety of other compound classes. To our knowledge, this is the largest multi-metabolite study ever undertaken to analyzefruits and vegetables. We believe that both the extraction and analytical methods developed for this study could be easily applied to analyze other types of foods. Many of the compounds studied in this work were experimentally characterized for the first time as normal constituents for many of the fruits and vegetables selected for this study. For those compounds that had been measured in previously reported studies, we found very good agreement between the concentrations we found and those reported elsewhere. This was somewhat surprising given the expected differences in growing conditions, the varietals used and the measurement techniques.

All of the metabolites that we experimentally identified and/or quantified as well as the metabolites we identified through extensive literature analysis have been deposited into a web-enabled database called Alberta Food Composition Database (AFCDB). The AFCDB contains detailed compound descriptions, extensive chemical composition data, chemical concentration

data, associated references or citations, physico-chemical data, structure data, spectral data as well as data on the known or presumptive health benefits of each compound. The AFCDB is also linked to FooDB (http://foodb.ca), which provides perhaps the world's most complete and detailed information on food composition for another 1000 raw or partially processed foods.

Given the extent of coverage, the high level of reproducibility, the good agreement with prior studies and the ease with which quantitative, multi-metabolite measurements can now be made, we believe that metabolomics can, and should, be used much more widely in food composition analysis. To that end, we hope this study will inspire other researchers to employ quantitative metabolomic methods to characterize more food types and to expand the repertoire of quantitative assays available for food composition analysis.

Figure 2.1 Venn diagram showing the overlap of average fruit/vegetable metabolites detected by global NMR, FAMEs/GC– MS, ICP-MS, HPLC, and DFI/LC-MS/MS methods.

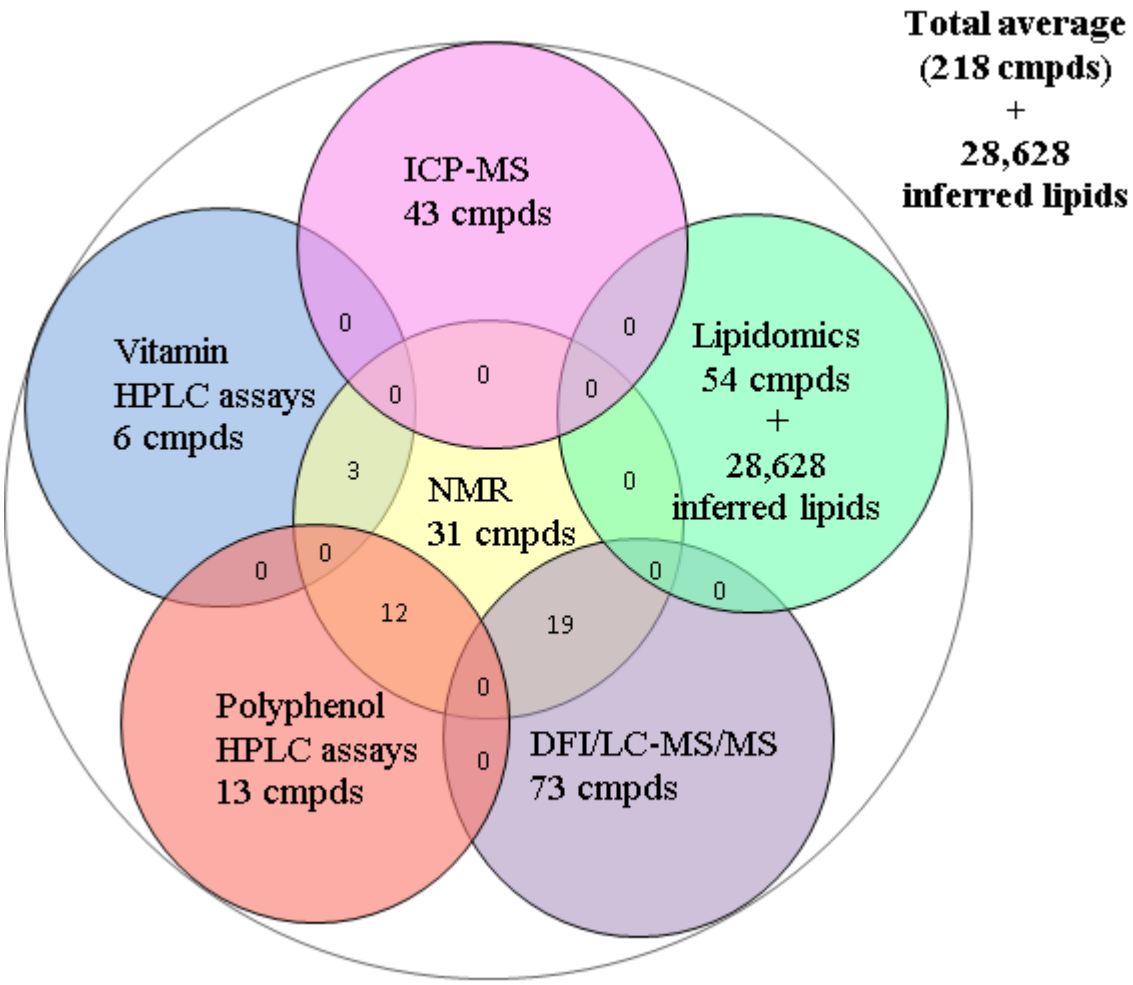


Figure 2.2 AFCDB (http://afcdb.ca) database allowing users to view the contents of the database from either a “FoodView” or a “ChemView”.

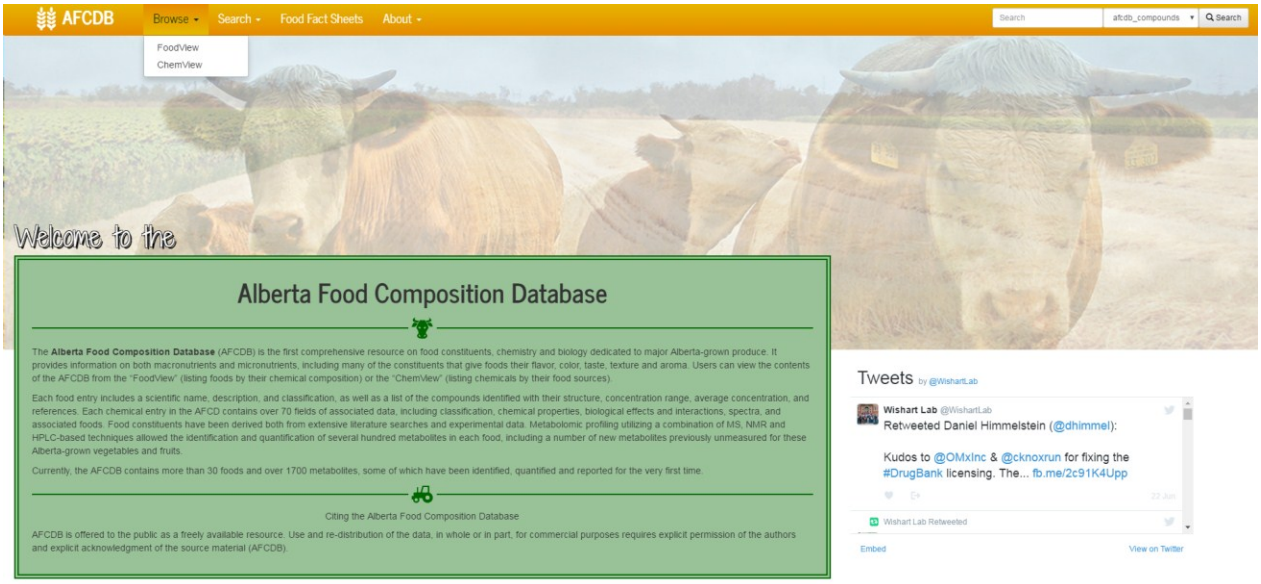


Figure 2.3 A sample of food entry in the AFDCB which provides the scientific name, description, classification, and chemical composition information.

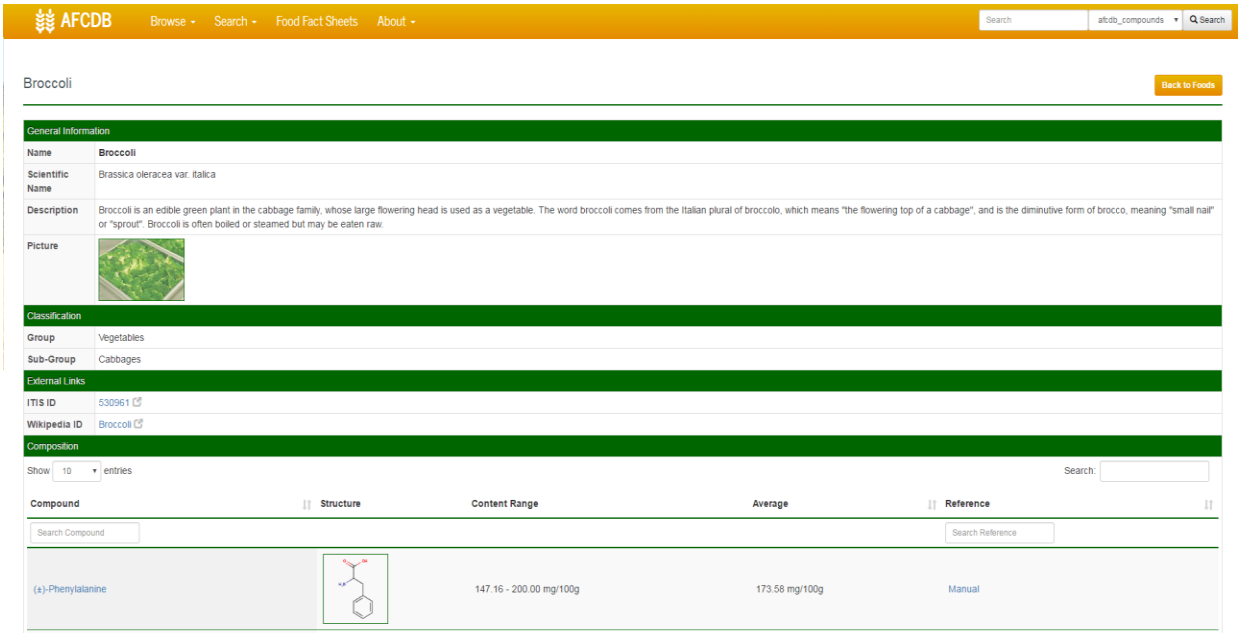


Table 2.1 List of fruits and vegetables selected for chemical and metabolic analysis.

English name	Scientific name	Family name	Analyzed part
Swiss chard	Beta vulgaris	Amaranthaceae	Leaf and stalk
Green bean	Phaseolus vulgaris	Leguminocae	Pod
Yellow wax bean	Phaseolus vulgaris	Leguminocae	Pod
Sunburst squash	Cucurbita pepo	Cucurbitaceae	Fruit with skin
Green bell pepper	Capsicum annuum	Solanaceae	Fruit- seedless
Red bell pepper	Capsicum annuum	Solanaceae	Fruit- seedless
Orange bell pepper	Capsicum annuum	Solanaceae	Fruit- seedless
Yellow bell pepper	Capsicum annuum	Solanaceae	Fruit- seedless
Red beetroot	Beta vulgaris	Amaranthaceae	Root
Spinach	Spinacia oleracea	Amaranthaceae	Leave
Onion	Allium cepa	Amaryllidaceae	Stem
Lettuce	Lactuca sativa	Asteraceae	Leaf
Cauliflower	Brassica oleracea	Brassicaceae	Flower
Parsnip	Pastinaca sativa	Umbelliferae	Root
Garlic	Allium sativum	Alliaceae	Leaf
Turnip	Brassica rapa	Brassicaceae	Root
White cabbage	Brassica oleracea capitata	Brassicaceae	Leaf
Japanese pumpkin	Cucurbita maxima	Cucurbitaceae	Flesh- skinless
Carrot	Daucus carota	Umbelifers	Root
Eggplant	Solanum melongena	Solanaceae	Fruit
Dill	Anethum graveolens	Umbelifers	Leaf
Broccoli	Brassica oleracea var. Italica	Cruciferacea	Flower
Italian sweet red pepper	Capsicum annuum	Solanaceae	Fruit- seedless
Persian cucumber	Cucumis sativus	Cucurbitaceae	Fruit with skin
Yellow zucchini	Cucurbita pepo	Cucurbitaceae	Fruit with skin
Green zucchini	Cucurbita pepo	Cucurbitaceae	Fruit with skin
Russet potato	Solanum tuberosum	Solanaceae	Tuber
Tomato	Solanum lycopersicum	Solanaceae	Fruit
Nanking cherry	Prunus tomentosa	Rosaceae	Fruit- seedless
Saskatoon berry	Amelanchier alnifolia	Rosaceae	Fruit
Raspberry	Rubus idaeus	Rosaceae	Fruit
Crab apple	Malus spp.	Rosaceae	Fruit- seedless

Table 2.2 Details of the gradient for the HPLC method used to determine polyphenols.

Time (min)	%B	%A	Flow rate(mL/min)
0	5	95	1
15	30	70	1
40	40	60	1
60	50	50	1
65	55	45	1
80	100	0	1
85	5	95	1
90	5	95	1

Table 2.3 Comprehensive food composition literature review for selected fruits and vegetables.

Food types	Number of studies	Number of compounds	Reported compounds on FooDB database	Reportded compounds + inferred lipids on FooDB database
Carrot	25	225	2,434	31,062
Onion	28	224	2,000	30,628
Lettuce	33	200	2,113	30,741
Parsnip	9	178	2,160	30,788
Potato	38	215	2,599	31,227
Spinach	37	185	2,276	30,904
Eggplant	41	214	2,219	30,847
Dill	12	214	2,279	30,907
Garlic	24	210	2,100	30,728
Cucumber	22	188	2,258	30,886
Green bean	16	210	2,190	30,818
Turnip	14	202	2,100	30,728
Tomato	39	209	2,176	30,804
Swiss chard	28	172	2,007	30,635
Sunburst squash	3	194	2,140	30,768
Italian red pepper	1	204	2,250	30,878
Japanese pumpkin	11	197	2,132	30,760
White cabbage	27	213	2,241	30,869
Orange bell pepper	21	193	2,310	30,938
Red bell pepper	45	183	2,503	31,131
Yellow bell pepper	26	205	2,527	31,155
Green bell pepper	45	202	2,440	31,068
Broccoli	29	198	2,280	30,908
Red beet root	31	217	2,142	30,770
Cauliflower	24	232	2,065	30,693
Raspberry	29	188	2,097	30,725
Wax bean	5	190	2,093	30,721
Nanking cherry	8	179	1,909	30,537

Table 2.4 Number of detected metabolites in Alberta-grown fruits and vegetables using various assays.

Food types	ICP-MS	DFI/LC-MS/MS	HPLC	GC-MS	NMR
Broccoli	47	76	22	20	31
Carrot	47	79	17	20	31
Cauliflower	39	75	21	56	31
Crab apple	45	61	10	165	29
Dill	49	76	19	165	30
Eggplant	42	60	18	35	38
Garlic	44	89	15	4	32
Green bean	42	81	23	56	28
Green bell pepper	44	71	20	84	32
Green zucchini	40	70	18	84	30
Italian red pepper	40	67	25	84	33
Japanese pumpkin	43	74	14	20	36
Lettuce	42	77	21	56	34
Nanking cherry	45	50	8	56	30
Onion	36	66	14	10	30
Orange bell pepper	35	89	17	20	31
Parsnip	44	59	21	56	32
Persian Cucumber	39	87	23	10	33
Potato	43	64	17	84	32
Raspberry	47	63	6	20	29
Red beet root	52	63	17	35	26
Red bell pepper	35	71	22	20	30
Saskatoon berry	47	65	4	20	30
Spinach	53	78	22	35	30
Sunburst squash	45	89	16	56	30
Swiss chard	43	54	19	35	31
Tomato	43	63	17	10	31
Turnip	45	65	16	84	31
Wax bean	39	78	22	56	31
White cabbage	46	77	16	120	31
Yellow bell pepper	35	103	20	20	31
Yellow zucchini	46	94	17	120	32

Table 2.5 Mineral content of fruits and vegetable as determined by ICP-MS (Conc. mg/100 g FW).

Metabolites	Broccoli	LV[1]	Carrot	LV
Li	0.005 (0.004-0.005)	-	0.00049(0.00048-0.00050)	-
B	1.2 (1.184-1.186)	-	0.47 (0.45-0.48)	-
Na	50.8 (42.3-59.4)	33.0	24.1 (20.8-27.4)	25.0
Mg	34.5 (34.2-34.9)	21.0	9.3(9.1-9.6)	12.0
Al	0.78 (0.73-0.83)	-	0.34 (0.32-0.37)	-
P	88.8 (76.9-100.7)	66.1	18.3 (16.8-19.8)	15.0
K	593.1 (542.3-643.7)	316.0	180.8(173.8-187.8)	170.0
Ca	46.5 (43.7-49.4)	47.00	17.5(17.1-18.1)	25.00
Ti	0.021 (0.0204-0.0215)	-	0.002(0.002-0.003)	-
V	0.0016 (0.0013-0.0019)	-	0.0008(0.0007-0.0010)	-
Cr	0.025 (0.021-0.028)	-	0.012(0.011-0.013)	-
Fe	1.3 (1.13-1.41)	0.73	0.33(0.33-0.34)	0.30
Mn	0.19 (0.15-0.22)	-	0.43(0.43-0.44)	0.50
Co	0.0018 (0.00183-0.00188)	-	0.0004(0.0003-0.0005)	-
Ni	0.014 (0.013-0.015)	-	0.004(0.001-0.007)	-
Cu	0.094 (0.091-0.096)	-	0.020(0.017-0.023)	0.020
Zn	0.49 (0.48-0.51)	0.41	0.25(0.22-0.28)	0.24
Ga	0.0008 (0.0008-0.0009)	-	0.0003(0.0002-0.0005)	-
Ge	0.0001 (0.00009-0.0001)	-	0.00002(0.00002-0.00003)	-
As	0.00044 (0.00043-0.00045)	-	0.0002 (0.0001-0.0002)	-
Se	0.006 (0.005-0.006)	-	0.0007(0.0006-0.0008)	-
Rb	0.75 (0.72-0.77)	-	0.06(0.057-0.058)	-
Sr	0.32 (0.25-0.38)	-	0.09 (0.08-0.11)	-
Y	0.00005(0.00005-0.00005)	-	0.00002(0.00002-0.00003)	-
Zr	0.0022(0.0021-0.0024)	-	0.0008(0.00084-0.00087)	-
Nb	0.00059 (0.00051-0.00067)	-	0.00007(0.00007-0.00008)	-
Mo	0.01 (0.009-0.01)	-	0.0006(0.0004-0.0008)	-
Ru	0.00004(0.00004-0.00004)	-	0.00002(0.00002-0.00002)	-
Pd	0.0008 (0.0006-0.0010)	-	0.00016(0.00016-0.00016)	-
Cd	0.0020 (0.0015-0.0025)	-	0.0010(0.0006-0.0015)	-
Sn	0.031 (0.029-0.032)	-	0.01(0.015-0.018)	-
Sb	0.00010 (0.00009-0.00020)	-	0.00003(0.00003-0.00004)	-
Cs	0.0014 (0.0014-0.0015)	-	0.000054(0.000051-0.000057)	-
Ba	0.10 (0.08-0.12)	-	0.11(0.104-0.106)	-
La	0.00010 (0.00007-0.00013)	-	0.00004(0.00003-0.00005)	-
Ce	0.0003 (0.0002-0.0004)	-	0.00006(0.00005-0.00007)	-
Pr	-	-	-	-

Continued.

[1] LV for Literature value. Literature references are provided in the AFCDB website.

Table 2.5.*Continued.*

Metabolites	Broccoli	LV	Carrot	LV
Nd	0.00005(0.00005-0.00006)	-	-	-
Sm	-	-	-	-
Eu	0.00004(0.00004-0.00005)	-	0.00005(0.00005-0.00005)	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.0003 (0.0002-0.0005)	-	0.00005 (0.00005-0.00006)	-
Ta	0.0007(0.0005-0.0009)	-	0.00013 (0.00012-0.00015)	-
W	0.0052 (0.0052-0.0053)	-	0.0018 (0.0017-0.0018)	-
Re	-	-	-	-
Os	0.0007 (0.0005-0.0009)	-	0.0002(0.0002-0.00022)	-
Pt	0.00021 (0.00020-0.00023)	-	0.00008(0.00008-0.00008)	-
Au	0.00071 (0.00065-0.00077)	-	0.00007(0.00007-0.00007)	-
Tl	0.00035 (0.00032-0.00037)	-	0.0005 (0.0004-0.0006)	-
Pb	0.00026 (0.00016-0.00036)	-	0.00003(0.00003-0.00004)	-
Th	0.00026 (0.00016-0.00036)	-	0.00003(0.00003-0.00004)	-
U	-	-	-	-
Metabolites	**Dill**	**LV**	**Eggplant**	**LV**
Nd	0.00016 (0.00014-0.00017)	-	-	-
Sm	-	-	-	-
Eu	0.00009 (0.00007-0.00010)	-	-	-
Gd	0.00004(0.00004-0.00004)	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.00006(0.00005-0.00008)	-	0.00002 (0.00002-0.00002)	-
Ta	0.0002(0.0002-0.0002)	-	0.00007 (0.00007-0.00008)	-
W	0.002(0.002-0.003)	-	0.0011 (0.0011-0.0012)	-
Re	0.0004(0.0003-0.0004)	-	-	-
Os	0.0004 (0.0003-0.0005)	-	0.00027 (0.00024-0.00030)	-
Pt	0.00013 (0.00012-0.00014)	-	0.00008(0.00008-0.00008)	-
Au	0.00004(0.00004-0.00005)	-	-	-
Tl	0.001 (0.0006-0.0010)	-	0.00014 (0.00008-0.00020)	-
Pb	0.00007(0.00006-0.00008)	-	-	-

Continued.

Table2.5.*Continued.*

Metabolites	Dill	LV	Eggplant	LV
Li	0.007(0.006-0.007)	-	0.0005 (0.0004-0.0005)	-
B	0.65 (0.64-0.66)	-	0.35 (0.33-0.37)	-
Na	36.1 (30.2-42.1)	61.0	0.53 (0.51-0.56)	-
Mg	32.21 (32.16-32.26)	55.0	6.9 (6.6-7.2)	14.0
Al	0.59 (0.54-0.65)	-	0.75 (0.66-0.83)	-
P	32.9 (26.9-38.9)	66.0	15.1(13.7-16.5)	24.0
K	567.4 (560-574.9)	738.0	141.1 (138.1-143.9)	229.0
Ca	169.7 (145.3-194.1)	208.00	9.6(8.8-10.4)	9.00
Ti	0.01 (0.013-0.014)	-	0.0020 (0.0019-0.0021)	-
V	0.001 (0.0011-0.0013)	-	0.0007 (0.0006-0.0007)	-
Cr	0.015 (0.015-0.016)	-	0.006 (0.006-0.007)	-
Fe	0.98 (0.94-1.01)	-	0.22 (0.21-0.22)	0.23
Mn	0.38 (0.37-0.39)	-	0.17 (0.15-0.18)	-
Co	0.001 (0.00113-0.00114)	-	0.00008(0.00007-0.00009)	-
Ni	0.025 (0.021-0.029)	-	0.0025 (0.0024-0.0025)	-
Cu	0.05 (0.049-0.051)	-	0.018 (0.014-0.021)	-
Zn	0.41 (0.39-0.43)	0.91	0.081 (0.076-0.086)	0.16
Ga	0.0004 (0.0003-0.0004)	-	0.00017(0.00016-0.00018)	-
Ge	0.00005(0.00005-0.00006)	-	0.00002(0.00002-0.00002)	-
As	0.0008 (0.00076-0.00083)	-	0.00009 (0.00009-0.0001)	-
Se	0.002 (0.0014-0.0021)	-	0.0004 (0.00035-0.00052)	-
Rb	0.16 (0.15-0.16)	-	0.064 (0.062-0.067)	-
Sr	0.51 (0.414-0.59)	-	0.062(0.051-0.073)	-
Y	0.0001 (0.0001-0.0001)	-	0.00002(0.00002-0.00002)	-
Zr	0.001 (0.0012-0.0014)	-	0.00077(0.00075-0.00078)	-
Nb	0.00009 (0.00006-0.00010)	-	0.00005 (0.00004-0.00007)	-
Mo	0.005 (0.0052-0.0055)	-	0.0024 (0.0022-0.0027)	-
Ru	0.0001 (0.00009-0.00020)	-	0.00003 (0.00003-0.00004)	-
Pd	0.0002 (0.0002-0.0003)	-	0.0001(0.00012-0.00015)	-
Cd	0.009 (0.008-0.009)	-	0.00005 (0.00005-0.00006)	-
Sn	0.021 (0.015-0.026)	-	0.015(0.014-0.016)	-
Sb	0.00007 (0.00007-0.00008)	-	0.00003 (0.00003-0.00004)	-
Cs	0.00006 (0.00006-0.00007)	-	0.00003(0.00003-0.00003)	-
Ba	0.19 (0.15-0.24)	-	0.006 (0.005-0.007)	-
La	0.0002 (0.0002-0.0002)	-	0.00001 (0.00001-0.00002)	-
Ce	0.0003 (0.00035-0.00035)	-	0.00003 (0.00003-0.00004)	-
Pr	0.00004 (0.00004-0.00004)	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Italian red pepper	LV	Russet potato	LV
Ge	-	-	-	-
As	0.00004(0.00003-0.00005)	-	0.0001(0.00007-0.00018)	-
Se	-	-	-	-
Rb	0.10(0.091-0.11)	-	0.25 (0.21-0.29)	-
Sr	0.012 (0.009-0.013)	-	0.03 (0.02-0.04)	-
Y	0.00002 (0.00002-0.00003)	-	0.00005 (0.00004-0.00007)	-
Zr	0.0010 (0.0007-0.0012)	-	0.0018 (0.0014-0.0021)	-
Nb	0.0001 (0.00009-0.0001)	-	0.00008 (0.00008-0.00009)	-
Mo	0.004(0.004-0.005)	-	0.0022(0.0021-0.0022)	-
Ru	0.00003(0.00003-0.00004)	-	0.00010(0.00007-0.00014)	-
Pd	0.0002(0.0002-0.0003)	-	0.0003 (0.0003-0.0004)	-
Cd	-	-	0.0009 (0.0008-0.001)	-
Sn	0.02 (0.01-0.02)	-	0.03(0.03-0.04)	-
Sb	0.00005(0.00004-0.00006)	-	0.0001(0.00010-0.00011)	-
Cs	0.00006 (0.00006-0.00007)	-	0.0003 (0.00024-0.00034)	-
Ba	0.0032(0.0029-0.0035)	-	0.04(0.02-0.05)	-
La	0.00002 (0.00002-0.00003)	-	0.0001 (0.00008-0.0002)	-
Ce	0.00005(0.00004-0.00006)	-	0.0004 (0.0002-0.0005)	-
Pr	-	-	-	-
Nd	-	-	0.00006 (0.00006-0.00007)	-
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.00006 (0.00005-0.00008)	-	0.00009(0.00008-0.00010)	-
Ta	0.00016 (0.00015-0.00017)	-	0.00019(0.00018-0.00019)	-
W	0.0009 (0.0008-0.0010)	-	0.0020(0.0016-0.0023)	-
Re	-	-	-	-
Os	0.0003(0.0002-0.0004)	-	0.00028(0.00027-0.00029)	-
Pt	0.00008 (0.00006-0.00010)	-	0.0002 (0.0001-0.0002)	-
Au	-	-	0.0003 (0.0002-0.0005)	-
Tl	0.0001 (0.0001-0.0002)	-	0.00032 (0.00032-0.00033)	-
Pb	0.00004(0.00003-0.00005)	-	0.00004 (0.00003-0.00006)	-
Th	-	-	-	-
U	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Italian red pepper	LV	Russet potato	LV
Li	0.00094(0.00092-0.00097)	-	0.001 (0.001-0.002)	-
B	0.53 (0.41-0.64)	-	0.86 (0.73-0.98)	-
Na	0.74 (0.56-0.92)	-	1.4 (1.18-1.68)	7.0
Mg	7.3(6.9-7.7)	-	12.2 (10.45-13.87)	17.0
Al	0.37(0.35-0.41)	-	1.04 (0.79-1.29)	-
P	11.8 (10.7-12.8)	-	24.6 (22.5-26.8)	37.0
K	141.2 (138.3-144.1)	-	284.8(235.3-334.4)	360.0
Ca	4.2 (3.5-4.9)	-	5.7 (5.1-6.5)	5.00
Ti	0.0020(0.0018-0.0021)	-	0.0044 (0.0038-0.0051)	-
V	0.0003 (0.0002-0.0003)	-	0.0007 (0.0006-0.0009)	-
Cr	0.01(0.01-0.011)	-	0.019 (0.018-0.021)	-
Fe	0.61 (0.53-0.68)	-	0.79 (0.65-0.94)	0.40
Mn	0.075(0.071-0.079)	-	0.067 (0.058-0.076)	-
Co	0.00006(0.00006-0.00007)	-	0.001 (0.001-0.002)	-
Ni	0.0023(0.0018-0.0029)	-	0.008 (0.006-0.009))	-
Cu	0.018 (0.014-0.021)	-	0.04 (0.03-0.06)	0.080
Zn	0.122(0.121-0.124)	-	0.18 (0.15-0.21)	-
Ga	0.00015(0.00014-0.00016)	-	0.00031 (0.00027-0.00035)	-
Metabolites	**Spinach**	**LV**	**Sunburst squash**	**LV**
Li	0.009 (0.0089-0.0092)	-	0.0005 (0.0005-0.0006)	-
B	0.99 (0.98-1.1)	-	0.29(0.28-0.29)	-
-	67.2 (62.7-71.7)	79.0	0.38 (0.38-0.39)	1.0
Mg	77.4 (70.7-84.1)	79.0	19.4 (19.1-19.7)	23.0
Al	1.2 (0.95-1.51)	-	8.9(8.7-9.07)	-
P	119.5 (113.4-125.6)	49.0	19.9(19.7-20.1)	36.0
K	936.4 (921.4-951.4)	558.0	210.5(210.21-210.8)	182.0
Ca	102.3 (93.9-110.8)	99.00	24.7(24.6-24.8)	19.00
Ti	0.03 (0.03-0.04)	-	0.003 (0.002-0.003)	-
V	0.003 (0.0031-0.0033)	-	0.0017 (0.0017-0.0018)	-
Cr	0.03 (0.025-0.031)	-	0.005(0.005-0.006)	-
Fe	2.9 (2.7-3.1)	2.71	0.29(0.29-0.31)	0.40
Mn	0.58 (0.55-0.62)	-	0.03(0.03-0.04)	-
Co	0.004 (0.0036-0.0037)	-	0.0003 (0.0002-0.0003)	-
Ni	0.03 (0.02-0.03)	-	0.012(0.012-0.013)	-
Cu	0.11 (0.11-0.12)	-	0.030 (0.030-0.031)	-
Zn	0.56 (0.48-0.63)	0.53	0.11(0.11-0.12)	0.29
Ga	0.001 (0.0013-0.0014)	-	0.0006 (0.0006-0.0007)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Spinach	LV	Sunburst squash	LV
Ge	0.00008(0.00008-0.00008)	-	0.00004(0.00004-0.00004)	-
As	0.001 (0.0008-0.001)	-	0.00017 (0.00014-0.0002)	-
Se	0.0006 (0.0006-0.0007)	-	0.0011 (0.0011-0.0012)	-
Rb	0.31 (0.22-0.39)	-	0.144 (0.143-0.144)	-
Sr	0.33 (0.29-0.37)	-	0.194 (0.194-0.195)	-
Y	0.001(0.0008-0.0012)	-	0.00002(0.00002-0.00002)	-
Zr	0.002 (0.0017-0.0028)	-	0.00023(0.00022-0.00024)	-
Nb	0.0003 (0.00016-0.00055)	-	0.00002 (0.00002-0.00003)	-
Mo	0.003 (0.0019-0.0034)	-	0.0021 (0.0021-0.0022)	-
Ru	0.00011 (0.00011-0.00012)	-	0.00004(0.00004-0.00005)	-
Pd	0.0006 (0.0005-0.0008)	-	0.00012(0.00011-0.00013)	-
Cd	0.009 (0.007-0.011)	-	0.00030(0.00028-0.00032)	-
Sn	0.033 (0.029-0.037)	-	0.011 (0.011-0.012)	-
Sb	0.00020(0.00020-0.00021)	-	0.00003 (0.00003-0.00004)	-
Cs	0.00019(0.00018-0.00020)	-	0.00014 (0.00014-0.00014)	-
Ba	0.21 (0.19-0.21)	-	0.0042 (0.0042-0.0043)	-
La	0.0013(0.0011-0.0016)	-	0.000052(0.000051-0.000053)	-
Ce	0.0026 (0.0021-0.0031)	-	0.000072(0.000071-0.000073)	-
Pr	0.00031(0.00025-0.00038)	-	-	-
Nd	0.0013 (0.0011-0.0015)	-	0.00002(0.00002-0.00002)	-
Sm	0.0002 (0.0002-0.0003)	-	-	-
Eu	0.00014(0.00013-0.00016)	-	-	-
Gd	0.00027(0.00021-0.00034)	-	-	-
Dy	0.00018(0.00014-0.00023)	-	-	-
Er	0.00009 (0.00007-0.00012)	-	-	-
Tm	-	-	-	-
Yb	0.00008 (0.00007-0.00010)	-	-	-
Lu	-	-	-	-
Hf	0.00009 (0.00006-0.00013)	-	-	-
Ta	0.00033(0.00031-0.00035)	-	0.00005(0.00004-0.00006)	-
W	0.0025 (0.0017-0.0022)	-	0.00063(0.00063-0.00064)	-
Re	-	-	0.00009(0.00009-0.00009)	-
Os	0.00017(0.00016-0.00018)	-	0.00021(0.00017-0.00026)	-
Pt	0.00016 (0.00014-0.00019)	-	0.000055(0.000050-0.000060)	-
Au	0.00047(0.00041-0.00054)	-	-	-
Tl	0.003 (0.003-0.004)	-	0.00018(0.00017-0.00018)	-
Pb	0.00039(0.00033-0.00045)	-	0.00022(0.00021-0.00023)	-
Th	0.0001 (0.00009-0.0001)	-	-	-
U	0.00011(0.00009-0.00012)	-	0.00005 (0.00005-0.00006)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Tomato	LV	White cabbage	LV
Li	0.00031 (0.00028-0.00033)	-	0.001 (0.0012-0.0017)	-
B	0.28 (0.22-0.33)	-	0.52 (0.29-0.74)	-
Na	1.05 (0.96-1.14)	9.0	6.1 (5.36-6.81)	18.0
Mg	4.6 (4.5-4.7)	7.0	9.5 (9.4-9.5)	12.0
Al	0.26 (0.26-0.26)	-	0.39 (0.36-0.42)	-
P	14.8 (14.5-15.19)	24.0	23.8 (23.3-24.3)	26.0
K	175.6 (163.5-187.7)	250.0	169.4 (164.7-174.1)	170.0
Ca	6.8 (6.4-7.2)	7.00	15.5 (13.7-17.2)	40.00
Ti	0.0015 (0.0013-0.0016)	-	0.005 (0.0052-0.0059)	-
V	0.00035 (0.00032-0.00038)	-	0.00025 (0.00023-0.00028)	-
Cr	0.0056 (0.0046-0.0067)	-	0.0065 (0.0061-0.0069)	-
Fe	0.26 (0.25-0.27)	0.50	0.29 (0.29-0.31)	0.47
Mn	0.065 (0.061-0.065)	-	0.11 (0.112-0.115)	-
Co	0.00004 (0.00004-0.00005)	-	0.002 (0.0019-0.0021)	-
Ni	0.001 (0.001-0.001)	-	0.005 (0.0047-0.0051)	-
Cu	0.012 (0.011-0.014)	0.010	0.01 (0.012-0.014)	-
Zn	0.045 (0.044-0.045)	-	0.092 (0.08-0.10)	0.18
Ga	0.00014 (0.00013-0.00015)	-	0.0002 (0.0002-0.0003)	-
Ge	0.00001 (0.00001-0.00001)	-	0.00001(0.000010-0.000011)	-
As	0.00006 (0.00005-0.00008)	-	0.00008 (0.00008-0.00009)	-
Se	0.00021 (0.00018-0.00024)	-	0.00080 (0.00079-0.00081)	-
Rb	0.035 (0.031-0.039)	-	0.03 (0.033-0.036)	-
Sr	0.008 (0.005-0.01)	-	0.04 (0.03-0.04)	-
Y	0.00001 (0.000010-0.000011)	-	0.00001 (0.00001-0.00002)	-
Zr	0.0005 (0.0004-0.0007)	-	0.00098 (0.00063-0.00133)	-
Nb	0.00008 (0.00007-0.00009)	-	0.00006 (0.00005-0.00007)	-
Mo	0.0042 (0.0042-0.0043)	-	0.006 (0.006-0.006)	-
Ru	0.00001 (0.00001-0.00002)	-	0.00005 (0.00005-0.00006)	-
Pd	0.00018 (0.00018-0.00019)	-	0.0002 (0.0001-0.0002)	-
Cd	0.00002 (0.00002-0.00003)	-	0.00050 (0.00049-0.00052)	-
Sn	0.009 (0.007-0.012)	-	0.012 (0.0099-0.0134)	-
Sb	0.00003 (0.00002-0.00005)	-	0.00003 (0.00003-0.00004)	-
Cs	0.000040 (0.000040-0.000041)	-	0.00005 (0.00005-0.00006)	-
Ba	0.0022 (0.0015-0.0026)	-	0.027 (0.022-0.031)	-
La	0.00001 (0.00001-0.00002)	-	0.00004 (0.00003-0.00005)	-
Ce	0.00003 (0.00002-0.00004)	-	0.00007 (0.00006-0.00008)	-
Pr	-	-	-	-
Nd	-	-	0.00002 (0.00002-0.00003)	-
Sm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Tomato	LV	White cabbage	LV
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.00005 (0.00003-0.00007)	-	0.00004(0.00003-0.00005)	-
Ta	0.00010 (0.00009-0.00012)	-	0.00010(0.00009-0.00012)	-
W	0.0005 (0.0004-0.0006)	-	0.00071 (0.00062-0.00081)	-
Re	-	-	0.00004(0.00003-0.00005)	-
Os	0.00030 (0.00025-0.00034)	-	0.00032(0.00026-0.00036)	-
Pt	0.00005 (0.00004-0.00006)	-	0.00010(0.00005-0.00015)	-
Au	-	-	-	-
Tl	-	-	0.00011(0.00010-0.00012)	-
Pb	0.00009 (0.00005-0.00014)	-	0.00017(0.00017-0.00018)	-
Th	0.00004 (0.00003-0.00005)	-	0.00003(0.00002-0.00004)	-
U	-	-	-	-
Metabolites	**Green bell pepper**	**LV**	**Japanese pumpkin**	**LV**
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.00004(0.00003-0.00005)	-	0.00001 (0.00001-0.00002)	-
Ta	0.00014(0.00011-0.00017)	-	0.0001 (0.00011-0.00012)	-
W	0.0009 (0.0008-0.001)	-	0.00092(0.00087-0.00096)	-
Re	-	-	-	-
Os	0.0003 (0.0003-0.0003)	-	0.00032(0.00029-0.00035)	-
Pt	-	-	-	-
Au	-	-	-	-
Tl	0.00026(0.00026-0.00027)	-	-	-
Pb	0.0002 (0.0002-0.0003)	-	0.0002 (0.0002-0.0003)	-
Th	0.00002 (0.00002-0.00003)	-	-	-
U	-	-	0.00004 (0.00004-0.00005)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Green bell pepper	LV	Japanese pumpkin	LV
Li	0.0051 (0.0049-0.0052)	-	0.00072(0.00058-0.00086)	-
B	0.55 (0.51-0.61)	-	0.48(0.41-0.57)	-
Na	1.1 (0.98-1.18)	3.0	0.58 (0.47-0.68)	-
Mg	8.5 (8.4-8.6)	10.0	13.4 (11.9-14.7)	-
Al	0.31 (0.30-0.31)	-	0.24 (0.16-0.31)	-
P	21.8(21.7-21.9)	20.0	13.3(11.8-14.8)	-
K	175.4 (171.8-178.9)	175.0	201.2(183.6-218.8)	-
Ca	9.9(9.1-10.7)	10.00	12.3 (10.9-13.7)	-
Ti	0.0032(0.0030-0.0033)	-	0.0027(0.0025-0.0029)	-
V	0.0003(0.00030-0.00031)	-	0.00042(0.00037-0.00046)	-
Cr	0.0093(0.0086-0.010)	-	0.011 (0.009-0.012)	-
Fe	0.54 (0.52-0.57)	0.34	0.33(0.29-0.35)	-
Mn	0.072 (0.071-0.074)	-	0.03 (0.025-0.031)	-
Co	0.002(0.0024-0.0025)	-	0.0003 (0.00031-0.00038)	-
Ni	0.021 (0.022-0.023)	-	0.010(0.0069-0.014)	-
Cu	0.061 (0.061-0.062)	-	0.07(0.066-0.079)	-
Zn	0.13 (0.11-0.15)	0.13	0.09 (0.077-0.11)	-
Ga	0.0002(0.00020-0.00021)	-	0.00013(0.00012-0.00015)	-
Ge	0.00001 (0.00001-0.00002)	-	0.00002(0.000020-0.000021)	-
As	0.00022 (0.00019-0.00024)	-	0.00013(0.00011-0.00015)	-
Se	0.0003 (0.0003-0.0003)	-	0.0008 (0.00077-0.001)	-
Rb	0.36 (0.36-0.37)	-	0.06 (0.055-0.065)	-
Sr	0.06 (0.058-0.065)	-	0.035 (0.031-0.038)	-
Y	0.00004(0.000040-0.000041)	-	0.00001(0.000010-0.000011)	-
Zr	0.00080(0.00072-0.00088)	-	0.00030(0.00029-0.00041)	-
Nb	0.00005(0.00004-0.00006)	-	0.00005 (0.00005-0.00006)	-
Mo	0.0018 (0.0017-0.0019)	-	0.0019 (0.0017-0.0021)	-
Ru	0.00006 (0.00006-0.00007)	-	0.00006(0.000060-0.000061)	-
Pd	0.00016(0.00014-0.00018)	-	0.00016(0.00016-0.00016)	-
Cd	0.001 (0.001-0.001)	-	0.0001 (0.0001-0.0001)	-
Sn	0.02 (0.015-0.02)	-	0.016 (0.015-0.017)	-
Sb	0.00005(0.000050-0.000051)	-	0.00005 (0.00004-0.00007)	-
Cs	0.0004(0.00040-0.00041)	-	0.00005(0.00004-0.00006)	-
Ba	0.033 (0.030-0.036)	-	0.02 (0.016-0.02)	-
La	0.00004 (0.00004-0.00005)	-	0.00003 (0.00003-0.00004)	-
Ce	0.00013(0.00012-0.00014)	-	0.0001 (0.00010-0.00014)	-
Pr	-	-	-	-
Nd	0.00003(0.000030-0.000031)	-	0.00002 (0.00002-0.00003)	-
Sm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Red beetroot	LV	Turnip	LV
As	0.00023(0.00019-0.00026)	-	0.0003 (0.0003-0.00031)	-
Se	0.00054(0.00037-0.00071)	-	0.0007 (0.0006-0.0008)	-
Rb	0.138(0.138-0.139)	-	0.21(0.20-0.21)	-
Sr	0.26(0.26-0.27)	-	0.11 (0.110-0.111)	-
Y	0.00032(0.00032-0.00033)	-	0.00005 (0.00005-0.00006)	-
Zr	0.001 (0.00106-0.00108)	-	0.0009(0.00076-0.0011)	-
Nb	0.00005(0.00004-0.00006)	-	0.0001(0.00006-0.00014)	-
Mo	0.002 (0.0019-0.002)	-	0.002 (0.0017-0.0021)	-
Ru	0.00009(0.000090-0.000091)	-	0.0001(0.0001-0.00011)	-
Pd	0.00025(0.00021-0.00029)	-	0.00042(0.00032-0.00053)	-
Cd	0.00092(0.0009-0.00095)	-	0.00057(0.00055-0.00059)	-
Sn	0.01(0.0101-0.0104)	-	0.012 (0.009-0.015)	-
Sb	0.00008(0.000080-0.000081)	-	0.00007 (0.00007-0.00008)	-
Cs	0.0001(0.00011-0.00012)	-	0.0003 (0.0003-0.00032)	-
Ba	0.44 (0.43-0.45)	-	0.11 (0.10-0.11)	-
La	0.0003 (0.00027-0.00028)	-	0.00006 (0.00006-0.00007)	-
Ce	0.0006 (0.00057-0.00058)	-	0.00017(0.00015-0.00019)	-
Pr	0.00008(0.00008-0.00008)	-	-	-
Nd	0.00035(0.00034-0.00036)	-	0.00005(0.000050-0.000051)	-
Sm	0.00009(0.00008-0.0001)	-	-	-
Eu	0.0002 (0.00019-0.0002)	-	0.00005(0.00004-0.00006)	-
Gd	0.00008 (0.00008-0.00009)	-	-	-
Dy	0.00006(0.000060-0.000061)	-	-	-
Er	0.00003(0.000030-0.000031)	-	-	-
Tm	-	-	-	-
Yb	0.00002(0.000020-0.000021)	-	-	-
Lu	-	-	-	-
Hf	0.00004 (0.00004-0.00005)	-	0.00009(0.00006-0.00012)	-
Ta	0.0001(0.00011-0.00014)	-	0.0003 (0.00021-0.00036)	-
W	0.0009 (0.00083-0.00104)	-	0.001 (0.00083-0.0013)	-
Re	-	-	-	-
Os	0.0003 (0.00026-0.00033)	-	0.0006(0.00038-0.00082)	-
Pt	-	-	-	-
Au	-	-	-	-
Tl	0.0003(0.00031-0.00032)	-	0.0003 (0.00027-0.0003)	-
Pb	0.0004(0.00045-0.00046)	-	0.0002(0.00022-0.00029)	-
Th	0.00004(0.00004-0.00004)	-	0.00007 (0.00004-0.00011)	-
U	0.00009(0.000090-0.000091)	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Red beetroot	LV	Turnip	LV
Li	0.021 (0.021-0.022)	-	0.001(0.0011-0.0012)	-
B	0.64 (0.58-0.71)	-	0.71 (0.62-0.79)	-
Na	39.9(39.1-40.8)	72 .8	4.8(4.6-5.1)	41
Mg	35.7 (35.1-36.2)	17.8	10.5(10.4-10.7)	9.5
Al	1.2(1.2-1.3)	-	0.56 (0.48-0.63)	-
P	39.4(39.4-39.5)	51.0	36.7(36.7-36.8)	34.9
K	192.1 (188.5-195.5)	380.0	193.8 (188.6-199.1)	236 .6
Ca	16.7(16.3-17.2)	18.2	29.5(28.4-30.5)	39.1
Ti	0.0054(0.0054-0.0055)	-	0.0068 (0.0065-0.0071)	-
V	0.00070 (0.00067-0.00074)	-	0.0006(0.0006-0.0007)	-
Cr	0.0138(0.0137-0.0139)	-	0.014(0.014-0.015)	-
Fe	0.56 (0.53-0.58)	0.80	0.35(0.31-0.39)	0.25
Mn	0.36(0.35-0.38)	-	0.048(0.046-0.049)	-
Co	0.0013(0.0013-0.0014)	-	0.0003 (0.00030-0.00031)	-
Ni	0.015(0.008-0.022)	-	0.002(0.0021-0.0022)	-
Cu	0.07(0.075-0.078)	0.020	0.018(0.017-0.019)	0.010
Zn	0.21 (0.21 -0.22)	0.35	0.12 (0.123-0.127)	0.27
Ga	0.00038(0.00037-0.00039)	-	0.0003(0.00030-0.00031)	-
Ge	0.00004(0.00003-0.00005)	-	0.00002(0.000020-0.000021)	-
Metabolites	**Yellow zucchini**	**LV**	**Parsnip**	**LV**
Li	0.0007 (0.00066-0.00075)	-	0.001(0.00096-0.00109)	-
B	0.31 (0.31-0.32)	-	0.97(0.91-1.1)	-
Na	0.33 (0.32-0.34)	-	6.7 (6.6-6.7)	10
Mg	26.4 (25.8-26.9)	18.0	29.3 (28.7-29.8)	26.4
Al	0.17 (0.15-0.18)	-	0.66 (0.57-0.75)	-
P	31.9 (30.9-32.8)	38.0	40.4(38.8-42.1)	72.5
K	364.3(354.1-374.6)	261.0	255.8(249.8-261.7)	412.5
Ca	21.1 (19.3-22.7)	16.00	22.8(22.4-23.2)	38.5
Ti	0.003(0.0031-0.0034)	-	0.004 (0.0036-0.0037)	-
V	0.0007 (0.00062-0.00076)	-	0.0005(0.0005-0.00057)	-
Cr	0.0083 (0.0082-0.0085)	-	0.02(0.019-0.027)	-
Fe	0.37 (0.36-0.38)	0.37	0.66(0.59-0.73)	0.595
Mn	0.09(0.095-0.099)	-	0.09(0.07-0.11)	-
Co	0.00038(0.000380-0.000381)	-	0.0006(0.00047-0.00073)	-
Ni	0.01(0.013-0.017)	-	0.02 (0.022-0.025)	-
Cu	0.04(0.045-0.046)	-	0.11 (0.09-0.11)	0.05
Zn	0.19(0.18-0.19)	0.32	0.21 (0.19-0.22)	0.59
Ga	0.00024(0.00023-0.00025)	-	0.0003 (0.00034-0.00036)	-
Ge	0.00003 (0.00003-0.00004)	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Yellow zucchini	LV	Parsnip	LV
As	0.00019(0.00018-0.00019)	-	0.0003 (0.00025-0.00028)	-
Se	0.001 (0.0009-0.001)	-	0.001(0.0014-0.0015)	-
Rb	0.69 (0.67-0.71)	-	0.28 (0.27-0.29)	-
Sr	0.23 (0.22-0.23)	-	0.13 (0.12-0.13)	-
Y	0.00002(0.00002-0.000021)	-	0.00009 (0.00007-0.00012)	-
Zr	0.00017(0.00015-0.00018)	-	0.001 (0.0014-0.0015)	-
Nb	0.00005(0.00004-0.00006)	-	0.00005(0.00005-0.00006)	-
Mo	0.0018 (0.0017-0.0018)	-	0.003 (0.0026-0.0031)	-
Ru	0.0001(0.00011-0.00014)	-	0.00007(0.00006-0.00007)	-
Pd	0.00023(0.00022-0.00024)	-	0.0006 (0.0004-0.0007)	-
Cd	0.0001 (0.00011-0.00011)	-	0.001 (0.001-0.002)	-
Sn	0.008 (0.006-0.009)	-	0.03(0.03-0.04)	-
Sb	0.00004(0.00004-0.000041)	-	0.00006 (0.00004-0.00007)	-
Cs	0.0005 (0.00051-0.00055)	-	0.0005(0.0005-0.00051)	-
Ba	0.02(0.0201-0.0202)	-	0.2 (0.19-0.21)	-
La	0.00004(0.00004-0.000041)	-	0.00007 (0.00007-0.00008)	-
Ce	0.00009 (0.00009-0.0001)	-	0.0001(0.00014-0.00015)	-
Pr	-	-	-	-
Nd	0.00003(0.00003-0.000031)	-	0.00006(0.00005-0.00007)	-
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.00002 (0.00002-0.00003)	-	0.00008(0.000080-0.000081)	-
Ta	0.0001(0.00012-0.00013)	-	0.0002 (0.00021-0.00022)	-
W	0.0006(0.0006-0.0007)	-	0.001(0.00145-0.00157)	-
Re	0.0001(0.00010-0.00011)	-	-	-
Os	0.0003(0.0003-0.0004)	-	0.00012 (0.00011-0.00012)	-
Pt	-	-	0.0001 (0.000120-0.000121)	-
Au	-	-	-	-
Tl	0.0001(0.00006-0.00015)	-	0.0004(0.00040-0.00047)	-
Pb	0.00009(0.00002-0.00016)	-	0.0004 (0.00037-0.0004)	-
Th	0.00008(0.00001-0.00015)	-	0.00004(0.000040-0.000041)	-
U	0.0001 (0.00010-0.00016)	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	White onion	LV	Green zucchini	LV
Li	0.002 (0.0021-0.0022)	-	0.0005 (0.00051-0.00053)	-
B	1.1 (0.93-1.1)	-	0.56 (0.55-0.56)	-
Na	3.3(3.2-3.4)	4.00	0.68(0.63-0.73)	8.00
Mg	11.7 (10.7-12.6)	10.00	19.4 (17.9-20.8)	18.00
Al	0.3 (0.21-0.37)	-	0.17 (0.16-0.17)	-
P	34.8(32.2-37.4)	29.00	32.3 (30.6-33.9)	38.00
K	165.5(149.3-181.7)	146.00	198.9(194.5-203.4)	261.00
Ca	20.1 (16.1-24.1)	23.00	16.5 (16.1-16.8)	16.00
Ti	0.005 (0.004-0.005)	-	0.001 (0.0014-0.0016)	-
V	0.0003 (0.00025-0.00027)	-	0.00007 (0.00007-0.00008)	-
Cr	0.02 (0.011-0.021)	-	0.007 (0.006-0.007)	-
Fe	0.32 (0.29-0.35)	0.21	0.35 (0.31-0.39)	0.37
Mn	0.07(0.06-0.08)	-	0.07 (0.075-0.077)	-
Co	0.0003(0.0003-0.0004)	-	0.0003 (0.00027-0.00028)	-
Ni	0.005(0.005-0.006)	-	0.01 (0.009-0.012)	-
Cu	0.03(0.025-0.036)	-	0.03 (0.031-0.032)	-
Zn	0.16(0.13-0.21)	-	0.19 (0.18-0.21)	0.32
Ga	0.0002 (0.00021-0.00023)	-	0.00014 (0.00014-0.00015)	-
Ge	-	-	-	-
As	0.0003 (0.00023-0.00036)	-	0.00008 (0.00007-0.0001)	-
Se	0.0005 (0.0004-0.0005)	-	0.0004 (0.00037-0.00038)	-
Rb	0.02 (0.014-0.018)	-	0.065(0.062-0.069)	-
Sr	0.1(0.08-0.11)	-	0.045(0.042-0.047)	-
Y	-	-	-	-
Zr	0.0006 (0.0005-0.0007)	-	0.00013(0.00013-0.00014)	-
Nb	0.0008 (0.00078-0.00079)	-	0.00044(0.00021-0.00067)	-
Mo	0.001 (0.0013-0.0014)	-	0.001 (0.0011-0.0016)	-
Ru	-	-	-	-
Pd	0.0006 (0.00057-0.00068)	-	0.0004 (0.0003-0.0006)	-
Cd	0.0003 (0.0003-0.0004)	-	0.00006 (0.00006-0.00007)	-
Sn	0.003 (0.0013-0.006)	-	0.0043(0.0036-0.0049)	-
Sb	0.00005(0.00005-0.00006)	-	-	-
Cs	-	-	0.00007(0.00007-0.000071)	-
Ba	0.05011(0.04165-0.05857)	-	0.02(0.019-0.022)	-
La	-	-	0.00002 (0.00002-0.00003)	-
Ce	0.00006(0.00005-0.00007)	-	0.00004(0.00004-0.00005)	-
Pr	-	-	-	-
Nd	-	-	0.00002(0.00002-0.000021)	-

Continued.

Table 2.5.*Continued.*

Metabolites	White onion	LV	Green zucchini	LV
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	-	-	0.00017(0.00016-0.00018)	-
Ta	0.0018 (0.0017-0.0019)	-	0.0005 (0.0004-0.0007)	-
W	0.0004 (0.0002-0.0006)	-	0.00018(0.00017-0.0002)	-
Re	-	-	0.00002 (0.00002-0.00003)	-
Os	0.001 (0.0007-0.002)	-	0.0002 (0.0001-0.0002)	-
Pt	-	-	0.00002(0.00002-0.00003)	-
Au	0.007(0.0050.009)	-	0.003 (0.002-0.004)	-
Tl	-	-	-	-
Pb	0.0004 (0.00034-0.00038)	-	0.00016(0.00016-0.00017)	-
Th	-	-	-	-
U	-	-	-	-
Metabolites	**Yellow bell pepper**	**LV**	**Red bell pepper**	**LV**
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	-	-	-	-
Ta	0.00070(0.00067-0.00074)	-	0.00084(0.00079-0.00089)	-
W	0.00020(0.00015-0.00025)	-	0.00023(0.00021-0.00025)	-
Re	-	-	-	-
Os	0.00029(0.00025-0.00033)	-	0.0002(0.0001-0.0002)	-
Pt	0.00002(0.00001-0.00002)	-	0.00002(0.00001-0.00002)	-
Au	0.004 (0.003-0.005)	-	0.004(0.002-0.005)	-
Tl	-	-	-	-
Pb	0.00034(0.00032-0.00036)	-	0.0004(0.0003-0.0005)	-
Th	-	-	-	-
U	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Yellow bell pepper	LV	Red bell pepper	LV
Li	0.002(0.0019-0.0022)	-	0.002 (0.0014-0.0018)	-
B	1.1 (1.09-1.1)	-	0.71 (0.64-0.76)	-
Na	1.6 (1.5-1.6)	2.00	1.1(1.1-1.2)	4.00
Mg	17.8(17.3-18.4)	12.00	13.8 (13.6-13.9)	12.00
Al	0.29(0.25-0.33)	-	0.21(0.19-0.23)	-
P	24.6(24.2-24.9)	24.00	27.2 (25.4-29.1)	26.00
K	291.2 (283.7-298.7)	212.00	241.6(234.4-248.8)	-
Ca	13.1(13.09-13.14)	11.00	7.3(7.3-7.4)	7.00
Ti	0.003 (0.0024-0.0031)	-	0.002 (0.0018-0.0021)	-
V	-	-	-	-
Cr	0.02 (0.015-0.016)	-	0.01(0.011-0.013)	-
Fe	0.12 (0.11-0.12)	0.17	0.1(0.11-0.13)	0.43
Mn	0.17(0.16-0.18)	-	0.1(0.11-0.12)	-
Co	0.0003 (0.00026-0.00029)	-	0.0002 (0.0001-0.0002)	-
Ni	0.01 (0.010-0.011)	-	0.0032(0.0026-0.0036)	-
Cu	0.04 (0.033-0.041)	-	0.027(0.026-0.028)	-
Zn	0.19(0.16-0.22)	0.25	0.11 (0.10-0.11)	-
Ga	0.00020(0.00017-0.00023)	-	0.0001(0.00012-0.00019)	-
Ge	-	-	-	-
As	0.00008 (0.00008-0.00009)	-	0.00008 (0.00008-0.00009)	-
Se	-	-	-	-
Rb	0.06 (0.060-0.064)	-	0.05 (0.049-0.053)	-
Sr	0.05 (0.052-0.053)	-	0.04(0.043-0.046)	-
Y	-	-	-	-
Zr	0.004 (0.003-0.005)	-	0.004 (0.0026-0.0049)	-
Nb	0.001 (0.0009-0.0013)	-	0.00052(0.00037-0.00067)	-
Mo	0.005 (0.005-0.006)	-	0.0028 (0.0027-0.0029)	-
Ru	-	-	-	-
Pd	0.00058(0.00057-0.0006)	-	0.0004 (0.0003-0.0004)	-
Cd	0.00005 (0.00004-0.00007)	-	0.00006(0.00005-0.00006)	-
Sn	0.003 (0.002-0.003)	-	0.003 (0.002-0.003)	-
Sb	-	-	-	-
Cs	0.00004 (0.00004-0.00005)	-	0.00003 (0.00003-0.00004)	-
Ba	0.006 (0.005-0.007)	-	0.004 (0.004-0.005)	-
La	-	-	-	-
Ce	0.00005 (0.00005-0.00006)	-	0.00005(0.00004-0.00005)	-
Pr	-	-	-	-
Nd	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Orange bell pepper	LV	Persian cucumber	LV
Ge	-	-	-	-
As	0.0001 (0.00012-0.00013)	-	0.00004 (0.00004-0.00005)	-
Se	-	-	0.00014(0.00012-0.00016)	-
Rb	0.071(0.069-0.074)	-	0.056(0.055-0.057)	-
Sr	0.032(0.031-0.033)	-	0.29(0.28-0.29)	-
Y	-	-	-	-
Zr	0.004(0.004-0.005)	-	0.001(0.001-0.0012)	-
Nb	0.003 (0.00031-0.00032)	-	0.00024(0.00021-0.00026)	-
Mo	0.004 (0.003-0.004)	-	0.0023 (0.0021-0.0025)	-
Ru	-	-	-	-
Pd	0.0005 (0.0004-0.0006)	-	0.00043(0.00033-0.00053)	-
Cd	0.00008(0.00007-0.00008)	-	0.00002 (0.00002-0.00003)	-
Sn	0.005 (0.004-0.005)	-	0.00059(0.00044-0.00074)	-
Sb	-	-	0.00001(0.00001-0.000011)	-
Cs	0.00006(0.00005-0.00006)	-	0.00004(0.00003-0.00004)	-
Ba	0.005(0.004-0.005)	-	0.01(0.01-0.011)	-
La	-	-	-	-
Ce	0.00008 (0.00008-0.00009)	-	0.00003(0.00002-0.00003)	-
Pr	-	-	-	-
Nd	-	-	-	-
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	-	-	-	-
Ta	0.0008 (0.0008-0.0009)	-	0.00039 (0.00037-0.00041)	-
W	0.0002 (0.0001-0.0002)	-	0.0004 (0.0003-0.0005)	-
Re	-	-	-	-
Os	0.0002 (0.0001-0.0002)	-	0.0009 (0.0004-0.0015)	-
Pt	0.00002(0.00001-0.00002)	-	0.00001(0.00001-0.000011)	-
Au	0.004 (0.002-0.005)	-	0.001 (0.0012-0.0019)	-
Tl	-	-	0.00003(0.00002-0.00003)	-
Pb	0.00038(0.0003-0.00047)	-	0.0009 (0.0009-0.001)	-
Th	-	-	-	-
U	-	-	0.00002(0.00002-0.00002)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Orange bell pepper	LV	Persian cucumber	LV
Li	0.002 (0.001-0.0012)	-	0.001(0.001-0.002)	-
B	1.3 (1.2-1.4)	-	0.48 (0.43-0.53)	-
Na	1.9 (1.7-2.2)	-	1.1 (1.0-1.1)	2.00
Mg	13.9 (13.1-14.7)	-	11.1 (11.0-11.1)	13.00
Al	0.39 (0.38-0.40)	-	0.13 (0.09-0.16)	-
P	27.2 (25.3-29.0)	-	26.9 (25.2-28.7)	24.00
K	315.0 (305.1-325.0)	-	135.7 (133.2-138.2)	147.00
Ca	7.2 (6.8-7.6)	-	14.3 (13.9-14.7)	16.00
Ti	0.003 (0.003-0.003)	-	0.001 (0.001-0.002)	-
V	-	-	-	-
Cr	0.02 (0.01-0.02)	-	0.005 (0.005-0.005)	-
Fe	0.15 (0.15-0.16)	-	0.23 (0.20-0.26)	0.28
Mn	0.13 (0.13-0.13)	-	0.11 (0.11-0.11)	-
Co	0.0003 (0.0003-0.0003)	-	0.00005 (0.00005-0.00005)	-
Ni	0.009 (0.005-0.01)	-	0.001 (0.0007-0.002)	-
Cu	0.04 (0.04-0.04)	-	0.02 (0.02-0.02)	-
Zn	0.17 (0.17-0.17)	-	0.14 (0.11-0.16)	0.20
Ga	0.0003 (0.0002-0.0003)	-	0.0001 (0.0001-0.0002)	-
Metabolites	**Romaine lettuce**	**LV**	**Swiss chard**	**LV**
Li	0.01 (0.01-0.01)	-	0.37 (0.34-0.40)	-
B	0.57 (0.41-0.73)	-	2.3 (2.2-2.4)	-
-	15.5 (14.8-16.3)	15.5	110.1 (105.6-114.6)	-
Mg	20.0 (18.9-21.1)	9.5	78.7 (68.0-89.4)	-
Al	0.23 (0.21-0.25)	-	0.68 (0.64-0.71)	-
P	13.3 (10.8-15.7)	28	141.3 (139.7-142.8)	-
K	131.4 (122.9-139.9)	207.2	312.2 (302.8-321.5)	-
Ca	46.1 (43.9-48.3)	32.5	27.0 (26.1-28.0)	-
Ti	0.002 (0.002-0.003)	-	0.02 (0.02-0.02)	-
V	0.0002 (0.0002-0.0002)	-	0.003 (0.002-0.003)	-
Cr	0.007 (0.007-0.007)	-	0.04 (0.04-0.04)	-
Fe	0.51 (0.51-0.51)	0.78	2.4 (2.2-2.5)	-
Mn	0.15 (0.15-0.15)	0.1	0.25 (0.22-0.27)	-
Co	0.0004 (0.0004-0.0004)	-	0.002 (0.002-0.002)	-
Ni	0.003 (0.003-0.003)	-	0.001 (0.001-0.001)	-
Cu	0.05 (0.05-0.05)	0.01	0.21 (0.20-0.23)	-
Zn	0.16 (0.15-0.17)	0.18	0.56 (0.54-0.58)	-
Ga	0.0001 (0.0001-0.0001)	-	0.0009 (0.0009-0.0009)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Romaine lettuce	LV	Swiss chard	LV
Ge	-	-	0.0002 (0.0001-0.0002)	-
As	0.0002 (0.0001-0.0002)	-	-	-
Se	0.0005 (0.0004-0.0007)	-	0.002 (0.001-0.002)	-
Rb	0.22 (0.21-0.22)	-	0.19 (0.18-0.19)	-
Sr	0.33 (0.30-0.36)	-	0.14 (0.11-0.17)	-
Y	-	-	0.00005 (0.00004-0.00005)	-
Zr	0.001 (0.0007-0.001)	-	0.003 (0.003-0.003)	-
Nb	0.0001 (0.0001 -0.0001)	-	0.0003 (0.0002-0.0003)	-
Mo	0.001(0.001-0.001)	-	0.05 (0.05-0.05)	-
Ru	-	-	-	-
Pd	0.0005 (0.0004-0.0006)	-	0.005 (0.004-0.006)	-
Cd	0.003 (0.003-0.003)	-	0.0005 (0.0005-0.0006)	-
Sn	0.0004 (0.0003-0.0004)	-	0.01(0.009-0.01)	-
Sb	0.00003 (0.00002-0.00003)	-	0.0002 (0.0002-0.0003)	-
Cs	0.0006 (0.0006-0.0006)	-	0.0001 (0.0001-0.0001)	-
Ba	0.05 (0.05-0.05)	-	0.30 (0.27-0.33)	-
La	0.0001 (0.0001-0.0001)	-	0.00003 (0.00003-0.00003)	-
Ce	0.0002 (0.0002-0.0002)	-	0.00008 (0.00006-0.00009)	-
Pr	-	-	-	-
Nd	0.0001 (0.0001-0.0001)	-	-	-
Sm	-	-	-	-
Eu	-	-	0.00009 (0.00008-0.00009)	-
Gd	-	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	-	-	0.0002 (0.0002-0.0002)	-
Ta	0.0005 (0.0003-0.0006)	-	0.0002 (0.0002-0.0003)	-
W	0.0005 (0.0002-0.0007)	-	0.004 (0.003-0.004)	-
Re	0.0001 (0.0001-0.0001)	-	-	-
Os	0.001 (0.001-0.002)	-	0.003 (0.003-0.003)	-
Pt	0.00001 (0.00001-0.00001)	-	0.0004 (0.0004-0.0004)	-
Au	0.003 (0.002-0.004)	-	-	-
Tl	0.00006 (0.00006-0.00006)	-	0.00009 (0.00008-0.0001)	-
Pb	0.0007 (0.0005-0.0009)	-	0.0005 (0.0005-0.0006)	-
Th	-	-	-	-
U	-	-	0.0001 (0.0001-0.0001)	-

Continued.

