UiT The Arctic University of Norway

Faculty of Health Sciences

Lipidomics of marine microalgae with industrial potential

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Master's thesis in Pharmacy, May 2021

Acknowledgement

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Torbjørn Myhre

Abstract

Background: Since 2014, The Arctic University of Norway (UIT) has been working with local industry in a project involving mass cultivation of microalgae. The algal biomass is cultivated where they can consume factory CO_2 emission and byproducts as inorganic nutrients to promote their growth. The biomass produced can potentially function as fish feed for aquaculture production. Microalgae are the main producers of the omega-3 long chained fatty acids eicosapentaenoic acid (EPA, 20:5) and docosahexaenoic acid (DHA, 22:6). To maximize the content of these fatty acids, this thesis investigates how cultivation in different light environments influences the EPA and DHA content of the microalgae, as well as changes in the lipid class composition.

Method: Two diatom species, *Porosira glacialis* and *Coscinodiscus radiatus*, were cultivated in three different light environments (red, blue and white light). After 7 days of growth the diatoms were harvested and the biomass was flash-frozen. The lipids were then extracted from the frozen biomass to prepare lipid analysis through High Performance Liquid Chromatography – Mass Spectrometry (HPLC-MS). A data dependent acquisition (DDA) method was used to gather identification information and measure the relative contents of the samples. Identification and relative quantification were thereafter done by the assistance of the software Lipidsearch.

Results: The content of both EPA and DHA were significantly increased when subjected to the blue light environment compared to both red- and white light for *P. glacialis*. Blue light represents a significant increase for DHA in *C. radiatus* compared to white light, and a non-significant increase for EPA. Blue light also had significant increase of both EPA and DHA compared to red light. White light had a significant increase on EPA content compared to red light, and a non-significant increase on DHA. Arachidonic acid (ARA) content was equal for blue- and white light, and significantly higher than red light for both species.

Conclusion: Our findings suggest blue light cultivation to be superior to both red- and white light for maximizing the LC-PUFA content of the microalgae.

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1 Introduction

1.1 Background

Since 2014, The Arctic University of Norway (UIT) has been engaged in a project with local industry involving mass cultivation of microalgae. As microalgae require CO_2, inorganic nutrients and trace metals to grow, and industry faces stricter demands towards their carbon footprint, the microalgae can be used to reduce the CO_2 emission along with any byproduct produced that the algae can utilize to grow. The microalgal fixation of CO_2 and possible byproducts results in the production of valuable biomass with a possible application as aquaculture fish-feed.

According to OECD reports (1) it is projected that by 2029 there will be a global increase in fish production for human consumption by 16,3% and that 90% of fish production will be consumed as food. It is also projected that aquaculture production will overtake capture fisheries in 2024 and that 52% of all production in 2029 will come from aquaculture. This rapid increase in aquaculture production creates a demand of high-quality fish-feed that reduces competition with human food resources. Diatom (microalgae) biomass is a renewable resource that fits the bill and algae derived fish-feed has been shown to surpass conventional fish-feed at weight gain in juvenile fish at lower costs (2).

The idea of algal mass cultivation for biomass harvesting is not novel as these products has several applications in the world, from biofuel to pharmaceutics (3). There are however large differences between the different species as to temperature tolerance and composition. And as the industry is located in northern Norway, using algae emanating from the north is wise, as this removes the energy need in maintaining a temperature to sustain algae from the southern hemisphere. The diatom *Porosira glacialis* was chosen for the project and its growth rate and fatty acid composition has been studied at different temperatures, finding that lipid content are influenced by temperature (4).

A natural continuation of this study is to try to understand the impact different lighting have on growth rate and lipid composition. Algal reproduction is dependent on light absorption as they are photosynthetic, and in its aquatic environment they will mainly be exposed to blue light. While growth rate will be studied for three light settings (blue, red and white) by The

Norwegian College for Fishery Science (NFH), this thesis focuses on the lipid content production of *Porosira glacialis* and a southern hemisphere diatom *Coscinodiscus radiatus*.

1.2 Diatom

Diatoms are small (10-200 µm) eukaryotic unicellular plant-like organisms (phytoplankton). They require sunlight as they are photosynthetic and 75% of the estimated 100.000 species can be found in photic (well-lit) areas of both marine- and freshwater bodies. They are a major group making up about 40% of all phytoplankton on earth and they account for about 20-25% of the CO_2 fixation and oxygen release in the world (5, p.131).

To grow, diatoms require sunlight, dissolved CO_2, inorganic nutrients and trace metals. They can utilize nitrate, phosphate, iron, copper, molybdenum and silica which alongside their ability to convert CO_2 into usable biomass and lipids make them ideal for wastewater treatment (6), and by extension, treatment of gaseous waste streams that can be filtered through water.

The growth rate of diatoms is divided into three phases. The first stage being the lag phase where the diatom is adapting to the environment. There is little to no increase in growth during this phase. The exponential growth phase happens after adaptation to the environment, and as the name implies this is a phase where there is rapid multiplication as long as there is a replete of inorganic nutrients (7). When inorganic nutrients deplete the diatom experiences nutrient stress, they alter their metabolism and they slow down their reproduction and increase their energy storage, which means accumulation of lipids (acylglycerols) within the cell (8). The growth rate can be calculated by measuring by the chlorophyll a (chl a) content of the algae (9).

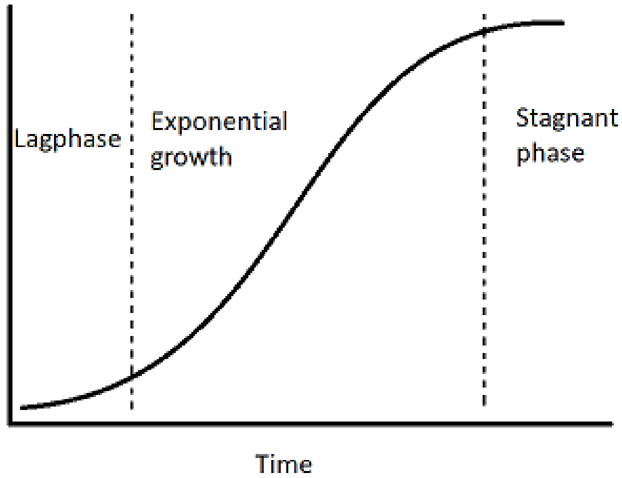

Figure 1: Illustration of growth rate phase of diatoms.

1.3 Lipid

Lipids is a collective term for a group of organic biomolecules and consists of fats (triacylglycerols) and fat-like compounds such as phospholipids, glycolipids, sphingolipids, steroids, carotenoids and waxes. They are characterized by their solubility in organic solvents and/or their insolubility in water. Their solubility depends upon the polarity of the head group of the molecule, with non-polar variants like the acylglycerols (e.g. triacylglycerol) being hydrophobic while more polar variants like the phospholipids (e.g. phosphatidylcholine) are amphipathic. The lipid classes are structurally different but have in common that they either partly consist of fatty acids, are derivatives of them, or closely relate to them biosynthetically or functionally.

A fatty acid is a carboxylic acid with an aliphatic hydrocarbon chain. Most fatty acids are even numbered carbon atom chains as biosynthesis starts with the substrates Acyl-CoA and Malonyl-CoA with further addition of Acyl-CoA for elongation (10). Bacteria, plants and algae however also produces odd numbered carbon chains believed to be due to reduction of Acyl-CoA to fatty aldehyde by the enzyme fatty acyl-CoA reductase (10, 11). Fatty acids can be saturated (SFA) which means having only single bonded carbon atoms, or unsaturated, which is the inclusion of one or more double bonds in the chain. Having one double bond in the chain makes the fatty acid a monounsaturated fatty acid (MUFA), while having two or more double bonds makes it a polyunsaturated fatty acid (PUFA).

1.3.1 Fatty acid nomenclature

To differentiate the fatty acids on their chain length, number of double bonds and position of these double bonds, they are given the designation C:D(n-x) where C is the number of carbon atoms present, D is the number of double bonds and n-x is the position of the first double bond from the aliphatic hydrocarbon end of the fatty acid (the omega side (ω)). E.g. Myristoleic acid has 14 carbon atoms and a single double bond placed between the fifth and sixth carbon from the omega side and is therefore designated 14:1(n-5).

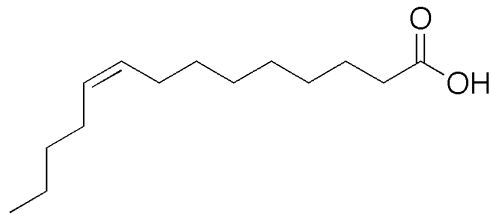

Figure 2: Structure of myristoleic acid 14:1(n-5).

1.3.2 Lipid classes

Lipids are essential for cellular functions such as energy management, cell-membranes and signaling. They are both complex and dynamic, meaning that there are tens to hundreds of thousands of compounds contained in the class of molecules, and that they are constantly changing with physiological and environmental conditions (12).

1.3.2.1 Acylglycerol

Acylglycerols consists of a glycerol bound to either one, two or three fatty acids with an ester bond to respectively form monoacylglycerol (MAG/MG), diacylglycerol (DAG/DG) or triacylglycerol (TAG/TG). These function as energy storage and the ester bonds hydrolyses when the organism is in need of energy, releasing free fatty acids (FFA) and glycerol.

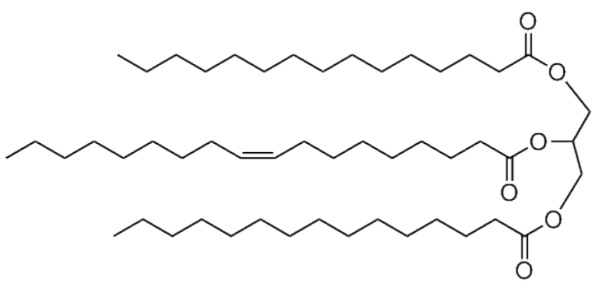

Figure 3: Structure of triacylglycerol (TAG) 15:0-18:1-15:0.

1.3.2.2 Phospholipid

Phospholipids closely resemble acylglycerols in that they consist of fatty acids bound to a glycerol. The difference between the two classes being the polar phosphate head group on one of the three binding sites on the glycerol. Their amphipathic nature with a polar head group and a hydrophobic carbon tail makes them ideal for lipid bilayers and they are therefore abundant in cell membranes. There is a variety of different phosphate head groups found in this lipid class, with the most common ones being phosphatidyl-choline (PC) and -ethanolamine (PE). Phospholipids with only one bound fatty acid is given the designation Lyso-.

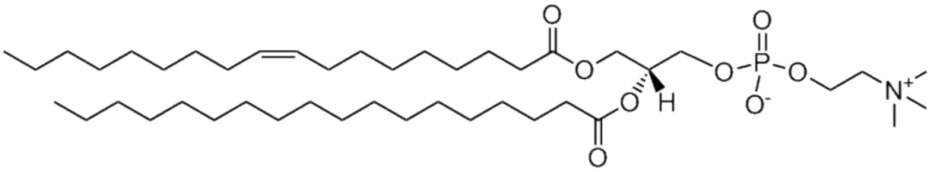

Figure 4: Structure of phosphatidylcholine (PC) 18:1-18:0

1.3.2.3 Glycolipid

Glycolipids are lipids conjugated with a carbohydrate. They are abundant on the extracellular membranes of cells and has crucial roles in cell recognition, cell-to-cell interaction and maintaining stability of the membrane. The most common glycolipids in microalgae are the galactolipids monogalactosyldiacylglyerol (MGDG) and digalactosyldiacylglycerol (DGDG). These lipids consist of fatty acids and the carbohydrate(s) galactose bound to a glycerol.

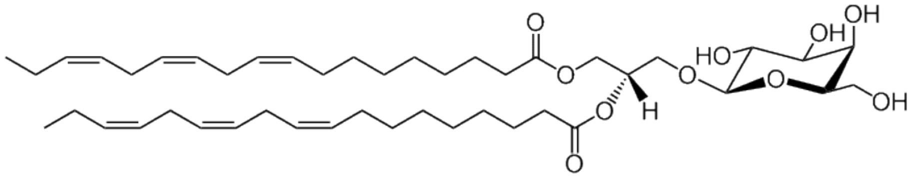

Figure 5: Structure of monogalactosyldiacylglycerol (MGDG) 18:3-18:3.

1.3.3 PUFA and health

All mammals, including humans, are incapable of *de novo* production of long chained polyunsaturated fatty acids (LC-PUFA), but are able to convert α-linolenic acid (ALA 18:3n-3) and linoleic acid (LA 18:2n-6) into some of the important LC-PUFA species such as arachidonic acid (AA 20:4n-6), eicosapentaenoic acid (EPA, 20:5n-3) and docosahexaenoic acid (DHA, 22:6n-3). This makes ALA and LA essential fatty acids and a dietary requirement

(13). The conversion rate of ALA and LA to n-3 and n-6 species is however slow, and it is therefore suggested that direct uptake of these species is more effective (14).

The omega-3 fatty acids EPA and DHA are well established to have protective effects on the development of cardiovascular diseases as well as promising antihypertensive, anticancer, antioxidant, antidepression, antiaging and antiarthritis effects (15). As marine microalgae are the primary producers of EPA and DHA, humans can acquire both fatty acids indirectly through them from consumption of marine fish. Higher EPA/DHA content in microalgae are suggested to have a positive impact on white muscle development in fish, and high contents of LC-PUFA in fish diet is suggested to be correlated to increased elongation activity of their fatty acids (16). The Atlantic salmon has also been shown to possess enzymes for endogenous production of both EPA and DHA from α-linolenic acid (ALA, 18:3(n-3)) (17).

The ratio of omega-3 to omega-6 is important to human health, as an overabundance of omega-6 fatty acids will reduce the production of LC-PUFA omega-3 due to these compounds competing for the same enzymes in their metabolic pathways (13). The typical western diet today contains unfavorable ratios of omega-3 to omega-6 paired with high omega-6 contents which promotes pathogenesis of several diseases like cardiovascular disease and autoimmune diseases (18). The ratio of omega-3 to omega-6 in fish-feed is also suggested to impact the fish content of omega-3 fatty acids (16), influencing how healthy the end product for human consumption will be.

1.3.4 Lipidomics

Lipidomics is the complete study of the lipid species and their function in a biological system. It aims to determine pathways and networks that exists in the lipidome (the complete lipid content of a cell) and how changes affect the organisms. It is a relatively new field of research driven by the rapid technological advancements in mass spectrometry (MS) and nuclear magnetic resonance (NMR). Lipidomics shows great potential in aiding our understanding of diseases such as metabolic syndrome and neurological disorders as well as being a predictive tool for both disease development and recovery (12).

1.4 Lipid extraction

A prerequisite for any lipid content analysis is extracting the lipid from their biomass. The extraction serves two purposes, one is to make ready lipid compounds for analysis and the other is washing away any non-lipid contaminants. There are several methods proposed to maximize both of these functions. The most used method is the Folch method of extraction, where the sample is mixed with chloroform/methanol (2:1) before adding 0.2 equivalents of water to induce phase separation. The method extracts lipids into the organic phase with a recovery of > 90% for the more polar lipids like triglycerides and 60-70% for phospholipids (19). Due to chloroform being linked to carcinogenic effects on humans, it has later been replaced by dichloromethane without loss of extraction efficiency (20).

For a higher sample throughput without loss of efficiency, a modified one-step version of the Folch method has been utilized. This method adds dichloromethane/methane and water to the sample in a centrifuge tube, which is then shaken vigorously and centrifuged (21). No cell disruption techniques needs to be applied to the sample as there are not significantly higher yield from disruption of flash-frozen algal biomass (22).

1.5 HPLC-MS

High Performance Liquid Chromatography – Mass Spectrometry (HPLC-MS) is an analytical method combining the chromatographic separation capability of HPLC with the mass analysis capabilities of MS. In HPLC, chromatographic separation is achieved through utilizing differences in the physicochemical properties of compounds in a manner that gives them different retention times through an analytical column. The coupled MS can provide structural and quantitative information of the compounds through analysis of mass and fragmentation.

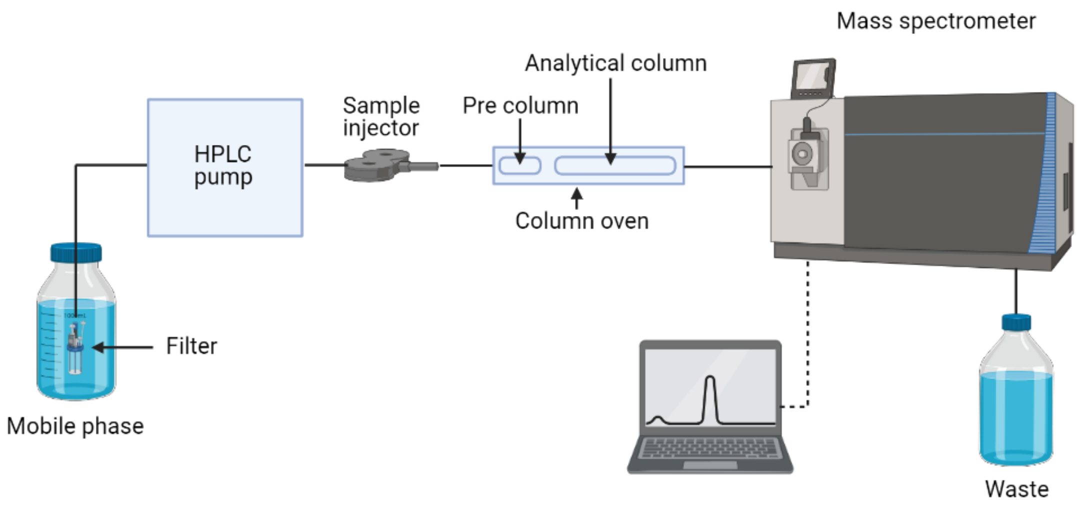

Figure 6: Simplified schematic of HPLC setup. Figure created in biorender.com

1.5.1 High performance liquid chromatography (HPLC)

The principle of HPLC is that a sample of soluble compounds are injected into a stream of mobile phase, which is also a liquid, in advance of a separation column. Different compounds (analytes) will have different affinity to the column particles and therefore the interaction between column and analyte will differ. This interaction between column and analyte is the deciding factor of how much time the analyte will need to pass through the column. When eluting from the column a detector can record the intensity of the signal and present it as intensity over time, a curve of which the area represents the relative quantity of the analyte. However, a requirement for this to be true is a need for a linear relationship between signal and quantity. The linear relationship can be decided experimentally. Depending on analytes and the matrix they are within, a variety of columns and mobile phases can be used to achieve separation.

1.5.1.1 Column and mobile phases

The reverse phase column is a chromatography column that contain a non-polar stationary phase (the columns packed particles). The stationary phase usually consists of silica with covalently bonded alkyl chains which has a strong affinity to hydrophobic, less polar molecules. A polar aqueous mobile phase serves as the weak mobile phase, eluting polar molecules while having minimal interaction with hydrophobic ones. An organic solvent miscible with water serves as the strong mobile phase, breaking interactions between analytes and the stationary phase and elutes hydrophobic analytes when the concentration is high enough. Stronger interactions between stationary phase and the analyte will require higher concentration of organic solvent to elute the analyte. A gradient between the two mobile phases can be employed to elute all analytes over a period of time.

Other factors influencing the retention time of analytes are pH, flow rate, temperature, stationary phase particle size and the dimensions of the column itself. Adjustment of pH can apply charge to analytes which in a reverse phase system will reduce retention time by increasing interaction between analyte and weak mobile phase, while removing charge has the opposite effect. The relationship between column dimension, particle size and flowrate decide the amount of backpressure generated in the HPLC system. Flow rate needs to be set so it gives the analyte enough time to interact with the stationary phase but balanced with reasonable runtimes while keeping within the pressure limits of the instrument. The role of temperature is to control viscosity of mobile phases, with higher temperatures reducing viscosity and thus reducing backpressure.

Conventional HPLC uses particle sizes of 3-5 µM and operates at pressures around 2000-4000 PSI. Newer systems, called Ultra High Performance Liquid Chromatography (UHPLC), uses particle sizes from 1.5-3 µM and operates at pressures from 6000 to above 20000 PSI. The newer system generates better signal-to-noise ratio (S/N) due to reduction in band broadening (narrower peaks) which also reduces ion suppression as co-eluting becomes less frequent (23).

1.5.2 Mass spectrometry (MS)

Mass spectrometry is a technique of measuring the mass over charge (m/z) ratio of one or more molecules present in a sample. The ability to measure m/z ratio is dependent on the molecules having at least one charge, which makes an ionization source a necessity in all MS instruments. The ionization source needs to fill two functions, one is applying a charge to the molecule, the other is transporting the molecule from the liquid mobile phase into a gaseous one. Once the molecule is in a gaseous phase and has a charge it can be moved through the system using electrical and/or magnetic forces. This makes it possible for a mass analyzer to separate molecules based on their m/z value and subsequently for an ion detection system to measure and record the intensity of each of these m/z values.

1.5.2.1 Ionization source

The electrospray ionization source (ESI) give charge to the molecules in the mobile phase by applying an electric current to the liquid (cone voltage). At the same time, there is pressure applied to the liquid as it is pushed through a capillary creating an aerosol. The aerosol containing charged molecules undergo rapid solvent evaporation often helped by a heated sheath gas. Evaporation causes a decrease in droplet volume which in turn increases the tension as the same charge molecules repel each other and ultimately exits the droplet through Coloumb fission, which is a series of droplet explosions creating smaller droplets (24). This is a soft ionization technique which leaves the molecular ions intact and causes minimal fragmentation, though some in-source fragmentation is possible depending on the cone voltage applied.