Table 2.5.*Continued.*

Metabolites	Cauliflower	LV	Green bean	LV
Li	0.001 (0.001-0.001)	-	0.0009 (0.0009-0.0009)	-
B	0.44 (0.42 -0.47)	-	0.89 (0.88-0.90)	-
Na	10.9 (10.7-11.3)	30	1.2 (1.2-1.2)	1.70
Mg	14.7 (14.4-14.9)	15.00	28.2 (27.9-28.6)	17.00
Al	0.09 (0.09-0.1)	-	0.22 (0.22-0.23)	-
P	30.9 (30.6-31.2)	44.00	45.6 (44.6-46.6)	39.00
K	339.1 (329.4-348.9)	299.00	365.9 (362.9-368.9)	237.00
Ca	25.9 (25.1-26.7)	22.00	45.2 (42.6-47.8)	60.00
Ti	0.003 (0.003-0.003)	-	0.002 (0.002-0.002)	-
V	0.00008 (0.00006-0.00009)	-	-	-
Cr	0.01(0.009-0.01)	-	0.02(0.01-0.02)	0.001
Fe	-	0.42	0.89(0.85-0.94)	1.00
Mn	0.12 (0.12-0.12)	-	0.23 (0.23-0.23)	0.25
Co	0.0009 (0.0009-0.0009)	-	0.003 (0.003-0.003)	-
Ni	0.005 (0.005-0.005)	-	0.05 (0.05-0.05)	0.014
Cu	0.05 (0.05-0.05)	-	0.05 (0.05-0.05)	0.057
Zn	0.28 (0.27-0.28)	0.27	0.36 (0.36-0.37)	0.39
Ga	0.0002 (0.0002-0.0002)	-	0.0004 (0.0004-0.0004)	-
Ge	0.00003 (0.00002-0.00003)	-	0.00008 (0.00007-0.00008)	-
As	-	-	-	-
Se	0.001 (0.001-0.001)	-	-	-
Rb	0.05 (0.05-0.05)	-	0.14 (0.14-0.14)	-
Sr	0.07 (0.06-0.07)	-	0.15 (0.15-0.15)	-
Y	0.00002 (0.00001-0.00002)	-	0.00009 (0.00009-0.00009)	-
Zr	0.0002 (0.0002-0.0002)	-	0.001 (0.001-0.001)	-
Nb	0.00005 (0.00004-0.00005)	-	0.0004 (0.0004-0.0004)	-
Mo	0.005 (0.005-0.005)	-	0.08 (0.08-0.08)	-
Ru	0.00005 (0.00004-0.00005)	-	0.0002 (0.0002-0.0002)	-
Pd	0.0004 (0.0004-0.0004)	-	0.002 (0.002-0.002)	-
Cd	0.001 (0.001-0.001)	-	0.00004 (0.00004-0.00004)	-
Sn	0.004 (0.002-0.005)	-	0.03(0.03-0.04)	-
Sb	0.00004 (0.00003-0.00004)	-	-	-
Cs	0.00008 (0.00008-0.00008)	-	0.00006 (0.00006-0.00006)	-
Ba	0.03 (0.03-0.03)	-	0.06 (0.06-0.06)	-
La	0.00002 (0.00001-0.00002)	-	0.0001 (0.0001-0.0001)	-
Ce	0.00003 (0.00002-0.00003)	-	0.0002 (0.0002-0.0002)	-
Pr	-	-	0.00003 (0.00003-0.00003)	-
Nd	-	-	0.0001 (0.0001-0.0001)	-
Sm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Cauliflower	LV	Green bean	LV
Eu	-	-	0.00004 (0.00003-0.00004)	-
Gd	-	-	0.00003 (0.00003-0.00003)	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	-	-	0.0004 (0.0003-0.0005)	-
Ta	0.00005 (0.00004-0.00005)	-	0.0006 (0.0005-0.0006)	-
W	0.002 (0.002-0.002)	-	0.005 (0.005-0.005)	-
Re	-	-	-	-
Os	0.002 (0.002-0.002)	-	0.006 (0.006-0.006)	-
Pt	0.0001 (0.00009-0.0001)	-	0.0002 (0.0002-0.0003)	-
Au	-	-	-	-
Tl	-	-	-	-
Pb	0.0007 (0.0007-0.0008)	-	0.0004 (0.0004-0.0004)	-
Th	-	-	-	-
U	-	-	-	-
Metabolites	**Saskatoon berry**	**LV**	**Crab apple**	**LV**
Al	6.9 (6.7-7.1)	12	9.9 (9.6-10.2)	11
P	76.3 (73.0-79.6)	77.00	115.9 (115.2-116.8)	107
K	-	-	0.0006 (0.0006-0.0006)	-
V	0.01 (0.009-0.01)	-	0.02 (0.02-0.02)	-
Cr	0.19 (0.19-0.19)	0.28	0.05 (0.05-0.05)	0.12
Fe	0.12 (0.11-0.12)	-	0.06 (0.05-0.06)	-
Mn	0.0006 (0.0006-0.0006)	-	0.0005 (0.0004-0.0005)	-
Co	0.008 (0.007-0.009)	-	0.007 (0.006-0.009)	-
Ni	0.03 (0.02-0.03)	-	0.04 (0.03-0.04)	-
Cu	22.4 (22.2-22.6)	6.00	7.1 (7.0-7.2)	6
Ca	0.09 (0.09-0.09)	0.16	0.05 (0.04-0.06)	0.04
Zn	0.0003 (0.0003-0.0004)	-	0.0004 (0.0003-0.0005)	-
Zr	0.26 (0.25-0.28)	-	0.06 (0.06-0.06)	-
Ba	-	-	-	-
Er	0.00006 (0.00006-0.00007)	-	0.00009 (0.00008-0.00009)	-
Pt	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Saskatoon berry	LV	Crab apple	LV
Au	0.00009 (0.00008-0.0001)	-	0.0001 (0.0001-0.0001)	-
Ga	0.00001 (0.00001-0.00001)	-	0.00001 (0.00001-0.00001)	-
Ge	-	-	-	-
As	0.00006 (0.00006-0.00006)	-	-	-
Se	0.05 (0.04-0.05)	-	0.04 (0.04-0.04)	-
Rb	0.07 (0.07-0.07)	-	0.03 (0.03-0.03)	-
Sr	0.00006 (0.00005-0.00007)	-	0.00001 (0.00001-0.00001)	-
Y	0.002 (0.002-0.002)	-	0.001(0.001-0.001)	-
Mo	0.00003 (0.00003-0.00004)	-	0.00009 (0.00009-0.0001)	-
Ru	0.0005 (0.0004-0.0007)	-	0.001 (0.001-0.002)	-
Pd	0.0006 (0.0006-0.0007)	-	0.00004 (0.00004-0.00004)	-
Cd	0.002 (0.002-0.003)	-	0.003 (0.001-0.004)	-
Sn	0.00002 (0.00002-0.00002)	-	0.00003 (0.00003-0.00004)	-
Sb	0.00006 (0.00006-0.00007)	-	0.00005 (0.00005-0.00006)	-
Cs	0.00012(0.00011-0.00014)	-	0.00006 (0.00005-0.00007)	-
Ce	0.00001 (0.00001-0.00002)	-	-	-
Pr	0.00004 (0.00002-0.00006)	-	0.00002 (0.00002-0.00002)	-
Nd	-	-	-	-
Sm	0.00007 (0.00007-0.00007)	-	0.00001 (0.00001-0.00002)	-
Eu	0.00002 (0.00001-0.00002)	-	-	-
Gd	0.00001 (0.00001-0.00001)	-	-	-
Dy	-	-	-	-
Yb	-	-	-	-
Lu	0.00004 (0.00004-0.00004)	-	0.00009 (0.00007-0.0001)	-
Hf	0.00003 (0.00002-0.00005)	-	0.0002 (0.0001-0.0002)	-
Ta	0.0002(0.0001-0.0002)	-	0.0002 (0.0001-0.0003)	-
W	-	-	-	-
Re	0.0004 (0.0002-0.0006)	-	0.002 (0.002-0.002)	-
Os	-	-	-	-
Tl	0.0007 (0.0006-0.0008)	-	0.001 (0.001-0.001)	-
Pb	-	-	-	-
Th	0.00001 (0.00001-0.00001)	-	0.00002 (0.00002-0.00003)	-
U	0.0009 (0.0008-0.001)	-	0.0009 (0.0006-0.001)	-
Ti	0.00002 (0.00001-0.00002)	-	0.00005 (0.00005-0.00006)	-
Nb	0.00007 (0.00006-0.00007)	-	0.00004 (0.00003-0.00005)	-
La	-	-	-	-
Tm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Saskatoon berry	LV	Crab apple	LV
Be	-	-	0.00004 (0.00003-0.00004)	-
Ag	-	-	-	-
Te	-	-	-	-
Tb	-	-	-	-
Ho	-	-	-	-
Ir	0.60 (0.57-0.63)	-	0.91 (0.89-0.94)	-
Li	0.44 (0.44-0.46)	-	0.50 (0.48-0.52)	-
B	0.47 (0.46.48)	1.00	0.59 (0.59-0.60)	-
Na	9.5 (9.0-10.0)	6	4.9 (4.7-5.2)	1
Mg	0.11 (0.10-0.12)	-	4.5 (4.4-4.5)	5
Metabolites	**Nanking cherry**	**LV**	**Raspberry**	**LV**
Be	-	-	-	-
Ag	-	-	-	-
Te	-	-	-	-
Tb	-	-	-	-
Ho	0.00005 (0.00005-0.00006)	-	0.00002 (0.00001-0.00002)	-
Ir	2.3 (2.3-2.4)	-	0.21 (0.21-0.21)	-
Li	1.1 (0.94-1.3)	-	0.77 (0.75-0.79)	-
B	1.3 (1.1-1.6)	-	1.3 (1.2-1.4)	1.00
Na	10.8 (10.6-11.1)	11	17.6 (16.9-18.3)	20.5
Mg	3.9 (3.7-4.1)	-	0.99 (0.94-1.03)	-
Al	23.7 (21.5-25.8)	21	22.9 (21.1-24.8)	29
P	399.2 (384.9-413.5)	222.1	172.8 (161.4-184.2)	160.5
K	0.0002 (0.0002-0.0003)	-	-	-
V	0.04 (0.04-0.04)	-	0.02 (0.02-0.02)	-
Cr	0.53 (0.52-0.54)	0.36	0.38 (0.32-0.44)	0.69
Fe	0.23 (0.21-0.24)	-	0.27 (0.26-0.27)	-
Mn	0.0006 (0.0005-0.0007)	-	0.0006 (0.0006-0.0006)	-
Co	0.03 (0.03-0.03)	-	0.02 (0.02-0.02)	-
Ni	0.07 (0.07-0.07)	-	0.06 (0.05-0.06)	0.1
Cu	17.9 (17.2-18.5)	13.00	33.3 (32.2-34.4)	25.00
Ca	0.14 (0.13-0.15)	0.07	0.31 (0.27-0.36)	0.42
Zn	0.0009 (0.0006-0.001)	-	0.001(0.0009-0.001)	-
Zr	0.12 (0.11-0.12)	-	0.13 (0.13-0.14)	-
Ba	-	-	-	-
Er	0.0002 (0.0001-0.0002)	-	0.0001 (0.0001-0.0002)	-
Pt	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Nanking cherry	LV	Raspberry	LV
Au	0.0007 (0.0006-0.0008)	-	0.0002 (0.0002-0.0003)	-
Ga	0.00005 (0.00005-0.00005)	-	0.00003 (0.00003-0.00003)	-
Ge	-	-	-	-
As	-	-	0.00005 (0.00004-0.00005)	-
Se	0.22 (0.21-0.22)	-	0.12 (0.09-0.14)	-
Rb	0.08 (0.07-0.08)	-	0.13 (0.12-0.14)	-
Sr	0.00009 (0.00008-0.00009)	-	0.0001 (0.0001-0.0001)	-
Y	0.001 (0.0008-0.001)	-	0.008 (0.008-0.008)	-
Mo	0.0002 (0.0001-0.0002)	-	-	-
Ru	0.0008 (0.0007-0.0009)	-	0.001 (0.0008-0.002)	-
Pd	0.0004 (0.0003-0.0006)	-	0.0002 (0.0002-0.0003)	-
Cd	0.0004 (0.0003-0.0004)	-	0.002 (0.001-0.002)	-
Sn	0.00003 (0.00003-0.00003)	-	0.00003 (0.00002-0.00003)	-
Sb	0.0001 (0.00009-0.0002)	-	0.0001 (0.0001-0.0001)	-
Cs	0.0001 (0.00009-0.0001)	-	0.0003 (0.0003-0.0004)	-
Ce	-	-	0.00003 (0.00003-0.00004)	-
Pr	0.00004 (0.00003-0.00005)	-	0.0001 (0.0001-0.0002)	-
Nd	-	-	-	-
Sm	0.00003 (0.00003-0.00004)	-	0.00005 (0.00005-0.00005)	-
Eu	-	-	0.00003 (0.00003-0.00003)	-
Gd	-	-	0.00002 (0.00002-0.00002)	-
Dy	-	-	-	-
Yb	-	-	-	-
Lu	0.0001 (0.0001-0.0001)	-	0.00008 (0.00004-0.0001)	-
Hf	0.0001 (0.00009-0.0002)	-	0.0001 (0.0001-0.0001)	-
Ta	0.0003 (0.0002-0.0004)	-	0.0002 (0.0002-0.0002)	-
W	-	-	-	-
Re	0.0009 (0.0009-0.0009)	-	0.0003 (0.0002-0.0003)	-
Os	0.00003 (0.00002-0.00003)	-	-	-
Tl	0.0008 (0.0006-0.001)	-	0.0004 (0.0004-0.0005)	-
Pb	-	-	-	-
Th	0.00003 (0.00003-0.00003)	-	0.00002 (0.00002-0.00002)	-
U	0.002 (0.001-0.002)	-	0.002 (0.002-0.002)	-
Ti	0.00006 (0.00005-0.00007)	-	-	-
Nb	0.00009 (0.00009-0.00009)	-	0.0002 (0.0001-0.0002)	-
La	-	-	-	-
Tm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Yellow bean	LV	Garlic	LV
Li	0.001 (0.001-0.001)	-	0.0009 (0.0009-0.0009)	-
B	0.86 (0.92-0.81)	-	1.1 (0.99-1.2)	-
Na	1.4 (1.7-1.1)	-	2.9 (2.6-3.2)	2.7
Mg	16.3 (14.7-17.9)	-	21.6 (19.5-23.8)	25.0
Al	0.29 (0.26-0.32)	-	1.5 (1.3-1.6)	-
P	37.7 (37.6-37.9)	-	147.0 (119.3-174.8)	153.0
K	290.0 (249.1-330.9)	-	358.3 (348.5-368.1)	401.0
Ca	34.3 (32.3-36.6)	-	11.5 (11.1-11.9)	-
Ti	0.001 (0.001-0.002)	-	0.05 (0.04-0.05)	-
V	-	-	0.001 (0.001-0.001)	-
Cr	0.03 (0.02-0.03)	-	0.04 (0.04-0.04)	-
Fe	1.5 (1.3-1.7)	-	0.95 (0.87-1.0)	1.70
Mn	0.48 (0.46-0.49)	-	0.25 (0.18-0.32)	-
Co	0.001 (0.001-0.001)	-	0.0003 (0.0003-0.0004)	-
Ni	0.05 (0.04-0.05)	-	0.01 (0.009-0.01)	-
Cu	0.05 (0.05-0.06)	-	0.16 (0.16-0.16)	-
Zn	0.39 (0.37-0.41)	-	0.48 (0.46-0.50)	1.16
Ga	0.0004 (0.0004-0.0004)	-	0.001 (0.0008-0.001)	-
Ge	0.0003 (0.0003-0.0004)	-	0.00009 (0.00008-0.00009)	-
As	-	-	0.002 (0.001-0.003)	-
Se	-	-	0.02 (0.01-0.03)	-
Rb	0.09 (0.09-0.09)	-	0.06 (0.06-0.06)	-
Sr	0.35 (0.32-0.37)	-	0.07 (0.06-0.08)	-
Y	-	-	0.00005 (0.00004-0.00005)	-
Zr	0.0009 (0.0009-0.0009)	-	0.003 (0.003-0.003)	-
Nb	0.0005 (0.0005-0.0005)	-	0.0001 (0.0001-0.0001)	-
Mo	0.09 (0.09-0.09)	-	0.016 (0.01-0.02)	-
Ru	0.0002 (0.0002-0.0002)	-	0.00007 (0.00005-0.00009)	-
Pd	0.002 (0.002-0.002)	-	0.0004 (0.0004-0.0004)	-
Cd	0.00006 (0.0006-0.0007)	-	0.0005 (0.0005-0.0005)	-
Sn	0.07 (0.07-0.08)	-	0.06 (0.06-0.06)	-
Sb	-	-	0.0001 (0.0001-0.0001)	-
Cs	0.00005 (0.00005-0.00006)	-	0.00006 (0.00006-0.00006)	-
Ba	0.01 (0.009-0.01)	-	0.05 (0.05-0.05)	-
La	0.00005 (0.00004-0.00005)	-	0.00006 (0.00005-0.00006)	-
Ce	0.00003 (0.00003-0.00004)	-	0.0001 (0.0001-0.0001)	-
Pr	-	-	-	-
Nd	-	-	-	-
Sm	-	-	-	-

Continued.

Table 2.5.*Continued.*

Metabolites	Yellow bean	LV	Garlic	LV
Eu	0.00007 (0.00007-0.00008)	-	-	-
Gd	0.00001 (0.00001-0.00002)	-	-	-
Dy	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.001 (0.0009-0.001)	-	0.0001 (0.0001-0.0001)	-
Ta	0.0002 (0.0002-0.0003)	-	0.0003 (0.0003-0.0004)	-
W		-	0.003 (0.002-0.004)	-
Re	-	-	-	-
Os	0.0006 (0.0005-0.0007)	-	0.0007 (0.0006-0.0007)	-
Pt	-	-	0.0002 (0.0002-0.0003)	-
Au	-	-	-	-
Tl	-	-	0.0009 (0.0003-0.001)	-
Pb	0.01 (0.008-0.009)	-	-	-
Th	-	-	0.0001 (0.0001-0.0001)	-
U	-	-	0.0001 (0.0001-0.0001)	-

Table 2.6 Metabolite contents of fruits and vegetables as determined by NMR (Conc. mg/100 g FW).

Metabolites	Cucumber	LV[1]	Metabolites	Eggplant	LV
4-Aminobutyrate	21.2 (21.1-21.3)	-	**Acetoacetate**	23.4 (17.9-29)	-
Alanine	40.8 (40.1-41.5)	23	**4-Aminobutyrate**	15.0 (13.8-16.2)	-
Arginine	35.6 (34.2-37.1)	28	**Alanine**	31.3 (28.9-33.7)	47
Asparagine	31.1 (30.6-31.5)	-	**Arginine**	75.9 (68.1-83.7)	53
Aspartic acid	63.8 (59.6-68)	40	**Asparagine**	32.5 (32.3-32.6)	-
Choline	14.8 (14.7-15)	-	**Aspartic acid**	138.1 (122.3-154)	-
Citric acid	20.7 (20.4-21)	-	**Betaine**	45.3 (42.4-48.2)	-
Citrulline	71.3 (67.6-75)	-	**Chlorogenic acid**	72.6 (66.9-78.4)	-
Formic acid	12.9 (11.6-14.21)	-	**Choline**	79.3 (72.9-85.6)	-
Fructose	731(707.8-754.2)	710	**Citric acid**	6.2 (5.9-6.5)	-
Fumaric acid	8.2 (8.2-8.3)	-	**Formic acid**	13.9 (13.6-14.2)	-
Glucose	455.9 (452.8-459)	310	**Fructose**	1514 (1340-1688)	1400
Glutamic acid	145.9 (141.7-150.2)	220	**Fumaric acid**	10.2 (9.4-11.1)	-
Glutamine	281.9 (214.7-349.1)	-	**Galactose**	12.1 (11.8-12.3)	-
Glycine	25.3 (21.7-28.9)	-	**Glucose**	1356.2 (1179.2-1533.1)	1400
Histidine	23.2 (17.9-28.6)	-	**Glutamic acid**	155.1 (134.1-176.1)	170
Isoleucine	14.6 (24.5-24.7)	18	**Glutamine**	181.1 (168.1-194.1)	-
Leucine	17.2 (15.9-18.5)	28	**Glycine**	61.9 (60.1-63.8)	38
Lysine	14.8 (13.7-15.9)	-	**Histidine**	22.9 (22-23.9)	21
Malic acid	91.9 (86.1-97.7)	-	**Isoleucine**	49.1 (47.5-50.7)	42
Maltose	26.3 (26.3-26.4)	10	**Leucine**	36.1 (30.8-41.5)	60
Methionine	7.7 (6.3-9.0)	-	**Lysine**	20.5 (18.2-22.8)	44
Phenylalanine	23.9 (23.4-24.3)	17	**Malic acid**	91.9 (89.7-94.2)	-
Proline	14.2 (13-15.4)	13	**Myo-inositol**	63.3 (58.9-67.7)	-
Pyroglutamate	19.4 (18.9-19.8)	-	**Ornithine**	7.1 (6.7-7.4)	-
Serine	37.2 (36.6-37.8)	25	**Phenylalanine**	38.1 (36.6-39.7)	41
Sucrose	39.5 (39.1-39.8)	30	**Proline**	41.1 (40.3-41.9)	41
Threonine	20.8 (20.7-20.9)	16	**Pyruvic acid**	12.1 (12.1-12.1)	-
Trigonelline	14.8 (13.4-16.2)	-	**Serine**	39.1 (37.4-40.8)	39
Tryptophan	4.1 (4.1-4.1)	5	**Succinic acid**	19.5 (17.2-21.7)	-
Tyrosine	10.2 (9.9-10.4)	10	**Sucros**	222 (196.9-247.2)	-
UDP-glucose	15.3 (14.1-16.6)	-	**Threonine**	21.8 (21-22.7)	35
Valine	15.4 (13.3-17.5)	22	**Trigonelline**	13.3 (11.7-14.9)	-
			Tryptophan	7.3 (6.9-7.7)	8
			Tyrosine	18.2 (17.9-18.5)	26
			UDP-glucose	13.4 (12.8-13.7)	-
			Valine	26. 4 (23.2-29.5)	50
			Xylose	48.1 (44.8-51.3)	-

[1] LV for Literature value. References for the LV's are provided in the AFCDB website.

Table 2.6.*Continued.*

Metabolites	Japanese pumpkin	LV	Metabolites	Potato	LV
4-aminobutyrate	51.6 (47.9-55.3)	-	**4-Aminobutyrate**	414 (412.4-415.6)	-
Alanine	17.8 (16-19.5)	-	**Alanine**	78.2 (72.2-84.3)	-
Arginine	106.1 (99.1-112.9)	-	**Allantoin**	62.9 (62.6-63.2)	-
Asparagine	46 (41.3-50.7)	-	**Arginine**	253.9 (253.8-254.1)	180
Aspartic acid	131.2 (118.7-143.7)	-	**Asparagine**	187 (182.1-191.9)	-
Betaine	0.7 (0.7-0.8)	-	**Asparatic acid**	403.4 (396.5-410.3)	410
Choline	48.2 (44.3-52.1)	-	**Choline**	66.3 (63.2-69.4)	-
Citric acid	12.8 (12.7-13.)	9	**Formic acid**	15.3 (14.8-15.7)	-
Formic acid	8 (7.8-8.2)	-	**Fructose**	73.9 (68.1-79.7)	70
Fructose	1574.5 (1485.3-1663.8)	-	**Fumaric acid**	7.5 (7.1-7.9)	-
Fructose	786.1 (760-812.2)	-	**Galactose**	42.4 (42.2-42.5)	-
Formic acid	8.9 (8.6-9.2)	-	**Glucose**	146.1 (136-156.3)	180
Fumaric acid	10.5 (9.8-11.3)	-	**Glutamic acid**	267.1(260-274.2)	260
Galactose	64 (59.6-68.4)	-	**Glutamine**	620.2 (576.1-664.3)	-
Glucose	1286.4 (1229.2-1343.6)	-	**Histidine**	70.8 (68.2-73.4)	70
Glutamic acid	93.8 (81.3-106.2)	-	**Isoleucine**	72.8 (71.5-74)	71
Glutamine	481.4 (405.1-557.8)	-	**Leucine**	85.6 (84.4-86.8)	110
Glycine	15.2 (13.5-17)	-	**Lysine**	220.8 (218.7-222.9)	256
Histidine	4.1 (3.3-4.9)	-	**Methionine**	24.15 (21.9-26.4)	29
Isoleucine	28.9 (24.9-33)	-	**O-Acetylcholine**	38.4 (37.3-39.5)	-
Leucine	25.6 (25.3-26)	-	**Phenylalanine**	145.1 (144.9-145.3)	77
Lysine	12.8 (11.1-14.5)	-	**Proline**	91.6 (90.5-92.7)	68
Malic acid	65.3 (60.2-70.4)	-	**Pyroglutamate**	282.5 (262.3-302.7)	-
Methionine	5.9 (5.3-6.4)	-	**Pyruvic acid**	21.7 (20.9-22.5)	-
Myo-inositol	79.2 (76.4-82.1)	-	**Serine**	103.1 (98.3-107.9)	68
Phenylalanine	233.1 (197.3-268.8)	-	**Succinic acid**	23.9 (21.1-26.6)	-
Proline	11.8 (11.1-12.7)	12	**Sucrose**	1572 (1519.3-1624.8)	-
Pyruvic acid	8.1 (7.8-8.3)	-	**Threonine**	80.7 (79.5-82)	65
Serine	30.5 (29.4-31.5)	-	**Tryptophan**	35.4 (35-35.9)	29
Succinic acid	10.3 (9-11.6)	-	**Tyramine**	32.5 (31.3-33.7)	-
Sucros	378.8 (344.9-412.8)	-	**Tyrosine**	121.3 (98.4-144.3)	-
Threonine	10 (9.8-10.3)	-	**Valine**	205 (204.8-205.1)	110
Trigonelline	12.4 (12.1-12.7)	-			
Tryptophan	9.8 (9.3-10.2)	-			
Tyrosine	38.9 (36.1-41.6)	-			
Valine	16.7 (16.1-17.2)	-			

Continued.

Table 2.6.*Continued.*

Metabolites	Lettuce	LV	Metabolites	Swiss chard	LV
4-Aminobutyrate	63.6 (59.8-67.4)	-	**4-Aminobutyrate**	59.8 (56.8-62.6)	-
Alanine	46.8 (44.9-48.7)	55	**Acetic acid**	8 (7.9-8.1)	-
Arginine	41 (38.8-43.2)	53	**Acetoacetate**	98.7 (95.7-101.6)	-
Asparagine	434.1 (403.5-464.8)	-	**Alanine**	103.9 (99.8-107.9)	-
Aspartic acid	146.5 (144.1-149)	140	**Asparagine**	108.6 (104.5-112.7)	-
Betaine	116.1 (112.2-119.9)	-	**Aspartic acid**	73.9 (69.3-78.6)	-
Chlorogenic acid	45.3 (40.3-50.4)	-	**Betaine**	189.7 (187.3-192.1)	-
Choline	125.4 (117.5-133.2)	-	**Choline**	78.5 (67.1-89.9)	-
Ferulate	4.1 (3.9-4.2)	-	**Citric acid**	375.1 (347.9-402.2)	-
Formic acid	13.1 (12.8-13.5)	-	**Ferulate**	14.8 (11.2-18.4)	8.5
Fructose	493.5 (487.9-499.1)	458.6	**Formic acid**	15.5 (15.1-15.9)	-
Fumaric acid	16.7 (15.9-17.5)	-	**Fructose**	340.9 (383.2-298.6)	-
Galactose	24.9 (23-26.7)	-	**Glucose**	530.9 (524.6-537.2)	-
Glucose	418.6 (399.6-437.6)	389.8	**Glutamic acid**	322.7 (298.1-347.3)	-
Glutamic acid	116.2 (110.3-122.2)	180	**Glutamine**	78.4 (77.2-79.6)	-
Glutamine	417.7 (392.2-443.2)	-	**Glycine**	37.4 (36.5-38.3)	-
Histidine	21.05 (19.8-22.3)	-	**Histidine**	31.3 (29.8-32.7)	35
Homoserine	66.8 (65.8-67.8)	-	**Hypoxanthine**	7.8 (7.7-8.8)	-
Isoleucine	43.2 (42.4-44.1)	45	**Isoleucine**	92 (87.7-96.3)	150
Leucine	47.1 (44.5-49.7)	77	**Leucine**	120.7 (113.2-128.2)	130
Lysine	59.6 (54.4-64.8)	63	**Lysine**	79.5 (72.6-86.3)	98
Malic acid	887 (803.7-970.2)	-	**Malonic acid**	62.2 (51.1-73.3)	-
Maltose	96.8 (84.5-109)	-	**Phenylalanine**	92.8 (88.4-97.2)	110
Phenylalanine	47.7 (44.6-50.9)	65	**Proline**	38.8 (32.8-44.7)	-
Proline	23.75 (22.9-24.6)	-	**Pyruvic acid**	50.5 (48.3-52.6)	-
Pyruvic acid	9.1 (7.4-10.9)	-	**Serine**	247.5 (241.7-253.3)	-
Serine	48.8 (42.6-55.0)	-	**Succinic acid**	188.5 (185.4-191.6)	-
Succinic acid	55.7 (52.4-58.9)	-	**Sucrose**	219.4 (221.1-217.8)	-
Sucrose	948.8 (891.6-1005.9)	-	**Threonine**	53.9 (47.6-60.2)	84
Threonine	41.8 (36.2-47.4)	43	**Tyrosine**	57.5 (53.6-61.4)	-
Tryptophan	9.9 (9.1-10.7)	10	**Valine**	101.1 (100.01-102.2)	-
Tyrosine	25.1 (21.7-28.5)	26			
Valine	34.8 (34.2-35.4)	55			
Xylose	58.6 (56.8-60.4)	-			

Continued.

Tabe 2.6.*Continued.*

Metabolites	Italian red pepper	LV	Metabolites	Carrot	LV
4-aminobutyrate	50.8 (47.8-53.8)	-	**4-aminobutyrate**	35.2 (32.9-37.6)	-
Alanine	58.5 (60-61.4)	-	**Alanine**	83.1 (78.1-88)	77
Arginine	34.2 (35.7-37.1)	-	**Arginine**	46.4 (44.3-48.6)	-
Ascorbic Acid	49.05 (47.8-50.3)		**Asparagine**	100.3 (89.5-111.1)	-
Asparagine	88.5 (78.5-83.5)	-	**Aspartic acid**	133.4 (130.5-136.3)	-
Aspartic acid	189.4 (212.6-235.7)	-	**Chlorogenic acid**	78.5 (74.4-82.6)	-
Betaine	77.1 (84.5-91.8)	-	**Choline**	12.5 (11.2-13.8)	-
Choline	28.8 (30.1-31.4)	-	**Citric acid**	13.3 (12.5-14)	-
Dimethylsulfone	33 (30.2-31.6)	-	**Ethanol**	12.6 (12.5-12.7)	-
Formic acid	26.8 (27.7-28.6)	-	**Formic acid**	14.2 (13.3-15.1)	-
Fructose	2214 (2419.1-2008.9)	-	**Fructose**	1514.4 (1542.1-1486.7)	1900
Glucose	1999.6 (2020.1-2040.5)	-	**Glucose**	2255 (2253.8-2256.2)	2560
Glutamic acid	85.1 (79.2-82.2)	-	**Glutamic acid**	164.7 (164.1-165.3)	180
Glutamine	148.7 (143.9-146.3)	-	**Glutamine**	462.4 (455.9-469)	-
Glycine	48.1 (55.3-62.5)	-	**Glycine**	14.4 (14-14.9)	27
Histidine	12.5 (11.7-13.3)	-	**Histidine**	20.35 (17.8-21.9)	-
Isobutyric acid	10.2 (6.2-8.2)	-	**Isoleucine**	41 (38.3-43.7)	29
Isoleucine	39.5 (36.1-37.8)	-	**Leucine**	37.6 (32.5-42.8)	38
Leucine	33.8 (34.6-35.3)	-	**Lysine**	33.8 (33.1-34.6)	35
Lysine	36.4 (29.5-33)	-	**Methionine**	13.3 (11.8-14.7)	9
Malonic acid	22.5 (22.5-22.6)	-	**Ornithine**	8.8 (7.6-10)	-
Methionine	10 (10.3-10.5)	-	**Phenylalanine**	43.3 (42.2-44.4)	26
Ornithine	8.2 (9.3-10.4)	-	**Proline**	38.7 (37.3-40.1)	-
Phenylalanine	33.3 (36.3-39.3)	-	**Pyruvic acid**	32.2 (28.1-36.2)	-
Proline	49.1 (48.1-50.2)	-	**Serine**	31.8 (29.1-34.4)	35
Serine	174.8 (175.7-176.6)	-	**Succinic acid**	43.6 (42-45.1)	-
Succinic acid	5.1 (5.9-6.6)	-	**Sucrose**	2395.3 (2080-2710.6)	-
Sucrose	211.1 (207.4-214.9	-	**Threonine**	30.6 (30.4-30.8)	26
Threonine	126.9 (127-127.1)	-	**Tryptophan**	11.3 (10.6-11.9)	9
Tryptophan	13 (12.6-13.3)	-	**Tyrosine**	17.7 (17.2-18.1)	14
Tyrosine	13.8 (14.4-15)	-	**Valine**	24.3 (21.2-27.3)	43
Valine	74 (76-78)	-			
4-aminobutyrate	50.8 (47.8-53.8)	-			

Continued.

Table 2.6.*Continued.*

Metabolites	Tomato	LV	Metabolites	Garlic	LV
4-Aminobutyrate	38.3 (33.9-42.7)	-	**4-Aminobutyrate**	18.9 (17.2-20.5)	-
Alanine	30.4 (28.9-31.9)	27	**Alanine**	189.2 (187.8-190.6)	130
Ascorbic acid	22.1 (20.7-23.5)	13.7	**Arginine**	280 (273.6-286.4)	640
Asparagine	155 (153.8-156.1)	-	**Ascorbic acid**	26.8 (26.4-27.3)	31
Asparatic acid	188.4 (185.7-191)	135	**Asparagine**	50 (48.8-51.1)	-
Betaine	40 (38.4-41.5)	-	**Asparatic Acid**	143.7 (129-158.4)	490
Choline	55.2 (55.1-55.2)	-	**Betaine**	38.5 (35.8-41.3)	-
Formic acid	13.5 (13.4-13.6)	-	**Butyrate**	16.3 (16.2.2-16.5)	-
Fructose	1067.8 (1052.3-1083.2)	1420	**Choline**	44.2 (40.9-47.5)	-
Fumaric acid	11.9 (11.6-12.2)	-	**Formic acid**	15.7 (15.5-15.9)	-
Galactose	24.8 (22.2-27.4)	-	**Fructose**	11.8 (8.9-14.6)	-
Glucose	1053.9 (987.7-1120.2)	1130	**Fumaric acid**	14.5 (14.4-14.6)	-
Glucose-1-phosphate	29.7 (29.6-29.8)	-	**Galactose**	208.9 (187.5-230.2)	220
Glutamic acid	447.5 (413.7-481.3)	431	**Glutamic acid**	349.3 (318.1-380.5)	810
Glutamine	492.8 (468.7-516.9)	-	**Glutamine**	45.2 (42.6-47.9)	77
Glycine	30.4 (28.7-32.1)	20	**Glycine**	261.8 (233.4-290.3)	210
Histidine	16.6 (14.9-18.3)	12	**Histidine**	45.1 (44.6-45.7)	
Isoleucine	16.1 (15.6-16.5)	18	**Isoleucine**	208.9 (187.5-230.2)	220
Leucine	23.7 (21.1-26.3)	28	**Leucine**	188.9 (188.5-189.3)	180
Lysine	51 (44.2-57.8)	34	**Lysine**	349.3 (318.1-380.5)	280
Maltose	118.1 (105.1-131)	-	**Maltose**	442.2 (413.1-471.2)	100
Phenylalanine	50.9 (50-51.8)	29	**Methionine**	15.2 (12.6-17.9)	-
Proline	38.7 (37.2-40.1)	23	**Phenylalanine**	72.5 (72-72.9)	180
Putrescine	27 (26.5-27.5)	-	**Proline**	161.16 (137.4-184.9)	100
Serine	18.8 (17.8-19.9)	26	**Pyruvic acid**	72.5 (72-72.9)	-
Succinic acid	6.8 (6.7-6.9)	-	**Serine**	388.4 (380.6-396.2)	200
Sucrose	396.8 (379-414.6)	-	**Succinic acid**	124.5 (123.2-125.8)	150
Threonine	53.8 (52.1-55.4)	-	**Sucrose**	79.2 (78.7-79.7)	67
Tryptophan	17.6 (16.2-18.9)	-	**Threonine**	107.7 (100.9-114.4)	82-150
Tyrosine	23.7 (22.7-24.7)	26	**Tryptophan**	100.8 (100.1-101.6)	67
Valine	22.1 (20.7-23.5)	21	**Tyrosine**	107.7 (101.7-113.6)	82
			Valine	200.9 (184.3-217.4)	300

Continued.

Table 2.6.*Continued.*

Metabolites	Onion	LV	Metabolites	Raspberry	LV
Alanine	36.5 (34.7-38.4)	35	**Acetic acid**	6.4 (6.2-7.5)	-
Arginine	228.2 (228.1-228.2)	210	**Alanine**	41.8 (28.7-54.9)	-
Ascorbic acid	5.1 (4.8-5.3)	-	**Arginine**	17.9 (17.7-18.2)	-
Aspartic acid	133 (122.5-143.5)	93	**Ascorbic acid**	34.6 (34.2-35.1)	26.2
Betaine	3.3 (3-3.5)	-	**Asparagine**	35.6 (35.1-36.2)	-
Choline	19.1 (18.3-20.1)	-	**Aspartic acid**	95.2 (94.9-95.5)	-
Citric acid	7.6 (6.3-8.9)	7.4	**Betaine**	26.9 (19.3-34.6)	-
Formic acid	8.7 (8.1-9.3)	-	**Choline**	13.0 (12.2-13.8)	15.1
Fructose	1587 (1563.2-1610.8)	1830	**Citric acid**	11.9 (6.4-17.3)	-
Glucose	1961.1 (1747-2175.1)	2240	**Epicatechin**	20.1 (18.8-21.3)	-
Glutamic acid	230.3 (214.8-245.9)	330	**Fructose**	1209.7 (1208-1211.3)	1220
Glutamine	336.3 (294.5-378.1)	-	**Glucose**	933.2 (906.2-960.3)	750
Glycine	61.4 (60.5-62.3)	33	**Glutamic acid**	24.5 (23.4-25.6)	-
Histidine	11.8 (10.2-13.5)	18	**Glutamine**	30.7 (30-31.3)	-
Isobutyric acid	13.1 (12.3-14)	-	**Glycine**	12.8 (12.3-13.3)	-
Isoleucine	43.5 (40.9-46.1)	30	**Isoleucine**	13.7 (11.9-15.5)	-
Leucine	63 (62.7-63.2)	53	**Leucine**	7.4 (6.7-8.2)	-
Lysine	60 (58.6-61.4)	50	**Lysine**	6.7 (6.7-6.7)	-
Methionine	24 (22.3-25.6)	12	**Methionine**	5.2 (3.1-7.3)	-
Ornithine	8.2 (8.2-8.2)	-	**Ornithine**	11.3 (8.7-13.9)	-
Phenylalanine	48.7 (48.6-48.9)	35	**Phenylalanine**	14.9 (12.7-17)	-
Proline	18.2 (17.6-18.8)	21	**Proline**	19.2 (16.2-22.2)	-
Pyruvic acid	39.6 (39-40.1)	-	**Pyruvic acid**	7.9 (6.3-9.5)	-
Serine	41.5 (40.3-42.6)	28	**Serine**	34.2 (31.9-36.4)	-
Succinic acid	24.4 (21.2-27.5)	-	**Sucrose**	271.5 (243.7-299.4)	203
Sucrose	914.9 (880.1-949.8)	-	**Threonine**	13.4 (9.4-17.4)	-
Threonine	40.3 (37.8-42.9)	-	**Tryptophan**	11.6 (11-12.2)	-
Tryptophan	36.3 (35.5-37.1)	19	**Tyrosine**	25.2 (22.9-27.6)	-
Tyrosine	63.5 (61-66)	-	**Valine**	11.1 (9.3-12.8)	-
Valine	42.1 (38.7-45.5)	-			

Continued.

Table 2.6.*Continued.*

Metabolites	Red bell pepper	LV	Metabolites	Green bell pepper	LV
4-aminobutyrate	108.2 (99.3-117.1)	-	**4-aminobutyrate**	139.4 (134.7-144.1)	-
Alanine	63.7(60.1-67.3)	50	**Alanine**	63.7 (59.9-67.4)	35
Arginine	61.1(54.9-67.2)	50	**Arginine**	90 (87.5-92.5)	35
Ascorbic acid	105 (97.8-112.2)	50	**Ascorbic acid**	67 (68.3-70.2)	50
Asparagine	172.2 (144.6-199.8)	-	**Asparagine**	47.8 (47.4.-48.2)	-
Aspartic acid	120.5 (102.3-138.7)	170	**Aspartic acid**	108.7 (96.7-120.7)	120
Betaine	66.6 (61.5-71.7)	-	**Betaine**	77.3 (74.4-80.2)	-
Choline	8.8 (7.9-9.7)	-	**Choline**	14 (14-14.1)	-
Citric acid	46.6 (37.7-55.5)	-	**Citric acid**	19.1 (17.7-20.5)	-
Formic acid	36.6 (27.6-45.6)	-	**Formic acid**	14 (13.2-14.8)	-
Fructose	2010.5 (2009.3-2011.8)	2430	**Fructose**	1249.4 (1210.6-1288.3)	1040
Glucose	1829.9 (1793.3-1866.4)	1570	**Glucose**	875.4 (821.8-929)	840
Glutamic acid	135.6 (124.8-146.5)	180	**Glutamic acid**	81.3 (74.7-87.9)	120
Glutamine	437.9 (434.2-441.7)	380	**Glutamine**	363.8 (353.5-374.1)	-
Glycine	29.6 (27.5-31.7)	44	**Glycine**	34.4 (31.9-37)	30
Guanidoacetate	76.9 (72.3-81.6)	-	**Guanidoacetate**	63.15 (58.4-67.6)	-
Histidine	22.5 (21.4-23.6)	21	**Histidine**	28.8 (20.7-36.8)	-
Isoleucine	33.7 (29.8-37.5)	40	**Isoleucine**	45.5 (45.4-45.6)	27
Leucine	57.3 (54.9-59.6)	52	**Leucine**	27 (26.2-27.8)	36
Lysine	34.4 (32.7-36.1)	60	**Lysine**	38.2 (37.4-39)	42
Methionine	12.5 (11.7-13.2)	10	**Malic acid**	85.5 (82.3-89.4)	-
Phenylalanine	33.9 (33.7-34.1)	40	**Methionine**	15.9 (14.8-17)	7
Proline	43 (42.1-43.8)	33	**Phenylalanine**	31.7 (31.6-31.8)	27
Pyruvic acid	5.7 (5.2-6.2)	-	**Proline**	17.4 (16.7-18.1)	23
Serine	130.7 (119.1-142.2)	62	**Pyruvic acid**	12.5 (11.7-13.2)	-
Sucrose	347.6 (318.9-376.3	-	**Serine**	120.8 (107.9-133.6)	43
Threonine	124.4 (98.6-150.1)	42	**Succinic acid**	9.6 (9.6-9.7)	-
Tryptophan	10.5 (9.5-11.4)	7	**Sucrose**	302.5 (293.1-311.8	-
Tyrosine	22.7 (19.6-25.8)	-	**Threonine**	14.8 (12.8-16.8)	29
Valine	96.2 (88.3-104.1)	60	**Tryptophan**	11.5 (11.9-12.6)	-
			Tyrosine	22.9 (21.2-24.6)	13
			Valine	45.4 (44-46.7)	42

Continued.

Table 2.6.*Continued.*

Metabolites	Yellow bell pepper	LV	Metabolites	Orange bell pepper	LV
4-Aminobutyrate	58.9 (58.7-59.1)	-	**4-Aminobutyrate**	28 (27.5-28.5)	-
Alanine	33.5 (32.1-35)	-	**Alanine**	131.3 (129.7-132.9)	-
Arginine	39.4 (38.6-40.1)	-	**Arginine**	41.1 (39.6-42.7)	-
Ascorbic acid	184.3 (170.1-198.6)	-	**Ascorbic acid**	94.2 (88.9-99.6)	-
Asparagine	203 (196-210.1)	-	**Asparagine**	246.1 (241.6-250.6)	-
Asparatic acid	308.6 (288.8-328.5)	-	**Asparatic acid**	123.8 (118.2-129.3)	-
Betaine	81 (78-84.1)	-	**Betaine**	76.2 (74.6-77.8)	-
Choline	8.9 (8.9-9)	-	**Choline**	5.5 (5.2-5.8)	-
Formic acid	27.6 (25.8-29.4)	-	**Formic acid**	35.6 (32.4-38.8)	-
Fructose	637 (625-649.1)	-	**Fructose**	3022.7 (2951-3094.5)	-
Glucose	1531.8 (1412.7-1650.9)	-	**Glucose**	2193.7 (2065.8-2321.7)	-
Glutamic acid	21.1 (19.8-22.4)	-	**Glutamic acid**	172.7 (148.2-197.2)	-
Glutamine	318.8 (305.6-331.9)	-	**Glutamine**	215.9 (214.6-217.2)	-
Glycine	32.5 (31-33.9)	-	**Glycine**	15.1 (14.7-15.5)	-
Guanidoacetate	81.2 (60.7-101.8)	-	**Guanidoacetate**	124.4 (123.6-125.2)	-
Histidine	9.5 (8.9-10.1)	-	**Histidine**	19.9 (19.2-20.7)	-
Isoleucine	14.4 (11.2-17.5)	-	**Isoleucine**	16.4 (16.1-16.6)	-
Leucine	16.1 (15.1-17.0)	-	**Leucine**	36.9 (34.7-39.1)	-
Lysine	19.6 (19.3-19.9)	-	**Lysine**	38.15 (36.4-39.9)	-
Maltose	326 (271.6-380.4)	-	**Maltose**	237.5 (225.8-249.2)	-
Methionine	8.2 (7.7-8.6)	-	**Methionine**	7.5 (5.8-9.2)	-
Phenylalanine	12.7 (11.4-14.1)	-	**Phenylalanine**	20.8 (20.2-21.4)	-
Proline	10.9 (9.1-12.6)	-	**Proline**	20.6 (18.8-22.4)	-
Pyruvic acid	5.6 (5-6.1)	-	**Pyruvic acid**	3.8 (3.7-3.8)	-
Serine	71.9 (68.7-75.1)	-	**Serine**	54.6 (53.8-55.5)	-
Succinic acid	3.4 (2.9-3.8)	-	**Succinic acid**	2.2 (2-2.3)	-
Sucrose	473.9 (455.8-492.1)	-	**Sucrose**	428 (417-438.9)	-
Threonine	74.8 (73.9-75.6)	-	**Threonine**	124.8 (123-126.7)	-
Tyrosine	9.1 (8.2-9.9)	-	**Tryptophan**	5.9 (5.6-6.2)	-
Tryptophan	11.4 (10.7-12.2)	-	**Tyrosine**	10.1 (9.6-10.6)	-
Valine	25 (23.9-26.1)	-	**Valine**	65.1 (63.3-67)	-

Continued.

Table 2.6.*Continued.*

Metabolites	Dill	LV	Metabolites	Wax bean	LV
4-aminobutyrate	78.9 (78.3-79.6)	-	**4-aminobutyrate**	60.2 (55.6-64.9)	-
Acetic acid	168.1 (166.4-169.7)	-	**Alanine**	83.8 (79.8-87.8)	84
Alanine	68 (66.4-69.7)	-	**Arginine**	26.1 (23.8-28.4)	77
Arginine	318 (287.2-348.9)	-	**Ascorbic acid**	29.7 (27.6-31.9)	21
Ascorbic acid	31.1 (27.9-34.4)	-	**Asparagine**	5.3 (5-5.5)	-
Asparagine	99 (98.7-99.3)	-	**Aspartic acid**	437.5 (421.6-453.5)	-
Aspartic acid	436.8 (353.9-519.7)	-	**Betaine**	7.1 (7-7.2)	-
Betaine	85.7 (75.9-95.4)	-	**Choline**	62 (41-83)	-
Choline	130.3 (114.7-145.9)	-	**Citric acid**	34.7 (29.1-40.2)	-
Citric acid	151.7 (142.5-160.8)	-	**Formic acid**	20.7 (19.6-21.8)	-
Formic acid	12.8 (12.1-13.5)	-	**Fructose**	533.4 (517.6-549.3)	-
Fructose	289.2 (286.3-292.1)	-	**Glucose**	494.2 (452.1-536.4)	-
Glucose	486.9 (474.4-499.5)	-	**Glutamic acid**	248.9 (242.3-255.4)	220
Glutamic acid	185.6 (179.2-192)	-	**Glutamine**	393.2 (363.3-423.2)	-
Glutamine	176.2 (164.3-188.1)	-	**Glycine**	12.5 (19.9-221)	-
Glycine	120 (111.2-128.8)	-	**Histidine**	35.7 (11.1-60.2)	33
Histidine	67.1 (64.9-69.3)	-	**Isoleucine**	135.2 (78.8-191.7)	81
Hypoxanthine	9.5 (9.1-9.9)	-	**Leucine**	193 (172.1-213.9)	120
Isoleucine	204.3 (193.7-214.8)	-	**Lysine**	143 (129.1-157)	110
Leucine	90.7 (81.3-100.1)	-	**Methionine**	22.4 (21.5-23.2)	28
Lysine	292.2 (273.4-311.1)	-	**Ornithine**	15.1 (13.8-16.4)	-
Methionine	12 (6.8-17.2)	-	**Phenylalanine**	14.3 (14.2-14.3)	57
Phenylalanine	40.7 (37-44.3)	-	**Proline**	2.9 (2.2-3.6)	-
Proline	151.6 (141.2-162)	-	**Pyruvic acid**	16.9 (14.8-19)	-
Pyruvic acid	41.2 (36-46.5)	-	**Serine**	300.7 (288-313.3)	170
Serine	209.9 (181.8-238.1)	-	**Succinic acid**	81.4 (81.4-81.4)	-
Threonine	52.8 (41.9-63.5)	-	**Sucrose**	249.5 (210.7-288.3	-
Tryptophan	15.6 (14.7-16.6)	-	**Threonine**	80.8 (66.1-95.6)	31
Tyrosine	88.8 (78.9-99.8)	-	**Tryptophan**	8.9 (7.8-9.9)	-
Valine	254.3 (233.6-275)	-	**Tyrosine**	69.3 (68-70.6)	47
			Valine	48 (43.2-52.7)	100

Continued.

Table 2.6.*Continued.*

Metabolites	Crab apple	LV	Metabolites	Parsnip	LV
4-aminobutyrate	84.1 (79.8-88.3)	-	**Acetic acid**	8.7 (8.6-8.7)	-
Acetic acid	7.4 (6.7-8.1)	-	**4-aminobutyrate**	48 (45.7-50.3)	-
Alanine	17.4 (17.1-17.8)	-	**Alanine**	65.3 (63.1-67.5)	81
Arginine	35.3 (31.2-39.5)	-	**Arginine**	216.8 (213-220.7)	200
Ascorbic acid	9.4 (8.7-10.1)	-	**Ascorbic acid**	18.5 (17.8-19.2)	17
Asparagine	116 (109.7-122.2)	-	**Asparagine**	111 (103.7-118.4)	-
Aspartic acid	51.1 (49.5-52.7)	-	**Aspartic acid**	188.8 (188.7-189)	230
Betaine	14.2 (12.3-15.1)	-	**Betaine**	40.9 (40.1-41.8)	-
Choline	7.9 (7.5-8.4)	-	**Choline**	35.2 (33.3-37.1)	-
Citric acid	23.2 (21.6-24.8)	-	**Citric acid**	419.6 (414.1-425.2)	-
Formic acid	17.1 (15.2-20.1)	-	**Formic acid**	17.6 (17.6-17.7)	-
Fructose	2513.7 (2017.6-2009.8)	-	**Fructose**	1245.1 (1203.2-1286.9)	-
Glucose	1639.5 (1568-1711.1)	-	**Glucose**	1150.2 (1073.1-1227.2)	-
Glutamic acid	61.1 (58.4-63.7)	-	**Glutamic acid**	196.2 (192.8-199.6)	200
Glutamine	271.6 (255.1-288)	-	**Glutamine**	212.7 (207.1-218.3)	-
Histidine	22.7 (20.1-25.2)	-	**Glycine**	56.5 (53.6-59.4)	54
Isoleucine	22.2 (20.9-23.5)	-	**Histidine**	24.9 (21.2-28.6)	34
Leucine	23.7 (22.4-25)	-	**Isoleucine**	37.4 (35-39.7)	71
Lysine	40.6 (39.2-42)	-	**Leucine**	80.2 (86.3-74.1)	97
Phenylalanine	33.8 (28.2-39.3)	-	**Lysine**	168.4 (149.7-188.6)	91
Proline	31.2 (29.8-32.7)	-	**Malic acid**	39.5 (34.8-44.2)	-
Pyruvic acid	6.6 (6.6-6.6)	-	**Methionine**	20.9 (20.5-21.2)	21
Serine	32.1 (30.7-33.5)	-	**Phenylalanine**	54.2 (53.9-54.5)	-
Succinic acid	5.7 (5.5-5.9)	-	**Proline**	185.1 (173.2-197)	-
Sucrose	862.7 (846.3-879.2)	-	**Pyruvic acid**	36.9 (36.8-37.1)	-
Threonine	20.4 (20.4-20.5)	-	**Serine**	56.4 (56.4-56.5)	77
Tryptophan	10.6 (10.3-10.8)	-	**Succinic acid**	24.1 (20.1-28.1)	-
Tyrosine	27.9 (26.1-29.8)	-	**Sucrose**	1901.8 (1870.1-1933.6)	-
Valine	68.1 (66.3-69.9)	-	**Threonine**	41.6 (41.1-42.1)	64
			Tryptophan	18.1 (17.8-18.4)	21
			Tyrosine	44 (43.3-44.7)	-
			Valine	39.9 (38.1-41.6)	91

Continued.

Table 2.6.*Continued.*

Metabolites	Broccoli	LV	Metabolites	White cabbage	LV
4-aminobutyrate	57.6 (55.7-59.6)	-	**4-aminobutyrate**	41.3 (37.6-44.9)	
Alanine	31.3 (30.4-32.3)	-	**Alanine**	54.8 (54.3-55.3)	61
Arginine	237.5 (219.7-255.4)	330	**Arginine**	45.9 (36.8-55)	67
Ascorbic acid	82.6 (72.1-93.2)	89.2	**Ascorbic acid**	28.1 (27.2-29.1)	36
Asparagine	238.7 (217.6-259.9)	-	**Asparagine**	108.4 (95.3-121.5)	-
Aspartic acid	319.6 (304.7-334.6)	-	**Aspartic acid**	143.6 (111.4-175.9)	110
Betaine	21.6 (16.9-26.2)	-	**Betaine**	18.7 (15.5-21.9)	-
Choline	69.8 (62.7-76.8)	-	**Choline**	23.4 (17.3-29.5)	-
Citric acid	32.3 (29.9-34.8)	-	**Citric acid**	30.9 (25.1-36.7)	-
Formic acid	13.2 (12.4-13.9)	-	**Fructose**	1688.3 (1654.9-1721.7)	1300
Fructose	1993.2 (1849.9-2136.6)	2020	**Glucose**	1326.3 (1074.6-1577.9)	1600
Fructose	1493.8 (1408.1-1579.6)	1300	**Glutamic acid**	345.2 (265.8-424.5)	290
Glucose	988.6 (887-1090.2)	800	**Glutamine**	118.8 (99.4-138.3)	-
Glutamic acid	179.4 (150.2-208.6)	-	**Glycine**	20 (17.1-22.9)	27
Glutamine	467.3 (466-468.6)	-	**Histidine**	46.5 (45.7-47.3)	-
Glycine	175.2 (157.7-192.7)	-	**Isoleucine**	36 (30.6-41.5)	27
Histidine	65.7 (59.5-71.9)	120	**Leucine**	40.3 (32.8-47.8)	35
Isoleucine	193.1 (165.8-220.4)	200	**Lysine**	19.1 (15.3-22.9)	35
Leucine	167.2 (138.7-195.8)	280	**Methionine**	9.9 (9.7-10.1)	9
Lysine	209.3 (256.7-261.9)	270	**Phenylalanine**	29 (22.6-35.4)	22
Methionine	151.4 (128.9-173.8)	76	**Proline**	65 (43.2-86.8)	57
Phenylalanine	281.7 (252.6-310.8)	200	**Pyruvic acid**	13.4 (12.7-14)	-
Proline	93.4 (78.1-108.7)	-	**Serine**	68.3 (52.9-83.7)	51
Pyruvic acid	16.6 (14.8-18.4)	-	**Sucrose**	572.6 (550.6-594.7)	-
Serine	136.7 (119.5-153.8)	-	**Threonine**	36.5 (29.7-43.2)	24
Succinic acid	8 (6.9-9.1)	-	**Tryptophan**	12.2 (10.7-12.8)	9
Sucrose	689 (644.8- 733.2	-	**Tyrosine**	9.5 (9-9.9)	12
Threonine	258.4 (219-297.9)	230	**Valine**	42.5 (42.9-42.9)	45
Tryptophan	54.5 (52.3-56.7)	59	**Alanine**	54.8 (54.3-55.3)	61
Tyrosine	20.9 (17.8-24.1)	-	**Arginine**	45.9 (36.8-55)	67
Valine	179.1 (170.3-188.0)	250	**Ascorbic acid**	28.1 (27.2-29.1)	36

Continued.

Table 2.6.*Continued.*

Metabolites	Turnip	LV	Metabolites	Spinach	LV
4-Aminobutyrate	11 (10-12.1)	-	**4-Aminobutyrate**	49.3 (48.1-50.5)	-
Alanine	29.0 (27.8-30.2)	28	**Alanine**	109.1 (107.7-110.4)	110
Arginine	17.3 (15.4-19.1)	10	**Arginine**	165.3 (163.2-167.4)	-
Ascorbic acid	31.95 (30.8-33.1)	-	**Ascorbic acid**	27.3 (26.9-27.7)	-
Asparagine	14.6 (13.4-15.7)	-	**Asparagine**	201.8 (198.4-205.2)	-
Aspartic acid	26.6 (26.4-26.9)	35	**Aspartic acid**	250.7 (230.5-270.9)	230
Betaine	54.9 (54.4-55.3)	-	**Betaine**	132.5 (131.8-133.3)	-
Choline	12.3 (12.2-12.4)	-	**Choline**	127.9 (127.6-128.2)	-
Formic acid	7.5 (7.2-7.9)	-	**Formic acid**	11.2 (10.5-11.8)	-
Fructose	969 (967.6-970.4)	-	**Fructose**	77.6 (77.1-78)	90
Fumaric acid	8.9 (8.6-9.2)	-	**Fumaric acid**	8.3 (8-8.7)	-
Galactose	32.5 (21.4-43.7)	-	**Glucose**	101 (100.5-101.4)	110
Glucose	854.7 (832.9-876.6)	-	**Glutamic acid**	163.6 (158.6-168.6)	290
Glutamic acid	50.1 (47.7-52.6)	56	**Glutamine**	424.0 (402.7-445.3)	-
Glutamine	118.1 (113.7-122.5)	-	**Glycine**	89.9 (87.4-92.5)	110
Glycine	101.9 (93.7-110.2)	-	**Histidine**	58.05 (57.1-59.0)	46
Histidine	14.3 (13.9-14.7)	5	**Isoleucine**	73.2 (72.9-73.5)	84
Homoserine	25 (21.8-28.2)	-	**Leucine**	122.7 (121.7-123.8)	150
Isoleucine	27.6 (27.2-28)	15	**Lysine**	130 (122.7-148.9)	-
Leucine	10.3 (10.2-10.4)	25	**Malic acid**	739.6 (709.8-769.4)	-
Lysine	36.9 (33.7-40.1)	-	**Phenylalanine**	85.9 (83.5-88.3)	120
Malic acid	15.6 (14.1-17.1)	-	**Proline**	120.5 (111.1-130.0)	84
Phenylalanine	12.5 (10.6-14.5)	12	**Proline**	23.4 (22.1-24.7)	21
Proline	23.4 (22.1-24.7)	-	**Serine**	94.5 (92.7-96.3)	100
Serine	20.2 (17.6-22.9)	-	**Sucrose**	104 (102.8-105.2)	-
Sucrose	97.7 (82.7-112.7)	-	**Threonine**	60 (59.1-60.9)	92
Sucrose	695.2 (688.2-602.1)	-	**Trigonelline**	12.4 (11.7-131)	-
Threonine	19.9 (19.7-20.1)	17	**Tryptophan**	44.7 (40.8-48.7)	42
Tryptophan	8.7 (7.9-9.5)	8	**Tyrosine**	92.9 (91.2-94.7)	63
Tyrosine	9.5 (8.7-10.3)	9	**Valine**	107.9 (101.8-113.9)	120
Valine	14.4 (13.1-15.6)	15			

Continued.

Table 2.6.*Continued.*

Metabolites	Yellow zucchini	LV	Metabolites	Green zucchini	LV
4-Aminobutyrate	18.3 (17.2-19.4)	-	**4-Aminobutyrate**	37.4 (36.8-38)	-
Alanine	39.25 (39.2-39.3)	62	**Alanine**	51.5 (41.2-61.8)	62
Arginine	50.25 (44.8-55.7)	50	**Arginine**	67.4 (54.8-80.1)	50
Ascorbic acid	17.05 (16.3-17.8)	18	**Ascorbic acid**	14.8 (13.9-15.8)	17.9
Asparagine	167.95 (162.7-173.2)	-	**Asparagine**	376.5 (350.6-402.4)	-
Aspartic acid	197.65 (191.5-203.8)	-	**Aspartic acid**	74.4 (70.4-78.4)	-
Betaine	9.2 (9.2-9.2)	-	**Betaine**	47.1 (36.9-57.4)	-
Choline	14.1 (12.5-15.8)	15	**Choline**	23.5 (22.9-24.1)	18
Formic acid	9.3 (9.2-9.4)	-	**Formic acid**	10.3 (7.8-12.9)	-
Fructose	1449.6 (1270.9-1628.3)	1380	**Fructose**	1808.1 (1803-1813.2)	1380
Fumaric acid	13.8 (13.7-13.9)	-	**Fumaric acid**	23.2 (21.7-24.8)	-
Galactose	18.75 (18-19.5)	-	**Galactose**	84.5 (82.3-86.7)	-
Glucose	1465.5 (1367.4-1563.6)	1070	**Glucose**	1183.4 (1138.3-1228.4)	1070
Glutamic acid	70 (62.1-77.9)	130	**Glutamic acid**	38 (33.1-42.9)	-
Glutamine	351.5 (337.3-365.7)	129	**Glutamine**	131 (96.8-165.3)	129
Glycine	66.8 (63.4-70.2)	47	**Glycine**	6.2 (5.2-7.3)	-
Histidine	35.9 (33.7-38.1)	25	**Histidine**	24.6 (21.3-27.9)	-
Homoserine	45.7 (41.5-49.9)	-	**Homoserine**	39.4 (33.3-45.6)	-
Isoleucine	25.7 (25.4-26)	45	**Isoleucine**	22 (20.7-23.4)	45
Leucine	25 (24.8-25.2)	72	**Leucine**	83.4 (82.2-84.7)	72
Lysine	56.5 (52.8-60.3)	68	**Lysine**	18.4 (17.0-19.8)	-
Malic acid	1073.65 (1018.7-1128.6)	-	**Malic acid**	1073.6 (992.9-1154.3)	-
Maltose	188.85 (137.2-240.5)	-	**Maltose**	74 (63.5-84.6)	-
Methionine	17.7 (15.6-19.9)	18	**Phenylalanine**	38.5 (35.2-41.7)	-
Phenylalanine	46.4 (42.7-50.1)	43	**Serine**	58.1 (47.3-69.0)	100
Proline	36.9 (36.2-37.7)	37	**Sucrose**	415.9 (378.6-453.3)	43
Serine	49.9 (40.8-59.1)	49	**Threonine**	20.9 (19.9-21.9)	-
Sucrose	355.35 (317.4-393.3)	-	**Tryptophan**	22.6 (22.3-22.9)	-
Threonine	21.15 (20.9-21.4)	29	**Tyrosine**	31.9 (31.7-32.1)	-
Tryptophan	8 (7-9)	10	**Valine**	39.4 (29.2-49.6)	54
Tyrosine	30.6 (30.5-30.7)	31			
Valine	38 (38-38)	54			

Continued.

Table 2.6.*Continued.*

Metabolites	Red beetroot	LV	Metabolites	Green bean	LV
4-aminobutyrate	58.1 (52.8-63.3)	-	**4-aminobutyrate**	83.9 (79.8-88.1)	-
Alanine	78.4 (77.1-79.8)	41	**Alanine**	103.7 (101.7-105.7)	94
Arginine	34.6 (33.3-35.8)	32	**Arginine**	35 (31.5-38.6)	70
Ascorbic acid	5.1 (4.8-5.4)	4.9	**Ascorbic acid**	16.9 (16.1-17.7)	12.1
Asparagine	53 (51.4-54.5)	-	**Asparagine**	45.7 (42.4-49)	-
Asparatic acid	63.9 (62.3-65.5)	86	**Aspartic acid**	264.8 (264.1-265.4)	260
Betaine	110.1 (109.0-112.2)	129	**Choline**	84.9 (70.9-99)	-
Choline	70.8 (69.9-71.8)	-	**Citric acid**	20 (17-23)	17
Formic acid	13.7 (13.14-4)	-	**Formic acid**	14.5 (14.2-14.8)	-
Fructose	248.9 (187.8-310.1)	290	**Fructose**	619.2 (532.7-714.8)	690
Glucose	374.3 (368.5-380.1)	350	**Glucose**	558.1 (448.6-667.6)	460
Glutamic acid	388 (384.9-391.1)	490	**Glutamic acid**	134 (122.4-145.6)	200
Glutamine	240.5 (225.2-255.8)	-	**Glutamine**	220.8 (208.1-233.4)	-
Glycine	32 (31.7-32.2)	30	**Glycine**	20.2 (19.1-21.4)	64
Histidine	8.9 (8.2-9.6)	18	**Isoleucine**	33.9 (33.2-34.6)	73
Isoleucine	29.4 (28.2-30.7)	32	**Leucine**	38 (34.6-41.5)	110
Leucine	25.0 (18.0-31.9)	35	**Lysine**	123.4 (114.8-132)	120
Lysine	65.8 (60.3-71.4)	140	**Methionine**	14.8 (11.5-18.1)	28
Phenylalanine	17.8 (17.4-18.1)	16	**Ornithine**	8.7 (7.8-9.7)	-
Proline	16.7 (15.6-17.8)	19	**Phenylalanine**	40.1 (36.3-43.9)	52
Serine	60.5 (60.3-60.7)	51	**Proline**	14.1 (12.9-15.2)	58
Sucrose	467.7 (44.62-489.3)	-	**Pyruvic acid**	9.8 (8.3-11.2)	-
Threonine	23.8 (22.2-25.3)	30	**Serine**	136 (135-136.9)	130
Tyrosine	17.6 (17-18.2)	14	**Succinic acid**	34.1 (31.4-36.7)	-
Tryptophan	8.5 (8.3-8.7)	9	**Sucrose**	227.3 (188.2-266.3	-
Valine	24 (23.9-24.1)	43	**Threonine**	84.9 (84.6-85.2)	79
			Tyrosine	60 (59.8-60.2)	40
			Valine	69.6 (65-74.2)	94

Continued.

Table 2.6.*Continued.*

Metabolites	Nanking cherry	LV	Metabolites	Saskatoon berry	LV
4-Aminobutyrate	48.1 (44.9-51.2)	-	**Acetic acid**	8.9 (8.6-9.3)	-
Acetic acid	12.2 (12-12.4)	-	**Alanine**	70.7 (67.3-74.2)	-
Alanine	12.1 (11.2-13)	-	**Alanine**	38.8 (38.2-39.4)	-
Arginine	37.4 (37.2-37.7)	-	**Arginine**	35.1 (32.4-37.7)	-
Ascorbic acid	24.1 (22.7-25.4)	-	**Ascorbic acid**	26.85 (23.8-29.9)	-
Asparagine	143.6 (125.5-161.7)	-	**Asparagine**	52.7 (47.2-58.3)	-
Aspartic acid	938.5 (866.6-1010.4)	-	**Aspartic acid**	34.3 (28.5-40)	-
Betaine	33.1 (32.4-33.8)	-	**Betaine**	42.2 (40.2-44.2)	-
Choline	14.1 (13.8-14.5)	-	**Choline**	8.5 (8.3-8.6)	-
Citric acid	23.2. (20.9-25.5)	-	**Citric acid**	39.1 (36.5-41.7)	-
Formic acid	18.0 (17.8-18.1)	-	**Formic acid**	7.7 (7.7-7.8)	
Fructose	673 (634.2-711.8)	-	**Fructose**	2157.1 (1944.4-2369.8)	-
Glucose	739.9 (704.2-775.6)	-	**Glucose**	2021.6 (1953.6-2089.7)	-
Glutamic acid	31.2 (28.3-34.2)	-	**Glutamine**	46.1 (38.4-53.8)	-
Glutamine	33.5 (32.7-34.2)	-	**Glycine**	28.6 (28.5-28.8)	-
Glycine	8.4 (8.1-8.7)	-	**Histidine**	10 (9.7-10.3)	-
Leucine	7.1 (5.5-8.6)	-	**Leucine**	34.8 (32.2-37.5)	-
Lysine	26.5 (25.7-27.3)	-	**Lysine**	23.5 (19-27.9)	-
Methionine	12.9 (11.7-14.1)		**Methionine**	14.8 (14-15.6)	-
Ornithine	10.1 (9.2-11.1)	-	**Ornithine**	73.4 (68.1-78.8)	-
Phenylalanine	17.2 (16.5-18)	-	**Phenylalanine**	22 (20.6-23.4)	-
Proline	34.2 (33-35.5)	-	**Proline**	13.2 (12.54-13.9)	-
Pyruvic acid	25.1 (24.9-25.3)	-	**Pyruvic acid**	16.5 (14.9.1-18.1)	-
Serine	62.6 (59.7-65.4)	-	**Serine**	23.2 (22.9-23.5)	-
Succinic acid	5.2 (4.5-5.9)	-	**Succinic acid**	6.6 (6.6-6.7)	-
Sucrose	235.9 (217.1-254.8)		**Sucrose**	549.5 (532.4-566.7)	-
Threonine	32.7 (32-33.4)	-	**Threonine**	10.1 (9.2-11.1)	-
Tryptophan	7.8 (7.4-8.3)	-	**Tryptophan**	8.5 (7.1-9.8)	-
Tyrosine	20.9 (19.3-22.6)	-	**Tyrosine**	12.7 (11.1-14.3)	-
Valine	17.8 (17.1-18.5)	-	**Valine**	30.9 (27.4-34.5)	-

Continued.

Table 2.6.*Continued.*

Metabolites	Cauliflower	LV	Metabolites	Sunburst squash	LV
4-Aminobutyrate	25.5 (21.7-29.4)	-	**4-aminobutyrate**	74.1 (67.9-80.3)	-
Acetic acid	11.9 (11.7-12.1)	-	**Alanine**	59.6 (57.5-61.7)	71
Alanine	170.1 (164.2-175.9)	180	**Arginine**	51.4 (50.5-52.3)	58
Arginine	50.3 (49.8-50.9)	91	**Asparagine**	161.3 (158.4-164.3)	-
Asparagine	175.2 (159.6-190.9)	-	**Aspartic acid**	134.8 (122.9-146.8)	160
Aspartic acid	186.2 (180.4-191.9)	190	**Betaine**	21.7 (20.9-22.5)	-
Betaine	14.6 (13-16.3)	-	**Choline**	53.8 (50.7-56.9)	-
Choline	40.9 (33.9-47.8)	-	**Citric acid**	44.9 (44.4-45.5)	-
Citric acid	21.2 (20.4-22)	-	**Ethanolamine**	12.3 (11.9-12.7)	-
Formic acid	21.4 (21.1-21.6)	-	**Formic acid**	15 (14.4-15.6)	-
Fructose	991.7 (902.6-1080.8)	1310	**Fructose**	1257.2 (1214.8-1299.7)	-
Glucose	798.9 (748-849.9)	510	**Glucose**	1081 (1027.6-1134.5)	700
Glutamic acid	116.8 (115.3-118.2)	260	**Glutamic acid**	164.6 (158.4-170.7)	140
Glutamine	235.2 (213-257.3)	-	**Glutamine**	258.6 (247.2-269.9)	-
Glycine	106.8 (100.3-113.4)	84	**Glycine**	58.8 (53.4-64.3)	51
Histidine	88.6 (87.7-89.5)	42	**Histidine**	70.8 (67.8-73.9)	-
Isoleucine	64.3 (63.8-64.7)	84	**Hypoxanthine**	9.4 (8.8-10)	-
Leucine	38.6 (33.3-43.9)	130	**Isoleucine**	45.9 (40.4-51.3)	49
Lysine	95.8 (85.2-106.3)	110	**Leucine**	72.3 (69.1-75.6)	80
Methionine	22.1 (20.4-23.7)	29	**Lysine**	74.8 (72.1-77.5)	
Ornithine	10.5 (9.1-11.8)	-	**Methionine**	20.1 (18.7-21.5)	20
Phenylalanine	58.6 (54.2-62.9)	80	**Ornithine**	13.7 (13.6-13.7)	-
Proline	84.5 (84.3-84.7)	100	**Phenylalanine**	40.6 (38.7-42.5)	47
Pyruvic acid	13.7 (12.2-15.2)	-	**Proline**	63.4 (45.8-81)	42
Serine	167.8 (165.1-170.4)	120	**Serine**	78 (68.2-87.8)	56
Succinic acid	4.9 (4.6-5.2)	-	**Sucrose**	150.8 (143.6-157.9)	-
Sucrose	326.4 (314.2-338.7)	-	**Threonine**	58.9 (58.6-59.2)	-
Threonine	91.8 (86.4-97.2)	80	**Tryptophan**	10.8 (9.9-11.8)	13
Tryptophan	22.5 (21.3-23.8)	27	**Tyrosine**	28.8 (27.9-29.8)	36
Tyrosine	27 (24.2-29.8)	49	**Valine**	75.4 (69.4-81.3)	60
Valine	128.9 (124.1-133.7)	110			

Table 2.7 Metabolite contents of fruits and vegetables as determined by DFI/LC-MS/MS (Conc. mg/100 g FW).

Metabolites	Green bell pepper	Green zucchini	Swiss chard
DL-Carnitine	0.12 (0.12-0.12)	-	-
Decanoyl-L carnitine	0.02 (0.01-0.03)	-	0.01 (0.008-0.01)
Decenoyl-L-carnitine	-	0.007 (0.006-0.008)	-
Decadienyl-L-carnitine	0.01 (0.009-0.02)	0.003 (0.002-0.004)	0.007 (0.006-0.008)
Dodecanoyl-L-carnitine	0.01 (0.009-0.01)	0.004 (0.002-0.006)	0.006 (0.005-0.007)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.05 (0.05-0.06)	-	-
Tetradecanoyl-L-carnitine	-	-	-
Tetradecenoyl-L-carnitine	0.001 (0.0009-0.001)	-	-
Hydroxytetradecenoyl-L-carnitine	0.001 (0.001-0.001)	0.0009 (0.0006-0.001)	-
Tetradecadienyl-L-carnitine	0.001 (0.001-0.001)	0.0006 (0.0005-0.0007)	-
Hydroxytetradecadienyl-L-carnitine	-	0.0008 (0.0006-0.001)	-
Hexadecanoyl-L-carnitine	-	0.001 (0.0005-0.002)	-
Hydroxyhexadecanoyl-L-carnitine	-	-	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.002 (0.002-0.002)	0.0005 (0.0004-0.0006)	-
Hydroxyhexadecadienyl-L-carnitine	0.003 (0.003-0.003)	-	-
Octadecanoyl-L-carnitine	0.001 (0.001-0.002)	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	-	-
Octadecadienyl-L-carnitine	0.001 (0.0009-0.001)	-	0.001 (0.001-0.001)
Acetyl-L-carnitine	-	-	0.004 (0.002-0.005)
Propionyl-L-carnitine	-	0.007 (0.006-0.008)	-
Malonyl-L-carnitine	-	0.003 (0.002-0.004)	-
Hydroxypropionyl-L-carnitine	0.002 (0.0008-0.002)	0.001 (0.001-0.002)	-
Propenyl-L-carnitine	-	0.003 (0.002-0.004)	0.005 (0.003-0.007)
Butyryl-L-carnitine	0.001 (0.001-0.001)	0.002 (0.002-0.002)	0.003 (0.002-0.004)
Butenyl-L-carnitine	0.008 (0.007-0.009)	0.003 (0.002-0.003)	0.004 (0.003-0.005)
Fumaryl-L-carnitine	-	-	-
Valeryl-L-carnitine	-	0.002 (0.002-0.003)	-
Methylglutaryl-L-carnitine	0.004 (0.003-0.004)	0.005 (0.005-0.006)	-
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.001 (0.001-0.002)	0.001 (0.0009-0.001)	-
Glutaryl-L-carnitine	0.003 (0.002-0.004)	-	-
Hexenoyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.002-0.002)	-
Pimelyl-L-carnitine	-	0.002 (0.002-0.003)	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.002 (0.001-0.003)	-	-

Continued.

[1] LV for Literature value. References for the LV's are provided in the AFCDB website.

Table 2.7.*Continued.*

Metabolites	Red bell pepper	Dill	Green bean
DL-Carnitine	0.18 (0.15-0.21)	-	0.21 (0.21-0.21)
Decanoyl-L carnitine	0.03 (0.02-0.04)	-	0.02 (0.01-0.02)
Decenoyl-L-carnitine	-	-	-
Decadienyl-L-carnitine	0.02 (0.01-0.02)	0.005 (0.005-0.005)	0.008 (0.008-0.008)
Dodecanoyl-L-carnitine	0.01 (0.01-0.01)	0.009 (0.009-0.009)	0.009 (0.009-0.009)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.02 (0.02-0.03)	-	0.03 (0.02-0.03)
Tetradecanoyl-L-carnitine	0.002 (0.001-0.003)	-	-
Tetradecenoyl-L-carnitine	0.002 (0.002-0.002)	0.001 (0.001-0.002)	-
Hydroxytetradecenoyl-L-carnitine	0.002 (0.001-0.002)	-	0.002 (0.002-0.002)
Tetradecadienyl-L-carnitine	0.002 (0.001-0.002)	0.001 (0.001-0.002)	0.002 (0.002-0.002)
Hydroxytetradecadienyl-L-carnitine	-	-	0.002 (0.001-0.002)
Hexadecanoyl-L-carnitine	0.002 (0.002-0.003)	0.002 (0.002-0.002)	0.003 (0.003-0.003)
Hydroxyhexadecanoyl-L-carnitine	0.004 (0.001-0.007)	0.001 (0.001-0.002)	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.003 (0.003-0.004)	0.001 (0.0009-0.001)	0.002 (0.002-0.002)
Hydroxyhexadecadienyl-L-carnitine	0.004 (0.003-0.004)	-	0.02 (0.01-0.02)
Octadecanoyl-L-carnitine	0.002 (0.002-0.002)	-	0.002 (0.002-0.002)
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	-	-
Octadecadienyl-L-carnitine	0.001 (0.001-0.001)	0.004 (0.001-0.007)	0.001 (0.001-0.002)
Acetyl-L-carnitine	-	-	0.008 (0.007-0.008)
Propionyl-L-carnitine	-	0.007 (0.006-0.008)	0.008 (0.008-0.008)
Malonyl-L-carnitine	-	0.003 (0.003-0.004)	1.4 (0.97-1.8)
Hydroxypropionyl-L-carnitine	0.003 (0.001-0.004)	-	0.002 (0.001-0.003)
Propenyl-L-carnitine	0.003 (0.001-0.005)	0.003 (0.002-0.003)	0.005 (0.003-0.006)
Butyryl-L-carnitine	0.003 (0.002-0.003)	0.002 (0.001-0.003)	0.004 (0.003-0.005)
Butenyl-L-carnitine	0.008 (0.005-0.01)	0.002 (0.001-0.002)	0.05 (0.01-0.09)
Fumaryl-L-carnitine	-	-	-
Valeryl-L-carnitine	-	-	0.005 (0.005-0.005)
Methylglutaryl-L-carnitine	0.006 (0.005-0.007)	-	-
Methylmalonyl-L-carnitine	-	-	0.007 (0.005-0.01)
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.002 (0.001-0.002)	0.001 (0.001-0.002)	0.002 (0.002-0.003)
Glutaryl-L-carnitine	0.003 (0.003-0.004)	0.002 (0.002-0.002)	0.002 (0.002-0.002)
Hexenoyl-L-carnitine	0.003 (0.002-0.004)	0.002 (0.001-0.002)	0.003 (0.003-0.003)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.003 (0.003-0.003)	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Japanese pumpkin	Saskatoon berry	Cucumber
DL-Carnitine	-	-	0.065 (0.060-0.070)
Decanoyl-L carnitine	0.02 (0.02-0.02)	0.12 (0.10-0.14)	0.007 (0.005-0.009)
Decenoyl-L-carnitine	0.02 (0.009-0.02)	0.07 (0.07-0.07)	-
Decadienyl-L-carnitine	0.01 (0.01-0.02)	0.05 (0.05-0.05)	0.005 (0.005-0.006)
Dodecanoyl-L-carnitine	0.09 (0.08-0.10)	0.06 (0.05-0.07)	0.003 (0.002-0.003)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.03 (0.03-0.04)	0.14 (0.10-0.18)	-
Tetradecanoyl-L-carnitine	0.008 (0.006-0.01)	0.02 (0.01-0.02)	-
Tetradecenoyl-L-carnitine	0.002 (0.001-0.002)	0.009 (0.008-0.009)	-
Hydroxytetradecenoyl-L-carnitine	0.004 (0.004-0.004)	0.02 (0.02-0.03)	-
Tetradecadienyl-L-carnitine	0.002 (0.001-0.002)	0.01 (0.009-0.01)	-
Hydroxytetradecadienyl-L-carnitine	0.004 (0.004-0.004)	0.008 (0.006-0.009)	-
Hexadecanoyl-L-carnitine	0.004 (0.004-0.005)	0.02 (0.02-0.03)	-
Hydroxyhexadecanoyl-L-carnitine	0.005 (0.004-0.005)	0.02 (0.02-0.02)	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	0.002 (0.002-0.003)	0.02 (0.02-0.02)	-
Hexadecadienyl-L-carnitine	0.001 (0.0008-0.002)	0.006 (0.004-0.007)	0.0007 (0.0004-0.001)
Hydroxyhexadecadienyl-L-carnitine	0.004 (0.003-0.005)	0.03 (0.03-0.03)	-
Octadecanoyl-L-carnitine	0.002 (0.002-0.002)	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	0.005 (0.004-0.005)	0.01 (0.01-0.02)	-
Octadecadienyl-L-carnitine	0.001 (0.001-0.001)	0.007 (0.007-0.007)	-
Acetyl-L-carnitine	-	0.08 (0.06-0.11)	-
Propionyl-L-carnitine	-	0.03 (0.02-0.03)	0.003 (0.003-0.003)
Malonyl-L-carnitine	0.01 (0.007-0.01)	0.13 (0.10-0.16)	0.03 (0.02-0.04)
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	0.003 (0.002-0.005)	0.02 (0.01-0.02)	0.001 (0.001-0.002)
Butyryl-L-carnitine	-	0.009 (0.009-0.009)	0.001 (0.001-0.001)
Butenyl-L-carnitine	0.004 (0.003-0.004)	0.05 (0.03-0.07)	0.005 (0.004-0.005)
Fumaryl-L-carnitine	0.008 (0.007-0.009)	-	-
Valeryl-L-carnitine	-	-	-
Methylglutaryl-L-carnitine	0.01 (0.01-0.01)	0.04 (0.04-0.04)	0.002 (0.002-0.003)
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.001 (0.001-0.002)	0.04 (0.02-0.07)	0.0008 (0.0008-0.0009)
Glutaryl-L-carnitine	0.003 (0.003-0.003)	0.05 (0.0-0.09)	0.001 (0.001-0.001)
Hexenoyl-L-carnitine	0.005 (0.005-0.006)	0.04 (0.02-0.06)	0.001 (0.001-0.001)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.004 (0.003-0.004)	0.06 (0.05-0.06)	-

Continued.

Table 2.7.*Continued.*

Metabolites	White cabbage	Carrot	Yellow bean
DL-Carnitine	0.08 (0.05-0.12)	0.26 (0.22-0.30)	0.27 (0.14-0.40)
Decanoyl-L carnitine	0.03 (0.02-0.04)	0.04 (0.03-0.04)	0.02 (0.01-0.03)
Decenoyl-L-carnitine	0.004 (0.003-0.005)	-	-
Decadienyl-L-carnitine	0.004 (0.003-0.006)	0.005 (0.004-0.005)	0.008 (0.008-0.009)
Dodecanoyl-L-carnitine	0.01 (0.01-0.02)	0.05 (0.05-0.05)	0.01 (0.009-0.01)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.01 (0.01-0.02)	0.02 (0.02-0.02)	0.03 (0.03-0.04)
Tetradecanoyl-L-carnitine	-	0.002 (0.002-0.002)	0.003 (0.002-0.004)
Tetradecenoyl-L-carnitine	0.0007 (0.0005-0.0009)	-	-
Hydroxytetradecenoyl-L-carnitine	-	-	0.001 (0.001-0.002)
Tetradecadienyl-L-carnitine	-	0.001 (0.001-0.001)	0.002 (0.001-0.002)
Hydroxytetradecadienyl-L-carnitine	-	-	-
Hexadecanoyl-L-carnitine	0.001 (0.001-0.002)	-	0.003 (0.002-0.004)
Hydroxyhexadecanoyl-L-carnitine	-	-	0.001 (0.001-0.002)
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.0005 (0.0005-0.0005)	0.0006 (0.0006-0.0006)	0.001 (0.001-0.002)
Hydroxyhexadecadienyl-L-carnitine	-	-	0.01 (0.01-0.01)
Octadecanoyl-L-carnitine	-	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	-	0.002 (0.002-0.002)
Octadecadienyl-L-carnitine	0.001 (0.001-0.001)	0.0006 (0.0006-0.0007)	-
Acetyl-L-carnitine	-	-	-
Propionyl-L-carnitine	0.002 (0.001-0.002)	-	0.006 (0.004-0.008)
Malonyl-L-carnitine	0.05 (0.05-0.05)	0.006 (0.006-0.006)	2.9 (2.7-3.0)
Hydroxypropionyl-L-carnitine	0.002 (0.001-0.002)	-	0.002 (0.001-0.003)
Propenyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.001-0.002)	0.004 (0.003-0.004)
Butyryl-L-carnitine	0.001 (0.001-0.002)	0.002 (0.001-0.003)	0.005 (0.005-0.006)
Butenyl-L-carnitine	0.006 (0.005-0.007)	0.01 (0.008-0.01)	0.02 (0.01-0.03)
Fumaryl-L-carnitine	-	0.005 (0.004-0.006)	0.003 (0.002-0.005)
Valeryl-L-carnitine	0.001 (0.001-0.002)	0.003 (0.002-0.004)	0.004 (0.004-0.004)
Methylglutaryl-L-carnitine	0.003 (0.002-0.003)	0.007 (0.006-0.008)	0.005 (0.005-0.005)
Methylmalonyl-L-carnitine	-	-	0.01 (0.01-0.02)
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.0009 (0.0009-0.001)	0.002 (0.002-0.002)	0.004 (0.004-0.005)
Glutaryl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.001-0.002)	0.002 (0.002-0.002)
Hexenoyl-L-carnitine	0.003 (0.003-0.003)	0.004 (0.003-0.005)	0.002 (0.002-0.003)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Sunburst squash	Nanking cherry	Broccoli
DL-Carnitine	-	-	-
Decanoyl-L carnitine	-	0.02 (0.01-0.02)	0.006 (0.006-0.006)
Decenoyl-L-carnitine	0.01 (0.01-0.01)	0.01 (0.01-0.01)	0.007 (0.005-0.009)
Decadienyl-L-carnitine	0.005 (0.003-0.006)	0.006 (0.005-0.007)	0.007 (0.007-0.008)
Dodecanoyl-L-carnitine	0.02 (0.02-0.03)	0.02 (0.01-0.02)	0.008 (0.008-0.008)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.02 (0.02-0.02)	0.02 (0.01-0.03)	-
Tetradecanoyl-L-carnitine	-	-	-
Tetradecenoyl-L-carnitine	0.002 (0.001-0.002)	-	0.002 (0.002-0.002)
Hydroxytetradecenoyl-L-carnitine	0.002 (0.002-0.002)	-	-
Tetradecadienyl-L-carnitine	0.002 (0.002-0.002)	-	0.001 (0.001-0.002)
Hydroxytetradecadienyl-L-carnitine	0.001 (0.001-0.002)	-	-
Hexadecanoyl-L-carnitine	0.002 (0.002-0.002)	-	0.0034(0.0028-0.0041)
Hydroxyhexadecanoyl-L-carnitine	0.001 (0.0009-0.001)	-	0.001 (0.001-0.001)
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.0007 (0.0007-0.0007)	-	0.001 (0.001-0.001)
Hydroxyhexadecadienyl-L-carnitine	0.002 (0.001-0.002)	-	-
Octadecanoyl-L-carnitine	-	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	0.001 (0.001-0.002)	0.003 (0.002-0.004)	-
Octadecadienyl-L-carnitine	0.002 (0.001-0.002)	-	0.0007 (0.0006-0.0008)
Acetyl-L-carnitine	-	0.004 (0.002-0.006)	-
Propionyl-L-carnitine	0.008 (0.008-0.008)	-	0.003 (0.003-0.003)
Malonyl-L-carnitine	-	-	0.05 (0.02-0.07)
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	0.003 (0.003-0.003)	0.002 (0.002-0.003)	0.003 (0.002-0.004)
Butyryl-L-carnitine	0.002 (0.002-0.002)	0.001 (0.0009-0.001)	0.002 (0.002-0.002)
Butenyl-L-carnitine	0.007 (0.007-0.007)	0.007 (0.004-0.009)	0.002 (0.002-0.003)
Fumaryl-L-carnitine	-	-	-
Valeryl-L-carnitine	0.002 (0.001-0.003)	-	0.004 (0.003-0.005)
Methylglutaryl-L-carnitine	0.006 (0.006-0.006)	0.004 (0.004-0.005)	-
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.001-0.002)	0.001 (0.001-0.001)
Glutaryl-L-carnitine	0.001 (0.001-0.002)	-	0.003 (0.003-0.003)
Hexenoyl-L-carnitine	0.002 (0.001-0.002)	0.003 (0.002-0.004)	0.002 (0.001-0.002)
Pimelyl-L-carnitine	0.001 (0.001-0.002)	-	0.002 (0.001-0.002)
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	-	0.01 (0.01-0.01)	-

Continued.

Table 2.7.*Continued.*

Metabolites	Turnip	Onion	Lettuce
DL-Carnitine	0.28 (0.20-0.37)	-	0.13 (0.09-0.17)
Decanoyl-L carnitine	0.06 (0.02-0.10)	0.01 (0.0113-0.0134)	0.009 (0.008-0.01)
Decenoyl-L-carnitine	0.02 (0.01-0.03)	-	-
Decadienyl-L-carnitine	0.07 (0.06-0.07)	0.01 (0.0101-0.0202)	0.004 (0.004-0.005)
Dodecanoyl-L-carnitine	0.06 (0.02-0.10)	0.16 (0.117-0.214)	0.005 (0.004-0.005)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.13 (0.12-0.13)	0.07 (0.071-0.0733)	0.01 (0.01-0.01)
Tetradecanoyl-L-carnitine	0.006 (0.005-0.007)	-	-
Tetradecenoyl-L-carnitine	0.003 (0.003-0.004)	-	-
Hydroxytetradecenoyl-L-carnitine	-	-	-
Tetradecadienyl-L-carnitine	0.002 (0.001-0.003)	-	0.002 (0.001-0.002)
Hydroxytetradecadienyl-L-carnitine	-	-	-
Hexadecanoyl-L-carnitine	0.004 (0.002-0.005)	-	-
Hydroxyhexadecanoyl-L-carnitine	-	-	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.002 (0.001-0.002)	0.001 (0.0012-0.0018)	0.0005 (0.0005-0.0005)
Hydroxyhexadecadienyl-L-carnitine	-	-	-
Octadecanoyl-L-carnitine	-	-	-
Octadecenoyl-L-carnitine	-	0.009 (0.0085-0.0093)	-
Hydroxyoctadecenoyl-L-carnitine	-	0.005 (0.0036-0.0058)	-
Octadecadienyl-L-carnitine	0.008 (0.003-0.01)	0.0009 (0.0007-0.0011)	-
Acetyl-L-carnitine	0.02 (0.007-0.03)	0.01 (0.0083-0.0113)	-
Propionyl-L-carnitine	-	0.08 (0.074-0.079)	0.003 (0.003-0.003)
Malonyl-L-carnitine	0.10 (0.02-0.18)	0.03 (0.024-0.033)	0.002 (0.002-0.003)
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	0.004 (0.004-0.005)	0.002 (0.0016-0.0024)	0.002 (0.002-0.003)
Butyryl-L-carnitine	0.004 (0.004-0.005)	0.002 (0.0022-0.0028)	0.001 (0.001-0.001)
Butenyl-L-carnitine	0.05 (0.04-0.05)	0.004 (0.0037-0.0045)	0.006 (0.005-0.006)
Fumaryl-L-carnitine	-	0.007 (0.0072-0.0076)	-
Valeryl-L-carnitine	0.01 (0.01-0.01)	-	-
Methylglutaryl-L-carnitine	0.01 (0.007-0.02)	0.02 (0.0155-0.018)	0.003 (0.003-0.003)
Methylmalonyl-L-carnitine	-	0.04 (0.0353-0.0408)	-
Tiglyl-L-carnitine	-	0.003 (0.003-0.0033)	-
Glutaconyl-L-carnitine	0.006 (0.006-0.006)	0.001 (0.001-0.0017)	0.001 (0.0009-0.001)
Glutaryl-L-carnitine	-	0.005 (0.002-0.0071)	0.001 (0.001-0.001)
Hexenoyl-L-carnitine	0.03 (0.02-0.03)	-	0.001 (0.001-0.002)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	-	-	0.002 (0.001-0.002)

Continued.

Table 2.7.*Continued.*

Metabolites	Potato	Raspberry	Yellow zucchini
DL-Carnitine	0.37 (0.32-0.42)	-	-
Decanoyl-L carnitine	-	0.02 (0.01-0.02)	0.04 (0.04-0.05)
Decenoyl-L-carnitine	-	0.01 (0.009-0.01)	0.01 (0.01-0.01)
Decadienyl-L-carnitine	0.03 (0.02-0.04)	0.01 (0.009-0.01)	0.009 (0.009-0.009)
Dodecanoyl-L-carnitine	0.02 (0.01-0.02)	0.01 (0.01-0.02)	0.01 (0.01-0.02)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	-	0.03 (0.02-0.03)	0.02 (0.02-0.02)
Tetradecanoyl-L-carnitine	0.008 (0.006-0.009)	0.003 (0.003-0.003)	-
Tetradecenoyl-L-carnitine	-	0.002 (0.002-0.002)	-
Hydroxytetradecenoyl-L-carnitine	-	0.004 (0.004-0.005)	0.003 (0.003-0.003)
Tetradecadienyl-L-carnitine	0.003 (0.002-0.003)	0.002 (0.002-0.002)	0.002 (0.002-0.003)
Hydroxytetradecadienyl-L-carnitine	-	0.002 (0.001-0.002)	0.002 (0.002-0.003)
Hexadecanoyl-L-carnitine	0.004 (0.003-0.004)	0.004 (0.003-0.005)	0.002 (0.002-0.003)
Hydroxyhexadecanoyl-L-carnitine	-	0.003 (0.002-0.003)	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	0.003 (0.002-0.003)	-
Hexadecadienyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.001-0.003)	0.001 (0.001-0.002)
Hydroxyhexadecadienyl-L-carnitine	-	0.007 (0.005-0.009)	-
Octadecanoyl-L-carnitine	-	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	0.003(0.003-0.003)	-
Octadecadienyl-L-carnitine	-	0.002 (0.001-0.002)	0.001 (0.001-0.001)
Acetyl-L-carnitine	0.02 (0.01-0.02)	0.03 (0.03-0.03)	-
Propionyl-L-carnitine	-	0.004 (0.004-0.005)	0.01 (0.01-0.01)
Malonyl-L-carnitine	0.02 (0.01-0.02)	0.03 (0.03-0.04)	0.006 (0.004-0.008)
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	0.004 (0.004-0.004)	0.003 (0.002-0.004)	0.006 (0.005-0.007)
Butyryl-L-carnitine	0.004 (0.004-0.004)	0.002 (0.002-0.002)	0.003 (0.002-0.003)
Butenyl-L-carnitine	-	0.01 (0.01-0.01)	0.01 (0.01-0.01)
Fumaryl-L-carnitine	-	-	-
Valeryl-L-carnitine	-	-	-
Methylglutaryl-L-carnitine	-	0.006 (0.005-0.007)	0.01 (0.01-0.02)
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.002 (0.002-0.002)	0.006 (0.005-0.006)	0.003 (0.003-0.003)
Glutaryl-L-carnitine	0.006 (0.005-0.007)	-	-
Hexenoyl-L-carnitine	0.004 (0.003-0.005)	0.004 (0.004-0.005)	0.004 (0.004-0.004)
Pimelyl-L-carnitine	-	-	0.004 (0.003-0.005)
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	-	0.02 (0.01-0.02)	-

Continued.

Table 2.7.*Continued.*

Metabolites	Yellow bell pepper	Garlic	Eggplant
DL-Carnitine	0.09 (0.09-0.09)	1.9 (1.6-2.3)	-
Decanoyl-L carnitine	0.03 (0.01-0.06)	-	0.008 (0.007-0.009)
Decenoyl-L-carnitine	-	0.04 (0.03-0.05)	-
Decadienyl-L-carnitine	0.02 (0.02-0.02)	0.05 (0.05-0.05)	0.005 (0.005-0.006)
Dodecanoyl-L-carnitine	0.01 (0.01-0.02)	0.10 (0.10-0.10)	0.01 (0.01-0.01)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.02 (0.01-0.02)	0.09 (0.09-0.10)	-
Tetradecanoyl-L-carnitine	0.002 (0.002-0.003)	0.01 (0.01-0.01)	0.002 (0.002-0.003)
Tetradecenoyl-L-carnitine	0.001 (0.001-0.002)	-	-
Hydroxytetradecenoyl-L-carnitine	0.001 (0.0009-0.001)	0.02 (0.01-0.03)	-
Tetradecadienyl-L-carnitine	0.001 (0.0009-0.001)	0.005 (0.004-0.005)	-
Hydroxytetradecadienyl-L-carnitine	0.0009 (0.0009-0.0009)	0.004 (0.003-0.005)	-
Hexadecanoyl-L-carnitine	0.002 (0.002-0.002)	0.006 (0.004-0.007)	-
Hydroxyhexadecanoyl-L-carnitine	0.002 (0.001-0.002)	0.008 (0.006-0.01)	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	0.007 (0.006-0.007)	-
Hexadecadienyl-L-carnitine	0.002 (0.002-0.003)	0.006 (0.005-0.007)	-
Hydroxyhexadecadienyl-L-carnitine	0.002 (0.002-0.003)	0.05 (0.01-0.10)	-
Octadecanoyl-L-carnitine	0.001 (0.001-0.001)	0.01 (0.01-0.01)	-
Octadecenoyl-L-carnitine	-	0.02 (0.02-0.03)	-
Hydroxyoctadecenoyl-L-carnitine	0.001 (0.001-0.001)	0.009 (0.008-0.01)	-
Octadecadienyl-L-carnitine	0.002 (0.002-0.002)	0.008 (0.007-0.008)	-
Acetyl-L-carnitine	-	0.06 (0.05-0.06)	-
Propionyl-L-carnitine	-	0.02 (0.01-0.02)	-
Malonyl-L-carnitine	-	0.06 (0.05-0.07)	-
Hydroxypropionyl-L-carnitine	0.003 (0.003-0.003)	-	-
Propenyl-L-carnitine	-	0.009 (0.008-0.009)	0.003 (0.002-0.003)
Butyryl-L-carnitine	0.001 (0.001-0.001)	0.01 (0.01-0.01)	-
Butenyl-L-carnitine	0.01 (0.01-0.01)	-	0.005 (0.004-0.005)
Fumaryl-L-carnitine	-	-	-
Valeryl-L-carnitine	-	0.03 (0.02-0.04)	-
Methylglutaryl-L-carnitine	0.004 (0.003-0.004)	0.01 (0.01-0.02)	-
Methylmalonyl-L-carnitine	0.004 (0.004-0.004)	0.03 (0.03-0.03)	-
Tiglyl-L-carnitine	-	0.01 (0.01-0.01)	-
Glutaconyl-L-carnitine	0.001 (0.001-0.001)	0.02 (0.02-0.02)	0.0008(0.0007-0.0009)
Glutaryl-L-carnitine	0.004 (0.004-0.004)	0.01 (0.01-0.02)	-
Hexenoyl-L-carnitine	0.003 (0.002-0.003)	0.03 (0.02-0.03)	0.002 (0.002-0.002)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.002 (0.002-0.002)	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Spinach	Crab apple	Tomato
DL-Carnitine	-	0.14 (0.11-0.17)	0.11 (0.08-0.13)
Decanoyl-L carnitine	-	-	0.007 (0.006-0.008)
Decenoyl-L-carnitine	0.01 (0.01-0.01)	-	-
Decadienyl-L-carnitine	0.006 (0.005-0.007)	0.01 (0.01-0.02)	0.002 (0.002-0.003)
Dodecanoyl-L-carnitine	0.009 (0.009-0.009)	0.007 (0.005-0.008)	0.06 (0.05-0.08)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	-	-	0.02 (0.02-0.03)
Tetradecanoyl-L-carnitine	-	0.003 (0.002-0.003)	0.004 (0.004-0.004)
Tetradecenoyl-L-carnitine	-	-	-
Hydroxytetradecenoyl-L-carnitine	0.002 (0.001-0.002)	-	-
Tetradecadienyl-L-carnitine	0.002 (0.002-0.002)	0.001 (0.0009-0.001)	-
Hydroxytetradecadienyl-L-carnitine	-	-	-
Hexadecanoyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.002-0.002)	-
Hydroxyhexadecanoyl-L-carnitine	0.002 (0.001-0.002)	-	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	0.002 (0.002-0.002)	-	-
Hexadecadienyl-L-carnitine	0.001 (0.0009-0.001)	0.0007 (0.0006-0.0008)	0.0008 (0.0006-0.001)
Hydroxyhexadecadienyl-L-carnitine	0.007 (0.005-0.009)	-	-
Octadecanoyl-L-carnitine	-	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	0.002 (0.002-0.002)	-	0.003 (0.003-0.003)
Octadecadienyl-L-carnitine	0.0008 (0.0008-0.0009)	-	-
Acetyl-L-carnitine	-	0.007 (0.007-0.008)	-
Propionyl-L-carnitine	-	-	-
Malonyl-L-carnitine	0.01 (0.007-0.01)	0.01 (0.01-0.01)	-
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	0.005 (0.003-0.006)	0.002 (0.002-0.002)	0.002 (0.002-0.002)
Butyryl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.002-0.002)	-
Butenyl-L-carnitine	0.001 (0.001-0.001)	-	-
Fumaryl-L-carnitine	-	-	0.01 (0.008-0.01)
Valeryl-L-carnitine	-	-	-
Methylglutaryl-L-carnitine	-	-	0.01 (0.01-0.02)
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.001 (0.0007-0.001)	0.0009 (0.0008-0.001)	0.0006 (0.0004-0.0007)
Glutaryl-L-carnitine	-	0.003 (0.003-0.003)	-
Hexenoyl-L-carnitine	0.002 (0.002-0.002)	0.003 (0.002-0.003)	-
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.003 (0.002-0.003)	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Orange bell pepper	Red beet root	Parsnip
DL-Carnitine	0.15 (0.14-0.16)	0.17 (0.16-0.18)	-
Decanoyl-L carnitine	0.03 (0.02-0.04)	0.01 (0.01-0.01)	0.04 (0.04-0.04)
Decenoyl-L-carnitine	-	-	-
Decadienyl-L-carnitine	0.01 (0.01-0.01)	0.004 (0.004-0.004)	0.04 (0.03-0.05)
Dodecanoyl-L-carnitine	0.01 (0.01-0.01)	0.14 (0.11-0.17)	0.25 (0.24-0.25)
Dodecanedioyl-L-carnitine	-	-	-
Dodecenoyl-L-carnitine	0.03 (0.03-0.03)	0.03 (0.03-0.03)	0.10 (0.08-0.12)
Tetradecanoyl-L-carnitine	0.004 (0.004-0.004)	0.007 (0.006-0.007)	0.03 (0.02-0.03)
Tetradecenoyl-L-carnitine	-	-	-
Hydroxytetradecenoyl-L-carnitine	0.002 (0.001-0.003)	-	-
Tetradecadienyl-L-carnitine	0.002 (0.002-0.002)	-	0.002 (0.002-0.002)
Hydroxytetradecadienyl-L-carnitine	-	-	-
Hexadecanoyl-L-carnitine	0.002 (0.002-0.002)	-	0.01 (0.009-0.01)
Hydroxyhexadecanoyl-L-carnitine	0.002 (0.002-0.002)	-	-
Hexadecenoyl-L-carnitine	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-
Hexadecadienyl-L-carnitine	0.002 (0.002-0.003)	0.001 (0.0008-0.001)	-
Hydroxyhexadecadienyl-L-carnitine	0.004 (0.004-0.004)	-	-
Octadecanoyl-L-carnitine	0.002 (0.001-0.002)	-	-
Octadecenoyl-L-carnitine	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	0.003 (0.003-0.004)	0.006 (0.005-0.007)
Octadecadienyl-L-carnitine	0.001 (0.001-0.002)	-	-
Acetyl-L-carnitine	-	-	-
Propionyl-L-carnitine	-	-	-
Malonyl-L-carnitine	-	-	-
Hydroxypropionyl-L-carnitine	-	-	-
Propenyl-L-carnitine	-	0.003 (0.002-0.004)	0.01 (0.01-0.02)
Butyryl-L-carnitine	0.002 (0.002-0.002)	-	0.009 (0.004-0.01)
Butenyl-L-carnitine	0.01 (0.01-0.02)	-	0.007 (0.007-0.008)
Fumaryl-L-carnitine	-	0.01 (0.01-0.01)	0.02 (0.02-0.03)
Valeryl-L-carnitine	-	-	-
Methylglutaryl-L-carnitine	0.005 (0.004-0.006)	0.01 (0.01-0.02)	0.04 (0.04-0.04)
Methylmalonyl-L-carnitine	-	-	-
Tiglyl-L-carnitine	-	-	-
Glutaconyl-L-carnitine	0.002 (0.001-0.002)	0.001 (0.001-0.001)	0.006 (0.006-0.006)
Glutaryl-L-carnitine	0.003 (0.003-0.003)	-	0.01 (0.0-0.01)
Hexenoyl-L-carnitine	0.003 (0.003-0.003)	-	0.008 (0.007-0.009)
Pimelyl-L-carnitine	-	-	-
Octanoyl-L-carnitine	-	-	-
Nonayl-L-carnitine	0.002 (0.002-0.003)	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Italian red pepper	Cauliflower
DL-Carnitine	0.17 (0.15-0.18)	0.49 (0.47-0.50)
Decanoyl-L carnitine	0.05 (0.05-0.06)	0.03 (0.02-0.03)
Decenoyl-L-carnitine	-	0.02 (0.02-0.02)
Decadienyl-L-carnitine	0.05 (0.05-0.05)	0.03 (0.02-0.03)
Dodecanoyl-L-carnitine	0.02 (0.02-0.02)	0.03 (0.03-0.04)
Dodecanedioyl-L-carnitine	-	-
Dodecenoyl-L-carnitine	0.03 (0.03-0.04)	-
Tetradecanoyl-L-carnitine	0.003 (0.002-0.004)	-
Tetradecenoyl-L-carnitine	0.002 (0.002-0.002)	0.009 (0.008-0.009)
Hydroxytetradecenoyl-L-carnitine	0.001 (0.001-0.001)	-
Tetradecadienyl-L-carnitine	0.002 (0.001-0.002)	0.005 (0.004-0.006)
Hydroxytetradecadienyl-L-carnitine	-	-
Hexadecanoyl-L-carnitine	0.003 (0.002-0.003)	0.02 (0.01-0.02)
Hydroxyhexadecanoyl-L-carnitine	0.002 (0.001-0.002)	0.005 (0.004-0.006)
Hexadecenoyl-L-carnitine	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-
Hexadecadienyl-L-carnitine	0.003 (0.003-0.004)	0.004 (0.003-0.004)
Hydroxyhexadecadienyl-L-carnitine	0.004 (0.004-0.004)	-
Octadecanoyl-L-carnitine	0.002 (0.002-0.002)	-
Octadecenoyl-L-carnitine	-	-
Hydroxyoctadecenoyl-L-carnitine	-	-
Octadecadienyl-L-carnitine	0.002 (0.002-0.002)	0.002 (0.002-0.003)
Acetyl-L-carnitine	-	-
Propionyl-L-carnitine	-	0.01 (0.01-0.01)
Malonyl-L-carnitine	-	0.28 (0.25-0.31)
Hydroxypropionyl-L-carnitine	0.006 (0.004-0.008)	-
Propenyl-L-carnitine	0.002 (0.002-0.003)	0.006 (0.006-0.007)
Butyryl-L-carnitine	0.002 (0.002-0.002)	0.008 (0.007-0.009)
Butenyl-L-carnitine	0.01 (0.01-0.01)	0.01 (0.01-0.01)
Fumaryl-L-carnitine	-	-
Valeryl-L-carnitine	-	0.01 (0.01-0.01)
Methylglutaryl-L-carnitine	0.007 (0.006-0.009)	-
Methylmalonyl-L-carnitine	-	-
Tiglyl-L-carnitine	-	-
Glutaconyl-L-carnitine	0.002 (0.002-0.003)	0.004 (0.004-0.005)
Glutaryl-L-carnitine	0.003 (0.001-0.005)	0.01 (0.01-0.01)
Hexenoyl-L-carnitine	0.006 (0.005-0.006)	0.007 (0.006-0.007)
Pimelyl-L-carnitine	-	0.006 (0.005-0.007)
Octanoyl-L-carnitine	-	-
Nonayl-L-carnitine	0.003 (0.003-0.004)	-

Continued.

Table 2.7.*Continued.*

Metabolites	Green bell pepper	Green zucchini	Japanese pumpkin
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.08 (0.08-0.09)	0.15 (0.14-0.16)	0.68 (0.68-0.68)
lysoPhosphatidylcholine acyl C16:1	0.01 (0.01-0.01)	0.005 (0.004-0.006)	0.01 (0.01-0.02)
lysoPhosphatidylcholine acyl C17:0	-	0.012 (0.004-0.02)	0.008 (0.007-0.009)
lysoPhosphatidylcholine acyl C18:0	0.02 (0.01-0.03)	0.01 (0.01-0.01)	0.02 (0.02-0.02)
lysoPhosphatidylcholine acyl C18:1	-	0.01 (0.01-0.01)	1.7 (1.5-1.8)
lysoPhosphatidylcholine acyl C18:2	0.42 (0.33-0.51)	0.05 (0.01-0.08)	0.43 (0.005-0.86)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	0.003 (0.002-0.004)	0.002 (0.002-0.002)	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	0.001 (0.001-0.001)	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	-	-	-
Phosphatidylcholine diacyl C 34:1	0.009 (0.009-0.009)	-	0.06 (0.06-0.06)
Phosphatidylcholine diacyl C 34:2	0.15 (0.11-0.18)	0.02 (0.01-0.03)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 34:3	0.04 (0.03-0.04)	0.02 (0.01-0.02)	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 34:4	0.001 (0.001-0.001)	0.0006 (0.0004-0.0007)	-
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	0.03 (0.01-0.04)	-	0.05 (0.03-0.06)
Phosphatidylcholine diacyl C 36:3	0.01 (0.01-0.01)	-	0.02 (0.01-0.02)
Phosphatidylcholine diacyl C 36:4	0.05 (0.04-0.06)	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 36:5	0.02 (0.02-0.02)	0.007 (0.006-0.009)	0.003 (0.003-0.003)
Phosphatidylcholine diacyl C 36:6	0.008 (0.007-0.009)	0.003 (0.003-0.004)	-
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	-	-	-
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	-
Phosphatidylcholine diacyl C 40:3	-	-	-
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Swiss chard	Red bell pepper	Dill
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.03 (0.02-0.05)	0.15 (0.12-0.18)	0.08 (0.08-0.08)
lysoPhosphatidylcholine acyl C16:1	-	0.009 (0.009-0.009)	-
lysoPhosphatidylcholine acyl C17:0	-	-	-
lysoPhosphatidylcholine acyl C18:0	0.01 (0.01-0.02)	0.03 (0.02-0.04)	0.01 (0.01-0.01)
lysoPhosphatidylcholine acyl C18:1	0.03 (0.03-0.04)	0.01 (0.01-0.02)	-
lysoPhosphatidylcholine acyl C18:2	0.26 (0.23-0.29)	0.31 (0.20-0.41)	0.10 (0.01-0.18)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	0.03 (0.02-0.03)	0.004 (0.003-0.005)	0.002 (0.002-0.003)
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	0.002 (0.001-0.003)	-	0.003 (0.003-0.003)
Phosphatidylcholine diacyl C 34:1	0.01 (0.01-0.01)	-	0.03 (0.02-0.05)
Phosphatidylcholine diacyl C 34:2	0.06 (0.06-0.06)	0.04 (0.04-0.04)	0.39 (0.39-0.40)
Phosphatidylcholine diacyl C 34:3	0.03 (0.03-0.03)	0.01 (0.01-0.02)	0.16 (0.15-0.17)
Phosphatidylcholine diacyl C 34:4	-	-	0.009 (0.006-0.01)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	-	-	0.11 (0.03-0.18)
Phosphatidylcholine diacyl C 36:3	0.06 (0.008-0.10)	0.006 (0.006-0.007)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 36:4	0.04 (0.04-0.05)	0.03 (0.02-0.03)	0.30 (0.21-0.38)
Phosphatidylcholine diacyl C 36:5	0.02 (0.02-0.02)	0.01(0.01-0.01)	0.21 (0.12-0.29)
Phosphatidylcholine diacyl C 36:6	0.007 (0.005-0.008)	-	0.09 (0.04-0.14)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	-	-	0.004 (0.002-0.005)
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	-
Phosphatidylcholine diacyl C 40:3	-	-	-
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Green bell pepper	Green zucchini	Japanese pumpkin
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	-	0.007 (0.007-0.008)	0.03 (0.01-0.05)
Phosphatidylcholine diacyl C 42:2	0.01 (0.01-0.02)	0.004 (0.004-0.005)	0.005 (0.005-0.006)
Phosphatidylcholine diacyl C 42:4	-	0.0007 (0.0005-0.0008)	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	-	0.002 (0.001-0.002)	-
Phosphatidylcholine acyl-alkyl C 34:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:3	-	-	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.003 (0.002-0.003)	0.003 (0.003-0.003)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 36:3	0.001 (0.001-0.001)	0.001 (0.001-0.001)	-
Phosphatidylcholine acyl-alkyl C 36:4	0.004 (0.002-0.006)	-	-
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	-
Phosphatidylcholine acyl-alkyl C 38:3	-	-	0.001 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 38:4	0.01 (0.01-0.02)	-	-
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	-
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.11 (0.06-0.15)	0.05 (0.05-0.05)	0.07 (0.07-0.07)
Phosphatidylcholine acyl-alkyl C 42:1	0.008 (0.006-0.01)	0.004 (0.004-0.004)	-
Phosphatidylcholine acyl-alkyl C 42:2	-	0.001 (0.001-0.001)	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 42:3	0.001 (0.001-0.002)	0.001 (0.001-0.001)	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.003 (0.002-0.005)	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 44:4	0.002 (0.001-0.003)	0.004 (0.003-0.004)	0.005 (0.005-0.006)
Phosphatidylcholine acyl-alkyl C 44:5	0.007 (0.006-0.008)	-	0.004 (0.004-0.005)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Swiss chard	Red bell pepper	Dill
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	-	0.001 (0.001-0.002)	0.004 (0.003-0.004)
Phosphatidylcholine diacyl C 42:2	0.01 (0.01-0.02)	0.004 (0.002-0.01)	0.006 (0.005-0.006)
Phosphatidylcholine diacyl C 42:4	-	-	0.002 (0.001-0.003)
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	-	-	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 34:2	-	-	0.008 (0.008-0.008)
Phosphatidylcholine acyl-alkyl C 34:3	-	-	0.009 (0.004-0.01)
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.003 (0.002-0.003)	0.003 (0.001-0.004)	0.005 (0.001-0.01)
Phosphatidylcholine acyl-alkyl C 36:3	0.001 (0.001-0.001)	-	0.005 (0.004-0.005)
Phosphatidylcholine acyl-alkyl C 36:4	0.004 (0.002-0.006)	-	0.005 (0.004-0.006)
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 38:3	-	-	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 38:4	0.01 (0.01-0.02)	-	0.003 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.11 (0.06-0.15)	0.04 (0.02-0.06)	0.11 (0.07-0.14)
Phosphatidylcholine acyl-alkyl C 42:1	0.01 (0.01-0.01)	0.01 (0.01-0.02)	-
Phosphatidylcholine acyl-alkyl C 42:2	-	0.002 (0.001-0.002)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 42:3	0.001 (0.001-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.003 (0.002-0.005)	0.005 (0.003-0.007)	0.001 (0.001-0.001)
Phosphatidylcholine acyl-alkyl C 44:4	0.002 (0.001-0.003)	0.01 (0.01-0.01)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 44:5	0.007 (0.006-0.008)	0.007 (0.004-0.01)	0.04(0.003-0.004)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Saskatoon berry	Nanking cherry	Broccoli
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	3.0 (2.2-3.8)	0.13 (0.12-0.14)	0.04 (0.04-0.05)
lysoPhosphatidylcholine acyl C16:1	-	-	0.02 (0.02-0.02)
lysoPhosphatidylcholine acyl C17:0	0.06 (0.05-0.07)	-	0.004 (0.003-0.004)
lysoPhosphatidylcholine acyl C18:0	0.53 (0.39-0.67)	0.05 (0.04-0.05)	0.009 (0.06-0.01)
lysoPhosphatidylcholine acyl C18:1	0.18 (0.08-0.28)	0.02 (0.02-0.03)	0.02 (0.02-0.03)
lysoPhosphatidylcholine acyl C18:2	1.6 (0.98-2.3)	0.15 (0.12-0.19)	0.03 (0.02-0.03)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	0.002 (0.002-0.003)
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	0.0004 (0.0-0.0008)
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	0.006 (0.005-0.007)	-	-
Phosphatidylcholine diacyl C 34:1	0.05 (0.03-0.08)	-	-
Phosphatidylcholine diacyl C 34:2	0.62 (0.36-0.88)	0.06 (0.04-0.07)	0.02 (0.01-0.03)
Phosphatidylcholine diacyl C 34:3	0.57 (0.45-0.68)	0.008 (0.007-0.009)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 34:4	0.01 (0.01-0.01)	-	0.002 (0.002-0.002)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	0.25 (0.24-0.27)	-	-
Phosphatidylcholine diacyl C 36:3	0.13 (0.08-0.19)	0.02 (0.01-0.02)	0.003 (0.002-0.005)
Phosphatidylcholine diacyl C 36:4	0.46 (0.43-0.50)	0.04 (0.03-0.04)	0.005 (0.001-0.009)
Phosphatidylcholine diacyl C 36:5	0.37 (0.32-0.42)	0.008 (0.006-0.009)	0.005 (0.003-0.008)
Phosphatidylcholine diacyl C 36:6	0.15 (0.08-0.21)	-	0.006 (0.005-0.007)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	-	-	0.002 (0.001-0.002)
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	-
Phosphatidylcholine diacyl C 40:3	-	-	0.001 (0.001-0.001)
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Yellow bean	Cucumber	Green bean
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.16 (0.07-0.25)	0.08 (0.07-0.09)	0.22 (0.12-0.33)
lysoPhosphatidylcholine acyl C16:1	0.007 (0.005-0.01)	0.01 (0.01-0.01)	0.04 (0.01-0.07)
lysoPhosphatidylcholine acyl C17:0	0.006 (0.005-0.007)	-	0.006 (0.004-0.008)
lysoPhosphatidylcholine acyl C18:0	0.02 (0.01-0.03)	0.01 (0.01-0.01)	0.03 (0.02-0.04)
lysoPhosphatidylcholine acyl C18:1	0.06 (0.04-0.09)	0.01 (0.01-0.01)	0.09 (0.09-0.09)
lysoPhosphatidylcholine acyl C18:2	0.90 (0.85-0.95)	0.16 (0.13-0.19)	0.67 (0.49-0.86)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	0.003 (0.002-0.003)	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	0.002 (0.001-0.002)	0.0005 (0.0004-0.0005)	0.0005 (0-0.0009)
Phosphatidylcholine diacyl C 32:0	-	0.006 (0.002-0.009)	-
Phosphatidylcholine diacyl C 32:1	-	0.003 (0.0007-0.005)	-
Phosphatidylcholine diacyl C 32:2	-	0.002 (0.002-0.002)	-
Phosphatidylcholine diacyl C 32:3	-	0.001 (0.0008-0.002)	0.002 (0.002-0.002)
Phosphatidylcholine diacyl C 34:1	-	0.07 (0.06-0.08)	-
Phosphatidylcholine diacyl C 34:2	0.04 (0.03-0.05)	0.04 (0.005-0.07)	0.03 (0.01-0.04)
Phosphatidylcholine diacyl C 34:3	0.05 (0.04-0.05)	0.03 (0.02-0.03)	0.03 (0.02-0.03)
Phosphatidylcholine diacyl C 34:4	-	0.002 (0.002-0.002)	0.001 (0.001-0.001)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	0.02 (0.01-0.03)	-
Phosphatidylcholine diacyl C 36:2	-	0.04 (0.04-0.04)	-
Phosphatidylcholine diacyl C 36:3	0.008 (0.008-0.008)	0.03 (0.02-0.03)	0.005 (0.002-0.007)
Phosphatidylcholine diacyl C 36:4	0.008 (0.007-0.008)	0.01 (0.01-0.01)	0.009 (0.008-0.009)
Phosphatidylcholine diacyl C 36:5	0.01 (0.01-0.01)	0.01 (0.01-0.01)	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 36:6	0.005 (0.005-0.006)	0.004 (0.001-0.007)	0.006 (0.002-0.009)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	0.003 (0.001-0.004)	-
Phosphatidylcholine diacyl C 38:4	-	0.004 (0.004-0.004)	-
Phosphatidylcholine diacyl C 38:5	-	0.004 (0.003-0.004)	-
Phosphatidylcholine diacyl C 38:6	-	0.003 (0.002-0.003)	0.002 (0.0-0.004)
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	-
Phosphatidylcholine diacyl C 40:3	0.003 (0.002-0.003)	0.0005 (0.0005-0.0005)	-
Phosphatidylcholine diacyl C 40:4	-	0.002 (0.001-0.002)	0.002 (0.002-0.002)
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Yellow bean	Cucumber	Green bean
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	-	0.01 (0.01-0.01)	0.006 (0.005-0.008)
Phosphatidylcholine diacyl C 42:2	0.006 (0.006-0.006)	0.004 (0.004-0.004)	0.01 (0.009-0.01)
Phosphatidylcholine diacyl C 42:4	-	0.0006 (0.0005-0.0006)	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	0.003 (0.003-0.003)	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.002 (0.002-0.003)	0.01 (0.009-0.009)	-
Phosphatidylcholine acyl-alkyl C 34:2	0.003 (0.002-0.003)	0.01 (0.01-0.01)	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 34:3	-	0.004 (0.004-0.005)	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	0.003 (0.003-0.003)	-
Phosphatidylcholine acyl-alkyl C 36:2	0.005 (0.004-0.007)	0.005 (0.004-0.005)	0.006 (0.005-0.007)
Phosphatidylcholine acyl-alkyl C 36:3	0.001 (0.001-0.001)	0.005 (0.005-0.006)	0.002 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 36:4	0.002 (0.001-0.002)	0.008 (0.008-0.008)	-
Phosphatidylcholine acyl-alkyl C 36:5	-	0.002 (0.001-0.003)	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	-
Phosphatidylcholine acyl-alkyl C 38:3	-	0.002 (0.002-0.002)	-
Phosphatidylcholine acyl-alkyl C 38:4	-	0.005 (0.004-0.005)	-
Phosphatidylcholine acyl-alkyl C 38:5	-	0.004 (0.001-0.007)	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 38:6	-	0.003 (0.003-0.004)	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	0.005 (0.002-0.007)	-	0.003 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	0.001 (0.001-0.001)	0.005 (0.0008-0.008)	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	-	-	0.08 (0.07-0.08)
Phosphatidylcholine acyl-alkyl C 42:1	0.01 (0.01-0.01)	0.005 (0.004-0.006)	0.01 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 42:2	0.002 (0.001-0.002)	-	0.003 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 42:3	0.002 (0.001-0.002)	0.002 (0.001-0.002)	0.002 (0.001-0.003)
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.003 (0.002-0.003)	0.0006 (0.0006-0.0006)	0.003 (0.002-0.004)
Phosphatidylcholine acyl-alkyl C 44:4	0.01 (0.01-0.01)	0.002 (0.002-0.003)	0.01 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 44:5	0.004 (0.003-0.004)	-	0.003 (0.001-0.005)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	White cabbage	Carrot	Sunburst squash
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.04 (0.04-0.05)	0.13 (0.13-0.14)	0.11 (0.09-0.14)
lysoPhosphatidylcholine acyl C16:1	0.007 (0.006-0.007)	-	0.007 (0.006-0.009)
lysoPhosphatidylcholine acyl C17:0	0.002 (0.001-0.004)	-	0.02 (0.01-0.02)
lysoPhosphatidylcholine acyl C18:0	0.008 (0.008-0.008)	0.01 (0.01-0.01)	0.02 (0.02-0.03)
lysoPhosphatidylcholine acyl C18:1	0.01 (0.01-0.01)	0.03 (0.02-0.03)	0.006 (0.002-0.01)
lysoPhosphatidylcholine acyl C18:2	0.04 (0.04-0.05)	0.52 (0.52-0.52)	0.06 (0.05-0.06)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	0.02 (0.01-0.02)
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	0.004 (0.003-0.006)	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	0.001 (0.0-0.001)
Phosphatidylcholine diacyl C 32:0	-	0.006 (0.005-0.006)	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	0.0007 (0.0006-0.0007)	-	0.001(0.0004-0.0017)
Phosphatidylcholine diacyl C 34:1	-	0.05 (0.03-0.06)	0.008 (0.004-0.01)
Phosphatidylcholine diacyl C 34:2	0.01 (0.01-0.01)	0.77 (0.66-0.88)	0.07 (0.01-0.13)
Phosphatidylcholine diacyl C 34:3	0.02 (0.02-0.02)	0.01 (0.01-0.02)	0.11 (0.01-0.21)
Phosphatidylcholine diacyl C 34:4	0.0007 (0.0007-0.0008)	0.01 (0.01-0.01)	0.003 (0.0006-0.005)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	-	0.07 (0.06-0.08)	-
Phosphatidylcholine diacyl C 36:3	-	0.04 (0.04-0.04)	0.02 (0.02-0.03)
Phosphatidylcholine diacyl C 36:4	0.005 (0.005-0.006)	0.43 (0.33-0.53)	0.06 (0.05-0.07)
Phosphatidylcholine diacyl C 36:5	0.009 (0.008-0.009)	0.02 (0.02-0.03)	0.04 (0.04-0.05)
Phosphatidylcholine diacyl C 36:6	0.005 (0.004-0.005)	0.006 (0.006-0.006)	0.03 (0.02-0.04)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	0.002 (0.002-0.002)	-	0.003 (0.003-0.004)
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	0.003 (0.003-0.003)	-
Phosphatidylcholine diacyl C 40:3	-	-	-
Phosphatidylcholine diacyl C 40:4	-	-	0.003 (0.002-0.004)
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	White cabbage	Carrot	Potato
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.04 (0.04-0.05)	0.13 (0.13-0.14)	0.05 (0.05-0.05)
lysoPhosphatidylcholine acyl C16:1	0.007 (0.006-0.007)	-	0.02 (0.01-0.02)
lysoPhosphatidylcholine acyl C17:0	0.002 (0.001-0.004)	-	-
lysoPhosphatidylcholine acyl C18:0	0.008 (0.008-0.008)	0.01 (0.01-0.01)	0.03 (0.03-0.03)
lysoPhosphatidylcholine acyl C18:1	0.01 (0.01-0.01)	0.03 (0.02-0.03)	-
lysoPhosphatidylcholine acyl C18:2	0.04 (0.04-0.05)	0.52 (0.52-0.52)	0.04 (0.04-0.05)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	0.004 (0.003-0.006)	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	-
Phosphatidylcholine diacyl C 32:0	-	0.006 (0.005-0.006)	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	0.0007 (0.0006-0.0007)	-	-
Phosphatidylcholine diacyl C 34:1	-	0.05 (0.03-0.06)	-
Phosphatidylcholine diacyl C 34:2	0.01 (0.01-0.01)	0.77 (0.66-0.88)	0.07 (0.07-0.08)
Phosphatidylcholine diacyl C 34:3	0.02 (0.02-0.02)	0.01 (0.01-0.02)	0.05 (0.05-0.05)
Phosphatidylcholine diacyl C 34:4	0.0007 (0.0007-0.0008)	0.01 (0.01-0.01)	0.002 (0.001-0.002)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	-	0.07 (0.06-0.08)	-
Phosphatidylcholine diacyl C 36:3	-	0.04 (0.04-0.04)	0.01 (0.01-0.02)
Phosphatidylcholine diacyl C 36:4	0.005 (0.005-0.006)	0.43 (0.33-0.53)	0.03 (0.02-0.03)
Phosphatidylcholine diacyl C 36:5	0.009 (0.008-0.009)	0.02 (0.02-0.03)	0.03 (0.03-0.03)
Phosphatidylcholine diacyl C 36:6	0.005 (0.004-0.005)	0.006 (0.006-0.006)	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	0.002 (0.002-0.002)	-	-
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	0.003 (0.003-0.003)	-
Phosphatidylcholine diacyl C 40:3	-	-	-
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Sunburst squash	Nanking cherry	Broccoli
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.004 (0.003-0.004)	-	0.01 (0.01-0.02)
Phosphatidylcholine diacyl C 42:2	0.005 (0.004-0.006)	0.005 (0.005-0.005)	0.005 (0.005-0.005)
Phosphatidylcholine diacyl C 42:4	-	-	0.001 (0.001-0.001)
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	0.002 (0.001-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.002 (0.002-0.002)	-	0.003 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 34:2	0.003 (0.002-0.004)	-	-
Phosphatidylcholine acyl-alkyl C 34:3	0.005 (0.005-0.005)	-	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.003 (0.002-0.004)	0.004 (0.004-0.004)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 36:3	0.004 (0.003-0.004)	-	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 36:4	0.003 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 36:5	0.002 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	0.004 (0.002-0.005)	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	-
Phosphatidylcholine acyl-alkyl C 38:3	0.003 (0.002-0.004)	-	-
Phosphatidylcholine acyl-alkyl C 38:4	-	-	-
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	-
Phosphatidylcholine acyl-alkyl C 40:3	0.003 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	0.001 (0.001-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.06 (0.06-0.06)	-	0.04 (0.03-0.05)
Phosphatidylcholine acyl-alkyl C 42:1	0.006 (0.005-0.007)	0.004 (0.003-0.005)	0.008 (0.006-0.01)
Phosphatidylcholine acyl-alkyl C 42:2	-	-	0.002 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 42:3	0.002 (0.002-0.002)	-	0.001 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.002 (0.002-0.002)	0.004 (0.002-0.005)	-
Phosphatidylcholine acyl-alkyl C 44:4	0.004 (0.004-0.005)	0.009 (0.006-0.01)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 44:5	0.004 (0.004-0.005)	0.005 (0.003-0.007)	-
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Raspberry	Yellow bell pepper	Garlic
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	-	0.15 (0.10-0.19)	2.1 (2.1-2.2)
lysoPhosphatidylcholine acyl C16:1	-	0.02 (0.01-0.03)	0.05 (0.04-0.05)
lysoPhosphatidylcholine acyl C17:0	-	0.005 (0.004-0.005)	0.04 (0.04-0.05)
lysoPhosphatidylcholine acyl C18:0	-	0.03 (0.02-0.03)	0.04 (0.03-0.06)
lysoPhosphatidylcholine acyl C18:1	-	0.03 (0.03-0.03)	0.70 (0.62-0.78)
lysoPhosphatidylcholine acyl C18:2	-	0.33 (0.31-0.35)	2.8 (2.0-3.7)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	0.002 (0.001-0.003)	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	0.0004 (0.0003-0.0005)	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	0.02 (0.01-0.02)	-
Phosphatidylcholine diacyl C 32:2	-	0.005 (0.004-0.01)	-
Phosphatidylcholine diacyl C 32:3	-	0.002 (0.002-0.003)	-
Phosphatidylcholine diacyl C 34:1	-	0.03 (0.03-0.04)	0.15 (0.13-0.16)
Phosphatidylcholine diacyl C 34:2	-	0.31 (0.30-0.31)	1.6 (1.3-1.9)
Phosphatidylcholine diacyl C 34:3	0.006 (0.006-0.007)	0.07 (0.07-0.08)	0.11 (0.09-0.14)
Phosphatidylcholine diacyl C 34:4	-	0.003 (0.002-0.003)	0.008 (0.007-0.008)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	0.008 (0.008-0.009)	-
Phosphatidylcholine diacyl C 36:2	-	0.11 (0.08-0.13)	-
Phosphatidylcholine diacyl C 36:3	-	0.06 (0.05-0.06)	0.37 (0.37-0.39)
Phosphatidylcholine diacyl C 36:4	0.009 (0.008-0.009)	0.20 (0.19-0.21)	1.2 (0.93-1.5)
Phosphatidylcholine diacyl C 36:5	0.004 (0.004-0.005)	0.05 (0.05-0.06)	0.28 (0.25-0.32)
Phosphatidylcholine diacyl C 36:6	-	0.006 (0.006-0.006)	0.03 (0.03-0.03)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	0.006 (0.006-0.007)	-
Phosphatidylcholine diacyl C 38:4	-	0.004 (0.003-0.006)	0.01 (0.01-0.02)
Phosphatidylcholine diacyl C 38:5	-	0.004 (0.004-0.004)	-
Phosphatidylcholine diacyl C 38:6	-	0.002 (0.001-0.003)	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	0.003 (0.0004-0.006)	-
Phosphatidylcholine diacyl C 40:3	-	0.001 (0.001-0.002)	-
Phosphatidylcholine diacyl C 40:4	-	0.002 (0.001-0.002)	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	0.03 (0.02-0.04)

Continued.

Table 2.7.*Continued.*

Metabolites	Turnip	Onion	Lettuce
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.10 (0.10-0.10)	0.07(0.049-0.093)	0.02 (0.003-0.04)
lysoPhosphatidylcholine acyl C16:1	0.05 (0.03-0.06)	0.01(0.0113-0.0122)	0.004 (0.004-0.004)
lysoPhosphatidylcholine acyl C17:0	-	-	-
lysoPhosphatidylcholine acyl C18:0	0.02 (0.02-0.02)	0.007(0.0055-0.0079)	0.007 (0.006-0.007)
lysoPhosphatidylcholine acyl C18:1	0.03 (0.03-0.03)	0.11(0.096-0.1189)	-
lysoPhosphatidylcholine acyl C18:2	0.06 (0.05-0.07)	0.17(0.114-0.2245)	0.05 (0.05-0.06)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	0.001 (0.001-0.002)
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	-	-	0.002 (0.001-0.003)
Phosphatidylcholine diacyl C 34:1	-	0.02(0.0131-0.026)	0.007 (0.004-0.009)
Phosphatidylcholine diacyl C 34:2	0.06 (0.05-0.06)	0.06(0.052-0.061)	0.25 (0.20-0.30)
Phosphatidylcholine diacyl C 34:3	0.03 (0.002-0.06)	0.01(0.0102-0.0132)	0.15 (0.12-0.18)
Phosphatidylcholine diacyl C 34:4	-	-	0.003 (0.001-0.004)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	-	-	-
Phosphatidylcholine diacyl C 36:2	-	-	0.05 (0.04-0.05)
Phosphatidylcholine diacyl C 36:3	0.03 (0.02-0.03)	0.03(0.022-0.032)	0.05 (0.04-0.05)
Phosphatidylcholine diacyl C 36:4	0.05 (0.04-0.05)	0.05(0.045-0.055)	0.17 (0.14-0.19)
Phosphatidylcholine diacyl C 36:5	0.03 (0.03-0.03)	0.008(0.0061-0.0096)	0.07 (0.06-0.08)
Phosphatidylcholine diacyl C 36:6	0.03 (0.03-0.04)	0.003(0.0024-0.0033)	0.04 (0.03-0.05)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	0.006 (0.005-0.006)
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	-	-	0.002 (0.001-0.002)
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	0.002 (0.002-0.003)
Phosphatidylcholine diacyl C 40:3	-	-	0.001 (0.001-0.001)
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Potato	Raspberry	Saskatoon berry
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.06 (0.05-0.06)	0.002 (0.002-0.002)	-
Phosphatidylcholine diacyl C 42:2	0.02 (0.01-0.02)	0.01 (0.01-0.01)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 42:4	-	-	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	0.005 (0.003-0.007)
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	0.003 (0.002-0.004)	-
Phosphatidylcholine acyl-alkyl C 34:1	0.006 (0.006-0.007)	-	0.01 (0.01-0.01)
Phosphatidylcholine acyl-alkyl C 34:2	-	-	0.04 (0.02-0.07)
Phosphatidylcholine acyl-alkyl C 34:3	-	-	0.02 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.01 (0.01-0.01)	0.004 (0.003-0.005)	0.03 (0.03-0.04)
Phosphatidylcholine acyl-alkyl C 36:3	0.002 (0.001-0.003)	-	0.01 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 36:4	-	-	-
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	0.02 (0.02-0.02)
Phosphatidylcholine acyl-alkyl C 38:3	-	-	0.01 (0.01-0.01)
Phosphatidylcholine acyl-alkyl C 38:4	-	-	-
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	-
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	0.006 (0.005-0.007)
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.20 (0.15-0.25)	0.13 (0.08-0.19)	-
Phosphatidylcholine acyl-alkyl C 42:1	0.07 (0.01-0.13)	0.004 (0.002-0.006)	-
Phosphatidylcholine acyl-alkyl C 42:2	0.006 (0.005-0.006)	-	-
Phosphatidylcholine acyl-alkyl C 42:3	0.003 (0.003-0.004)	-	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.002 (0.001-0.003)	0.002 (0.002-0.003)	0.006 (0.006-0.007)
Phosphatidylcholine acyl-alkyl C 44:4	0.02 (0.01-0.03)	0.005 (0.005-0.005)	0.02 (0.02-0.02)
Phosphatidylcholine acyl-alkyl C 44:5	0.007 (0.007-0.008)	0.01 (0.01-0.01)	0.02 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Turnip	Onion	Lettuce
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.06 (0.05-0.07)	0.03 (0.032-0.032)	0.006 (0.006-0.006)
Phosphatidylcholine diacyl C 42:2	0.02 (0.01-0.02)	0.004 (0.0018-0.0065)	0.005 (0.005-0.006)
Phosphatidylcholine diacyl C 42:4	-	-	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	0.0009 (0.0009-0.0009
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.005 (0.003-0.006)	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 34:2	-	-	0.006 (0.005-0.007)
Phosphatidylcholine acyl-alkyl C 34:3	-	-	0.004 (0.004-0.005)
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	0.003 (0.003-0.004)
Phosphatidylcholine acyl-alkyl C 36:2	0.007 (0.006-0.008)	0.0037 (0.0035-0.0039)	0.005 (0.005-0.006)
Phosphatidylcholine acyl-alkyl C 36:3	-	0.0014 (0.0008-0.0021)	0.001 (0.0003-0.002)
Phosphatidylcholine acyl-alkyl C 36:4	-	-	0.002 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 38:3	-	-	0.003 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 38:4	-	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	-
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.20 (0.20-0.21)	0.080 (0.071-0.089)	-
Phosphatidylcholine acyl-alkyl C 42:1	-	0.0073 (0.0055-0.0091)	-
Phosphatidylcholine acyl-alkyl C 42:2	0.005 (0.004-0.005)	0.0020 (0.0011-0.0030)	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 42:3	-	0.0015 (0.0011-0.0019)	0.001 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	-	-	0.001 (0.001-0.002)
Phosphatidylcholine acyl-alkyl C 44:4	0.02 (0.01-0.02)	0.0068 (0.0053-0.0083)	0.003(0.002-0.003)
Phosphatidylcholine acyl-alkyl C 44:5	0.01 (0.01-0.01)	0.0071 (0.007-0.0073)	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Eggplant	Parsnip	Yellow zucchini
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.12 (0.1208-0.1218)	0.26 (0.23-0.28)	0.41 (0.38-0.44)
lysoPhosphatidylcholine acyl C16:1	0.005 (0.004-0.006)	-	0.01 (0.01-0.02)
lysoPhosphatidylcholine acyl C17:0	0.005 (0.005-0.006)	-	0.01 (0.01-0.02)
lysoPhosphatidylcholine acyl C18:0	0.16 (0.15-0.17)	0.03 (0.02-0.03)	0.03 (0.02-0.04)
lysoPhosphatidylcholine acyl C18:1	0.06 (0.06-0.06)	0.02 (0.02-0.03)	0.02 (0.01-0.02)
lysoPhosphatidylcholine acyl C18:2	0.89 (0.86-0.91)	0.50 (0.50-0.50)	0.15 (0.12-0.18)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	0.004 (0.004-0.004)
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	-
Phosphatidylcholine diacyl C 32:0	-	-	0.02 (0.01-0.02)
Phosphatidylcholine diacyl C 32:1	-	-	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 32:2	-	-	0.008 (0.008-0.009)
Phosphatidylcholine diacyl C 32:3	-	-	0.009 (0.009-0.009)
Phosphatidylcholine diacyl C 34:1	0.006 (0.005-0.007)	-	0.06 (0.05-0.07)
Phosphatidylcholine diacyl C 34:2	0.05 (0.04-0.07)	1.2 (1.1-1.2)	1.0 (0.98-1.1)
Phosphatidylcholine diacyl C 34:3	0.02 (0.01-0.02)	0.05 (0.04-0.05)	3.1 (2.8-3.4)
Phosphatidylcholine diacyl C 34:4	0.005 (0.001-0.008)	0.02 (0.01-0.03)	0.02 (0.01-0.02)
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	0.005 (0.004-0.005)	-	0.008 (0.008-0.008)
Phosphatidylcholine diacyl C 36:2	0.04 (0.03-0.04)	0.08 (0.08-0.08)	0.09 (0.09-0.10)
Phosphatidylcholine diacyl C 36:3	0.01 (0.01-0.02)	0.11 (0.10-0.12)	0.24 (0.21-0.26)
Phosphatidylcholine diacyl C 36:4	0.02 (0.01-0.04)	1.1 (1.0-1.2)	0.43 (0.39-0.46)
Phosphatidylcholine diacyl C 36:5	0.02 (0.01-0.03)	0.06 (0.05-0.07)	0.36 (0.31-0.41)
Phosphatidylcholine diacyl C 36:6	0.002 (0.002-0.003)	0.04 (0.01-0.06)	0.76 (0.75-0.77)
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 38:4	-	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 38:5	-	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-
Phosphatidylcholine diacyl C 40:2	-	0.01 (0.01-0.01)	0.008 (0.007-0.009)
Phosphatidylcholine diacyl C 40:3	-	-	0.004 (0.0006-0.007)
Phosphatidylcholine diacyl C 40:4	-	-	0.002 (0.002-0.003)
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6		-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Yellow bell pepper	Garlic	Cauliflower
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.002 (0.001-0.002)	0.39 (0.31-0.48)	0.15 (0.15-0.15)
Phosphatidylcholine diacyl C 42:2	0.007 (0.007-0.008)	0.03 (0.02-0.03)	0.07 (0.06-0.07)
Phosphatidylcholine diacyl C 42:4	-	0.004 (0.003-0.005)	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 42:5	-	-	0.02 (0.02-0.03)
Phosphatidylcholine diacyl C 42:6	-	-	0.07 (0.06-0.07)
Phosphatidylcholine acyl-alkyl C 30:0	-	-	0.10 (0.09-0.11)
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	0.01 (0.01-0.01)
Phosphatidylcholine acyl-alkyl C 32:1	0.0008 (0.0005-0.001)	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.001 (0.001-0.001)	0.008 (0.008-0.008)	-
Phosphatidylcholine acyl-alkyl C 34:2	0.003 (0.002-0.003)	0.02 (0.01-0.02)	-
Phosphatidylcholine acyl-alkyl C 34:3	-	-	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	0.005 (0.005-0.006)	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.01 (0.01-0.02)	0.02 (0.01-0.03)	0.008 (0.003-0.01)
Phosphatidylcholine acyl-alkyl C 36:3	0.002 (0.002-0.003)	0.006 (0.005-0.007)	-
Phosphatidylcholine acyl-alkyl C 36:4	0.003 (0.002-0.004)	0.008 (0.007-0.009)	-
Phosphatidylcholine acyl-alkyl C 36:5	0.002 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	0.002 (0.002-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 38:2	0.003 (0.002-0.004)	-	0.05 (0.04-0.06)
Phosphatidylcholine acyl-alkyl C 38:3	0.003 (0.002-0.004)	0.007 (0.007-0.007)	0.08 (0.07-0.08)
Phosphatidylcholine acyl-alkyl C 38:4	0.004 (0.003-0.004)	-	0.006 (0.005-0.008)
Phosphatidylcholine acyl-alkyl C 38:5	0.002 (0.001-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	0.001 (0.001-0.002)	-	0.02 (0.02-0.02)
Phosphatidylcholine acyl-alkyl C 40:3	-	-	0.03 (0.03-0.04)
Phosphatidylcholine acyl-alkyl C 40:4	-	-	0.04 (0.03-0.04)
Phosphatidylcholine acyl-alkyl C 40:5	0.0005 (0.0004-0.0006)	-	0.02 (0.02-0.02)
Phosphatidylcholine acyl-alkyl C 40:6	-	0.03 (0.02-0.03)	-
Phosphatidylcholine acyl-alkyl C 42:0	-	0.34(0.27-0.41)	-
Phosphatidylcholine acyl-alkyl C 42:1	0.005 (0.004-0.005)	0.03 (0.02-0.03)	-
Phosphatidylcholine acyl-alkyl C 42:2	0.004 (0.003-0.004)	0.009 (0.008-0.009)	-
Phosphatidylcholine acyl-alkyl C 42:3	0.001 (0.0008-0.001)	0.004 (0.004-0.005)	0.006 (0.005-0.006)
Phosphatidylcholine acyl-alkyl C 42:4	-	0.15 (0.09-0.21)	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.001 (0.001-0.001)	0.01 (0.01-0.01)	-
Phosphatidylcholine acyl-alkyl C 44:4	0.003 (0.002-0.003)	0.03 (0.02-0.03)	0.005 (0.005-0.005)
Phosphatidylcholine acyl-alkyl C 44:5	0.003 (0.003-0.004)	-	-
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Eggplant	Parsnip	Yellow zucchini
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.003 (0.002-0.003)	0.009 (0.008-0.009)	0.003 (0.002-0.003)
Phosphatidylcholine diacyl C 42:2	0.005 (0.005-0.005)	0.03 (0.01-0.05)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 42:4	-	-	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.002 (0.002-0.002)	-	0.005 (0.005-0.005)
Phosphatidylcholine acyl-alkyl C 34:2	0.001 (0.001-0.002)	0.04 (0.03-0.05)	0.02 (0.02-0.02)
Phosphatidylcholine acyl-alkyl C 34:3	-	-	0.04 (0.03-0.04)
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	-	-	-
Phosphatidylcholine acyl-alkyl C 36:2	0.002 (0.001-0.003)	0.02 (0.02-0.02)	0.02 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 36:3	0.001 (0.001-0.001)	0.004 (0.003-0.005)	0.02 (0.01-0.03)
Phosphatidylcholine acyl-alkyl C 36:4	-	-	0.006 (0.005-0.006)
Phosphatidylcholine acyl-alkyl C 36:5	-	-	0.002 (0.001-0.003)
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	-
Phosphatidylcholine acyl-alkyl C 38:3	0.001 (0.001-0.001)	0.005 (0.005-0.005)	0.007 (0.006-0.008)
Phosphatidylcholine acyl-alkyl C 38:4	-	-	0.008 (0.007-0.008)
Phosphatidylcholine acyl-alkyl C 38:5	-	-	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	-	-	0.005 (0.005-0.005)
Phosphatidylcholine acyl-alkyl C 40:3	-	-	0.007 (0.006-0.007)
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	0.001 (0.0-0.002)
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	-	-	0.18 (0.10-0.26)
Phosphatidylcholine acyl-alkyl C 42:1	0.005 (0.004-0.006)	-	0.008 (0.007-0.009)
Phosphatidylcholine acyl-alkyl C 42:2	0.005 (0.0007-0.009)	0.005 (0.004-0.005)	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 42:3	-	-	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.002 (0.001-0.003)	0.003 (0.002-0.003)	0.007 (0.006-0.008)
Phosphatidylcholine acyl-alkyl C 44:4	0.002 (0.001-0.003)	0.02 (0.01-0.03)	0.003 (0.002-0.004)
Phosphatidylcholine acyl-alkyl C 44:5	0.002 (0.002-0.002)	0.02 (0.01-0.04)	-
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Orange bell pepper	Red beet root	Cauliflower
lysoPhosphatidylcholine acyl C14:0	-	-	0.06 (0.05-0.07)
lysoPhosphatidylcholine acyl C16:0	0.05 (0.004-0.10)	0.04 (0.02-0.06)	0.02 (0.02-0.02)
lysoPhosphatidylcholine acyl C16:1	-	-	0.004 (0.004-0.004)
lysoPhosphatidylcholine acyl C17:0	-	-	-
lysoPhosphatidylcholine acyl C18:0	0.03 (0.03-0.04)	0.01 (0.01-0.02)	-
lysoPhosphatidylcholine acyl C18:1	0.02 (0.01-0.02)	-	-
lysoPhosphatidylcholine acyl C18:2	0.62 (0.55-0.69)	0.05 (0.04-0.06)	-
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	0.002 (0.001-0.003)	-	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	0.006 (0.004-0.007)
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 30:0	-	-	0.008 (0.006-0.009)
Phosphatidylcholine diacyl C 30:2	0.002 (0.001-0.002)	-	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	0.005 (0.004-0.006)	-	-
Phosphatidylcholine diacyl C 32:3	-	-	-
Phosphatidylcholine diacyl C 34:1	0.04 (0.04-0.04)	0.01 (0.009-0.01)	-
Phosphatidylcholine diacyl C 34:2	1.03 (0.93-1.1)	0.39 (0.05-0.74)	-
Phosphatidylcholine diacyl C 34:3	0.16 (0.12-0.20)	0.09 (0.09-0.09)	-
Phosphatidylcholine diacyl C 34:4	0.01 (0.01-0.02)	0.01 (0.01-0.01)	-
Phosphatidylcholine diacyl C 36:0	-	-	-
Phosphatidylcholine diacyl C 36:1	0.02 (0.01-0.02)	0.008 (0.008-0.008)	-
Phosphatidylcholine diacyl C 36:2	0.32 (0.28-0.36)	0.06 (0.02-0.11)	-
Phosphatidylcholine diacyl C 36:3	0.13 (0.10-0.17)	0.07 (0.06-0.09)	-
Phosphatidylcholine diacyl C 36:4	0.98 (0.93-1.0)	0.69 (0.61-0.78)	-
Phosphatidylcholine diacyl C 36:5	0.21 (0.21-0.21)	0.09 (0.08-0.09)	-
Phosphatidylcholine diacyl C 36:6	0.03 (0.03-0.04)	0.03 (0.03-0.03)	0.19 (0.17-0.20)
Phosphatidylcholine diacyl C 38:0	-	-	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 38:1	-	-	0.002 (0.0003-0.003)
Phosphatidylcholine diacyl C 38:3	0.01 (0.01-0.01)	-	0.004 (0.003-0.005)
Phosphatidylcholine diacyl C 38:4	0.006 (0.006-0.006)	-	-
Phosphatidylcholine diacyl C 38:5	-	-	-
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	0.01 (0.009-0.01)
Phosphatidylcholine diacyl C 40:2	0.02 (0.02-0.03)	0.02 (0.01-0.03)	-
Phosphatidylcholine diacyl C 40:3	0.003 (0.003-0.003)	-	-
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	0.06 (0.05-0.07)
Phosphatidylcholine diacyl C 40:6	-	-	0.02 (0.02-0.02)

Continued.