1.5.2.2 Mass analyzer

The quadrupole is the most used mass analyzer in MS. It consists of four parallel metal rods which can be applied an electric current. It is able to select molecules of a given m/z value by alternating positive and negative charge along pairs of rods which gives desired molecules a stable trajectory to continue into the system, while molecules of higher or lower m/z will be offset by unstable trajectories and will ultimately collide with the rods. The quadrupole generally operates at the transmission range 50 – 2000 m/z and can select ions precursors within 0.5 atomic mass units (AMU).

1.5.2.3 Ion trap

A linear quadrupole ion trap is a device which has the ability to trap ions and hold them. By rapidly swapping positive and negative charge along the rods and by a stopping potential on plates covering each end, the ions are kept within the device. The ion trap can eject all ions in a given range for fullscan, or only ions with a selected m/z by resonance ejection. It is also used as a collision cell for fragmentation and can analyze fragment m/z values (25).

Additionally, instruments like the Orbitrap are equipped with a similar device called the C-trap, which has the function of holding ions until the orbitrap is ready for injection. It operates by allowing a fixed number of ions (automatic gain control (AGC)), or as many ions as possible in a given time period (maximum injection time), before injecting the ion packet into the orbitrap. The control function for ion trap contents is called a microscan. A microscan is a complete scan by the ion trap of the stored ions which give information used to produce a orbitrap scan. Increasing the number of microscans can have a positive effect on the signal-to-noise (S/N) ratio but will increase scan time. One microscan is generally considered sufficient (26).

1.5.2.4 Ion detection system

The orbitrap mass spectrometer is a high resolution – accurate mass (HRAM) instrument. It operates by oscillating orbitally trapped ions along an electric field around a central spindle. The axial frequency of ion oscillations is measured by acquisition of time-domain image currents and the signal is transformed into a corresponding m/z value by Fourier transformation (27). The mass accuracy of measurement depends on the number of oscillations the ions undergo which is limited by time. The trade-off of increased mass accuracy is fewer points of measurement pr. unit of time. Quantification of compounds is improved by increasing the amount of measurements in any given chromatographic peak, while identification is improved by reducing the amount of points of measurements so that the orbitrap can oscillate ions for a longer period of time.

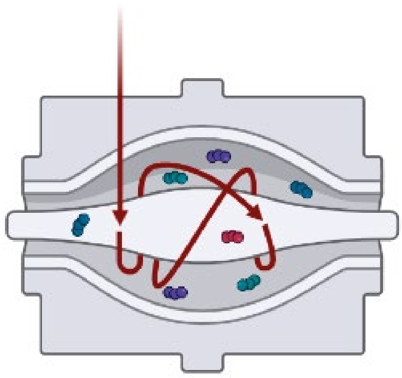

Figure 7: Illustration of ion oscillation in Orbitrap. Figure created in biorender.com.

1.5.2.5 MS^n fragmentation

In identification of compounds it is not sufficient with accurate mass measurement and retention times as there usually is an abundance of possibilities of elemental composition for any given exact mass measured. Fragmentation of ions make it possible to compare fragments with theoretical fragmentation and/or fragment databases which adds invaluable information towards positive identification. The two most commonly used techniques in omics are collision induced dissociation (CID) and higher energy collisional dissociation (HCD).

CID fragmentation happens when ions are accelerated from a low energy to their final user-defined maximum energy within a collision cell. While being accelerated the ions collide with an inert gas (often helium, nitrogen or argon) which can break weaker bonds in the compound (depending on selected final energy). Resonance CID that happens in an ion trap will only accelerate precursor ions within the ion trap, meaning that fragmented product ions do not continue colliding after initial fragmentation. In HCD fragmentation the ions are exposed to a larger energy giving both weak and stronger bonds the chance to break, and the product ions remain excited leaving the possibility of further fragmenting into smaller product ions (28).

1.6 Identification of lipids

AcquireX (Thermo Fisher Scientific, Waltham, MA, USA) is a MS data collection software that can help generate the data needed for lipidomic analysis. Data-dependent acquisition (DDA) can be done by scanning a control sample (Qc) that contains all compounds in the individual samples prepared. This fullscan can find all peak intensities over a user-defined threshold and add them to an inclusion reference list. By also scanning a blank sample containing only solvent, it can identify peaks that can be considered noise and creates an exclusion list for these. MS^n scanning thereafter inspects all inclusion reference peak intensities that is not present on the exclusion list. After an object on the inclusion reference has been inspected, it gets added to the exclusion list to avoid data redundancy. As the inclusion reference list size is dependent on the contents of the sample and the capacity of MS^n is time-limited, several injections of the control sample may be necessary to inspect all the entries of the inclusion reference list. The amount of injections should therefore be experimentally decided to allow a full analysis of the inclusion reference list.

Lipidsearch (Thermo Fisher Scientific, Waltham, MA, USA) is a program designed to help identify and quantify lipids. It operates by superimposing the identification data generated from

AcquireX on to fullscans of each individual sample. After identification, the program can integrate the area under the curve (AUC) for each compound to assign relative abundance of analytes within sample. The program contains a set of user-defined parameters for positive identification in mass deviation in parts per million (PPM) and retention time tolerance in minutes, alongside an arbitrary unit for fragment similarity (m-score) to avoid false positives. This m-score is a set of parameters needed for positive identification, and includes measurement of the lipid head group, the neutral loss of one or more fatty acids, and typical fragments observed when fragmenting some lipid species. Retention time tolerance is a setting that decides what difference in retention time is acceptable for inclusion under any given positive identification generated by the MS^n scan.

2 The aim of the thesis

The main aim of this thesis was to investigate the long chain omega-3 fatty acid content of diatoms cultivated in three different light environments. Secondarily, to investigate potential differences in lipid class composition arising from cultivation in these different light environments.

2 Materials and methods

2.1 Diatom cultivation

Table 1: Chemicals used in the cultivation of diatoms.

Chemicals	Supplier
Guillard's F2 Marine water enrichment solution (50x) Sodium metasilicate nonahydrate (≥98%)	Sigma Aldrich (St. Louis, MO, USA)

The monoculture of *Porosira glacialis* was isolated from a sediment sample collected in the Barents Sea (N 76° 27.54′, E 033° 03.54′) on a cruise in 2014 and was identified by SEM-imaging and rcbL-gene barcoding (29). *Coscinodiscus radiatus* was acquired from SAMS (CCAP 1013/11).

The cultivation of both these cultures was performed in 4-liter polycarbonate flasks (Nalgene, Rochester, NY, USA). *P. glacialis* was incubated at 8°C and *C. radiatus* at 20°C, and their growth media was enriched with Guillard's F2 with added silicate. For both diatom strains 9 flasks of cell culture was made and placed in groups of 3 into rooms illuminated with red, blue or white light (figure 8). The rooms were fitted with LED strips (Co/tech Model 36-7237, Surrey, UK) which was adjusted to 35 µmol m^{-2} s^{-1} using LI-250A light meter (LI-COR, Cambridge, UK) coupled with a Walz US-SQS/L sensor (Heinz Walz GMBH, Effeltrich, Germany). The peak wavelengths were 629 nm for red light, 457 nm for blue light, and 457, 521 and 629 nm for white light, recorded using a BLACK-Comet Fluorescence Spectrophotometer (StellarNet, Tampa, FL, USA).

Figure 8: The setup for cultivation under different light setting.

Prior to the experiment, inoculums of both strains were acclimatized to their environment (red, blue or white light) for 7 days. After these 7 days they were diluted to a starting concentration of $1*10^6$ cells/L for *P. glacialis* and $5*10^5$ cells/L for *C. radiatus*. The difference in starting concentration is due to the physical size difference of the species, and the starting concentrations were decided experimentally as to fulfill the need for 7 days of exponential growth.

2.1.1 Harvesting

After 7 days the cultures were harvested by filtration through a 10 µm plankton net (KC Denmark AS, Silkeborg, Denmark) and the samples placed into 50 mL centrifugation tubes (Corning Science, Reynosa, Mexico) for centrifugation at 2000 G for 4 minutes (Heraeus Multifuge 1S-R, Danau, Germany). The supernatant was discarded and the remaining mass was flash-frozen in liquid nitrogen and stored at -80°C.

2.2 Lipid extraction

Table 2: Chemicals used in the lipid extraction

Chemicals	Supplier
Dichloromethane (99.8%) Methanol (99.9%)	Sigma Aldrich (St. Louis, MO, USA)

The extraction procedure was a modified Folch using dichloromethane (DCM) and methanol (MeOH) as the extractant. Each sample tube (18 in total) was added 2mL of DCM/MeOH (2:1 v/v) and 2mL 5% NaCl in MiliQ water (w/v). The sample tubes were gently shaken before centrifugation at 2000 G for 5 minutes (Heraeus Multifuge 1S-R, Danau, Germany). The organic phase was thereafter transferred to pre-weighed dram glasses. After repeating this extraction method twice to increase the yield, the samples were evaporated under nitrogen gas and the total lipid content was decided gravimetrically. All samples were resuspended in 2-propanol to 1 mg/mL or 2 mg/mL for *C. radiatus* and *P. glacialis* respectively and then stored in -80°C.

2.3 Sample preparation

Table 3: Chemicals used in sample preparation.

Chemicals	Supplier
2-Propanol (100%)	Merck KGaA (Darmstadt, Germany)

A sample concentration of 0.5 mg/mL was experimentally decided to be the ideal concentration to find low abundance lipids without losing chromatographic quality in high abundance lipids. Samples with a concentration of 0.5 mg/mL was prepared by diluting the resuspended samples with 2-propanol into vials and vortexing each for 10 seconds. The vials used were Waters screw top vial 12,32 mm with cap and pre-slit PTFE-silicone septa (Waters, Milford, MA, USA).

Qc sample: For control, a Qc sample was prepared by pipetting 20 µL of each of the prepared 0.5 mg/mL samples into a separate vial and vortexing for 10 seconds. Hence, the Qc sample is an average of all samples to be analysed.

Blank sample: To follow the process of the lipid samples, an empty vial was added 2mL of DCM/MeOH (2:1 v/v) and 2mL 5% NaCl in MiliQ water (w/v). The vial was then evaporated under liquid nitrogen and resuspended with 2-propanol and vortexed for 10 seconds.

2.4 UHPLC-MS

Table 4: Chemicals used in UHPLC-MS.

Chemicals	Supplier
Acetonitrile	Sigma Aldrich (St. Louis, MO, USA)
2-Propanol	
Formic acid (97,5-98,5%)	Merck KGaA (Darmstadt, Germany)
Ammonium formate (≥99%)	

2.4.1 UHPLC Configuration

UHPLC was performed on a Vanquish Horizon UHPLC (Thermo Fisher Scientific, Waltham, MA, USA) with a Waters Aquity Premier 100mm x 2,1mm 1,7µm C18 reverse phase column (Waters, Milford, MA, USA). The flow rate was set to 0,6 ml/min. The mobilephase configuration used was; A: Equal amounts of MiliQ-water and acetonitrile (50%/50%) with 1mM ammonium formate (NH4FA) and 0,01% formic acid (FA). B: Equal amounts of 2-Propanol and acetonitrile (49,5%/49,5%) with 1% MiliQ-water, 1mM NH4FA and 0,01% FA. The ammonium formate was added to the mobile phases as triglycerides need ammonium to form ammonium adducts (+NH4). Formic acid was added to mobile phases as it has the ability to improve peak shapes (30). The mobile phase gradients are shown in figures below.

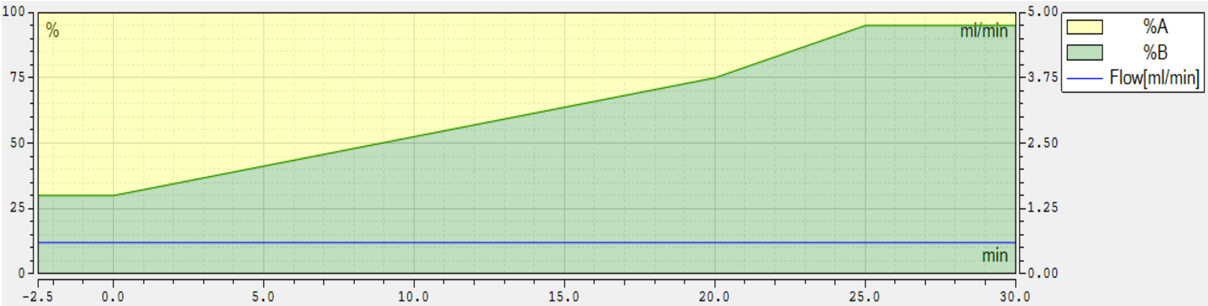

Figure 9: Flow setting and gradient of mobile phases in the method.

No	Time	Flow [ml/min]	%B	Curve
1	-2.500	Equilibration		
2	-2.500	0.600	30.0	5
3	0.000	0.600	30.0	5
4	*New Row*			
5	0.000	Run		
6	0.000	0.600	30.0	5
7	20.000	0.600	75.0	5
8	25.000	0.600	95.0	5
9	*New Row*			
10	30.000	Stop Run		

Figure 10: Flow setting and gradient of mobile phases in the method.

The temperature in the sampler module was set to 5°C and the column temperature was set to 60°C. Both draw speed and dispense speed was set at 5 µl/s. Needle wash was set for 5 seconds with 10 µl/s MiliQ-water/MeOH (3:1 v/v).

2.4.2 MS Configuration

MS was performed on an Orbitrap ID-X Tribrid MS (Thermo Fisher Scientific, Waltham, MA, USA) with electrospray ionization (figure 11).

Ion Source

Ion Source Type: **H-ESI**
Spray Voltage: **Static**
Positive Ion (V): **3500**
Negative Ion (V): **2500**
Sheath Gas (Arb): **60**
Aux Gas (Arb): **15**
Sweep Gas (Arb): **2**
Ion Transfer Tube Temp (°C): **350**
Vaporizer Temp (°C): **350**
APPI Lamp: **Not in Use**
Use Ion Source Settings from Tune: **False**

Figure 11: Ion source settings for the method.

2.4.2.1 Fullscan setup

The fullscan method in the experiment is used for inclusion reference, exclusion reference and sample scans. It is also configured as the masterscan in the MS^n method which will be shown in the next segment.

MS OT

Detector Type: **Orbitrap**
Orbitrap Resolution: **120000**
Use Quadrupole Isolation: **True**
Scan Range (m/z): **250-1500**
RF Lens (%): **40**
AGC Target: **Standard**
Maximum Injection Time Mode: **Custom**
Maximum Injection Time (ms): **50**
Microscans: **1**
Data Type: **Profile**
Polarity: **Positive**
Source Fragmentation: **Disabled**
Use EASY-IC™: **True**

Figure 12: Configuration of MS in the fullscan of samples.

2.4.2.2 MS^n setup

The MS^n configuration was set up to do one masterscan (as shown in previous segment as fullscan) every 1.5 seconds. The orbitrap mass scan (MS OT) was executed and data was checked with both the exclusion list and the dynamic exclusion list and if not present in these lists, the targeted mass from the inclusion reference list were then fragmented with a HCD fragmentation (figure 13). Following the HCD fragmentation came CID fragmentation and possibly further CID fragmentation for MS^3 if a targeted mass loss is recorded. A targeted mass loss is a user defined list of m/z loss from precursor ion, and in this method the neutral loss triggering MS^3 was the loss of a fatty acid.

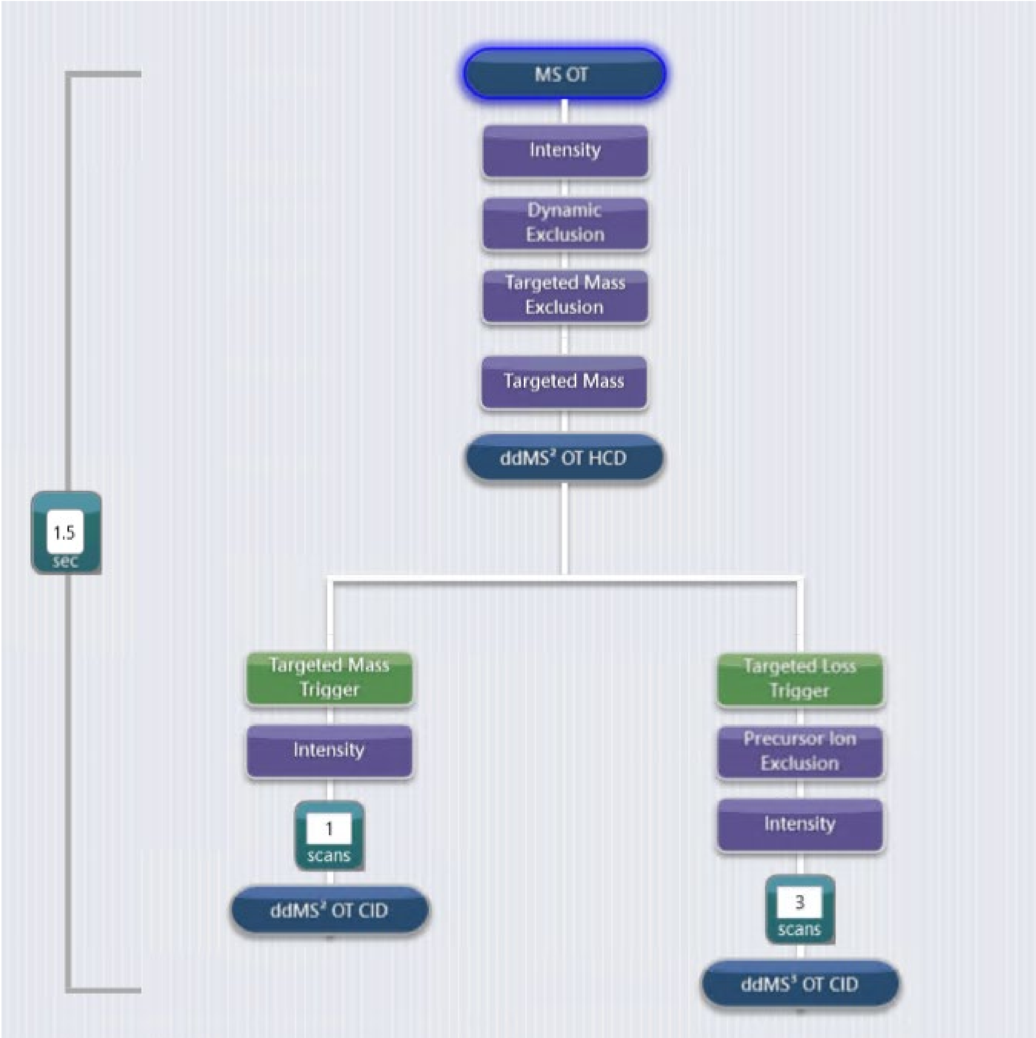

Figure 13: MS scan and fragmentation workflow. Orbitrap mass spec (MS OT) records intensity and checks exclusion references before starting fragmentation of ions in inclusion reference list. Targeted mass loss can start further MS^n analysis.

Figure 14: Configuration of HCD and CID fragmentation and scan in the MS^n method.

2.4.3 Acquisition setup

As the MS^n setup has one obvious limiting factor in time usage and therefore the number of scans it is able to do at any given time of the chromatography, an acquisition setup was needed to improve data collection.

Acquisition was done with AcquireX with an inclusion reference threshold for peak intensity set to 1.0e5. The common adducts to identify by was set to hydrogen (+H), sodium (+Na) or ammonium (+NH4) and the program was set to re-inspect objects moved from inclusion list to exclusion list if reappearing with an intensity difference of 5 or greater of the original inspected peak.

The injection sequence was setup to first flush the system with blank sample four times and use the fifth blank to generate the exclusion list. The control sample (Qc) was then used to create the inclusion and subsequent MS^n scans. A repeat sequence of all individual samples was then injected (figure 15). A total of 52 injections gave a runtime of 26 hours per species.

Figure 15: Injection sequence of samples in AcquireX. All injections were 2µl unless otherwise stated.

2.5 Analysis of lipids

The RAW files from AcquireX identification were imported to Lipidsearch. In lipidsearch, each fullscan was aligned with the MS^n scans to assign identity to compounds. The arbitrary mScore was set to 5 to avoid false positives, and mass accuracy threshold was set to 5 PPM for both parent- and product ion. The intensity threshold for product ions was set to 1.0% of parent and retention time tolerance was set to 2.0 min to reduce the occurrence of isomer identification of each analyzed m/z. After identification of compounds and integration of their AUC in Lipidsearch, the data was exported for further analysis using R. In R, the total AUC for aggregated light environment samples was normalized to a value of 100 so that the mean and standard deviation (SD) in each environment could be effectively compared. This also made the AUC for each lipid count correspond to its actual percent of the total lipid production (TLP).

Table 5: List of lipid species included in Lipidsearch analysis of RAW files.