Table 2.7.*Continued.*

Metabolites	Spinach	Crab apple	Tomato
lysoPhosphatidylcholine acyl C14:0	-	-	-
lysoPhosphatidylcholine acyl C16:0	0.08 (0.07-0.08)	0.03 (0.02-0.03)	0.02 (0.02-0.02)
lysoPhosphatidylcholine acyl C16:1	0.01 (0.01-0.02)	0.02 (0.01-0.03)	-
lysoPhosphatidylcholine acyl C17:0	-	-	-
lysoPhosphatidylcholine acyl C18:0	0.007 (0.007-0.007)	0.02 (0.01-0.02)	0.007 (0.006-0.007)
lysoPhosphatidylcholine acyl C18:1	0.08 (0.07-0.08)	-	-
lysoPhosphatidylcholine acyl C18:2	0.19 (0.16-0.21)	0.03 (0.02-0.03)	0.04 (0.03-0.04)
lysoPhosphatidylcholine acyl C20:3	-	-	-
lysoPhosphatidylcholine acyl C20:4	-	-	-
lysoPhosphatidylcholine acyl C24:0	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-
Phosphatidylcholine diacyl C 30:2	-	-	-
Phosphatidylcholine diacyl C 32:0	-	-	-
Phosphatidylcholine diacyl C 32:1	-	-	-
Phosphatidylcholine diacyl C 32:2	-	-	-
Phosphatidylcholine diacyl C 32:3	-	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 34:1	-	0.04 (0.03-0.05)	0.53 (0.45-0.62)
Phosphatidylcholine diacyl C 34:2	0.15 (0.15-0.16)	0.03 (0.02-0.03)	0.07 (0.07-0.08)
Phosphatidylcholine diacyl C 34:3	0.02 (0.008-0.04)	0.0007 (0.0006-0.0008)	0.005 (0.005-0.006)
Phosphatidylcholine diacyl C 34:4	0.002 (0.002-0.003)	-	-
Phosphatidylcholine diacyl C 36:0	-	-	0.006 (0.006-0.007)
Phosphatidylcholine diacyl C 36:1	-	-	0.08 (0.08-0.08)
Phosphatidylcholine diacyl C 36:2	0.02 (0.02-0.03)	0.007 (0.006-0.008)	0.05 (0.05-0.06)
Phosphatidylcholine diacyl C 36:3	0.02 (0.02-0.03)	0.007 (0.004-0.01)	0.59 (0.54-0.65)
Phosphatidylcholine diacyl C 36:4	0.16 (0.15-0.16)	0.02 (0.01-0.03)	0.05 (0.04-0.06)
Phosphatidylcholine diacyl C 36:5	0.02 (0.02-0.03)	0.006 (0.005-0.007)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 36:6	0.02 (0.02-0.03)	-	-
Phosphatidylcholine diacyl C 38:0	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-
Phosphatidylcholine diacyl C 38:3	-	-	-
Phosphatidylcholine diacyl C 38:4	-	-	-
Phosphatidylcholine diacyl C 38:5	-	-	-
Phosphatidylcholine diacyl C 38:6	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	0.006 (0.006-0.007)
Phosphatidylcholine diacyl C 40:2	-	-	-
Phosphatidylcholine diacyl C 40:3	-	-	-
Phosphatidylcholine diacyl C 40:4	-	-	-
Phosphatidylcholine diacyl C 40:5	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Orange bell pepper	Red beet root	Italian red pepper
Phosphatidylcholine diacyl C 42:0	-	-	-
Phosphatidylcholine diacyl C 42:1	0.003 (0.003-0.003)	-	0.15 (0.15-0.16)
Phosphatidylcholine diacyl C 42:2	0.015 (0.013-0.02)	0.01 (0.01-0.01)	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 42:4	-	0.002 (0.002-0.002)	-
Phosphatidylcholine diacyl C 42:5	-	-	0.05 (0.04-0.06)
Phosphatidylcholine diacyl C 42:6	-	-	0.03 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 30:0	-	-	0.59 (0.59-0.60)
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	0.006 (0.006-0.006)
Phosphatidylcholine acyl-alkyl C 32:1	0.002 (0.002-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.004 (0.003-0.005)	-	-
Phosphatidylcholine acyl-alkyl C 34:2	0.01 (0.01-0.02)	0.01 (0.01-0.01)	-
Phosphatidylcholine acyl-alkyl C 34:3	0.005 (0.005-0.005)	0.004 (0.004-0.005)	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	0.005 (0.004-0.007)	0.02 (0.01-0.04)	-
Phosphatidylcholine acyl-alkyl C 36:2	0.02 (0.005-0.04)	0.01 (0.01-0.01)	-
Phosphatidylcholine acyl-alkyl C 36:3	0.05 (0.01-0.09)	0.002 (0.001-0.002)	-
Phosphatidylcholine acyl-alkyl C 36:4	0.004 (0.003-0.004)	0.003 (0.002-0.004)	-
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	0.002 (0.001-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 38:2	0.008 (0.007-0.008)	-	0.06 (0.05-0.06)
Phosphatidylcholine acyl-alkyl C 38:3	0.007 (0.007-0.007)	0.002 (0.002-0.003)	0.01 (0.01-0.01)
Phosphatidylcholine acyl-alkyl C 38:4	0.003 (0.003-0.003)	0.007 (0.006-0.008)	-
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	0.004 (0.004-0.004)	0.002 (0.001-0.002)	0.009 (0.008-0.009)
Phosphatidylcholine acyl-alkyl C 40:3	-	-	0.02 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 40:4	-	-	0.009 (0.008-0.009)
Phosphatidylcholine acyl-alkyl C 40:5	-	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.07 (0.06-0.07)	0.13 (0.08-0.18)	-
Phosphatidylcholine acyl-alkyl C 42:1	-	0.005 (0.004-0.006)	-
Phosphatidylcholine acyl-alkyl C 42:2	0.009 (0.009-0.009)	0.003 (0.003-0.003)	-
Phosphatidylcholine acyl-alkyl C 42:3	0.002 (0.002-0.002)	-	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.003 (0.002-0.004)	0.003 (0.002-0.004)	-
Phosphatidylcholine acyl-alkyl C 44:4	0.007 (0.006-0.007)	0.006 (0.005-0.007)	-
Phosphatidylcholine acyl-alkyl C 44:5	0.01 (0.01-0.02)	0.01 (0.01-0.01)	-
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Spinach	Crab apple	Tomato
Phosphatidylcholine diacyl C 42:0	-	0.03 (0.02-0.03)	-
Phosphatidylcholine diacyl C 42:1	0.004 (0.003-0.004)	0.005 (0.005-0.005)	0.008 (0.008-0.009)
Phosphatidylcholine diacyl C 42:2	0.01 (0.007-0.01)	-	0.001 (0.001-0.001)
Phosphatidylcholine diacyl C 42:4	0.001 (0.001-0.001)	-	-
Phosphatidylcholine diacyl C 42:5	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	-	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	-	0.003 (0.003-0.003)	-
Phosphatidylcholine acyl-alkyl C 34:1	0.003 (0.002-0.004)	-	0.01 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 34:2	0.004 (0.003-0.004)	-	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 34:3	0.003 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 36:0	-	-	0.008(0.007-0.008)
Phosphatidylcholine acyl-alkyl C 36:1	-	0.005 (0.005-0.006)	0.009 (0.008-0.009)
Phosphatidylcholine acyl-alkyl C 36:2	0.004 (0.003-0.005)	0.002 (0.002-0.002)	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 36:3	0.003 (0.002-0.004)	-	0.002 (0.002-0.003)
Phosphatidylcholine acyl-alkyl C 36:4	0.002 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	-	-	0.002 (0.002-0.002)
Phosphatidylcholine acyl-alkyl C 38:3	-	-	0.008 (0.006-0.009)
Phosphatidylcholine acyl-alkyl C 38:4	0.002 (0.002-0.003)	-	-
Phosphatidylcholine acyl-alkyl C 38:5	-	-	-
Phosphatidylcholine acyl-alkyl C 38:6	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	0.003 (0.002-0.004)
Phosphatidylcholine acyl-alkyl C 40:2	-	-	-
Phosphatidylcholine acyl-alkyl C 40:3	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	-	-	-
Phosphatidylcholine acyl-alkyl C 40:6	-	0.08 (0.07-0.08)	0.07(0.07-0.08)
Phosphatidylcholine acyl-alkyl C 42:0	0.12 (0.08-0.16)	0.005 (0.005-0.006)	0.004 (0.004-0.004)
Phosphatidylcholine acyl-alkyl C 42:1	0.006 (0.005-0.006)	0.003 (0.003-0.003)	0.003 (0.003-0.003)
Phosphatidylcholine acyl-alkyl C 42:2	-	0.002 (0.001-0.004)	-
Phosphatidylcholine acyl-alkyl C 42:3	0.001 (0.001-0.001)	-	-
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	0.002 (0.001-0.002)	0.001 (0.001-0.001)
Phosphatidylcholine acyl-alkyl C 44:3	0.0008 (0.0006-0.001)	0.005 (0.005-0.005)	0.005 (0.005-0.006)
Phosphatidylcholine acyl-alkyl C 44:4	0.005 (0.005-0.005)	0.003 (0.003-0.003)	0.007 (0.007-0.008)
Phosphatidylcholine acyl-alkyl C 44:5	0.005 (0.005-0.005)	-	-
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Italian red pepper
lysoPhosphatidylcholine acyl C14:0	0.002 (0.002-0.003)
lysoPhosphatidylcholine acyl C16:0	0.01 (0.01-0.01)
lysoPhosphatidylcholine acyl C16:1	-
IysoPhosphatidylcholine acyl C17:0	-
IysoPhosphatidylcholine acyl C18:0	-
lysoPhosphatidylcholine acyl C18:1	-
IysoPhosphatidylcholine acyl C18:2	-
lysoPhosphatidylcholine acyl C20:3	-
IysoPhosphatidylcholine acyl C20:4	-
IysoPhosphatidylcholine acyl C24:0	-
IysoPhosphatidylcholine acyl C26:0	-
IysoPhosphatidylcholine acyl C26:1	-
lysoPhosphatidylcholine acyl C28:0	-
lysoPhosphatidylcholine acyl C28:1	-
Phosphatidylcholine diacyl C 24:0	-
Phosphatidylcholine diacyl C 26:0	-
Phosphatidylcholine diacyl C 28:1	0.006 (0.005-0.007)
Phosphatidylcholine diacyl C 30:0	-
Phosphatidylcholine diacyl C 30:2	-
Phosphatidylcholine diacyl C 32:0	-
Phosphatidylcholine diacyl C 32:1	-
Phosphatidylcholine diacyl C 32:2	-
Phosphatidylcholine diacyl C 32:3	-
Phosphatidylcholine diacyl C 34:1	-
Phosphatidylcholine diacyl C 34:2	-
Phosphatidylcholine diacyl C 34:3	-
Phosphatidylcholine diacyl C 34:4	-
Phosphatidylcholine diacyl C 36:0	-
Phosphatidylcholine diacyl C 36:1	-
Phosphatidylcholine diacyl C 36:2	-
Phosphatidylcholine diacyl C 36:3	-
Phosphatidylcholine diacyl C 36:4	-
Phosphatidylcholine diacyl C 36:5	-
Phosphatidylcholine diacyl C 36:6	0.10 (0.09-0.11)
Phosphatidylcholine diacyl C 38:0	0.008 (0.008-0.009)
Phosphatidylcholine diacyl C 38:1	0.001 (0.001-0.002)
Phosphatidylcholine diacyl C 38:3	-
Phosphatidylcholine diacyl C 38:4	-
Phosphatidylcholine diacyl C 38:5	-
Phosphatidylcholine diacyl C 38:6	0.003 (0.002-0.003)
Phosphatidylcholine diacyl C 40:1	0.008 (0.007-0.009)
Phosphatidylcholine diacyl C 40:2	0.005 (0.005-0.006)
Phosphatidylcholine diacyl C 40:3	-
Phosphatidylcholine diacyl C 40:4	-
Phosphatidylcholine diacyl C 40:5	0.002 (0.002-0.003)
Phosphatidylcholine diacyl C 40:6	0.01 (0.01-0.01)

Continued.

Table 2.7 *Continued.*

Metabolites	Yellow pepper	LV[1]	Green pepper	LV	Broccoli	LV
Alanine	32.9 (30.1-35.7)	-	80.9 (66.6-95.3)	35	64.8 (53.1-76.5)	-
Arginine	38.5 (37.9-39.1)	-	67.2 (66.2-68.2)	35	≥ 73.6	330
Asparagine	≥ 52.8	-	62.5 (55.8-69.3)	-	≥ 52.8	-
Asparatic Acid	≥ 53.2	-	≥ 53.2	120	≥ 53.2	-
Citrulline	5.40 (4.6-6.3)	-	1.49 (1.34-1.65)	-	2.2 (1.7-2.7)	-
Glutamine	≥ 233.8	-	≥ 233.8	-	≥ 233.8	-
Glutamic Acid	25.1 (22.5-27.7)	-	89.3 (85.6-93.1)	120	≤ 2.2	-
Glycine	49.7 (46.1-53.3)	-	11.9 (10.5-13.3)	30	133.3 (133.1-133.5)	100
Histidine	13.0 (13.0-13.0)	-	30.6 (25.4-35.9)		70.1 (69.7-70.5)	120
Isoleucine	15.5 (13.9-17.1)	-	41.9 (40.2-43.5)	27	136.3 (133.6-138.9)	200
Leucine	15.6 (14.9-16.2)	-	33.0 (32.6-33.4)	36	123.6 (121.5-125.7)	280
Lysine	13.7 (10.6-16.8)	-	56.7 (56.1-57.3)	42	149.0 (106.8-191.2)	270
Methionine	6.2 (5.5-6.9)	-	≤15	7	151.6 (117.2-186.0)	76
Ornithine	1.5 (1.4-1.6)	-	34.1 (31.4-36.8)	27	1.5 (1.4-1.6)	-
Phenylalanine	16.3 (14.0-18.7)	-	35.0 (34.9-35.1)	27	221.3 (210.6-231.9)	200
Proline	10.6 (9.6-11.6)	-	8.9 (8.3-9.5)	-	45.0 (40.2-49.9)	-
Serine	96.5 (90.1-102.9)	-	14.7 (12.9-16.5)	43	≥ 105.1	-
Threonine	62.5 (59.4-65.6)	-	12.3 (11.5-13.2)	13	272.9 (266.5-279.5)	230
Tryptophan	6.2 (5.9-6.5)	-	10.8 (9.8-11.8)	29	49.0 (43.4-54.6)	59
Tyrosine	8.2 (7.5-8.9)	-	16.8 (16.1-17.6)	13	29.3 (28.9-29.6)	-
Valine	46.9 (34.3-59.7)	-	103.3 (84.4-122.2)	42	129.7 (121.4-138.1)	250
Acetylornithine	-	-	-	-	0.70 (0.55-0.85)	-
Dimethylarginine	0.28 (0.27-0.29)	-	0.62 (0.44-0.80)	-	0.97 (0.79-1.2)	-
Alpha-aminoadipic acid	-	-	0.80 (0.56-1.0)	-	1.53 (1.46-1.61)	-
Carnosine	-	-	-	-	-	-
Creatinine	0.13 (0.11-0.15)	-	-	-	-	-
Levodopa	0.05 (0.03-0.06)	-	0.12 (0.10-0.13)	-	0.14 (0.14-0.15)	-
Dopamine	-	-	0.11 (0.08-0.14)	-	0.02 (0.02-0.02)	-
Histamine	-	-	-	-	-	-
Kynurenine	0.36 (0.34-0.38)	-	-	-	-	-
Methioninesulfoxide	-	-	-	-	0.56 (0.54-0.58)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
Hydroxyproline	-	-	4.8 (4.3-5.3)	-	0.27 (0.19-0.36)	-
Phenylethylamine	-	-	-	-	0.07 (0.05-0.09)	-
Putrescine	-	-	-	-	0.50 (0.46-0.53)	-
Serotonin	0.32 (0.28-0.35)	-	-	-	-	-
Taurine	-	-	0.81 (0.66-0.95)	-	-	-

Continued.

Table 2.7 *Continued.*

Metabolites	Green zucchini	LV	Potato	LV	Yellow zucchini	LV
Alanine	69.4 (64.5-74.4)	62	76.5 (66.0-86.9)	-	61.3 (59.6-63.0)	62
Arginine	54.6 (53.6-55.7)	-	≥70	80.0	61.3 (55.4-67.2)	50
Asparagine	≥ 52.8	-	≥ 52.8	-	≥ 52.8	-
Asparatic Acid	64.7 (62.1-67.3)	-	≥ 53.2	410	≥ 53.2	150
Citrulline	10.2 (8.6-11.9)	-	8.0 (7.50-8.56)	-	3.7 (3.4-4.0)	-
Glutamine	138.3 (138.1-138.5)	129	788.7 (626.0-951.5)	-	400.5 (361.8-439.2)	-
Glutamic acid	52.2 (43.4-61.1)	-	161.1 (136.6-185.6)	-	93.1 (87.7-98.5)	130
Glycine	10.9 (10.2-11.6)	-	116.2 (99.4-133.2)	-	72.6 (62.3-82.8)	47
Histidine	25.6 (23.4-27.7)	-	61.9 (49.8-73.9)	-	35.0 (32.6-37.5)	25
Isoleucine	26.6 (25.6-27.6)	45	107.7 (97.1-118.2)	71.0	61.7 (45.2-78.2)	45
Leucine	130.4 (126.1-134.7)	72	55.0 (49.2-60.8)	110	39.6 (36.5-42.7)	72
Lysine	20.8 (18.4-23.3)	-	181.4 (171.3-191.5)	-	43.7 (42.1-45.3)	68
Methionine	5.4 (4.7-5.9)	-	17.2 (15.4-18.9)	-	11.3 (10.2-12.5)	18
Ornithine	6.5 (5.9-7.1)	-	13.4 (12.9-13.9)	-	≤ 1.3	-
Phenylalanine	39.2 (37.7-40.7)	-	135.4 (116.9-153.9)	77.0	38.5 (37.7-39.2)	43
Proline	5.6 (5.1-6.1)	-	102.9 (101.7-104.0)	70.0	38.3 (34.9-41.7)	37
Serine	53.2 (48.6-57.9)	100	107.2 (100.1-114.4)	60.0	54.9 (54.2-55.6)	49
Threonine	29.5 (25.6-33.5)	29	78.7 (76.5-80.9)	65.0	20.6 (18.9-22.3)	29
Tryptophan	22.7 (20.4-24.9)	-	43.4 (39.4-47.4)	29.0	12.2 (11.6-12.8)	10
Tyrosine	43.4 (40.4-46.4)	31	124.6 (124.5-124.6)	-	24.1 (20.6-27.5)	31
Valine	31.8 (29.8-33.7)	54	245.0 (233.9-256.1)	110	41.8 (32.5-51.2)	54
Acetylornithine	2.9 (2.6-3.3)	-	0.69 (0.52-0.86)	-	3.4 (2.0-4.8)	-
Dimethylarginine	0.97 (0.79-1.2)	-	0.45 (0.38-0.52)	-	0.92 (0.85-0.99)	-
Alpha-aminoadipic acid	4.8 (4.6-4.9)	-	1.59 (1.34-1.85)	-	0.57 (0.45-0.68)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	-	-	0.28 (0.25-0.32)	-	0.17(0.17-0.17)	-
Dopamine	0.08 (0.07-0.09)	-	-	-	-	-
Histamine	-	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	0.54 (0.49-0.59)	-	1.7 (1.0-2.4)	-	0.49 (0.40-0.58)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	0.96 (0.76-1.2)	-	0.55 (0.53-0.57)	-	0.42 (0.38-0.46)	-
Phenylethylamine	-	-	-	-	-	-
Putrescine	-	-	-	-	-	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Garlic	LV	Yellow bean	LV	Eggplant	LV
Alanine	165.1 (143.5-186.7)	130.0	79.3 (70.9-87.7)	84.0	34.5 (34.2-34.8)	47.0
Arginine	≥70	640.0	19.4 (18.5-20.3)	77.0	46.1 (37.5-54.6)	53.0
Asparagine	≥52.8	-	≥52.8	-	33.6 (33.0-34.1)	-
Asparatic Acid	≥53.2	490.0	198.9 (175.6-222.2)	-	120.8 (111.8-129.4)	150.0
Citrulline	5.1 (4.8-5.5)	-	6.7 (4.8-8.7)	-	2.7(1.8-3.7)	-
Glutamine	67.6 (62.2-73.1)	-	389.6 (331.6-447.5)	-	153.8 (119.3-188.4)	-
Glutamic acid	448.0 (436.6-459.5)	810.0	249.4 (241.5-257.3)	220	176.5 (174.6-178.4)	170
Glycine	201.2 (179.4-222.9)	210.0	19.3 (14.3-24.3)	-	55.9 (55.7-56.2)	38.0
Histidine	84.8 (78.5-91.0)	110.0	41.8 (40.8-42.9)	33.0	21.9 (20.1-23.7)	21.0
isoleucine	236.9 (231.8-242.2)	220.0	83.8 (81.8-85.7)	81.0	40.6 (39.6-41.7)	42.0
Leucine	408.5 (330.6-486.5)	310.0	138.4 (136.1-140.6)	120.0	38.8 (37.4-30.3)	60.0
Lysine	311.9 (305.8-318.1)	280.0	85.5 (82.2-88.7)	110	12.1 (7.9-16.4)	44.0
Methionine	12.8 (11.61-13.9)	77.0	15.6 (13.4-17.8)	28.0	≤1.5	10.0
Ornithine	50.4 (49.2-51.6)	-	≤ 1.3	-	≤1.3	-
Phenylalanine	84.4 (77.7-91.1)	180.0	14.1 (10.1-18.2)	57.0	35.2 (32.9-37.6)	41.0
Proline	284.6 (279.9-289.3)	100.0	8.3 (6.3-10.2)	-	39.9 (39.6-40.2)	41.0
Serine	435.9 (432.7-439.1)	200.0	≥105.1	170	44.7 (40.4-49.1)	39.0
Threonine	114.1 (106.8-121.3)	150.0	53.9 (48.3-59.6)	31.0	25.1 (22.8-27.5)	35.0
Tryptophan	79.2 (70.6-87.8)	67.0	≤6.1	-	≤6.1	8.0
Tyrosine	126.1 (115.5-136.7)	82.0	59.8 (50.6-68.9)	47.0	15 (13.6-16.4)	26.0
Valine	174.3 (163.3-185.3)	300.0	58.0 (43.2-72.8)	100	19.9 (17.7-22.3)	50.0
Acetylornithine	1.24 (1.18-1.30)	-	3.0 (2.4-3.6)	-	1.2 (1.1-1.3)	-
Dimethylarginine	1.6 (1.4-1.7)	-	0.10 (0.10-0.10)	-	0.11 (0.11-0.11)	-
Alpha-aminoadipic acid	2.09 (1.69-2.50)	-	2.4 (2.2-2.6)	-	1.3 (0.97-1.5)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	0.45 (0.42-0.48)	-	0.15 (0.05-0.26)	-	-	-
Dopamine	-	-	0.03 (0.02-0.04)	-	-	-
Histamine	-	-	-	-	1.7 (1.6-1.8)	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	1.1 (0.99-1.2)	-	-	-	-	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	-	-	-	-	-	-
Phenylethylamine	-	-	-	-	0.03 (0.02-0.04)	-
Putrescine	0.92 (0.81-1.0)	-	-	-	-	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	0.15 (0.13-0.18)	-

Continued.

Table 2.7.*Continued.*

Metabolites	Cucumber	LV	Swiss chard	LV	Green bean	LV
Alanine	43.2 (37.9-48.3)	23	135.7 (114.6-156.7)	-	121.6 (111.9-131.4)	94
Arginine	≥70	-	≥70	-	32.7 (31.7-33.7)	70
Asparagine	35.5 (31.0-39.8)	-	112.1 (107.9-116.2)	-	≥ 52	-
Asparatic Acid	80.1 (72.7-87.6)	-	83.7 (82.6-84.9)	-	≥ 53.2	260
Citrulline	≤ 0.9	-	≤ 0.9	-	10.7 (8.7-12.8)	-
Glutamine	≥ 233.8	-	82.1 (82.1-82.1)	-	≥ 233.8	-
Glutamic acid	123.0 (120-127.1)	-	378.2 (358.3-398.1)	-	74.7 (73.4-75.9)	200
Glycine	36.2 (29.2-43.2)	-	70.1 (53.8-86.3)	-	25.6 (19.9-31.4)	64
Histidine	25.3 (23.7-26.9)	-	35.8 (34.6-37.0)	35	20.5 (19.1-21.8)	36
isoleucine	25.6 (20.4-30.9)	-	88.8 (82.3-95.4)	150	36.7 (35.0-38.4)	73
Leucine	22.3 (19.6-25.1)	-	118.1 (101.8-134.4)	130	36.6 (34.1-39.1)	110
Lysine	11.7 (10.3-13.1)	-	97.4 (93.5-101.4)	98	113.2 (111.3-115.1)	120
Methionine	8.2 (8.1-8.4)	-	≤ 1.5	-	19.2 (18.8-19.6)	28
Ornithine	4.0 (3.1-4.9)	-	≤1.3	-	≤1.3	-
Phenylalanine	23.2 (21.7-24.6)	17	103.5 (97.8-109.2)	110	16.5 (0.0-33.0)	52
Proline	8.9 (7.1-10.6)	13	47.7 (38.7-56.7)	-	16.7 (15.2-18.1)	58
Serine	25.5 (24.9-25.9)	25	294.1 (225.7-362.6)	-	≥105.1	130
Threonine	25.6 (25.4-25.8)	16	63.1 (62.7-63.4)	84	116.5 (110.1-122.9)	79
Tryptophan	7.6 (6.3-9.0)	10	≤ 6.1	-	≤ 6.1	21
Tyrosine	11.9 (11.1-12.7)	10	75.1 (60.9-89.2)	-	63.7 (53.4-73.9)	40
Valine	21.5 (18.7-24.3)	-	121.9 (102.0-141.8)	-	80.4 (64.8-96.1)	94
Acetylornithine	0.50 (0.37-0.63)	-	-	-	3.8 (2.9-4.6)	-
Dimethylarginine	0.15 (0.15-0.15)	-	0.7 (0.60-0.71)	-	0.13 (0.13-0.14)	-
Alpha-aminoadipic acid	11.2 (10.9-11.5)	-	11.4 (10.8-12.0)	-	3.8 (3.4-4.1)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	0.05 (0.03-0.06)	-	2.7 (2.2-3.2)	-	0.23 (0.03-0.42)	-
Dopamine	-	-		-	0.05 (0.04-0.06)	-
Histamine	-	-	3.0 (2.6-3.3)	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	1.3 (1.2-1.3)	-	-	-	0.93 (0.92-0.94)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	0.07 (0.0-0.14)	-	-	-	0.23 (0.17-0.28)	-
Phenylethylamine	-	-	-	-	-	-
Putrescine	-	-	039 (0.086-0.69)	-	-	-
Serotonin	-	-	0.58 (0.39-0.77)	-	-	-
Taurine	-	-	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Parsnip	LV	Red pepper	LV	Carrot	LV
Alanine	72.4 (68.1-76.7)	81	69.8 (69.7-69.9)	50	(68.3-74.9)	77
Arginine	223.4 (217.0-229.9)	200	44.3 (42.4-46.2)	50	49.9 (49.0-50.9)	-
Asparagine	≥52.8	-	≥52.8	-	≥52.8	-
Asparatic Acid	67.3 (57.9-76.7)	230	≥53.2	170	≥53.2	-
Citrulline	≤0.9	-	15.4 (13.8-16.9)	-	5.4 (4.0-6.9)	-
Glutamine	218.9 (215.1-222.7)	-	≥ 233.8	-	352.5 (341.5-363.4)	-
Glutamic acid	193.4 (192.8-194.0)	200	80.4 (72.9-87.9)	180	255.1 (248.2-261.9)	180
Glycine	55.5 (55.2-55.7)	54	42.7 (41.3-44.1)	44	15.2 (10.1-20.4)	27
Histidine	20.5 (20.2-20.8)	34	27.4 (24.7-30.1)	21	19.4 (15.2-23.7)	-
isoleucine	37.5 (34.6-40.5)	71	45.4 (44.8-46.0)	40	42.8 (40.5-45.02)	29
Leucine	34.9 (32.2-37.5)	97	32.4 (30.5-34.3)	52	45.7 (30.2-61.1)	38
Lysine	123.0 (121.9-124.2)	91	34.8 (34.2-35.3)	60	25.9 (24.1-27.6)	35
Methionine	≤1.5	21	7.3 (6.7-8.0)	10	8.6 (8.3-8.9)	9
Ornithine	≤1.3	-	≤1.3	-	≤1.3	-
Phenylalanine	59.5 (56.7-62.4)	64	42.0 (38.9-45.0)	40	37.6 (32.9-42.2)	26
Proline	197.2 (182.0-213.5)	120	46 (42.7-49.3)	33	31.8 (28.06-35.5)	
Serine	50.1 (46.6-53.6)	77	≥ 105.1	62	37.5 (36.7-38.4)	35
Threonine	38.5 (32.6-44.4)	64	≥ 119.1	42	35.1 (32.8-37.4)	26
Tryptophan	≤ 7	11	15.2 (12.2-18.2)	7	25.0 (12.2-37.8)	9
Tyrosine	44.5 (42.8-46.1)	33	21.6 (13.8-29.4)	19	19.6 (18.4-20.8)	14
Valine	39.6 (35.5-43.8)	91	75.6 (63.7-87.4)	60	59.2 (53.9-64.5)	-
Acetylornithine	-	-	-	-	12.0 (10.9-13.1)	-
Dimethylarginine	0.22 (0.16-0.28)	-	0.38 (0.37-0.39)	-	0.52 (0.32-0.72)	-
Alpha-aminoadipic acid	0.52 (0.0-1.0)	-	0.36 (0.25-0.47)	-	0.62 (0.47-0.77)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	-	-	0.15 (0.13-0.16)	-	-	-
Dopamine	-	-	0.11 (0.11-0.11)	-	0.04 (0.03-0.06)	-
Histamine	-	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	-	-	0.54 (0.46-0.62)	-	0.50 (0.49-0.50)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	-	-	1.1 (0.99-1.3)	-	0.18 (0.0-0.36)	-
Phenylethylamine	-	-	-	-	-	-
Putrescine	-	-	-	-	0.84 (0.82-0.86)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	0.58 (0.47-0.69)	-	1.6 (1.2-2.0)	-

Continued.

Table 2.7.*Continued.*

Metabolites	Red beetroot	LV	Onion	LV	White cabbage	LV
Alanine	101.9 (81.0-122.0)	41	30.9 (28.4-33.4)	35	54.82 (54.0-55.6)	61
Arginine	39.3 (34.9-43.8)	32	≥ 70	210	60.1 (57.9-62.3)	67
Asparagine	56.4 (55.4-57.4)	-	≥ 52.8	-	≥52.8	-
Asparatic Acid	56.4 (49.4-63.4)	86	≥ 53.2	93	≥ 53.2	-
Citrulline	≤ 0.9	-	6.7 (6-7.3)	-	1.6 (1.4-1.8)	-
Glutamine	≥ 233.8	-	≥ 233.8	-	≥ 233.8	-
Glutamic acid	388 (384.9-391.1)	490	246 (233.7-258.3)	330	≥300	-
Glycine	32.1 (29.4-34.7)	30	45.5 (43.1-47.9)	-	17.8 (17.1-18.4)	27
Histidine	11.9 (9.3-14.5)	18	21.8 (19.3-24.3)	18	50.9 (46.8-55.0)	
isoleucine	28.4 (21.9-35.0)	32	34.6 (30.3-38.8)	30	30.6 (29.7-31.5)	27
Leucine	33.0 (27.6-38.3)	35	87.5 (86.1-88.9)	53	40.6 (38.7-42.6)	35
Lysine	83.4 (82.3-84.5)	140	20.8 (19.9-31.7))	50	27.8 (26.0-29.7)	35
Methionine	≤15	8	≤15	12	≤15	9
Ornithine	≤1.3	-	9.6 (7.8-11.4)	-	≤1.3	-
Phenylalanine	9.1 (7.1-11.1)	16	54.3 (49.8-58.8)	35	20.6 (19.5-21.7)	22
Proline	13.1 (10.2-16.0)	19	9.8 (7.8-11.7)	21	39.3 (38.8-39.7)	57
Serine	103.3 (64.7-141.9)	51	31.6 (28.8-34.3)	28	92.6 (79.9-105.3)	51
Threonine	26.9 (23.7-30.1)	30	46.4 (43.1-49.7)	-	23.4 (21.6-25.1)	24
Tryptophan	≤6.1	9	35.5 (33.5-37.5)	-	12.7 (10.8-14.5)	9
Tyrosine	16.9 (16.8-17.1)	14	64.0 (60.4-67.6)	18	7.2 (6.2-8.2)	12
Valine	29.6 (22.3-36.9)	43	43.3 (42.1-44.5)	38	58.1 (56.6-59.7)	45
Acetylornithine	-	-	4.0 (3.8-4.2)	-	0.52 (0.26-0.79)	-
Dimethylarginine	-	-	-	-	0.30 (0.26-0.33)	-
Alpha-aminoadipic acid	0.72 (0.68-0.75)	-	2.0 (1.8-2.2)	-	0.83 (0.62-0.10)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	0.59 (0.41-0.78)	-	0.2 (0.1-0.2)	-	0.13 (0.08-0.19)	-
Dopamine		-	0.2 (0-0.4)	-	-	-
Histamine	-	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	0.76 (0.69-0.84)	-	-	-	0.55 (0.50-0.61)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	-	-	-	-	0.54 (0.35-0.73)	-
Phenylethylamine	-	-	-	-	0.06 (0.04-0.09)	-
Putrescine	0.32 (0.31-0.33)	-	1.0 (0.9-1.1)	-	0.54 (0.43-0.65)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Dill	LV	Orange pepper	LV	Turnip	LV
Alanine	178.3 (118.5-239.1)	227	137.6 (131.8-143.3)	-	29.3 (28.9-29.7)	28
Arginine	523.5 (517.9-529.1)	142	67.6 (64.7-70.4)	-	13.7 (0.0-13.7)	10
Asparagine	≥52.8	-	≥52.8	-	≥52.8	-
Asparatic Acid	≥53.2	343	≥53.2	-	≥53.2	35
Citrulline	≤ 0.9	-	15.5 (12.6-18.3)	-	≥ 0.9	-
Glutamine	≥ 233.8	-	≥ 23.8	-	102.2 (100.1-104.3)	-
Glutamic acid	155.0 (133.9-176.7)	290	70.4 (64.4-76.4)	-	51.6 (50.3-52.8)	56
Glycine	146.2 (102.5-190.0)	169	12.4 (11.7-13.1)	-	89.1 (88.2-91.0)	15
Histidine	55.0 (51.1-59.0)	71	25.6 (25.5-25.7)	-	6.1 (6.0-6.2)	5
isoleucine	118.5 (116.5-120.5)	195	27.3 (25.6 -29.0)	-	23.4 (17.4-29.4)	15
Leucine	79.1 (57.0-101.2)	159	30.3 (28.1-32.5)	-	17.7 (15.9-19.6)	25
Lysine	364.1 (343.2-385.0)	246	40.5 (40.0-40.9)	-	11.4 (10.9-11.9)	12
Methionine	15.5 (14.2-16.9)	11	7.4 (7.3-7.6)	-	-	7
Ornithine	≤ 1.3	-	≤ 1.3	-	≤ 1.3	-
Phenylalanine	46.8 (39.3-54.3)	65	27.4 (26.3-28.5)	-	11.5 (11.5-11.6)	12
Proline	≥ 115.1	248	13.1 (9.4-16.8)	-	20.2 (20.1-20.3)	21
Serine	≥ 105.1	158	52.9 (52.1-53.7)	-	14.4 (14.3-14.5)	20
Threonine	152.8 (141.9-163.5)	68	162.7 (151.6-173.0)	-	16.6 (16.1-17.0)	17
Tryptophan	15.9 (15.6-16.3)	14	≤ 6.1	-	8.2 (6.5-10.0)	8
Tyrosine	81.4 (76.0-86.9)	96	12.2 (11.8-12.5)	-	6.8 (5.9-7.6)	9
Valine	171.1 (162.6-179.7)	154	89.7 (78.5-100.8)	-	14.2 (12.7-15.7)	15
Acetylornithine	3.3 (1.6-5.0)	-	-	-	-	-
Dimethylarginine	0.35 (0.21-0.49)	-	0.72 (0.59-0.86)	-	0.12 (0.09-0.14)	-
Alpha-aminoadipic acid	1.57 (1.23-1.91)	-	-	-	1.7 (1.3-2.2)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	0.22 (0.20-0.24)	-	0.13 (0.06-0.19)	-	0.06 (0.05-0.06)	-
Dopamine	0.14 (0.11-0.16)	-	0.10 (0.08-0.12)	-	-	-
Histamine	0.25 (0.24-0.25)	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	0.80 (0.72-0.87)	-	0.46 (0.34-0.58)	-	0.15 (0.13-0.17)	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	0.64 (0.56-0.71)	-	0.91 (0.84-0.97)	-	0.71 (0.60-0.81)	-
Phenylethylamine	-	-	0.03 (0.03-0.03)	-	0.07 (0.05-0.10)	-
Putrescine	-	-	-	-	0.07 (0.06-0.08)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	0.69 (0.54-0.83)	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Spinach	LV	Sunburst squash	LV	Cauliflower	LV
Alanine	90.2 (76.4-104.0)	110	69.6 (66.2-72.9)	-	124.5 (123.6-125.4)	180
Arginine	≥ 70	140	55.7 (52.9-58.6)	58	≥ 70	91
Asparagine	≥ 52.8	-	≥52.8	-	≥52.8	-
Asparatic Acid	≥ 53.2	230	≥53.2	-	≥53.2	-
Citrulline	2.6 (2.5-2.6)	-	52.3 (42.5-62.1)		3.4 (2.8-3.9)	
Glutamine	405.1 (399.7-410.4)	-	≥ 233.8	-	≥ 233.8	-
Glutamic acid	173.4 (164.9-181.8)	290	173.5 (170.2-176.9)	-	≥ 300	-
Glycine	45.7 (42.7-48.8)	110	43.8 (41.8-45.7)	-	199.1 (197.9-200.2)	84
Histidine	50.2 (45.1-55.3)	46	109.1 (103.8-114.2)	-	122.5 (116.8-128.1)	42
isoleucine	83.7 (72.4-95.1)	84	69.4 (60.4-78.4)	-	60.3 (51.4-69.2)	84
Leucine	115.5 (102.6-128.5)	150	74.5 (71.6-77.4)	-	28.2 (25.9-30.4)	130
Lysine	87.9 (84.0-91.7)	120	80.2 (79.4-81.0)	-	30.4 (30.1-30.7)	110
Methionine	5.7(4.9-6.4)	26	27.8 (26.5-29.2)	-	25.7 (25.6-25.9)	29
Ornithine	2.4 (2.3-2.5)	-	7.4 (6.0-8.8)	-	≤1.3	-
Phenylalanine	68.3 (63.9-72.8)	120	59.9 (42.5-77.3)	-	47.4 (45.7-49.1)	80
Proline	126.7 (111.2-142.2)	84	59.9 (42.5-77.3)	-	93.6 (84.7-102.4)	100
Serine	74.7 (60.2-89.1)	100	73.5 (73.3-73.8)	-	231.1 (228.5-233.7)	120
Threonine	48.1 (46.4-49.8)	92	46.3 (42.9-49.8)	-	75.5 (52.7-98.4)	80
Tryptophan	49.3 (43.3-55.4)	42	30.8 (30.0-31.6)	-	21.6 (18.6-24.7)	27
Tyrosine	79.7 (69.2-90.1)	63	73.1 (52.0-94.2)	-	16.9 (15.5-18.4)	49
Valine	114.1 (112.4-115.9)	120	51.14 (42.5-59.8)	-	134.9 (133.9-136.0)	140
Acetylornithine	1.0 (0.85-1.2)	-	1.5 (1.2-1.7)	-	0.57(0.55-0.59)	-
Dimethylarginine	0.32 (0.21-0.43)	-	1.1 (0.70-1.6)	-	0.62 (0.60-0.64)	-
Alpha-aminoadipic acid	0.73 (0.64-0.82)	-	-	-	0.16 (0.14-0.17)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	1.1 (0.86-1.4)	-	0.10 (0.09-0.11)	-	-	-
Dopamine	0.06 (0.05-0.08)	-	-	-	-	-
Histamine	17.1 (16.4-17.8)	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	0.44 (0.38-0.49)	-	1.7 (1.6-1.8)	-	-	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	0.46 (0.37-0.54)	-	1.9 (1.8-2.1)	-	-	-
Phenylethylamine	0.07 (0.05-0.09)	-	-	-	-	-
Putrescine	-	-	-	-	1.3 (1.2-1.4)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Japanese pumpkin	LV	Lettuce	LV	Tomato	LV
Alanine	16.9 (15.8-18.0)	12	43.6 (40.2-47.1)	55	36.8 (33.4-40.3)	19
Arginine	≥ 70	32	39.5 (37.5-41.5)	53	17.9 (17.3-18.4)	27
Asparagine	51.7 (47.2-56.3)	-	≥ 52.8	-	114.2 (100.1-128.3)	-
Asparatic Acid	≥ 53.2	120	139.9 (136.7-143.1)	140	137.9 (131.6-144.2)	82
Citrulline	1.8 (1.8-1.9)	-	≤ 0.9	-	≤ 0.9	-
Glutamine	382.8 (327.9-437.5)	-	≥ 233.8	-	≥ 233.8	-
Glutamic acid	95.6 (93.5-97.68)	100	113.7 (109.6-117.8)	180	86.7 (78.7-94.7)	200
Glycine	19.5 (19.4-19.7)	15	2.7 (2.4-3.0)		28.3 (27.9-28.8)	21
Histidine	3.6 (2.7-4.5)	7	14.8 (13.8-15.8)		14.8 (14.3-15.3)	12
isoleucine	23.7 (22.4-24.9)	21	37.1 (31.1-43.1)	45	15.1 (11.0-19.2)	34
Leucine	21.5 (17.5-25.4)	24	28.7 (27.4-30.0)	77	23.4 (18.9-27.8)	29
Lysine	7.2 (4.3-10.1)	19	56.1 (42.9-69.4)	63	99.9 (77.3-122.7)	34
Methionine	6.8 (6.2-7.4)	7	≤15	-	≤15	8
Ornithine	≤ 1.3	-	≤ 1.3	-	≤ 1.3	-
Phenylalanine	209.6 (199.5-219.7)	150	46.2 (45.5-46.9)	65	33.7 (31.7-35.6)	20
Proline	9.8 (9.7-10.0)	12	13.2 (11.9-14.5)	-	46.2 (40.0-52.4)	23
Serine	36.4 (35.9-36.8)	37	40.3 (31.1-49.5)	-	29.9 (29.4-30.6)	26
Threonine	13.2 (11.6-14.9)	11	31.3 (28.8-33.7)	43	23.3 (22.8-23.7)	20
Tryptophan	10.2 (9.0-11.4)	9	10.7 (9.1-12.3)	10	7.3(6.9-7.7)	7
Tyrosine	37.2 (31.9-42.4)	12	18.9 (15.9-22.1)	26	27.2 (26.3-28.1)	27
Valine	7.2 (6.5-7.8)	22	36.5 (32.5-40.56)	55	12.0 (11.2-12.8)	21
Acetylornithine	4.5 (3.6-5.5)	-	0.43 (0.41-0.47)	-	-	-
Dimethylarginine	2.9 (2.7-3.0)	-	0.08 (0.07-0.09)	-	-	-
Alpha-aminoadipic acid	3.2 (2.5-3.9)	-	1.3 (0.0-2.5)	-	0.35 (0.31-0.39)	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	0.15 (0.12-0.18)	-	-	-	-	-
Dopamine	-	-	-	-	-	-
Histamine	-	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	0.53 (0.48-0.57)	-	0.16 (0.13-0.19)	-	-	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans 4-Hydroxyproline	-	-	0.17 (0.15-0.18)	-	-	-
Phenylethylamine	-	-	-	-	-	-
Putrescine	-	-	-	-	0.17 (0.16-0.19)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Italian red pepper	LV	Nanking cherry	LV
Alanine	60.4 (58.9-61.9)	-	14.0 (13.4-14.6)	-
Arginine	34.4 (32.9-35.9)	-	35.7 (35.2-36.3)	-
Asparagine	80.8 (79-6-82.1)	-	≥52.8	-
Asparatic Acid	150.3 (149.3-151.3)	-	≥53.2	-
Citrulline	13.2 (12.0-14.4)	-	≤ 1	-
Glutamine	136.4 (131.8-140.9)	-	56.2(53.7-58.7)	-
Glutamic acid	55.4 (49.3-61.6)	-	29.9 (28.1-31.8)	-
Glycine	67.7 (62.6-72.9)	-	5.8 (3.6-8.1)	-
Histidine	14.2 (2.9-25.5)	-	1.7 (1.5-1.9)	-
isoleucine	39.9 (37.8-42.2)	-	≤2.6	-
Leucine	29.4 (28.3-30.5)	-	7.3 (5.3-9.3)	-
Lysine	28.4 (27.2-29.6)	-	35.4 (33.4-36.4)	-
Methionine	≤15	-	≤15	-
Ornithine	≤13	-	≤13	-
Phenylalanine	50.9 (43.7-58.1)	-	21.1 (19.9-22.2)	-
Proline	42.5 (40.7-44.3)	-	35.2 (30.9-39.4)	-
Serine	180.5 (180.5-180.5)	-	52.9 (49.3-56.4)	-
Threonine	122.4 (117.8-127.0)	-	45.8 (44.2-47.4)	-
Tryptophan	14.9 (14.4-15.4)	-	≤6	-
Tyrosine	12.9 (12.7-13.1)	-	19 (18.1-19.9)	-
Valine	66.7 (59.0-74.5)	-	19.8 (18.8-20.9)	-
Acetylornithine	-	-	12.8 (9.6-16.1)	-
Dimethylarginine	0.34 (0.31-0.37)	-	-	-
Alpha-aminoadipic acid	0.38 (0.35-0.40)	-	-	-
Carnosine	-	-	-	-
Creatinine	-	-	-	-
Levodopa	-	-	-	-
Dopamine	-	-	-	-
Histamine	-	-	-	-
Kynurenine	-	-	-	-
Methioninesulfoxide	-	-	-	-
cis 4-Hydroxyproline	-	-	-	-
trans 4-Hydroxyproline	-	-	5.5 (2.7-8.3)	-
Phenylethylamine	-	-	0.03 (0.02-0.04)	-
Putrescine	-	-	-	-
Serotonin	-	-	0.43 (0.29-0.57)	-
Taurine	-	-	-	-

Continued.

Table 2.7.*Continued.*

Metabolites	Raspberry	LV	Crab apple	LV	Saskatoon berry	LV
Alanine	39.2 (38.7-39.6)	-	19.8 (19.8-19.9)	-	93.4 (91.7-95.2)	-
Arginine	15.9 (13.0-18.8)	-	43.5 (42.3-44.8)	-	33.1 (32.8-33.3)	-
Asparagine	73.5 (64.6-82.4)	-	≥ 52.8	-	≥ 52.8	-
Asparatic Acid	62.1 (59.8-64.4)	-	62.5 (60.3-64.7)	-	21.4 (13.5-29.4)	-
Citrulline	1.2 (0.51-1.9)	-	25.7 (25.6-25.7)	-	≤ 0.9	-
Glutamine	106.3 (102.4-110.3)	-	292.0 (291.2-292.8)	-	59.9 (56.5-63.3)	-
Glutamic acid	27.9 (27.5-28.4)	-	55.7 (55.5-55.8)	-	161.4 (154.3-168.5)	-
Glycine	13.5 (12.0-15.0)	-	3.9 (3.9-3.9)	-	22.6 (18.9-26.4)	-
Histidine	2.8 (1.7-4.0)	-	22.5 (22.5-22.6)	-	12.4 (10.1-14.8)	-
Isoleucine	10.7 (10.4-11.1)	-	28.0 (27.9-28.0)	-	≤ 2.6	-
Leucine	12.1 (11.7-12.5)	-	201.0 (20.9-21.02)	-	35.6 (35.5-35.8)	-
Lysine	3.1 (3.0-3.2)	-	38.9 (38.8-39.1)	-	17.0 (15.5-18.6)	-
Methionine	11.3 (11.1-11.6)	-	≤15	-	12.4 (12.1-12.7)	-
Ornithine	14.5 (14.2-14.8)	-	4.0 (4.0-4.1)	-	69.8 (69.2-70.4)	-
Phenylalanine	25.7 (25.3-26.1)	-	22.0 (21.9-22.1)	-	20.0 (18.3-21.8)	-
Proline	14.7 (13.5-16.0)	-	31.1 (31.0-31.2)	-	23.8 (22.0-25.5)	-
Serine	44.0 (31.8-56.3)	-	28 (27.9-28.1)	-	21.3 (14.2-28.4)	-
Threonine	23.4 (23.3-23.6)	-	24.3 (24.2-24.3)	-	13.6 (13.0-14.2)	-
Tryptophan	9.1 (8.9-9.3)	-	11.7 (11.7-11.7)	-	≤6.1	-
Tyrosine	23(22.7-23.3)	-	23.5 (23.2-23.9)	-	9.8 (8.7-10.8)	-
Valine	10.5 (8.5-12.5)	-	70.2 (70.0-70.4)	-	42.4 (36.4-48.3)	-
Acetylornithine	7.3 (4.6-9.9)	-	2.6 (2.5-2.6)	-	11.1 (10.5-11.6)	-
Dimethylarginine	-	-	0.11 (0.11-0.11)	-	0.31 (0.21-0.41)	-
Alpha-aminoadipic acid	-	-	0.52 (0.51-0.52)	-	-	-
Carnosine	-	-	-	-	-	-
Creatinine	-	-	-	-	-	-
Levodopa	-	-	-	-	-	-
Dopamine	-	-	-	-	-	-
Histamine	-	-	-	-	-	-
Kynurenine	-	-	-	-	-	-
Methioninesulfoxide	-	-	-	-	-	-
cis 4-Hydroxyproline	-	-	-	-	-	-
trans4-Hydroxyproline	-	-	-	-	-	-
Phenylethylamine	0.38 (0.35-0.42)	-	-	-	-	-
Putrescine	0.62 (0.61-0.63)	-	0.99 (0.99-1.0)	-	2.2 (1.8-2.7)	-
Serotonin	-	-	-	-	-	-
Taurine	-	-	-	-	-	-

Table 2.8 Polyphenol contents of fruits and vegetables as determined by HPLC (Conc. mg/100 g FW).

Metabolites	Cucumber	LV[1]	Onion	LV
Gallic Acid	0.009 (0.009-0.01)	-	0.41 (0.31-0.51)	-
3, 4-Dihydroxybenzoic acid	0.03 (0.02-0.03)	-	0.61 (0.56-0.66)	-
Catechin	0.002 (0.002-0.002)	-	-	-
Chlorogenic Acid	0.004 (0.003-0.005)	-	-	-
Caffeic Acid	0.06 (0.05-0.07)	-	0.04 (0.03-0.04)	-
Vanillic Acid	0.03 (0.02-0.03)	-	0.49 (0.39-0.58)	-
Syringic Acid	0.006 (0.005-0.007)	-	-	-
Coumaric Acid	0.001 (0.001-0.001)	-	-	-
Benzoic Acid	-	-	0.67 (0.51-0.83)	-
Ferulic Acid	0.001 (0.001-0.001)	-	0.12 (0.12-0.12)	-
Sinapic Acid	-	-	20.8 (15.8-25.8)	-
Rutin	0.002 (0.002-0.003)	-	0.53 (0.41-0.66)	-
Resveratrol	0.008 (0.006-0.009)	-	0.15 (0.12-0.18)	-
Myricetin	-	-	16.2(15.3-17.23)	29.9
Quercetin	0.03 (0.03-0.03)	0.04	0.03 (0.03-0.03)	0.03
Luteolin	0.001 (0.001-0.001)	0.0015	-	-
Kaempferol	0.06 (0.06-0.06)	0.06	-	-
Isorhamnetin	0.001 (0.001-0.001)	-	5.1 (4.8-5.3)	-
Apigenin	-	0.0005	-	-
Polyphenols	**Carrot**	**LV**	**Green zucchini**	**LV**
Gallic Acid	0.15 (0.14-0.17)	-	1.0 (0.99-1.1)	-
3, 4-Dihydroxybenzoic acid	0.56 (0.53-0.60)	-	0.02 (0.01-0.03)	-
Catechin	-	-	-	-
Chlorogenic Acid	-	0.15	-	-
Caffeic Acid	-	0.02	0.47 (0.43-0.51)	-
Vanillic Acid	3.2 (3.1-3.3)	-	0.48 (0.47-0.50)	-
Syringic Acid	-	-	0.04 (0.04-0.04)	-
Coumaric Acid	-	-	-	-
Benzoic Acid	0.03 (0.03-0.03)	-	0.10 (0.10-0.11)	-
Ferulic Acid	-	-	0.94 (0.92-0.95)	-
Sinapic Acid	-	-	0.57 (0.55-0.58)	-
Rutin	-	-	-	-
Resveratrol	0.14 (0.13-0.15)	-	-	-
Myricetin	-	-	-	-
Quercetin	0.35 (0.33-0.37)	-	0.02 (0.02-0.03)	-
Luteolin	2.3 (2.2-2.5)	-	0.27 (0.26-0.28)	-
Kaempferol	2.2 (2.1-2.3)	-	-	-
Isorhamnetin	0.39 (0.30-0.48)	-	-	-
Apigenin	-	-	-	-

[1] LV for Literature value. References for LV's are reported in the AFCDB website.*Continued.*

Table 2.8.*Continued.*

Polyphenols	Tomato	LV	Italian red pepper	LV
Gallic Acid	0.46 (0.43-0.49)	-	1.7 (1.5-1.9)	-
3, 4-Dihydroxybenzoic acid	0.01 (0.01-0.01)	-	0.09 (0.08-0.10)	-
Catechin	-	-	-	-
Chlorogenic Acid	0.009 (0.009-0.009)	-	0.11 (0.10-0.12)	-
Caffeic Acid	0.13 (0.13-0.13)	0.38 ± 0.106	0.30 (0.27-0.34)	-
Vanillic Acid	0.02 (0.02-0.02)	-	1.2 (1.0-1.3)	-
Syringic Acid	0.01 (0.01-0.01)	-	0.19 (0.18-0.22)	-
Coumaric Acid	-	-	0.02 (0.02-0.02)	-
Benzoic Acid	0.001 (0.001-0.001)	-	10.6 (9.5-11.7)	-
Ferulic Acid	-	-	0.25 (0.24-0.25)	-
Sinapic Acid	0.61 (0.59-0.62)	-	0.88 (0.79-0.97)	-
Rutin	0.002 (0.001-0.002)	-	0.06 (0.06-0.06)	-
Resveratrol	0.001 (0.001-0.002)	-	0.01 (0.01-0.01)	-
Myricetin	0.001 (0.001-0.001)	-	0.006 (0.006-0.007)	-
Quercetin	0.009 (0.009-0.009)	0.00423	0.07 (0.06-0.08)	-
Luteolin	-	-	0.003 (0.003-0.004)	-
Kaempferol	-	-	-	-
Isorhamnetin	0.005 (0.005-0.006)	-	0.02 (0.02-0.02)	-
Apigenin	-	-	0.09 (0.08-0.10)	-
Polyphenols	**Turnip**	**LV**	**Japanese pumpkin**	**LV**
Gallic Acid	1.6 (1.3-2.3)	-	0.10 (0.10-0.11)	-
3, 4-Dihydroxybenzoic acid	0.03 (0.03-0.03)	-	0.06 (0.05-0.08)	-
Catechin	-	-	0.45 (0.44-0.46)	-
Chlorogenic Acid	-	-	0.37 (0.35-0.39)	-
Caffeic Acid	0.03 (0.02-0.03)	-	-	-
Vanillic Acid	0.13 (0.10-0.15)	-	-	-
Syringic Acid	0.05 (0.04-0.06)	-	-	-
Coumaric Acid	-	-	0.03 (0.03-0.03)	-
Benzoic Acid	0.02 (0.01-0.02)	-	-	-
Ferulic Acid	0.56 (0.47-0.65)	-	0.13 (0.11-0.15)	-
Sinapic Acid	0.10 (0.09-0.11)	-	0.16 (0.15-0.17)	-
Rutin	0.02 (0.01-0.02)	-	-	-
Resveratrol	0.07 (0.06-0.09)	-	0.01 (0.01-0.01)	-
Myricetin	-	-	0.08 (0.08-0.08)	-
Quercetin	0.03 (0.02-0.04)	-	0.33 (0.21-0.44)	-
Luteolin	0.001 (0.001-0.001)	-	-	-
Kaempferol	0.005 (0.005-0.006)	-	-	-
Isorhamnetin	-	-	-	-
Apigenin	-	-	-	-

Continued.

Table 2.8.*Continued.*

Polyphenols	Garlic	LV	Parsnip	LV
Gallic Acid	0.61 (0.60-0.62)	-	8.2 (6.8-9.6)	-
3, 4-Dihydroxybenzoic acid	0.04 (0.04-0.04)	-	-	-
Catechin	-	-	-	-
Chlorogenic Acid	-	-	-	-
Caffeic Acid	0.01 (0.01-0.01)	-	0.75 (0.64-0.87)	-
Vanillic Acid	0.18 (0.17-0.18)	-	1.4 (1.2-1.7)	-
Syringic Acid	-	-	1.1 (1.0-1.2)	-
Coumaric Acid	0.26 (0.26-0.26)	-	26.2 (24.3-28.1)	-
Benzoic Acid	-	-	0.32 (0.31-0.33)	-
Ferulic Acid	-	-	1.2 (1.1-1.3)	-
Sinapic Acid	5.2 (4.9-5.5)	-	1.4 (1.3-1.6)	-
Rutin	0.01 (0.01-0.01)	-	0.15 (0.13-0.17)	-
Resveratrol	-	-	0.21 (0.17-0.25)	-
Myricetin	-	-	0.04 (0.04-0.04)	-
Quercetin	0.03 (0.02-0.03)	-	0.62 (0.57-0.66)	-
Luteolin	0.22 (0.21-0.22)	-	0.30 (0.30-0.31)	-
Kaempferol	-	-	-	-
Isorhamnetin	0.02 (0.01-0.02)	-	0.20 (0.17-0.23)	-
Apigenin	0.61 (0.60-0.62)	-	0.10 (0.09-0.10)	-
Polyphenols	**Eggplant**	**LV**	**Yellow bean**	**LV**
Gallic Acid	0.12 (0.11-0.13)	0.14	1.7 (1.3-2.0)	-
3, 4-Dihydroxybenzoic acid	0.03 (0.02-0.04)	-	0.73 (0.70-0.76)	-
Catechin	-	-	-	-
Chlorogenic Acid	0.09 (0.09-0.10)	-	-	-
Caffeic Acid	0.22 (0.15-0.29)	0.38	0.08 (0.07-0.08)	-
Vanillic Acid	0.16 (0.13-0.18)	-	2.9 (2.4-3.3)	-
Syringic Acid	0.02 (0.02-0.03)	-	0.71 (0.70-0.72)	-
Coumaric Acid	-	-	0.17 (0.15-0.19)	-
Benzoic Acid	0.02 (0.01-0.02)	-	0.01 (0.01-0.01)	-
Ferulic Acid	0.59 (0.51-0.68)	0.22	-	-
Sinapic Acid	-	-	0.15 (0.12-0.19)	-
Rutin	0.01 (0.01-0.01)	-	0.28 (0.22-0.35)	-
Resveratrol	-	-	0.32 (0.30-0.35)	-
Myricetin	0.003 (0.002-0.003)	-	0.33 (0.25-0.40)	-
Quercetin	0.007 (0.005-0.009)	-	0.12 (0.10-0.14)	-
Luteolin	-	-	1.71 (1.64-1.78)	-
Kaempferol	-	-	-	-
Isorhamnetin	0.07 (0.01-0.13)	-	0.15 (0.14-0.16)	-
Apigenin	-	-	1.7 (1.3-2.0)	-

Continued.

Table 2.8.*Continued.*

Polyphenols	Red bell pepper	LV	Yellow pepper	LV
Gallic Acid	0.24 (0.21-0.27)	-	0.08 (0.07-0.09)	-
3, 4-Dihydroxybenzoic acid	0.008 (0.008-0.008)	-	0.50 (0.44-0.55)	-
Catechin	0.05 (0.04-0.06)	-	0.06 (0.05-0.06)	-
Chlorogenic Acid	0.07 (0.06-0.08)	-	0.16 (0.13-0.18)	-
Caffeic Acid	1.8 (1.6-1.9)	-	0.83 (0.74-0.92)	-
Vanillic Acid	0.13 (0.12-0.15)	-	0.28 (0.25-0.31)	-
Syringic Acid	0.11 (0.10-0.12)	-	0.15 (0.13-0.17)	-
Coumaric Acid	0.06 (0.05-0.08)	-	0.19 (0.16-0.23)	-
Benzoic Acid	0.07 (0.07-0.07)	-	-	-
Ferulic Acid	0.02 (0.02-0.02)	-	0.03 (0.02-0.04)	-
Sinapic Acid	-	-	0.01 (0.01-0.02)	-
Rutin	0.10 (0.10-0.10)	-	-	-
Resveratrol	-	-	0.05 (0.05-0.06)	-
Myricetin	0.12 (0.12-0.13)	-	0.11 (0.10-0.13)	-
Quercetin	0.03 (0.03-0.04)	-	1.7 (1.6-1.9)	-
Luteolin	1.2 (1.0-1.4)	-	2.2 (1.9-2.4)	-
Kaempferol	-	-	-	-
Isorhamnetin	0.007 (0.007-0.007)	-	-	-
Apigenin	0.04 (0.04-0.04)	-	-	-
Polyphenols	**Green bean**	**LV**	**Lettuce**	**LV**
Gallic Acid	1.7 (1.2-2.2)	-	0.001 (0.001-0.001)	-
3, 4-Dihydroxybenzoic acid	-	-	1.4 (1.2-1.5)	-
Catechin	0.60 (0.59-0.61)	0.4	0.004 (0.004-0.005)	-
Chlorogenic Acid	-	-	2.3 (2.1-2.5)	-
Caffeic Acid	-	-	0.03 (0.03-0.04)	-
Vanillic Acid	1.3 (1.2-1.4)	-	0.76 (0.66-0.85)	-
Syringic Acid	0.30 (0.23-0.37)	-	0.001 (0.001-0.001)	-
Coumaric Acid	0.30 (0.28-0.32)	-	0.75 (0.67-0.83)	-
Benzoic Acid	-	-	-	-
Ferulic Acid	0.29 (0.19-0.39)	-	0.004 (0.003-0.004)	-
Sinapic Acid	0.24 (0.10-0.38)	-	0.74 (0.66-0.81)	-
Rutin	-	-	-	-
Resveratrol	0.34 (0.33-0.36)	-	0.003 (0.002-0.003)	-
Myricetin	0.72 (0.54-0.89)	-	0.04 (0.04-0.04)	-
Quercetin	0.53 (0.52-0.54)	-	0.001 (0.001-0.001)	-
Luteolin	2.3 (1.7-2.9)	-	0.15 (0.14-0.16)	-
Kaempferol	1.9 (1.3-2.6)	-	-	-
Isorhamnetin	0.31 (0.12-0.49)	-	0.72 (0.64-0.80)	-
Apigenin	-	-	-	-

Continued.

Table 2.8.*Continued.*

Polyphenols	Spinach	LV	Red beetroot	LV
Gallic Acid	2.8 (2.8-2.8)	-	0.60 (0.48-0.71)	-
3, 4-Dihydroxybenzoic acid	14.9 (12.7-17.1)	-	0.92 (0.78-1.1)	-
Catechin	-	-	0.56 (0.46-0.66)	-
Chlorogenic Acid	0.10 (0.09-0.11)	-	0.03 (0.03-0.03)	0.018
Caffeic Acid	0.58 (0.53-0.63)	-	-	0.037
Vanillic Acid	4.3 (4.2-4.4)	-	2.8 (2.6-3.1)	-
Syringic Acid	0.21 (0.19-0.23)	-	0.60 (0.57-0.63)	-
Coumaric Acid	0.69 (0.11-1.27)	-	1.3 (1.2-1.5)	-
Benzoic Acid	-	-	0.19 (0.17-0.20)	-
Ferulic Acid	0.92 (0.83-1.0)	-	2.0 (1.4-2.7)	-
Sinapic Acid	0.03 (0.02-0.04)	-	0.21 (0.19-0.24)	-
Rutin	-	-	1.2 (1.1-1.3)	-
Resveratrol	0.37 (0.35-0.39)	-	-	-
Myricetin	0.17 (0.16-0.19)	0.37	-	-
Quercetin	2.0 (1.9-2.2)	1.96	0.16 (0.14-0.17)	0.134
Luteolin	-	-	-	-
Kaempferol	2.02 (1.85-2.2)	1.53	-	-
Isorhamnetin	-	-	0.36 (0.29-0.44)	-
Apigenin	20.2 (18.2-22.3)	-	-	-
Polyphenols	**Potato**	**LV**	**Swiss chard**	**LV**
Gallic Acid	0.16 (0.13-0.18)	-	1.7 (1.7-1.7)	-
3, 4-Dihydroxybenzoic acid	0.90 (0.86-0.95)	-	2.3 (2.2-2.4)	-
Catechin	0.14 (0.12-0.16)	-	-	-
Chlorogenic Acid	1.3 (1.3-1.3)	-	0.26 (0.22-0.29)	-
Caffeic Acid	-	-	0.32 (0.27-0.36)	0.2
Vanillic Acid	2.1 (2.0-2.1)	-	1.7 (1.6-1.9)	-
Syringic Acid	0.95 (0.95-0.96)	-	30.6 (29.4-31.9)	25.75
Coumaric Acid	0.24 (0.22-0.25)	-	2.9 (2.9-2.9)	4.4
Benzoic Acid	0.20 (0.18-0.21)	-	0.06 (0.05-0.06)	-
Ferulic Acid	0.17 (0.15-0.19)	-	8.7 (7.9-9.4)	6.85 ± 1.7
Sinapic Acid	0.10 (0.10-0.10)	-	0.01 (0.01-0.02)	-
Rutin	2.3 (2.1-2.5)	-	0.28 (0.23-0.32)	-
Resveratrol	-	-	-	-
Myricetin	-	-	-	-
Quercetin	-	-	0.33 (0.32-0.35)	0.5
Luteolin	-	-	0.12 (0.07-0.17)	-
Kaempferol	-	-	1.7 (1.0-2.3)	1.7
Isorhamnetin	-	-	0.05 (0.04-0.06)	-
Apigenin	-	-	1.7 (1.7-1.8)	-

Continued.

Table 2.8.*Continued.*

Polyphenols	Orange pepper	LV	White cabbage	LV
Gallic Acid	0.40 (0.36-0.44)	-	0.44 (0.43-0.45)	-
3, 4-Dihydroxybenzoic acid	0.17 (0.15-0.18)	-	0.57 (0.55-0.58)	-
Catechin	0.15 (0.15-0.16)	-	-	-
Chlorogenic Acid	-	-	-	-
Caffeic Acid	-	-	-	-
Vanillic Acid	1.0 (0.93-1.1)	-	0.23 (0.19-0.27)	-
Syringic Acid	-	-	0.30 (0.26-0.34)	-
Coumaric Acid	0.97 (0.85-1.1)	-	-	-
Benzoic Acid	0.04 (0.03-0.04)	-	0.07 (0.06-0.09)	-
Ferulic Acid	-	-	-	-
Sinapic Acid	-	-	0.30 (0.27-0.34)	-
Rutin	0.84 (0.77-0.92)	-	-	-
Resveratrol	-	-	0.15 (0.11-0.20)	-
Myricetin	1.1 (1.0-1.1)	-	-	-
Quercetin	-	-	0.15 (0.10-0.20)	0.16
Luteolin	3.3 (3.0-3.5)	1.07	-	-
Kaempferol	-	-	-	-
Isorhamnetin	0.18 (0.16-0.20)	-	-	-
Apigenin	-	-	0.04 (0.03-0.04)	0.04
Polyphenols	**Dill**	**LV**	**Sunburst squash**	**LV**
Gallic Acid	0.39 (0.38-0.40)	-	0.35 (0.30-0.39)	-
3, 4-Dihydroxybenzoic acid	2.1 (1.9-2.3)	-	0.01 (0.0-0.02)	-
Catechin	0.08 (0.08-0.09)	-	-	-
Chlorogenic Acid	1.1 (1.0-1.3)	-	-	-
Caffeic Acid	0.62 (0.60-0.64)	-	0.20 (0.17-0.22)	-
Vanillic Acid	1.7 (1.7-1.7)	-	0.65 (0.65-0.65)	-
Syringic Acid	0.14 (0.13-0.14)	-	0.07 (0.06-0.09)	-
Coumaric Acid	0.24 (0.22-0.27)	-	-	-
Benzoic Acid	1.5 (1.4-1.5)	-	0.01 (0.01-0.01)	-
Ferulic Acid	0.35 (0.30-0.39)	-	0.34 (0.33-0.35)	-
Sinapic Acid	0.38 (0.34-0.41)	-	0.78 (0.77-0.79)	-
Rutin	-	-	0.01 (0.01-0.01)	-
Resveratrol	-	-	-	-
Myricetin	0.71 (0.68-0.74)	0.7	-	-
Quercetin	7.9 (7.6-8.3)	5	0.04 (0.03-0.05)	-
Luteolin	0.3 (0.29-0.35)	-	0.46 (0.36-0.56)	-
Kaempferol	-	-	-	-
Isorhamnetin	22.4 (20.5-24.3)	43.5	-	-
Apigenin	-	-	-	-

Continued.

Table 2.8.*Continued.*

Polyphenols	Cauliflower	LV	Green pepper	LV
Gallic Acid	0.59 (0.51-0.67)	0.69	1.4 (1.3-1.4)	-
3, 4-Dihydroxybenzoic acid	1.6 (1.4-1.8)	-	0.03 (0.02-0.03)	-
Catechin	-	-	0.37 (0.33-0.41)	-
Chlorogenic Acid	0.55 (0.50-0.61)	-	-	-
Caffeic Acid	0.01 (0.01-0.01)	0.01	-	-
Vanillic Acid	0.51 (0.49-0.52)	-	1.2 (1.1-1.4)	-
Syringic Acid	1.3 (1.2-1.4)	1.13	0.24 (0.21-0.27)	-
Coumaric Acid	0.29 (0.28-0.30)	-	0.52 (0.43-0.61)	-
Benzoic Acid	0.01 (0.01-0.01)	-	-	-
Ferulic Acid	0.67 (0.62-0.71)	0.53	0.46 (0.46-0.47)	-
Sinapic Acid	3.6 (3.1-4.1)	4.28	0.11 (0.10-0.11)	-
Rutin	0.07 (0.05-0.10)	-	-	-
Resveratrol	0.78 (0.71-0.85)	-	0.37 (0.32-0.41)	-
Myricetin	-	-	0.58 (0.53-0.63)	-
Quercetin	0.31 (0.28-0.33)	-	1.7 (1.6-1.9)	2.16
Luteolin	-	-	3.0 (2.6-3.4)	2.11
Kaempferol	-	-	2.8 (2.5-3.2)	-
Isorhamnetin	0.11 (0.11-0.12)	-	0.56 (0.55-0.57)	-
Apigenin	0.07 (0.06-0.07)	-	-	-
Polyphenols	**Broccoli**	**LV**	**Yellow zucchini**	**LV**
Gallic Acid	0.03 (0.03-0.03)	-	0.79 (0.65-0.93)	-
3, 4-Dihydroxybenzoic acid	2.6 (2.4-2.8)	-	0.02 (0.01-0.04)	-
Catechin	1.8 (1.7-2.0)	-		-
Chlorogenic Acid	2.6 (2.4-2.8)	-		-
Caffeic Acid	0.27 (0.27-0.27)	-	0.57 (0.50-0.64)	-
Vanillic Acid	1.8 (1.7-2.0)	-	0.40 (0.33-0.48)	-
Syringic Acid	0.42 (0.38-0.46)	-	0.04 (0.04-0.05)	-
Coumaric Acid		-	-	-
Benzoic Acid	0.33 (0.31-0.36)	-	0.06 (0.06-0.06)	-
Ferulic Acid	11.6 (11.0-12.1)	-	0.78 (0.60-0.96)	-
Sinapic Acid	2.3 (2.2-2.5)	-	0.52 (0.38-0.66)	-
Rutin	-	-	-	-
Resveratrol	-	-		-
Myricetin		-		-
Quercetin	0.92 (0.87-0.96)	1.54	0.02 (0.02-0.03)	-
Luteolin	0.52 (0.48-0.57)	-	0.23 (0.18-0.28)	-
Kaempferol	5.1 (4.6-5.5)	3.08		-
Isorhamnetin	-	-	0.004 (0.003-0.005)	-
Apigenin	-	-	-	-

Table 2.9 Composition of fatty acids in vegetables and fruits as determined by GC-MS (molar%). Note that: GL is for glycolipids, PL is for phospholipids, CE is for cholesteryl esters, TG is for triglycerides and FF is for free fatty acids.

Lipids	Broccoli lipids					Red beetroot lipids				
	GL[1]	PL[2]	Neutral lipids			GL	PL	Neutral lipids		
			CE[3]	TG[4]	FF[5]			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	2.33	-	4.04	2.68	4.95	1.83	0.98	1.40	-	4.27
C15:0	1.63	0.67	-	-	1.56	3.10	3.43	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	-	48.65	17.80	24.75	21.82	13.39	86.48	22.90	16.34	49.32
C16:1(9)	1.55	-	-	-	-	-	1.37	-	-	-
C17:0	4.35	2.76	24.87	-	5.74	4.72	2.23	14.60	3.86	22.64
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	7.42	2.74	24.85	-	11.11	4.49	2.95	18.65	4.46	-
C18:1(9)	-	-	-	-	-	-	-	1.92	-	3.46
C18:2(9,12)	6.17	5.10	9.94	4.38	6.96	9.59	-	33.06	48.87	16.78
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	10.16	5.74	-	-	5.04	-	-	-	-	-
C18:3(9,12,15)	66.03	33.84	14.36	68.19	40.46	59.97	-	7.07	26.46	2.80
C20:1(11)	-	-	-	-	-	-	-	0.42	-	-
C21:0	-	-	-	-	0.31	-	-	-	-	-
C20:2(11,14)	-	0.25	-	-	-	1.21	0.97	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.37	0.26	-	-	0.73	0.63	0.53	-	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	4.13	-	0.36	0.35	0.35	-	-	0.73
C23:0	-	-	-	-	-	0.14	0.26	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	-	-	0.97	0.57	0.43	-	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

[1] GL for glycolipids
[2] PL for phospholipids
[3] CE for cholesteryl esters
[4] TG for triglycerides
[5] FF for free fatty acids

Table 2.9.*Continued.*

Lipids	Dill lipids					Eggplant lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.39	-	5.23	1.65	3.84	2.04	-	0.98	8.12	1.52
C15:0	0.65	-	-	3.31	-	3.69	-	-	-	0.85
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	66.47	-	31.26	28.21	38.35	-	36.60	33.39	-	36.17
C16:1(9)	-	-	-	-	-	-	-	-	-	-
C17:0	6.08	13.38	9.67	-	22.71	10.02	3.83	8.97	7.70	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	2.52	4.03	6.52	9.95	18.43	16.97	-	20.97	76.70	20.01
C18:1(9)		-	-	1.25	-	-	1.40	1.74	-	-
C18:2(9,12)	8.87	60.44	24.92	32.47	9.86	24.92	40.07	25.34	-	32.44
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	7.89	-	7.17	0.55	-	39.30	3.51	1.37	6.37	2.79
C18:3(9,12,15)	4.91	22.15	13.85	22.12	6.13	-	14.37	7.23	-	6.23
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	1.02	-	-	-	0.67	3.06	0.21	-	1.11	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.70	0.49	-	-	-	-	-	-
C23:0	0.20	-	-	-	-	-	-	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	0.68	-	-	-	-	-	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Garlic lipids					Green bean lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	0.42	-	1.51	16.81	1.27	0.91	-	1.92	3.98	6.74
C15:0	0.86	0.53	1.59	-	-	0.62	-	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	45.40	43.93	5.33	83.19	21.91	11.86	39.13	9.03	37.41	51.14
C16:1(9)	-	-	-	-	-	-	-	-	-	-
C17:0	3.53	-	7.61	-	16.25	3.71	-	9.64	11.91	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	4.89	-	35.39	-	12.82	1.79	-	16.14	-	-
C18:1(9)	1.00	3.42	-	-	-	-	-	-	12.89	-
C18:2(9,12)	10.99	44.55	40.59	-	37.76	5.01	29.41	16.09	8.80	8.23
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	0.97	-	1.41	10.48	0.43	3.67	-	18.40
C18:3(9,12,15)	32.40	7.29	2.98	-	7.16	63.53	30.88	39.02	25.01	-
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	1.31
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.23	0.17	1.36	-	1.42	1.42	0.14	3.35	-	7.68
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	0.12	-	0.77	-	-	-	-	0.45	-	-
C23:0	0.15	0.12	1.07	-	-	0.19	-	0.69	-	0.83
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	0.83	-	-	0.48	-	-	-	5.68
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Green bell pepper lipids					Green zucchini lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.41	0.52	2.86	2.73	1.67	3.02	1.16	8.23	1.33	4.27
C15:0	0.47	0.66	-	2.05	-	6.65	6.04	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	29.94	15.24	46.01	18.05	49.31	32.85	-	10.35	13.96	16.95
C16:1(9)	-	-	-	-	-	10.45	-	-	-	-
C17:0	2.23	2.29	16.05	-	24.05	-	7.28	29.78	8.47	34.70
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	-	-	-	11.43	-	-	13.81	39.48	9.33	33.59
C18:1(9)	-	-	-	1.01	-	-	-	-	3.91	-
C18:2(9,12)	6.75	-	7.58	9.95	9.72	20.40	42.06	7.56	12.17	8.30
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	15.36	11.59	3.12	-	-	-	1.98	1.26	-	-
C18:3(9,12,15)	42.30	66.64	18.57	54.78	14.27	18.84	21.21	-	50.84	-
C20:1(11)	-	-	-	-	-	-		-	-	-
C21:0	-	0.79	-	-	-	-	0.19	-	-	-
C20:2(11,14)	-	-	-	-	-	-	0.56	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.98	2.26	5.30	-	0.98	5.71	4.69	1.57	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	-	-	-		-	1.77	-	2.19
C23:0	0.21	-	0.52	-	-	-	0.51	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	0.34	-	-	-	-	2.09	0.50	-	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Japanese pumpkin lipids					Lettuce lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	7.70	-	1.94	25.58	5.69	4.37	0.79	6.05	2.59	5.38
C15:0	-	-	-	5.78	-	-	3.03	0.97	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	-	5.54	26.12	49.00	51.88	22.99	-	28.58	16.16	48.54
C16:1(9)	-	0.55	-	-	-	-	-	-	-	-
C17:0	-	0.63	3.19	19.65	0.86	7.28	2.48	3.84	3.90	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	22.07	5.96	9.64	-	-	-	7.74	17.99	3.98	41.60
C18:1(9)	20.48	3.74	10.03	-	-	-	-	-	-	-
C18:2(9,12)	14.86	41.61	20.88	-	5.00	17.27	11.95	13.05	16.05	4.48
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	0.85	1.74	-	6.17	-	6.13	3.66	-	-
C18:3(9,12,15)	-	39.46	25.39	-	27.20	16.02	65.10	17.66	57.32	-
C20:1(11)	-	-	-	-	1.20	-	-	-	-	-
C21:0	31.79	-	-	-	-	25.57	-	-	-	-
C20:2(11,14)	-	-	-	-	-	-	0.59	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	3.11	0.99	0.60	-	1.76	4.81	1.43	4.09	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.37	-	-	-	-	1.02	-	-
C23:0	-	0.37	-	-	-	1.68	-	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	0.29	0.11	-	0.23	-	0.46	3.10	-	-
C24:1(15)	-	-	-	-	-	-	0.31	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Italian red pepper lipids					Onion lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	1.79	0.72	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	2.70	0.53	7.85	31.46	10.11	1.77	0.38	1.31	-	2.09
C15:0	-	-	-	-	-	3.18	1.61	-	2.00	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	36.55	27.43	32.49	39.86	31.85	56.12	59.11	19.35	47.16	31.30
C16:1(9)	1.33	-	-	-	-	-	-	-	-	-
C17:0	-	1.81	12.63	-	7.70	0.92	1.89	9.97	-	27.34
C17:1(10)	-	-	-	-	-	-	-	16.46	-	-
C18:0	16.92	12.43	20.47	-	25.19	-	1.32	2.09	-	25.71
C18:1(9)	-	-	0.8	-	-	5.55	21.61	46.61	-	4.23
C18:2(9,12)	2.30	45.64	3.81	-	18.86	-	7.93	-	-	6.85
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	4.53	1.87	12.36	-	0.70	1.03	-	-	-	-
C18:3(9,12,15)	35.28	9.75	-	-	4.24	26.85	4.44	3.21	50.85	1.45
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	1.40	23.41	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	-	0.69	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.39	0.53	6.47	3.72	0.24	2.39	1.05	0.38	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.34	-	0.22	-	-	-	-	1.04
C23:0	-	-	0.81	0.51	0.18	0.29	0.14	0.62	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	0.58	0.38	-	1.20	0.50	-	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Potato lipids					Red bell pepper lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	0.78	0.67	2.30	1.59	7.94	9.25	0.53	2.53	25.86	27.48
C15:0	-	1.50	-	0.99	-	-	-	-	2.35	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	6.81	75.96	22.19	39.02	92.06	81.10	41.62	28.36	-	35.75
C16:1(9)	-	-	-	-	-	-	-	-	17.26	-
C17:0	3.118	3.86	9.75	1.25	-	5.59	3.63	2.08	-	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	24.40	2.01	13.69	-	-	-	20.21	14.57	-	19.98
C18:1(9)	-	-	-	-	-	-	-	-	-	-
C18:2(9,12)	11.24	1.97	23.27	3.65	-	-	7.14	27.43	-	10.11
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	8.09	4.66	0.36	4.12	-	-	3.00	5.61	54.52	-
C18:3(9,12,15)	43.55	8.46	27.60	49.38	-	-	23.04	13.82	-	5.37
C20:1(11)	0.23	-	-	-	-	-	-	-	-	-
C21:0	-	0.29	-	-	-	0.59	0.20	0.70	-	-
C20:2(11,14)	0.25	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.56	0.62	-	-	-	2.23	0.62	3.12	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	0.25	-	0.84	-	-	0.34	-	0.56	-	1.31
C23:0	0.40	-	-	-	-	0.38	-	0.65	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	0.25	-	-	-	-	0.53	-	0.58	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Yellow zucchini lipids					Yellow bell pepper lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	6.66	0.64	3.93	10.29	-	7.34	0.68	18.60	50.87	6.10
C15:0	6.65	1.44	0.90	-	-	1.21	-	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	16.07	61.57	39.54	19.10	2.80	12.72	24.75	5.29	20.99	35.33
C16:1(9)	-	1.10	-	-	-	-	-	9.11	14.67	-
C17:0	7.68	1.58	7.58	4.06	-	5.77	2.37	-	-	8.59
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	-	6.14	36.45	26.68	12.47	41.57	17.51	-	-	28.81
C18:1(9)	-	-	-	-	-	-	-	-	-	-
C18:2(9,12)	-	3.31	6.74	12.00	16.33	8.04	45.47	1.93	-	13.09
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	19.82	1.61	15.11	7.15	11.25	2.87	-	-	1.33
C18:3(9,12,15)	24.28	2.11	1.51	11.21	53.93	9.43	5.60	42.97	-	4.69
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	24.91	-	-	-	1.00	-	0.21	18.48	-	-
C20:2(11,14)	-	-	-	1.55	-	-	-	0.47	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	9.28	1.34	1.49	-	5.79	1.51	0.54	2.38	13.47	1.06
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.25	-	-	-	-	-	-	0.56
C23:0	1.14	0.43	-	-	-	0.36	-	0.39	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	3.33	0.52	-	-	0.52	0.81	-	0.37	-	0.43
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Turnip lipids					Tomato lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.08	-	0.69	1.43	3.13	0.89	0.57	3.97	24.62	2.97
C15:0	3.15	1.5	-	-	-	-	0.64	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	40.70	51.98	32.85	63.07	42.09	30.22	49.68	24.40	56.51	30.29
C16:1(9)	3.05	-	-	-	-	-	-	-	-	-
C17:0	7.96	2.77	9.26	4.48	10.34	4.51	4.74	7.02	18.78	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	7.41	1.85	4.69	5.77	44.44	8.53	2.06	9.36	-	36.15
C18:1(9)	-	-	-	-	-	-	-	-	-	-
C18:2(9,12)	17.52	34.85	12.66	11.63	-	35.63	7.44	36.39	-	19.20
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	-	-	-	-	33.03	1.44	-	2.03
C18:3(9,12,15)	13.10	6.90	37.12	13.22	-	20.00	1.68	9.43	-	6.61
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	-	-	1.75	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.29	-	-	-	-	0.21	-	1.19	-	1.61
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	1.89	0.40	-	-	-	0.72	-	0.67
C23:0	-	-	-	-	-	-	0.15	2.81	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	0.15	0.33	-	-	-	-	1.54	-	0.47
C24:1(15)	-	-	0.51	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Swiss chard lipids					Sunburst squash lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	16.50	0.52	2.02	4.37	4.28	3.63	-	1.95	4.31	6.31
C15:0	11.11	1.19	-	-	-	3.35	1.56	0.74	1.28	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	-	2.95	32.65	36.86	38.31	52.35	36.43	11.15	15.50	37.40
C16:1(9)	-	-	-	-	-	-	1.02	-	-	-
C17:0	-	3.90	10.65	13.38	8.31	5.87	1.86	6.38	4.14	6.88
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	31.67	1.35	34.87	9.49	43.62	-	1.68	22.40	-	30.22
C18:1(9)	-	2.75	-	-	-	-	-	-	-	-
C18:2(9,12)	-	6.66	9.09	-	3.79	7.77	5.46	23.49	10.51	6.12
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	-	-	-	12.35	2.88	0.59	-	-
C18:3(9,12,15)	-	79.36	9.34	35.90	-	8.83	47.06	31.05	64.26	8.78
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	-	-	-	-	-
C20:2(11,14)	15.91	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	11.48	0.91	-	-	-	3.28	1.43	1.33	-	2.79
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	4.40	-	1.37	-	1.70	0.48	-	0.92	-	0.82
C23:0	2.03	-	-	-	-	0.59	0.21	-	-	0.69
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	6.90	0.39	-	-	-	1.52	0.41	-	-	0.88
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Spinach lipids					Cauliflower lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	0.98	0.42	3.5	-	5.43	1.06	-	2.23	2	3.20
C15:0	1.49	0.70	1.22	-	-	1.22	-	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	41.62	50.82	27.68	27.15	45.02	8.41	39.36	26.35	9.75	40.03
C16:1(9)	11.40	4.61	-	-	-	1.35	-	-	-	-
C17:0	3.64	2.11	11.32	5.80	-	7.81	0.48	10.65	4.37	-
C17:1(10)	0.66	-	-	-	-	-	-	-	-	-
C18:0	-	1.86	14.92	5.10	43.90	-	0.46	19.23	5.30	-
C18:1(9)	-	-	-	-	-	-	-	-	-	2.19
C18:2(9,12)	5.12	34.77	6.60	27.21	-	16.94	3.97	6.15	7.86	6.82
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	10.08	-	-	8.43	-	-	-	-
C18:3(9,12,15)	33.65	4.28	19.89	34.75	4.45	54.78	55.73	34.84	70.73	47.76
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	0.48	-	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.70	0.27	3.44	-	1.19	-	-	-	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	0.21	-	-	-	-	-	-	0.55	-	-
C23:0	0.53	-	0.33	-	-	-	-	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	D	0.17	0.54	-	-	-	-	-	-	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Cucumber lipids					Orange bell pepper lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	1.45
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	2.51	0.43	1.10	-	20.80	6.83	0.47	25.61	34.80	6.30
C15:0	0.85	0.69	-	-	14.10	-	-	0.96	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	80.20	49.67	23.01	86.74	25.83	31.43	43.75	-	29.13	36.56
C16:1(9)	1.88	-	-	-	-	-	-	-	-	-
C17:0	1.08	3.35	4.75	5.14	-	6.19	1.98	-	4.51	7.40
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	7.56	18.86	12.80	8.12	-	-	15.32	29.81	-	26.81
C18:1(9)	-	-	-	-	-	-	0.44	-	-	-
C18:2(9,12)	-	-	22.73	-	-	20.20	4.62	13.81	-	10.06
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	-	-	-	26.70	2.81	20.59	31.53	10.87
C18:3(9,12,15)	-	25.15	35.90	-	-	5.58	29.84	-	-	-
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	0.45	0.21	1.41	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.27	1.02	-	-	12.56	1.72	0.33	5.60	-	-
C20:4(5,8,11,14)	3.72	0.63	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.72	-	-	-	-	-	-	-
C23:0	-	-	-	-	2.75	0.34	0.09	1.45	-	-
C20:5(5,8,11,14,17)	1.81	-	-	-	-	-	-	-	-	-
C24:0	0.11	0.20	-	-	23.96	0.57	0.13	0.76	-	0.55
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Raspberry lipids					Nanking cherry lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.17	1.55	0.86	3.84	3.03	0.92	0.43	2.44	2.63	23.46
C15:0	-	-	-	-	-	0.40	0.51	-	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	20.33	20.14	26.92	62.16	22.39	5.35	5.81	27.77	19.41	-
C16:1(9)	-	4.09	-	-	-	-	-	-	-	-
C17:0	4.11	1.13	1.76	-	5.12	7.39	1.48	6.37	-	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	10.50	5.37	11.40	-	18.52	25.26	28.48	25.83	4.62	-
C18:1(9)	-	21.89	-	-	-	1.08	3.40	-	2.90	19.02
C18:2(9,12)	22.12	41.51	33.75	-	50.06	5.78	42.95	13.08	58.90	44.65
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	2.75	-	19.02	-	-	2.66	9.59	4.76	-	-
C18:3(9,12,15)	38.44	4.18	-	-	-	50.26	5.99	-	11.54	12.87
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	0.32	33.05	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	-	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.35	0.15	4.13	0.95	0.89	0.39	1.00	7.84	-	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	0.56	-	-	0.28	-	1.07	-	-
C23:0	-	-	0.23	-	-	-	-	3.88	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	0.22	-	1.05	-	-	-	0.37	6.96	-	-
C24:1(15)	-	-	-	-	-	0.24	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Crab apple lipids					Saskatoon berry Lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	1.12		-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.59	-	-	-	1.09	0.73	-	0.56	2.33	1.18
C15:0	-	0.38	1.18	0.67	0.87	-	-	0.56	-	-
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	9.80	54.69	30.49	22.83	-	5.19	68.85	-	49.7	19.6
C16:1(9)	-	-	-	-	-	-	-	-	-	-
C17:0	19.50	2.11	4.00	7.18	29.7	3.87	3.46	-	3.87	11.2
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	43.15	7.15	3.00	57.18	44.8	12.89	11.85	39.80	-	42.0
C18:1(9)	8.31	-	-	7.07	19.6	-	-	-	-	-
C18:2(9,12)	17.66	3.30	-	-	-	2.97	8.26	27.45	-	23.1
C18:3(6,9,12)	-	32.37	-	-	-	-	-	-	-	-
C20:0	-	-	1.92	2.13	-	28.53	2.15	13.62	44.1	1.80
C18:3(9,12,15)	-	-	-	1.09	3.83	22.05	5.13	-	-	-
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	0.73	-	2.08	-	3.12	-	-
C20:2(11,14)	-	-	-	-	-	-	0.30	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	-	-	-	-	-	18.63	-	11.7	-	0.42
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	-	-	-	0.17	-	-	-	-
C23:0	-	-	-	-	-	1.01	-	2.17	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	-	-	-	1.97	-	1.02	-	0.74
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Carrot Lipids					Parsnip Lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.66	0.47	4.60	-	3.13	1.31	-	2.43	1.78	8.03
C15:0	3.06	7.00	-	-	8.12	1.80	0.75	5.13	-	0.89
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	82.47	16.02	18.20	32.36	59.06	48.16	77.42	12.03	37.07	78.99
C16:1(9)	-	-	-	-	-	-	-	-	-	-
C17:0	5.06	5.42	15.60	-	-	2.98	4.77	5.90	-	-
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	-	17.61	53.95	6.22	-	0.67	2.53	11.73	-	-
C18:1(9)	-	2.55	-	-	-	-	-	-	-	-
C18:2(9,12)	-	12.14	5.92	1.66	-	2.17	14.52	9.11	3.66	
C18:3(6,9,12)	-	-	-	-	-	-	-	-	52.18	-
C20:0	2.86	5.34	-	-	16.49	0.69	-	3.30	4.18	-
C18:3(9,12,15)	-	23.05	-	59.76	-	40.24	-	46.73	-	-
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	1.06	2.34	-	-	5.00	0.29	-	-	1.13	9.55
C20:2(11,14)	0.67	1.38	-	-	0.75	-	-	-	-	-
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	1.94	4.79	-	-	6.03	1.16	-	2.13	-	2.10
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	0.27	-	1.73	-	0.67	-	-	-	-	-
C23:0	0.57	1.28	-	-	0.43	0.24	-	1.17	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	0.39	0.6	-	-	0.32	0.30	-	0.34	-	0.44
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

Continued.

Table 2.9.*Continued.*

Lipids	Yellow bean Lipids					White cabbage Lipids				
	GL[1]	PL[2]	Neutral lipids			GL	PL	Neutral lipids		
			CE[3]	TG[4]	FF[5]			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	0.80	-	3.19	6.26	3.80	0.86	-	2.11	3.3	2.09
C15:0	0.64	0.68	-	-	1.05	-	0.51	-	-	1.18
C15:1(10)	-	-	-	-	-	-	-	-	-	-
C16:0	27.85	3.88	45.36	20.99	50.88	4.75	71.57	26.82	32.11	35.14
C16:1(9)	-	-	-	-	-	-	-	-	-	-
C17:0	4.08	3.92	-	-	-	10.67	2.23	7.43	-	12.77
C17:1(10)	-	-	-	-	-	-	-	-	-	-
C18:0	11.57	9.42	36.54	17.09	-	14.27	2.68	22.1	7.21	-
C18:1(9)	-	-	-	8.17	-	-	-	-	-	-
C18:2(9,12)	3.63	69.07	-	21.73	5.58	5.54	2.35	2.11	6.13	7.11
C18:3(6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	3.54	1.92	8.82	-	21.80	-	0.63	-	0.34	-
C18:3(9,12,15)	46.78	10.09	-	25.76	8.29	63.04	18.35	39.12	50.24	41.18
C20:1(11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	-	-	-	-	-	-
C20:2(11,14)	-	-	-	-	0.67	0.88	1.28	-	-	0.53
C20:3(8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	0.80	0.70	5.29	-	4.68	-	0.26	-	0.18	-
C20:4(5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1(13)	-	-	-	-	-	-	-	-	-	-
C23:0	-	-	-	-	0.63	-	-	-	-	-
C20:5(5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	0.31	0.32	0.79	-	2.62	-	0.15	0.31	0.49	-
C24:1(15)	-	-	-	-	-	-	-	-	-	-
C22:6(4,7,10,13,16,19)	-	-	-	-	-	-	-	-	-	-

[1] GL for glycolipids
[2] PL for phospholipids
[3] CE for cholesteryl esters
[4] TG for triglycerides
[5] FF for free fatty acids

Table 2.10 Estimation of the upper limit triglyceride concentrations using the CLR method.

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C12:0/C12:0/C12:0)	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	22.73	8.82	7.3	0	0	8.33	18.26
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	4.38	16.34	22.12	0	0	8.8	9.95
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	12.37	8.17	14.10	0	0	18.70	9.02
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	12.37	8.17	14.10	0	0	18.70	9.02
TG(C16:0/C16:0/C16:0)	8.25	5.44	9.40	0	27.73	12.47	6.01
TG(C16:0/C16:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	2.19	24.43	16.23	0	0	4.4	4.97
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))	2.19	24.43	16.23	0	0	4.4	4.97
TG(C14:0/C14:0/C16:0)[iso3]	1.34	0	0.82	0	8.405	1.99	1.36
TG(C14:0/C16:0/C16:0)[iso3]	1.34	0	0.82	0	8.405	1.99	1.36
TG(C18:0/C18:0/C18:0)	0	1.48	3.31	25.56	0	0	3.81
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C16:0/C16:0/C17:0)[iso3]	0	3.86	0	0	0	11.91	0
TG(C16:0/C17:0/C17:0)[iso3]	0	3.86	0	0	0	11.91	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	1.46	16.29	10.82	0	0	2.93	3.31
TG(C14:0/C16:0/C17:0)[iso6]	0	0	0	0	0	3.98	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	4.38	8.17	14.10	0	0	8.80	9.02
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	4.38	8.17	14.10	0	0	8.80	9.02
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	4.46	9.95	0	0	0	11.43
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	4.46	9.95	0	0	0	9.95
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	4.46	9.95	0	0	0	9.95
TG(C20:0/C20:0/C20:0)	0	0	0.18	2.12	0	0	0
TG(C14:0/C14:0/C14:0)	0.89	0	0.55	2.70	5.60	1.32	0.91
TG(C14:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	0	4.46	9.95	0	0	0	9.025
TG(C16:0/C18:0/C18:0)[iso3]	0	4.46	9.95	0	0	0	9.025
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0.55	4.06	0	0	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0.55	4.06	0	0	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	3.86	0	0	0	11.91	0
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0	0	0	4.06	0	1.99	0
TG(C14:0/C17:0/C17:0)[iso3]	0	0	0	4.06	0	1.99	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	1.25	0	0	12.89	1.01
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	1.25	0	0	12.89	1.01
TG(C16:0/C17:0/C18:0)[iso6]	0	3.86	0	0	0	0	0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	2.23	4.97	0	0	0	5.71
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	2.23	4.97	0	0	0	5.71
TG(C14:0/C14:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	2.23	4.97	0	0	0	5.71
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	2.23	4.97	0	0	0	5.71
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.25	0	0	12.89	1.01
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	3.86	0	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	3.86	0	0	0	8.8	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	3.86	0	0	0	8.8	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0.55	6.37	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini
TG(C12:0/C12:0/C12:0)	0.59	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	0	16.95	0	19.10	16.46	0	3.73
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	16.05	3.65	0	11.21
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	0	23.58	0	8.08	19.51	0	9.55
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	23.58	0	8.08	19.51	0	9.55
TG(C16:0/C16:0/C16:0)	13.28	15.72	16.33	5.38	13.00	0	6.36
TG(C16:0/C16:0/C21:0)[iso3]	19.93	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	19.93	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	0	0	0	8.02	1.825	0	6
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	8.02	1.825	0	6
TG(C14:0/C14:0/C16:0)[iso3]	15.73	0	12.79	1.29	0.795	0	5.14
TG(C14:0/C16:0/C16:0)[iso3]	15.73	0	12.79	1.29	0.795	0	5.14
TG(C18:0/C18:0/C18:0)	0	0	0	1.32	0	0	8.89
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	0	1.59	0	10.29
TG(C16:0/C16:0/C17:0)[iso3]	0	0	19.65	3.9	1.25	0	4.06
TG(C16:0/C17:0/C17:0)[iso3]	0	0	19.65	3.9	1.25	0	4.06
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0	0	4.12	0	9.55
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0	0	4.12	0	9.55
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0	0	0	5.35	1.21	0	4
TG(C14:0/C16:0/C17:0)[iso6]	0	0	19.65	2.59	1.25	0	4.06
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0	0	0	8.08	3.65	0	9.55
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	8.08	3.65	0	9.55
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	3.98	0	0	11.21
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	0	0	3.98	0	0	12
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	3.98	0	0	11.21
TG(C20:0/C20:0/C20:0)	0	0	0	0	1.37	18.17	5.03
TG(C14:0/C14:0/C14:0)	10.486	0	8.52	0.86	0.53	8.62	3.43
TG(C14:0/C16:0/C21:0)[iso6]	23.41	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	0	0	0	3.98	0	0	9.55
TG(C16:0/C18:0/C18:0)[iso3]	0	0	0	3.98	0	0	9.55
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	0	0.79	12.93	5.145
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0	0.79	12.93	5.14
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	3.9	1.25	0	4.06
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	12.93	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	12.93	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0	0	12.79	1.29	0.79	0	4.06
TG(C14:0/C17:0/C17:0)[iso3]	0	0	12.79	1.29	0.79	0	4.06
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	17.26	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	0	0	0	3.9	0	0	4.06
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	0	0	1.99	0	0	12
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	1.99	0	0	12
TG(C14:0/C14:0/C21:0)[iso3]	15.73	0	0	0	0	0	0
TG(C14:0/C21:0/C21:0)[iso3]	15.73	0	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	0	0	1.99	0	0	11.21
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	1.99	0	0	11.21
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	15.11
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	3.9	0	0	4.06
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	0	0	3.9	1.25	0	4.06
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	3.9	1.25	0	4.06
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0	0	0	0	13.34

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower
TG(C12:0/C12:0/C12:0)	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	4.40	0	11.96	21.42	11.58	23.57
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	11.63	0	0	10.51	27.15	7.86
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	13.22	0	18.43	7.75	13.575	4.875
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	13.22	0	18.43	7.75	13.575	4.875
TG(C16:0/C16:0/C16:0)	21.02	18.83	12.28	5.16	9.05	3.25
TG(C16:0/C16:0/C21:0)[iso3]	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	5.81	0	0	5.25	13.605	3.93
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	5.81	0	0	5.25	13.605	3.93
TG(C14:0/C14:0/C16:0)[iso3]	0.71	12.31	2.185	2.15	0	1
TG(C14:0/C16:0/C16:0)[iso3]	0.71	12.31	2.185	2.15	0	1
TG(C18:0/C18:0/C18:0)	1.92	0	3.16	0	1.7	1.76
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0
TG(C16:0/C16:0/C17:0)[iso3]	4.48	18.78	13.38	4.14	5.8	4.37
TG(C16:0/C17:0/C17:0)[iso3]	4.48	18.78	13.38	4.14	5.8	4.37
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0	0	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	3.87	0	0	3.50	9.07	2.62
TG(C14:0/C16:0/C17:0)[iso6]	1.43	18.78	4.37	4.14	0	2
TG(C16:0/C16:0/C18:2(9,12))[iso3]	11.63	0	0	7.75	13.57	4.87
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	11.63	0	0	7.75	13.57	4.87
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	5.77	0	9.49	0	5.1	5.3
TG(C16:0/C18:0/C18:2(9,12))[iso6]	5.77	0	0	0	5.1	5.3
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	5.77	0	0	0	5.1	5.3
TG(C20:0/C20:0/C20:0)	0	0	0	0	0	0
TG(C14:0/C14:0/C14:0)	0.47	8.20	1.45	1.43	0	0.66
TG(C14:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	5.77	0	9.49	0	5.1	4.875
TG(C16:0/C18:0/C18:0)[iso3]	5.77	0	9.49	0	5.1	4.875
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	0	0	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	4.48	0	13.38	4.14	5.8	4.37
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0.71	12.31	2.18	2.155	0	1
TG(C14:0/C17:0/C17:0)[iso3]	0.71	12.31	2.18	2.155	0	1
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	4.48	0	9.49	0	5.1	4.37
TG(C18:0/C18:0/C18:2(9,12))[iso3]	2.88	0	0	0	2.55	2.65
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	2.88	0	0	0	2.55	2.65
TG(C14:0/C14:0/C21:0)[iso3]	0	0	0	0	0	0
TG(C14:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	2.88	0	4.74	0	2.55	2.65
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	2.88	0	4.74	0	2.55	2.65
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	4.48	0	9.49	0	5.1	4.37
TG(C16:0/C17:0/C18:2(9,12))[iso6]	4.48	0	0	4.14	5.8	4.37
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	4.48	0	0	4.14	5.8	4.37
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean
TG(C12:0/C12:0/C12:0)	0	0	0.37	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	0	3.84	0.36	0	19.92	0	8.58
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	11.54	0	0	1.66	0	20.99
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	0	9.70	1.09	0	16.18	0	10.49
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	9.70	1.09	0	16.18	0	10.49
TG(C16:0/C16:0/C16:0)	20.72	6.47	7.61	16.56	10.78	12.35	6.99
TG(C16:0/C16:0/C21:0)[iso3]	31.08	0	0.73	0	0	1.13	0
TG(C16:0/C21:0/C21:0)[iso3]	31.08	0	0.73	0	0	1.13	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	0	11.54	0	0	0.83	0	10.86
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))[iso3	0	11.54	0	0	0.83	0	10.86
TG(C14:0/C14:0/C16:0)[iso3]	1.92	1.315	0	1.165	0	0.89	3.13
TG(C14:0/C16:0/C16:0)[iso3]	1.92	1.315	0	1.165	0	0.89	3.13
TG(C18:0/C18:0/C18:0)	0	1.54	19.06	0	2.07	0	5.69
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	2.33	0	1.78	0
TG(C16:0/C16:0/C17:0)[iso3]	0	0	7.18	3.87	0	0	0
TG(C16:0/C17:0/C17:0)[iso3]	0	0	7.18	3.87	0	0	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	2.13	24.85	0	4.18	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	2.13	24.85	0	4.18	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0	19.63	0	0	0.55	1.22	7.24
TG(C14:0/C16:0/C17:0)[iso6]	0	0	0	2.33	0	0	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0	9.70	0	0	1.66	3.66	10.49
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	9.70	0	0	1.66	3.66	10.49
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	4.62	1.09	0	6.22	0	17.09
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	4.62	0	0	1.66	0	17.09
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	4.62	0	0	1.66	0	17.09
TG(C20:0/C20:0/C20:0)	0	0	0.71	14.7	0	1.39	0
TG(C14:0/C14:0/C14:0)	1.28	0.87	0	0.77	0	0.59	2.08
TG(C14:0/C16:0/C21:0)[iso6]	3.84	0	0	0	0	1.13	0
TG(C16:0/C16:0/C18:0)[iso3]	0	4.62	11.41	0	6.22	0	10.49
TG(C16:0/C18:0/C18:0)[iso3]	0	4.62	11.41	0	6.22	0	10.49
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	1.16	0	0.89	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	1.16	0	0.89	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	18.53	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	18.53	0
TG(C14:0/C14:0/C17:0)[iso3]	0	0	0	1.16	0	0	0
TG(C14:0/C17:0/C17:0)[iso3]	0	0	0	1.16	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	17.39	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	2.9	7.07	0	0	0	8.17
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	2.9	7.07	0	0	0	8.17
TG(C16:0/C17:0/C18:0)[iso6]	0	0	7.18	0	0	0	0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	2.31	0	0	1.66	0	8.54
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	2.31	0	0	1.66	0	8.54
TG(C14:0/C14:0/C21:0)[iso3]	1.92	0	0	0	0	0.89	0
TG(C14:0/C21:0/C21:0)[iso3]	1.92	0	0	0	0	0.89	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	2.31	1.09	0	3.11	0	8.54
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	2.31	1.09	0	3.11	0	8.54
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	2.9	1.09	0	0	0	8.17
TG(C16:0/C18:0/C20:0)[iso6]	0	0	2.13	0	0	0	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	2.13	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Green zucchini	Yellow pepper	Orange pepper	White cabbage	Cucumber
TG(C12:0/C12:0/C12:0)	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	16.94	0	0	16.74	0
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	12.17	0	0	6.13	0
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	6.98	0	0	16.05	0
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	6.98	0	0	16.05	0
TG(C16:0/C16:0/C16:0)	4.65	6.99	9.71	10.70	28.91
TG(C16:0/C16:0/C21:0)[iso3]	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	6.08	0	0	3.06	0
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	6.08	0	0	3.06	0
TG(C14:0/C14:0/C16:0)[iso3]	0.66	20.99	17.4	1.65	0
TG(C14:0/C16:0/C16:0)[iso3]	0.66	20.99	17.4	1.65	0
TG(C18:0/C18:0/C18:0)	3.11	0	0	2.40	2.70
TG(C14:0/C16:0/C20:0)[iso6]	0	0	29.13	0.34	0
TG(C16:0/C16:0/C17:0)[iso3]	6.98	0	4.51	0	5.14
TG(C16:0/C17:0/C17:0)[iso3]	6.98	0	4.51	0	5.14
TG(C16:0/C16:0/C20:0)[iso3]	0	0	14.56	0.34	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	14.56	0.34	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	4.05	0	0	2.04	0
TG(C14:0/C16:0/C17:0)[iso6]	1.33	0	4.51	0	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	6.98	0	0	6.13	0
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	6.98	0	0	6.13	0
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	9.33	0	0	7.21	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	9.33	0	0	6.13	0
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	9.33	0	0	6.13	0
TG(C20:0/C20:0/C20:0)	0	0	10.51	0.11	0
TG(C14:0/C14:0/C14:0)	0.44	16.95	11.6	1.1	0
TG(C14:0/C16:0/C21:0)[iso6]	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	6.98	0	0	7.21	8.12
TG(C16:0/C18:0/C18:0)[iso3]	6.98	0	0	7.21	8.12
TG(C14:0/C14:0/C20:0)[iso3]	0	0	17.4	0.34	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	17.4	0.34	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	8.47	0	0	0	0
TG(C14:0/C14:0/C16:1(9))[iso3]	0	14.67	0	0	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	14.67	0	0	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0.66	0	4.51	0	0
TG(C14:0/C17:0/C17:0)[iso3]	0.66	0	4.51	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	3.91	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	3.91	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	8.47	0	0	0	5.14
TG(C18:0/C18:0/C18:2(9,12))[iso3]	4.66	0	0	3.60	0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	4.66	0	0	3.60	0
TG(C14:0/C14:0/C21:0)[iso3]	0	0	0	0	0
TG(C14:0/C21:0/C21:0)[iso3]	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	4.66	0	0	3.60	0
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	4.66	0	0	3.60	0
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	3.91	0	0	0	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0	0.34	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	8.47	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	8.47	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	8.47	0	0	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	14.67	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0	0.34	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0.55	6.37	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	11.91	0
TG(C14:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C21:0)	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	2.68	0	1.65	0	0	3.98	2.73
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	2.68	0	1.65	0	0	3.98	2.73
TG(C14:0/C16:0/C18:2(9,12))[iso6]	2.68	0	1.65	0	0	3.98	2.73
TG(C14:0/C16:0/C18:0)[iso6]	0	0	1.65	0	0	0	2.73
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	0	1.65	0	0	0	2.73
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	1.65	0	0	0	2.73
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	11.91	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	1.25	0	0	8.8	1.01
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	1.25	0	0	8.8	1.01
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	3.86	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0.55	6.37	0	0	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.55	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0.55	0	0	0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	1.25	0	0	0	1.01
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	1.25	0	0	0	1.01
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	1.25	0	0	0	1.01
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.55	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.55	0	0	0	0
TG(C17:0/C17:0/C17:0)	0	1.28	0	2.56	0	3.97	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	1.93	0	0	0	5.95	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	1.93	0	0	0	5.95	0
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	7.7	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0	1.93	0	3.85	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0	1.93	0	3.85	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	8.8	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	1.25	0	0	0	1.01
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.25	0	0	0	1.01
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	6.37	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	1.93	0	0	0	5.95	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.93	0	0	0	5.95	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	3.98	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0.27	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.27	0	0	0	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0	0	0	5.95	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	5.95	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	1.25	0	0	3.98	1.01
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	1.25	0	0	3.98	1.01
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.25	0	0	3.98	1.01
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0.62	0	0	6.44	0.50

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	13.34
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C22:0)[iso6]	3.72	0	0	0	0	0	0
TG(C14:0/C14:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C21:0)	7.80	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	2.59	1.59	0	10.29
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	2.59	1.59	0	10.29
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0	0	0	2.59	1.59	0	10.29
TG(C14:0/C16:0/C18:0)[iso6]	0	0	0	2.59	0	0	10.29
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	2.59	0	0	10.29
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	3.65	0	12
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	0	2.59	0	0	10.29
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	3.9	0	0	4.06
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	12
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	10.29
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	4.12	0	11.21
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	3.65	0	11.21
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	11.21
TG(C16:0/C16:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	1.59	0	10.29
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	1.59	0	10.29
TG(C17:0/C17:0/C17:0)	0	0	6.55	1.3	0.41	0	1.35
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	0	0	1.95	0.625	0	2.03
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	1.95	0.625	0	2.03
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	2.59	0	0	4.06
TG(C17:0/C17:0/C18:0)[iso3]	0	0	0	1.95	0	0	2.03
TG(C17:0/C18:0/C18:0)[iso3]	0	0	0	1.95	0	0	2.03
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0	1.25	0	4.06
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	8.63	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	8.63	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	1.95	0.62	0	2.03
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	1.95	0.62	0	2.03
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	2.59	1.25	0	4.06
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0	0	2.06	0	7.55
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	2.06	0	7.55
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0

Continued

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C21:0)	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	1.43	0	4.37	4.31	0	2	0
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	1.43	0	0	4.31	0	2	0
TG(C14:0/C16:0/C18:2(9,12))[iso6]	1.43	0	0	4.31	0	2	0
TG(C14:0/C16:0/C18:0)[iso6]	1.43	0	4.37	0	0	2	0
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	1.43	0	4.37	0	0	2	0
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	1.43	0	0	0	0	2	0
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	4.48	0	0	0	5.1	4.37	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C17:0)	1.49	6.26	4.46	1.38	1.93	1.45	1.71
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	2.24	0	6.69	2.07	2.9	2.18	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	2.24	0	6.69	2.07	2.9	2.18	0
TG(C14:0/C17:0/C18:0)[iso6]	1.43	0	4.37	0	0	2	0
TG(C17:0/C17:0/C18:0)[iso3]	2.24	0	6.69	0	2.9	2.18	2.57
TG(C17:0/C18:0/C18:0)[iso3]	2.24	0	6.69	0	2.9	2.18	2.57
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	2.24	0	0	2.07	2.9	2.18	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	2.24	0	0	2.07	2.9	2.18	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	1.43	0	4.37	4.14	0	2	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean
TG(C18:0/C20:0/C20:0)[iso3]	0	0	2.13	0	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	7.07	0	0	0	0
TG(C14:0/C16:0/C22:0)[iso6]	0.95	0	0	0	0	0	0
TG(C14:0/C14:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C21:0)	11.01	0	0.24	0	0	0.37	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0	2.63	0	0	0	1.78	6.26
TG(C14:0/C16:0/C18:0)[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	2.63	0	0	0	0	6.26
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	3.66	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	2.63	0	0	0	0	6.26
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	2.9	0	0	0	0	8.17
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	2.9	0	0	0	0	8.17
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	2.9	7.07	0	0	0	8.17
TG(C18:0/C18:0/C18:1(9))[iso3]	0	2.31	7.07	0	0	0	8.17
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	2.31	7.07	0	0	0	8.17
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	1.78	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C17:0)	0	0	2.39	1.29	0	0	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	0	1.09	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	1.09	0	0	0	0
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0	0	3.59	0	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0	0	3.59	0	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	2.9	0	0	0	0	8.17
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	2.9	1.09	0	0	0	8.17
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	2.33	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	7.07	0	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	1.06	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	1.06	0	0	0	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	3.59	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	3.59	0	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	2.63	0	0	0	0	6.26
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	1.45	1.09	0	0	0	4.08

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Green zucchini	Yellow pepper	Orange pepper	White cabbage
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0	0.34
TG(C16:0/C17:0/C18:1(9))[iso6]	3.91	0	0	0
TG(C14:0/C16:0/C22:0)[iso6]	0	13.47	0	0.18
TG(C14:0/C14:0/C22:0)[iso3]	0	13.47	0	0.18
TG(C14:0/C22:0/C22:0)[iso3]	0	13.47	0	0.18
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	13.47	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	13.47	0	0
TG(C21:0/C21:0/C21:0)	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	1.33	0	0	3.3
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	1.33	0	0	3.3
TG(C14:0/C16:0/C18:2(9,12))[iso6]	1.33	0	0	3.3
TG(C14:0/C16:0/C18:0)[iso6]	1.33	0	0	3.3
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	1.33	0	0	3.3
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0.34
TG(C14:0/C18:0/C18:2(9,12))[iso6]	1.33	0	0	3.3
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	3.91	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	3.91	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	3.91	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	8.47	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0.34
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0.34
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0.34
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0.34
TG(C16:0/C18:0/C18:1(9))[iso6]	3.91	0	0	0
TG(C18:0/C18:0/C18:1(9))[iso3]	3.91	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	3.91	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0.34
TG(C16:0/C16:0/C22:0)[iso3]	0	10.49	0	0.18
TG(C16:0/C22:0/C22:0)[iso3]	0	10.49	0	0.18
TG(C16:0/C16:0/C16:1(9))[iso3]	0	10.49	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	10.49	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0.34
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0.34
TG(C17:0/C17:0/C17:0)	2.82	0	1.50	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	4.23	0	0	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	4.23	0	0	0
TG(C14:0/C17:0/C18:0)[iso6]	1.33	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	4.23	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	4.23	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	3.91	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	3.91	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	3.91	0	0	0
TG(C14:0/C17:0/C20:0)[iso6]	0	0	4.51	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	4.23	0	0	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	4.23	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	1.33	0	0	0
TG(C17:0/C18:0/C18:1(9))[iso6]	3.91	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0	0.17
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0.17
TG(C17:0/C17:0/C18:1(9))[iso3]	3.91	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	3.91	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	1.33	0	0	0
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	1.33	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	1.33	0	0	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	1.95	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.62	0	0	6.44	0.50
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0.62	0	0	6.44	0.50
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0.62	0	0	6.44	0.50
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	6.37	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	3.98	0
TG(C14:0/C14:0/C18:0)[iso3]	0	0	0.82	4.06	0	0	1.36
TG(C14:0/C18:0/C18:0)[iso3]	0	0	0.82	4.06	0	0	1.36
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	1.25	0	0	0	1.01
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	1.34	0	0.82	0	0	1.99	1.36
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	1.34	0	0.82	0	0	1.99	1.36
TG(C14:0/C14:0/C18:2(9,12))[iso3]	1.34	0	0.82	0	0	1.99	1.36
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	1.34	0	0.82	0	0	1.99	1.36
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0.82	0	0	0	1.36
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0.82	0	0	0	1.36
TG(C14:0/C15:0/C16:0)[iso6]	0	0	1.65	0	0	0	2.05
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0.41	0	0	4.29	0.33
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	3.85	0	0	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	3.85	0	0	0
TG(C22:0/C22:0/C22:0)	0	0	0	0.37	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	3.31	0	0	0	2.05
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	3.98	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	3.31	0	0	0	2.05
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	3.31	0	0	0	2.05
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0.82	0	0	1.99	1.01
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.82	0	0	1.99	1.01
TG(C15:0/C16:0/C18:0)[iso6]	0	0	3.31	0	0	0	2.05
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	3.31	0	0	0	2.05
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	3.31	0	0	0	2.05
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C16:0/C16:0)[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	1.65	0	0	0	2.05
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	1.65	0	0	0	2.05
TG(C14:0/C15:0/C18:0)[iso6]	0	0	1.65	0	0	0	2.05
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	1.10	0	0	0	0.68
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0.62	0	0	6.44	0.50

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Green zucchini	Yellow pepper	Orange pepper	White cabbage
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	1.95	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	1.95	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	1.95	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	4.89	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	7.33	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	7.33	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	1.33	0	0	0
TG(C14:0/C14:0/C18:0)[iso3]	0.66	0	0	1.65
TG(C14:0/C18:0/C18:0)[iso3]	0.66	0	0	1.65
TG(C16:0/C17:0/C20:0)[iso6]	0	0	4.51	0
TG(C14:0/C18:0/C18:1(9))[iso6]	1.33	0	0	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0.66	0	0	1.65
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0.66	0	0	1.65
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0.66	0	0	1.65
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.66	0	0	1.65
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0.34
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0.34
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	1.30	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	2.255	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	2.255	0
TG(C22:0/C22:0/C22:0)	0	4.49	0	0.06
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	1.33	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0.66	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0.66	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0	0
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	1.95	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	4.06
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	5.75	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	2.59	1.25	0	4.06
TG(C14:0/C14:0/C18:0)[iso3]	0	0	0	1.29	0	0	5.14
TG(C14:0/C18:0/C18:0)[iso3]	0	0	0	1.29	0	0	5.14
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	1.25	0	4.06
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	0	0	1.29	0.79	0	5.145
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	1.25	0.79	0	5.145
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	0	0	1.95	0.75	0	5.145
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	1.29	0.79	0	5.145
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	1.82	0	6
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	1.82	0	6
TG(C14:0/C14:0/C15:0)[iso3]	0	0	5.78	0	0.79	2.35	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	5.78	0	0.79	2.35	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	5.78	0	0.99	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	5.78	0	0.99	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	5.78	0	0.99	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	0	0.62	0	2.03
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	0	0.62	0	2.03
TG(C22:0/C22:0/C22:0)	1.24	0	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	2	0	0	0.99	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	1.25	0	4.06
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	1.25	0	4.06
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0.99	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0.99	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	3.72	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	3.72	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	3.72	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	1	2.89	0	0.49	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	1	2.89	0	0.49	0	0
TG(C15:0/C15:0/C17:0)[iso3]	0	0	2.89	0	0.49	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	2.89	0	0.49	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0	0.99	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0.99	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0	0.99	2.35	0
TG(C15:0/C15:0/C15:0)	0	0.66	1.92	0	0.33	0.783	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	2.35	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	1.43	0	0	4.14	0	2	0
TG(C14:0/C14:0/C18:0)[iso3]	0.715	0	2.185	0	0	1	0
TG(C14:0/C18:0/C18:0)[iso3]	0.715	0	2.185	0	0	1	0
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0.715	0	2.185	2.155	0	1	0
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0.715	0	2.185	2.155	0	1	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0.715	0	0	2.155	0	1	0
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.715	0	0	2.155	0	1	0
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	1.28	0	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	1.28	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C22:0/C22:0/C22:0)	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	1.28	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	1.28	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	1.28	0	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0.64	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0	0.42	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	1.45	1.09	0	0	0	4.08
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	1.45	0	0	0	0	4.08
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.45	0	0	0	0	4.08
TG(C17:0/C18:0/C20:0)[iso6]	0	0	2.13	0	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:0)[iso3]	0	1.31	0	0	0	0	3.13
TG(C14:0/C18:0/C18:0)[iso3]	0	1.31	0	0	0	0	3.13
TG(C16:0/C17:0/C20:0)[iso6]	0	0	2.13	3.87	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	2.63	0	0	0	0	6.26
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	1.31	0	0	0	0	3.13
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	1.31	0	0	0	0	3.13
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	1.31	0	0	0	0.89	3.13
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.31	0	0	0	0.89	3.13
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	1.83	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	1.83	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0.67	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0.96	2.35	0	0	0	2.72
TG(C17:0/C17:0/C20:0)[iso3]	0	0	2.13	1.93	0	0	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	2.13	1.93	0	0	0
TG(C22:0/C22:0/C22:0)	0.31	0	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	4.18	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	4.18	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	4.18	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	1.31	0	0	0	0	3.13
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	1.31	0	0	0	0	3.13
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0.95	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0.95	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0.95	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	3.66	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	3.66	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0.33	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0.22	0	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	1.65	0	0	0	1.02
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C15:0/C18:0)[iso3]	0	0	1.65	0	0	0	1.02
TG(C15:0/C18:0/C18:0)[iso3]	0	0	1.65	0	0	0	1.02
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	1.25	0	0	0	1.01
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	1.25	0	0	0	1.01
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.25	0	0	0	1.01
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	1.25	0	0	0	1.01
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	1.25	0	0	0	1.01
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	1.25	0	0	0	1.01
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	1.25	0	0	0	1.01
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	White cabbage	Orange pepper	Yellow pepper	Green zucchini
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Yellow zucchini	Japanese pumpkin	Lettuce	Potato	Red pepper
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	2.35
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	1	0	0	0	0.49	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	1	0	0	0	0.49	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0	0	0.49	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0.49	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	1.79	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	1.79	0	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	1.79	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	1.79	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	1.79	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	1.79	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.99	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.99	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	1.55	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	1.55	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0.64	0	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0.64	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	1.28	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	1.28	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.33	0	0	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	2.13	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	2.13	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	2.13	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	2.13	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	2.13	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0.335	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0.335	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0.73	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	1.83	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	1.83	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	1.78	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	1.78	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	1.78	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0.55	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0.55	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0.55	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.55	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	1.11	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0.55	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	1.11	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	1.11	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	1.11	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	White cabbage	Green zucchini	Yellow pepper	Orange pepper	Orange pepper	Yellow pepper	Green zucchini
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[iso3	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0.18	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0.18	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0.18	0	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0.18	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0.18	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0.17	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0.17	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	1.55
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	1.55
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	1.55
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[iso3]	0	0	0	0	0	0	1.55
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0.49	1.17	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0.49	1.17	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0.99	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0.99	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0.99	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	1.17	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	1.17	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0.99	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	1.55

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0.33	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0.73	0	0	1.13	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0.73	0	0	1.13	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0.73	0	0	1.13	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0.67	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	1.13	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	1.13	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	1.13	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	1.13	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	1.13	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	1.12	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	1.12	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	1.09	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0.55	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0.49	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C12:0/C14:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0.89	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0.89	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0.4	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	1.09	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0.89	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0.89	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0.73	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.73	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0.67	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.67	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0	0	0.49	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0.55	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0.55	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0.49	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0.51	0
TG(C12:0/C12:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber
TG(C14:0/C16:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0.4	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0.4	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0.56	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.56	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)[iso3]	0	0	0.54	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0.54	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0.49	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.49	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C21:0/C22:0/C23:0)[iso6]	0.51	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0.51	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0.51	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13	0	0	0	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:1(13))[iso3]	0.4	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0.4	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0.4	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6	0.4	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0.4	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)[iso3	0	0	0	0	0	0	0	0.49
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.49
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.09
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.09
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0.27	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.27	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0.16	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.34
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.34
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.34
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.34
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0.34
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0.33	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0.33	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0	0	0	0	0	0.16
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0.18
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)	0	0	0	0	0	0	0	0.18
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0.18
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)	0	0	0	0	0	0	0	0.18
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0.18
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0.18
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.17
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0.17
TG(C23:0/C23:0/C23:0)	0	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C12:0/C23:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0.38	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0.38	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0.25	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0.25	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0.12	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0.17	0	0	0	0	0	0	0

Continued.

Table 2.10*Continued.*

Upper limit triglyceride concentrations	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0.13	0	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0	0	0	0	0	0	0

Table 2.11.The most probable triglyceride concertation values using the CLR method (in molar).

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C12:0/C12:0/C12:0)	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:0)	1.51	0.43	2.24	0	57.57	5.23	0.58	0.27
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15)	31.70	1.85	1.08	0	0	1.56	16.43	13.13
TG(C18:0/C18:0/C18:0)	0	0.01	0.09	45.12	0	0	0.14	0.08
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0.008	11.67	3.42	0	0	0.06	0.09	0.18
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	11.50	1.14	1.38	0	0	2.33	5.41	3.60
TG(C20:0/C20:0/C20:0)	0	0	1.66	0.02	0	0	0	0
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	4.17	0.70	1.76	0	0	3.50	1.78	0.99
TG(C14:0/C16:0/C16:0)[iso3]	0.16	0	0.13	0	11.63	0.55	0.08	0.02
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C14:0)	0.002	0	0.0004	0.05	0.47	0.006	0.002	0.0002
TG(C16:0/C16:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0.04	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0.001	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))	2.03	3.42	1.58	0	0	0.55	2.98	3.14
TG(C14:0/C14:0/C16:0)[iso3]	0.01	0	0.007	0	2.35	0.05	0.01	0.002
TG(C16:0/C16:0/C17:0)[iso3]	0	0.10	0	0	0	1.6	0	0.16
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0.032	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.04	3.90	2.97	0	0	0.28	0.17	0.20
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	0.13	6.32	2.33	0	0	0.19	0.54	0.75
TG(C16:0/C18:0/C18:0)[iso3]	0	0.03	0.27	0	0	0	0.23	0.12
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	0	0.11	0.79	0	0	0	0.37	0.18
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0.26	1.30	2.58	0	0	1.23	0.32	0.23
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.31	0.48	0	0	0	3.42	2.41
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0.0001	0.04	0	0	0	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0	0.007	0	4.52	0	0	0	0.07
TG(C14:0/C18:0/C18:0)[iso3]	0	0	0.016	4.77	0	0	0.03	0.01
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.73	2.11	2.02	0	0	0.82	0.98	0.86
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0.005	3.74	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.27	0	0	0	0.74	0	2.18
TG(C21:0/C21:0/C21:0)	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0.17	0	0.01
TG(C14:0/C14:0/C22:0)[iso3]	0	0	0	0.007	0	0	0	0
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0.002	0	0	0	0	0
TG(C14:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C17:0)[iso3]	0	0.02	0	0	0	0.53	0	0.10
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	1.24	0	0.08	0	0	0.24	0.81	0.34
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	0.19	0.62	0	0	0	1.13	0.66
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	0.01	0	0	0	0.01	0.03
TG(C14:0/C14:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.06	1.04	0	0	0	0.11	0.13
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	0.16	0	0	0	1.11	0	0.60
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	0.09	0	0	1.80	0.03	0.07
TG(C14:0/C14:0/C17:0)[iso3]	0	0	0	0.05	0	0.02	0	0.001
TG(C14:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0.57	0.71	0	0	0	0.62	0.57
TG(C14:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0.26	0	0	0	0.06	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	0.35	0.91	0	0	0	0.20	0.15

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C12:0/C12:0/C12:0)	0.0005	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:0)	6.19	10.48	11.7	0.42	5.94	0	0.69	0.92
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15))	0	13.14	0	18.83	12.04	0	0.14	0
TG(C18:0/C18:0/C18:0)	0	0	0	0.006	0	0	1.89	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0	0	0	0.41	0.004	0	0.17	0
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	12.19	0	5.30	9.51	0	0.24	0
TG(C20:0/C20:0/C20:0)	0	0	0	0	0.006	16.20	0.34	0
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	0	11.30	0	1.49	7.51	0	0.40	0
TG(C14:0/C16:0/C16:0)[iso3]	4.88	0	6.14	0.06	0.24	0	0.37	2.24
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C14:0)	3.04	0	1.67	0.001	0.0004	1.72	0.10	13.16
TG(C16:0/C16:0/C21:0)[iso3]	3.63	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0	0	0.62	0	0.55	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0	0	0.06	0	0.43	0
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))[iso3	0	0	0	5.27	0.89	0	0.15	0
TG(C14:0/C14:0/C16:0)[iso3]	3.85	0	3.20	0.01	0.009	0	0.20	5.43
TG(C16:0/C16:0/C17:0)[iso3]	0	0	4.717	0.10	0.19	0	0.14	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0	0.002	7.68	0.23	0
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0.41	0.05	0	0.27	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))[iso3]	0	0	0	1.47	0.06	0	0.16	0
TG(C16:0/C18:0/C18:0)[iso3]	0	0	0	0.02	0	0	1.35	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	2.13	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	0	0	0	0.11	0	0	0.97	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0	0	0	0.41	0.55	0	0.43	0
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	1.30	0	0	0.33	0
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	0	0.001	3.64	0.15	0
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	5.13	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0	0	0	0.006	0	0	0.28	0
TG(C14:0/C18:0/C18:0)[iso3]	0	0	0	0.004	0	0	0.73	0
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	1.48	0.70	0	0.25	0
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	1.15	0	3.79
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0	0	0	0	1.07	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	1.28	0.31	0	0.05	0
TG(C21:0/C21:0/C21:0)	1.25	0	0	0	0	0	0	0
TG(C14:0/C16:0/C17:0)[iso6]	0	0	2.46	0.016	0.007	0	0.08	0
TG(C14:0/C14:0/C22:0)[iso3]	0.35	0	0	0	0	0	0	3.48
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	0	0.02	0	0.29	0
TG(C14:0/C16:0/C21:0)[iso6]	2.87	0	0	0	0	0	0	0
TG(C16:0/C17:0/C17:0)[iso3]	0	0	1.89	0.02	0.006	0	0.03	0
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0.85	0.38	0	0.13	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	2.43	0	0
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0.36	0	0	0.571	0
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C21:0)[iso3]	2.26	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0.10	0	0	0.38	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0.36	0.245	0	0.08	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0	0	1.28	0.002	0.0003	0	0.04	0
TG(C14:0/C21:0/C21:0)[iso3]	1.68	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	1.62	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	1.56
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0.36	0	0	0.35	0
TG(C14:0/C16:0/C22:0)[iso6]	0.45	0	0	0	0	0	0	1.43
TG(C15:0/C16:0/C16:0)[iso3]	0	0.44	1.38	0	0.15	0	0	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0.10	0	0	0.61	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C12:0/C12:0/C12:0)	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:0)	25.08	18.07	5.01	0.37	2.01	0.09	65.26	2.47
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,15	0.23	0	4.62	26.53	4.19	35.37	0	0
TG(C18:0/C18:0/C18:0)	0.02	0	0.08	0	0.01	0.01	0.05	0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0.16	0	0	0.11	2.01	0.05	0	0
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	1.11	0	4.75	6.40	3.25	4.87	0	0
TG(C20:0/C20:0/C20:0)	0	0	0	0	0	0	0	3.13
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	5.25	0	4.87	1.54	2.56	0.67	0	0
TG(C14:0/C16:0/C16:0)[iso3]	0.56	7.87	0.59	0.10	0	0.02	0	2.95
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C14:0)	0.0002	1.49	0.008	0.008	0	0.0008	0	4.21
TG(C16:0/C16:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0	0	0	0	0	2.67
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	2.89
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))	0.20	0	0	4.33	3.28	3.93	0	0
TG(C14:0/C14:0/C16:0)[iso3]	0.01	3.43	0.07	0.02	0	0.003	0	3.52
TG(C16:0/C16:0/C17:0)[iso3]	1.78	6.01	1.81	0.09	0.42	0.04	3.86	0.38
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	3.46
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.85	0	0	0.17	2.01	0.06	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))	0.17	0	0	0.70	2.57	0.43	0	0
TG(C16:0/C18:0/C18:0)[iso3]	0.20	0	0.33	0	0.07	0.027	0.57	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C18:0)[iso3]	2.26	0	1.28	0	0.37	0.05	6.10	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	4.62	0	0	0.25	2.01	0.07	0	0
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0.11	0	1.22	0	0.61	2.65	0	0
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	0	0	0	0	3.82
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0.01	0	0.12	0	0.01	0.01	0.03	0
TG(C14:0/C18:0/C18:0)[iso3]	0.004	0	0.04	0	0	0.005	0	0
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.96	0	0	1.04	2.56	0.54	0	0
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0.07	0	1.72	1.70	0.70	2.18	0	0
TG(C21:0/C21:0/C21:0)	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C17:0)[iso6]	0.04	2.61	0.21	0.02	0	0.008	0	0.45
TG(C14:0/C14:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0	3.19
TG(C14:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C17:0)[iso3]	0.12	1.99	0.65	0.02	0.09	0.018	0.23	0.06
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0.02	0	0.567	1.77	0	1.00	0	0
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0.48	0	1.25	0	0.48	0.36	0	0
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.08	0	0	0	0.37	0.03	0	0
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0.37	0	1.77	0.41	0.54	0.30	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C17:0)[iso3]	0.001	1.14	0.02	0.007	0	0.001	0	0.54
TG(C14:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.08	0	0	0	0.48	0.29	0	0
TG(C14:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0	0.03	0	0	0	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0.42	0	0	0	0.37	0.04	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C12:0/C12:0/C12:0)	0	0	0.001	0	0	0	0	0
TG(C16:0/C16:0/C16:0)	24.01	0.73	1.18	12.27	3.38	5.09	0.92	3.31
TG(C18:3(9,12,15)/C18:3(9,12,15)/C18:3(9,12,1	0	0.15	0.0001	0	21.34	0	1.71	12.6
TG(C18:0/C18:0/C18:0)	0	0.009	18.69	0	0.024	0	0.49	0.03
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0	20.43	0	0	0.0004	0.004	1.02	0.02
TG(C16:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.25	0.002	0	11.55	0	1.39	8.10
TG(C20:0/C20:0/C20:0)	0	0	0.001	8.57	0	0.007	0	0
TG(C16:0/C16:0/C18:3(9,12,15))[iso3]	0	0.43	0.05	0	6.25	0	1.13	5.18
TG(C14:0/C16:0/C16:0)[iso3]	1.48	0.09	0	0.57	0	0.24	0.27	0.34
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0	0	0	0	0	14.20	0	0
TG(C14:0/C14:0/C14:0)	0.005	0.001	0	0.001	0	0.0005	0.02	0.003
TG(C16:0/C16:0/C21:0)[iso3]	12.77	0	0.03	0	0	0.15	0	0
TG(C16:0/C16:0/C20:0)[iso3]	0	0	0.11	10.89	0	0.57	0	0.03
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	10.09	0	0
TG(C16:0/C20:0/C20:0)[iso3]	0	0	0.01	9.66	0	0.06	0	0.0003
TG(C18:2(9,12)/C18:3(9,12,15)/C18:3(9,12,15))	0	0.78	0	0	0.59	0	1.44	1.54
TG(C14:0/C14:0/C16:0)[iso3]	0.09	0.013	0	0.026	0	0.01	0.08	0.03
TG(C16:0/C16:0/C17:0)[iso3]	0	0	0.37	0.95	0	0	0	0
TG(C14:0/C20:0/C20:0)[iso3]	0	0	0	0.45	0	0.003	0	0
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	6.73	0	0	0.008	0.04	0.99	0.12
TG(C18:2(9,12)/C18:2(9,12)/C18:3(9,12,15))	0	4.00	0	0	0.01	0	1.21	0.18
TG(C16:0/C18:0/C18:0)[iso3]	0	0.04	7.46	0	0.12	0	0.61	0.16
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	7.17	0	0
TG(C16:0/C21:0/C21:0)[iso3]	6.78	0	0.001	0	0	0.005	0	0
TG(C16:0/C16:0/C18:0)[iso3]	0	0.17	2.98	0	0.65	0	0.75	0.74
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0	2.21	0	0	0.17	0.50	0.95	0.63
TG(C18:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.06	0.006	0	2.22	0	1.13	1.81
TG(C14:0/C14:0/C20:0)[iso3]	0	0	0	0.02	0	0.001	0	0.0003
TG(C16:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:0)[iso3]	0	0	2.34	0	0	0	0	0
TG(C14:0/C18:0/C18:0)[iso3]	0	0.005	0	0	0	0	0.18	0.017
TG(C16:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	1.31	0	0	0.32	0	1.17	0.98
TG(C14:0/C14:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:0)[iso3]	0	0	0.69	0	0	0	0	0.002
TG(C17:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.0008	0	0	0	0	0
TG(C21:0/C21:0/C21:0)	3.61	0	0	0	0	0.0001	0	0
TG(C14:0/C16:0/C17:0)[iso6]	0	0	0	0.04	0	0	0	0
TG(C14:0/C14:0/C22:0)[iso3]	0.001	0	0	0	0	0	0	0.0002
TG(C14:0/C16:0/C20:0)[iso6]	0	0	0	0.51	0	0.03	0	0.003
TG(C14:0/C16:0/C21:0)[iso6]	0.78	0	0	0	0	0.007	0	0
TG(C16:0/C17:0/C17:0)[iso3]	0	0	0.11	0.07	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.03	0	0	0	0	0.41	0.83
TG(C14:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:3(9,12,15))[iso6]	0	0.10	0.14	0	1.21	0	0.92	1.16
TG(C18:0/C18:0/C18:1(9))[iso3]	0	0.006	2.31	0	0	0	0.24	0
TG(C14:0/C14:0/C21:0)[iso3]	0.05	0	0	0	0	0.0003	0	0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.61	0	0	0.002	0	0.81	0.02
TG(C16:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0.02	0	0	0	0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0.11	0.36	0	0	0	0.36	0
TG(C14:0/C14:0/C17:0)[iso3]	0	0	0	0.002	0	0	0	0
TG(C14:0/C21:0/C21:0)[iso3]	0.42	0	0	0	0	0.0002	0	0
TG(C16:1(9)/C16:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0.31	0	0	0.06	0	0.95	0.22
TG(C14:0/C16:0/C22:0)[iso6]	0.02	0	0	0	0	0	0	0.002
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0.03	0	0	0	0	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	0.53	0	0	0.03	0	0.78	0.14

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.06	0	0	0.80	0.30	1.01
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	0.05	0.21	0	0	0	0.71	0.44
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C17:0)[iso3]	0	0	0	0.04	0	0.05	0	0.009
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.078	0	0	1.21	0.09	0.27
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	0	0.02	0	0	0	0	0	0.11
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	0.09	0.32	0	0	0	0.13	0.11
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0.13	0	0	0.09	0.01	0.06
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0.45	0	0.11	0	0	0.37	0.27	0.09
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.02	0	0	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C17:0)	0	0.005	0	0.04	0	0.17	0	0.06
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0.92	0	0	0	0.09	0	0.12
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0.49	0	0	0	0.26	0	0.52
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	0.03	0	0	0	0.02	0.05
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.005	0	0.17	0	0	0.03	0.02	0.02
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0.16	0	0	0	0.62	0
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	0	0	0	0.001	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	0.03	0	0	0	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.03	0	0	0	0	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0.01	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	0.04	0	0	0	0.35	0	0.36
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0.015	0	0	0	0.01	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0.0001	0	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	0.31	0	0	0	0.39	0	0.14
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0.0003	0.31	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0.65	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.004	0	0	0.62	0.002	0.02
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0.11	0	0	0.42	0.02	0.06
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	0.04	0	0	0	0	0	0.40
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0.09	0	0	0.28	0.05	0.24
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0.57	0	0.04
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0.2	0	0	0	0.21	0
TG(C14:0/C16:0/C18:0)[iso6]	0	0	0.04	0	0	0	0.05	0.02
TG(C14:0/C14:0/C18:0)[iso3]	0	0	0.003	0.51	0	0	0.008	0.002
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0.001	0.39	0	0	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0	0.006	0	0.45	0	0	0	0.06
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.08	0	0.12	0	0	0.08	0.15	0.08
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0.04	0	0	0	0
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	0.48	0	0	0	0.01
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0.02	0	0	0	0	0
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0.03	0	0.15	0	0	0.14	0.049	0.02
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0.036	0	0	0	0.17	0.06
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.01	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0.003	0	0	0.41	0.005	0.07
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	0	0	0.09	0	0	0.79	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0.77	0	1.09
TG(C14:0/C17:0/C17:0)[iso3]	0	0	0.98	0.004	0.0002	0	0.01	0
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	0	0	0	0.02	0	0	0.21	0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	0	0	0.02	0	0	0.85	0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0.24	0.31	0	0.22	0
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	1.01	0	0.19	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	1.01
TG(C17:0/C17:0/C17:0)	0	0	0.76	0.006	0.0002	0	0.006	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0.11	0.001	0	0.06	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0.36	0.02	0	0.05	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0.06	0.002	0	0.14	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0.51	0	0	0.24	0	0	0
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	0.02	0	0.12	0
TG(C14:0/C22:0/C22:0)[iso3]	0.04	0	0	0	0	0	0	0.92
TG(C16:0/C16:0/C22:0)[iso3]	0.57	0	0	0	0	0	0	0.59
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	0	0.002	0	0.09	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0.79	0	0.32	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0.76	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	0	0	0.09	0.007	0	0.02	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0.73	0	0.006	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0.001	0.69	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0.11	0.01	0	0.09	0
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0.61	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0.64
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0.08	0	0	0.12	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0.51	0	0.31
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0.47	0	0	0.19	0	0	0
TG(C14:0/C16:0/C18:0)[iso6]	0	0	0	0.01	0	0	0.52	0
TG(C14:0/C14:0/C18:0)[iso3]	0	0	0	0.002	0	0	0.28	0
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0.41	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0.55	0	0.004	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0	0	0	0.006	0	0	0.04	0
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0.24	0.03	0	0.14	0
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0	0.001	0	0.06	0
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	0.004	0	0	0.11	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0.48	0
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0.06	0.02	0	0.23	0
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0.05	0	0	0.31	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0.45
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0.45	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0.41