Species	
Phosphatidic acid (PA)	Lysophosphatic acid (LPA)
Phosphatidylcholine (PC)	Lysophosphatidylcholine (LPC)
Phosphatidylethanolamine (PE)	Lysophosphatidylethanolamine (LPE)
Phosphatidylglycerol (PG)	Lysophosphatidylglycerol (LPG)
Phosphatidylinositol (PI)	Lysophosphatidylinositol (LPI)
Phosphatidylserine (PS)	Lysophosphatidylserine (LPS)
Monoglyceride (MG)	
Diglyceride (DG)	
Triglyceride (TG)	
Monogalactosyldiacylglycerol (MGDG)	
Digalactosyldiacylglycerol (DGDG)	
Sulfoquiovosyldiacylglycerol (SQDG)	

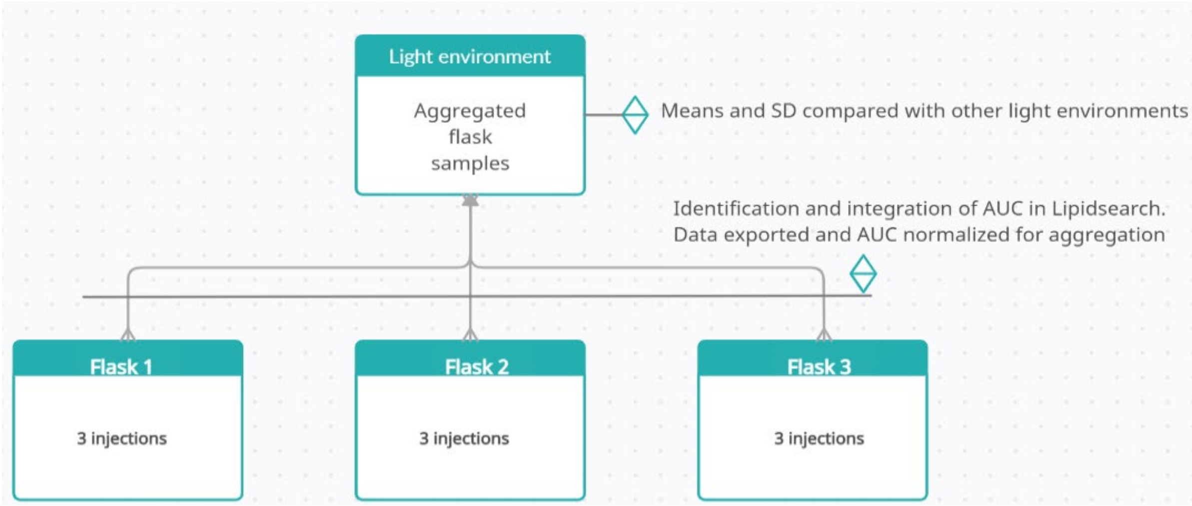

Figure 16: Shows how experiment was set up for collecting data and aggregating data before comparison.

2.6 Statistical analysis

All samples are presented with mean and one standard deviation (SD) in figures the in the results and discussion chapter. Homogeneity of variance (Levene's test) and normal distribution (Shapiro-Wilks test) tested in selected samples as export output did not include individual residuals. Data was analyzed with ANOVA. All analyses were performed using R.

3 Results and discussion

3.1 Diatom cultivation and harvesting

The project group had a method set up from previous cultivations of *P. glacialis* and applied the same method to *C. radiatus*.

As diatoms might stop their growth if the culture is diluted too much, starting concentrations were set high enough to reduce the chance of this issue occurring while still being able to grow for 7 days without reaching the stagnant phase. It seems however that two of the flasks might have reached the stagnant phase and accumulated triglycerides, which resulted in a very different lipid profile than their two other parallels and they were therefore removed from the project. This loss of parallels could have been avoided if the runtime of cultivation were altered, and we suggest harvest on day 6 to still be in the exponential growth phase for future cultivation projects. The difference observed in triglyceride levels for *Porosira glacialis* can be seen in figure 17 with S1 (flask 1, red light) showing very high triglyceride levels compared to S2 and S3 (the other two flasks). The other flask removed from the dataset was from the white light cultivation of *Coscinodiscus radiatus* (flask 1, white light). Data not shown.

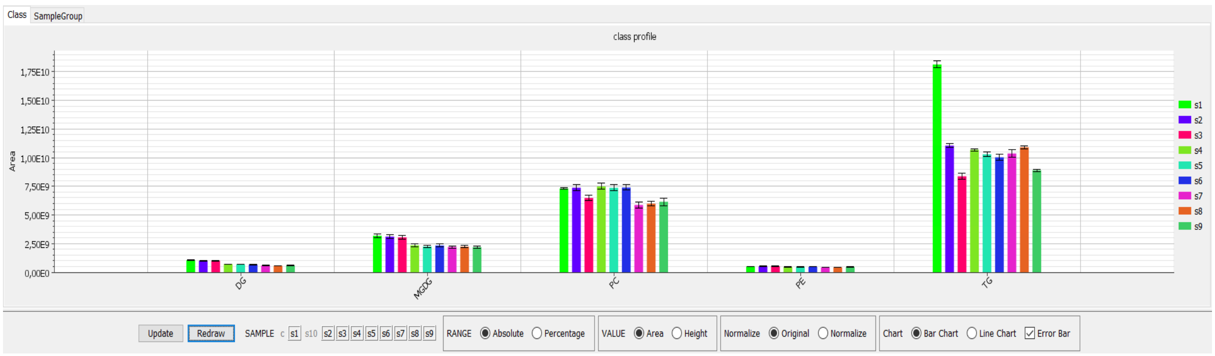

Figure 17: User interface of Lipidsearch showing quantification bins of lipid classes in samples. This data belongs to Porosira glacialis and S1-S3 represents red color, S4-S6 represents blue color and S7-S9 represents white color.

By measuring the chlorophyll a (chl a) contents of each flask 4 times daily during the duration of diatom cultivation, an average growth rate was calculated for each light setting (figure 18, 19). These figures might suggest that a shorter duration of cultivation would have been a better choice as differences in the growth curves were observed towards the end of the cultivation. As this is an average of all flasks it does not investigate the differences within each group, which could have been accomplished by monitoring the growth of each flask separately. Red light *P.*

glacialis and white light *C. radiatus* shows the largest variance of growth rate, which is consistent with our hypothesis of differences within these light settings.

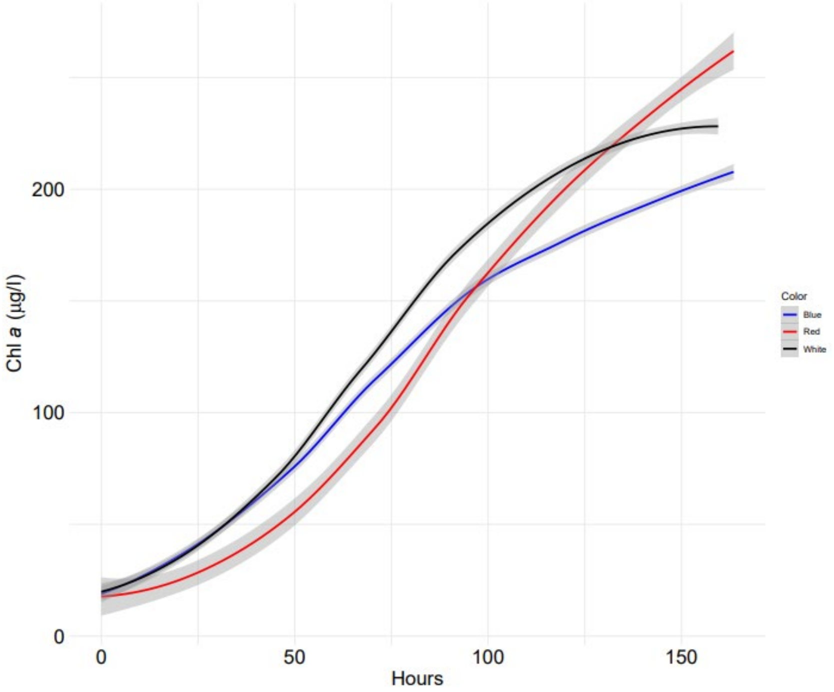

Figure 18: The growth rate of Porosira glacialis recorded by the content of chlorophyll a (chl a). The gray area around lines show the 95% confidence interval.

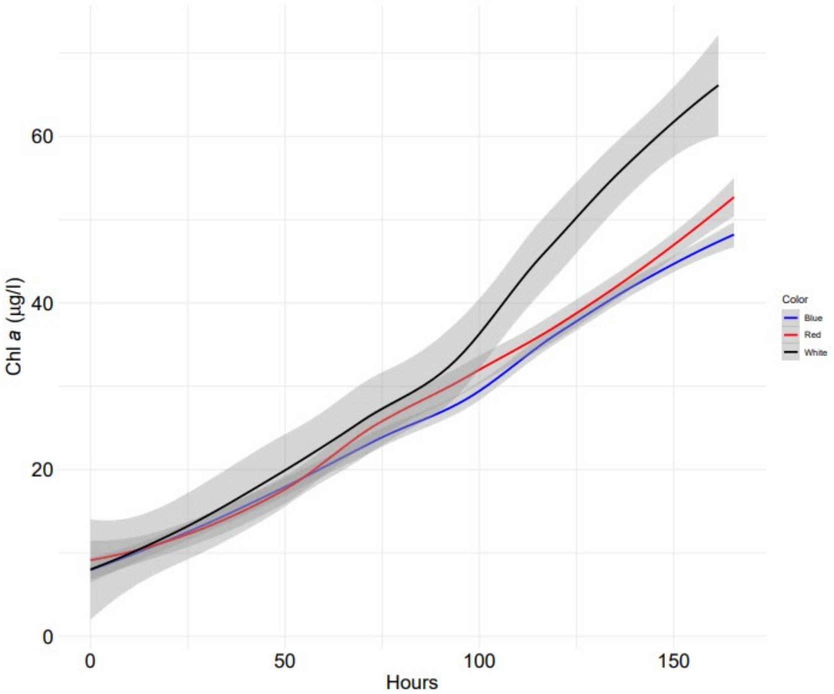

Figure 19: The growth rate of Coscinodiscus radiatus recorded by the content of chlorophyll a (chl a). The gray area around lines show the 95% confidence interval.

3.2 UHPLC-MS and analysis of lipids

The initial testing of both the UHPLC-MS method and the following lipid analysis in Lipidsearch was done by injecting a mix of known lipid standards to see their retention time through the column, the mass accuracy measured by the orbitrap and to see if Lipidsearch provided the correct identification. As the main lipid classes observed in the old samples of P. glacialis were triglycerides (TG), phosphatidylethanolamine (PE), phosphatidylcholine (PC) and monogalactosyldiacylglycerol (MGDG) the standards used for identification testing were TG 18:1-18:1-18:1, PE 14:0-14:0, PC 14:0-14:0 and a mix of MGDG, mainly 16:3-18:3 and 18:3-18:3 (Avanti Polar Lipids, Alabaster, AL, USA).

Interestingly, the MGDG standards were identified as 16:0-18:0 and 18:0-18:0. But as the MGDG standard was labelled with 3 months stability and the standard used in this experiment were bought in January 2019, these results were overlooked as the sample was considered to have undergone some oxidation deformation. Figure 20 shows identification parameters for MGDG 16:0-18:0, and in order these are:

ProductIon	Type	ObsMz	Intensity	Delta(Da)
M-16:0-18:0+Na	HCD	243.0835	1	-0.0004
M-18:0+Na	HCD	497.309	26.3	0.0005
M-16:0+Na	HCD	525.3404	12.9	0.0006
M+Na	HCD	781.5802	100	0.0002

Figure 20: Identification parameters of MGDG 16:0-18:0 from the Lipidsearch interface.

1. The sodium (Na) adduct of parent ion after loss of both fatty acids (M-16:0-18:0+Na) with an intensity of 1% of the precursor ion (most intense ion) and a mass error of -0.0004 Dalton (Da).
2. The sodium (Na) adduct of parent ion after loss of 18:0 fatty acid (M-18:0+Na) with an intensity of 26.3% of the precursor ion and a mass error of 0.0005 Da.
3. The sodium (Na) adduct of parent ion after loss of 16:0 fatty acid (M-16:0+Na) with an intensity of 12.9% of precursor ion and a mass error of 0.0006 Da.
4. The precursor ion at 100% intensity with a mass error of 0.0002 Da.

The rest of the standard mixtures were however successfully identified by Lipidsearch (figure 21), giving validation to the method so that the analysis could progress to diatom lipid samples.

ID	LipidGroup	Grade	Scan	Formula	ObsMz	CalcMz
PC(14:0_14:0)+H	PC(28:0)+H	A	MS2	C36 H73 O8 N1 P1	678.5064	678.5068
TG(18:1_18:1_18:1)+NH4	TG(54:3)+NH4	A	MS2	C57 H108 O6 N1	902.8211	902.8171
PE(14:0_14:0)+H	PE(28:0)+H	A	MS2	C33 H67 O8 N1 P1	636.4599	636.4599

Figure 21: Successful identification of lipid standards PC 14:0-14:0, TG 18:1-18:1-18:1 and PE 14:0-14:0.

The first trial runs using diatom samples were done on a 100mm x 2,1mm 1,9µm C18 reverse phase column (Thermo Fisher Scientific, Waltham, MA, USA) which resulted in problems identifying some compounds. There was a retention time shift for compounds eluting between the 9 and 19 minutes, along with an interference later identified to be polydimethylsiloxane (PDMS) that affected some of the peaks in this window. To combat this problem, the column was swapped to a Waters Aquity Premier 100mm x 2,1mm 1,7µm C18 reverse phase column (Waters, Milford, MA, USA) and the HPLC vials were swapped to a pre-slit septa cap variant to reduce the cap puncture upon injection, which was suspected to add PDMS as the interference signal increased for each successive injection. This was a great improvement to the analysis, and even though the PDMS signal did not disappear from these changes, its effect on identification appeared to be reduced.

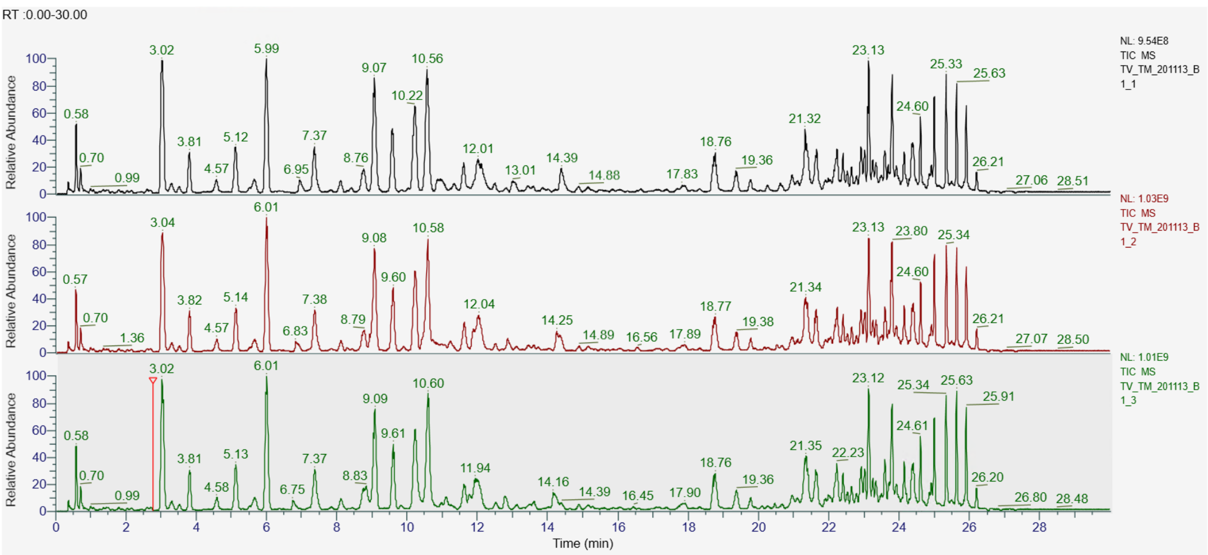

Figure 22: Chromatography on new 1.7µm column. 3 injections of flask 1, blue light P. glacialis.

To further improve the identification of lipids in Lipidsearch, the setting of retention time tolerance was increased from an initial 0.2 min. to 2.0 min. Increasing this setting allowed the software to include a larger portion of isomers with identical m/z to be included under the identification of the main isomer peak (the most intense isomer signal). This greatly reduced the count of compounds detected by the software, but this reduction was due to loss of replicates, not of unique lipid counts (figure 23).

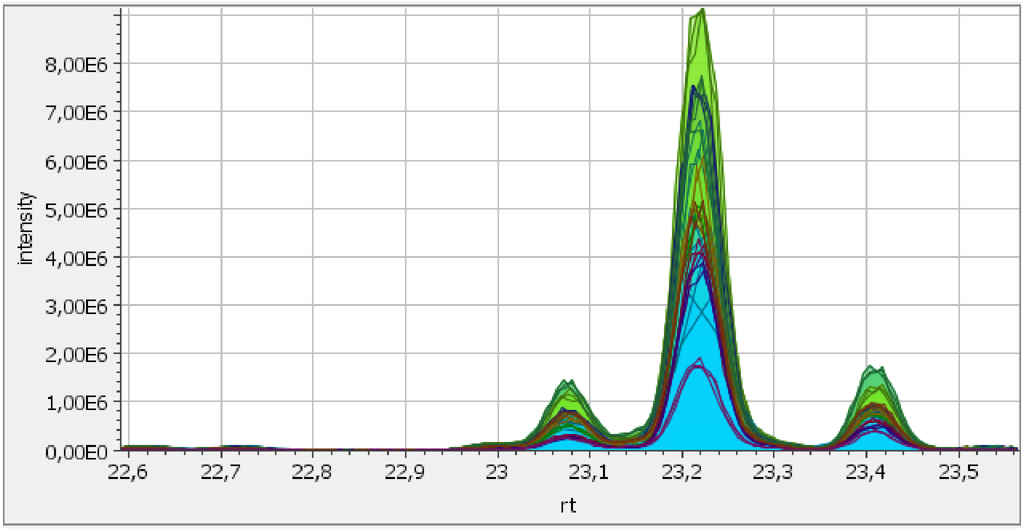

Figure 23: Integration of 3 isomers of TG 20:5-18:2-20:5 as one compound in the Lipidsearch interface. The graph shows 18 superimposed curves injected from 6 vials.

This did however make it necessary to manually integrate the AUC for all lipid counts both because the software algorithm was unable to find a natural cutoff when including several peaks under one umbrella, and to exclude obvious interference peaks in the integration.

There were some attempts at increasing the unique lipid count in the experiments, mainly by lowering the inclusion threshold mentioned in the mass spectrometry part of the method section. This setting was initially set to 1.0e5 as producer recommendation. Lowering this to the producers recommended minimum settings of 2.5e4 did not discover lipids not present in the first run and were hence restored to the initial recommended settings.

The linear relationship between quantity and signal were confirmed in the range 5e4 (lowest AUC in analysis) to 2.2e9 (highest AUC in analysis) with a dilution series of the TG 18:1-18:1-18:1 standard. Results not shown.

3.3 Fragmentation

Some problems encountered in the study was the inability for the method to fragment some compounds to achieve sufficient identification parameters. This means that some of the compounds got assigned fatty acid group key where the head group has been successfully identified but the rest of the molecule is sparsely identified as the total number of carbons and double bonds of the attached fatty acids (figure 24).

MGDG(22:6_22:6)	13.445
MGDG(32:5)	12.863

Figure 24: Two compounds identified in Lipidsearch, one complete identification (MGDG(22:6-22:6)) and one partial identification (MGDG(32:5)), and their retention time.

ProductIon	Type	ObsMz	Intensity	Delta(Da)
M-14:0+H	HCD	493.28	22	0.0004
M+H	HCD	721.4901	100	0.0016

Figure 25: There was a recorded a loss of a fatty acid 14:0 for compound MGDG(32:5)(figure 23), but partial identification remains.

This identification leaves several possibilities of what fatty acids may be contained in the molecules, which in turn leaves a possibility for DHA and EPA not being recognized. The reason this happened was because fragmentation produced an identifiable head group but lost both fatty acids, or that the neutral loss of one fatty acid not reach the threshold value of 1% of precursor ion. This might have resulted in parts of DHA/EPA content being hidden which could influence the result, but it seems unlikely as the fatty acids were uniformly distributed among the isomers. A lot of the identification entries are replicates, meaning that isomers of the same compounds have triggered identification scans with one being granted fatty acid identity and others getting group keys of combined fatty acid contents. This seems to have resulted in some isomers getting assigned a complete identification, while others only getting assigned a partial identification. Due to limitations in Lipidsearch we were unable to manually override this happening, but all isomer peak integration was done the same way between sample environments (Figure 26).

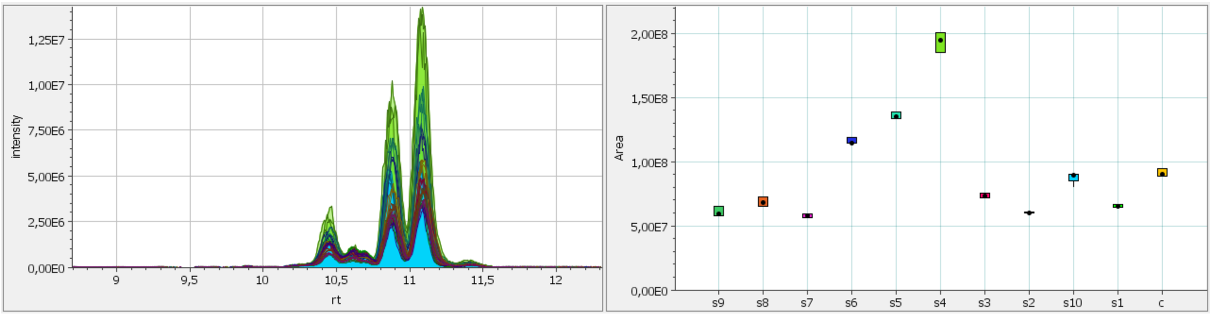

Figure 26: Integration of PC (14:0-20:5) in Lipidsearch. Figure shows all isomers of lipid included in integration with area designation on right pane. S1-S3 represent red light, S4-S6 represent blue light, and S7-S9 represent white light. C is control (Qc) and S10 belongs to identification files.

3.4 Lipid class composition

After integration of lipid compounds in Lipidseach, data was exported, normalized to the same AUC and aggregated to represent the growth environment light color of which they were cultivated. Data was then grouped by lipid class and the production of each lipid class was compared.

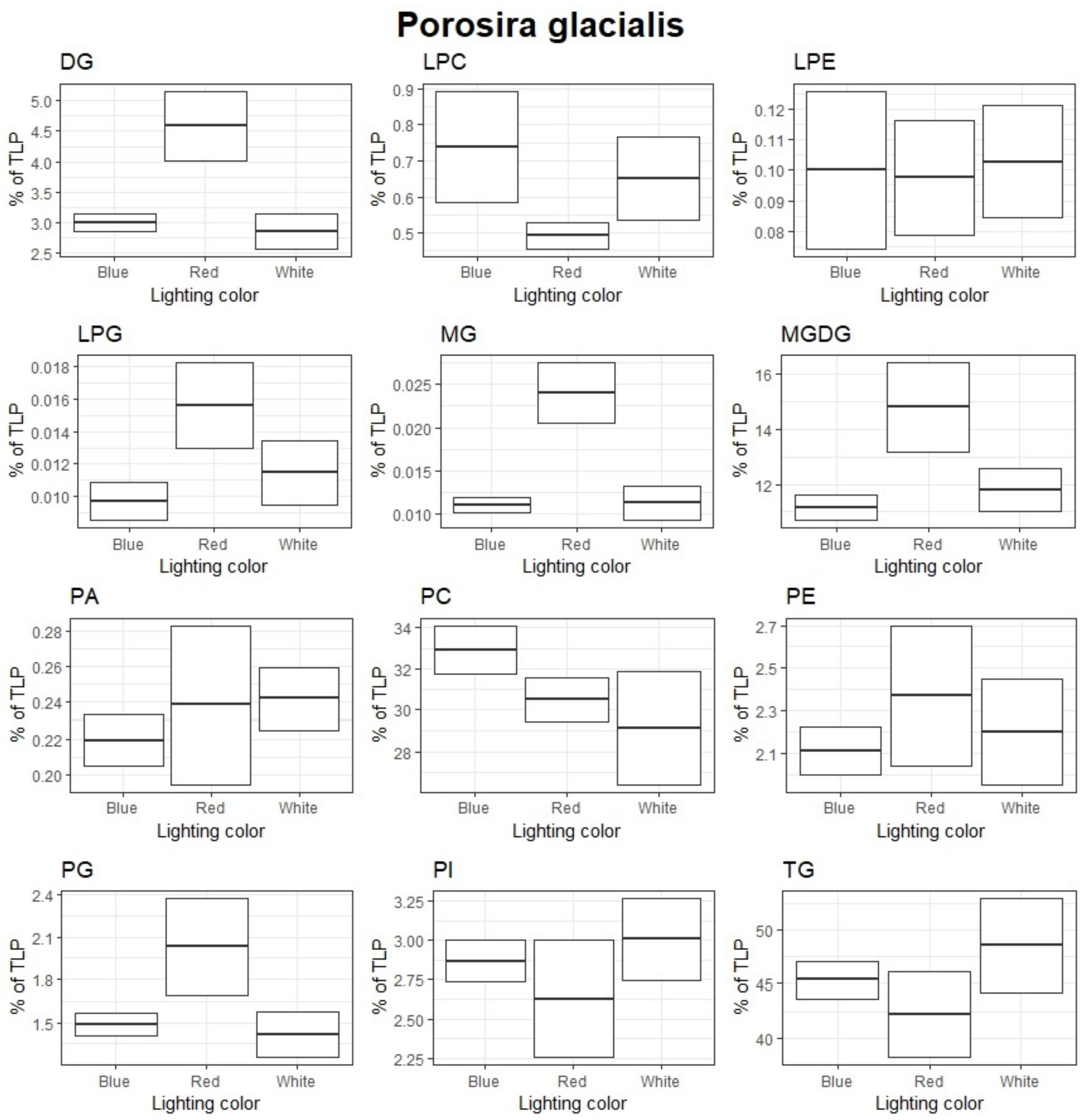

Figure 27: Boxplot of lipid class composition comparison of species Porosira glacialis. Boxplot show mean value +/- 1 SD. TLP = Total lipid production.

We observed 12 different lipid classes within the species *Porosira glacialis* (figure 27). The diglyceride (DG) content was 50% higher for red light (≈ 4.5%) compared to blue and white light (≈ 3%) ($p < 0.05$ for both). This is the same trend found in monoglyceride (MG) with red light (≈ 0.0125%) being higher than both blue- and white light (both ≈ 0.011%) ($p < 0.05$ for both). Triglyceride (TG) are however different than the other acylglycerols with white light having the highest content (≈ 48%) while blue light was lower (≈ 45.5%) and red light had the lowest content (≈ 42.5%), significant only between red- and white light ($p = 0.023$).

The contents of phosphatidylcholine (PC) and lysophosphatidylcholine (LPC) are quite similar with blue light producing most (PC ≈ 33%, LPC ≈ 0.75%) while red light has the second highest PC and the lowest LPC (PC ≈ 30.5%, LPC ≈ 0.5%). White light recorded the lowest PC content and the second lowest LPC content (PC ≈ 29.2%, LPC ≈ 0.65%). For PC there was a significant difference between white and blue light ($p = 0.0045$) and between white and red light ($p = 0.038$). The only significant finding in LPC was between the red and blue ($p = 0.011$).

The phosphatidylethanolamine (PE) content recorded a higher production for red light (≈ 2.4%) than white (≈ 2.2%) and blue (≈ 2.1%), but the large variance within each environment gives the intervals a considerable overlap and no significant differences were found. The lysophosphatidylethanolamine (LPE) content showed no difference between the environments.

Phosphatidylglycerol (PG) and lysophosphatidylglycerol (LPG) show similar patterns and has red light as producing most (PG ≈ 2%, LPG ≈ 0.016%). There is no difference between blue light (PG ≈ 1.5%, LPG ≈ 0.01%) and white light (PG ≈ 1.48%, LPG ≈ 0.011%). Red light was significantly higher than both blue- and white light for both PG and LPG ($p < 0.05$ for all).

Both phosphatidic acid (PA) and phosphatidylinositol (PI) show marginally higher content for white- (PA ≈ 0.24%, PI ≈ 3%) than blue light (PA ≈ 0.22%, 2.82%). Red light (PA ≈ 0.24, PI ≈ 2.63) seemed quite similar but had a large variance compared to the other environments which gave no significant finding.

The monogalactosyldiacylglycerol (MGDG) contents are highest for red light (≈ 15%), with white light (≈ 12%) recording second highest content and blue light recording the lowest content (≈ 11%). The difference was significant between both red- and blue light ($p = 2.6e\text{-}5$) and between red- and white light ($p = 0.004$).

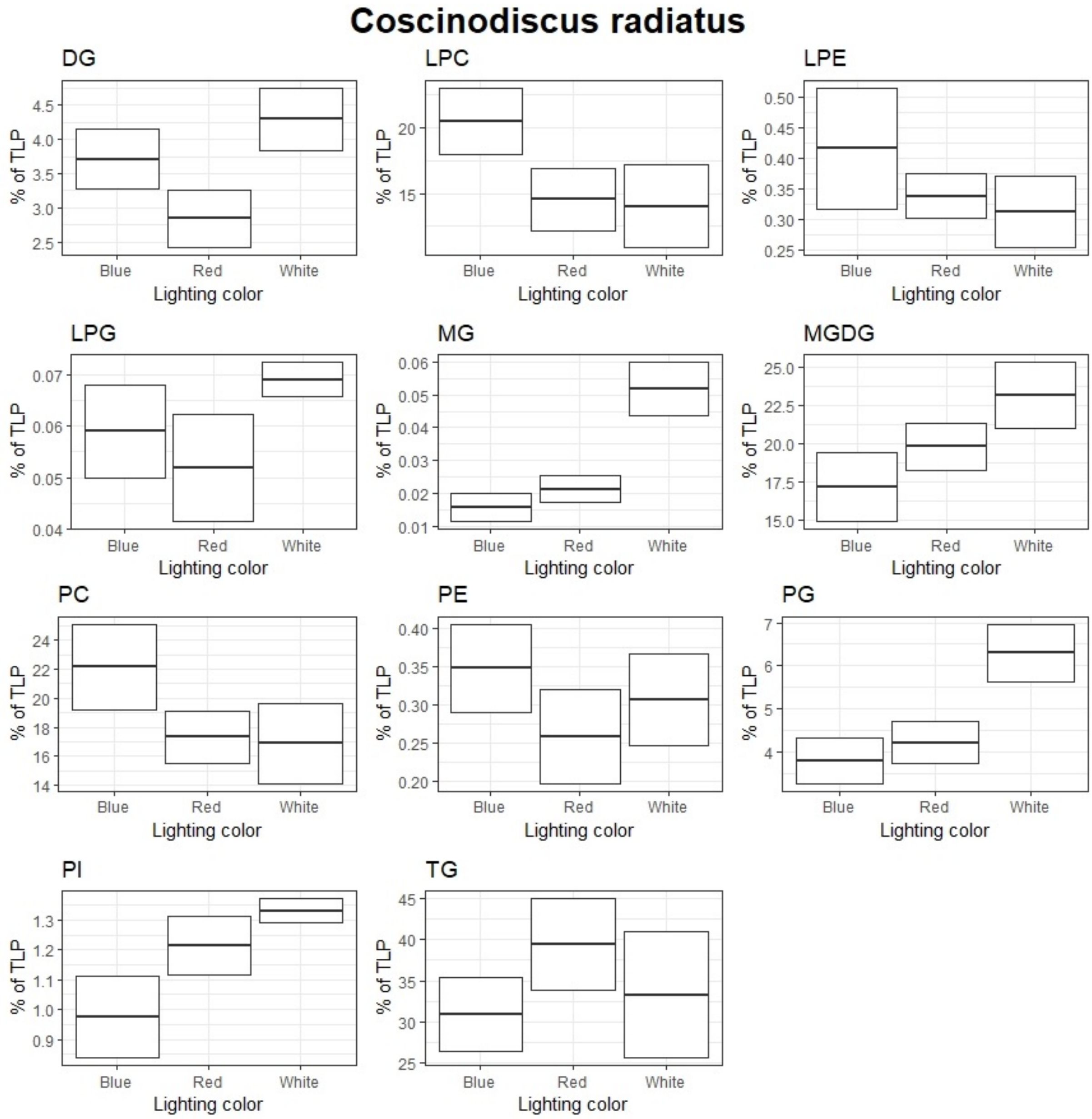

Figure 28: Boxplot of lipid class composition comparison of species Coscinodiscus radiatus. Boxplot of mean value +/- 1 SD. TLP = Total lipid production

We observed 11 different lipid classes within the species *Coscinodiscus radiatus* (figure 28). Phosphatidic acid (PA) was only observed in *P. glacialis.*

Diglyceride (DG) production was highest for white light (≈ 4.3%), followed by blue light (≈ 3.75%) and red light (≈ 2.8%), all differences was significant ($p < 0.05$ for all). The monoglyceride (MG) also show highest production for white light (≈ 0.052%), but here red light (≈ 0.02%) had higher contents than blue light (≈ 0.015%). White light had significantly higher contents than both blue- ($p = 5e-15$) and red light ($p= 2.6e-11$). Triglyceride (TG) production was highest for red light (≈ 40%) followed by white light (≈ 34%) and lowest for blue light (≈ 32%). There was however a large overlap of the intervals leaving no significant findings.

The phosphatidylcholine (PC) and lysophosphatidylcholine (LPC) showed very similar contents. Blue environment was the highest producer (PC ≈ 22%, LPC ≈ 21 %) while red- (PC ≈ 17.5%, LPC ≈ 15%) and white light (PC ≈ 17%, LPC ≈ 14%) were lower and had similar production to each other. The differences between blue light and both the red- ($p = 0.0028$) and white light ($p = 0.005$) environments was found to be significant.

Phosphatidylethanolamine (PE) and lysophosphatidylethanolamine (LPE) also showed similar characteristics as seen in PC and LPC. Blue produced more (PE ≈ 0.35%, LPE ≈ 0.43%) with red- (PE ≈ 0.26%, LPE ≈ 0.34%) and white light (PE ≈ 0.33%, LPE ≈ 0.34%) being lower and similar. These groups also showed a large overlap of intervals and the only significant finding were between the red- and blue light PE ($p = 0.027$)

Phosphatidylglycerol (PG) and lysophosphatidylglycerol (LPG) showed highest production for white light (PG ≈ 6.5%, LPG ≈ 0.07%) while red- (PG ≈ 4.4%, LPG ≈ 0.05%) and blue light (PG ≈ 3.8%, LPG ≈ 0.06%) were lower and similar each other. White light PG content was significantly higher than both red- and blue light ($p < 0.05$ for both) while the only significant finding for LPG was between the white- and red light ($p = 0.005$).

Phosphatidylinositol (PI) production was highest for white light (≈ 1.35%). Red light had second highest (≈ 1.22%) and blue light was lowest (≈ 1%). The content in the red light sample was significantly higher than both blue- and white light ($p < 0.05$ for both).

The monogalactosyldiacylglycerol (MGDG) content was highest in the white light sample (≈ 23%), followed by red light (≈ 20%) and lowest were the blue light environment (≈ 17.5%). Significant differences in MGDG content were found between white- and blue light ($p = 1.3e-6$) and between white- and red light ($p = 0.005$).

Comparison of the two species *P. glacialis* and *C. radiatus* showed that the diglyceride (DG) class had the same content range for both (2.5-4.5%), but that red light was the highest producing light environment for *P. glacialis* while it was white light for *C. radiatus.* The SD was similar in all samples. The monoglyceride (MG) class showed the same trend in which was the most producing light environment, but the content range (0.01-0.025% for *P. glacialis* and 0.015-0.06 for *C. radiatus)* was not quite as similar as in DG. This class also had similar SD for all samples. The content range for the triglyceride (TG) class was higher in *P. glacialis* (38-55%) with the highest content recorded in red light compared to *C. radiatus* (25-45%) that had the highest content recorded in white light. The SD was also similar in this class, with the largest difference being approximately 2x for white- and red light compared to blue light for *P. glacialis*.

For Phosphatidylcholine (PC), *P. glacialis* had a higher content range (26-34%) than *C. radiatus* (14-25%), but both showed blue light to give the highest content. Lysophosphatidylcholine (LPC) on the other hand was much lower in *P. glacialis* (0.4-0.9%) than in *C. radiatus* (12-25%) which can be of interest as this class has shown to be a better transporter of DHA (31) to the brain of mice than any other lipid class. This combined with the relatively high DHA content of *C. radiatus* (discussed later) makes it a good candidate for any direct food supplement aimed at human consumption, while the effect might not be as high if using intermediates such as fish (16). The SD intervals show that there had been large variation of content within color samples from *P. glacialis* for both PC with white light SD being almost three times the size of red light SD, and for LPC with blue light SD being almost four times the size of red light SD. For *C. radiatus* there were no noteworthy variation as the SDs are quite similar for all samples.

For phosphatidylethanolamine (PE) the contents were higher in *P. glacialis* (2.0-2.7%) with the highest content belonging to the red sample while *C. radiatus* (0.2-0.4%) had the highest content in the blue light sample. There was also some variation within these samples for *P. glacialis* as the SD for red light is three times that of blue. *C. Radiatus* had similar SD for all samples. Lysophosphatidylethanolamine (LPE) content was a little higher for *C. radiatus* (0.35-0.50%) than for *P.glacialis* (0.08-0.12%). There was no difference observed between colors in *P. glacialis* in neither content nor in SD size, while *C. radiatus* had higher content for blue light than the others, but also twice the size of SD for this sample.

The contents of phosphatidylglycerol (PG) were higher in *C. radiatus* (3.5-7%) with white light producing most. The SD for these samples were similar. In *P. glacialis* (1.2-2.4%) red light had the highest content. The SD was about four times higher for red than in the blue samples.

Phosphatidylinositol (PI) had a higher content in *P. glacialis* (2.25-3.25%) with white light having the highest content. There was also a lot of variation in these samples as the SD for red light is approximately three times bigger than that of blue light. In *C. radiatus* (0.8-1.4%) white light had the highest content. The SD was three times higher for blue light than that of white.

The monogalactosyldiacylglycerol (MGDG) content was highest in *C. radiatus* (15-25%) where white light produced the most. The SD for this class was similar for all samples. *P. glacialis* (11-17%) showed red light producing the highest content. The SD was more than three times higher for red light than for blue, showing a lot of variation within samples. MGDG content in this study is consistent with findings from the cyanobacteria Anacystis nidulans and in cucumber cotyledons that show increased accumulation when exposed to red or white light compared to blue (32, 33).

The large variation of contents within some of the samples are nothing new when working with biological samples. It can be a result of several factors ranging from bacterial growth in the medium of diatoms, or other contaminants, to simply being differences due to self-shadowing or similar phenomenon common in such cultivation. Controllable factors should however be considered for the future, and better control of growth phase (as mentioned earlier) is one of the key points to reducing the variation. Another key point might be to add more replicates to the study, which can improve the statistical strength as well as reduce the impact removal of one parallel has.

3.5 Fatty acid content of lipids

After comparing the lipid class differences between the different light environments, all lipid compounds were grouped by fatty acid components, and filtered by the inclusion of at least one DHA (22:6) fatty acid. Then a similar approach was done for EPA (20:5) and the content of lipids containing these fatty acids was compared. DHA and EPA were the main points of interest in this thesis and their content and distribution in lipid classes are shown in this chapter along with the contents of a known omega-6 fatty acid arachidonic acid (ARA 20:4n-6). Including the omega-6 ARA made it possible to inspect ratio of DHA:EPA/ARA. Ideally, this should have been done on all fatty acids found in the study, a work on which we started. But due to limited time, only these omega-3 EPA/DHA and the omega-6 acid ARA was included.

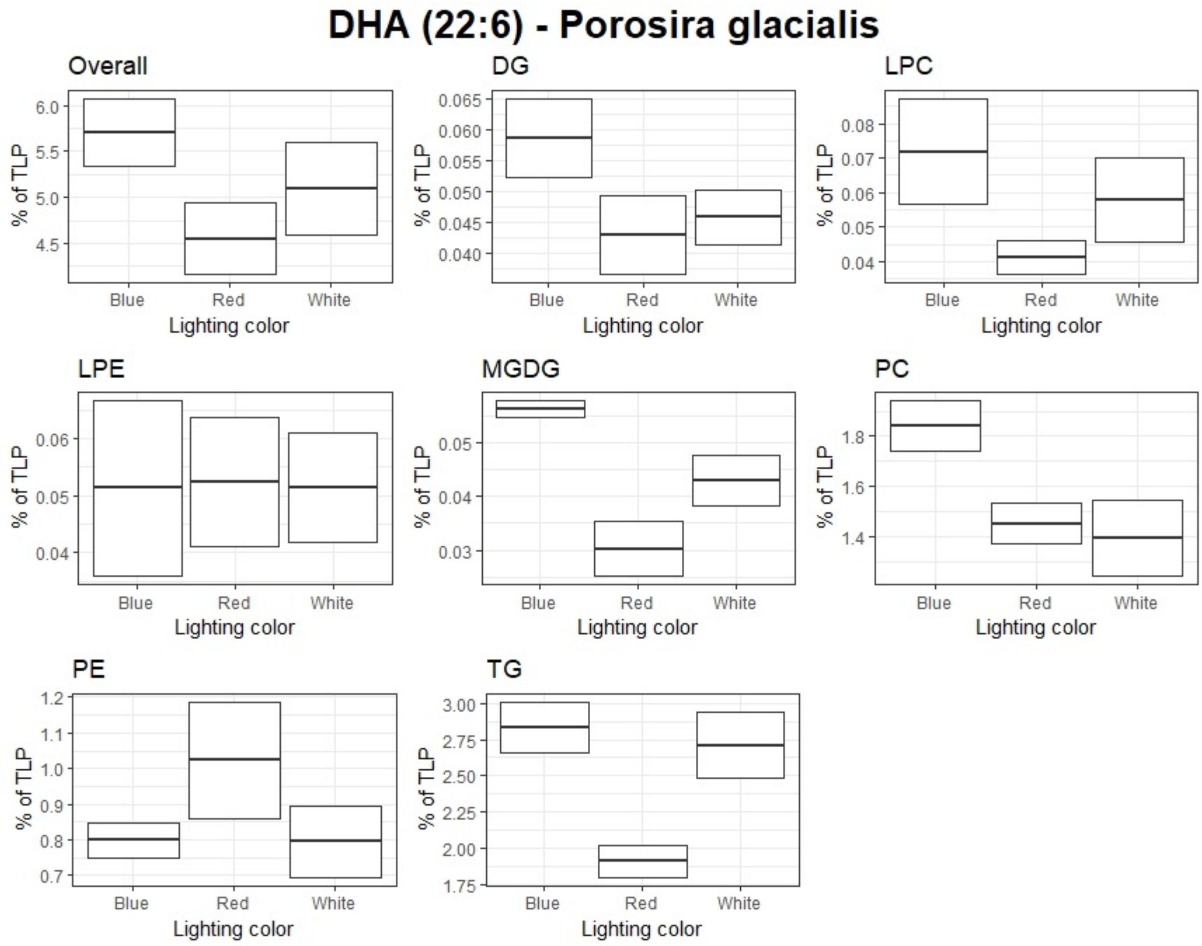

Figure 29: Boxplot of DHA content of species Porosira glacialis. Boxplot show mean value +/- 1 SD. TLP = Total lipid production

We observed DHA (22:6) and the distribution of this fatty acid in the lipid classes in *P. glacialis* (figure 29). For the overall content of DHA, the blue light (≈ 5.73%) represented a significant increase compared to both white (≈ 5.2%) and red light (≈ 4.6%) ($p < 0.05$ for both). White light showed higher content of DHA than red light, but this finding was not significant ($p > 0.05$).