Continued

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0.04	0	0.32	0	0.09	0.19	0	0
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C17:0)[iso3]	0.003	0.89	0.07	0.007	0	0.003	0	0.07
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:0)[iso6]	0.16	0	0.47	0	0.08	0.02	0.36	0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0.04	0	0	0	0.07	0.02	0	0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0.12	0	0.58	0.43	0	0.13	0	0
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C17:0)	0.009	0.66	0.24	0.007	0.02	0.008	0.01	0.01
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.06	0	0	0.04	0.43	0.02	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.07	0	0	0.28	0.55	0.24	0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.02	0	0	0.05	0	0.01	0	0
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0.53	0	0	0	0
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0.41
TG(C14:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0.45
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0.02	0	0.64	0.11	0.12	0.13	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	0.008	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0.33	0	0	0.07	0.43	0.03	0	0
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0.03	0	0.45	0	0.11	0.17	0	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0.13	0	0	0	0
TG(C14:0/C16:0/C18:0)[iso6]	0.05	0	0.15	0	0	0.01	0	0
TG(C14:0/C14:0/C18:0)[iso3]	0.001	0	0.02	0	0	0.002	0	0
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0	0.008	0	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0.01	0	0.17	0	0.02	0.01	0.02	0
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0.02	0	0	0.29	0	0.11	0	0
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0.49
TG(C14:0/C17:0/C18:0)[iso6]	0.004	0	0.05	0	0	0.005	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0.11	0	0	0.07	0	0.01	0	0
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0.01	0	0.15	0	0	0.07	0	0
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C18:1(9)/C18:3(9,12,15)/C18:3(9,12,15))	0	0.03	0.001	0	0	0	0.54	0
TG(C18:0/C18:0/C18:3(9,12,15))[iso3]	0	0.02	0.35	0	0.23	0	0.75	0.26
TG(C14:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C17:0)[iso3]	0	0	0	0.003	0	0	0	0
TG(C16:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0.06	0.02	0	0	0	0.44	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C20:0)[iso3	0	0	0	0	0	1.14	0	0
TG(C16:0/C17:0/C18:0)[iso6]	0	0	0.93	0	0	0	0	0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0	0.12	0	0	0.006	0	0.63	0.03
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0	1.01	0	0	0	0	0.38	0
TG(C14:0/C16:0/C18:3(9,12,15))[iso6]	0	0.05	0	0	0	0	0.33	0.53
TG(C20:0/C18:3(9,12,15)/C18:3(9,12,15))	0	0	0.0002	0	0	0	0	0.08
TG(C14:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C17:0)	0	0	0.03	0.005	0	0	0	0
TG(C17:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12)	0	0	0	0	0	0.99	0	0
TG(C17:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0.02	0.92	0	0	0	0.29	0
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0.91	0	0	0	0.002	0.29	0.01
TG(C15:0/C18:3(9,12,15)/C18:3(9,12,15))	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:0)[iso6]	0	0	0.03	0.84	0	0	0	0
TG(C14:0/C22:0/C22:0)[iso3]	0.0003	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:0)[iso3]	0.37	0	0	0	0	0	0	0.02
TG(C17:0/C20:0/C20:0)[iso3]	0	0	0.003	0.75	0	0	0	0
TG(C16:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.005	0	0	0	0	0.05
TG(C16:0/C18:0/C20:0)[iso6]	0	0	0.272	0	0	0	0	0.008
TG(C16:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0.81	0	0
TG(C17:0/C17:0/C18:3(9,12,15))[iso3]	0	0	0.005	0	0	0	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0.71	0	0
TG(C15:0/C20:0/C20:0)[iso3]	0	0	0.0003	0	0	0	0	0
TG(C16:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:0)[iso3]	0	0	0.03	0	0	0	0	0
TG(C18:0/C18:0/C22:0)[iso3]	0	0	0	0	0	0	0	0.001
TG(C16:0/C16:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0.01	0.11	0	0	0	0.14	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0.33	0	0	0	0	0.37	0
TG(C17:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0.04	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C18:3(9,12,15))	0	0.19	0	0	0	0	0.45	0
TG(C16:1(9)/C16:1(9)/C16:1(9))	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C18:1(9))[iso6]	0	0	0.11	0	0	0	0	0
TG(C15:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0.001	0	0	0	0	0
TG(C14:0/C16:0/C18:0)[iso6]	0	0.02	0	0	0	0	0.22	0.07
TG(C14:0/C14:0/C18:0)[iso3]	0	0.003	0	0	0	0	0.06	0.008
TG(C14:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0.0008
TG(C15:0/C16:0/C17:0)[iso6]	0	0	0.01	0	0	0	0	0
TG(C17:0/C17:0/C18:0)[iso3]	0	0	0.29	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0.17	0	0	0	0	0.35	0.10
TG(C14:0/C17:0/C20:0)[iso6]	0	0	0	0.04	0	0	0	0
TG(C14:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3	0	0	0	0	0	0.48	0	0
TG(C18:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0.001
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0	0.30	0	0	0	0.02	0.28	0.06
TG(C14:0/C18:0/C18:3(9,12,15))[iso6]	0	0.014	0	0	0	0	0.27	0.12
TG(C16:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.01	0	0	0	0	0.01
TG(C18:1(9)/C18:1(9)/C18:3(9,12,15))[iso3]	0	0.009	0.005	0	0	0	0.17	0
TG(C16:0/C16:1(9)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.007	0	0	0.045	0.003	0.006
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.107	0	0	0	0.023	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0.038	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0.002	0	0	0	0.003	0.005
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0.001	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0.002	0	0	0	0.001	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0.066	0	0.002
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0.069	0	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.042	0	0.014
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0.066	0	0	0	0
TG(C22:0/C22:0/C22:0)	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	0.061	0	0.004
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0.054	0	0	0	0
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0.045	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0.052	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0.012	0	0	0	0.031	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0.031	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.024	0	0	0	0.023	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0.020	0.001	0.001
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0.036	0	0	0	0.004	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	0	0.035	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0.002	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0	0	0	0.110	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.105	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0	0.001	0	0.025	0
TG(C16:0/C22:0/C22:0)[iso3]	0.096	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0.085	0	0	0.014	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0.079	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0.079	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0.059	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0.002	0	0.074	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0	0	0.025	0	0.069	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0.070	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0.016	0.001	0	0.050	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0.066	0	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C22:0)	0.063	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0.062	0
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0.057	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0	0	0	0	0.050	0
TG(C12:0/C14:0/C16:0)[iso6]	0.049	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0.008	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0.047	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0.047	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0.046	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0.045	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0.043	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0.020	0	0	0.005	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0.037	0	0	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0.037	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0.036	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0.035	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0.035	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0	0.006	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Caulifl ower	Cucumber	Orange pepper
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0	0.064
TG(C16:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0.001	0	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0.007	0	0	0.019	0	0.007	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0	0.001	0	0	0	0
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C22:0)	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C20:0)[iso6]	0.029	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0.005	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0.035	0	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:1(9))[iso3]	0.033	0	0	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0.011	0	0	0	0
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0	0.002	0	0	0	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0.006	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0.034	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C17:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.005	0	0	0	0	0
TG(C17:0/C18:0/C20:0)[iso6]	0	0	0.08	0	0	0	0	0
TG(C14:0/C14:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0.01	0.04	0	0	0	0.36	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0.07	0	0	0	0	0.23	0.01
TG(C16:0/C21:0/C22:0)[iso6]	0.19	0	0	0	0	0	0	0
TG(C16:0/C22:0/C22:0)[iso3]	0.005	0	0	0	0	0	0	0.000
TG(C12:0/C18:0/C18:0)[iso3]	0	0	0.36	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0.05	0	0.006
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0	0	0.34	0	0
TG(C14:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0	0.07	0	0	0	0	0.30	0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C21:0)[iso3]	0	0	0	0	0	0.30	0	0
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0	0.004	0.28	0	0	0	0.11	0
TG(C17:0/C18:0/C18:1(9))[iso6]	0	0	0.29	0	0	0	0	0
TG(C14:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:1(9)/C16:1(9)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C16:0)[iso3]	0	0	0.05	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0.006	0	0.00007
TG(C15:0/C18:2(9,12)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C22:0)[iso6]	0.012	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C18:3(9,12,15))[iso3]	0	0	0.0004	0	0	0	0	0.0006
TG(C16:1(9)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C22:0)	0.00008	0	0	0	0	0	0	0
TG(C18:0/C18:0/C21:0)[iso3]	0	0	0.23	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:0)[iso3]	0	0	0	0	0	0.005	0	0.001
TG(C15:0/C17:0/C17:0)[iso3]	0	0	0.003	0	0	0	0	0
TG(C21:0/C21:0/C22:0)[iso3]	0.11	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0.21	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0	0.002	0.03	0	0	0	0.05	0
TG(C12:0/C14:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0.21	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0.015	0	0	0	0	0.11	0
TG(C18:2(9,12)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0.01
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0	0.05	0	0	0	0	0.14	0
TG(C14:0/C14:0/C18:3(9,12,15))[iso3]	0	0.008	0	0	0	0	0.11	0.05
TG(C17:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.03	0	0	0	0	0
TG(C17:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0.003	0	0.0007
TG(C17:0/C17:0/C18:1(9))[iso3]	0	0	0.03	0	0	0	0	0
TG(C17:0/C17:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0.008	0	0	0	0	0.13	0
TG(C14:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0.005
TG(C12:0/C14:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0.001	0	0	0	0	0
TG(C12:0/C16:0/C21:0)[iso6]	0	0	0.002	0	0	0	0	0
TG(C16:0/C16:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	0.04	0	0	0	0.001	0.08	0.006
TG(C12:0/C16:0/C18:0)[iso6]	0	0	0.14	0	0	0	0	0
TG(C15:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0.004	0	0	0	0	0
TG(C17:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0.08	0	0	0	0	0
TG(C12:0/C14:0/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0.007	0	0	0.045	0.003	0.006
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0.107	0	0	0	0.023	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	0.038	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0.002	0	0	0	0.003	0.005
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0.001	0	0	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0.002	0	0	0	0.001	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0.066	0	0.002
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0.069	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.042	0	0.014
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0.066	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0.061	0	0.004
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0.054	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.045	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0.052	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0.012	0	0	0	0.031	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.031	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0.024	0	0	0	0.023	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0	0.020	0.001	0.001
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0.036	0	0	0	0.004	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.035	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0.002	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.110
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0.105	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	0	0	0.001	0	0.025
TG(C12:0/C21:0/C21:0)[iso3]	0	0.096	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	0.085	0	0	0.014	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0.079	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.079
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0	0.059	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0.002	0	0.074
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.025	0	0.069
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0.070	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0.016	0.001	0	0.050
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0.066	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0.063	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.062
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.057
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.050
TG(C14:0/C14:0/C23:0)[iso3]	0	0.049	0	0	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.008	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0.047	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0.047	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.046
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.045
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.043
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0.020	0	0	0.005	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0.037	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0.037	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.036
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.035
TG(C16:0/C21:0/C24:0)[iso6]	0	0.035	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.006	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0.001	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0.007	0	0	0.019	0	0.007
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0	0	0.001	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.029	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))	0	0	0.005	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.035	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.033	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0.011	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0	0	0.002	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.006	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.034	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0.045	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C24:0)	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C16:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:0)[iso3]	0	0.064	0	0	0	0.011	0.066	0
TG(C12:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0.095	0	0
TG(C18:3(6,9,12)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0.004	0	0	0
TG(C18:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0.086	0	0
TG(C14:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0.002	0	0	0
TG(C16:0/C16:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.002	0	0
TG(C15:0/C16:1(9)/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C16:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0.046	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:0)	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0.045	0	0
TG(C16:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0	0.002	0	0	0
TG(C14:0/C14:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.001	0	0
TG(C16:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0.034	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0.001	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0.004	0	0	0	0.002	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0	0	0.024	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0.004	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0.014	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14)	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0.004	0	0	0	0.001	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0.018	0	0	0	0.006	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0.005	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.016	0	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0.012	0	0	0	0.004	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0.009	0	0	0	0.011	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0.013	0	0	0	0.002	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0.011	0	0	0	0.005	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.011	0	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.033
TG(C21:0/C22:0/C22:0)[iso3]	0	0.032	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.030
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0	0	0.030	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.028
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0.027	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0.027	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.026
TG(C12:0/C16:0/C22:0)[iso6]	0	0.026	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.024
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.022
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.021
TG(C12:0/C14:0/C22:0)[iso6]	0	0.020	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.020	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0.020	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))	0	0	0	0	0	0	0	0.019
TG(C15:0/C15:0/C15:0)	0	0	0.001	0.019	0	0	0.001	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.019
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.001	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.018
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.017
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0.016	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.016
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0.015	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0.012	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.012
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Orange pepper
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))[iso	0	0	0.007	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14))[iso	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0.015	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,14))[i	0	0	0	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.006	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.003	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0.011	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.003	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C22:0)[iso3]	0	0	0	0.003	0	0	0	0
TG(C14:0/C16:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0.030	0	0
TG(C18:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0.030	0	0
TG(C16:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:0)[iso6]	0	0	0	0	0	0.028	0	0
TG(C14:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0	0	0.027	0	0
TG(C20:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C20:2(11,14)	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C21:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C20:2(11,1	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C15:0)	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C17:0)[iso6]	0	0	0	0	0	0.018	0	0
TG(C12:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0.018	0	0
TG(C14:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0.004	0	0
TG(C18:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0.003	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0	0	0.011	0	0
TG(C16:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.001	0	0
TG(C12:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0.014	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C16:0)[iso3]	0	0	0	0	0	0.003	0	0
TG(C16:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0.012	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0	0	0.003	0	0
TG(C16:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0.012	0	0
TG(C16:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0.011	0	0
TG(C18:1(9)/C18:1(9)/C20:0)[iso3]	0	0	0	0	0	0.011	0	0
TG(C14:0/C18:3(6,9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0.009	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0.002	0	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0.005	0	0	0	0.006	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0.007	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0.006	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0.006	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0.006	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0.005	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.005	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0.005	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0.004	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0.004	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.003	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0.0005	0	0	0	0.0002	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0.0000 4	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C12:0/C12:0/C14:0)[iso3]	0	0.009	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0.009	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.009
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.007
TG(C16:0/C22:0/C23:0)[iso6]	0	0.007	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0.007	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.007
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0.006
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.006
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0.006	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.0004	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0.005	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.004
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0.004	0	0	0	0	0	0
TG(C21:0/C22:0/C23:0)[iso6]	0	0.004	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.003
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0.003	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0.003	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Orange pepper
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0.005	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)[iso6	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0.001	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0.003	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C12:0/C12:0/C14:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C16:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0.008	0	0
TG(C15:0/C18:0/C20:0)[iso6]	0	0	0	0	0	0.008	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C21:0)[iso3]	0	0	0	0	0	0.00009	0	0
TG(C12:0/C12:0/C18:0)[iso3]	0	0	0	0	0	0.007	0	0
TG(C17:0/C18:3(9,12,15)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.007	0	0
TG(C14:0/C17:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(6,9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C20:2(11,14))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C17:0)[iso3]	0	0	0	0	0	0.005	0	0
TG(C14:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0.005	0	0
TG(C12:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0.005	0	0
TG(C15:0/C17:0/C18:2(9,12))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:3(9,12,15)/C22:0)[iso6	0	0	0	0	0	0	0	0
TG(C16:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C20:0)[iso6]	0	0	0	0	0	0.005	0	0
TG(C17:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0.005	0	0
TG(C16:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.004	0	0
TG(C20:0/C20:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:0)[iso6]	0	0	0	0	0	0.004	0	0
TG(C14:0/C16:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C21:0)[iso3]	0	0	0	0	0	0.004	0	0
TG(C17:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0.004	0	0
TG(C18:1(9)/C18:1(9)/C21:0)[iso3]	0	0	0	0	0	0.004	0	0
TG(C20:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C18:1(9))[iso6]	0	0	0	0	0	0.003	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0	0	0.003	0	0
TG(C21:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C20:0)[iso3]	0	0	0	0	0	0.003	0	0
TG(C18:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0.003	0	0
TG(C14:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[is	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0.002	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0.001	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0.002	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0.001	0	0	0	0.0004	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.001	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0007	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0.0002	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0.0009	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0.0009	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0.0006	0	0	0	0.0006	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0.0008	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.003
TG(C12:0/C14:0/C23:0)[iso6]	0	0.003	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))[iso3	0	0	0	0	0	0	0	0.002
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0.002	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.002
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.002
TG(C12:0/C22:0/C22:0)[iso3]	0	0.002	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0.002	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0.002	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0.001	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0.001	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0.0005	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0.001	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0.001
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0.0005	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Orange pepper
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.0007	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0.002	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.0007	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.001	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0.001	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0	0
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0.0003	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C18:2(9,12)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:0/C21:0)[iso6]	0	0	0	0	0	0.003	0	0
TG(C12:0/C16:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.003	0	0
TG(C18:3(9,12,15)/C20:2(11,14)/C20:2(11,14	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C16:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C17:0/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:2(9,12)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.002	0	0
TG(C18:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C14:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C21:0)[iso3]	0	0	0	0	0	0.0003	0	0
TG(C18:1(9)/C18:2(9,12)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.002	0	0
TG(C18:2(9,12)/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C16:0)[iso6]	0	0	0	0	0	0.002	0	0
TG(C12:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0.00171	0	0
TG(C12:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0.002	0	0
TG(C15:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C21:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0	0	0.0003	0	0
TG(C18:1(9)/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C20:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C15:0/C16:0/C21:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C17:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C18:1(9)/C20:0/C21:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C17:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0.001	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C20:2(11,14)/C20:2(11,14))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C17:0)[iso3]	0	0	0	0	0	0.0009	0	0
TG(C12:0/C12:0/C18:1(9))[iso3]	0	0	0	0	0	0.0009	0	0
TG(C12:0/C17:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.00088	0	0
TG(C18:2(9,12)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.0008	0	0
TG(C14:0/C18:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0.0008	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0.0008	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0.0007	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.0006	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0.0006	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3]	0	0	0.0005	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0.0005	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0.0003	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0.0003	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0002	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.0002	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0.0001	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0.0008	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0.0007	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0.0007	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0.0006	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0.0006	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0.0005	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0.0004	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0.0004	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0.0004
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0.0003	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0.0003	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0.0002	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0.0001	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0.0008	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0.0002	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3	0	0	0.0002	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0.0003	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0003	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0.0003	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.0003	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0.0003	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0.0003	0	0	0	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0.0003	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.0003	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0.0003	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0.0004	0	0	0	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0.0004	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0.0004	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0.0004	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0.0004	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C17:0/C17:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C22:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C18:2(9,12)/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0.0006	0	0
TG(C12:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0.0006	0	0
TG(C17:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.0006	0	0
TG(C18:3(9,12,15)/C22:1(13)/C22:1(13))[iso3	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.0005	0	0
TG(C20:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0.0001	0	0
TG(C12:0/C15:0/C17:0)[iso6]	0	0	0	0	0	0.0005	0	0
TG(C15:0/C15:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:1(9))[iso6]	0	0	0	0	0	0.0005	0	0
TG(C22:0/C22:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C20:0)[iso3]	0	0	0	0	0	0.0005	0	0
TG(C18:2(9,12)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C21:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C17:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0.0004	0	0
TG(C18:1(9)/C21:0/C21:0)[iso3]	0	0	0	0	0	0.0004	0	0
TG(C20:2(11,14)/C20:2(11,14)/C20:2(11,14))	0	0	0	0	0	0	0	0
TG(C14:0/C18:2(9,12)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C17:0/C21:0)[iso6]	0	0	0	0	0	0.0003	0	0
TG(C15:0/C18:1(9)/C21:0)[iso6]	0	0	0	0	0	0.0003	0	0
TG(C12:0/C22:0/C23:0)[iso6]	0	0	0	0	0	0	0	0
TG(C21:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C15:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C20:0)[iso3]	0	0	0	0	0	0.0003	0	0
TG(C12:0/C20:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.0002	0	0
TG(C14:0/C17:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C16:0/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0.0002	0	0
TG(C18:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.0002	0	0
TG(C18:3(9,12,15)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C20:0)[iso6]	0	0	0	0	0	0.0002	0	0
TG(C12:0/C12:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C14:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C18:3(9,12,15))[iso3]	0	0	0	0	0	0.0001	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Broccoli	Red beetroot	Dill	Eggplant	Garlic	Green bean	Green pepper	Green zucchini
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15))[iso3]	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0.0001	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.0001	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0.00009	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.00008	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0.00008	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.00004	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0.00004	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0.00003	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0.00003	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0.00001	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0.00001	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.00001	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Raspberry	Nanking cherry	Crab apple	Saskatoon berry	Carrot	Parsnip	Wax bean	White cabbage
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15	0	0	0	0	0	0.0001	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0.0001	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.0001	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0	0	0	0	0	0	0.0001	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0.0001	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0.0001	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0.0001	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0.0001	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0.0001	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0.0001	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	4	0	0
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	3	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued

Table 2.11*Continued.*

Lipid compositions	Italian pepper	Onion	Japanese pumpkin	Lettuce	Potato	Red pepper	Yellow zucchini	Yellow pepper
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15)	0	0	0	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0.0001	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0.00009	0	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)	0	0	0	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0.00007	0	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0.00005	0	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0.00005	0	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C23:0/C24:0)[iso6]	0	0.00003	0	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0.00003	0	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0.00001	0	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0.00001	0	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0.00001	0	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0.00001	0	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0	0	0	0	0	0

Continued.

Table 2.11*Continued.*

Lipid compositions	Turnip	Tomato	Swiss chard	Sunburst squash	Spinach	Cauliflower	Cucumber	Orange pepper
TG(C12:0/C18:3(9,12,15)/C18:3(9,12,15)	0	0	0.0004	0	0	0	0	0
TG(C18:0/C20:0/C24:0)[iso6]	0	0	0.0004	0	0	0	0	0
TG(C12:0/C12:0/C24:0)[iso3]	0	0	0.0004	0	0	0	0	0
TG(C14:0/C18:1(9)/C20:0)[iso6]	0	0	0.0004	0	0	0	0	0
TG(C15:0/C20:0/C21:0)[iso6]	0	0	0.0004	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C24:0)[iso6]	0	0	0.0005	0	0	0	0	0
TG(C14:0/C18:1(9)/C22:1(13))[iso6]	0	0	0.0005	0	0	0	0	0
TG(C22:0/C23:0/C23:0)[iso3]	0	0	0.0005	0	0	0	0	0
TG(C15:0/C20:0/C22:1(13))[iso6]	0	0	0.0005	0	0	0	0	0
TG(C12:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.0005	0	0	0	0	0
TG(C18:3(9,12,15)/C18:3(9,12,15)/C21:0)	0	0	0.0005	0	0	0	0	0
TG(C12:0/C12:0/C15:0)[iso3]	0	0	0.0005	0	0	0	0	0
TG(C12:0/C15:0/C18:3(9,12,15))[iso6]	0	0	0.0005	0	0	0	0	0
TG(C15:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0005	0	0	0	0	0
TG(C18:1(9)/C18:1(9)/C22:1(13))[iso3]	0	0	0.0005	0	0	0	0	0
TG(C17:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0006	0	0	0	0	0
TG(C22:0/C23:0/C24:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C18:0/C22:0/C24:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C18:3(9,12,15)/C21:0/C21:0)[iso3]	0	0	0.0006	0	0	0	0	0
TG(C14:0/C20:0/C24:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C12:0/C15:0/C21:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C24:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C15:0/C18:3(9,12,15)/C21:0)[iso6]	0	0	0.0006	0	0	0	0	0
TG(C22:0/C24:0/C24:0)[iso3]	0	0	0.0006	0	0	0	0	0
TG(C12:0/C15:0/C15:0)[iso3]	0	0	0.0006	0	0	0	0	0
TG(C12:0/C23:0/C23:0)[iso3]	0	0	0.0007	0	0	0	0	0
TG(C14:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0007	0	0	0	0	0
TG(C14:0/C20:0/C22:1(13))[iso6]	0	0	0.0007	0	0	0	0	0
TG(C18:2(9,12)/C20:0/C22:0)[iso6]	0	0	0.0007	0	0	0	0	0
TG(C15:0/C21:0/C21:0)[iso3]	0	0	0.0007	0	0	0	0	0
TG(C12:0/C23:0/C24:0)[iso6]	0	0	0.0007	0	0	0	0	0
TG(C18:1(9)/C20:0/C22:1(13))[iso6]	0	0	0.0007	0	0	0	0	0
TG(C15:0/C15:0/C21:0)[iso3]	0	0	0.0007	0	0	0	0	0
TG(C18:1(9)/C22:1(13)/C22:1(13))[iso3]	0	0	0.0007	0	0	0	0	0
TG(C12:0/C24:0/C24:0)[iso3]	0	0	0.0007	0	0	0	0	0
TG(C18:2(9,12)/C22:0/C22:0)[iso3]	0	0	0.0008	0	0	0	0	0
TG(C20:0/C20:0/C22:1(13))[iso3]	0	0	0.0008	0	0	0	0	0
TG(C22:1(13)/C22:1(13)/C22:1(13))	0	0	0.0008	0	0	0	0	0
TG(C20:0/C22:1(13)/C22:1(13))[iso3]	0	0	0.0008	0	0	0	0	0
TG(C23:0/C23:0/C23:0)	0	0	0.0008	0	0	0	0	0
TG(C24:0/C24:0/C24:0)	0	0	0.0008	0	0	0	0	0
TG(C23:0/C23:0/C24:0)[iso3]	0	0	0.0008	0	0	0	0	0
TG(C20:0/C24:0/C24:0)[iso3]	0	0	0.0008	0	0	0	0	0
TG(C23:0/C24:0/C24:0)[iso3]	0	0	0.0008	0	0	0	0	0
TG(C20:0/C20:0/C24:0)[iso3]	0	0	0.0008	0	0	0	0	0
TG(C20:0/C22:0/C24:0)[iso6]	0	0	0.0009	0	0	0	0	0

Table 2.12. Inferred lipids consisting of all the possible chain lengths of the fatty acids in lipids and the number of acyl chains for the specific lipid classes.

Lipid Types	Lipid count
CDP-diacylglycerols	527
Glycerophosphoethanolamines	438
Glycerophosphocholines	438
Glycerophosphoglycerols	477
Phosphoglycerolphosphates	477
Glycerophosphoinositols	438
Glycerophosphoserines	438
Cardiolipins	22,775
Triacylglycerols	1,771
Monoacylglycerols	46
Diacylglycerols	527
Sphingolipids	276
Total	**28,628**

Table 2.93 Vitamin content of fruits and vegetables as determined by HPLC (Conc. mg/100 g FW).

Vitamins	Swiss chard	LV[1]	Sunburst squash	LV
Vitamin C	38.2 (25.9-50.4)	30	22.7 (18.9-26.5)	-
Vitamin B1	0.03 (0.03-0.03)	0.04	0.03 (0.03-0.03)	-
Vitamin B2	0.21 (0.17-0.25)	0.09	0.61 (0.60-0.63)	-
Vitamin B5	-	0.172	0.55 (0.55-0.56)	-
Vitamin B7	-	-	-	-
Vitamin B9	-	0.014	-	-
Vitamin B12	0.05 (0.04-0.05)	-	0.02 (0.02-0.02)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.03 (0.02-0.04)	-	-	-
Vitamin K	-	0.83	-	-
	Green bean	**LV**	**Yellow bean**	**LV**
Vitamin C	16.1 (15.7-16.5)	4.6	32.3 (6.8-57.8)	21
Vitamin B1	0.13 (0.12-0.13)	0.535	0.10 (0.09-0.11)	0.69
Vitamin B2	0.41 (0.32-0.49)	0.221	0.61 (0.36-0.85)	0.33
Vitamin B5	-	0.05	0.009 (0.009-0.01)	0.05
Vitamin B7	-	0.0007	0.003(0.002-0.004)	0.0007
Vitamin B9	0.23 (0.20-0.26)	0.399	0.20 (0.18-0.21)	0.389
Vitamin B12	0.009 (0.008-0.009)	-	-	-
Vitamin D2	0.04 (0.04-0.04)	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.12 (0.11-0.12)	-	0.14 (0.13-0.14)	-
Vitamin K	0.02 (0.02-0.02)	-	0.005 (0.005-0.006)	-
	Green bell pepper	**LV**	**Red bell pepper**	**LV**
Vitamin C	65.7 (53.4-77.9)	80.4	51.2 (50.6-51.7)	127.7
Vitamin B1	0.03 (0.03-0.04)	0.057	0.03 (0.03-0.03)	0.054
Vitamin B2	0.05 (0.05-0.05)	0.028	0.13 (0.12-0.14)	0.085
Vitamin B5	-	0.23	0.30 (0.29-0.32)	0.27
Vitamin B7	-	-	-	-
Vitamin B9	0.01 (0.01-0.01)	0.01	-	0.046
Vitamin B12	-	-	0.005 (0.005-0.005)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.65 (0.53-0.76)	0.37	1.3 (1.1-1.5)	1.58
Vitamin K	-	0.0074	-	4.9

[1] LV for Literature value

Continued.

Table 2.13.*Continued.*

Vitamins	Orange bell pepper	LV	Yellow bell pepper	LV
Vitamin C	50.9 (49.16-52.7)	-	56.1 (52.9-59.25)	183.5
Vitamin B1	0.02 (0.02-0.02)	-	0.04 (0.04-0.04)	0.028
Vitamin B2	0.02 (0.02-0.03)	-	0.04 (0.04-0.04)	0.025
Vitamin B5	-	-	-	-
Vitamin B7	-	-	-	-
Vitamin B9	0.48(0.48-0.48)	-	0.02 (0.01-0.02)	0.026
Vitamin B12	0.03 (0.03-0.03)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	0.21 (0.18-0.24)	-
Vitamin E	-	-	0.30 (0.29-0.31)	-
Vitamin K	1.0 (0.97-1.1)	-	-	-
	Red beetroot	**LV**	**Spinach**	**LV**
Vitamin C	5.5 (1.5-9.5)	4.9	28.5 (27.3-29.7)	28.1
Vitamin B1	0.03 (0.03-0.03)	0.031	0.06 (0.05-0.06)	0.078
Vitamin B2	-	0.04	0.18 (0.18-0.18)	0.189
Vitamin B5	-	0.15	0.28 (0.27-0.29)	0.3
Vitamin B7	-	-	-	0.00016
Vitamin B9	-	0.109	0.18 (0.17-0.19)	0.194
Vitamin B12	0.05 (0.05-0.05)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	-	0.04	1.2 (1.2-1.3)	2.03
Vitamin K	0.003 (0.003-0.003)	0.0002	0.60 (0.59-0.60)	0.4829
	Onion	**LV**	**Lettuce**	**LV**
Vitamin C	-	7.4	-	4
Vitamin B1	0.01 (0.01-0.02)	0.046	0.02 (0.01-0.02)	0.072
Vitamin B2	-	0.27	0.04 (0.04-0.04)	0.067
Vitamin B5	0.14 (0.05-0.23)	0.13	-	-
Vitamin B7	-	0.0009	0.10 (0.10-0.11)	0.142
Vitamin B9	-	0.019	0.30 (0.24-0.36)	0.136
Vitamin B12	0.04 (0.03-0.05)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	-	0.02	-	0.13
Vitamin K	-	0.0004	0.04 (0.03-0.04)	0.1025

Continued.

Table 2.13.*Continued.*

Vitamins	Cauliflower	LV	Parsnip	LV
Vitamin C	18.1 (17.1-19.1)	48.2	-	17
Vitamin B1	0.02 (0.01-0.02)	0.05	0.15 (0.12-0.18)	0.09
Vitamin B2	0.06 (0.05-0.07)	0.06	-	0.05
Vitamin B5	0.58 (0.49-0.67)	0.6	0.27 (0.23-0.31)	0.6
Vitamin B7	-	0.0015	-	0.0001
Vitamin B9	0.12 (0.12-0.12)	0.057	0.08 (0.07-0.09)	0.067
Vitamin B12	1.9 (1.8-1.9)	-	0.02 (0.01-0.02)	-
Vitamin D2	-	-	0.006 (0.006-0.006)	-
Vitamin D3	-	-	-	-
Vitamin E	-	0.08	0.15 (0.13-0.16)	0.15
Vitamin K	-	0.0155	-	0.0225
	Garlic	**LV**	**Turnip**	**LV**
Vitamin C	26.8 (25.9-27.7)	31.2	18.9 (18.6-19.2)	21
Vitamin B1	0.064 (0.06-0.06)	0.2	0.03 (0.03-0.03)	0.04
Vitamin B2	0.16 (0.16-0.17)	0.11	-	0.03
Vitamin B5	0.8 (0.74-086)	0.596	-	0.2
Vitamin B7	-	-	-	0.0001
Vitamin B9	-	0.003	0.02 (0.02-0.02)	0.015
Vitamin B12	0.19 (0.17-0.21)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	0.05 (0.04-0.07)	-
Vitamin E	-	0.08	-	0.03
Vitamin K	-	0.0017	-	0.1
	White cabbage	**LV**	**Japanese pumpkin**	**LV**
Vitamin C	7.4 (6.0-8.8)	4.2-36	11.8 (114.8-114.8)	9
Vitamin B1	0.05(0.05-0.06)	0.061	0.04 (0.04-0.04)	0.05
Vitamin B2	-	0.04	-	0.11
Vitamin B5	0.18 (0.18-0.18)	0.21	-	0.4
Vitamin B7	-	0.0012	-	0.0004
Vitamin B9	0.02 (0.01-0.02)	0.043	0.02 (0.02-0.03)	0.016
Vitamin B12	0.18 (0.18-0.18)	-	0.08 (0.08-0.08)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	-	0.15	-	1.06
Vitamin K	0.59 (0.51-0.68)	0.076	-	0.0011

Continued.

Table 2.13.*Continued.*

Vitamins	Carrot	LV	Eggplant	LV
Vitamin C	7.7 (7.2-8.2)	5.9	2.3(2.1-2.5)	2.2
Vitamin B1	0.08 (0.08-0.08)	0.066	0.03 (0.02-0.04)	0.039
Vitamin B2	0.02 (0.01-0.02)	0.058	-	0.037
Vitamin B5	0.29 (0.27-0.30)	0.28	-	0.22
Vitamin B7	0.006 (0.006-0.006)	0.0034	0.04 (0.04-0.04)	-
Vitamin B9	-	0.019	0.04 (0.04-0.04)	0.022
Vitamin B12	0.14 (0.13-0.15)	-	0.05 (0.05-0.06)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	0.04 (0.03-0.05)	-
Vitamin E	0.45 (0.45-0.46)	0.66	-	0.3
Vitamin K	-	0.0132	-	0.0035
	Dill	**LV**	**Broccoli**	**LV**
Vitamin C	24.1 (23.6-24.7)	-	66.6 (63.3-69.8)	89.2
Vitamin B1	0.03 (0.03-0.03)	0.058	0.05 (0.04-0.05)	0.071
Vitamin B2	0.19 (0.17-0.20)	0.296	0.09 (0.09-0.09)	0.117
Vitamin B5	-	0.3	0.79 (0.76-0.81)	1
Vitamin B7	-	0.004	0.004 (0.004-0.004)	0.005
Vitamin B9	-	0.15	0.04 (0.04-0.04)	0.063
Vitamin B12	0.21 (0.21-0.21)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.23 (0.25-0.21)	-	1.7 (1.6-1.8)	0.78
Vitamin K	-	-	0.21 (0.20-0.22)	-
	Italian red pepper	**LV**	**Russet potato**	**LV**
Vitamin C	45.4 (45.1-45.73)	-	19.9 (17.5-22.5)	26.4
Vitamin B1	0.05 (0.05-0.05)	-	0.05 (0.05-0.05)	0.055
Vitamin B2	0.25 (0.22-0.28)	-	0.02(0.02-0.02)	0.063
Vitamin B5	0.05 (0.05-0.06)	-	-	0.38
Vitamin B7	0.007 (0.006-0.008)	-	0.002 (0.002-0.002)	0.00047
Vitamin B9	0.35 (0.31-0.38)	-	-	0.036
Vitamin B12	-	-	0.02 (0.02-0.03)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.24 (0.21-0.26)	-	-	-
Vitamin K	-	-	-	0.016

Continued.

Table 2.13.*Continued.*

Vitamins	Green zucchini	LV	Yellow zucchini	LV
Vitamin C	12.8 (12.5-13.0)	17.9	13.5 (11.6-15.4)	-
Vitamin B1	0.03 (0.02-0.03)	0.045	0.02 (0.02-0.02)	-
Vitamin B2	-	0.094	-	-
Vitamin B5	0.17 (0.16-0.19)	-	-	-
Vitamin B7	0.73 (0.58-0.89)	0.155	0.03 (0.02-0.03)	-
Vitamin B9	0.02 (0.02-0.02)	0.024	0.05 (0.04-0.05)	-
Vitamin B12	-	-	0.06 (0.06-0.06)	-
Vitamin D2	0.07 (0.05-0.09)	-	-	-
Vitamin D3	0.01 (0.01-0.01)	-	-	-
Vitamin E	0.16 (0.14-0.18)	0.12	-	-
Vitamin K	-	0.0043	-	-
	Tomato	**LV**	**Nanking cherry**	**LV**
Vitamin C	25.6 (24.5-26.8)	13.7	8.1 (7.7-8.6)	-
Vitamin B1	0.02 (0.02-0.02)	0.037	0.01 (0.01-0.01)	-
Vitamin B2	-	0.019	0.05 (0.05-0.06)	-
Vitamin B5	-	0.33	0.19 (0.18-0.20)	-
Vitamin B7	-	-	0.0006 (0.0006-0.0006)	-
Vitamin B9	-	-	0.001 (0.001-0.001)	-
Vitamin B12	0.02 (0.02-0.02)	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.55 (0.55-0.55)	0.54	0.30 (0.30-0.30)	-
Vitamin K	-	0.0079	-	-
	Raspberry	**LV**	**Saskatoon berry**	**LV**
Vitamin C	37.4 (36.2-38.5)	26.2	29.2 (28.0-30.3)	-
Vitamin B1	0.03 (0.03-0.03)	0.032	0.04 (0.04-0.04)	-
Vitamin B2	-	0.038	-	-
Vitamin B5	0.18 (0.16-0.19)	0.24	0.02 (0.01-0.03)	-
Vitamin B7	-	0.0019	-	-
Vitamin B9	0.02 (0.02-0.03)	0.021	-	-
Vitamin B12	-	-	-	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.61 (0.59-0.62)	0.87	-	-
Vitamin K	0.005 (0.005-0.005)	0.0078	-	-

Continued.

Table 2.13.*Continued.*

Vitamins	Crab apple	LV	Cucumber	LV
Vitamin C	9.5 (9.3-9.6)	-	7.5 (4.5-10.6)	2.8
Vitamin B1	0.04 (0.03-0.04)	-	0.04 (0.04-0.04)	0.027
Vitamin B2	0.008 (0.007-0.009)	-	-	0.033
Vitamin B5	0.08 (0.07-0.09)	-	-	0.3
Vitamin B7	0.0003 (0.0003-0.0003)	-	-	0.004
Vitamin B9	0.006 (0.006-0.007)	-	0.01 (0.009-0.01)	0.007
Vitamin B12	0.01(0.01-0.02)	-	0.12 (0.11-0.12)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.004 (0.003-0.005)	-	-	0.03
Vitamin K	0.001 (0.001-0.001)	-	0.04 (0.04-0.04)	0.0164

Table 2.14. Cross checking NMR and DFI/LC-MS/MS assays.

Yellow zucchini metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	39.25 (39.2-39.3)	61.3 (59.6-63.0)	62
Arginine	50.25 (44.8-55.7)	61.3 (55.4-67.2)	50
Asparagine	167.95 (162.7-173.2)	≥ 52.8	-
Asparatic Acid	197.65 (191.5-203.8)	≥ 53.2	150
Glutamine	351.5 (237.3-365.7)	400.5 (361.8-439.2)	-
Glutamic acid	70 (62.1-77.9)	93.1 (87.7-98.5)	130
Glycine	66.8 (63.4-70.2)	72.6 (62.3-82.8)	47
Histidine	35.9 (33.7-38.1)	35.0 (32.6-37.5)	25
Isoleucine	25.7 (25.4-26)	61.7 (45.2-78.2)	45
Leucine	25 (24.8-25.2)	39.6 (36.5-42.7)	72
Lysine	56.5 (52.8-60.3)	43.7 (42.1-45.3)	68
Methionine	17.7 (15.6-19.9)	11.3 (10.2-12.5)	18
Phenylalanine	46.4 (42.7-50.1)	38.5 (37.7-39.2)	43
Proline	36.9 (36.2-37.7)	38.3 (34.9-41.7)	37
Serine	49.9 (40.8-59.1)	54.9 (54.2-55.6)	49
Threonine	21.15 (20.9-21.4)	20.6 (18.9-22.3)	29
Tryptophan	8.1 (7.2-9.0)	12.2 (11.6-12.8)	10
Tyrosine	30.6 (30.5-30.7)	24.1 (20.6-27.5)	31
Valine	38.4 (38.2-38.7)	41.8 (32.5-51.2)	54
Yellow bell pepper Metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	33.5 (32.1-35)	32.9 (30.1-35.7)	-
Arginine	39.4 (38.6-40.1)	38.5 (37.9-39.1)	-
Asparagine	203 (196-210.1)	≥ 52.8	-
Asparatic Acid	308.6 (288.8-328.5)	≥ 53.2	-
Glutamine	318.8 (305.6-331.9)	≥ 233.8	-
Glutamic acid	21.1 (19.8-22.4)	25.1 (22.5-27.7)	-
Glycine	32.5 (31-33.9)	49.7 (46.1-53.3)	-
Isoleucine	14.4 (11.2-17.5)	15.5 (13.9-17.1)	-
Leucine	16.1 (15.1-17.0)	15.6 (14.9-16.2)	-
Lysine	19.6 (19.3-19.9)	16.7 (16.6-16.8)	-
Methionine	8.2 (7.7-8.6)	6.2 (5.5-6.9)	-
Phenylalanine	12.7 (11.4-14.1)	16.3 (14.0-18.7)	-
Proline	10.9 (9.1-12.6)	10.6 (9.6-11.6)	-
Serine	71.9 (68.7-75.1)	96.5 (90.1-102.9)	-
Threonine	74.8 (73.9-75.6)	62.5 (59.4-65.6)	-
Tryptophan	11.4 (10.7-12.2)	6.2 (5.9-6.5)	-
Tyrosine	9.1 (8.2-9.9)	8.2 (7.5-8.9)	-
Valine	25 (23.9-26.1)	46.9 (34.3-59.7)	-

Table 2.14.*Continued.*

Green bell pepper Metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	63.7 (59.9-67.4)	80.9 (66.6-95.3)	35
Arginine	90 (87.5-92.5)	67.2 (66.2-68.2)	35
Asparagine	47.8 (47.4.-48.2)	62.5 (55.8-69.3)	-
Asparatic Acid	108.7 (96.7-120.7)	≥ 53.2	120
Glutamine	363.8 (353.5-374.1)	≥ 233.8	-
Glutamic acid	81.3 (74.7-87.9)	89.3 (85.6-93.1)	120
Glycine	34.4 (31.9-37)	11.9 (10.5-13.3)	30
Histidine	28.8 (20.7-36.8)	30.6 (25.4-35.9)	
Isoleucine	45.5 (45.4-45.6)	41.9 (40.2-43.5)	27
Leucine	27 (26.2-27.8)	33.0 (32.6-33.4)	36
Lysine	38.2 (37.4-39)	56.7 (56.1-57.3)	42
Phenylalanine	31.7 (31.6-31.8)	35.0 (34.9-35.1)	27
Proline	31.7 (31.6-31.8)	8.9 (8.3-9.5)	-
Serine	12.5 (11.7-13.2)	14.7 (12.9-16.5)	43
Threonine	14.8 (12.8-16.8)	12.3 (11.5-13.2)	13
Tryptophan	11.5 (11.9-12.6)	10.8 (9.8-11.8)	29
Tyrosine	22.9 (21.2-24.6)	16.8 (16.1-17.6)	13
Valine	45.4 (44-46.7)	103.3 (84.4-122.2)	42
Green zucchini metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	51.5 (41.2-61.8)	69.4 (64.5-74.4)	62
Arginine	67.4 (54.8-80.1)	54.6 (53.6-55.7)	-
Asparagine	376.5 (350.6-402.4)	≥ 52.8	-
Asparatic Acid	74.4 (70.4-78.4)	64.7 (62.1-67.3)	-
Glutamine	131 (96.8-165.3)	138.3 (138.1-138.5)	129
Glutamic acid	38 (33.1-42.9)	52.2 (43.4-61.1)	-
Glycine	6.2 (5.2-7.3)	10.9 (10.2-11.6)	-
Histidine	24.6 (21.3-27.9)	25.6 (23.4-27.7)	-
Isoleucine	22 (20.7-23.4)	26.6 (25.6-27.6)	45
Leucine	83.4 (82.2-84.7)	130.4 (126.1-134.7)	72
Lysine	18.4 (17.0-19.8)	20.8 (18.4-23.3)	-
Phenylalanine	38.5 (35.2-41.7)	39.2 (37.7-40.7)	-
Serine	58.1 (47.3-69.0)	53.2 (48.6-57.9)	100
Threonine	20.9 (19.9-21.9)	29.5 (25.6-33.5)	29
Tryptophan	22.6 (22.3-22.9)	22.7 (20.4-24.9)	-
Tyrosine	31.9 (31.7-32.1)	43.4 (40.4-46.4)	31
Valine	39.4 (29.2-49.6)	31.8 (29.8-33.7)	54

Continued.

Table 2.14.*Continued.*

Garlic metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	189.2 (187.8-190.6)	165.1 (143.5-186.7)	130
Arginine	280 (273.6-286.4)	≥70	640
Asparatic Acid	143.7 (129-158.4)	≥53.2	490
Citrulline	3.8 (3.4-4.2)	5.1 (4.8-5.5)	-
Glutamine	45.2 (42.6-47.9)	67.6 (62.2-73.1)	77
Glutamic acid	349.3 (318.1-380.5)	448.0 (436.6-459.5)	810
Glycine	261.8 (233.4-290.3)	201.2 (179.4-222.9)	210
Histidine	50.2 (44.2-56.8)	84.8 (78.5-91.0)	110
isoleucine	208.9 (187.5-230.2)	236.9 (231.8-242.2)	220
Leucine	188.9 (188.5-189.3)	408.5 (330.6-486.5)	180-310
Lysine	349.3 (318.1-380.5)	311.9 (305.8-318.1)	280
Phenylalanine	72.5 (72-72.9)	84.4 (77.7-91.1)	180
Proline	161.16 (137.4-184.9)	284.6 (279.9-289.3)	100
Serine	388.4 (380.6-396.2)	435.9 (432.7-439.1)	200
Threonine	107.7 (100.9-114.4)	114.1 (106.8-121.3)	82-150
Tryptophan	100.8 (100.1-101.6)	79.2 (70.6-87.8)	67
Tyrosine	101.7-113.6	126.1 (115.5-136.7)	82
Valine	200.9 (184.3-217.4)	174.3 (163.3-185.3)	300
Eggplant metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	31.3 (28.9-33.7)	34.5 (34.2-34.8)	47
Arginine	75.9 (68.1-83.7)	46.1 (37.5-54.6)	53
Asparagine	32.5 (32.3-32.6)	33.6 (33.0-34.1)	-
Asparatic Acid	138.1 (122.3-154)	120.8 (111.8-129.4)	150
Glutamine	181.1 (168.1-194.1)	153.8 (119.3-188.4)	-
Glutamic acid	155.1 (134.1-176.1)	176.5 (174.6-178.4)	170
Histidine	22.9 (22-23.9)	21.9 (20.1-23.7)	21
isoleucine	49.1 (47.5-50.7)	40.6 (39.6-41.7)	42
Leucine	36.1 (30.8-41.5)	38.8 (37.4-30.3)	60
Lysine	20.5 (18.2-22.8)	12.1 (7.9-16.4)	44
Phenylalanine	38.1 (36.6-39.7)	35.2 (32.9-37.6)	41
Proline	41.1 (40.3-41.9)	39.9 (39.6-40.2)	41
Serine	39.1 (37.4-40.8)	44.7 (40.4-49.1)	39
Threonine	21.8 (21-22.7)	25.1 (22.8-27.5)	35
Tyrosine	18.2 (17.9-18.5)	15 (13.6-16.4)	26
Valine	26. 4 (23.2-29.5)	19.9 (17.7-22.3)	50

Continued.

Table 2.14.*Continued.*

Wax bean metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	83.8 (79.8-87.8)	79.3 (70.9-87.7)	84
Arginine	26.1 (23.8-28.4)	19.4 (18.5-20.3)	-
Asparatic Acid	437.5 (421.6-453.5)	198.9 (175.6-222.2)	-
Glutamine	393.2 (363.3-423.2)	389.6 (331.6-447.5)	-
Glutamic acid	248.9 (242.3-255.4)	249.4 (241.5-257.3)	220
Glycine	12.5 (1.9-2.2)	19.3 (14.3-24.3)	-
Histidine	35.7 (11.1-60.2)	41.8 (40.8-42.9)	33
isoleucine	135.2 (78.8-191.7)	83.8 (81.8-85.7)	81
Leucine	193 (172.1-213.9)	138.4 (136.1-140.6)	120
Lysine	143 (129.1-157)	85.5 (82.2-88.7)	110
Methionine	22.4 (21.5-23.2)	15.6 (13.4-17.8)	28
Phenylalanine	14.3 (14.2-14.3)	14.1 (10.1-18.2)	57
Proline	2.9 (2.2-3.6)	8.3 (6.3-10.2)	-
Serine	300.7 (288-313.3)	≥105.1	170
Threonine	80.8 (66.1-95.6)	53.9 (48.3-59.6)	31
Tyrosine	69.3 (68-70.6)	59.8 (50.6-68.9)	47
Valine	48 (43.2-52.7)	58.0 (43.2-72.8)	100
Red beetroot metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	78.4 (77.1-79.8)	101.9 (81.0-122.0)	41
Arginine	34.6 (33.3-35.8)	39.3 (34.9-43.8)	32
Asparagine	53 (51.4-54.5)	56.4 (55.4-57.4)	-
Asparatic Acid	63.9 (62.3-65.5)	56.4 (49.4-63.4)	86
Glutamic acid	388 (384.9-391.1)	369.4 (363.5-375.2)	490
Glycine	32 (31.7-32.2)	32.1 (29.4-34.7)	30
Histidine	8.9 (8.2-9.6)	11.9 (9.3-14.5)	18
isoleucine	29.4 (28.2-30.7)	28.4 (21.9-35.0)	32
Leucine	25.0 (18.0-31.9)	33.0 (27.6-38.3)	35
Lysine	65.8 (60.3-71.4)	83.4 (82.3-84.5)	140
Phenylalanine	17.8 (17.4-18.1)	9.1 (7.1-11.1)	16
Proline	16.7 (15.6-17.8)	13.1 (10.2-16.0)	19
Serine	60.5 (60.3-60.7)	103.3 (64.7-141.9)	51
Threonine	23.8 (22.2-25.3)	26.9 (23.7-30.1)	30
Tryptophan	8.5 (8.3-8.7)	≤6.1	9
Tyrosine	17.6 (17-18.2)	16.9 (16.8-17.1)	14
Valine	24 (23.9-24.1)	29.6 (22.3-36.9)	43

Continued.

Table 2.14.*Continued.*

Cucumber metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	40.8 (40.1-41.5)	43.2 (37.9-48.3)	23
Arginine	35.6 (34.2-37.1)	≥70	28
Asparagine	31.1 (30.6-31.5)	35.5 (31.0-39.8)	-
Asparatic Acid	63.8 (59.6-68)	80.1 (72.7-87.6)	40
Glutamine	81.9 (214.7-349.1)	≥ 233.8	-
Glutamic acid	145.9 (141.7-150.2)	123.0 (120-127.1)	220
Glycine	25.3 (21.7-28.9)	36.2 (29.2-43.2)	-
Histidine	23.2 (17.9-28.6)	25.3 (23.7-26.9)	-
isoleucine	14.6 (24.5-24.7)	25.6 (20.4-30.9)	18
Leucine	17.2 (15.9-18.5)	22.3 (19.6-25.1)	28
Lysine	14.8 (13.7-15.9)	11.7 (10.3-13.1)	-
Methionine	7.7 (6.3-9.0)	8.2 (8.1-8.4)	-
Phenylalanine	23.9 (23.4-24.3)	23.2 (21.7-24.6)	17
Proline	14.2 (13-15.4)	8.9 (7.1-10.6)	13
Serine	37.2 (36.6-37.8)	25.5 (24.9-25.9)	25
Threonine	20.8 (20.7-20.9)	25.6 (25.4-25.8)	16
Tryptophan	4.1 (4.1-4.1)	7.6 (6.3-9.0)	5.6
Tyrosine	10.2 (9.9-10.4)	11.9 (11.1-12.7)	10
Valine	15.4 (13.3-17.5)	21.5 (18.7-24.3)	-
Swiss chard metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	103.9 (99.8-107.9)	135.7 (114.6-156.7)	-
Asparagine	108.6 (104.5-112.7)	112.1 (107.9-116.2)	-
Asparatic Acid	73.9 (69.3-78.6)	83.7 (82.6-84.9)	-
Glutamine	78.4 (77.2-79.6)	82.1 (82.1-82.1)	-
Glutamic acid	322.7 (298.1-347.3)	378.2 (358.3-398.1)	-
Glycine	37.4 (36.5-38.3)	70.1 (53.8-86.3)	-
Histidine	31.3 (29.8-32.7)	35.8 (34.6-37.0)	35
isoleucine	92 (87.7-96.3)	88.8 (82.3-95.4)	150
Leucine	120.7 (113.2-128.2)	118.1 (101.8-134.4)	130
Lysine	79.5 (72.6-86.3)	97.4 (93.5-101.4)	98
Phenylalanine	92.8 (88.4-97.2)	103.5 (97.8-109.2)	110
Proline	38.8 (32.8-44.7)	47.7 (38.7-56.7)	-
Serine	247.5 (241.7-253.3)	294.1 (225.7-362.6)	-
Threonine	53.9 (47.6-60.2)	63.1 (62.7-63.4)	84
Tyrosine	57.5 (53.6-61.4)	75.1 (60.9-89.2)	-
Valine	101.1 (100.01-102.2)	121.9 (102.0-141.8)	-

Continued.

Table 2.14.*Continued.*

Parsnip metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	65.3 (63.1-67.5)	72.4 (68.1-76.7)	81
Arginine	216.8 (213-220.7)	223.4 (217.0-229.9)	200
Asparagine	111 (103.7-118.4)	≥52.8	-
Asparatic Acid	188.8 (188.7-189)	67.3 (57.9-76.7)	230
Glutamine	212.7 (207.1-218.3)	218.9 (215.1-222.7)	-
Glutamic acid	196.2 (192.8-199.6)	193.4 (192.8-194.0)	200
Glycine	56.5 (53.6-59.4)	55.5 (55.2-55.7)	54
Histidine	24.9 (21.2-28.6)	20.5 (20.2-20.8)	34
isoleucine	37.4 (35-39.7)	37.5 (34.6-40.5)	71
Leucine	74.1 (68.4-79.9)	80.2 (86.3-74.1)	97
Lysine	168.4 (149.7-188.6)	123.0 (121.9-124.2)	91
Methionine	20.9 (20.5-21.2)	≤1.5	21
Phenylalanine	54.2 (53.9-54.5)	59.5 (56.7-62.4)	64
Proline	185.1 (173.2-197)	197.2 (182.0-213.5)	120
Serine	56.4 (56.4-56.5)	50.1 (46.6-53.6)	77
Threonine	41.6 (41.1-42.1)	38.5 (32.6-44.4)	64
Tyrosine	44 (43.3-44.7)	44.5 (42.8-46.1)	33
Valine	39.9 (38.1-41.6)	39.6 (35.5-43.8)	37.8
Onion metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	36.5 (34.7-38.4)	30.9 (28.4-33.4)	35
Arginine	228.2 (228.1-228.2)	≥ 70	210
Asparatic Acid	133 (122.5-143.5)	≥ 53.2	93
Glutamine	336.3 (294.5-378.1)	≥ 233.8	-
Glutamic acid	230.3 (214.8-245.9)	246 (233.7-258.3)	330
Glycine	61.4 (60.5-62.3)	45.5 (43.1-47.9)	-
Histidine	11.8 (10.2-13.5)	21.8 (19.3-24.3)	18
isoleucine	43.5 (40.9-46.1)	34.6 (30.3-38.8)	30
Leucine	63 (62.7-63.2)	87.5 (86.1-88.9)	53
Lysine	60 (58.6-61.4)	20.8 (19.9-31.7)	50
Methionine	24 (22.3-25.6)	≤15	12
Ornithine	8.2 (8.2-8.2)	9.6 (7.8-11.4)	-
Phenylalanine	48.7 (48.6-48.9)	54.3 (49.8-58.8)	35
Proline	18.2 (17.6-18.8)	13.1 (10.2-16.0)	21
Serine	41.5 (40.3-42.6)	31.6 (28.8-34.3)	28
Threonine	37.8 (37.2-38.3)	46.4 (43.1-49.7)	-
Tryptophan	36.3 (35.5-37.1)	35.5 (33.5-37.5)	-
Tyrosine	63.5(61-66)	64.0 (60.4-67.6)	-
Valine	42.1(38.7-45.5)	43.3 (42.1-44.5)	38

Continued.

Table 2.14.*Continued.*

Red bell pepper metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	63.7(60.1-67.3)	69.8 (69.7-69.9)	50
Arginine	61.1(54.9-67.2)	44.3 (42.4-46.2)	50
Asparagine	172.2(144.6-199.8)	≥52.8	-
Asparatic Acid	120.5(102.3-138.7)	≥53.2	170
Glutamine	437.9 (434.2-441.7)	≥ 233.8	380
Glutamic acid	135.6 (124.8-146.5)	80.4 (72.9-87.9)	180
Glycine	29.6 (27.5-31.7)	42.7 (41.3-44.1)	44
Histidine	22.5 (21.4-23.6)	27.4 (24.7-30.1)	21
isoleucine	33.7 (29.8-37.5)	45.4 (44.8-46.0)	40
Leucine	57.3(54.9-59.6)	32.4 (30.5-34.3)	52
Lysine	34.4(32.7-36.1)	34.8 (34.2-35.3)	60
Methionine	12.5(11.7-13.2)	7.3 (6.7-8.0)	10
Phenylalanine	33.9(33.7-34.1)	42.0 (38.9-45.0)	40
Proline	43(42.1-43.8)	46 (42.7-49.3)	33
Serine	130.7(119.1-142.2)	≥ 105.1	62
Threonine	124.4(98.6-150.1)	≥ 119.1	42
Tryptophan	10.5(9.5-11.4)	15.2 (12.2-18.2)	7
Tyrosine	22.7(19.6-25.8)	21.6 (13.8-29.4)	19
Valine	96.2(88.3-104.1)	75.6 (63.7-87.4)	60
Carrot metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	83.1 (78.1-88)	71.6 (68.3-74.9)	77
Arginine	46.4 (44.3-48.6)	49.9 (49.0-50.9)	-
Asparagine	100.3 (89.5-111.1)	≥52.8	-
Asparatic Acid	133.4 (130.5-136.3)	≥53.2	-
Glutamine	462.4 (455.9-469)	352.5 (341.5-363.4)	-
Glutamic acid	164.7 (164.1-165.3)	255.1 (248.2-261.9)	180
Glycine	14.4 (14-14.9)	15.2 (10.1-20.4)	27
Histidine	20.35 (17.8-21.9)	19.4 (15.2-23.7)	-
isoleucine	41 (38.3-43.7)	42.8 (40.5-45.02)	29
Leucine	37.6 (32.5-42.8)	45.7 (30.2-61.1)	38
Lysine	33.8 (33.1-34.6)	25.9 (24.1-27.6)	35
Methionine	13.3 (11.8-14.7)	8.6 (8.3-8.9)	9
Ornithine	8.8 (7.6-10)	≤1.3	-
Phenylalanine	43.3 (42.2-44.4)	37.6 (32.9-42.2)	26
Proline	38.7 (37.3-40.1)	31.8 (28.06-35.5)	
Serine	31.8 (29.1-34.4)	37.5 (36.7-38.4)	35
Threonine	30.6 (30.4-30.8)	35.1 (32.8-37.4)	26
Tryptophan	11.3 (10.6-11.9)	25.0 (12.2-37.8)	9

Continued.

Table 2.14.*Continued.*

Carrot metabolites	NMR	DFI/LC-MS/MS	Literature values
Tyrosine	17.7 (17.2-18.1)	19.6 (18.4-20.8)	14
Valine	24.3 (21.2-27.3)	59.2 (53.9-64.5)	-
White cabbage metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	54.8 (54.3-55.3)	54.82 (54.0-55.6)	61
Arginine	45.9 (36.8-55)	60.1 (57.9-62.3)	67
Asparagine	108.4 (95.3-121.5)	≥52.8	-
Asparatic Acid	143.6 (111.4-175.9)	≥ 53.2	-
Glutamine	118.8 (99.4-138.3)	≥ 233.8	-
Glutamic acid	345.2 (265.8-424.5)	≥300	-
Glycine	20 (17.1-22.9)	17.8 (17.1-18.4)	27
Histidine	46.5 (45.7-47.3)	50.9 (46.8-55.0)	-
isoleucine	36 (30.6-41.5)	30.6 (29.7-31.5)	27
Leucine	40.3 (32.8-47.8)	40.6 (38.7-42.6)	35
Lysine	19.1 (15.3-22.9)	27.8 (26.0-29.7)	35
Methionine	9.9 (9.7-10.1)	≤15	9
Phenylalanine	29 (22.6-35.4)	20.6 (19.5-21.7)	22
Proline	65 (43.2-86.8)	39.3 (38.8-39.7)	57
Serine	68.3 (52.9-83.7)	92.6 (79.9-105.3)	51
Threonine	36.5 (29.7-43.2)	23.4 (21.6-25.1)	24
Tryptophan	12.2 (10.7-12.8)	12.7 (10.8-14.5)	9
Tyrosine	9.5 (9-9.9)	7.2 (6.2-8.2)	12
Valine	42.5 (42.9-42.9)	58.1 (56.6-59.7)	45
Dill metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	168.1 (166.4-169.7)	178.3 (118.5-239.1)	227
Arginine	318 (287.2-348.9)	523.5 (517.9-529.1)	142
Asparagine	99 (98.7-99.3)	≥52.8	-
Asparatic Acid	436.8 (353.9-519.7)	≥53.2	343
Glutamine	176.2 (164.3-188.1)	≥ 233.8	-
Glutamic acid	185.6 (179.2-192)	155.0 (133.9-176.7)	290
Glycine	120 (111.2-128.8)	146.2 (102.5-190.0)	169
Histidine	67.1 (64.9-69.3)	55.0 (51.1-59.0)	71
isoleucine	204.3 (193.7-214.8)	118.5 (116.5-120.5)	195
Leucine	90.7 (81.3-100.1)	79.1 (57.0-101.2)	159
Lysine	292.2 (273.4-311.1)	364.1 (343.2-385.0)	246
Methionine	12 (6.8-17.2)	15.5 (14.2-16.9)	11

Continued.

Table 2.14. Continued.

Dill metabolites	NMR	DFI/LC-MS/MS	Literature values
Phenylalanine	40.7 (37-44.3)	46.8 (39.3-54.3)	65
Proline	151.6 (141.2-162)	≥ 115.1	248
Serine	209.9 (181.8-238.1)	≥ 105.1	158
Threonine	70.6 (62.4-78.9)	52.8 (41.9-63.5)	68
Tryptophan	15.6 (14.7-16.6)	15.9 (15.6-16.3)	14
Tyrosine	88.8 (78.9-99.8)	81.4 (76.0-86.9)	96
Valine	254.3 (233.6-275)	171.1 (162.6-179.7)	154
Orange bell pepper	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	131.3 (129.7-132.9)	137.6 (131.8-143.3)	-
Arginine	41.1 (39.6-42.7)	67.6 (64.7-70.4)	-
Asparagine	246.1 (241.6-250.6)	≥52.8	-
Asparatic Acid	123.8 (118.2-129.3)	≥53.2	-
Glutamine	215.9 (214.6-217.2)	≥ 23.8	-
Glutamic acid	172.7 (148.2-197.2)	70.4 (64.4-76.4)	-
Glycine	15.1 (14.7-15.5)	12.4 (11.7-13.1)	-
Histidine	19.9 (19.2-20.7)	25.6 (25.5-25.7)	-
isoleucine	16.4 (16.1-16.6)	27.3 (25.6 -29.0)	-
Leucine	36.9 (34.7-39.1)	30.3 (28.1-32.5)	-
Lysine	38.15 (36.4-39.9)	40.5 (40.0-40.9)	-
Methionine	7.5 (5.8-9.2)	7.4 (7.3-7.6)	-
Phenylalanine	20.8 (20.2-21.4)	27.4 (26.3-28.5)	-
Proline	20.6 (18.8-22.4)	13.1 (9.4-16.8)	-
Serine	54.6 (53.8-55.5)	52.9 (52.1-53.7)	-
Threonine	124.8 (123-126.7)	162.7 (151.6-173.0)	-
Tryptophan	5.9 (5.6-6.2)	≤ 6.1	-
Tyrosine	10.1 (9.6-10.6)	12.2 (11.8-12.5)	-
Valine	65.1 (63.3-67)	89.7 (78.5-100.8)	-
Turnip metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	29.0 (27.8-30.2)	29.3 (28.9-29.7)	-
Arginine	17.3 (15.4-19.1)	13.7 (0.0-13.7)	10
Asparagine	14.6 (13.4-15.7)	≥52.8	-
Asparatic Acid	26.6 (26.4-26.9)	≥53.2	35
Glutamine	118.1 (113.7-122.5)	102.2 (100.1-104.3)	100
Glutamic acid	50.1 (47.7-52.6)	51.6 (50.3-52.8)	56
Glycine	101.9 (93.7-110.2)	89.1 (88.2-91.0)	100
Histidine	14.3 (13.9-14.7)	6.1 (6.0-6.2)	5
isoleucine	27.6 (27.2-28)	23.4 (17.4-29.4)	15
Leucine	10.3 (10.2-10.4)	17.7 (15.9-19.6)	25
Lysine	36.9 (33.7-40.1)	11.4 (10.9-11.9)	12
Proline	23.4 (22.1-24.7)	20.2 (20.1-20.3)	21

Continued.

Table 2.14.*Continued.*

Turnip metabolites	NMR	DFI/LC-MS/MS	Literature values
Phenylalanine	12.5 (10.6-14.5)	11.5 (11.5-11.6)	12
Serine	20.2 (17.6-22.9)	14.4 (14.3-14.5)	20
Threonine	19.9 (19.7-20.1)	16.6 (16.1-17.0)	17
Tryptophan	8.7 (7.9-9.5)	8.2 (6.5-10.0)	8
Tyrosine	9.5 (8.7-10.3)	6.8 (5.9-7.6)	9
Valine	14.4 (13.1-15.6)	14.2 (12.7-15.7)	15
Spinach metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	109.1 (107.7-110.4)	90.2 (76.4-104.0)	110
Arginine	165.3 (163.2-167.4)	≥ 70	140
Asparagine	201.8 (198.4-205.2)	≥ 52.8	-
Asparatic Acid	250.7 (230.5-270.9)	≥ 53.2	230
Glutamine	424.0 (402.7-445.3)	405.1 (399.7-410.4)	-
Glutamic acid	163.6 (158.6-168.6)	173.4 (164.9-181.8)	290
Glycine	89.9 (87.4-92.5)	45.7 (42.7-48.8)	110
Histidine	58.05 (57.1-59.0)	50.2 (45.1-55.3)	46
isoleucine	73.2 (72.9-73.5)	83.7 (72.4-95.1)	84
Leucine	122.7 (121.7-123.8)	115.5 (102.6-128.5)	150
Lysine	130 (122.7-148.9)	87.9 (84.0-91.7)	120
Phenylalanine	85.9 (83.5-88.3)	68.3 (63.9-72.8)	120
Proline	120.5 (111.1-130.0)	126.7 (111.2-142.2)	84
Serine	94.5 (92.7-96.3)	74.7 (60.2-89.1)	100
Threonine	60 (59.1-60.9)	48.1 (46.4-49.8)	92
Tryptophan	44.7 (40.8-48.7)	49.3 (43.3-55.4)	42
Tyrosine	92.9 (91.2-94.7)	79.7 (69.2-90.1)	63
Valine	107.9 (101.8-113.9)	114.1 (112.4-115.9)	120
Sunburst squash	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	59.6 (57.5-61.7)	69.6 (66.2-72.9)	71
Arginine	51.4 (50.5-52.3)	55.7 (52.9-58.6)	58
Asparagine	161.3 (158.4-164.3)	≥52.8	-
Asparatic Acid	134.8 (122.9-146.8)	≥53.2	160
Glutamine	258.6 (247.2-269.9)	≥ 233.8	-
Glutamic acid	164.6 (158.4-170.7)	173.5 (170.2-176.9)	140
Glycine	58.8 (53.4-64.3)	43.8 (41.8-45.7)	51
Histidine	70.8 (67.8-73.9)	109.1 (103.8-114.2)	-
isoleucine	45.9 (40.4-51.3)	69.4 (60.4-78.4)	49

Continued.

Table 2.14.*Continued.*

Sunburst squash metabolites	NMR	DFI/LC-MS/MS	Literature values
Leucine	72.3 (69.1-75.6)	74.5 (71.6-77.4)	80
Lysine	74.8 (72.1-77.5)	80.2 (79.4-81.0)	-
Methionine	20.1 (18.7-21.5)	27.8 (26.5-29.2)	20
Phenylalanine	40.6 (38.7-42.5)	59.9 (42.5-77.3)	47
Proline	63.4 (45.8-81)	59.9 (42.5-77.3)	42
Serine	78 (68.2-87.8)	73.5 (73.3-73.8)	56
Threonine	58.9 (58.6-59.2)	46.3 (42.9-49.8)	-
Tryptophan	10.8 (9.9-11.8)	30.8 (30.0-31.6)	13
Tyrosine	28.8 (27.9-29.8)	73.1 (52.0-94.2)	36
Valine	75.4 (69.4-81.3)	51.14 (42.5-59.8)	60
Cauliflower metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	170.1 (164.2-175.9)	124.5 (123.6-125.4)	180
Arginine	50.3 (49.8-50.9)	≥ 70	91
Asparagine	175.2 (159.6-190.9)	≥52.8	-
Asparatic Acid	186.2 (180.4-191.9)	≥53.2	-
Glutamine	235.2 (213-257.3)	≥ 233.8	-
Glutamic acid	116.8 (115.3-118.2)	≥ 300	260
Glycine	106.8 (100.3-113.4)	199.1 (197.9-200.2)	84
Histidine	88.6 (87.7-89.5)	122.5 (116.8-128.1)	42
isoleucine	64.3 (63.8-64.7)	60.3 (51.4-69.2)	84
Leucine	38.6 (33.3-43.9)	28.2 (25.9-30.4)	130
Lysine	95.8 (85.2-106.3)	30.4 (30.1-30.7)	110
Methionine	22.1 (20.4-23.7)	25.7 (25.6-25.9)	29
Ornithine	10.5 (9.1-11.8)	≤1.3	-
Phenylalanine	58.6 (54.2-62.9)	47.4 (45.7-49.1)	80
Proline	84.5 (84.3-84.7)	93.6 (84.7-102.4)	100
Serine	167.8 (165.1-170.4)	231.1 (228.5-233.7)	120
Threonine	91.8 (86.4-97.2)	75.5 (52.7-98.4)	80
Tryptophan	22.5 (21.3-23.8)	21.6 (18.6-24.7)	27
Tyrosine	27 (24.2-29.8)	16.9 (15.5-18.4)	49
Valine	128.9 (124.1-133.7)	134.9 (133.9-136.0)	140
Japanese pumpkin	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	17.8 (16-19.5)	16.9 (15.8-18.0)	12
Arginine	106.1 (99.1-112.9)	≥ 70	32
Asparagine	46 (41.3-50.7)	51.7 (47.2-56.3)	-
Asparatic Acid	131.2 (118.7-143.7)	≥ 53.2	120
Glutamine	481.4 (405.1-557.8)	382.8 (327.9-437.5)	-

Continued.