Blue light was found to have the highest content of DHA in diglyceride (DG), lyso-phosphatidylcholine (LPC), monogalactosyldiacylglycerol (MGDG), phosphatidylcholine (PC) and triglyceride (TG). Lysophosphatidylethanolamine (LPE) showed the same content for all lights, while phosphatidylethanolamine (PE) showed a higher content of DHA in the red light sample. DHA was not observed in lysophosphatidylglycerol (LPG), monoglyceride (MG), phosphatidic acid (PA), phosphatidylglycerol (PG) or phosphatidylinositol (PI).

The majority of DHA contents were found in triglyceride (TG) (1.8-3%), phosphatidylcholine (PC) (1.3-1.9%) and phosphatidylethanolamine (PE) (0.7-0.18%).

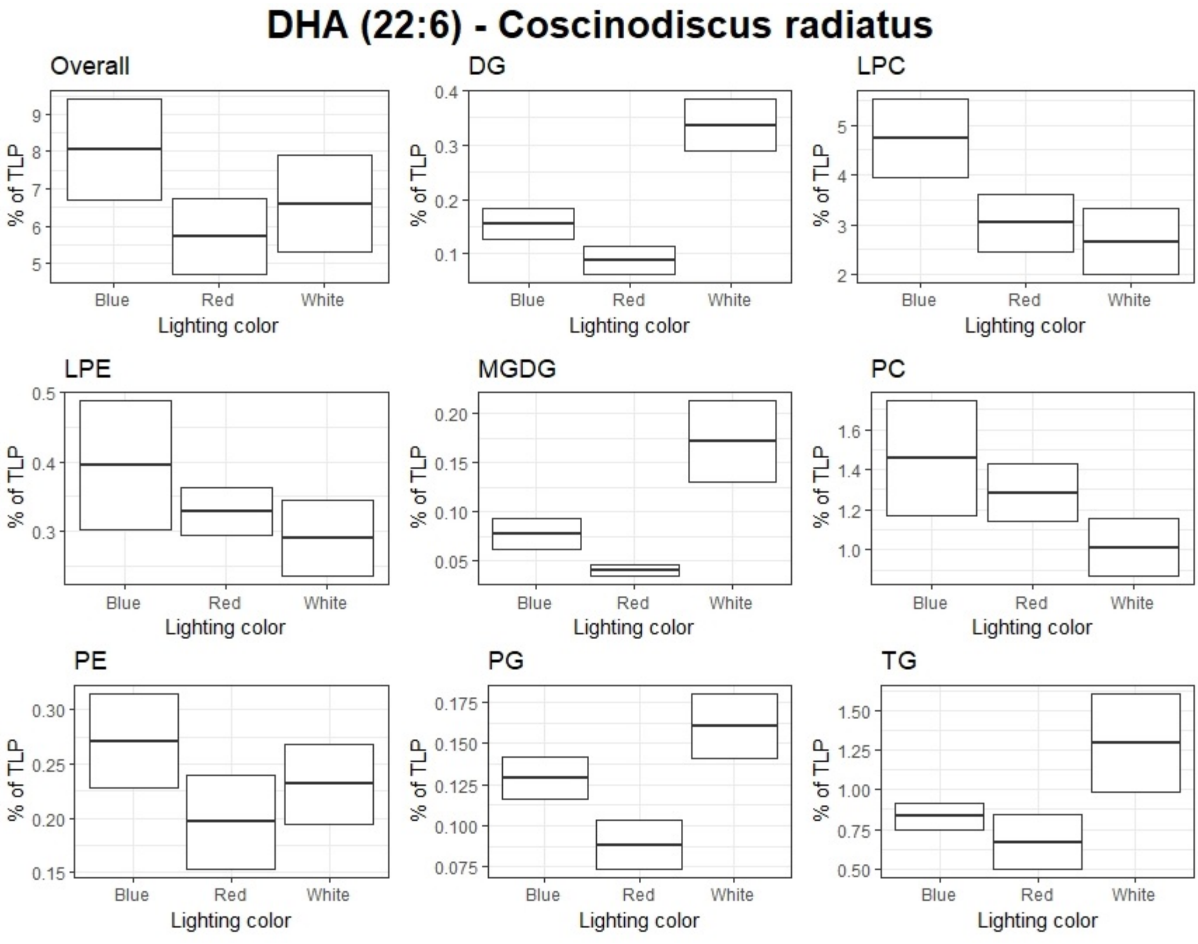

Figure 30: Boxplot of DHA content of species Coscinodiscus radiatus. Boxplot show mean value +/- 1 SD. TLP = Total lipid production

We observed DHA (22:6) and the distribution of this fatty acid in the lipid classes in *C. radiatus* (figure 30). For the overall content of DHA, the blue light (≈ 8%) show significantly higher contents of DHA compared to both white- (≈ 6.5%) and red light (≈ 5.7%) ($p < 0.05$ for both). The white light contents are higher than red light, but not significantly so ($p > 0.05$).

Blue light was found to have the highest content of DHA in phosphatidylcholine (PC), lysophosphatidylcholine (LPC), phosphatidylethanolamine (PE) and lysophosphatidylethanolamine (LPE) while white light was found to have the higher contents in diglyceride (DG), monogalactosyldiacylglycerol (MGDG), phosphatidylglycerol (PG) and triglyceride (TG).

The majority of DHA content was found in lysophosphatidylcholine (LPC) (2-5.5%), phosphatidylcholine (PC) (0.9-1.7%) and triglyceride (0.5-1.6%).

DHA was not observed in lysophosphatidylglycerol (LPG), monoglyceride (MG) or phosphatidylinositol (PI).

Comparison of the two species showed that more of the lipids in *C. radiatus* (4.5-9.5%) contain DHA than was found in *P. glacialis* (4-6%). The largest difference was seen in the class lysophosphatidylcholine (LPC) which was recorded to be < 0.1% in *P. glacialis* and 2-5.5% in *C. radiatus.*

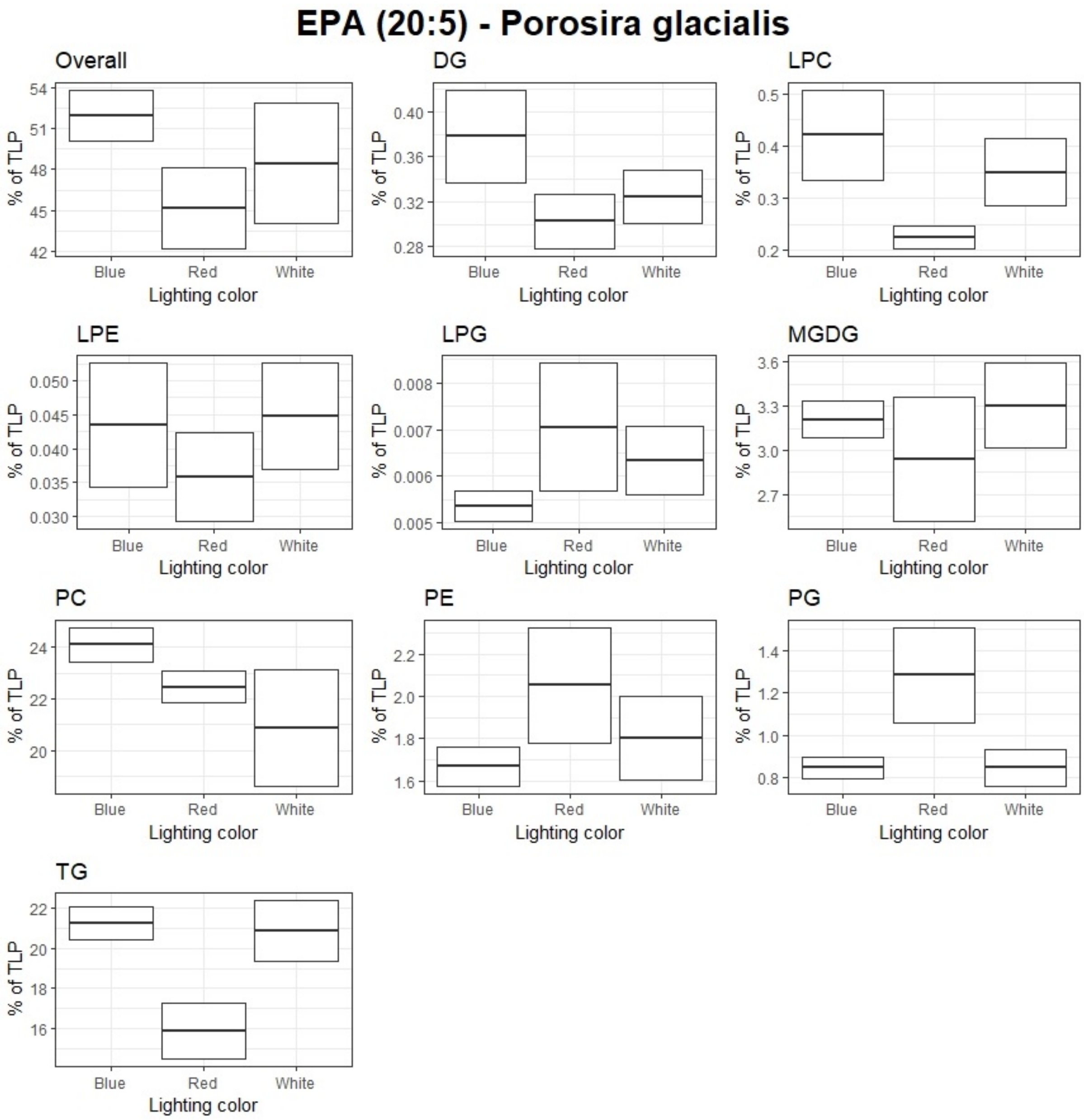

Figure 31: Boxplot of EPA content of species Porosira glacialis. Boxplot show mean value +/- 1 SD. TLP = Total lipid production.

We observed EPA (20:5n-3) and the distribution of this fatty acid in the lipid classes in *P. glacialis* (figure 31). For the overall contents, blue light (≈ 52%) represents a significant increase compared to white light (≈ 48), and white light is significantly higher than red light (≈ 45.5%) ($p < 0.05$ for all).

Blue light was found to have the highest EPA content in diglyceride (DG), lysophosphatidylcholine (LPC), and phosphatidylcholine (PC). Triglyceride (TG) showed similar contents for blue (≈ 21%) and white light (≈ 21%), with red light producing less (≈

16%). This was also the case with monogalactosyldiacylglycerol (MGDG) but the SD for red (≈ 2.9%) light overlaps all of blue- (≈ 3.2%) and most of white light (≈ 3.3%) contents. For lysophosphatidylethanolamine (LPE), blue- (≈ 0.044%) and white light (≈ 0.045) were similar and higher than red light (≈ 0.035%). For phosphatidylethanolamine (PE), red light (≈ 2.1%) had the highest content, white light (≈ 1.84) had the second highest, and blue light had the lowest content (≈ 1.68%). Phosphatidylglycerol (PG) also showed higher content for red light (≈ 1.29%) than blue- (≈ 0.85%) and white light (≈ 0.85%) which were similar.

The majority of lipids containing EPA was found in phosphatidylcholine (PC) (18-25%), triglyceride (TG) (14.5-22.5%) and monogalactosyldiacylglycerol (MGDG) (2.55-36%).

EPA was not observed in monoglyceride (MG), phosphatidic acid (PA) or phosphatidylinositol (PI).

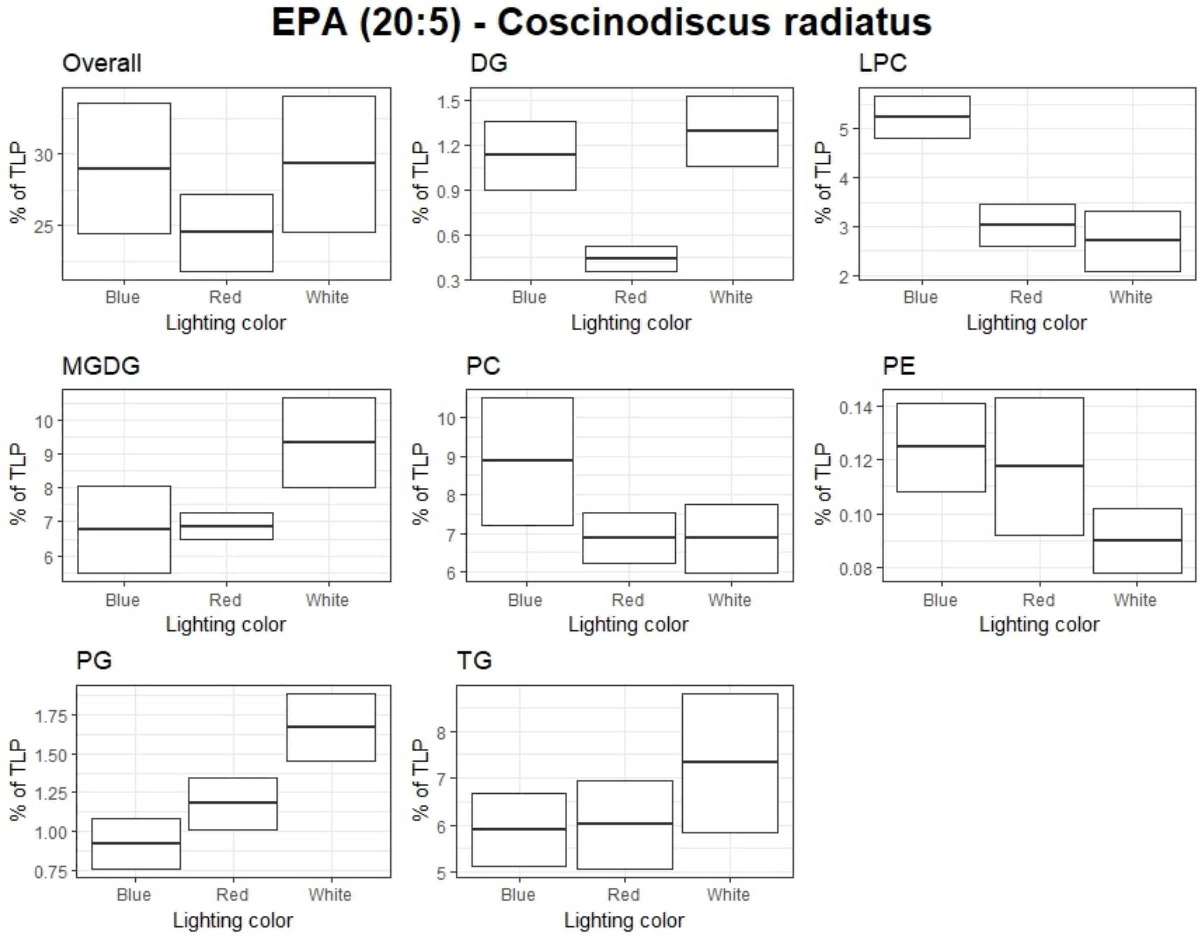

Figure 32: Boxplot of EPA content of species Coscinodiscus radiatus. Boxplot show mean value +/- 1 SD. TLP = Total lipid production

The overall contents of EPA in *C. radiatus* show a non-significant increase for blue light (≈ 29%) compared to white light (≈ 29%) ($p > 0.05$) while both blue light and white light had significantly higher contents than red light (≈ 25%) ($p < 0.05$ for both). Means of blue and white light appear equal at 29%, but blue showed a higher content when accounting for double or triple counts of EPA (figure 33).

Blue light (≈ 5.3%) was found to have the highest EPA content in lysophosphatidylcholine (LPC), with red- (≈ 3%) and white light (≈ 2.73%) being lower and similar each other. The same were true for phosphatidylcholine (PC) with blue light (≈ 9%) recording the highest content and red- (≈ 6.9%) and white light (≈ 6.9%) were lower and similar each other as well.

White light (≈ 9.4%) produced the highest EPA content in monogalactosyldiacylglycerol (MGDG) while red- (≈ 6.9%) and blue light (≈ 6.9%) were lower but quite similar each other. White light (≈ 1.3%) also recorded the highest EPA content in diglyceride (DG), but the blue light sample (≈ 1.1%) were close while red light (≈ 0.45%) produced less. White light (≈ 1.65%) also had the highest content of EPA in the classes phosphatidylglycerol (PG) with red light (≈ 1.2%) being higher than blue light (≈ 0.9%). Triglyceride (TG) showed white as having the highest EPA content (≈ 7.3%), with blue- and red light (both ≈ 6%) being lower.

EPA was not observed in lysophosphatidylethanolamine (LPE), monoglyceride (MG), phosphatidic acid (PA) or phosphatidylinositol (PI).

Comparison of the species show a larger percentage of EPA lipids in *P. glacialis* (42-54%) than in *C. radiatus* (22-33%). Phosphatidylcholine (PC) and triglyceride (TG) had the higher content range for *P. glacialis* with 18.5-25% and 14.5-22% compared to 6-11% and 5-9.5% for *C. radiatus* respectively. *C. radiatus* had a higher content of EPA in monogalactosyldiacylglycerol (MGDG) (5.5-11.5%) compared to *P. glacialis* (2.5-3.6%), along with a ten times higher lysophosphatidylcholine (LPC) EPA content (2-5.7% vs. 0.2-0.5%)

The figures (Figure 29, 30, 31, 32) all show the AUC for lipid species that has at least one EPA/DHA attached. It did not distinguish between double or triple counts of these fatty acids. For the relative content comparison of the fatty acids we therefore made a model where we multiplied the AUC of each lipid containing the fatty acid of interest by the count of this fatty acid (figure 35 and 36, appendix) and the P-values were generated from these models (figure 38, 39, 40 and 41, appendix). And to make sure that the figures containing DHA/EPA would be a good proxy to the real relative contents of fatty acids, we inspected lipid species containing 2 or 3 of these fatty acids to see if they had equal trends to the figures shown above, which was found to be true (Figure 33).

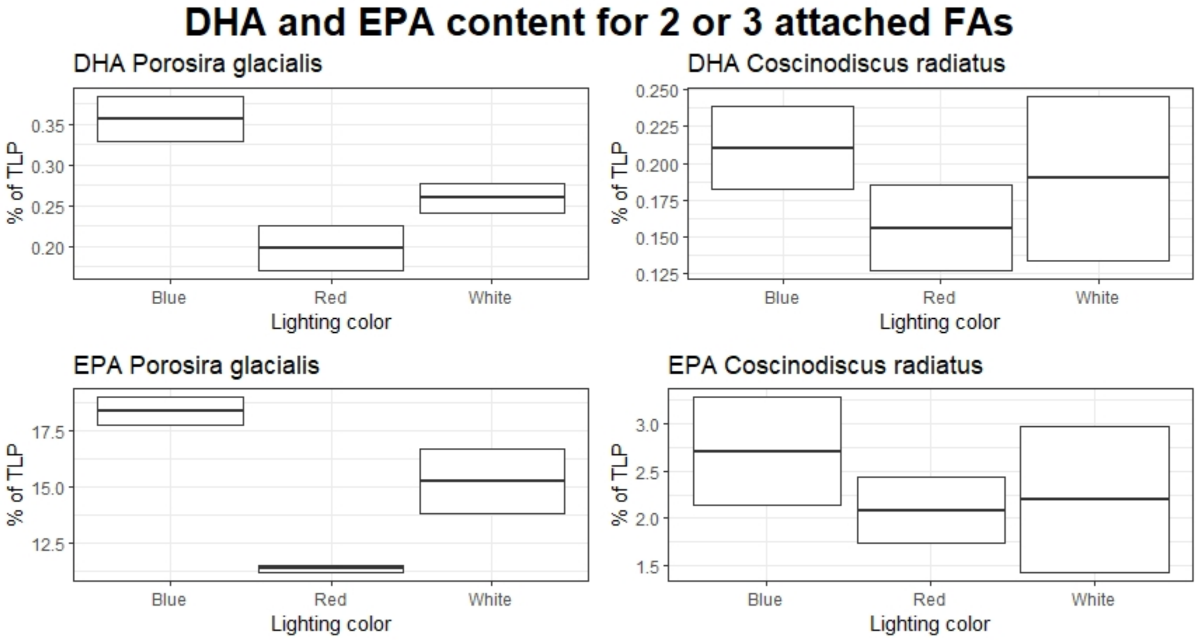

Figure 33: Boxplot for overall contents of P. glacialis and C. radiatus containing 2 or 3 DHA or EPA fatty acids. Boxplot show mean value +/- 1 SD. TLP = Total lipid production.

When inspecting lipid compounds that consist of 2 or 3 DHA or EPA fatty acids, we found that differences in both DHA and EPA were increased for *P. glacialis,* while *C. radiatus* only recorded a small increase in differences in both fatty acids.

Our findings suggest that both DHA and EPA are increased in blue light growth environment for both species of diatoms and that red light has the lowest content of these fatty acids.

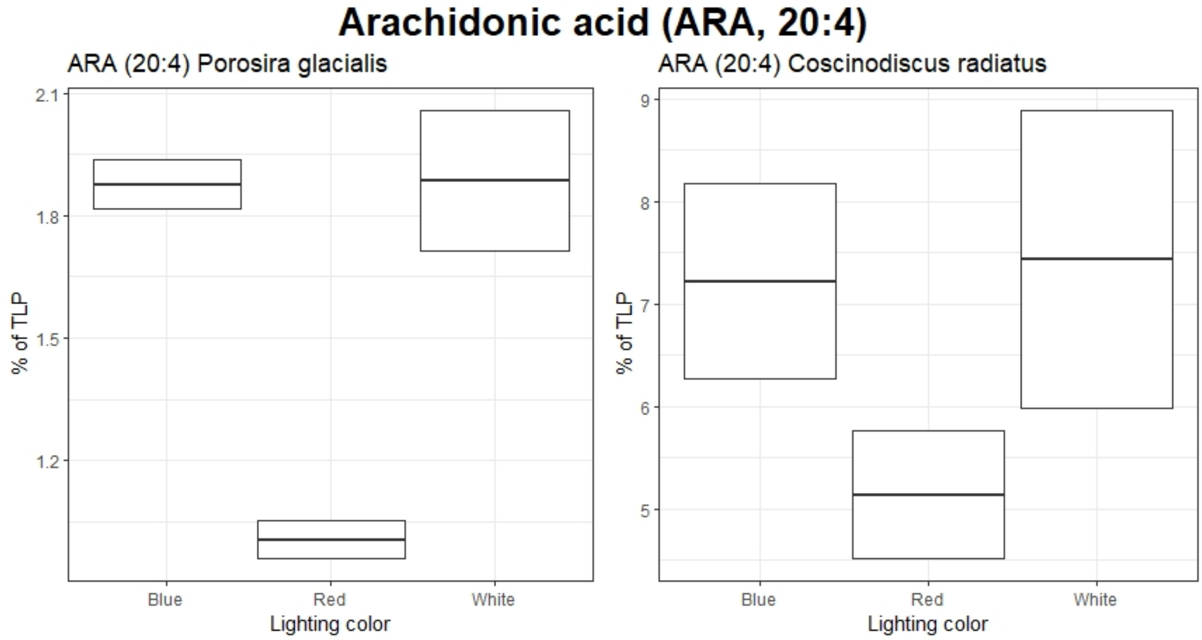

Figure 34: Boxplot of arachidonic acid (ARA) content of both species. Boxplot show mean value +/- 1 SD. TLP = Total lipid production

As the ratio of omega-3 to omega-6 play a role in maximizing the omega-3 content in fish, we compared the contents of the omega-6 arachidonic acid (20:4n-6) to see how the different lighting influenced this production (figure 34). For *P. glacialis,* there were no difference in content between blue light and white light (≈ 1.88 for both). Both were however significantly higher in content than was found in red light (≈ 0.95, p = 0.05 for both). We found the same characteristic in *C. radiatus* when inspecting significance, but the content range was found to be higher with blue- and white light contents recorded between 7.3-7.5% while red light recorded a content of approximately 5.2%.

Table 6: Ratio of DHA/ARA and EPA/ARA for P. glacialis and C. radiatus DHA = docosahexaenoic acid, EPA = eicosapentaenoic acid and ARA = arachidonic acid.

Species and fatty acids	Blue light	Red light	White light
P. glacialis DHA/ARA	3.0	4.8	2.7
P. glacialis EPA/ARA	27.6	47.8	25.5
C. radiatus DHA/ARA	1.1	1.1	0.86
C. radiatus EPA/ARA	3.9	4.8	3.8

Assuming that all of the 20:4 fatty acid observed in the samples was arachidonic acid, all of 20:5 was eicosapentaenoic acid and all of 22:6 was docosahexaenoic acid, the ratio of these fatty acids were calculated (table 1). Despite recording the lowest content of all the LC-PUFAs, red light was the one that showed the highest DHA/EPA:ARA ratio in all cases, except for *C. radiatus* DHA/ARA where blue light was equal. Blue light had a slightly higher ratio in all cases than that of white light. This was not an accurate representation of the total omega-3 to omega-6 content in the samples as just a few of the fatty acids were included, but it is nevertheless an interesting observation.

3.6 Limitations

Regrettably, no internal standards were included in the experiment. Trials with samples from older cultivation projects showed that we could compare relative abundancy in lipid profiles by normalizing the area under the curve. Though such comparison does not rely on information from internal standards, the addition of internal standards could have provided very useful information in this experiment.

Firstly, a triglyceride internal standard could have been used to verify that the large variance in triglyceride levels were in fact due to difference in the cultivated samples and not due to faulty extraction.

Secondly, internal standards could have helped decide the extraction efficiency of each class. A class specific extraction yield percentage could have helped estimate the absolute lipid contents of the diatom and, depending on the standards used, made quantification possible for some lipids.

Finally, the internal validity of an experiment using internal standards is far greater than without. Even if conducted properly, the experiments findings are put to a disadvantage in their lack of certainty by the exclusion of internal standards.

4 Conclusion and future perspectives

The content of EPA and DHA was found to be significantly increased for diatoms cultivated in a blue light environment compared to both red- and white light for *P. glacialis*. The ARA content was equal for blue- and white light who had a significantly higher content than red light. The white light cultivation showed a significant increase in EPA and ARA content over red light, but the small increase in DHA was not significant.

For *C. radiatus* only EPA was significantly higher in the blue light sample than in the white light, while all LC-PUFA were significantly higher for blue light compared to red light. White light had a significantly higher content of EPA and ARA than that of red light, but the increase of DHA was not significant.

The findings suggest that a blue light growth environment is superior to both red- and white light when it comes to maximizing the content of LC-PUFA. The ratio of omega-3 to omega-6 is however suggested to be higher in the red light environment based of the ratio of EPA and DHA to ARA.

A future prospect might be reproducing the work done in this thesis and including techniques such as gas chromatography with picolinyl derivatization of fatty acids to allow the identification of double bonds, and to more accurately find the omega-3 to omega-6 ratio.

If reproduced, it would also be wise to include an internal standard for each major lipid class. These standards should include PUFAs like EPA (20:5n-3) and/or DHA (22:6n-3) as this was a point of interest in the experiment and could have made absolute quantification possible for some of these compounds. An increase of natural replicates of each color setting and a reduced cultivation time would also be advised.

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Appendix

Table 7: P-values for differences in lipid classes for both species.

Species	*Lipid*	*lhs*	*estimate*	*std.error*	*statistic*	*p.value*
Porosira	MAG	White - Red	-0.0142407370	0.001979998	-7.19230035	1.143863e-12
Porosira	MAG	Red - Blue	0.0143718176	0.001979998	7.25850274	1.926315e-11
Porosira	DAG	White - Red	-0.3857708809	0.065596949	-5.88092721	7.853860e-09
Porosira	DAG	Red - Blue	0.3022179944	0.065596949	4.60719592	1.442796e-05
Porosira	MGDG	Red - Blue	2.9392639198	0.666696040	4.40870163	2.605335e-05
Porosira	LPG	Red - Blue	0.0066128698	0.001637903	4.03740092	1.532109e-04
Porosira	PG	White - Red	-0.6836743919	0.180192895	-3.79412513	4.511720e-04
Porosira	MGDG	White - Red	-2.3318322084	0.666696040	-3.49759421	1.372717e-03
Porosira	PG	Red - Blue	0.6043094248	0.180192895	3.35368064	2.274990e-03
Porosira	PC	White - Blue	-3.7025551351	1.168710634	-3.16806832	4.534004e-03
Porosira	LPG	White - Red	-0.0047940459	0.001637903	-2.92694182	9.568569e-03
Porosira	LPC	Red - Blue	-0.2677849731	0.092843608	-2.88425857	1.093674e-02
Porosira	TAG	White - Red	6.3684918959	2.415463363	2.63655081	2.287382e-02
Porosira	PC	White - Red	-3.1957942059	1.306658212	-2.44577670	3.828283e-02
Porosira	PE	Red - Blue	0.3979760214	0.179407537	2.21827928	6.793102e-02
Porosira	LPC	White - Red	0.1664596310	0.092843608	1.79290351	1.714508e-01
Porosira	PE	White - Red	-0.2951377121	0.179407537	-1.64506864	2.262577e-01
Porosira	PI	White - Red	0.3718746159	0.231010116	1.60977633	2.408424e-01
Porosira	TAG	White - Blue	3.1159420797	2.160456110	1.44226123	3.185355e-01
Porosira	DAG	White - Blue	-0.0835528865	0.058671695	-1.42407488	3.277457e-01
Porosira	TAG	Red - Blue	-3.2525498162	2.415463363	-1.34655316	3.686949e-01
Porosira	LPG	White - Blue	0.0018188239	0.001464985	1.24153102	4.279279e-01
Porosira	LPC	White - Blue	-0.1013253421	0.083041848	-1.22017206	4.404658e-01
Porosira	PI	Red - Blue	-0.2353608643	0.231010116	-1.01883359	5.642723e-01
Porosira	MGDG	White - Blue	0.6074317114	0.596311067	1.01864907	5.644071e-01
Porosira	PI	White - Blue	0.1365137516	0.206621729	0.66069407	7.858584e-01
Porosira	PE	White - Blue	0.1028383093	0.160466979	0.64086898	7.971215e-01
Porosira	PG	White - Blue	-0.0793649671	0.161169425	-0.49243190	8.746563e-01
Porosira	PC	Red - Blue	-0.5067609292	1.306658212	-0.38782975	9.202690e-01
Porosira	LPE	White - Red	0.0044180392	0.017054102	0.25906020	9.635982e-01
Porosira	LPE	White - Blue	0.0021225743	0.015253653	0.13915187	9.893573e-01
Porosira	LPE	Red - Blue	-0.0022954649	0.017054102	-0.13459899	9.900388e-01
Porosira	MAG	White - Blue	0.0001310806	0.001770964	0.07401653	9.969772e-01
Coscinodiscus	DAG	White - Red	1.437311200	0.165836677	8.66702846	0.000000e+00
Coscinodiscus	MAG	White - Blue	0.039820909	0.005048429	7.88778172	4.996004e-15
Coscinodiscus	MAG	White - Red	0.034031225	0.005048429	6.74095302	2.646339e-11
Coscinodiscus	DAG	Red - Blue	-0.987834247	0.148328833	-6.65975876	4.330314e-11
Coscinodiscus	PG	White - Blue	2.110997444	0.350941020	6.01524850	5.353014e-09
Coscinodiscus	PI	White - Blue	0.358407620	0.063555350	5.63929896	4.423195e-08
Coscinodiscus	MGDG	White - Blue	5.975751004	1.172505359	5.09656605	1.287630e-06
Coscinodiscus	PG	White - Red	1.561310215	0.350941020	4.44892482	2.199393e-05
Coscinodiscus	PI	Red - Blue	0.212700553	0.056845633	3.74172193	5.028291e-04
Coscinodiscus	LPC	Red - Blue	-7.059908597	2.139679150	-3.29951741	2.842108e-03
Coscinodiscus	LPG	White - Red	0.019404118	0.006185070	3.13725111	4.860949e-03
Coscinodiscus	LPC	White - Blue	-7.474446563	2.392234014	-3.12446296	4.922447e-03
Coscinodiscus	MGDG	White - Red	3.639471633	1.172505359	3.10401279	5.324905e-03
Coscinodiscus	DAG	White - Blue	0.449476954	0.165836677	2.71035914	1.831606e-02
Coscinodiscus	PE	Red - Blue	-0.095503530	0.037242607	-2.56436210	2.752615e-02
Coscinodiscus	PI	White - Red	0.145707067	0.063555350	2.29260113	5.670828e-02
Coscinodiscus	MGDG	Red - Blue	2.336279371	1.048720675	2.22774226	6.642026e-02
Coscinodiscus	PC	Red - Blue	-3.156206441	1.439722839	-2.19223197	7.215910e-02
Coscinodiscus	TAG	Red - Blue	8.300414688	3.893503119	2.13186286	8.320075e-02
Coscinodiscus	PC	White - Blue	-3.247862874	1.609659068	-2.01773341	1.075844e-01
Coscinodiscus	LPE	White - Blue	-0.121631281	0.066812928	-1.82047524	1.624415e-01
Coscinodiscus	PG	Red - Blue	0.549687229	0.313891191	1.75120311	1.857997e-01
Coscinodiscus	LPG	White - Blue	0.010350790	0.006185070	1.67351220	2.148456e-01
Coscinodiscus	LPG	Red - Blue	-0.009053328	0.005532095	-1.63650985	2.296553e-01
Coscinodiscus	LPE	Red - Blue	-0.096365382	0.059759299	-1.61255876	2.397124e-01
Coscinodiscus	TAG	White - Red	-6.344920499	4.353068823	-1.45757413	3.109191e-01
Coscinodiscus	PE	White - Blue	-0.056358193	0.041638500	-1.35351159	3.649109e-01
Coscinodiscus	MAG	Red - Blue	0.005789684	0.004515453	1.28219347	4.045061e-01
Coscinodiscus	PE	White - Red	0.039145337	0.041638500	0.94012360	6.142160e-01
Coscinodiscus	TAG	White - Blue	1.955494189	4.353068823	0.44922198	8.945245e-01
Coscinodiscus	LPE	White - Red	-0.025265899	0.066812928	-0.37815884	9.240413e-01
Coscinodiscus	LPC	White - Red	-0.414537966	2.392234014	-0.17328487	9.835446e-01
Coscinodiscus	PC	White - Red	-0.091656433	1.609659068	-0.05694152	9.982099e-01

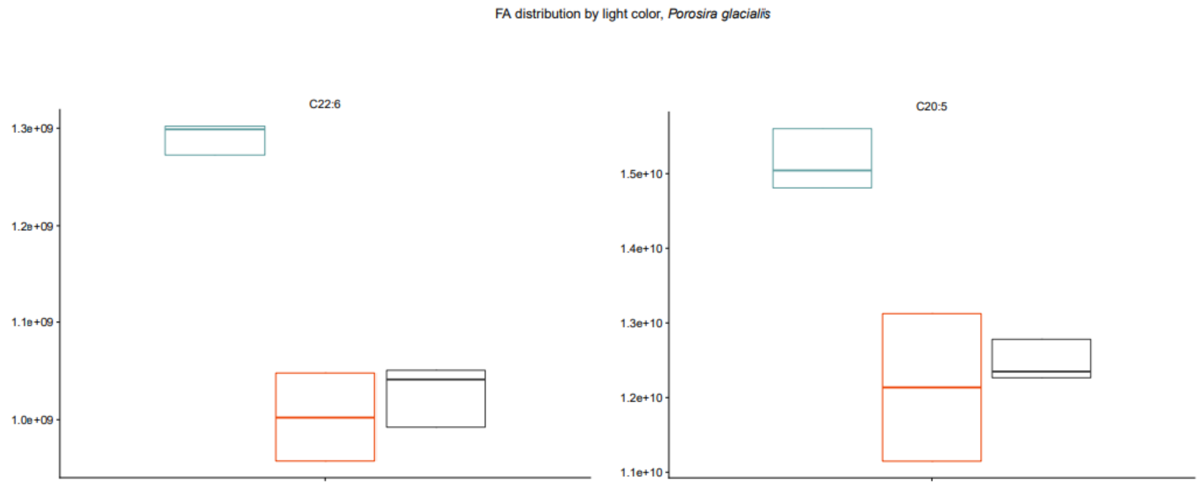

Figure 35: Area of DHA and EPA for P. glacialis when multiplying by the fatty acid count of DHA/EPA in the molecules.

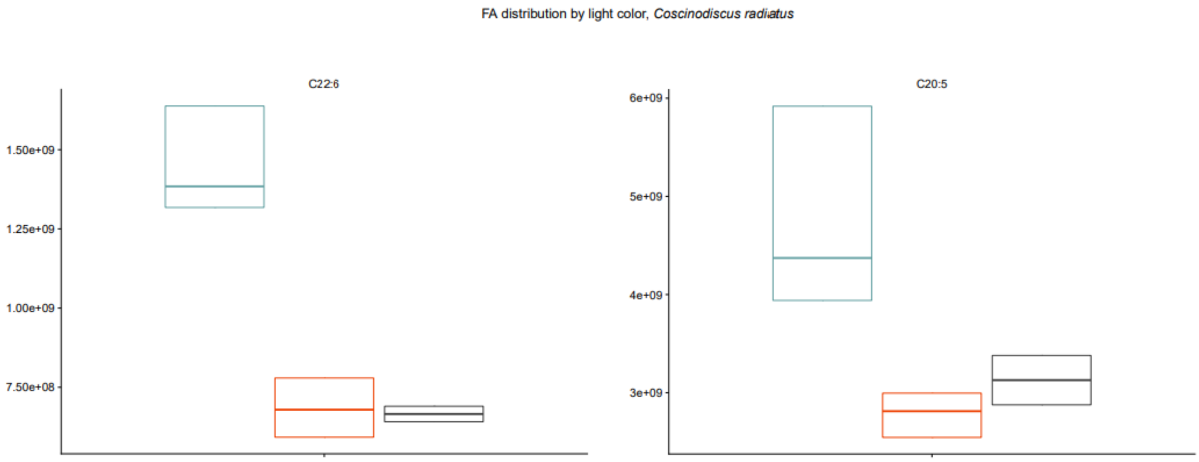

Figure 36: Area of DHA and EPA for C. radiatus when multiplying by the fatty acid count of DHA/EPA in the molecules.

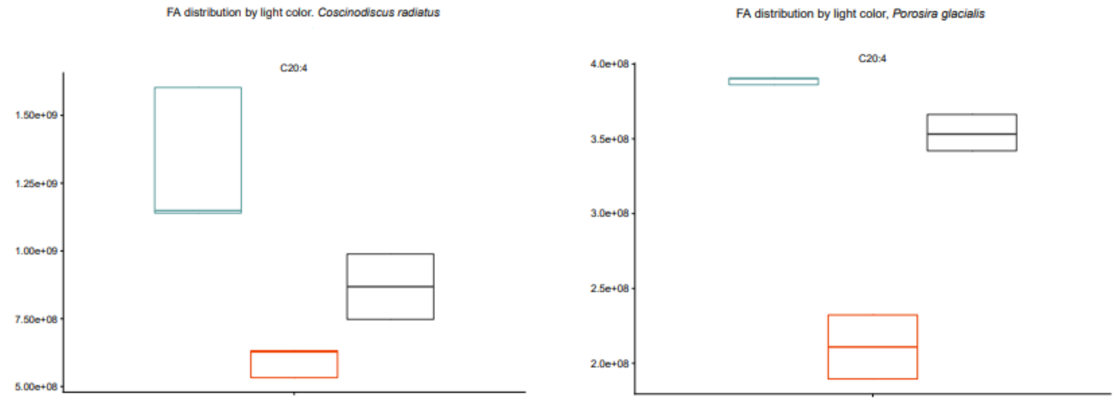

Figure 37: Area of ARA for both species when multiplying by the fatty acid count of ARA in the molecules.

```
```{r Tukey's test Porosira, main fatty acids}
FA.tukeys.porosira <- AllFA_sum %>%
   filter(Species == "Porosira") %>%
  #filter(freq > 1) %>%
  filter(FA1 == "C22:6" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.porosira

```
```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C22:6	Red - Blue	0	-0.5953879	0.09286826	-6.411103	1.093224e-09
C22:6	White - Blue	0	-0.3815799	0.08306390	-4.593811	1.120908e-05
C22:6	White - Red	0	0.2138081	0.09286826	2.302273	5.521140e-02

3 rows

Figure 38: P-values for P. glacialis DHA content.

```{r Tukey's test Coscinodiscus, main fatty acids}
FA.tukeys.cos <- AllFA_sum %>%
  filter(Species == "Cos") %>%
  #filter(freq > 1) %>%
  filter(FA1 == "C22:6" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.cos

```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C22:6	Red - Blue	0	-1.5690492	0.3104663	-5.053847	1.427912e-06
C22:6	White - Blue	0	-1.2042412	0.3471118	-3.469318	1.573243e-03
C22:6	White - Red	0	0.3648079	0.3471118	1.050981	5.439992e-01

3 rows

Figure 39: P-values for C. radiatus DHA content.

```{r Tukey's test Porosira, main fatty acids}
FA.tukeys.porosira <- AllFA_sum %>%
  filter(Species == "Porosira") %>%
  #filter(freq > 1) %>%
  filter(FA1 == "C20:5" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.porosira

```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C20:5	Red - Blue	0	-6.260306	0.7894668	-7.929790	1.554312e-14
C20:5	White - Blue	0	-3.518475	0.7061206	-4.982825	2.444176e-06
C20:5	White - Red	0	2.741831	0.7894668	3.473016	1.424979e-03

3 rows

Figure 40:P-values for P.glacialis EPA content.

```
```{r Tukey's test Coscinodiscus, main fatty acids}
FA.tukeys.cos <- AllFA_sum %>%
   filter(Species == "Cos") %>%
  #filter(freq > 1) %>%
  filter(FA1 == "C20:5" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.cos

```
```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C20:5	White - Red	0	3.4026421	0.9552496	3.5620452	0.001032597
C20:5	Red - Blue	0	-2.6725504	0.8544012	-3.1279807	0.004824526
C20:5	White - Blue	0	0.7300917	0.9552496	0.7642942	0.724433205

3 rows

Figure 41: P-values for C. radiatus EPA content.

```
```{r Tukeys test, porosira}
FA.tukeys.porosira.EPA <- AllFA_sum %>%
   filter(Species == "Porosira") %>%
  #filter(freq > 2) %>%
  filter(FA1 == "C20:4" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.porosira.EPA

```
```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C20:4	Red - Blue	0	-0.37829481	0.02526332	-14.9740734	0.0000000
C20:4	White - Red	0	0.36587245	0.02526332	14.4823583	0.0000000
C20:4	White - Blue	0	-0.01242235	0.02259620	-0.5497541	0.8462887

3 rows

Figure 42: P-values for P.glacialis ARA content.

```
```{r Tukeys test, coscinodiscus}
FA.tukeys.coscinodiscus.ARA <- AllFA_sum %>%
   filter(Species == "Cos") %>%
  #filter(freq > 2) %>%
  filter(FA1 == "C20:4" ) %>%
  group_by(FA1) %>%
  do(
    glm(freq ~ Light, family = "gaussian", data = .) %>% glht(linfct = mcp(Light = "Tukey")) %>%
      summary %>%
      tidy()
    ) %>%
  arrange(p.value)

FA.tukeys.coscinodiscus.ARA

```
```

FA1 <fctr>	lhs <chr>	rhs <dbl>	estimate <dbl>	std.error <dbl>	statistic <dbl>	p.value <dbl>
C20:4	Red - Blue	0	-1.4254501	0.09113428	-15.641206	0.00000000
C20:4	White - Red	0	1.6475226	0.10189123	16.169426	0.00000000
C20:4	White - Blue	0	0.2220725	0.10189123	2.179506	0.07434588

3 rows

Figure 43: P-values for C.radiatus ARA content.