Table 2.14.*Continued.*

Japanese pumpkin	NMR	DFI/LC-MS/MS	Literature values
Glutamic acid	93.8 (81.3-106.2)	95.6 (93.5-97.68)	100
Glycine	15.2 (13.5-17)	19.5 (19.4-19.7)	15
Histidine	4.1 (3.3-4.9)	3.6 (2.7-4.5)	7
isoleucine	28.9 (24.9-33)	23.7 (22.4-24.9)	21
Leucine	25.6 (25.3-26)	21.5 (17.5-25.4)	24
Lysine	12.8 (11.1-14.5)	7.2 (4.3-10.1)	19
Methionine	5.9 (5.3-6.4)	6.8 (6.2-7.4)	7
Phenylalanine	233.1 (197.3-268.8)	209.6 (199.5-219.7)	150
Proline	11.8 (11.1-12.7)	9.8 (9.7-10.0)	12
Serine	30.5 (29.4-31.5)	36.4 (35.9-36.8)	37
Threonine	10 (9.8-10.3)	13.2 (11.6-14.9)	11
Tryptophan	9.8 (9.3-10.2)	10.2 (9.0-11.4)	9
Tyrosine	38.9 (36.1-41.6)	37.2 (31.9-42.4)	12
Valine	16.7 (16.1-17.2)	7.2 (6.5-7.8)	22
Lettuce metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	46.8 (44.9-48.7)	43.6 (40.2-47.1)	55
Arginine	41 (38.8-43.2)	39.5 (37.5-41.5)	53
Asparagine	434.1 (403.5-464.8)	≥ 52.8	-
Asparatic Acid	146.5 (144.1-149)	139.9 (136.7-143.1)	140
Glutamine	417.7 (392.2-443.2)	≥ 233.8	-
Glutamic acid	116.2 (110.3-122.2)	113.7 (109.6-117.8)	180
Histidine	21.05 (19.8-22.3)	14.8 (13.8-15.8)	-
isoleucine	43.2 (42.4-44.1)	37.1 (31.1-43.1)	45
Leucine	47.1 (44.5-49.7)	28.7 (27.4-30.0)	77
Lysine	59.6 (54.4-64.8)	56.1 (42.9-69.4)	63
Phenylalanine	47.7 (44.6-50.9)	46.2 (45.5-46.9)	65
Proline	23.75 (22.9-24.6)	13.2 (11.9-14.5)	-
Serine	48.8 (42.6-55.0)	40.3 (31.1-49.5)	-
Threonine	41.8 (36.2-47.4)	31.3 (28.8-33.7)	43
Tryptophan	9.9 (9.1-10.7)	10.7 (9.1-12.3)	10
Tyrosine	25.1 (21.7-28.5)	18.9 (15.9-22.1)	26
Valine	34.8 (34.2-35.4)	36.5 (32.5-40.56)	55
Tomato metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	30.4 (28.9-31.9)	36.8 (33.4-40.3)	19
Asparagine	155 (153.8-156.1)	114.2 (100.1-128.3)	-
Asparatic Acid	188.4 (185.7-191)	137.9 (131.6-144.2)	82
Glutamine	492.8 (468.7-516.9)	≥ 233.8	-

Continued.

Table 2.14.*Continued.*

Tomato metabolites	NMR	DFI/LC-MS/MS	Literature values
Glutamic acid	447.5 (413.7-481.3)	86.7 (78.7-94.7)	200
Glycine	30.4 (28.7-32.1)	28.3 (27.9-28.8)	21
Histidine	16.6 (14.9-18.3)	14.8 (14.3-15.3)	12
isoleucine	16.1 (15.6-16.5)	15.1 (11.0-19.2)	34
Leucine	23.7 (21.1-26.3)	23.4 (18.9-27.8)	29
Lysine	51 (44.2-57.8)	99.9 (77.3-122.7)	34
Phenylalanine	50.9 (50-51.8)	33.7 (31.7-35.6)	20
Proline	38.7 (37.2-40.1)	46.2 (40.0-52.4)	23
Serine	18.8 (17.8-19.9)	29.9 (29.4-30.6)	26
Threonine	53.8 (52.1-55.4)	23.3 (22.8-23.7)	20
Tryptophan	17.6(16.2-18.9)	7.3(6.9-7.7)	7
Tyrosine	23.7(22.7-24.7)	27.2 (26.3-28.1)	27
Valine	22.1 (20.7-23.5)	12.0 (11.2-12.8)	21
Italian red pepper	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	58.5 (60-61.4)	60.4 (58.9-61.9)	-
Arginine	34.2 (35.7-37.1)	34.4 (32.9-35.9)	-
Asparagine	88.5 (78.5-83.5)	80.8 (79-6-82.1)	-
Asparatic Acid	189.4 (212.6-235.7)	150.3 (149.3-151.3)	-
Glutamine	148.7 (143.9-146.3)	136.4 (131.8-140.9)	-
Glutamic acid	85.1 (79.2-82.2)	55.4 (49.3-61.6)	-
Glycine	48.1 (55.3-62.5)	67.7 (62.6-72.9)	-
Histidine	12.5 (11.7-13.3)	14.2 (2.9-25.5)	-
isoleucine	39.5 (36.1-37.8)	39.9 (37.8-42.2)	-
Leucine	33.8 (34.6-35.3)	29.4 (28.3-30.5)	-
Lysine	36.4 (29.5-33)	28.4 (27.2-29.6)	-
Methionine	10 (10.3-10.5)	≤15	-
Ornithine	8.2 (9.3-10.4)	≤13	-
Phenylalanine	33.3 (36.3-39.3)	50.9 (43.7-58.1)	-
Proline	49.1 (48.1-50.2)	42.5 (40.7-44.3)	-
Serine	174.8 (175.7-176.6)	180.5 (180.5-180.5)	-
Threonine	126.9 (127-127.1)	122.4 (117.8-127.0)	-
Tryptophan	13 (12.6-13.3)	14.9 (14.4-15.4)	-
Tyrosine	13.8 (14.4-15)	12.9 (12.7-13.1)	-
Valine	74 (76-78)	66.7 (59.0-74.5)	-

Continued.

Table 2.14.*Continued.*

Nanking cherry metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	12.1 (11.2-13)	14.0 (13.4-14.6)	-
Arginine	37.4 (37.2-37.7)	35.7 (35.2-36.3)	-
Asparagine	143.6 (125.5-161.7)	≥52.8	-
Asparatic Acid	938.5 (866.6-1010.4)	≥53.2	-
Glutamine	33.5 (32.7-34.2)	56.2(53.7-58.7)	-
Glutamic acid	31.2 (28.3-34.2)	29.9 (28.1-31.8)	-
Glycine	8.4 (8.1-8.7)	5.8 (3.6-8.1)	-
Leucine	7.1 (5.5-8.6)	7.3 (5.3-9.3)	-
Lysine	26.5 (25.7-27.3)	35.4 (33.4-36.4)	-
Methionine	12.9 (11.7-14.1)	≤15	-
Ornithine	10.1 (9.2-11.1)	≤13	-
Phenylalanine	17.2 (16.5-18)	21.1 (19.9-22.2)	-
Proline	34.2 (33-35.5)	35.2 (30.9-39.4)	-
Serine	62.6 (59.7-65.4)	52.9 (49.3-56.4)	-
Threonine	32.7 (32-33.4)	45.8 (44.2-47.4)	-
Tryptophan	7.8 (7.4-8.3)	≤6	-
Tyrosine	20.9 (19.3-22.6)	19 (18.1-19.9)	-
Valine	17.8 (17.1-18.5)	19.8 (18.8-20.9)	-
Raspberry metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	41.8 (28.7-54.9)	39.2 (38.7-39.6)	-
Arginine	17.9 (17.7-18.2)	15.9 (13.0-18.8)	-
Asparagine	35.6 (35.1-36.2)	73.5 (64.6-82.4)	-
Asparatic Acid	95.2 (94.9-95.5)	62.1 (59.8-64.4)	-
Glutamine	30.7 (30-31.3)	106.3 (102.4-110.3)	-
Glutamic acid	24.5 (23.4-25.6)	27.9 (27.5-28.4)	-
Glycine	12.8 (12.3-13.3)	13.5 (12.0-15.0)	-
Isoleucine	13.7 (11.9-15.5)	10.7 (10.4-11.1)	-
Leucine	7.4 (6.7-8.2)	12.1 (11.7-12.5)	-
Lysine	6.7 (6.7-6.7)	3.1 (3.0-3.2)	-
Methionine	5.2 (3.1-7.3)	11.3 (11.1-11.6)	-
Ornithine	11.3 (8.7-13.9)	14.5 (14.2-14.8)	-
Phenylalanine	14.9 (12.7-17)	25.7 (25.3-26.1)	-
Proline	19.2 (16.2-22.2)	14.7 (13.5-16.0)	-
Serine	34.2 (31.9-36.4)	44.0 (31.8-56.3)	-
Threonine	13.4 (9.4-17.4)	23.4 (23.3-23.6)	-

Continued.

Table 2.14.*Continued.*

Raspberry metabolites	NMR	DFI/LC-MS/MS	Literature values
Tryptophan	11.6 (11-12.2)	9.1 (8.9-9.3)	-
Tyrosine	25.2 (22.9-27.6)	23(22.7-23.3)	-
Valine	11.1 (9.3-12.8)	10.5 (8.5-12.5)	-
Potato Metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	78.2 (72.2-84.3)	76.5 (66.0-86.9)	-
Arginine	253.9 (253.8-254.1)	≥70	180
Asparagine	187 (182.1-191.9)	≥ 52.8	-
Asparatic Acid	403.4 (396.5-410.3)	≥ 53.2	410
Glutamine	620.2 (576.1-664.3)	788.7 (626.0-951.5)	-
Glutamic acid	267.1(260-274.2)	161.1 (136.6-185.6)	260
Glycine	72.8 (71.5-74)	116.2 (99.4-133.2)	120
Histidine	70.8 (68.2-73.4)	61.9 (49.8-73.9)	70
Isoleucine	72.8 (71.5-74)	107.7 (97.1-118.2)	71
Leucine	85.6 (84.4-86.8)	55.0 (49.2-60.8)	110
Lysine	220.8 (218.7-222.9)	181.4 (171.3-191.5)	256
Methionine	24.15 (21.9-26.4)	17.2 (15.4-18.9)	29
Phenylalanine	145.1 (144.9-145.3)	135.4 (116.9-153.9)	77
Proline	91.6 (90.5-92.7)	102.9 (101.7-104.0)	68
Serine	103.1 (98.3-107.9)	107.2 (100.1-114.4)	68
Threonine	80.7 (79.5-82)	78.7 (76.5-80.9)	65
Tryptophan	35.4 (35-35.9)	43.4 (39.4-47.4)	29
Tyrosine	121.3 (98.4-144.3)	124.6 (124.5-124.6)	-
Valine	205 (204.8-205.1)	245.0 (233.9-256.1)	110
Green bean metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	103.7 (101.7-105.7)	121.6 (111.9-131.4)	94
Arginine	35 (31.5-38.6)	32.7 (31.7-33.7)	70
Asparagine	45.7 (42.4-49)	≥ 52	-
Asparatic Acid	264.8 (264.1-265.4)	≥ 53.2	260
Glutamine	220.8 (208.1-233.4)	≥ 233.8	-
Glutamic acid	134 (122.4-145.6)	74.7 (73.4-75.9)	200
Glycine	20.2 (19.1-21.4)	25.6 (19.9-31.4)	64
isoleucine	33.9 (33.2-34.6)	36.7 (35.0-38.4)	73
Leucine	38 (34.6-41.5)	36.6 (34.1-39.1)	110
Lysine	123.4 (114.8-132)	113.2 (111.3-115.1)	120
Methionine	14.8 (11.5-18.1)	19.2 (18.8-19.6)	28

Continued.

Table 2.14.*Continued.*

Green bean metabolites	NMR	DFI/LC-MS/MS	Literature values
Ornithine	8.7 (7.8-9.7)	≤1.3	-
Phenylalanine	40.1 (36.3-43.9)	16.5 (0.0-33.0)	52
Proline	14.1 (12.9-15.2)	16.7 (15.2-18.1)	58
Serine	136 (135-136.9)	≥105.1	130
Threonine	84.9 (84.6-85.2)	116.5 (110.1-122.9)	79
Tyrosine	60 (59.8-60.2)	63.7 (53.4-73.9)	40
Valine	69.6 (65-74.2)	80.4 (64.8-96.1)	94
Crab apple metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	17.4 (17.1-17.8)	19.8 (19.8-19.9)	-
Arginine	35.3 (31.2-39.5)	43.5 (42.3-44.8)	-
Asparagine	116 (109.7-122.2)	≥ 52.8	-
Asparatic Acid	51.1 (49.5-52.7)	62.5 (60.3-64.7)	-
Glutamine	271.6 (255.1-288)	292.0 (291.2-292.8)	-
Glutamic acid	61.1 (58.4-63.7)	55.7 (55.5-55.8)	-
Histidine	22.7 (20.1-25.2)	22.5 (22.5-22.6)	-
Isoleucine	22.2 (20.9-23.5)	28.0 (27.9-28.0)	-
Leucine	23.7 (22.4-25)	201.0 (20.9-21.02)	-
Lysine	40.6 (39.2-42)	38.9 (38.8-39.1)	-
Phenylalanine	33.8 (28.2-39.3)	22.0 (21.9-22.1)	-
Proline	31.2 (29.8-32.7)	31.1 (31.0-31.2)	-
Serine	32.1 (30.7-33.5)	28 (27.9-28.1)	-
Threonine	20.4 (20.4-20.5)	24.3 (24.2-24.3)	-
Tryptophan	10.6 (10.3-10.8)	11.7 (11.7-11.7)	-
Tyrosine	27.9 (26.1-29.8)	23.5 (23.2-23.9)	-
Valine	68.1 (66.3-69.9)	70.2 (70.0-70.4)	-
Saskatoon berry	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	70.7 (67.3-74.2)	93.4 (91.7-95.2)	-
Arginine	35.1 (32.4-37.7)	33.1 (32.8-33.3)	-
Asparagine	52.7 (47.2-58.3)	≥ 52.8	-
Asparatic Acid	34.3 (28.5-40)	21.4 (13.5-29.4)	-
Glutamine	46.1 (38.4-53.8)	59.9 (56.5-63.3)	-
Glutamic acid	143.6 (137.4-149.8)	161.4 (154.3-168.5)	-
Glycine	28.6 (28.5-28.8)	22.6 (18.9-26.4)	-
Histidine	10 (9.7-10.3)	12.4 (10.1-14.8)	-
Leucine	34.8 (32.2-37.5)	35.6 (35.5-35.8)	-

Continued.

Table 2.14.*Continued.*

Saskatoon berry	NMR	DFI/LC-MS/MS	Literature values
Lysine	23.5 (19-27.9)	17.0 (15.5-18.6)	-
Methionine	14.8 (14-15.6)	12.4 (12.1-12.7)	-
Ornithine	73.4 (68.1-78.8)	69.8 (69.2-70.4)	-
Phenylalanine	22 (20.6-23.4)	20.0 (18.3-21.8)	-
Proline	13.2 (12.54-13.9)	23.8 (22.0-25.5)	-
Serine	23.2 (22.9-23.5)	21.3 (14.2-28.4)	-
Threonine	10.1 (9.2-11.1)	13.6 (13.0-14.2)	-
Tryptophan	8.5 (7.1-9.8)	≤6.1	-
Tyrosine	12.7 (11.1-14.3)	9.8 (8.7-10.8)	-
Valine	30.9 (27.4-34.5)	42.4 (36.4-48.3)	-
Broccoli metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	31.3 (30.4-32.3)	64.8 (53.1-76.5)	-
Arginine	237.5 (219.7-255.4)	≥ 73.6	330
Asparagine	238.7 (217.6-259.9)	≥ 52.8	-
Asparatic Acid	319.6 (304.7-334.6)	≥ 53.2	-
Glutamine	467.3 (466-468.6)	≥ 233.8	-
Glycine	175.2 (157.7-192.7)	133.3 (133.1-133.5)	100
Histidine	65.7 (59.5-71.9)	70.1 (69.7-70.5)	120
Isoleucine	193.1 (165.8-220.4)	136.3 (133.6-138.9)	200
Leucine	167.2 (138.7-195.8)	123.6 (121.5-125.7)	280
Lysine	209.3 (156.7-261.9)	149.0 (106.8-191.2)	270
Methionine	151.4 (128.9-173.8)	151.6 (117.2-186.0)	76
Phenylalanine	281.7 (252.6-310.8)	221.3 (210.6-231.9)	200
Proline	93.4 (78.1-108.7)	45.0 (40.2-49.9)	-
Serine	136.7 (119.5-153.8)	≥ 105.1	-
Threonine	258.4 (219-297.9)	272.9 (266.5-279.5)	230
Tryptophan	54.5 (52.3-56.7)	49.0 (43.4-54.6)	59
Tyrosine	20.9 (17.8-24.1)	29.3 (28.9-29.6)	-
Valine	179.1 (170.3-188.0)	129.7 (121.4-138.1)	250

Table 2.15. Cross checking NMR and HPLC-UV assays for Vitamin C.

Food samples	NMR	HPLC	Literature values
Yellow zucchini	17.05 (16.3-17.8)	13.5 (11.6-15.4)	18
Yellow bell pepper	184.3 (170.1-198.6)	56.1 (52.9-59.25)	-
Green bell pepper	67 (68.3-70.2)	65.7 (53.4-77.9)	-
Green zucchini	14.8 (13.9-15.8)	12.8 (12.5-13.0)	17.9
Garlic	26.8 (26.4-27.3)	26.8 (25.9-27.7)	31
Eggplant	2.9 (2.8-3.1)	2.3 (2.1-2.5)	2.2
Wax bean	29.7 (27.6-31.9)	32.3 (6.8-57.8)	21
Red beetroot	5.1 (4.8-5.4)	5.5 (1.5-9.5)	4.9
Cucumber	5.8 (4.9-6.7)	7.5 (4.5-10.6)	2.8
Swiss chard	37.6 (34.9-40.2)	38.2 (25.9-50.4)	30
Red bell pepper	105 (97.8-112.2)	51.2 (50.6-51.7)	127.7
Carrot	7.0 (6.6-7.4)	7.7 (7.2-8.2)	5.9
White cabbage	28.1 (27.2-29.1)	7.4 (6.0-8.8)	36
Dill	31.1 (27.9-34.4)	24. (23.6-24.7)	21
Orange bell pepper	94.2 (88.9-99.6)	50.9 (49.16-52.7)	-
Spinach	27.3 (26.9-27.7)	28.5 (27.3-29.7)	28.1
Sunburst squash	19.4 (19.3-19.7)	22.7 (18.9-26.5)	-
Cauliflower	39.6 (38.9-40.3)	18.1 (17.1-19.1)	48.2
Japanese pumpkin	12.8 (12.7-13.)	11.8 (11.2-12.4)	9
Tomato	18.55 (17.8-19.3)	25.6 (24.5-26.8)	13.7
Italian red pepper	49.05 (47.8-50.3)	45.4 (45.1-45.73)	-
Potato	20.8 (19.4-22.3)	19.9 (17.5-22.5)	26.4
Nanking cherry	13 (12.7-13.3)	8.1 (7.7-8.6)	
Green bean	16.9 (16.1-17.7)	16.1 (15.7-16.5)	-
Saskatoon berry	26.85 (23.8-29.9)	29.2 (28.0-30.3)	-
Raspberry	34.6 (34.2-35.1)	37.4 (36.2-38.5)	26.2
Crab apple	9.4 (8.7-10.1)	9.5 (9.3-9.6)	-
Broccoli	82.6 (72.1-93.2)	66.6 (63.3-69.8)	-

Chapter 3. The Application of Multi-platform Metabolomics Methods for the Characterization of the Chemical Composition of Common Cereal Grains

3.1 Introduction

Cereal grains are calorie rich, nutrient dense food sources. Their high yield and low cost, combined with their broad climate/soil compatibility and multiple uses (for carbohydrates, oils, fibre, etc.) have made cereal grains the main energy source in the human diet (Fao 2012). Cereal grains are not only important for caloric purposes, they have a number of important health benefits as well. For instance, the USDA's Food Guide Pyramid suggests at least 3 servings a day of whole cereal grains are needed for healthy living. Epidemiological studies have found that the high intake of whole grains is associated with a reduced risk of cardiovascular disease, obesity, type II diabetes, gastrointestinal, and hormone-related cancers (Ross et al., 2004; Truswell, 2006).Many of these benefits arise from the unique phytochemicals found in cereals and cereal grains. Some of these include phenolics, carotenoids, vitamin E-related compounds, lignans, β-glucan, and inulin (Liu, 2007). Unfortunately, the precise chemical composition of many cereal grains is not well known and standard food composition tables only provide data on a few dozen highly abundant chemical constituents (Ragaee et al., 2006; Zieliński & Kozłowska, 2000). They rarely provide much data on the many of the lower abundance chemicals (organic acids, esters, biogenic amines, vitamins, trace metals or fatty acids) that are responsible for the flavour, aroma, taste, colour and many of the key health benefits of cereal grains.Given the growing interest among food producers, consumers, nutritionists, and dieticians on the micronutrient content of many foods (including cereal grains and oils), there is a clear unmet need for the development of

more comprehensive food composition information and more in-depth food characterization techniques.

Over the past two decades, a number of efforts have been made to remedy this situation (Cevallos-Cevallosa et al., 2009; Herrero et al., 2011). Some of these include the development of improved analytical technologies and specially targeted assays aimed at characterizing certain classes of compounds such as polyphenols, phytosterols or terpenoids (Hamm et al., 2003; Lagarda et al., 2006; Motilva et al., 2013; Naczka & Shahidi, 2004; Moreaua et al., 2002). These targeted or class-specific phytochemical techniques have enabled the routine identification of perhaps 20-30 more chemicals in cereal grains. More recently, advances in the field of metabolomics, have made it possible to identify and quantify not just hundreds, but thousands of compounds in biological matrices. These developments suggest that it may be possible to use metabolomics to more completely characterize the chemical constituents of foods, especially cereal grains.

Metabolomics as a branch of omics science uses techniques such as nuclear magnetic resonance spectroscopy (NMR), liquid chromatography (LC), gas chromatography (GC) and mass spectrometry (MS) to separate, identify and/or quantify large numbers of small molecules from complex mixtures and matrices. When properly performed, untargeted metabolomics assays can lead to the detection of >10,000 features and the identification or quantification of >1000 compounds in biological samples (Scalbert et al., 2009). Consequently, when metabolomics is used in food science it has the potential to provide "ultra-comprehensive" food composition analysis (Wishart, 2008).

However, despite its promise and the many potential advantages of metabolomics over existing food composition analysis techniques, the application of metabolomics to food analysis

(especially with regard to cereal grains) is not particularly widespread. A review of PubMed and Google Scholar indicates that fewer than a dozen papers on cereal grain characterization have been published with the word “metabolomics”or other modern analytical techniquesin the title. Furthermore, almost all published papers describing the application of metabolomics towards cereal grain characterization have been restricted to a single metabolomics platform such as MS, LC, or NMR (Abdel-Aal et al., 2007) or a single type of compound (Smeds et al., 2009).

Therefore we decided to conduct a comprehensive, multi-platform quantitative metabolomic study on a several common cereal grains. More specifically, we chose to analyze a total of 4common cereal crops: oats, wheat, barley and rye (Table 3.1) using a combination of NMR spectroscopy, GC-MS, DFI/LC-MS, ICP-MS (Inductive Coupled Plasma Mass Spectrometry), lipidomics and several targeted HPLC-based assays. In addition to these experimental metabolomic techniques, we also conducted a comprehensive literature review (covering approximately 200 papers) of published food composition data for each these cereal crops. This literature review was done to both validate the experimental results and to extend the overall chemical coverage for these fruits and vegetables.

In conducting such a comprehensive metabolomics assessment we wanted to: 1) gain a more complete picture of the chemical composition of many common cereals; 2) assess the utility of different metabolomics platforms for cereal grain analysis; 3) determine the maximum degree of chemical coverage attainable by multiple, quantitative metabolomic methods for cereal grains; 4) compare the coverage obtained by metabolomics methods with other food analysis techniques and 5) extend our experimental analyses using literature mining and make all of the data available through a public, web-accessible database called the Alberta Food Composition Database (AFCDB: http://afcdb.ca). In undertaking this study and in describing the results, it is particularly

important to emphasize that this is both a feasibility study (for metabolomics) and survey study on general cereal grain composition. It was not designed to look at variables such as location, farming practice, soil, temperature, sunlight, moisture, harvesting or storage conditions on compound concentrations. Such a study would be addressing fundamentally different questions.

Overall, we found this multi-platform metabolomics approach to be remarkably effective. Typically in each cereal grain we could identify and/or quantify an average of 198 metabolites using our multi-platform approach. This included an average of 33 compounds by NMR, 96 compounds by DFI/LC-MS/MS, 40 trace elements using ICP-MS, 9 vitamins by HPLC-UV, and 20lipids via GC-MS assays. Data that was experimentally measured in Alberta-grown cereal grains was combined with literature-derived data and led to the identification of ~2000 metabolites (~30,628 metabolites considering inferred lipids) for each cereal grain. All the steps involved in data collection, materials, methods, analysis, and results are given below.

All of the information compiled from this study, along with the previous literature-derived information on concentration values, physiological effects, presumptive health effects, chemistry and biochemistry of cereal grain compositions are freely available through the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca). Indeed, the intent of this work is to demonstrate the feasibility of metabolomics in performing ultra-comprehensive cereal grain analysis using data gathered from various resources and applying various technologies.

3.2 Materials and Methods

3.2.1 Materials

This study was designed to provide a broad survey of the metabolite composition of 4 common grown cereals from the Edmonton region in the province of Alberta, Canada. The Edmonton

region has a humid continental climate with relatively low precipitation and falls into the USDA plant hardiness zone 4a (latitude; 53° 33' N). Small grain cereals are a major constituent of the Canadian prairie landscape with mainly spring-sown cereals being grown in the Alberta region. The most important cereal crops found in western Canada are: wheat, barley, oats, and rye.As a result, these are the cereal grains on which we chose to focus. All cereal crops were grown, harvested and sampled at the University of Alberta research farm (Alberta, Canada). Air-dried cereal grains were stored at room temperature for 1-2 months prior to analysis. Whole grain cereals consist of the inner kernel and outer husk layers were used for all the extraction procedures. Metabolomic studies were conducted at The Metabolomic Innovation Centre (TMIC) at the University of Alberta.

3.2.2 Extraction of Trace Minerals from Cereal Grains

Four types of cereal grains, including two biological replicates (independent samples which were grown in the same farm) were used for trace metal extraction. The extraction was conducted according to the method of Jabeen et al. (2014) with some minor modifications. Previously dried samples were lyophilized for 48 hours. The lyophilized whole-grain cereal samples were covered in liquid nitrogen and ground thoroughly to a fine powder in an agate mortar. After the liquid nitrogen evaporated, six hundred microliters of hydrogen peroxide (Fisher Scientific, Ontario) was mixed with 10 mg of each sample in a 50 ml Falcon tube and vortexed thoroughly. The mixture was then sonicated (at 234 watts) in an ultrasonic water bath for 10 min (Branson Model 2210 ultrasonic bath; Ultrasonics Corporation, Danbury, CT) in order to obtain a homogeneous dispersion. The mixture was then subjected to acid digestion by adding 2 ml of 8 M HNO_3(Fisher Scientific) and maintained over a hot plate and boiled for 10 minutes followed by centrifuging for

10 min, at 3000 rpm (Beckman-GPKR Centrifuge; Beckman Coulter). Prior to conducting Inductively Coupled Plasma mass spectrometry (ICP-MS), the supernatant was taken and filtered through Whatman (grade 2) filter paper. The resulting filtrate was dried and used for ICP-MS based elemental analysis of 63 trace minerals. A detailed description of the ICP-MS analysis method is given in section 3.2.6.

3.2.3 Extraction of Polar Metabolites from Cereal Grains

Four types of cereal grains, including two biological replicates (a total of 8 samples) were used for extraction. Our extraction protocol is based on the method described previously by Wu et al. (2008) with some minor modifications.It is an efficient extraction procedure for rapid and high throughput NMR- and MS-based metabolomic analysis. Grain cereal samples were first homogenized into a fine powder by grinding in a liquid-nitrogen-filled agate mortar.Then 100 mg of the fine, visually homogeneous frozen tissue was mixed with 3 ml of boiling isopropanol andtransferred to a 30 ml glass tube. The extraction solvent, including 4 ml cold HPLC grade methanol and 0.85 ml cold HPLC grade water (Fisher Scientific, Ontario) was added to each sample. Samples were then vortexed and sonicated in an ice bath sonicator for 10 min at 234 watts (Branson Model 2210 ultrasonic bath). After the sonication step, 4 ml chloroform and 4.4 ml HPLC grade water were added to each sample, followed by adding 2.5 ml of 0.88% KCl to the vial. The mixture was kept for 60 min on a shaker (Lab-Line Shaker, Model #4626, VWR Ontario, Canada) and left on ice for 10 min, followed by centrifugation in a Beckman Coulter centrifuge equipped with GH3.7 swinging bucket rotor for 30 minutes at 3000 rpm and 4 °C. The upper layer was lyophilized and kept for analysis by both DFI/LC-MS/MS and nuclear magnetic resonance spectroscopy (NMR) (see section 3.2.7 and 3.2.8). The lower layer was taken and

placed in another tube and stored at -20 °C to be used for further non-polar metabolite analysis (see section 3.2.9). The middle layer containing insoluble material was discarded. The reproducibility, relative simplicity, high yield, and rapid sample throughput makes this technique a good method of choice for total polar metabolite extraction.

3.2.4 Extraction of Lipids and Non-polar Metabolites from Cereal Grains

As described earlier, extraction of polar metabolites by methanol, water, isopropanol, and chloroform resulted in two layers, a polar layer on top and a nonpolar chloroform layer on the bottom, which was collected for lipid analysis. The non-polar extract was concentrated with a stream of nitrogen. Fractionation of total lipid extract was then accomplished using silica Sep-Pak cartridges (3ml, 500-mg matrix, Supelco, St. Louis, MO, USA) and based on a method developed by Hamilton and Comai (1984) with some modifications. The total lipid extract was fractionated into glycolipid, phospholipid, and neutral lipid fractions by column chromatography. Briefly, 10 ml of chloroform was passed through the Sep-Pak column to eliminate any residual lipid before fractionation of the total lipids. Then 10 ml of 100% chloroform was added to the Sep-Pak cartridge to wash off the neutral lipids and the eluate was saved. After draining the first solvent, glycolipids (GL) were eluted from the column by adding 15 ml of acetone and methanol (9:1 v/v). Finally, the column was eluted successively with 15 ml of 100% methanol to elute off phospholipids (PL) from the column. All the eluted fractions were evaporated to dryness under nitrogen and dissolved in small amount of chloroform (for neutral lipids) or 2:1 of chloroform: methanol (other fractions). The neutral lipids were further fractionated into four classes including, cholesterol esters (CE), triglycerides (TG), free fatty acids (FFA), and hydrocarbons using the method described by Christie (2003). Hydrocarbons were eluted first by adding 3 ml of hexane. Cholesterol esters and triglycerides were then washed from the column with 6 ml of

hexane:diethyl ether solution (99:1) and then 5 ml of hexane:diethyl ether solution (95:5), respectively. Subsequently, free fatty acids were separated by adding 5 ml of a hexane:diethylether solution (92:8). Eluates were saved and the solvents were evaporated to dryness with a gentle stream of pure nitrogen. The resulting dried materialwas redissolved in a small amount of chloroform. The identification and quantification of the lipids and other non-polar molecules is described in section 3.2.9.

3.2.5 Vitamin Extraction of Cereal Grains

Four types of cereal grains, including two biological replicates (a total of 8 samples) were used for vitamin extraction. Water and fat-soluble vitamin analysis was performed by employing a previously described method (Santosa et al., 2012). Briefly, cereal grain samples were homogenized into a fine powder in a liquid-nitrogen-filled mortar. After weighing 0.5 g of each cereal grain sample, the frozen tissues were spiked with 40 μL of a mixture of selected internal standards (isotopically labeled fat-soluble vitamins A, E and K). Dry powdered samples were then transferred into a 50 ml Falcon tube and treated with 16 ml of 10mM ammonium acetate/methanol (50:50, v/v) containing 0.1% butylated hydroxytoluene. The mixture was then shaken using a Lab-Line tabletop shaker (15 min at 450 rpm), positioned in the ice bath and sonicated for 15 min(Branson Model 2210 ultrasonic bath). The homogenates were centrifuged at 4000 rpm for 15 min in a Beckman GPKR centrifuge. The upper layer containing all the water-soluble vitamins was dried in a micro centrifuge tube in a Savant Speed Vac vacuum centrifuge. The residue was then dissolved in 1 mL 50/50 HPLC grade methanol/water and applied to Supelclean LC-C18 cartridges (500 mg/3 mL), prior to use. The bottom layer including all fat-soluble vitamins was collected and re-extracted 3 times with 12 ml of a mixture consisting of ethyl acetate and 0.1% butylated hydroxytoluene 50:50 (v/v). The mixture was shaken vigorously for 15 min at 450 rpm

and treated in an ultrasonic bath (Branson Model 2210)for 15 min, followed by centrifugation (Beckman-GPKR Centrifuge; Beckman Coulter)for 15 min at 3000 rpm. The combined supernatants, containing all the water-soluble vitamins, were then dried in a Savant Speed-Vac concentrator.The resultant material was dissolved in 500 µL of ethyl acetate and then placed into an HPLC system coupled with a mass spectrometer. The identification and quantification of the vitamins is described in more detail in section 3.2.10.

3.2.6 Trace Element Analysis Using ICP-MS

In total 4 different cereal grains, using 2 biological replicates, were analyzed individually by ICP-MS for 63 minerals including Li, Be, B, Na, Mg, Al, Si, P, K, Ca, Ti, V, Cr, Fe, Mn, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Rb, Sr, Y, Zr, Nb, Mo, Ru, Pd, Ag, Cd, Sn, Sb, Te, Cs, Ba, La, Ce, Pr, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Tl, Pb, Th, and U. The ICP-MS analysis was performed using a Perkin Elmer Sciex Elan 6000 quadrupole ICP-MS with a dual detector mode (Perkin-Elmer, Norwalk, CT, USA). The ICP-MS unit operates at an RF power of the ICP of 1300 W. The sample uptake flow rate was approximately 1 ml/min. The runs used 35 sweeps per reading, one reading per replicate and three replicates. Dwell times were 10–20 ms for all elements with the exception of Se which was 150 ms. The integration time was calculated as dwell-time times number of sweeps (in this case was 35). The integration times were 700 ms for all elements with exception of Se which was 5250 ms and 350 ms for Al, K, Cu, Zn and Sr. The relative standard deviation (%R.S.D.) for As, Ni, Pb, and Zn ranged between 5 and 10 %. The accuracy of the analytical procedure was assessed through the analysis of certified reference standard materials (whole rock powders) BE-N and DR-N available from the SARM laboratory at the CRPG (Centre de Recherches Petrographiques et Geologiques). Blank subtraction was

undertaken and 3 internal standards containing Bi, Sc and Inwere used for absolute qauntfiacation. Quantification of all 63 elements was done by four point calibration curves (0, 0.25, 0.50 and 1.00 ppm for Na, Ca, Mg, Fe, K, P, and 0, 0.005, 0.010, and 0.020 ppm for other remaining elements).

3.2.7 Compound Identification and Quantification by NMR

In total 4 different cereal grains, using 2 biological replicates, were analyzed individually by NMR. Each prepared extract (using the protocol described in 3.2.3) was lyophilized and 50 mg of dried material was transferred to a 1.5 ml Eppendorf tube. The extract was dissolved in 470 µL of HPLC-grade water, 70 µL D_2O, and 60 µL of a standard NMR buffer solution (11.667 mM disodium-2,2 dimethyl 2-silapentane-5-sulphonate, 730 mM imidazole, and 0.47% NaN_3 in H_2O). The sample was then loaded to a standard thin-walled 5 mm cylindrical glass NMR tube (Wilmad, Buena, NJ, USA) for furthur analysis. All ^{1}H-NMR spectra were acquired on a 500 MHz Inova spectrometer (Varian Inc., Palo Alto, California) witha 5 mm pulsed field gradient cold-probe at 25°C. Spectra were collected using the first transient of the tnnoesy-presaturation pulse sequence which has previously been shown to provide a uniformly high level of precision and accuracy (Saude et al., 2006; Bouatra et al., 2013). All spectra were acquired with 256 transients collected with a 4 second acquisition time and a recycle delay of 1 second. Prior to spectral analysis, all FIDs were zero-filled to 64,000 data points and line broadened by 0.5 Hz. The methyl singlet produced by the DSS methyl groups was usedas an internal standard for chemical shift referencing (set to 0 ppm) and for quantification. All one-dimensional ^{1}H-NMR spectra were processed and analyzed using the Chenomx NMR Suite Professional software package version 7.7 (Chenomx Inc., Edmonton, AB).

3.2.8 DFI/LC-MS/MS Compound Identification and Quantification

Unambiguous metabolite identification and absolute quantification was done for all 4 grain samples (2 biological replicates) using the commercially available AbsoluteIDQ^{TM} p180 kit (BIOCRATES Life Sciences AG- Austria). The p180 kit was used in combination with an ABI 4000 Q-Trap (Applied Biosystems/MDS Sciex) mass spectrometer to quantitatively measure up to 186 metabolites including amino acids, acylcarnitines, biogenic amines, and glycerophospholipids. The kit was originally designed for plasma and has been used to investigate metabolites in plasma, serum, urine, saliva, and recently for fruits and vegetables (Bouatra et al., 2013; Dame et al., 2015; Saleem et al., 2012). Cross validation of the cereal grain extracts measured by the Biocrates kit with other techniques (NMR) showed excellent concordance, which gave us the confidence to use the kit for our cereal extract samples (Table 3.10). This assay involves direct derivatization and measurement of analytes using multiplexed multiple reaction monitoring mass spectrometry (MRM-MS) to quantitatively profile complex biological matrices. Isotopically-labeled internal standards were integrated into the filter plate for absolute metabolite quantification. The exact methods have been described in detail elsewhere (Bouatra et al., 2013; Psychogios et al., 2011; Mandal et al., 2012).

The total polar extracts of all 8 samples (4 cereal grainsand 2 biological replicates) were analyzed by the procedure described in the AbsoluteIDQ p180 user manual. Briefly, 10 microliters of each extract (prepared in Section 3.2.3) was loaded into the kit's wells and samples were concentrated to dryness by placing the plate under a stream of nitrogen for 30 min. Subsequently, 20 μL of the derivatization solution containing 5% v/v phenylisothiocyanate (PIT) was injected to each well. The plate was incubated for 20 min followed by drying under a stream

of nitrogen for an hour. Extraction of the metabolites was then achieved by adding 300 µL of methanol containing 5 mM ammonium acetate and shaking vigorously for 30 min (at 450 rpm). All wells were diluted by 400 µL using the provided running solvent. The extracts were analyzed on an ABI 4000 Q-Trap (Applied Biosystems/MDS Sciex) mass spectrometer equipped with a solvent delivery system. A standard flow injection protocol consisting of two 20 µL injections (one for the positive and one for the negative ion detection mode) was applied for all measurements. MRM detection was used for quantification. Data acquisition, processing, and calculations were performed using Analyst and MetIDQ software. The kit included MetIDQ software for managing the entire kit workflow, from sample registration to automated calculation of metabolite concentrations to the export of data into other data analysis programs.

3.2.9 GC-MS Analysis of Cereal Grain Extracts

Identifcation and quantification of lipid metabolites for the 4 types of cereal grains (and their 2 replicates) for all the lipid fractions extracted as described in section 3.2.4 was performed using GC-MS and the method described by Christie (2010).The transesterification of the lipids and fatty acids was done by adding 1ml of 2% H_2SO_4 in methanol to each fraction. All the lipid fractions were incubated at 86°C for 1 hr followed by cooling on ice for 5 min. Subsequently, 0.5 ml of 0.5% sodium chloride solution and 2 ml of hexane were added to each sample, followed by extensive vortexing. The hexane layer was taken and 2 ml of hexane was added to the lower layer followed by vortexing. The upper layers were combined in a 2 ml vial and the solvent was evaporated under a stream of nitrogen gas and subsequently dissolved in hexane. The extracts were then subjected to gas chromatographic analysis for simultaneous determination of the fatty acid methyl esters (FAMES). GC–MS was performed with an Agilent 7890-5975 instrument

(Agilent technologies) using an Agilent HP-88 column (100 × 0.25 mm ID, 0.2-μm film thickness). The oven temperature was set at 70 °Cfor 1 min, which was raised to 76 °Cat 1 °C/min and then decreased to 250 °C at a rate of 6.1 °C/min. The flow rate was set to 11.6 cm/s (helium). The programmable splitless/split injector was set with a split ratio of 10:1. The quadrupole temperature and the detector temperature were set at 185 and 250 °C, respectively. Confirmation of each fatty acid for each lipid class was performed by comparing the observed EI-MS spectra and retention times to laboratory standards (Sigma-Aldrich, St Louis, MO, USA). Quantification of the lipids and fatty acids was achieved using defined fatty acid methyl ester standards (FAMES) and CLR method was used to regenerate the structures and estimate the most probable concentrations of the triacylglycerols.

3.2.10 Characterization of Vitamins using HPLC-UV

The prepared extracts (from each of the 4 grain samples and their 2 biological replicates) from the protocol described in section 3.2.5 were analyzed using an Agilent 1100 HPLC system equipped with an Agilent G1315B diode array detector (with a scanning wavelength between 190 and 500 nm), a reversed-phase HPLC column Kinetex C18 (2.6 μm-particle size, 3.0x100 mm, 100A) and an automatic injector. The injection volume was 10 μL and the mobile phases were a mixture of 20 mM ammonium formate in water with 0.1% formic acid (solvent A) and 100% methanol (solvent B). The oven temperature was set to 40°C and the flow-rate of 0.5 mL/min was used throughout the test procedure.

For the determination of water soluble vitamins, a chromatographic gradient profile started at 95:5 (A:B) and was linearly decreased to 85:5 in the first 3 min. It was then followed by a linear decrease to 40:60 (A:B) during the next 3 min. The profile was completed by a further linear

gradient to 95:5 (A:B) in the next 2 min interval and kept at 95:5 in the last 2 min of separation. The total run time was 10 min. For the determination of fat-soluble vitamins, the gradient profile started at 70:30 (B:A) and linearly increased to 100 (B) in the next 2 min and was kept at 100 for the next 5 min. Finally the gradient was set back to 70:30 (B:A) for 5 min and kept at that state for another 3 min to bring the total run time to10 min.

This protocol allowed us to identify and quantify a total of 9 water soluble vitamins and 5 fat soluble vitamins including vitamin C, B1, B2, B3, B5, B6, B7, B9, B12, A, D2, D3, E, and K. Quantitation was carried out using 5 to 8 point calibration curves for each standard, covering a concentration range of 0.01–100 mg/mL. Calibration curves were prepared by plotting peak areas vs concentration. The curves were judged linear if the agreement coefficient was more than 0.99 as calculated by the weighted linear regression. The absolute concentrations of 14 vitamins were determined using the calibration curves and the corresponding regression equation.

3.2.11 Literature Analysis, Text Mining and Compound Annotation

A literature review was performed for cereal grain compositionusing PubMed and Google Scholar by searching for all of their relevant literature including scientific names and synonyms along with the terms including “metabolomics”, “metabolome”, “metabonomics”, “chemical composition”, “secondary metabolites”, “nutrient constituents”, “nutritional composition”, “nutrient composition”, “metabolite profiling”, “metabolomics assays”, “NMR”, “GC-MS, “MS/MS”, “pytochemical”, “polyphenols”, “aminoacids”, “vitamins”, “lipids”, and “fatty acids”. Our literature review results can be seen in Table 3.1. This comprehensive literature review yielded about 200 articles related to the chemical composition of barley, wheat, oats and rye. Additional data was also compiled from various textbooks including the Dictionary of Food Compounds, The Composition of Foods, and other textbooks was also used(Panda, 2013; Miller,

1958; McCance, 2002; Yanna, 2012). Further compositional data were collected from online National food composition tables and databases including the USDA National Nutrient Database (NND), the DTU (the Danish Food Composition Databank), Health Canada's food composition tables as well as FooDB, HMDB, Phenol-Explorer, KNApSAcK, MetaboLights, and Dr. Duke's Phytochemical database (Wishart, 2015; Wishart et al., 2013; Neveu et al., 2010; Nakamura et al., 2013; Haug et al., 2013; Duke, 2000). The entireset of manually-derived literature data was further annotated using the DataWrangler program, which automatically generates names, synonyms, descriptions, structures, chemical taxonomies, organoleptic features, physiological effects, presumptive health effects, chemistry and biochemistry of each identified food compound. All the datacompiled or assembled by DataWrangler was manually checked and then placed into the Alberta Food Composition Database (with regard to descriptions and health/biological effects). All the cereal grain composition (and related) dataare available through the AFCDB website (http://afcdb.ca).

3.3 Results and Discussion

In this study we employed a quantitative metabolomics approach for multi-platform characterization of the common grown cereal grains including wheat, barley, oats, and rye. The content of minerals, lipids, vitamins, amino acids, sugars and other metabolites were determined using a variety of quantitative assays and several analytical platforms including NMR spectroscopy, ICP-MS, DFI/LC–MS/MS, GC-MS, HPLC, and GC-MS based lipidomics (Table 3.2). Compound identification was confirmed using authentic reference standards, standardized reference spectra, and comprehensive virtual libraries. We also performed quantitative analysis

using the assembled/purchased external standards and carefully preparingappropriate calibration curves for each standard.

The central objectives of this study on "ultra-comprehensive" cereal composition analysis were to: 1) provide a more complete picture of the chemical composition of common cereal grains;2) assess the utility of various metabolomics assays for cereal grain analysis; 3) determine the maximum metabolome coverage for cereal grains which is attainable by multiple metabolomic methods; 4) compare the coverage obtained in this study by metabolomics methods and techniques with other food analysis methods and previous published studies on cereal grains; and 5) create a fully web accessible database that contains both the experimental and literature-compiled data as well as health effects, chemistry, and biology informationon Alberta-grown cereals, called the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca). The results concerning each of these objectives are outlined below:

3.3.1 Assessing Different Metabolomics Platforms

A total of five different metabolomics assays and compound class-specific were used in this study: 1) ICP-MS; 2) NMR; 3) DFI/LC-MS/MS; 4) GC-MS (fatty acids/lipids); 5) Vitamin assays.ICP-MS identified and quantified an average of 40 (range = 38-41) compounds (metals); NMR spectroscopy was able to identify and quantify an average of 33 (range = 32-34) compounds; DFI/LC-MS/MS identified and quantified and average of 96 (range = 77-120) metabolites; GC-MS based lipidomics identified and quantified an average of 20 (range = 1-56) fatty acid compounds; and the vitamin assays identified and quantified an average of 8 (range = 8-9) compounds. The Venn diagram in Figure 3.1 summarizes these results and shows that there is relatively little overlap between the different platforms. The Venn diagram also shows that the

DFI/LC-MS/MS approach provided the largest average number of metabolites identified and quantified, while the specialized assays such as the vitamin assay provided the fewest. A more detailed description of what was found for each platform or method is given below.

3.3.1.1 – ICP-MS Results

Inductively coupled plasma mass spectrometry (ICP-MS) was used to provide the quantitative results for 63 trace minerals for the 4 cereal grains as shown in Table 3.3. Measured concentrations for all detected trace elements are also reported in the AFCDB website. Our findings demonstrated the power of ICP-MS as a promising analytical tool, which is capable of rapid and precise determination of trace element abundance in a variety of targets or matrices. Previous studies on mineral content of cereal grains were mostly investigated the high abundance elements (Demirbas, 2005; Shimbo et al., 2001). In this study, the cereals that were most fully characterized by ICP-MS were oats and rye with 41 metal ions identified and quantified. The cereal grain that yielded the lowest number of ICP-MS-identifiable trace elements was barley, which had 38 metal ions identified and quantified. We found that the most abundant minerals were P, K, Ca, Mg, Si, Fe, Mn, Na, and B. The lowest concentration we found was 44 ng/100 grams fresh weight, for lanthanum in wheat. The highest concentration we found was 757.8 mg/ 100 grams fresh weight for potassium in rye. According to our data, cereal grains are excellent sources of potassium, phosphate, magnesium, calcium, aluminum, and sodium. Across all cereal grains, the most abundant ions were potassium (up to to 758 mg/100 g FW), phosphorous (up to to 471.9 mg/100 g FW), magnesium (up to to 155.8 mg/100 g FW), and calcium (up to to 81.5 mg/100 g FW). Our data also confirms that cereal grains are good sources of zinc, iron, and manganese with an average amount of 4.2, 3.3,and 2.5 mg/100g FW respectively. Based on our

data, rye is the best source of zinc (5.4 mg/100 g FW)and barley is the best source of iron (3.5 mg/100 g FW). These results align with data from other on-line nutrient databases such as USDA-NND and the Danish Food Composition Databank.As can be seen in Table 3.3, only 10-12 elemental ions dominate while the other ions are present only as trace amounts.

To the best of our knowledge, this is the largest multi-elemental study on cereal grains ever conducted using ICP-MS. Our experimental results show a very good agreemenet (83.7%) between the metal ions we measured compared to previously published studies by considering ± 50% of threshold value. However a little variation is always expected due to biotic and abiotic factors that may influence content of minerals and trace. It has been demonstrated that geographical and environmental factors can affect mineral values in cereal products (Shimbo et al., 2001). The concentration of minerals is also strongly correlated with soil type (Effiom, 2015; Steadmana et al., 2001). As can be seen in Table 3.3, a large number of the minerals we identified and quantified are being reported for the very first time in this study.

3.3.1.2 – NMR Results

NMR was used for identification and quantification of a wide range of water-soluble metabolites including sugars, alcohols, amino acids, organic acids and various phytochemicals. In this study, NMR provided quantitative data for an average of 33 high-concentration (>1 μM), water-soluble compounds as shown in Table 3.4. Other previous published studies and online national food composition tables report no more than 18 compounds in this category. Measured concentrations for all detected compounds for Alberta-grown cereal grains are also provided at the AFCDB website,along with the literature-derived values and their associated citations. Typically about 70% of the peak area in any given cereal grain NMR spectrum could be assigned. This suggests

that another 10-20 compoupnds compounds could be identified if reference NMR spectra existed for these “unknown” compounds.The cereal grain that was most fully characterized by NMR was wheat which had 34 compounds identified and quantified. The cereal grain that yielded the lowest number of NMR-characterized metabolites was barley which had 32 compounds identified and quantified. The lowest concentration we found by NMR in cereal grains was 14.6 mg/100 grams fresh weight for formate in barley. The highest concentration we found by NMR was 3.1 grams/100 grams fresh weight, for glutamic acid in wheat.Note that all amino acid values reported here represent the concentrations of free amino acids. Protein hydrolysis was not performed, so the total amino acid content reported for this kind of analysis will differ from those provided by somefood databases which typically use protein hydrolysis to obtain amino acid values. However, inspection of Table 3.4 and 3.5 shows that the agreement with literature-reported values (which likely didn’t include protein hydrolysis in the quantitation process) is actually quite good.It should be noted that leucine published literature values include protein hydrolysis and thus our experimental results appear to differ slightly from those reported values.Among our cereal grain samples, the most common NMR-detectable compounds were glucose, fructose, leucine, isoleucine, tyrosine, glutamine, serine, alanine, and phenylalanine. Across all cereal grains, glutamate (up to 3.1 g/100 g FW), asparatate (up to 1.2 g/100 g FW), and proline (up to 1.1 g/100 g FW) were the most abundant NMR-detectable compounds. According to our data, wheat is the best source of serine and arginine with concentrationsof 0.95 and 0.59g/100 g FW, oats are the best source of asparagine, glutamine, andcysteine with concentrations of 1.1, 0.99, and 7.98g/100 g FW, rye is the best source of asparatate, choline, and, fumarate with concentrations of 0.81, 0.72, and 0.83 respectively. Unlike the situation with ICP-MS, the results from our NMR study showed a much narrower range of concentrations (varying by 3 orders of magnitude) compared to

ICP-MS, which exhibited variations of 6 orders of magnitude. This reflects the differing sensitivity of the measuring systems.

We believe this is the largest and most comprehensive food composition study on cereal grains ever conducted using NMR spectrometry. In general we found very good overall quantitative agreement between the Alberta grown cereatl grains and previously reported values from other studies. In particular, the percentage of agreement was 94%, using a ± 50% threshold cutoff. However, it is also important to remember that these values can be influenced by a number of factors including, the local environment, level of fertilization, irrigation, and plant cultivar, as well as various analytical or extraction methods and different technologies from different periods in history (Hopkins & Elsen, 1959; Hattori & Chino, 2001; Sharma & Rao, 2013; Pietola, 2000; Balint et al. 2001). Therefore we would, and should not, expect a perfect match between our NMR results and those in the literature that were measured using other technologies. We also compared the concentrations of the compounds measured by NMR spectroscopywith the same metabolites measured via other assays (DFI/LC-MS/MS, vitamins, polyphenols) as well as the reported literature values.These are indicated in Table 3.10. Overall, the agreement between the NMR values and other assays conducted in our laboratory (using similar or identical biological samples) is excellent.

3.3.1.3 – Direct flow injection/LC-MS/MS Results

We optimized a cereal grain extraction method for the identification and quantification of biogenic amines, amino acids, fatty acids and lipids using DFI/LC-MS/MS via the Biocrates AbsolutIDQ™ p180 Kit (BIOCRATES Life Sciences AG, Innsbruck). The lower and upper limits of quantification were determined experimentally by Biocrates AbsoluteIDQ™ kit. To the best of

our knowledge, this is the first and largest food composition study on cereal grains ever conducted using the Biocrates AbsoluteIDQ kit. This assay provided quantitative results for an average of 96 compounds, as shown in Table 3.5. The most fully characterized cereal grain was wheat with 120 compounds identified and quantified using this LC-MS assay. The cereal grain with the lowest number of DFI/LC-MS/MS-identifiable metabolites was oat, which had 77 compounds. The lowest concentration we found via DFI/LC-MS/MS was 4 μg/100 grams FW for octadecadienyl-L-carnitine in wheat. The highest concentration we found was 2.74 g/100 grams FW for glutamic acid in wheat. Note that all amino acid values reported here represent the concentrations of free amino acids. Protein hydrolysis was not performed, so the total amino acid content reported for this kind of analysis will differ slightly from those provided by some national food tables which typically use protein hydrolysis to obtain amino acid values. Across all cereal grain species, the most ambundant compounds were glutamic acid (up to 3.4 g/100 g FW), proline (up to 1.5 g/100 g FW), asparatic acid (up to 1.2 g/100 g FW), and serine (up to 0.84 g/100 g FW). According to our data on Table 3.5, oats are the best sources of asparatic acid, serine, alanine, lysine, and asparagine (with concentraions greather than 0.5 grams/100 g FW). Rye is the best source of proline with concentration of 1 gram/100 grams FW. Wheat and barley are the best sources of glutamic acid and valine respectively.The amount of glutamic acid in wheat was2.7 grams/100 g FW and the valine concentration in barley was 0.6 grams/100 g FW. These results are in moderately good agreement with data from other on-line nutrient databases such as the Danish Food Composition Databank.Overall, the percentage of agreement between the concentrations for the compounds we measured andthose reported in previously published studies was 65.5% (using a cutoff of ± 50% of the value we measured).

This is the first food composition study on cereal grains ever conducted using the Biocrates AbsoluteIDQ kit. Comparing the results we obtained via this kit with previous studies proved to be difficult as essentially no other studies provided data on phospholipids, biogenic amines or acyl carnitines. Comparisons to reported amino acid content values also proved to be difficult with some, as our analysis focused on the quantification of free amino acids, as opposed to total amino acids (obtained via protein hydrolysis combined with free amino acids).However, our results on Table 3.10show good cross-platform agreement with identical metabolites measured by other methods and assays such as NMR, GC-MS, and other data from previously reported studies (available values for amino acids and biogenic amines).

3.3.1.4 – GC-MS Lipidomics Results

The lipid and fatty acid composition of the four cereal grains were examined using a combination of lipid extraction, solid phase separation and GC-FAMES. A technique known as Combinatorial Lipid Reconstruction (CLR) (Psychogios et al., 2011) was used to computationally regenerate precise lipid structures and to approximate the lipid concentration ranges (in mole percent) for 5 lipid classes: glycolipids (GL), phospholipids (PL), choleteryl esters (CE), triglycerides (CL) and free fatty acids. The results for the fatty acid composition for each of 5 different lipid classes are presented in Tables 3.6 and 3.7. A total of 13 different types of fatty acids were measurabe for these 5 lipid classes. Unfortunately, insufficient data was collected to obtain fully quantitative information about some of these lipid classes (with the possible exception of the cholesteryl esters).

Using both direct measurements for fatty acid compositions and the CLR method for triglycerides we identified and quantified (or semi-quantified) 81 triacylglycerol compositions (an

average of 20) in 4 cereal grains (Table 3.7). Lipid concentrations are substantially different among different cereal grains.Our study, along with other previous studies, have demonstrated that the composition of lipid classes is often quite consistent between selected cereals (Morrison, 1977; Morrison, 1988). Oats were the most fully characterized samples by GC-MS with56triacylglycerol compositiondetected. Rye yielded the lowest number of compounds detectable by GC-MS, which had just 1 triacylglycerol.

Our results also show that the five most common fatty acids detected in cereal grains are medium-to-long chain fatty acids, including myristic acid (14:0), palmitic acid (16:0), margaric acid (17:0), stearic acid (18:0), and linoleic acid (18:2). Our data also confirm that cereal grains are a useful source of linoleic acid (Morrison, 1988). The most abundant fatty acid among all lipid classes and among all Alberta cereal grains was palmitic acid, which is consistent with previous studies (Price & Parsons, 1975).

Although cereal lipids do not appear to have been extensively studied by other investigators, our observations on the lipid and fatty acid content in Alberta cereals appear to be in good agreement with other published results (Morrison, 1988; Macmurray & Morrison, 1970). A little variation between the content of lipids and fatty acids in the cereal grains studied here and those reported in other studies would be expected given the different environmental conditions. Indeed there are a number of factors that might affect cereal lipid content, including the crop cultivar, growing seasons, growing temperature, fertilization, and storage conditions (Zhou et al., 1999).

3.3.1.5 – Vitamin Assay Results

In this study we used a reversed-phase high-performance liquid chromatographic (HPLC) with UV detection to identify and quantify water and fat-soluble vitamins in cereal grains. The quantitative results for 9 water-soluble vitamins and 5 fat-soluble vitamins are shown in Table 3.9. All the vitamin data, along with the literature-derived values and their associated citationshave also beenentered into AFCDB website.

As can be seen in Table 3.9, the highest numbers of detectable vitamins were found in rye and wheat, which had 9 vitamins. Oats and barley had 8 detectable vitamins. The lowest concentration was 2 μg/100 grams fresh weight found for vitamin K in wheat. The highest concentration we found by our HPLC assays was 7.14 mg/100 grams fresh weight, for vitamin B3 in barley. Across all cereal grains, barley and wheat had the highest amount of total vitamins. Vitamins D, C, and B12 were not detected in any of our selected cereal grains. This may be due to their concentrations being below the limit of detection for our assays or it may be due to the absence of these vitamins through chemical decomposition as part of the standard seed aging, drying, and cleaning process.The most abundant vitamins were vitamin B3 (up to to 7.14 mg/100g FW), vitamin E (up to to 1.52 mg/100g FW), vitamin B5 (up to to 1.33 mg/100g FW) and the least abundant vitamins were vitamin K (0.002 to 0.006 mg/100g FW), and vitamin B7 (0.0049 to 0.01 mg/100g FW). According to our data, wheat is the best source of vitamin B1, barley is the best source of vitamin B3 and vitamin B6, rye is the best source of vitamins E, B2, B5, and B9.

We also compared our results with previously reported vitamin values in various national food tables as well as other literature derived sources. These are presented in Table 3.9. Comparisons to these values show generally good agreement. The percentage of agreement was 80.4% using a ± 50% threshold. The table also shows that vitamin content values are probably the

most extensively covered and reported among measurable metabolites in cereal grops. However, there are several factors that may affect vitamin concentrations including, but not limited to growing season, geographic origin, presence of pathogens, fertilizer, irrigation, and storage condition (Jood & Kapoor, 1994; Hegedi et al., 1985).

3.3.2 Assessing the Extent of Compound Coverage

In this study, a total of 29,419 including (28,628 inferred lipids)separate chemical measurements were made over 4 different ceral grains corresponding to the identification of an average of 28,826 metabolites per sample. A total of 247 non-repetetive metabolites or metabolite species were identified experimentally.Five different analytical platforms or compound-specific methods were used, including NMR, DFI/LC-MS/MS, ICP-MS, HPLC-UV assays (for vitamins),and GC-MS-based lipidomics.The ICP-MS assay identified and quantified an average of 40 (range = 38-41) metabolites; NMR spectroscopy identified and quantified an average of 33 (range = 32-34) compounds; DFI/LC-MS/MS identified and quantified an average of 96 (range = 77-120) metabolites; GC-MS-based lipidomics detected an average of 20 (range = 1-56) compounds; and the HPLC-UV vitamin assay identified and quantified an average of 8 (range = 8-9) compounds for our 4 cereal grain samples. The most effective approach for generating completely novel or never-before reported data was ICP-MS (with an average of 80% of the metabolites having no prior literature value), followed by the DFI/LC-MS/MS method (with an average of 75% of the metabolites having no prior literature values). The assay that provided the least amount of novel or never-before-seen data was the vitamin assay, with an average of just 2 % of the vitamins have no prior literature value.

We estimate that our 5 platforms were capable of identifying a total of 2657 compounds (12 vitamins by HPLC-UV, 63 by ICP-MS, 400 by NMR, 182 by DFI/LC-MS/MS, and about 2000 by GC-MS). This suggests that we were able to detect about 15% of all potentially measurable compounds. Rye had the lowest level of characterization with 178 unique compounds identified and quantified, while oat had the highest level of characterization with the total of 247unique compounds identified and quantified. As far as we are aware, these numbers represent the highest number of cereal grain metabolites ever identified and quantified in a single cereal grain study.

A summary of our results can be seen in the Venn diagram (Figure 3.1). From this figure it is evidentthat some methods provide completely unique data (ICP-MS, in particular), while other methods exhibit some modest overlap (DFI/LC-MS/MS, NMR, and the vitamin assay).As clearly indicated in this study, and as shown in many other studies (Bouatra et al., 2013; Psychogios et al., 2011; Wishart et al., 2008) multiple methods should be used in metabolomic studies in order to maximize metabolome coverage.

3.3.3 Compound Coverage: Literature Comparison

As noted above, Tables 3.3-3.8 provide comparisons between our experimentally measured values and those reported in the literature and online food composition tables.The exact literature sources and associated references are provided in the AFCDBwebsite (there is insufficient space to provide this information in the attached tables). In many cases, only a single literature value was found, however, when 3 or more values were obtainable, an average and a standard deviation are provided. In evaluating the nutritional value of cereal grains we categorized nutritional constituents to 4 parts including 1) trace elements; 2) water-soluble metabolites; 3) fatty acids and/or lipids; 4) and vitamins.

A comparison of the extent of trace element coverage for previously reported studies relative to our data is presented in Table 3.3. It can be seen from this table that most sources report values for an average of 7 most abundant metals or trace minerals, including sodium, magnesium, phosphorous, potassium, calcium, iron, etc. In our literature review we identified~15 studies that provided modest or reasonably extensive trace metal analysis using atomic absorption spectroscopy, flame ionization spectroscopy, and ICP-MS. The ICP-MS studies typically reported highest number of trace elements (Ekholm et al.,2007). Many of these studies did not report absolute concentrations but rather simply reported detection. Overall, most of these trace element studies on cereal grains achieved only relatively modest coverage with an average of 8 minerals reported for 1-14 different cereal grains (Demirbas, 2005; Zhao et a.l, 2009; Ekholm et al., 2009; Kirchmann et al., 2009; White & Broadley, 2005). The most complete metal ion study we could find was that reported by Demirbas (2005). He studied 14 cereal grains and achieved an average coverage of 12 trace elements. Table 3.3 shows that our study achieved an average coverage of 40 trace element values for 4 cereal grains.

We also used NMR for quantitative profiling of polar metabolites in cereal grains and our results are presented in Table 3.4. As can be seen from this table, previously published studies typically reported values for up to 10 water-soluble metabolites in cereal grains. There are quite a few NMR studies on cereal grains. These studies mainly describe application of metabolomics towards a single cereal grain (Morgan et al., 1999; Outrup, 1981) or a single NMR-detectable compound (Cui et al., 2000). The most complete NMR study on cereal grains that we could find was reported by Broyart et al. (2009). They identified and quantified a total of 18 compounds in maize. While NMR spectroscopy has enabled the identification of several compounds in cereal grains, as far as we are aware, our study appears to be the largest and most complete NMR

studyon cereal grains, with an average coverage of 31 NMR-detected metabolites for each of the 4 cereal grains.

Relatively large number of studiesconfirms that LC-MS/MS is generally the preferred method for identifying and quantifying plant metabolites. Almost all published papers have been restricted to application of DFI/LC-MS/MS towards the characterization of a single metabolite (Hanhineva et al., 2011; Sorensen et al., 2008) or a particular toxin (Blesa et al., 2004; Tanaka et al., 2007; Granby et al., 2003) in cereal grains. In terms of compound identification for cereal grains, the most extensive LC-MS study we found was a survey conducted by Bruce et al (2010) who performed LC-MS/MS on a total of 32 cereal flours and cereal fractions to identify and quantify just two compounds: choline and betaine. Table 3.5 presents the quantitative results for amino acids, acylcarnitines, glycerophospholipids, and hexose with an average coverage of 76 metabolites in the 4 cereal grains. Our LC-MS study also demonstrated that it is possible to determine the concentration of water-soluble compounds in cereal grains using LC-MS/MS via the Biocrates AbsolutIDQ™ p180 kit. However, some caution is warranted. In particular there were a number of mammalian-specific compounds (sphingomyelins, creatinine, carnosine) which had to be manually excluded after the initial analysis. This is because the kit would occasionally misidentify these compounds in the plant matrix (likely due to the existence of as-yet unidentified plant compounds with identical molecular weights (to sphingomyelins or creatinine) and similar retention times.The Biocrates AbsolutIDQ kits have already been applied to other types of biological samples for metabolic investigations of bovine ruminal fluid, human urine, human saliva, and, most recently, for fruits and vegetables (Bouatra et al., 2013; Dame et al., 2015; Saleem et al., 2012). The Biocrates system offers a number of advantages over manual LC-MS/MS analysis and other technologies, including higher separation efficiencies, better detection

limits, absolute quantification of metabolites, decreased solvent consumption, and reduced costs for targeted metabolomics. This assay was also able to detect/quantify more compounds than GC–MS and NMR (Saleem et al., 2012).

The previously published studies mainly focused on the total lipid composition or the total fatty acid composition (Price & Parsons, 1975). Food composition tables typically report values for 8-11 fatty acids including palmitic acid (16:0), oleic acid (18:1), linolenic acid (18:2), rather than lipids.The majority of fatty acid composition studies on cereals were published by Morrison (1977; 1988; 2006). Notably, our study provided data on the fatty acid content of 5 lipid classes including glycolipids, phospholipids, cholesteryl esters, free fatty acids and triglycerides, as well as providing information on the identity and abundance of these lipids. Based on a detailed comparison of the literature, it is clear that our study is currently the "high-water" mark for lipid analysis of cereal grains.

Table 3.9 provides a comparison of the extent of vitamin coverage for different food composition databases and previously published values. As can be seen from this table, modern food composition tables achieved relatively good coverage of vitamins for cereal grains. Vitamin data reported in national food tables and other published scientific studies are generally more extensive than other groups of compounds.

Based on our literature surveys,vitamin E and B group vitamins have been the most extensively studied and a variety of techniques have been proposed for their characterization (Hegedi et al., 1985; Zielinski et al., 1999; Zielinski et al., 2001). The most detailed vitamin studies we could find for cereal grains were those reported by Hegedus et al. (1985) and Lebiedzinska & Szefer (2006). The Hegedus study (1985) identified and quantified 7 vitamins in 6 cereal types using a microbiological assay in combination with HPLC coupled to a fluorescence

detector. The Lebiedzinska and Szefer study (2006) reported 4 vitamins in 5 cereals using microbiological analytical methods. Compared to existing studies, our study yielded moderately good coverage with an average of 9 vitamin values (typically 7-10 vitamins) for 4 cereal grains. As can be seen from our experimental data our results are in good agreement with previous literature values(the percentage of agreement was 80.4% using a ± 50% threshold).

3.3.4 Literature Survey and Alberta Food Composition Database

Our literature survey identified a total of 8,205 metabolites and an average of 2,051 unique compoundsfrom 167 existing studies and 5 food databases, spanning all 4 cereal grains in our study. The cereal grain with the most literature-reported metabolites was barley, with 2090 compounds detected.The cereal grain with the fewest number of literature-reported metabolites was rye, with 1976 compounds detected. This compares to an average of 215 metabolitesfor our experimental work reported here. Experimentally, we found that oats had the largest numbr of identified and quantified metabolites whileryehad the fewest compounds. When combining the literature-derived data with the experimentally derived data, we obtained an average of 30,679 compounds for each cereal grain. This corresponds to an average of 28,628 lipids and 2,051 non-lipid molecules.

All of the data collected from this study, including both the experimentally measured and literature-derived data has been entered into the Alberta Food Composition Database (AFCDB: http://afcdb.ca) to provide a more accessible and more richly annotated version of all of the data presented here. The database is freely available, fully searchable, easily queried and web-enabled. Clicking on the “Search” button generates a tabular view that allows user to scroll through the database by compound names, nutrients, food contents or food types. The content of the AFCDB is accessible by browsing through the “FoodView” (listing foods by their chemical constituents)

and “ChemView” (listing chemicals by their food sources) to facilitate user searching. Each food metabolite entry in this database provides the scientific name, description, classification, and chemical composition information. Many of these associated data are hyperlinked to other databases such as the USDA NND, Phenol-Explorer, Dr. Duke's database, KNApSAcK, the Danish Food Composition Databank (DTU) and other online sources. The database can be fully downloaded by pressingthe 'Download' button.Overall, the AFCDB database contains nutritional information for nearly 40 Alberta-grown foods including 4 cereal grains and more than 17,000 content values.

3.4 Conclusion

By combining experimentally measured data with manual and computer-aided literature-derived data we were able to perform an ultra-comprehensive analysis of cereal grains. Our study led to theidentification and/or quantification of an average of 29,419compounds in Alberta grown cereals, which about 198compounds being experimentally validated and the other 28,628being obtained either through literature searches or genetic reconstructions of cereal grain metabolism. If we consider only non-lipid molecules, a total of202 experimentally determined non-repetetive metabolites or metabolite species and 151 literature-derived unique metabolites or metabolite species were obtained from our analysis. Comparisons to previously published studies and to existing food composition data tables, show that our experimental findings regarding the chemical composition of Alberta grown cereals is in generally good accordance with previous studies. However, only 21% of the metabolites we measured have had values previously reported in the literature. We believe the variation that exists between our data and that of other published studies can largely be explained by environmental factors and/or strain differences.

We believe that these results (and the data in the AFCDB) should be able to help food producers, food consumers, nutritional experts, and medical professionals become far more aware of some of the key ingredients and some of the compositional variations in wholegrain cereals. Furthermore, we believe that we have been able to successfully demonstrate, develop and refine a number of useful metabolite extraction and metabolitle detection techniques that should enable more complete chemical analysis of many other cereal grains in different jurisdictions or under different growth conditions. Overall, our results suggest that comprehensive metabolite profiling of cereals needs multiple analytical platforms and the use of multiple methods for extracting, separating or isolating metabolites.

Figure 3.1 Venn diagram showing the overlap of average cereal grain metabolites detected by global NMR, FAMEs/GC– MS, ICP-MS, HPLC, and DFI–MS/MS methods.

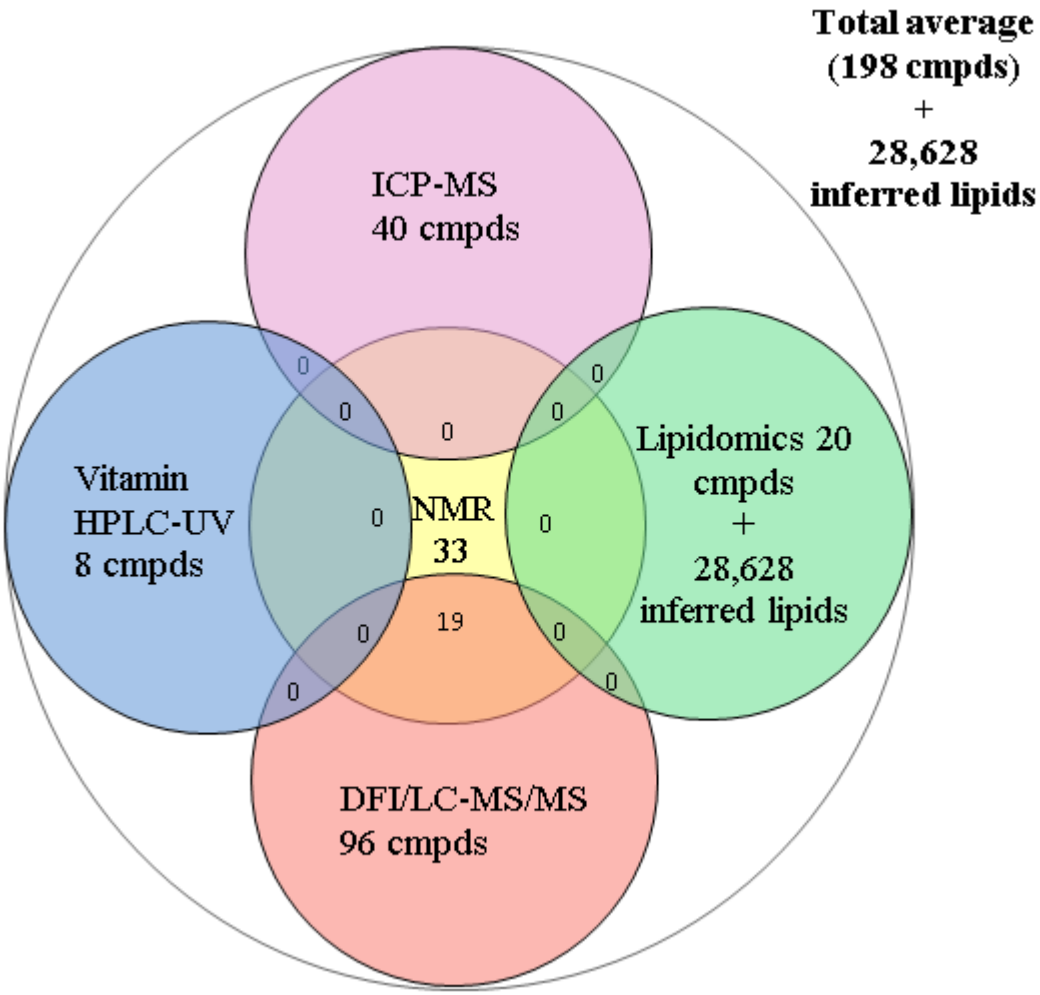


Table 3.1 Comprehensive food composition literature review for selected cereal grains.