Figure 44: The following pages contain the identification files for both species in the thesis and the area assigned to each of the lipids. The dataset is not complete, as that would require too much space.

Job Name	Glacialis_smart	
Sample		
c-1	Poros	TV_TM_201113_Rs_2.raw
c-2	Poros	TV_TM_201113_Rs_3.raw
c-3	Poros	TV_TM_201113_Rs_1.raw
s1-1	Poros	TV_TM_201113_R1_3.raw
s1-2	Poros	TV_TM_201113_R1_1.raw
s1-3	Poros	TV_TM_201113_R1_2.raw
s10-1	NY_II	TV_TM_201213_ID_05.raw
s10-2	NY_II	TV_TM_201213_ID_04.raw
s10-3	NY_II	TV_TM_201213_ID_03.raw
s10-4	NY_II	TV_TM_201213_ID_02.raw
s10-5	NY_II	TV_TM_201213_ID_01.raw
s2-1	Poros	TV_TM_201113_R2_2.raw
s2-2	Poros	TV_TM_201113_R2_3.raw
s2-3	Poros	TV_TM_201113_R2_1.raw
s3-1	Poros	TV_TM_201113_R3_3.raw
s3-2	Poros	TV_TM_201113_R3_2.raw
s3-3	Poros	TV_TM_201113_R3_1.raw
s4-1	Poros	TV_TM_201113_B1_3.raw
s4-2	Poros	TV_TM_201113_B1_1.raw
s4-3	Poros	TV_TM_201113_B1_2.raw
s5-1	Poros	TV_TM_201113_B2_3.raw
s5-2	Poros	TV_TM_201113_B2_2.raw
s5-3	Poros	TV_TM_201113_B2_1.raw
s6-1	Poros	TV_TM_201113_B3_2.raw
s6-2	Poros	TV_TM_201113_B3_3.raw
s6-3	Poros	TV_TM_201113_B3_1.raw
s7-1	Poros	TV_TM_201113_W1_3.raw
s7-2	Poros	TV_TM_201113_W1_1.raw
s7-3	Poros	TV_TM_201113_W1_2.raw
s8-1	Poros	TV_TM_201113_W2_3.raw
s8-2	Poros	TV_TM_201113_W2_2.raw
s8-3	Poros	TV_TM_201113_W2_1.raw
s9-1	Poros	TV_TM_201113_W3_3.raw
s9-2	Poros	TV_TM_201113_W3_2.raw
s9-3	Poros	TV_TM_201113_W3_1.raw
Result		

LipidMolec	Class	Calc Mass	MainArea[c]	MainArea[s1]	MainArea[s10	MainArea[s2]	MainArea[s3]	MainArea[s4]	MainArea[s5]	MainArea[s6]	MainArea[s7]	MainArea[s8]	MainArea[s9]
DG(14:0_14:0)	DG	512.4441	7.86E+05	8.24E+05	5.43E+05	7.55E+05	6.98E+05	8.77E+05	1.00E+06	1.06E+06	7.12E+05	6.43E+05	7.34E+05
DG(16:1_14:0)	DG	538.4597	1.96E+07	2.41E+07	1.50E+07	2.32E+07	2.43E+07	2.13E+07	2.07E+07	2.28E+07	1.61E+07	1.71E+07	1.84E+07
DG(16:1_14:0)	DG	538.4597	7.29E+06	9.21E+06	5.63E+06	8.56E+06	8.03E+06	7.76E+06	7.62E+06	7.78E+06	6.41E+06	6.48E+06	6.28E+06
DG(16:1_14:0)	DG	538.4597	4.07E+05	3.86E+05	2.84E+05	4.14E+05	4.02E+05	4.32E+05	4.83E+05	5.06E+05	3.79E+05	3.62E+05	4.08E+05
DG(16:1_16:1)	DG	564.4754	2.91E+07	4.49E+07	2.17E+07	4.15E+07	3.89E+07	2.53E+07	2.39E+07	2.60E+07	2.14E+07	2.36E+07	2.40E+07
DG(16:1_16:1)	DG	564.4754	7.87E+06	1.12E+07	6.17E+06	1.15E+07	1.04E+07	6.82E+06	6.54E+06	6.74E+06	6.58E+06	6.95E+06	6.25E+06
DG(16:1_20:5)	DG	612.4754	2.64E+07	3.53E+07	2.03E+07	2.64E+07	2.57E+07	3.00E+07	2.78E+07	2.90E+07	2.27E+07	2.36E+07	2.43E+07
DG(18:4_14:0)	DG	560.4441	2.87E+07	5.97E+07	1.85E+07	5.22E+07	5.03E+07	2.03E+07	1.88E+07	1.96E+07	2.03E+07	2.13E+07	1.88E+07
DG(18:4_14:0)	DG	560.4441	8.46E+06	1.95E+07	6.73E+06	1.16E+07	1.06E+07	6.24E+06	5.86E+06	5.71E+06	6.02E+06	6.60E+06	5.82E+06
DG(18:4_16:0)	DG	588.4754	3.18E+05	1.28E+06	2.50E+05	5.40E+05	5.06E+05	2.53E+05	2.31E+05	2.32E+05	3.34E+05	3.90E+05	2.83E+05
DG(18:4_16:1)	DG	586.4597	2.47E+07	3.80E+07	2.51E+07	3.58E+07	3.26E+07	2.13E+07	1.98E+07	2.30E+07	1.68E+07	1.82E+07	1.86E+07
DG(18:4_18:4)	DG	608.4441	2.96E+06	8.67E+06	1.98E+06	5.41E+06	5.79E+06	2.29E+06	1.88E+06	1.88E+06	1.92E+06	1.89E+06	1.73E+06
DG(18:4_20:5)	DG	634.4597	1.82E+07	3.33E+07	1.38E+07	2.08E+07	1.82E+07	2.03E+07	1.58E+07	1.45E+07	1.43E+07	1.42E+07	1.35E+07
DG(20:5_20:5)	DG	660.4754	2.60E+07	1.90E+07	2.10E+07	1.75E+07	1.76E+07	3.66E+07	3.02E+07	3.09E+07	2.40E+07	2.22E+07	2.33E+07
DG(22:6_22:6)	DG	712.5067	9.82E+06	7.60E+06	7.52E+06	8.73E+06	9.14E+06	1.32E+07	1.10E+07	1.23E+07	8.55E+06	8.28E+06	8.92E+06
DG(30:3)	DG	534.4284	5.64E+05	3.12E+05	4.20E+05	3.14E+05	2.78E+05	1.01E+06	9.63E+05	9.51E+05	4.52E+05	4.05E+05	4.60E+05
DG(32:3e)	DG	548.4805	4.39E+08	6.37E+08	3.07E+08	6.56E+08	6.80E+08	3.77E+08	3.77E+08	3.62E+08	3.48E+08	3.19E+08	3.45E+08
DG(34:6)	DG	584.4441	4.84E+06	6.45E+06	3.56E+06	5.07E+06	4.07E+06	4.60E+06	4.50E+06	4.69E+06	5.40E+06	5.78E+06	4.85E+06
DG(36:4e)	DG	602.5274	2.08E+07	1.41E+07	1.58E+07	1.58E+07	1.26E+07	3.33E+07	3.05E+07	3.00E+07	1.63E+07	1.39E+07	1.64E+07
DG(36:4e)	DG	602.5274	1.45E+06	9.52E+05	9.58E+05	1.00E+06	6.78E+05	2.67E+06	2.12E+06	1.84E+06	1.10E+06	8.35E+05	8.25E+05
DG(36:6)	DG	612.4754	4.56E+06	3.31E+06	3.20E+06	4.44E+06	5.26E+06	5.01E+06	4.85E+06	5.63E+06	4.16E+06	4.07E+06	4.49E+06
DG(36:7)	DG	610.4597	4.31E+05	3.80E+05	3.13E+05	2.49E+05	3.85E+05	6.14E+05	5.08E+05	5.41E+05	3.83E+05	3.23E+05	3.77E+05
DG(38:7)	DG	638.491	1.83E+06	1.96E+06	1.67E+06	1.78E+06	1.72E+06	2.75E+06	2.11E+06	2.32E+06	1.42E+06	1.27E+06	1.30E+06
LPC(16:0)	LPC	495.3325	9.76E+05	1.13E+06	9.75E+05	8.56E+05	6.16E+05	9.01E+05	1.12E+06	1.02E+06	1.24E+06	1.14E+06	9.48E+05
LPC(16:1)	LPC	493.3168	6.09E+06	3.45E+06	5.63E+06	3.94E+06	4.52E+06	7.05E+06	8.82E+06	8.51E+06	6.48E+06	5.27E+06	6.60E+06
LPC(18:1)	LPC	521.3481	2.24E+06	2.53E+06	2.06E+06	2.11E+06	2.32E+06	2.04E+06	2.50E+06	2.32E+06	2.46E+06	2.13E+06	2.37E+06
LPC(18:2)	LPC	519.3325	6.78E+05	1.40E+06	5.65E+05	1.20E+06	8.87E+05	5.32E+05	5.98E+05	6.79E+05	5.21E+05	3.91E+05	5.55E+05
LPC(18:3)	LPC	517.3168	1.89E+06	2.29E+06	1.78E+06	2.32E+06	1.96E+06	1.67E+06	2.26E+06	2.04E+06	1.72E+06	1.44E+06	1.70E+06
LPC(18:4)	LPC	515.3012	3.34E+07	5.43E+07	3.22E+07	3.76E+07	3.18E+07	2.81E+07	3.76E+07	3.25E+07	3.12E+07	2.77E+07	3.22E+07
LPC(19:1)	LPC	535.3638	3.94E+05	1.83E+05	3.70E+05	2.13E+05	2.14E+05	5.56E+05	6.71E+05	6.28E+05	3.77E+05	3.11E+05	4.14E+05
LPC(20:4)	LPC	543.3325	2.71E+06	1.57E+06	2.52E+06	1.67E+06	1.80E+06	2.62E+06	3.90E+06	3.26E+06	3.34E+06	2.76E+06	3.32E+06
LPC(20:5)	LPC	541.3168	6.66E+07	4.71E+07	6.04E+07	4.77E+07	4.65E+07	7.48E+07	9.72E+07	8.95E+07	6.77E+07	5.75E+07	7.08E+07
LPC(22:6)	LPC	567.3325	1.14E+07	7.93E+06	1.09E+07	8.59E+06	8.63E+06	1.27E+07	1.67E+07	1.52E+07	1.16E+07	9.20E+06	1.16E+07
LPE(16:1)	LPE	451.2699	6.69E+05	7.09E+05	7.03E+05	7.39E+05	8.60E+05	5.98E+05	7.78E+05	6.56E+05	6.49E+05	5.17E+05	6.43E+05
LPE(18:4)	LPE	473.2542	8.22E+05	2.43E+06	8.59E+05	1.25E+06	1.04E+06	3.65E+05	5.12E+05	3.85E+05	6.73E+05	7.21E+05	5.83E+05
LPE(20:5)	LPE	499.2699	8.10E+06	7.19E+06	7.51E+06	7.07E+06	7.77E+06	7.93E+06	1.04E+07	8.67E+06	8.80E+06	7.40E+06	8.87E+06
LPE(22:6)	LPE	525.2855	9.95E+06	9.98E+06	9.82E+06	1.00E+07	1.16E+07	9.04E+06	1.31E+07	9.67E+06	1.05E+07	8.41E+06	9.87E+06
LPG(16:0)	LPG	484.2801	6.62E+05	1.12E+06	6.63E+05	1.09E+06	1.23E+06	3.91E+05	4.96E+05	4.11E+05	5.42E+05	4.42E+05	4.97E+05
LPG(16:1)	LPG	482.2645	5.15E+05	7.24E+05	5.50E+05	6.47E+05	5.88E+05	3.96E+05	4.75E+05	5.16E+05	5.60E+05	3.57E+05	4.73E+05
LPG(20:5)	LPG	530.2645	1.21E+06	1.23E+06	8.73E+05	1.38E+06	1.54E+06	1.08E+06	1.13E+06	1.13E+06	1.24E+06	1.11E+06	1.20E+06

MG(16:1)	MG	328.2614	1.81E+06	3.37E+06	1.90E+06	2.89E+06	3.17E+06	1.28E+06	1.43E+06	1.42E+06	1.38E+06	1.10E+06	1.35E+06
MG(18:4)	MG	350.2457	1.39E+06	4.13E+06	1.26E+06	1.99E+06	1.92E+06	9.11E+05	9.31E+05	9.25E+05	8.91E+05	7.76E+05	8.47E+05
MGDG(12:0_16:4)	MGD	666.4343	1.38E+06	1.37E+06	9.25E+05	1.61E+06	1.51E+06	1.68E+06	1.48E+06	1.63E+06	1.22E+06	1.15E+06	1.25E+06
MGDG(14:0_14:0)	MGD	674.4969	2.05E+06	1.76E+06	1.23E+06	1.61E+06	1.54E+06	3.31E+06	2.78E+06	3.07E+06	1.49E+06	1.39E+06	1.55E+06
MGDG(14:0_15:3)	MGD	682.4656	3.99E+05	4.61E+05	3.58E+05	3.61E+05	3.59E+05	4.34E+05	4.28E+05	4.30E+05	3.52E+05	3.21E+05	3.60E+05
MGDG(14:0_16:2)	MGD	698.4969	2.94E+07	3.19E+07	2.35E+07	3.56E+07	2.83E+07	3.96E+07	3.80E+07	3.84E+07	3.36E+07	3.05E+07	3.02E+07
MGDG(14:0_16:3)	MGD	696.4812	6.35E+07	1.12E+08	7.72E+07	1.12E+08	1.16E+08	3.46E+07	3.16E+07	3.31E+07	2.92E+07	2.55E+07	2.83E+07
MGDG(14:0_16:4)	MGD	694.4656	3.32E+08	3.28E+08	2.66E+08	2.98E+08	3.08E+08	3.68E+08	3.60E+08	3.68E+08	3.19E+08	3.18E+08	3.22E+08
MGDG(14:0_17:4)	MGD	708.4812	6.59E+06	1.06E+07	7.82E+06	9.23E+06	8.54E+06	6.70E+06	6.60E+06	6.87E+06	4.86E+06	4.79E+06	5.03E+06
MGDG(14:1_16:4)	MGD	692.45	6.88E+06	4.91E+06	6.28E+06	4.11E+06	3.80E+06	9.77E+06	9.66E+06	1.01E+07	5.85E+06	5.60E+06	6.44E+06
MGDG(16:0_16:1)	MGD	728.5438	9.15E+06	1.70E+07	7.07E+06	1.25E+07	1.24E+07	8.12E+06	7.91E+06	8.04E+06	7.81E+06	8.00E+06	7.26E+06
MGDG(16:0_16:2)	MGD	726.5282	6.04E+07	8.70E+07	5.23E+07	8.91E+07	8.37E+07	5.47E+07	5.14E+07	5.08E+07	4.99E+07	5.17E+07	4.71E+07
MGDG(16:0_16:4)	MGD	722.4969	1.07E+08	1.83E+08	4.68E+07	1.45E+08	1.43E+08	7.10E+07	6.82E+07	6.89E+07	7.77E+07	8.66E+07	7.54E+07
MGDG(16:1_14:0)	MGD	700.5126	5.37E+07	7.46E+07	3.64E+07	6.63E+07	6.25E+07	6.08E+07	5.81E+07	5.60E+07	4.61E+07	4.47E+07	4.39E+07
MGDG(16:1_16:2)	MGD	724.5126	4.41E+07	4.84E+07	4.58E+07	6.16E+07	5.19E+07	3.73E+07	3.73E+07	3.87E+07	4.26E+07	4.69E+07	3.96E+07
MGDG(16:1_16:4)	MGD	720.4812	1.82E+08	2.63E+08	1.36E+08	2.62E+08	2.49E+08	1.33E+08	1.33E+08	1.27E+08	1.66E+08	1.74E+08	1.57E+08
MGDG(16:1_18:4)	MGD	748.5126	2.67E+07	4.02E+07	1.31E+07	3.39E+07	3.61E+07	2.48E+07	2.38E+07	2.68E+07	2.33E+07	2.58E+07	2.36E+07
MGDG(16:1_20:5)	MGD	774.5282	4.38E+07	3.17E+07	2.75E+07	4.38E+07	5.15E+07	4.43E+07	4.39E+07	5.33E+07	3.73E+07	3.66E+07	4.00E+07
MGDG(18:1_18:1)	MGD	782.5908	4.08E+05	1.79E+05	3.38E+05	1.97E+05	2.02E+05	7.44E+05	6.62E+05	6.64E+05	4.05E+05	3.56E+05	4.27E+05
MGDG(18:4_16:2)	MGD	746.4969	4.14E+07	5.46E+07	3.59E+07	4.48E+07	3.59E+07	3.71E+07	3.77E+07	3.84E+07	4.79E+07	5.11E+07	4.34E+07
MGDG(18:4_16:3)	MGD	744.4812	2.06E+08	3.48E+08	1.35E+08	3.12E+08	2.61E+08	1.35E+08	1.29E+08	1.32E+08	1.51E+08	1.63E+08	1.42E+08
MGDG(18:4_16:3)	MGD	744.4812	1.84E+07	2.25E+07	1.60E+07	2.15E+07	2.07E+07	1.05E+07	1.05E+07	8.34E+06	1.04E+07	6.21E+06	9.36E+06
MGDG(18:4_16:4)	MGD	742.4656	1.20E+08	1.48E+08	8.80E+07	1.22E+08	1.13E+08	1.34E+08	1.25E+08	1.32E+08	1.03E+08	1.06E+08	1.08E+08
MGDG(18:4_18:4)	MGD	770.4969	1.47E+08	2.28E+08	1.35E+08	2.33E+08	2.56E+08	9.12E+07	7.80E+07	8.25E+07	8.61E+07	8.11E+07	8.48E+07
MGDG(18:4_18:4)	MGD	770.4969	3.04E+07	4.69E+07	1.77E+07	4.12E+07	4.26E+07	2.58E+07	2.44E+07	2.87E+07	2.53E+07	2.79E+07	2.39E+07
MGDG(18:4_18:5)	MGD	768.4812	4.10E+07	5.55E+07	4.32E+07	4.60E+07	3.32E+07	3.91E+07	3.95E+07	4.05E+07	4.92E+07	5.25E+07	4.47E+07
MGDG(18:4_20:5)	MGD	796.5126	1.59E+07	2.30E+07	9.78E+06	1.74E+07	1.82E+07	1.60E+07	1.43E+07	1.59E+07	1.26E+07	1.46E+07	1.34E+07
MGDG(20:5_16:2)	MGD	772.5126	1.13E+08	4.71E+07	9.25E+07	8.52E+07	1.01E+08	1.27E+08	1.19E+08	1.34E+08	1.17E+08	1.09E+08	1.23E+08
MGDG(20:5_16:4)	MGD	768.4812	4.67E+08	4.39E+08	4.12E+08	4.52E+08	4.53E+08	4.84E+08	4.67E+08	4.76E+08	4.45E+08	4.45E+08	4.62E+08
MGDG(22:6_16:4)	MGD	794.4969	8.59E+06	8.71E+06	9.85E+06	6.04E+06	6.50E+06	1.18E+07	1.14E+07	1.18E+07	7.86E+06	7.77E+06	8.50E+06
MGDG(32:4)	MGD	722.4969	5.54E+07	7.64E+07	4.73E+07	6.82E+07	6.28E+07	6.08E+07	5.89E+07	5.89E+07	4.67E+07	4.62E+07	4.46E+07
MGDG(32:5)	MGD	720.4812	3.09E+07	3.25E+07	2.86E+07	3.63E+07	2.75E+07	4.17E+07	3.88E+07	3.91E+07	3.27E+07	2.94E+07	3.00E+07
MGDG(34:5)	MGD	748.5126	6.02E+07	9.24E+07	6.40E+07	9.22E+07	8.18E+07	5.38E+07	5.07E+07	5.17E+07	4.88E+07	5.20E+07	4.63E+07
MGDG(34:6)	MGD	746.4969	4.06E+07	4.59E+07	5.22E+07	5.92E+07	4.80E+07	3.25E+07	3.41E+07	3.56E+07	3.91E+07	4.53E+07	3.52E+07
MGDG(36:7)	MGD	772.5126	2.05E+06	5.47E+06	1.60E+06	3.16E+06	3.03E+06	1.49E+06	1.41E+06	1.44E+06	1.82E+06	1.98E+06	1.50E+06
MGDG(38:11)	MGD	792.4812	1.50E+08	2.25E+08	1.52E+08	2.33E+08	2.55E+08	9.14E+07	7.77E+07	8.31E+07	8.78E+07	8.27E+07	8.59E+07
MGDG(38:9)	MGD	796.5126	4.35E+07	3.19E+07	3.07E+07	4.48E+07	5.09E+07	4.29E+07	4.20E+07	5.33E+07	3.51E+07	3.46E+07	3.81E+07
MGDG(40:12)	MGD	818.4969	1.60E+07	2.27E+07	1.16E+07	1.77E+07	1.81E+07	1.60E+07	1.42E+07	1.62E+07	1.31E+07	1.50E+07	1.34E+07
MGDG(46:15)	MGD	896.5438	9.44E+05	8.89E+05	1.92E+06	8.18E+05	7.97E+05	9.28E+05	9.39E+05	9.50E+05	9.60E+05	1.00E+06	9.26E+05
PA(38:6)	PA	720.473	5.67E+06	3.68E+06	4.59E+06	2.30E+06	2.33E+06	6.64E+06	6.64E+06	7.16E+06	5.65E+06	5.70E+06	5.60E+06
PA(38:7)	PA	718.4574	4.14E+07	3.93E+07	3.08E+07	4.47E+07	4.96E+07	3.73E+07	3.84E+07	3.98E+07	3.92E+07	3.92E+07	4.07E+07