Cereal types	Number of studies	Number of compounds from Literature	Reported compounds on FooDB database	Reported compounds + inferred lipids on FooDB database
Wheat	44	130	2053	30681
Barley	39	105	2090	30718
Oat	51	128	2086	30714
Rye	33	151	1976	30604

Table 3.2 Number of detected metabolites in Alberta-grown cereal grains using various assays.

Food types	ICP-MS	DFI/LC-MS/MS	HPLC	GC-MS	NMR
Wheat	39	120	9	4	34
Barley	38	93	8	20	32
Oat	41	77	8	56	33
Rye	41	95	9	1	33

Table 3.3 Mineral contents of Alberta grown cereal grains as determined by ICP-MS (Conc. mg/100 g FW).

Minerals	Wheat	LV[1]	Barley	LV
Li	0.005 (0.004-0.005)	-	0.007 (0.007-0.007)	-
Be	-	-	-	-
B	1.4 (1.3-1.6)	-	2.0 (2.0-2.1)	-
Na	3.2 (2.8-3.5)	3.8±1.13	10.9 (10.5-11.2)	17.9±8.34
Mg	122.4 (104.0-140.9)	117	111.2 (110.0-112.4)	165±45.25
Al	0.65 (0.53-0.78)	-	19.0 (18.4-19.7)	
Si	9.0 (8.4-9.6)	-	7.5 (5.5-9.5)	
P	375.3 (303.2-447.3)	336±18.38	330.6 (315.7-345.5)	306.5±60.10
K	346.7 (335.3-358.0)	238±220.62	417.1 (415.9-418.3)	454.6±3.68
Ca	36.9 (34.9-38.9)	33	38.9 (37.3-40.4)	53.3±28.71
Ti	0.009 (0.006-0.01)	-	0.01 (0.01-0.02)	-
V	-	-	0.002 (0.0-0.001)	-
Cr	0.11 (0.08-0.15)	-	0.13 (0.10-0.16)	-
Fe	3.4 (2.9-3.9)	2.515±1.69	3.5 (0.62-6.3)	3.60
Mn	3.2 (2.8 -3.6)	0.515±0.01	1.5 (1.5-1.5)	-
Co	0.001 (0.001-0.001)	-	0.0008 (0.0006-0.001)	-
Ni	0.04 (0.03-0.05)	0.004	0.02 (0.01-0.02)	-
Cu	0.31 (0.27-0.36)	-	0.32 (0.32-0.32)	-
Zn	4.6 (4.2-5.0)	2.96	3.2 (2.8-3.5)	5.06±3.34
Ga	0.002 (0.002-0.003)	-	0.003 (0.002-0.004)	-
Ge	0.0002 (0.0002-0.0003)	-	0.0005 (0.0003-0.0007)	-
As	-	-	-	-
Se	0.001 (0.001-0.001)	0.002	0.0009 (0.0008-0.0009)	-
Rb	0.38 (0.32-0.44)	-	0.54 (0.51-0.56)	-
Sr	0.11 (0.09-0.13)	-	0.20 (0.19-0.21)	-
Y	0.0002 (0.00007-0.0002)	-	0.0003 (0.0002-0.0004)	-
Zr	0.001 (0.0008-0.002)	-	0.002 (0.001-0.002)	-
Nb	0.0001 (0.0001-0.0001)	-	0.0004 (0.0002-0.0006)	-
Mo	0.02 (0.01-0.02)	-	0.03 (0.03-0.04)	-
Ru	0.0002 (0.0-0.0002)	-	0.0002 (0.0-0.0002)	-
Pd	0.004 (0.002-0.007)	-	0.007 (0.004-0.009)	-
Ag	-	-	0.0005 (0.0004-0.0005)	-
Cd	0.002 (0.002-0.002)	-	0.002 (0.002-0.002)	-
Sn	0.005 (0.002-0.007)	-	0.008 (0.007-0.009)	-
Sb	0.00009 (0.00009-0.00009)	-	0.0001 (0.0001-0.0001)	-
Te	-	-	-	-
Cs	0.0003 (0.0002-0.0003)	-	0.0005 (0.0005-0.0005)	-

[1] LV for Literature value. References to the LV's are provided in the AFCDB. *Continued*

Table 3.3.*Continued.*

Minerals	Wheat	LV	Barley	LV
Ba	0.46 (0.39-0.53)	-	0.25 (0.24-0.26)	-
La	0.0001 (0.0001-0.0001)	-	0.0004 (0.0002-0.0006)	-
Ce	0.0003 (0.0003-0.0003)	-	0.0006 (0.0004-0.0009)	-
Pr	-	-	0.0001 (0.0001-0.0001)	-
Nd	0.0001 (0.0001-0.0001)	-	0.0003 (0.0002-0.0004)	-
Sm	-	-	-	-
Eu	0.0001 (0.0001-0.0001)	-	0.0001 (0.0001-0.0001)	-
Gd	-	-	-	-
Tb	-	-	-	-
Dy	-	-	-	-
Ho	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-
Lu	-	-	-	-
Hf	0.0002 (0.0002-0.0002)	-	0.0002 (0.0002-0.0002)	-
Ta	0.0003 (0.0003-0.0003)	-	0.0004 (0.0004-0.0004)	-
W	0.0025 (0.00030-0.0040)	-	0.005 (0.001-0.009)	-
Re	-	-	-	-
Os	0.0025 (0.0020-0.0030)	-	0.02 (0.01-0.03)	-
Ir	-	-	-	-
Pt	0.0004 (0.0004-0.0004)	-	0.0005 (0.0005-0.0005)	-
Tl	-	-	-	-
Pb	0.003 (0.002-0.005)	-	0.005 (0.004-0.006)	-
Th	-	-	-	-
U	-	-	0.0002 (0.0001-0.0002)	-
	Rye	**LV**	**Oat**	**LV**
Li	0.0035 (0.0030-0.0040)	-	0.007 (0.006-0.007)	-
Be	-	-	-	-
B	3.1 (3.0-3.2)	-	2.1 (1.8-2.5)	-
Na	6.1 (5.9-6.3)	2	6.6 (6.1-7.1)	2
Mg	150.9 (145.9-155.8)	110	123.5 (120.6-126.3)	177
Al	1.3 (1.3-1.4)	-	0.76 (0.72-0.80)	-
Si	12.3 (11.9-12.7)	-	11.5 (9.0-13.9)	-
P	457.1 (442.3-471.9)	332	353.7 (349.5-357.9)	523
K	733.9 (710.2-757.8)	510	444.3 (431.8-456.9)	429
Ca	55.3 (53.5-57.1)	24	81.4 (81.3-81.5)	54
Ti	0.01 (0.01-0.01)	-	0.01 (0.01-0.01)	-
V	-	-	-	-

Continued.

Table 3.3.*Continued.*

Minerals	Rye	LV	Oat	LV
Cr	0.21 (0.20-0.22)	-	0.14 (0.12-0.16)	-
Fe	2.2 (2.1-2.3)	2.63	3.9 (3.9-4.0)	4.72
Mn	3.6 (3.5-3.8)	-	1.7 (1.4-2.0)	-
Co	0.002 (0.001-0.002)	-	0.0009 (0.0008-0.0009)	-
Ni	0.05 (0.05-0.05)	-	0.30 (0.24-0.36)	-
Cu	0.53 (0.51-0.55)	-	0.24 (0.20-0.29)	-
Zn	5.4 (5.2-5.6)	-	3.5 (2.9-4.22)	-
Ga	0.003 (0.003-0.003)	-	0.0025 (0.0020-0.0030)	-
Ge	0.0003 (0.0003-0.0003)	-	0.0009 (0.0007-0.0010)	-
As	-	-	-	-
Se	-	-	-	-
Rb	1.2 (1.1-1.2)	-	0.69 (0.67-0.72)	-
Sr	0.15 (0.15-0.16)	-	0.17 (0.16-0.18)	-
Y	0.0005 (0.0005-0.0005)	-	0.0003 (0.0002-0.0003)	-
Zr	0.001 (0.001-0.002)	-	0.002 (0.001-0.003)	-
Nb	0.0005 (0.0005-0.0005)	-	0.0005 (0.0002-0.0007)	-
Mo	0.05 (0.05-0.05)	-	0.13 (0.12-0.14)	-
Ru	0.0002 (0.0002-0.0002)	-	0.001 (0.001-0.001)	-
Pd	0.009 (0.008-0.009)	-	0.01 (0.01-0.02)	-
Ag	-	-	0.0003 (0.0003-0.0003)	-
Cd	0.001 (0.001-0.001)	-	0.0005 (0.0005-0.0006)	-
Sn	0.02 (0.02-0.02)	-	0.008 (0.004-0.01)	-
Sb	-	-	0.0002 (0.0002-0.0002)	-
Te	-	-	-	-
Cs	0.0008 (0.0008-0.0008)	-	0.0004 (0.0004-0.0004)	-
Ba	0.44 (0.43-0.46)	-	0.18 (0.16-0.20)	-
La	0.0003 (0.0003-0.0003)	-	0.002 (0.002-0.002)	-
Ce	0.0005 (0.0004-0.0005)	-	0.003 (0.002-0.003)	-
Pr	-	-	-	-
Nd	0.0002 (0.0002-0.0002)	-	0.0001 (0.0001-0.0001)	-
Sm	-	-	-	-
Eu	-	-	-	-
Gd	-	-	-	-
Tb	-	-	-	-
Dy	-	-	-	-
Ho	-	-	-	-
Er	-	-	-	-
Tm	-	-	-	-
Yb	-	-	-	-

Continued.

Table 3.3.*Continued.*

Minerals	Rye	LV	Oat	LV
Lu	-	-	-	-
Hf	-	-	0.002 (0.002-0.002)	-
Ta	0.0005 (0.0004-0.0005)	-	0.003 (0.002-0.003)	-
W	0.007 (0.006-0.007)	-	0.02 (0.02-0.02)	-
Re	-	-	-	-
Os	0.01 (0.01-0.01)	-	0.02 (0.02-0.03)	-
Ir	-	-	0.002 (0.001-0.002)	-
Pt	0.0008 (0.0008-0.0009)	-	0.001 (0.0007-0.001)	-
Tl	-	-	-	-
Pb	0.003 (0.003-0.003)	-	0.002 (0.001-0.002)	-
Th	-	-	-	-
U	0.0003 (0.0003-0.0003)	-	-	-

Table 3.4 Metabolite contents of cereal grains as determined by NMR (Conc. mg/100 g FW).

Metabolites	Wheat	LV[1]	Metabolites	Barley	LV
Adenosine	122.5 (121.4-123.5)	-	**Adenosine**	176.3 (157.1-195.5)	-
Alanine	441.3 (437.8-444.9)	460	**Alanine**	604.4 (580.4-628.3)	410
Arginine	599.3 (544.2-654.4)	550	**Arginine**	325.0 (312.7-337.2)	440
Asparagine	412.4 (411.7-413.2)	-	**Asparagine**	494.3 (479.9-508.7)	-
Aspartate	1254.8 (1134.6-1375.0)	610	**Aspartate**	422.1 (411.7-432.4)	540
Betaine	57.7 (55.4-60.0)	73	**Betaine**	22.9 (20.3-25.5)	66
Choline	361.5 (358.5-364.5)	-	**Choline**	457.4 (435.3-479.5)	-
Cystine	655.6 (610.7-700.5)	-	**Ethanol**	17.4 (15.4-19.4)	-
Cytidine	67.4 (67.0-67.7)	-	**Formic acid**	14.6 (14.2-15.0)	-
Ethanol	52.9 (52.4-53.3)	-	**Fructose**	390.4 (378.7-402.0)	-
Formic acid	126.2 (126.1-126.4)	-	**Fumaric acid**	106.7 (97.9-115.5)	-
Fructose	119.2 (116.4-122.0)	-	**Glutamic acid**	2068.3 (2004.1-2132.5)	2400
Fumaric acid	223.9 (201.1-246.7)	-	**Glutamine**	323.3 (314.7-331.9)	-
Glucose	127.5 (126.4-128.6)	-	**Glycine**	356.1 (337-375.3)	360
Glutamic acid	3127.9 (3051.5-3204.2)	3400	**Histidine**	205.7 (203.1-208.3)	240
Glutamine	354.2 (327.4-381.0)	-	**Isoleucine**	224.0 (175.5-272.4)	410
Glycine	428.1 (426.0-430.2)	480	**Leucine**	284.4 (205.9-362.9)	740
Histidine	289.7 (287.1-292.3)	280	**Lysine**	318.5 (308.9-328.1)	350
Isoleucine	229.3 (226.8-231.9)	420	**Maltose**	503.6 (446.6-560.5)	-
Leucine	220.0 (218.0-221.9)	750	**Methionine**	117.9 (108.6-127.1)	160
Lysine	295.0 (294.5-295.5)	370	**Ornithine**	113.2 (109.1-117.3)	-
Methionine	445.8 (441.8-449.8)	-	**Phenylalanine**	285.0 (224.3-345.7)	540
Ornithine	191.3 (183.1-199.6)	-	**Proline**	1152.5 (1133.6-1171.4)	1200
Phenylalanine	480.5 (472.8-488.3)	520	**Pyroglutamate**	724.0 (697.5-750.5)	-
Proline	673.0 (652.1-693.8)	1000	**Serine**	610.9 (589.7-632.1)	470
Pyroglutamate	381.6 (378.3-384.9)	-	**Sucrose**	244.7 (218.0-271.4)	-
Serine	954.6 (946.4-962.9)	550	**Threonine**	318.9 (316.7-321.2)	330
Sucrose	337.0 (325.5-348.6)	-	**Trigonelline**	33.0 (29.3-36.8)	-
Threonine	426.2 (405.5-447.0)	350	**Tryptophan**	193.2 (172.0-214.4)	120
Trigonelline	519.8 (515.4-524.2)	-	**Tyrosine**	134.2 (119.0-149.3)	270
Tryptophan	159.7 (154.8-164.6)	150	**Valine**	477.6 (469.7-485.4)	570
Tyrosine	246.3 (209.7-283.0)	290	**β-Alanine**	42.7 (37.9-47.6)	-
Valine	511.3 (510.8-511.8)	570			

[1]LV for Literature value. References to the LV's are provided in the AFCDB. *Continued.*

Table 3.4.*Continued.*

Metabolites	Oat	LV	Metabolites	Rye	LV
Adenosine	215.8 (209.5-222.1)	-	**2-Aminoadipate**	183.4 (174.9-191.9)	-
Alanine	681.1 (680.2-682.0)	700	**Adenosine**	185.4 (123.6-247.2)	-
Arginine	595.8 (503.3-688.4)	910	**Alanine**	385.3 (379.7-390.8)	420
Asparagine	1137.0 (1108.4-1165.6)	-	**Arginine**	464.5 (435.7-493.2)	440
Aspartate	1206.8 (1166.3-1247.4)	1200	**Asparagine**	442.8 (412.9-472.8)	-
Betaine	26.1 (25.3-26.9)	31	**Aspartate**	805.8 (785.0-826.6)	650
Choline	636.7 (618.1-655.4)	-	**Betaine**	73.0 (69.6-76.4)	146.0
Cystine	798.2 (673.7-922.8)	390	**Carnitine**	2.2 (2.1-2.3)	-
Cytidine	117.6 (113.3-121.8)	-	**Choline**	725.2 (495.8-954.7)	-
Ethanol	93.1 (90.4-95.8)	-	**Ethanol**	208.7 (160.2-257.2)	-
Formic acid	220.8 (214.4-227.2)	-	**Formic acid**	219.7 (171.1-268.3)	-
Fructose	284.5 (209.3-359.6)	-	**Fructose**	433.7 (413.6-453.8)	-
Fumaric acid	398.8 (361.6-436.0)	-	**Fumaric acid**	833.6 (725.8-941.4)	-
Glucose	224.1 (216.9-231.3)	-	**Glucose**	336.2 (329.3-343.1)	-
Glutamic acid	2913.8 (2890.9-2936.8)	3000	**Glutamic acid**	1645.7 (1594.9-1696.5)	2000
Glutamine	992.3 (912.6-1072.1)	-	**Glutamine**	603.1 (568.9-637.1)	-
Glycine	768.2 (763.8-772.6)	770	**Glycine**	630.5 (599.8-661.3)	-
Histidine	259.8 (254.9-264.8)	320	**Histidine**	157.6 (126.1-189.1)	230
Isoleucine	253.7 (197.8-309.6)	570	**Isoleucine**	158.9 (145.7-172.1)	350
Leucine	462.1 (361.5-562.6)	1000	**Leucine**	166.7 (166.2-167.1)	610
Lysine	572.7 (556.1-589.3)	590	**Lysine**	301.2 (268.9-333.5)	380
Methionine	126.7 (105.3-148.2)	230	**Methionine**	188 (175.7-200.3)	-
Ornithine	78.1 (76.7-79.5)	-	**Ornithine**	160.3 (148.4-172.2)	-
Phenylalanine	700.8 (689.1-712.6)	750	**Phenylalanine**	260.7 (257.6-263.8)	420
Proline	1147.9 (1119.3-1176.4)	1100	**Proline**	686.8 (683.7-690.0)	790
Pyroglutamate	672.5 (653.0-692.1)	-	**Pyroglutamate**	279.2 (266.6-291.8)	-
Serine	823.7 (799.7-847.7)	770	**Sucrose**	204.0 (170.6-237.3)	-
Sucrose	563.8 (542.3-585.3)	-	**Serine**	325.7 (307.3-344.2)	560
Threonine	508.6 (493.6-523.5)	480	**Threonine**	267.9 (255.5-280.3)	330
Trigonelline	916.1 (889.5-942.6)	-	**Trigonelline**	118.4 (116.7-120.2)	-
Tryptophan	387.4 (280.6-494.2)	180	**Tryptophan**	149.4 (143.1-155.8)	110
Tyrosine	408.4 (377.0-439.8)	430	**Tyrosine**	216.9 (211.9-221.9)	230
Valine	452.6 (416.8-488.3)	840	**Valine**	345.7 (337.7-353.7)	510

Table 3.5 Metabolite contents of cereal grains as determined by DFI/LC-MS/MS (Conc. mg/100 g FW).

Metabolites	Wheat	Rye	Barley	Oat
DL-Carnitine	0.85 (0.85-0.86)	1.9 (1.8-2.1)	-	1.2 (1.1-1.2)
Decanoyl-L carnitine	-	-	-	-
Decenoyl-L-carnitine	-	-	0.07 (0.073-0.079)	-
Decadienyl-L-carnitine	0.02 (0.02-0.03)	0.06 (0.03-0.06)	-	0.03(0.02-0.04)
Dodecanoyl-L-carnitine	0.14 (0.09-0.2)	0.58 (0.53-0.63)	0.15 (0.11-0.21)	0.28(0.22-0.35)
Dodecanedioyl-L-carnitine	-	-	-	-
Dodecenoyl-L-carnitine	0.11(0.07-0.15)	0.62 (0.51-0.73)	0.19 (0.14-0.25)	-
Tetradecanoyl-L-carnitine	0.02 (0.01-0.03)	0.02 (0.01-0.02)	0.04 (0.03-0.05)	-
Tetradecenoyl-L-carnitine	0.005 (0.004-0.006)	-	-	0.01 (0.014-0.015)
Hydroxytetradecenoyl-L-carnitine	-	-	-	-
Tetradecadienyl-L-carnitine	-	0.01 (0.008-0.019)	-	-
Hydroxytetradecadienyl-L-carnitine	-	-	-	-
Hexadecanoyl-L-carnitine	0.01 (0.01-0.02)	-	-	-
Hydroxyhexadecanoyl-L-carnitine	0.005 (0.004-0.006)	0.01 (0.011-0.019)	0.01 (0.013-0.017)	0.01 (0.008-0.014)
Hexadecenoyl-L-carnitine	-	-	-	-
Hydroxyhexadecenoyl-L-carnitine	-	-	-	-
Hexadecadienyl-L-carnitine	-	0.01 (0.008-0.017)	-	-
Hydroxyhexadecadienyl-L-carnitine	-	-	-	-
Octadecanoyl-L-carnitine	0.007 (0.0072-0.008)	-	-	-
Octadecenoyl-L-carnitine	0.01 (0.009-0.02)	-	-	-
Hydroxyoctadecenoyl-L-carnitine	-	-	-	-
Octadecadienyl-L-carnitine	0.005 (0.004-0.005)	0.01 (0.011-0.012)	-	-
Acetyl-L-carnitine	0.02 (0.02-0.03)	-	-	-
Propionyl-L-carnitine	-	-	-	-
Malonyl-L-carnitine	0.01 (0.008-0.02)	0.14 (0.14-0.14)	0.14 (0.13-0.15)	0.06 (0.042-0.088)
Hydroxypropionyl-L-carnitine	-	-	-	-
Propenyl-L-carnitine	0.007 (0.006-0.008)	0.03 (0.025-0.031)	0.02 (0.016-0.023)	0.01 (0.013-0.019)
Butyryl-L-carnitine	0.02 (0.019-0.026)	0.013 (0.013-0.013)	-	0.01 (0.01-0.017)
Butenyl-L-carnitine	-	-	-	-
Fumaryl-L-carnitine	-	0.03 (0.02-0.04)	-	-
Valeryl-L-carnitine	-	-	-	-
Methylglutaryl-L-carnitine	0.015 (0.0143-0.015)	0.08 (0.07-0.09)	-	-
Methylmalonyl-L-carnitine	-	-	-	-
Tiglyl-L-carnitine	-	-	-	-
Glutaconyl-L-carnitine	-	0.01 (0.008-0.011)	-	-
Glutaryl-L-carnitine	-	-	-	-
Hexenoyl-L-carnitine	-	0.03 (0.021-0.031)	-	0.04 (0.023-0.066)
Pimelyl-L-carnitine	-	-	-	-
Octanoyl-L-carnitine	-	-	-	-
Nonayl-L-carnitine	-	-	-	-

[1] LV for Literature value. References for the LV's are provided in the AFCDB website. *Continued.*

Table 3.5.*Continued.*

Metabolites	Wheat	Rye	Barley	Oat
lysoPhosphatidylcholine acyl C14:0	-	-	-	0.11 (0.09-0.14)
lysoPhosphatidylcholine acyl C16:0	3.1 (1.9-4.4)	0.30 (0.16-0.45)	12.8 12.8-12.8)	2.5 (2.1-2.8)
lysoPhosphatidylcholine acyl C16:1	0.05 (0.05-0.05)	0.03 (0.01-0.04)	0.16 (0.16-0.17)	0.009 (0.006-0.01)
lysoPhosphatidylcholine acyl C17:0	0.04 (0.04-0.04)	0.20 (0.15-0.25)	0.09 (0.08-0.10)	0.005 (0.005-0.006)
lysoPhosphatidylcholine acyl C18:0	0.11 (0.09-0.14)	0.69 (0.66-0.72)	0.87 (0.83-0.92)	0.06 (0.06-0.07)
lysoPhosphatidylcholine acyl C18:1	0.64 (0.45-0.82)	0.07 (0.07-0.07)	1.6 (0.02-3.1)	0.37 (0.33-0.42)
lysoPhosphatidylcholine acyl C18:2	3.1 (2.4-3.7)	0.30 (0.10-0.50)	10.4 (0.03-20.8)	1.1 (0.91-1.4)
lysoPhosphatidylcholine acyl C20:3	-	-	-	-
lysoPhosphatidylcholine acyl C20:4	0.06 (0.05-0.06)	0.03 (0.02-0.04)	-	-
lysoPhosphatidylcholine acyl C24:0	-	-	-	-
lysoPhosphatidylcholine acyl C26:0	-	-	-	-
lysoPhosphatidylcholine acyl C26:1	-	-	-	-
lysoPhosphatidylcholine acyl C28:0	-	-	-	-
lysoPhosphatidylcholine acyl C28:1	-	-	-	-
Phosphatidylcholine diacyl C 24:0	-	-	-	-
Phosphatidylcholine diacyl C 26:0	-	-	-	-
Phosphatidylcholine diacyl C 28:1	-	-	-	-
Phosphatidylcholine diacyl C 30:0	-	-	-	-
Phosphatidylcholine diacyl C 30:2	-	0.007(0.006-0.008)	-	-
Phosphatidylcholine diacyl C 32:0	0.28 (0.22-0.33)	0.05 (0.05-0.06)	0.08 (0.08-0.08)	0.86 (0.74-0.98)
Phosphatidylcholine diacyl C 32:1	0.07 (0.06-0.09)	-	-	0.17 (0.15-0.20)
Phosphatidylcholine diacyl C 32:2	0.02 (0.02-0.02)	0.03 (0.02-0.05)	0.03 (0.02-0.05)	0.15 (0.14-0.16)
Phosphatidylcholine diacyl C 32:3	-	-	-	-
Phosphatidylcholine diacyl C 34:1	0.90 (0.11-1.7)	0.73 (0.58-0.87)	0.43 (0.28-0.57)	0.30 (0.18-0.42)
Phosphatidylcholine diacyl C 34:2	1.5 (0.14-2.8)	0.23 (0.18-0.31)	1.9 (0.03-3.8)	1.6 (1.3-1.8)
Phosphatidylcholine diacyl C 34:3	0.26 (0.23-0.28)	0.54 (0.43-0.64)	0.64 (0.51-0.78)	0.56 (0.34-0.78)
Phosphatidylcholine diacyl C 34:4	0.02 (0.02-0.03)	0.04 (0.04-0.04)	0.03 (0.02-0.04)	0.03 (0.02-0.03)
Phosphatidylcholine diacyl C 36:0	-	-	-	-
Phosphatidylcholine diacyl C 36:1	0.25 (0.20-0.30)	0.05 (0.04-0.06)	-	0.13 (0.02-0.24)
Phosphatidylcholine diacyl C 36:2	0.50 (0.41-0.59)	0.61 (0.60-0.62)	0.71 (0.71-0.71)	0.31 (0.27-0.36)
Phosphatidylcholine diacyl C 36:3	1.2 (0.96-1.3)	0.02 (0.02-0.03)	1.1 (0.99-1.3)	0.50 (0.41-0.60)
Phosphatidylcholine diacyl C 36:4	1.6 (0.62-2.5)	0.06 (0.05-0.07)	1.9 (0.01-3.8)	0.51 (0.41-0.61)
Phosphatidylcholine diacyl C 36:5	0.19 (0.09-0.28)	0.01 (0.01-0.02)	0.51 (0.42-0.60)	0.46 (0.40-0.53)
Phosphatidylcholine diacyl C 36:6	0.02 (0.02-0.03)	0.17 (0.12-0.21)	0.09 (0.08-0.10)	0.06 (0.05-0.06)
Phosphatidylcholine diacyl C 38:0	-	-	-	-
Phosphatidylcholine diacyl C 38:1	-	-	-	-
Phosphatidylcholine diacyl C 38:3	0.07 (0.06-0.09)	0.13 (0.12-0.13)	-	0.20 (0.10-0.29)
Phosphatidylcholine diacyl C 38:4	0.04 (0.04-0.04)	0.05 (0.04-0.07)	-	-
Phosphatidylcholine diacyl C 38:5	0.06 (0.05-0.07)	0.03 (0.02-0.04)	0.06 (0.05-0.06)	0.02 (0.01-0.03)
Phosphatidylcholine diacyl C 38:6	0.03 (0.02-0.04)	-	-	-
Phosphatidylcholine diacyl C 40:1	-	-	-	-
Phosphatidylcholine diacyl C 40:2	-	-	0.02 (0.01-0.031)	-
Phosphatidylcholine diacyl C 40:3	0.006 (0.005-0.007)	-	-	-
Phosphatidylcholine diacyl C 40:4	0.006 (0.005-0.008)	-	-	0.01 (0.01-0.02)
Phosphatidylcholine diacyl C 40:5	-	-	-	-
Phosphatidylcholine diacyl C 40:6	-	-	-	-

Continued.

Table 3.5.*Continued.*

Metabolites	Wheat	Rye	Barley	Oat
Phosphatidylcholine diacyl C 42:0	-	-	-	-
Phosphatidylcholine diacyl C 42:1	0.04 (0.03-0.05)	0.05 (0.04-0.05)	0.03 (0.03-0.04)	0.02 (0.02-0.02)
Phosphatidylcholine diacyl C 42:2	0.05 (0.03-0.07)	0.07 (0.07-0.08)	0.08 (0.07-0.08)	0.06 (0.06-0.07)
Phosphatidylcholine diacyl C 42:4	0.004 (0.003-0.005)	-	-	0.01 (0.01-0.01)
Phosphatidylcholine diacyl C 42:5	-	-	-	-
Phosphatidylcholine diacyl C 42:6	-	-	-	-
Phosphatidylcholine acyl-alkyl C 30:0	-	-	-	-
Phosphatidylcholine acyl-alkyl C 30:1	-	0.02 (0.01-0.03)	-	-
Phosphatidylcholine acyl-alkyl C 30:2	-	-	-	-
Phosphatidylcholine acyl-alkyl C 32:1	0.006 (0.006-0.007)	-	-	-
Phosphatidylcholine acyl-alkyl C 32:2	-	-	-	-
Phosphatidylcholine acyl-alkyl C 34:0	0.02 (0.02-0.03)	-	-	-
Phosphatidylcholine acyl-alkyl C 34:1	0.04 (0.04-0.04)	0.03 (0.02-0.03)	0.02 (0.01-0.02)	0.03 (0.01-0.04)
Phosphatidylcholine acyl-alkyl C 34:2	0.03 (0.03-0.04)	0.06 (0.05-0.07)	0.04 (0.03-0.05)	0.03 (0.02-0.04)
Phosphatidylcholine acyl-alkyl C 34:3	0.009 (0.009-0.01)	-	0.02 (0.01-0.02)	-
Phosphatidylcholine acyl-alkyl C 36:0	0.12 (0.10-0.15)	-	-	-
Phosphatidylcholine acyl-alkyl C 36:1	0.28 (0.26-0.30)	0.10 (0.10-0.10)	0.18 (0.12-0.25)	0.19 (0.12-0.26)
Phosphatidylcholine acyl-alkyl C 36:2	0.16 (0.13-0.19)	0.07 (0.06-0.08)	0.05 (0.03-0.07)	0.05 (0.05-0.05)
Phosphatidylcholine acyl-alkyl C 36:3	0.04 (0.03-0.05)	0.03 (0.03-0.03)	0.01 (0.009-0.01)	0.03 (0.03-0.03)
Phosphatidylcholine acyl-alkyl C 36:4	0.01 (0.009-0.01)	0.02 (0.01-0.03)	0.02 (0.01-0.02)	-
Phosphatidylcholine acyl-alkyl C 36:5	-	-	-	-
Phosphatidylcholine acyl-alkyl C 38:0	0.03 (0.01-0.05)	-	-	-
Phosphatidylcholine acyl-alkyl C 38:1	0.07 (0.05-0.09)	-	-	-
Phosphatidylcholine acyl-alkyl C 38:2	0.06 (0.05-0.07)	0.08 (0.08-0.08)	0.02 (0.01-0.03)	0.06 (0.06-0.07)
Phosphatidylcholine acyl-alkyl C 38:3	0.03 (0.0-0.06)	0.09 (0.009-0.18)	0.12 (0.09-0.15)	0.10 (0.09-0.11)
Phosphatidylcholine acyl-alkyl C 38:4	0.09 (0.09-0.09)	0.21 (0.16-0.27)	0.10 (0.10-0.10)	0.06 (0.04-0.08)
Phosphatidylcholine acyl-alkyl C 38:5	0.02 (0.01-0.02)	0.04 (0.02-0.06)	0.01 (0.01-0.02)	0.02 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 38:6	0.04 (0.03-0.04)	-	-	-
Phosphatidylcholine acyl-alkyl C 40:1	-	-	-	-
Phosphatidylcholine acyl-alkyl C 40:2	0.02 (0.01-0.02)	0.02 (0.02-0.02)	-	-
Phosphatidylcholine acyl-alkyl C 40:3	0.02 (0.01-0.02)	-	-	-
Phosphatidylcholine acyl-alkyl C 40:4	-	-	-	-
Phosphatidylcholine acyl-alkyl C 40:5	0.007 (0.005-0.009)	0.008 (0.008-0.009)	-	-
Phosphatidylcholine acyl-alkyl C 40:6	0.02 (0.02-0.02)	-	-	-
Phosphatidylcholine acyl-alkyl C 42:0	0.19 (0.11-0.28)	0.36 (0.08-0.63)	0.65 (0.59-0.71)	0.67 (0.66-0.68)
Phosphatidylcholine acyl-alkyl C 42:1	0.02 (0.01-0.02)	0.06 (0.06-0.06)	0.06 (0.05-0.06)	0.05 (0.05-0.06)
Phosphatidylcholine acyl-alkyl C 42:2	0.05 (0.01-0.09)	0.01 (0.01-0.01)	0.02 (0.02-0.02)	0.02 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 42:3	0.006 (0.005-0.007)	0.01 (0.01-0.01)	0.007 (0.006-0.008)	0.02 (0.01-0.02)
Phosphatidylcholine acyl-alkyl C 42:4	-	-	-	-
Phosphatidylcholine acyl-alkyl C 42:5	-	-	-	-
Phosphatidylcholine acyl-alkyl C 44:3	0.005 (0.002-0.007)	0.03 (0.03-0.03)	0.02 (0.02-0.03)	0.02 (0.02-0.03)
Phosphatidylcholine acyl-alkyl C 44:4	0.05 (0.03-0.08)	0.07 (0.07-0.07)	0.06 (0.05-0.07)	0.05 (0.05-0.05)
Phosphatidylcholine acyl-alkyl C 44:5	0.02 (0.02-0.02)	0.09 (0.07-0.11)	0.05 (0.04-0.07)	0.05 (0.04-0.05)
Phosphatidylcholine acyl-alkyl C 44:6	-	-	-	-

Continued.

Table 3.5.*Continued.*

Metabolites	Wheat	LV	Barley	LV [1]
Alanine	403.5 (374.4-432.7)	460	576.3 (549.8-602.7)	410
Arginine	647.5 (620.9-674)	550	≥ 70	440
Asparagine	256.7 (250.5-262.9)	-	452.8 (413.9-491.7)	-
Asparatic Acid	1047.5 (1015.7-1079.4)	610	489.7 (409.5-570)	540
Citrulline	67.7 (67.6-67.8)	-	47.9 (44.82-51.09)	-
Glutamine	339.8 (309.8-369.8)	-	261.3 (217.9-304.8)	-
Glutamic acid	≥ 300	3400	1919.1 (1752.2-2086)	2400
Glycine	453.4 (425.2-481.6)	480	340.3 (333.7-346.8)	360
Histidine	278.8 (258.1-299.5)	280	275.3 (264-286.7)	240
Isoleucine	≥262.4	420	≥262.4	410
Leucine	≥ 262.4	750	≥ 262.4	740
Lysine	302.7 (268.4-337.1)	370	424.4 (337.3-511.5)	350
Methionine	≥ 59.7	170	≥ 59.7	160
Ornithine	≥ 132.2	-	≥ 132.2	
Phenylalanine	435.6 (402.8-468.3)	520	375.2 (318.1-432.3)	540
Proline	642.1 (564.3-719.9)	1000	1461 (1278.7-1643.2)	1200
Serine	521.5 (240.4-802.7)	550	673.4 (581.9-764.9)	470
Threonine	449.6 (424.6-474.7)	350	≥ 119.1	330
Tryptophan	163.7 (120.6-206.8)	150	≥ 40.8	120
Tyrosine	≥ 181.2	290	≥ 181.2	270
Valine	527.3 (490.5-564.2)	570	626 (607.1-644.9)	570
Acetylornithine	153.9 (119-188.7)	-	47.8 (37.7-57.9)	-
Dimethylarginine	6.6 (4.6-8.5)	-	10.7 (9.9-11.6)	-
Alpha-aminoadipic acid	23.3 (9-37.7)	-	-	-
Carnosine	-	-	-	-
Creatinine	-	-	-	-
Levodopa	-	-	-	-
Dopamine	-	-	-	-
Histamine	-	-	-	-
Kynurenine	-	-	-	-
Methioninesulfoxide	-	-	-	-
cis 4-Hydroxyproline	-	-	-	-
trans4-Hydroxyproline	-	-	-	-
Phenylethylamine	-	-	-	-
Putrescine	-	-	63.7 (58.6-68.8)	-
Serotonin	-	-	-	-
Taurine	-	-	-	-

Table 3.5.*Continued.*

Metabolites	Oat	LV	Rye	LV
Alanine	643.2 (610.3-676.2)	690	513.3 (473.3-553.3)	390
Arginine	≥ 70	890	477.1 (466.1-488.2)	440
Asparagine	2384.5 (2274.5-2494.6)	-	421 (371.6-470.3)	-
Asparatic Acid	1503.2 (1229.6-1776.7)	1200	463 (452.2-473.9)	560
Citrulline	40.25 (39.9-40.6)	-	23.1 (22.7-23.4)	-
Glutamine	947.4 (901.4-993.4)	-	683.9 (675.8-691.9)	-
Glutamic acid	2647.5 (2435-2859.9)	2900	1620.2 (1296.3-1944)	3000
Glycine	≥ 375.5	760	≥ 375.5	-
Histidine	290.4 (259.1-321.7)	310	154.3 (144.6-164)	240
Isoleucine	≥262.4	560	≥262.4	-
Leucine	≥ 262.4	1000	≥ 262.4	-
Lysine	429 (338.3-519.6)	580	354.2 (351.4-356.9)	290
Methionine	≥ 59.7	220	≥ 59.7	-
Ornithine	≥ 132.2		≥ 132.2	-
Phenylalanine	670.9 (666.1-675.7)	740	190.3 (187.6-192.9)	520
Proline	1494.1 (1470.6-1517.5)	1100	1032 (1026.6-1037.4)	990
Serine	830.7 (817.1-844.3)	760	238.5 (237.2-239.8)	560
Threonine	≥ 119.1	470	≥ 119.1	-
Tryptophan	≥ 40.8	180	≥ 40.8	-
Tyrosine	≥ 181.2	420	≥ 181.2	-
Valine	≥117.1	820	≥117.1	-
Acetylornithine	-	-	-	-
Dimethylarginine	-	-	-	-
Alpha-aminoadipic acid	-	-	66.9 (66.7-67.1)	-
Carnosine	-	-	-	-
Creatinine	-	-	-	-
Levodopa	-	-	-	-
Dopamine	-	-	-	-
Histamine	-	-	-	-
Kynurenine	-	-	-	-
Methioninesulfoxide	-	-	-	-
cis 4-Hydroxyproline	-	-	-	-
trans4-Hydroxyproline	-	-	-	-
Phenylethylamine	-	-	-	-
Putrescine	27 (25.1-28.9)	-	50.1 (46.9-53.3)	-
Serotonin	10.8 (9.2-12.4)	-	-	-
Taurine	-	-	-	-

Table 3.6 Lipid contents of cereals as determined by GC-MS (molar%). Note that: GL is for glycolipids, PL is for phospholipids, CE is for cholesteryl esters, TG is for triglycerides and FF is for free fatty acids.

Lipids	Wheat lipids					Barley lipids				
	GL[1]	PL[2]	Neutral lipids			GL	PL	Neutral lipids		
			CE[3]	TG[4]	FF[5]			CE	TG	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	0.64	0.17	1.73	71.2	1.33	2.15	2.29	2.31	22.3	9.85
C15:0	0.52	-	-	28.7	-	0.66	0.85	-	-	1.62
C15:1 (10)	-	-	-	-	-	-	-	-	-	-
C16:0	68.6	34.0	6.98	-	39.0	46.3	50.1	54.8	53.7	44.8
C16:1 (9)	-	-	-	-	-	-	-	-	-	-
C17:0	2.08	2.45	13.0	-	6.37	7.43	8.22	8.15	18.0	10.8
C17:1 (10)	-	-	-	-	-	-	-	-	-	-
C18:0	2.84	1.98	14.0	-	2.25	9.80	10.0	-	-	-
C18:1 (9)	-	-	-	-	4.22	5.9	15.1	12.2	-	-
C18:2 (9,12)	3.91	56.0	55.1	-	41.2	5.38	13.2	2.71	-	-
C18:3 (6,9,12)	-	-	-	-	-	-	-	16.8	-	-
C20:0	-	-	1.09	-	0.27	-	-	1.65	-	3.87
C18:3 (9,12,15)	21.1	5.32	6.82	-	5.26	22.3	-	-	-	20.5
C20:1 (11)	-	-	-	-	-	-	-	1.24	-	2.13
C21:0	-	-	-	-	-	-	-	-	-	-
C20:2 (11,14)	-	-	-	-	-	-	-	-	-	0.66
C20:3 (8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	-	-	-	-	-	-	-	-	-	3.02
C20:4 (5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1 (13)	0.19	-	1.08	-	-	-	-	-	-	0.71
C23:0	-	-	-	-	-	-	-	-	5.93	0.6
C20:5 (5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	-	-	-	-	-	-	-	1.34
C24:1 (15)	-	-	-	-	-	-	-	-	-	-
C22:6	-	-	-	-	-	-	-	-	-	-

Continued.

[1] GL for glycolipids
[2] PL for phospholipids
[3] CE for cholesteryl esters
[4] TG for triglycerides
[5] FF for free fatty acids

Table 3.6.*Continued.*

Lipids	Oat lipids					Rye lipids				
	GL	PL	Neutral lipids			GL	PL	Neutral lipids		
			CE	TG	FF			CE	T	FF
C12:0	-	-	-	-	-	-	-	-	-	-
C13:0	-	-	-	-	-	-	-	-	-	-
C14:0	1.91	-	2.25	-	11.9	-	-	0.82	10	0.93
C15:0	-	-	-	-	11.2	-	-	-	-	-
C15:1 (10)	-	-	-	-	-	-	-	-	-	-
C16:0	59.9	68.9	32.0	36.1	46.2	21.2	57.8	42.0	-	37.6
C16:1 (9)	1.04	-	-	-	4.69	-	-	-	-	-
C17:0	3.40	4.90	26.6	11.7	4.63	1.93	4.80	9.77	-	-
C17:1 (10)	-	-	-	-	-	-	-	-	-	-
C18:0	4.59	2.33	37.7	12.0	-	4.95	1.03	12.4	-	10.5
C18:1 (9)	6.41	2.28	-	3.89	-	6.62	5.68		-	
C18:2 (9,12)	21.0	18.6	-	22.6	-	56.5	3.38	29.1	-	39.6
C18:3 (6,9,12)	-	-	-	-	-	-	-	-	-	-
C20:0	-	-	-	-	-	-	-	-	-	-
C18:3 (9,12,15)	1.40	2.92	1.27	13.5	-	8.70	27.3	4.81	-	10.8
C20:1 (11)	-	-	-	-	-	-	-	-	-	-
C21:0	-	-	-	-	17.5	-	-	-	-	-
C20:2 (11,14)	-	-	-	-	-	-	-	-	-	-
C20:3 (8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:0	-	-	-	-	2.27	-	-	0.49	-	-
C20:4 (5,8,11,14)	-	-	-	-	-	-	-	-	-	-
C22:1 (13)	0.28	-	-	-	1.31	-	-	0.51	-	0.39
C23:0	-	-	-	-	-	-	-	-	-	-
C20:5 (5,8,11,14,17)	-	-	-	-	-	-	-	-	-	-
C24:0	-	-	-	-	-	-	-	-	-	-
C24:1 (15)	-	-	-	-	-	-	-	-	-	-
C22:6	-	-	-	-	-	-	-	-	-	-

Table 3.7 Estimation of the upper limit triglyceride concentrations using the CLR method.

Upper limit triglyceride concentrations	Rye	Wheat	Oat	Barley
TG(C14:0/C14:0/C14:0)	33.3	23.7	0	7.4
TG(C14:0/C14:0/C15:0)[iso3]	0	28.8	0	0
TG(C14:0/C14:0/C16:0)[iso3]	0	0	0	11.2
TG(C14:0/C14:0/C17:1(10))[iso3]	0	0	0	11.2
TG(C14:0/C14:0/C18:0)[iso3]	0	0	0	0
TG(C14:0/C14:0/C18:1(9))[iso3]	0	0	0	0
TG(C14:0/C14:0/C18:2(9,12))[iso3]	0	0	0	0
TG(C14:0/C14:0/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C14:0/C14:0/C23:0)[iso3]	0	0	0	5.9
TG(C14:0/C15:0/C15:0)[iso3]	0	28.8	0	0
TG(C14:0/C15:0/C16:0)[iso6]	0	0	0	0
TG(C14:0/C15:0/C17:1(10))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:0)[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:1(9))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C15:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C15:0/C23:0)[iso6]	0	0	0	0
TG(C14:0/C16:0/C16:0)[iso3]	0	0	0	11.2
TG(C14:0/C16:0/C17:1(10))[iso6]	0	0	0	18.1
TG(C14:0/C16:0/C18:0)[iso6]	0	0	0	0
TG(C14:0/C16:0/C18:1(9))[iso6]	0	0	0	0
TG(C14:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C16:0/C23:0)[iso6]	0	0	0	5.9
TG(C14:0/C17:1(10)/C17:1(10))[iso3]	0	0	0	11.2
TG(C14:0/C17:1(10)/C18:0)[iso6]	0	0	0	0
TG(C14:0/C17:1(10)/C18:1(9))[iso6]	0	0	0	0
TG(C14:0/C17:1(10)/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C17:1(10)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C17:1(10)/C23:0)[iso6]	0	0	0	5.9
TG(C14:0/C18:0/C18:0)[iso3]	0	0	0	0
TG(C14:0/C18:0/C18:1(9))[iso6]	0	0	0	0
TG(C14:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C18:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C18:0/C23:0)[iso6]	0	0	0	0
TG(C14:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0
TG(C14:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0
TG(C14:0/C18:1(9)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C18:1(9)/C23:0)[iso6]	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0
TG(C14:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C14:0/C18:2(9,12)/C23:0)[iso6]	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C14:0/C18:3(6,9,12)/C23:0)[iso6]	0	0	0	0
TG(C14:0/C23:0/C23:0)[iso3]	0	0	0	5.9
TG(C15:0/C15:0/C15:0)	0	9.6	0	0
TG(C15:0/C15:0/C16:0)[iso3]	0	0	0	0
TG(C15:0/C15:0/C17:1(10))[iso3]	0	0	0	0
TG(C15:0/C15:0/C18:0)[iso3]	0	0	0	0
TG(C15:0/C15:0/C18:1(9))[iso3]	0	0	0	0
TG(C15:0/C15:0/C18:2(9,12))[iso3]	0	0	0	0
TG(C15:0/C15:0/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C15:0/C15:0/C23:0)[iso3]	0	0	0	0
TG(C15:0/C16:0/C16:0)[iso3]	0	0	0	0
TG(C15:0/C16:0/C17:1(10))[iso6]	0	0	0	0
TG(C15:0/C16:0/C18:0)[iso6]	0	0	0	0
TG(C15:0/C16:0/C18:1(9))[iso6]	0	0	0	0

Continued

Table 3.7*Continued.*

Upper limit triglyceride concentrations	Rye	Wheat	Oat	Barley
TG(C15:0/C16:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C15:0/C16:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C15:0/C16:0/C23:0)[iso6]	0	0	0	0
TG(C15:0/C17:1(10)/C17:1(10))[iso3]	0	0	0	0
TG(C15:0/C17:1(10)/C18:0)[iso6]	0	0	0	0
TG(C15:0/C17:1(10)/C18:1(9))[iso6]	0	0	0	0
TG(C15:0/C17:1(10)/C18:2(9,12))[iso6]	0	0	0	0
TG(C15:0/C17:1(10)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C15:0/C17:1(10)/C23:0)[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:0)[iso3]	0	0	0	0
TG(C15:0/C18:0/C18:1(9))[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:2(9,12))[iso6]	0	0	0	0
TG(C15:0/C18:0/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C15:0/C18:0/C23:0)[iso6]	0	0	0	0
TG(C15:0/C18:1(9)/C18:1(9))[iso3]	0	0	0	0
TG(C15:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	0	0
TG(C15:0/C18:1(9)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C15:0/C18:1(9)/C23:0)[iso6]	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	0	0
TG(C15:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	0	0
TG(C15:0/C18:2(9,12)/C23:0)[iso6]	0	0	0	0
TG(C15:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	0	0
TG(C15:0/C18:3(6,9,12)/C23:0)[iso6]	0	0	0	0
TG(C16:0/C16:0/C16:0)	0	0	12.0	17.9
TG(C16:0/C16:0/C17:1(10))[iso3]	0	0	11.8	18.1
TG(C16:0/C16:0/C18:0)[iso3]	0	0	12.0	0
TG(C16:0/C16:0/C18:1(9))[iso3]	0	0	3.9	0
TG(C16:0/C16:0/C18:2(9,12))[iso3]	0	0	18.1	0
TG(C16:0/C16:0/C18:3(6,9,12))[iso3]	0	0	13.6	0
TG(C16:0/C16:0/C23:0)[iso3]	0	0	0	5.9
TG(C16:0/C17:1(10)/C17:1(10))[iso3]	0	0	11.8	18.1
TG(C16:0/C17:1(10)/C18:0)[iso6]	0	0	11.8	0
TG(C16:0/C17:1(10)/C18:1(9))[iso6]	0	0	3.9	0
TG(C16:0/C17:1(10)/C18:2(9,12))[iso6]	0	0	11.8	0
TG(C16:0/C17:1(10)/C18:3(6,9,12))[iso6]	0	0	11.8	0
TG(C16:0/C17:1(10)/C23:0)[iso6]	0	0	0	5.9
TG(C16:0/C18:0/C18:0)[iso3]	0	0	12.0	0
TG(C16:0/C18:0/C18:1(9))[iso6]	0	0	3.9	0
TG(C16:0/C18:0/C18:2(9,12))[iso6]	0	0	12.0	0
TG(C16:0/C18:0/C18:3(6,9,12))[iso6]	0	0	12.0	0
TG(C16:0/C18:0/C23:0)[iso6]	0	0	0	0
TG(C16:0/C18:1(9)/C18:1(9))[iso3]	0	0	3.9	0
TG(C16:0/C18:1(9)/C18:2(9,12))[iso6]	0	0	3.9	0
TG(C16:0/C18:1(9)/C18:3(6,9,12))[iso6]	0	0	3.9	0
TG(C16:0/C18:1(9)/C23:0)[iso6]	0	0	0	0
TG(C16:0/C18:2(9,12)/C18:2(9,12))[iso3]	0	0	18.1	0
TG(C16:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0	0	13.6	0
TG(C16:0/C18:2(9,12)/C23:0)[iso6]	0	0	0	0
TG(C16:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0	0	13.6	0
TG(C16:0/C18:3(6,9,12)/C23:0)[iso6]	0	0	0	0
TG(C16:0/C23:0/C23:0)[iso3]	0	0	0	5.9
TG(C17:1(10)/C17:1(10)/C17:1(10))	0	0	3.9	6.0
TG(C17:1(10)/C17:1(10)/C18:0)[iso3]	0	0	5.9	0
TG(C17:1(10)/C17:1(10)/C18:1(9))[iso3]	0	0	3.9	0
TG(C17:1(10)/C17:1(10)/C18:2(9,12))[iso3]	0	0	5.9	0
TG(C17:1(10)/C17:1(10)/C18:3(6,9,12))[iso3]	0	0	5.9	0
TG(C17:1(10)/C17:1(10)/C23:0)[iso3]	0	0	0	5.9

Continued.

Table 3.7*Continued.*

Upper limit triglyceride concentrations	Rye	Wheat	Oat	Barley
TG(C17:1(10)/C18:0/C18:0)[iso3]	0.0	0.0	5.9	0.0
TG(C17:1(10)/C18:0/C18:1(9))[iso6]	0.0	0.0	3.9	0.0
TG(C17:1(10)/C18:0/C18:2(9,12))[iso6]	0.0	0.0	11.8	0.0
TG(C17:1(10)/C18:0/C18:3(6,9,12))[iso6]	0.0	0.0	11.8	0.0
TG(C17:1(10)/C18:0/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C17:1(10)/C18:1(9)/C18:1(9))[iso3]	0.0	0.0	3.9	0.0
TG(C17:1(10)/C18:1(9)/C18:2(9,12))[iso6]	0.0	0.0	3.9	0.0
TG(C17:1(10)/C18:1(9)/C18:3(6,9,12))[iso6]	0.0	0.0	3.9	0.0
TG(C17:1(10)/C18:1(9)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C17:1(10)/C18:2(9,12)/C18:2(9,12))[iso3]	0.0	0.0	5.9	0.0
TG(C17:1(10)/C18:2(9,12)/C18:3(6,9,12))[iso6]	0.0	0.0	11.8	0.0
TG(C17:1(10)/C18:2(9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C17:1(10)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0.0	0.0	5.9	0.0
TG(C17:1(10)/C18:3(6,9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C17:1(10)/C23:0/C23:0)[iso3]	0.0	0.0	0.0	5.9
TG(C18:0/C18:0/C18:0)	0.0	0.0	4.0	0.0
TG(C18:0/C18:0/C18:1(9))[iso3]	0.0	0.0	3.9	0.0
TG(C18:0/C18:0/C18:2(9,12))[iso3]	0.0	0.0	6.0	0.0
TG(C18:0/C18:0/C18:3(6,9,12))[iso3]	0.0	0.0	6.0	0.0
TG(C18:0/C18:0/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:0/C18:1(9)/C18:1(9))[iso3]	0.0	0.0	3.9	0.0
TG(C18:0/C18:1(9)/C18:2(9,12))[iso6]	0.0	0.0	3.9	0.0
TG(C18:0/C18:1(9)/C18:3(6,9,12))[iso6]	0.0	0.0	3.9	0.0
TG(C18:0/C18:1(9)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:0/C18:2(9,12)/C18:2(9,12))[iso3]	0.0	0.0	6.0	0.0
TG(C18:0/C18:2(9,12)/C18:3(6,9,12))[iso6]	0.0	0.0	12.0	0.0
TG(C18:0/C18:2(9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:0/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0.0	0.0	6.0	0.0
TG(C18:0/C18:3(6,9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:0/C23:0/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:1(9)/C18:1(9)/C18:1(9))	0.0	0.0	1.3	0.0
TG(C18:1(9)/C18:1(9)/C18:2(9,12))[iso3]	0.0	0.0	1.9	0.0
TG(C18:1(9)/C18:1(9)/C18:3(6,9,12))[iso3]	0.0	0.0	1.9	0.0
TG(C18:1(9)/C18:1(9)/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:1(9)/C18:2(9,12)/C18:2(9,12))[iso3]	0.0	0.0	1.9	0.0
TG(C18:1(9)/C18:2(9,12)/C18:3(6,9,12))[iso6]	0.0	0.0	3.9	0.0
TG(C18:1(9)/C18:2(9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:1(9)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0.0	0.0	1.9	0.0
TG(C18:1(9)/C18:3(6,9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:1(9)/C23:0/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:2(9,12)/C18:2(9,12)/C18:2(9,12))	0.0	0.0	7.6	0.0
TG(C18:2(9,12)/C18:2(9,12)/C18:3(6,9,12))[iso3]	0.0	0.0	11.3	0.0
TG(C18:2(9,12)/C18:2(9,12)/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:2(9,12)/C18:3(6,9,12)/C18:3(6,9,12))[iso3]	0.0	0.0	11.3	0.0
TG(C18:2(9,12)/C18:3(6,9,12)/C23:0)[iso6]	0.0	0.0	0.0	0.0
TG(C18:2(9,12)/C23:0/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C18:3(6,9,12))	0.0	0.0	4.5	0.0
TG(C18:3(6,9,12)/C18:3(6,9,12)/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C18:3(6,9,12)/C23:0/C23:0)[iso3]	0.0	0.0	0.0	0.0
TG(C23:0/C23:0/C23:0)	0.0	0.0	0.0	2.0

Table 3.8. Inferred lipids consisting of all the possible sizes of the fatty acids in lipids and the sizes of the lipids involved.

Lipid Types	Lipid count
CDP-diacylglycerols	527
Glycerophosphoethanolamines	438
Glycerophosphocholines	438
Glycerophosphoglycerols	477
Phosphoglycerolphosphates	477
Glycerophosphoinositols	438
Glycerophosphoserines	438
Cardiolipins	22,775
Triacylglycerols	1,771
Monoacylglycerols	46
Diacylglycerols	527
Sphingolipids	276
Total	**28,628**

Table 3.9 Vitamin content of cereals as determined by HPLC (mg/100 g FW).

Vitamins	Wheat	LV [1]	Barley	LV
Vitamin C	-	-	-	-
Vitamin B1	0.57 (0.53-0.61)	0.35±0.086	0.45 (0.43-0.47)	0.35±0.028
Vitamin B2	0.10 (0.09-0.11)	0.15±0.049	0.095 (0.09-0.10)	0.11
Vitamin B3	4.2 (3.9-4.4)	3.05±3.18	6.6 (6.1-7.1)	5.98±0.40
Vitamin B5	0.77 (0.56-0.97)	1.5	-	-
Vitamin B6	0.66 (0.59-0.73)	0.12±0.028	0.55 (0.52-0.57)	0.36±0.042
Vitamin B7	0.008 (0.007-0.008)	0.019	0.01 (0.009-0.01)	-
Vitamin B9	0.05 (0.05-0.05)	0.037±0.013	0.007 (0.006-0.008)	0.008
Vitamin B12	-	-	-	-
Vitamin A	-	-	0.002 (0.002-0.002)	-
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.87 (0.84-0.90)	0.53	0.64 (0.61-0.67)	0.57
Vitamin K	0.003 (0.002-0.004)	0.0019	0.004 (0.004-0.004)	0.0022
	Oat	**LV**	**Rye**	**LV**
Vitamin C	-	-	-	-
Vitamin B1	0.41 (0.38-0.44)	0.59±0.24	0.39 (0.40-0.40)	0.32±0.009
Vitamin B2	0.12 (0.11-0.13)	0.12±0.007	0.11 (0.17-0.17)	0.17±0.10
Vitamin B3	0.63 (0.57-0.69)	0.88±0.11	2.2 (2.2-2.2)	2.98±1.81
Vitamin B5	0.75 (0.72-0.77)	1.5	1.3 (1.1-1.1)	0.49
Vitamin B6	0.08 (0.07-0.09)	0.13±0.01	0.38 (0.38-0.38)	0.28±0.009
Vitamin B7	0.008 (0.007-0.008)	0.03 ±0.02	0.006 (0.006-0.006)	0.006
Vitamin B9	0.07 (0.07-0.07)	0.047	0.07 (0.07-0.07)	0.05±0.02
Vitamin B12	-	-	-	-
Vitamin A	-	-	-	0.001
Vitamin D2	-	-	-	-
Vitamin D3	-	-	-	-
Vitamin E	0.40 (0.37-0.42)	0.75	1.2 (1.23-1.23)	0.85
Vitamin K	-	-	0.006 (0.007-0.007)	0.0059

[1]LV for Literature value. References to the LV's are provided in the AFCDB.

Table 3.10. Cross checking NMR withDFI/LC-MS/MS results.

Wheat metabolites	NMR	DFI/LC-MS/MS	Literature values
Alanine	441.3 (437.8-444.9)	403.5 (374.4-432.7)	460
Arginine	599.3 (544.2-654.4)	647.5 (620.9-674)	550
Asparagine	412.4 (411.7-413.2)	256.7 (250.5-262.9)	-
Asparatic Acid	1254.8 (1134.6-1375.0)	1047.5 (1015.7-1079.4)	610
Glutamine	354.2 (327.4-381.0)	339.8 (309.8-369.8)	-
Glutamic acid	3127.9 (3051.5-3204.2)	≥ 300	3400
Glycine	428.1 (426.0-430.2)	453.4 (425.2-481.6)	480
Histidine	289.7 (287.1-292.3)	278.8 (258.1-299.5)	280
Isoleucine	393.3 (387.4-399.2)	≥262.4	420
Leucine	220.0 (218.0-221.9)	≥ 262.4	750
Lysine	295.0 (294.5-295.5)	302.7 (268.4-337.1)	370
Methionine	445.8 (441.8-449.8)	≥ 59.7	170
Ornithine	191.3 (183.1-199.6)	≥ 132.2	-
Phenylalanine	480.5 (472.8-488.3)	435.6 (402.8-468.3)	520
Proline	673.0 (652.1-693.8)	642.1 (564.3-719.9)	1000
Serine	554.6 (546.4-562.9)	521.5 (240.4-802.7)	550
Threonine	426.2 (405.5-447.0)	449.6 (424.6-474.7)	350
Tryptophan	159.7 (154.8-164.6)	163.7 (120.6-206.8)	150
Tyrosine	246.3 (209.7-283.0)	≥ 117.1	290
Valine	511.3 (510.8-511.8)	527.3 (490.5-564.2)	570
Barley metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	604.4 (580.4-628.3)	576.3 (549.8-602.7)	410
Arginine	325.0 (312.7-337.2)	≥ 70	440
Asparagine	494.3 (479.9-508.7)	452.8 (413.9-491.7)	-
Asparatic Acid	422.1 (411.7-432.4)	489.7 (409.5-570)	540
Glutamine	323.3 (314.7-331.9)	261.3 (217.9-304.8)	-
Glutamic acid	2068.3 (2004.1-2132.5)	1919.1 (1752.2-2086)	2400
Glycine	341.1 (337-345.3)	340.3 (333.7-346.8)	360
Histidine	205.7 (203.1-208.3)	275.3 (264-286.7)	240
Isoleucine	224.0 (175.5-272.4)	≥262.4	410
Leucine	284.4 (205.9-362.9)	≥ 262.4	740
Lysine	318.5 (308.9-328.1)	424.4 (337.3-511.5)	350
Methionine	117.9 (108.6-127.1)	≥ 59.7	160
Ornithine	113.2 (109.1-117.3)	≥ 132.2	-
Phenylalanine	285.0 (224.3-345.7)	375.2 (318.1-432.3)	540
Proline	1152.5 (1133.6-1171.4)	1461 (1278.7-1643.2)	1200
Serine	610.9 (589-632)	673.4 (581.9-764.9)	470
Threonine	318.9 (316.7-321.2)	≥ 119.1	330

Table 3.10.*Continued.*

Barley metabolites	NMR	DFI/LC-MS/MS	Literature values
Tryptophan	193.2 (172.0-214.4)	≥ 40.8	120
Tyrosine	134.2 (119.0-149.3)	≥ 181.2	270
Valine	477.6 (469.7-485.4)	626 (607.1-644.9)	570
Oat metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	681.1 (680.2-682.0)	643.2 (610.3-676.2)	690
Arginine	595.8 (503.3-688.4)	≥ 70	890
Asparagine	1137.0 (1108.4-1165.6)	2384.5 (2274.5-2494.6)	-
Asparatic Acid	1206.8 (1166.3-1247.4)	1503.2 (1229.6-1776.7)	1200
Glutamine	992.3 (912.6-1072.1)	947.4 (901.4-993.4)	-
Glutamic acid	2913.8 (2890.9-2936.8)	2647.5 (2435-2859.9)	2900
Glycine	768.2 (763.8-772.6)	≥ 375.5	760
Histidine	259.8 (254.9-264.8)	290.4 (259.1-321.7)	310
Isoleucine	253.7 (197.8-309.6)	≥262.4	560
Leucine	462.1 (361.5-562.6)	≥ 262.4	1000
Lysine	572.7 (556.1-589.3)	429 (338.3-519.6)	580
Methionine	126.7 (105.3-148.2)	≥ 59.7	220
Ornithine	78.1 (76.7-79.5)	≥ 132.2	-
Phenylalanine	700.8 (689.1-712.6)	670.9 (666.1-675.7)	750
Proline	1147.9 (1119.3-1176.4)	1494.1 (1470.6-1517.5)	1100
Serine	823.7 (799.7-847.7)	830.7 (817.1-844.3)	760
Threonine	508.6 (493.6-523.5)	≥ 119.1	470
Tryptophan	387.4 (280.6-494.2)	≥ 40.8	180
Tyrosine	408.4 (377.0-439.8)	≥ 181.2	420
Valine	452.6 (416.8-488.3)	≥117.1	820
Rye metabolites	**NMR**	**DFI/LC-MS/MS**	**Literature values**
Alanine	385.3 (379.7-390.8)	513.3 (473.3-553.3)	390
Arginine	464.5 (435.7-493.2)	477.1 (466.1-488.2)	440
Asparagine	442.8 (412.9-472.8)	421 (371.6-470.3)	-
Asparatic Acid	805.8 (785.0-826.6)	463 (452.2-473.9)	650
Glutamine	603.1 (568.9-637.1)	683.9 (675.8-691.9)	-
Glutamic acid	1645.7 (1594.9-1696.5)	1620.2 (1296.3-1944)	2000
Glycine	630.5 (599.8-661.3)	≥ 375.5	-
Histidine	157.6 (126.1-189.1)	154.3 (144.6-164)	240
Isoleucine	158.9 (145.7-172.1)	≥262.4	-
Leucine	166.7 (166.2-167.1)	≥ 262.4	-
Lysine	301.2 (268.9-333.5)	354.2 (351.4-356.9)	290
Methionine	188 (175.7-200.3)	≥ 59.7	-
Ornithine	160.3 (148.4-172.2)	≥ 132.2	-

Table 3.10.*Continued.*

Rye metabolites	NMR	DFI/LC-MS/MS	Literature values
Phenylalanine	260.7 (257.6-263.8)	190.3 (187.6-192.9)	520
Proline	686.8 (683.7-690.0)	1032 (1026.6-1037.4)	990
Serine	325.7 (307.3-344.2)	238.5 (237.2-239.8)	560
Threonine	267.9 (255.5-280.3)	≥ 119.1	-
Tryptophan	149.4 (143.1-155.8)	≥ 40.8	110
Tyrosine	216.9 (211.9-221.9)	≥ 181.2	230
Valine	345.7 (337.7-353.7)	≥117.1	510

Chapter 4. General Conclusions & Future Work

4.1 Conclusions

My thesis project had two overall aims: 1) use advanced metabolomics platforms such as NMR, HPLC, GC-MS, ICP-MS and DFI/LC-MS/MS to identify and quantify the more abundant food chemicals and micronutrients in Alberta's common vegetables, fruits and cereals; and 2) create a fully web accessible database that contains both experimentally derived values and literature-derived information on Alberta-grown foods, called the "Alberta Food Composition Database" (AFCDB: http://afcdb.ca). The AFCDB is intended provide not only detailed chemical composition data, but also rich information on the known or presumptive health effects (with full references and hyperlinks) as well as food organoleptic properties such as flavour, color, stability, aroma features, taste, and texture. As has been outlined in Chapters 2 and 3, I believe I have achieved both of these aims. In particular, with the help of a number of members in Dr. Wishart's lab, I have experimentally identified and quantified more than 387 unique compounds and another 2599 compounds via literature reviewsfor 32 Alberta-grown fruits and vegetables. I have also experimentally identified and quantified more than 247 unique compounds as well as another 2090 compounds via literature reviews for 4 Alberta-grown cereal grains. All of the data (and the associated references) have been placed in the AFCDB. The database, which was constructed with the assistance of several web developers in Dr. Wishart's lab, contains metabolite information on a total of 70,245 compounds for 36 different Alberta-grown foods. Each compound entry contains an average of 100 data fields. The entire database occupies nearly 402 megabytes. While some of the metabolites listed in the AFCDB (i.e. the literature-derived compounds) have already been identified in other studies, many food compounds in the AFCDB were experimentally identified, quantified and reported for the very first time.

In conducting these studies, I also wanted to explore the capabilities and feasibility of using a variety of different analytical platforms or metabolomic assays for food composition analysis. My experimental work showed that it was possible to use the BiocratesIDQ system to accurately identify and quantify between 75-100 different food constituents. I also demonstrated that the application of NMR spectroscopy can be very effective in identifying between 30-40 different chemical constituents in foods. More specialized assays, such as the vitamin and polyphenol assays, which I co-developed with several members of the Wishart lab, proved to be quite effective. Comparisons of the measured results between platforms (NMR, LC-MS, GC-MS, etc.) and against previously reported values in the literature showed a high degree of reproducibility. This result was both surprising and encouraging as we expected that foods grown in different areas (other than Alberta) might vary far more in composition and/or concentration than we observed. This is because the chemical constituents in plants are reported to be highly dependent on genetics, cultivars, and environmental factors such as light, temperature, soil compounds, fertilization, irrigation, storage conditions, biotic and abiotic stress. Overall, these results suggest that food composition is much more "stable" across cultivars and locations than might have been expected. Furthermore, these data indicate that the use of standard metabolomic techniques can be quite effective in food compositional analysis. They also suggest that the use of multiple analytical platforms enhances compound coverage, while at the same time providing internal validation.

Proper measurement of the chemical constituents in foods requires careful measurement on the appropriate analytical platforms and the development of effective, efficient chemical extraction protocols. In this thesis, I reviewed, modified and (with the help of many colleagues in the Wishart lab) optimized a number of chemical extraction protocols. I also was able to

participate in the optimization and adaptation of a numberof previously described analytical assays so that they could characterize food constituents. Consequently, several novel procedures for food constituent analysis were developed through the course of this project. I believe that some of these could prove to beparticularly useful for the food chemistry community with regard to saving time, reducing costs, and improving the accuracy and efficiency of chemical identification in foods.

4.2 Future Directions

The application of metabolomics to food composition analysis is relatively new and challenges still exist with regard to food metabolite identification. Given the relatively incomplete (~70% of observed spectral area) coverage we achievedby NMR spectroscopy, it is quite clear that both NMR compound libraries and NMR spectral libraries need to be expanded. This is true not only for NMR, but also for MS/MS and GC-MS libraries.Currently there is a real shortage of plant metabolite (especially secondary metabolite)spectra in public libraries or databases such as HMDB, NIST, Metlin, MoNA and MassBank. A sustained effort by the food analysis community or an improved system for exchanging or sharing compounds or compound information in food metabolomics studies would certainly help. In this regard, the development of the Food Compound Exchange (FoodComEx), an initiative by the JPI-BioNH program in France and Holland, could lead to substantial benefits for the food analysis community.

While improved databases would certainly help, the development of more automated data processing tools would certainly reduce the time and improve the accuracy of metabolomic-based food composition studies. One recently developed software program, called Bayesil, is now able to quickly and accurately identify and quantify metabolites using NMR spectra of plasma, serum

or cerebrospinal fluid (Ravanbakhsh et al. 2015). Obviously if Bayesil could be expanded to support the characterization of other substrates (plant or juice extracts) then food analysis by NMR could become somewhat easier. Likewise, recent developments in ESI-MS/MS and EI-MS spectrum prediction – such as CFM-ID (Allen et al. 2015) suggest that these tools could be used to facilitate much more comprehensive plant (and therefore food) metabolite identification by mass spectrometry. However, the current collection of predicted MS spectra offered by CFM-ID is restricted almost exclusively to mammalian metabolites. Expanding this spectral collection to include phytochemicals or known food constituents could greatly benefit the food analysis community. The development of other novel technologies aimed at addressing the incomplete coverage of the food metabolome or for accelerating the identification and quantification of food metabolites is certainly an area needing further development.

I believe the work outlined in this thesis could open the door to much deeper analysis of a much broader variety of foods. Currently the FooDB database (the world's largest and most comprehensive food constituent database) lists chemical constituent data for 900 different "raw" or partially processed foods grown around the world. My thesis reports data for just 36 different "raw" or partially processed foods that are grown just in Alberta. Applying the same principles and techniques used here, one can calculate that there is enough work for 25-30 graduate students (for 3 years of work each) to conduct a thorough, experimental characterization of all 900 commonly available raw or processed foods.

It is also important to note that the experimental compound coverage I achieved was somewhat modest (typically ~215 compounds per food item). With continued improvements to metabolomics technology and improvements to the databases and reference libraries, I believe it should be possible to achieve targeted identification and quantification of 800-1500 compounds

within the next 2-3 years. Certainly one are of metabolite coverage that could be expanded upon greatly would be GC-MS analysis of food volatiles. In many cases it is these volatile compounds that are responsible for the subtle taste and aromas of many food items (including fruits and vegetables). I believe that these metabolomic methods could also be extended to include analyzing the effect of cooking and processing on the content of food chemicals, as well as characterizing the phytochemical metabolites formed inside the body.

My hope is that this thesis will form a basis for a new perspective on food analysis and a broader acceptance of food metabolomics as a legitimate technique by the food chemistry community. By encouraging others to use more comprehensive, more robust and more accurate methods for food constituent analysis I would hope that a much greater understanding of the "foodome" will be achieved. Creating and annotating databases such as the AFCDB or the FooDB are an important step in this direction. However, it will also be important to tie this information about food chemistry to information regarding the health effects and organoleptic effects of these compounds. The methods and techniques to acquire and interpret this physiological information are still in their infancy and the "physiological consequence" data contained in AFCDB and FooDB is rather sparse. Nevertheless, this will be an important direction to pursue given thatfood metabolomics is predicted to become one of the main cornerstonesof diet-guided precision, preventative medicine (Hall 2007).

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