PC(14:0_18:3)	PC	727.5152	3.69E+07	1.32E+07	3.15E+07	2.08E+07	1.98E+07	5.06E+07	5.06E+07	5.33E+07	3.79E+07	3.63E+07	3.77E+07
PC(16:1_16:1)	PC	729.5309	4.23E+07	2.89E+07	3.57E+07	4.00E+07	3.89E+07	5.07E+07	4.95E+07	5.27E+07	3.91E+07	3.89E+07	3.92E+07
PC(16:1_18:2)	PC	755.5465	3.01E+07	3.25E+07	3.20E+07	4.04E+07	4.04E+07	2.70E+07	2.63E+07	2.95E+07	2.41E+07	2.35E+07	2.34E+07
PC(16:1_20:5)	PC	777.5309	5.61E+08	3.85E+08	3.04E+08	4.92E+08	4.75E+08	6.79E+08	6.84E+08	6.64E+08	4.92E+08	5.14E+08	5.49E+08
PC(17:1_17:1)	PC	757.5622	2.18E+07	2.13E+07	1.61E+07	2.02E+07	2.09E+07	2.34E+07	2.29E+07	2.25E+07	2.36E+07	2.38E+07	2.16E+07
PC(18:0_20:5)	PC	807.5778	1.43E+07	1.19E+07	1.25E+07	1.01E+07	9.23E+06	1.75E+07	1.84E+07	1.88E+07	1.69E+07	1.75E+07	1.59E+07
PC(18:1_18:1)	PC	785.5935	3.32E+07	1.59E+07	2.62E+07	1.72E+07	1.50E+07	5.93E+07	5.04E+07	4.65E+07	3.26E+07	2.64E+07	3.04E+07
PC(18:1_18:2)	PC	783.5778	3.16E+07	3.63E+07	2.59E+07	3.50E+07	2.99E+07	4.06E+07	3.77E+07	3.42E+07	2.78E+07	2.46E+07	2.65E+07
PC(18:1_20:5)	PC	805.5622	1.79E+08	2.31E+08	9.47E+07	2.28E+08	2.28E+08	1.63E+08	1.69E+08	1.74E+08	1.95E+08	1.93E+08	1.81E+08
PC(18:1_20:5)	PC	805.5622	3.83E+06	4.32E+06	3.45E+06	4.21E+06	3.53E+06	5.05E+06	4.75E+06	4.51E+06	3.35E+06	2.94E+06	3.15E+06
PC(18:1_22:6)	PC	831.5778	1.65E+07	2.08E+07	1.34E+07	2.05E+07	2.04E+07	1.34E+07	1.42E+07	1.38E+07	1.82E+07	1.75E+07	1.73E+07
PC(18:3_20:5)	PC	801.5309	1.05E+08	1.17E+08	9.31E+07	1.40E+08	1.19E+08	1.13E+08	1.12E+08	1.24E+08	8.01E+07	8.08E+07	8.56E+07
PC(18:4_14:0)	PC	725.4996	6.41E+07	9.21E+07	4.50E+07	7.98E+07	6.91E+07	6.48E+07	6.41E+07	6.49E+07	5.23E+07	5.28E+07	5.17E+07
PC(18:4_16:0)	PC	753.5309	3.36E+07	6.27E+07	2.65E+07	5.18E+07	4.60E+07	2.66E+07	2.63E+07	2.79E+07	2.82E+07	3.13E+07	2.62E+07
PC(18:4_16:1)	PC	751.5152	2.41E+08	3.31E+08	2.09E+08	2.80E+08	2.52E+08	2.33E+08	2.35E+08	2.50E+08	2.03E+08	2.16E+08	2.16E+08
PC(18:4_18:1)	PC	779.5465	1.67E+08	3.18E+08	1.40E+08	2.30E+08	1.75E+08	1.19E+08	1.23E+08	1.16E+08	1.57E+08	1.67E+08	1.40E+08
PC(18:4_18:4)	PC	773.4996	1.39E+08	2.95E+08	1.23E+08	2.54E+08	2.16E+08	9.32E+07	9.11E+07	9.28E+07	8.46E+07	8.89E+07	8.45E+07
PC(18:4_20:5)	PC	799.5152	1.22E+09	2.13E+09	9.87E+08	1.81E+09	1.50E+09	1.10E+09	1.04E+09	1.03E+09	8.86E+08	9.92E+08	9.87E+08
PC(18:5e)	PC	513.2855	9.14E+05	4.44E+05	8.88E+05	4.09E+05	4.78E+05	1.03E+06	1.49E+06	1.35E+06	9.60E+05	7.21E+05	1.01E+06
PC(19:1_18:4)	PC	793.5622	1.74E+07	2.02E+07	1.41E+07	2.11E+07	1.91E+07	1.69E+07	1.69E+07	1.76E+07	1.43E+07	1.46E+07	1.58E+07
PC(19:1_20:5)	PC	819.5778	2.21E+07	1.27E+07	1.83E+07	1.61E+07	1.40E+07	3.03E+07	3.13E+07	3.15E+07	2.03E+07	2.00E+07	2.28E+07
PC(19:3)	PC	545.3118	9.36E+05	5.00E+05	8.44E+05	6.39E+05	7.41E+05	1.40E+06	1.49E+06	1.60E+06	6.61E+05	5.22E+05	8.10E+05
PC(20:5_18:2)	PC	803.5465	1.76E+08	2.07E+08	2.11E+08	2.71E+08	2.35E+08	1.93E+08	1.78E+08	1.82E+08	1.20E+08	1.15E+08	1.33E+08
PC(20:5_20:4)	PC	827.5465	1.44E+08	9.33E+07	1.91E+08	1.22E+08	9.75E+07	1.75E+08	1.76E+08	1.80E+08	1.43E+08	1.34E+08	1.49E+08
PC(20:5_20:5)	PC	825.5309	1.78E+09	1.45E+09	1.26E+09	1.66E+09	1.41E+09	2.26E+09	2.20E+09	2.12E+09	1.56E+09	1.56E+09	1.73E+09
PC(20:5_22:6)	PC	851.5465	2.95E+08	2.26E+08	3.14E+08	2.95E+08	2.70E+08	3.63E+08	3.58E+08	3.81E+08	2.38E+08	2.34E+08	2.57E+08
PC(30:0)	PC	705.5309	9.92E+05	9.11E+05	1.31E+06	7.30E+05	5.06E+05	1.34E+06	1.21E+06	1.52E+06	1.16E+06	1.18E+06	9.09E+05
PC(30:1)	PC	703.5152	7.04E+06	4.10E+06	5.24E+06	4.68E+06	4.24E+06	1.12E+07	1.12E+07	1.11E+07	6.35E+06	5.92E+06	6.47E+06
PC(30:2)	PC	701.4996	4.23E+06	1.43E+06	3.67E+06	1.82E+06	1.46E+06	6.88E+06	7.05E+06	7.51E+06	3.85E+06	3.68E+06	3.87E+06
PC(30:3)	PC	699.4839	7.57E+05	1.10E+06	5.72E+05	1.15E+06	9.63E+05	1.00E+06	1.01E+06	1.05E+06	7.53E+05	7.05E+05	6.90E+05
PC(30:4)	PC	697.4683	2.85E+06	1.64E+06	2.31E+06	1.65E+06	1.40E+06	3.92E+06	4.18E+06	4.21E+06	2.82E+06	2.89E+06	2.61E+06
PC(32:0)	PC	733.5622	1.90E+06	6.75E+05	1.56E+06	4.18E+05	3.84E+05	2.09E+06	2.09E+06	2.07E+06	3.34E+06	3.07E+06	2.63E+06
PC(32:1)	PC	731.5465	1.22E+07	1.18E+07	1.09E+07	8.61E+06	8.16E+06	1.37E+07	1.39E+07	1.34E+07	1.47E+07	1.46E+07	1.22E+07
PC(32:5)	PC	723.4839	4.99E+07	2.80E+07	3.45E+07	3.63E+07	3.63E+07	5.20E+07	5.55E+07	5.94E+07	4.80E+07	4.97E+07	4.69E+07
PC(32:6)	PC	721.4683	8.91E+06	3.68E+06	7.55E+06	4.49E+06	4.92E+06	1.11E+07	1.13E+07	1.25E+07	9.65E+06	9.89E+06	9.29E+06
PC(32:7)	PC	719.4526	3.34E+06	2.80E+06	2.41E+06	3.51E+06	4.40E+06	2.98E+06	2.94E+06	3.17E+06	3.04E+06	3.03E+06	2.82E+06
PC(32:8)	PC	717.437	6.41E+06	2.04E+06	5.44E+06	2.54E+06	2.40E+06	7.75E+06	8.46E+06	9.09E+06	7.31E+06	7.65E+06	7.12E+06
PC(33:3)	PC	741.5309	5.77E+06	1.20E+07	4.40E+06	9.43E+06	9.04E+06	4.50E+06	4.11E+06	4.24E+06	4.24E+06	4.52E+06	4.04E+06
PC(33:4)	PC	739.5152	1.36E+05	3.19E+05	1.45E+05	2.38E+05	1.67E+05	1.04E+05	9.37E+04	8.75E+04	7.56E+04	1.02E+05	9.08E+04
PC(34:0)	PC	761.5935	8.04E+05	2.04E+05	6.86E+05	1.43E+05	1.64E+05	8.10E+05	8.90E+05	8.79E+05	1.61E+06	1.36E+06	1.26E+06
PC(34:1)	PC	759.5778	5.70E+06	5.54E+06	4.69E+06	3.14E+06	3.02E+06	6.82E+06	6.42E+06	6.43E+06	7.21E+06	7.44E+06	5.55E+06

PC(34:6)	PC	749.4996	5.38E+07	5.10E+07	4.44E+07	4.99E+07	4.50E+07	6.30E+07	6.15E+07	6.57E+07	5.03E+07	5.30E+07	5.24E+07
PC(34:7)	PC	747.4839	2.13E+07	4.51E+07	1.55E+07	3.54E+07	3.73E+07	1.63E+07	1.46E+07	1.56E+07	1.29E+07	1.37E+07	1.24E+07
PC(34:8)	PC	745.4683	3.10E+07	3.48E+07	2.52E+07	2.84E+07	2.79E+07	3.29E+07	3.30E+07	3.55E+07	2.88E+07	3.19E+07	2.99E+07
PC(34:9)	PC	743.4526	2.72E+06	7.21E+05	2.32E+06	9.38E+05	9.40E+05	3.84E+06	4.03E+06	4.35E+06	2.87E+06	3.19E+06	2.87E+06
PC(35:2)	PC	771.5778	2.51E+06	1.58E+06	2.42E+06	1.95E+06	2.01E+06	3.13E+06	3.13E+06	3.20E+06	2.15E+06	2.15E+06	2.35E+06
PC(35:5)	PC	765.5309	7.94E+06	1.07E+07	5.86E+06	1.04E+07	9.00E+06	9.67E+06	9.28E+06	9.72E+06	7.12E+06	7.66E+06	7.53E+06
PC(35:6)	PC	763.5152	6.17E+06	8.85E+06	3.73E+06	7.81E+06	6.62E+06	6.78E+06	6.54E+06	6.83E+06	5.90E+06	5.97E+06	5.68E+06
PC(36:1)	PC	787.6091	4.27E+05	5.19E+05	3.75E+05	3.12E+05	2.73E+05	4.67E+05	4.55E+05	4.41E+05	5.25E+05	6.18E+05	4.13E+05
PC(36:10)	PC	769.4683	5.43E+06	1.60E+07	4.74E+06	1.03E+07	1.10E+07	3.77E+06	2.95E+06	4.00E+06	2.66E+06	3.59E+06	2.08E+06
PC(36:4)	PC	781.5622	1.12E+07	1.70E+07	1.24E+07	1.52E+07	1.22E+07	9.06E+06	9.65E+06	9.48E+06	9.63E+06	1.06E+07	9.11E+06
PC(36:5)	PC	779.5465	2.50E+06	2.51E+06	2.21E+06	2.31E+06	1.98E+06	2.59E+06	2.59E+06	2.56E+06	2.75E+06	2.77E+06	2.44E+06
PC(36:5e)	PC	765.5672	1.01E+06	2.96E+05	6.45E+05	2.66E+05	2.67E+05	1.93E+06	1.99E+06	2.08E+06	6.17E+05	5.49E+05	7.60E+05
PC(36:7)	PC	775.5152	2.18E+08	9.22E+07	1.93E+08	1.21E+08	1.07E+08	2.93E+08	2.99E+08	3.16E+08	2.25E+08	2.22E+08	2.34E+08
PC(36:8)	PC	773.4996	4.34E+07	7.26E+07	3.79E+07	6.22E+07	4.56E+07	4.06E+07	4.23E+07	4.36E+07	3.67E+07	4.00E+07	3.92E+07
PC(36:9)	PC	771.4839	1.89E+08	1.04E+08	1.40E+08	1.27E+08	1.16E+08	2.34E+08	2.30E+08	2.35E+08	1.80E+08	1.88E+08	1.76E+08
PC(37:3)	PC	797.5935	2.35E+06	2.25E+06	1.89E+06	2.92E+06	2.50E+06	3.06E+06	2.88E+06	2.95E+06	1.78E+06	1.70E+06	1.89E+06
PC(37:4)	PC	795.5778	1.05E+06	1.04E+06	8.82E+05	1.36E+06	1.17E+06	1.28E+06	1.25E+06	1.22E+06	8.62E+05	8.28E+05	8.91E+05
PC(38:9)	PC	799.5152	6.45E+07	4.13E+07	5.90E+07	5.08E+07	4.66E+07	7.99E+07	7.99E+07	7.96E+07	6.70E+07	6.88E+07	6.63E+07
PC(39:7)	PC	817.5622	4.02E+06	2.79E+06	3.09E+06	3.86E+06	3.62E+06	5.21E+06	5.11E+06	5.47E+06	2.80E+06	2.67E+06	3.19E+06
PC(40:10)	PC	825.5309	2.79E+07	3.55E+07	3.91E+07	5.37E+07	4.07E+07	3.21E+07	2.90E+07	3.66E+07	1.96E+07	2.06E+07	1.92E+07
PC(40:6)	PC	833.5935	4.55E+05	3.91E+05	3.76E+05	4.16E+05	3.78E+05	5.39E+05	5.53E+05	5.74E+05	4.71E+05	4.73E+05	4.79E+05
PC(40:8)	PC	829.5622	2.46E+06	2.32E+06	2.52E+06	2.91E+06	2.78E+06	2.84E+06	2.75E+06	2.93E+06	2.05E+06	1.98E+06	2.03E+06
PC(41:7)	PC	845.5935	2.69E+06	2.01E+06	2.35E+06	2.90E+06	2.81E+06	3.21E+06	3.28E+06	3.24E+06	2.20E+06	2.11E+06	2.54E+06
PC(42:10)	PC	853.5622	5.12E+06	4.22E+06	4.01E+06	6.08E+06	6.30E+06	6.07E+06	6.04E+06	6.56E+06	3.81E+06	4.19E+06	4.24E+06
PC(42:5)	PC	863.6404	8.24E+05	9.91E+05	7.71E+05	6.83E+05	6.31E+05	1.03E+06	1.01E+06	1.07E+06	6.62E+05	6.92E+05	7.69E+05
PC(42:6)	PC	861.6248	8.60E+05	9.78E+05	8.75E+05	6.61E+05	4.56E+05	1.21E+06	1.18E+06	1.20E+06	7.04E+05	6.88E+05	7.20E+05
PC(44:6)	PC	889.6561	5.85E+06	5.29E+06	5.46E+06	2.98E+06	2.72E+06	8.15E+06	8.05E+06	8.91E+06	5.70E+06	5.80E+06	6.17E+06
PC(8:0e_10:2)	PC	519.3325	6.88E+05	1.41E+06	5.74E+05	1.21E+06	8.96E+05	5.41E+05	6.18E+05	6.98E+05	5.34E+05	4.01E+05	5.68E+05
PE(15:0_20:5)	PE	723.4839	2.05E+06	9.80E+05	1.56E+06	1.16E+06	1.14E+06	3.11E+06	3.03E+06	3.17E+06	2.11E+06	1.94E+06	2.24E+06
PE(16:0_20:5)	PE	737.4996	5.50E+06	3.24E+06	4.57E+06	2.12E+06	2.19E+06	6.57E+06	6.57E+06	7.09E+06	5.44E+06	5.40E+06	5.46E+06
PE(16:0_20:5)	PE	737.4996	2.17E+06	3.70E+06	1.56E+06	3.43E+06	2.84E+06	1.87E+06	1.97E+06	1.85E+06	2.01E+06	2.35E+06	1.92E+06
PE(16:1_14:0)	PE	661.4683	9.76E+06	3.34E+06	7.40E+06	4.06E+06	4.22E+06	1.54E+07	1.48E+07	1.54E+07	1.03E+07	9.09E+06	1.09E+07
PE(16:1_20:5)	PE	735.4839	4.24E+07	4.06E+07	3.17E+07	4.59E+07	5.09E+07	3.82E+07	3.94E+07	4.09E+07	4.02E+07	4.01E+07	4.16E+07
PE(18:1_18:2)	PE	741.5309	1.29E+06	5.09E+05	1.02E+06	6.23E+05	5.16E+05	1.74E+06	1.64E+06	1.59E+06	1.05E+06	9.10E+05	1.06E+06
PE(18:2_18:2)	PE	739.5152	7.35E+06	1.14E+07	5.54E+06	1.10E+07	1.53E+07	5.96E+06	6.03E+06	6.48E+06	5.53E+06	5.69E+06	5.65E+06
PE(18:2_18:2)	PE	739.5152	9.12E+05	4.21E+05	7.60E+05	4.85E+05	4.32E+05	1.33E+06	1.32E+06	1.29E+06	9.91E+05	8.75E+05	1.03E+06
PE(18:3_20:5)	PE	759.4839	2.54E+06	3.87E+06	1.85E+06	3.64E+06	3.29E+06	1.99E+06	2.05E+06	2.11E+06	2.28E+06	2.35E+06	2.19E+06
PE(18:4_14:0)	PE	683.4526	9.43E+05	1.38E+06	7.39E+05	8.73E+05	7.31E+05	9.75E+05	9.86E+05	1.00E+06	1.02E+06	1.04E+06	9.13E+05
PE(18:4_20:5)	PE	757.4683	2.92E+07	6.73E+07	2.47E+07	4.58E+07	3.81E+07	1.16E+07	1.22E+07	1.20E+07	2.03E+07	2.60E+07	1.82E+07
PE(20:5_20:5)	PE	783.4839	1.14E+08	1.13E+08	7.63E+07	1.14E+08	1.13E+08	1.14E+08	1.18E+08	1.14E+08	1.11E+08	1.13E+08	1.20E+08
PE(20:5_22:6)	PE	809.4996	1.67E+08	1.77E+08	1.29E+08	2.05E+08	2.19E+08	1.60E+08	1.65E+08	1.71E+08	1.44E+08	1.42E+08	1.59E+08

PE(28:0)	PE	635.4526	4.66E+05	2.68E+05	3.81E+05	3.23E+05	3.40E+05	6.63E+05	6.22E+05	7.41E+05	4.16E+05	3.92E+05	4.97E+05
PE(31:1)	PE	675.4839	4.28E+06	1.18E+06	3.51E+06	1.52E+06	1.51E+06	6.38E+06	6.41E+06	6.69E+06	4.23E+06	3.70E+06	4.65E+06
PE(31:2)	PE	673.4683	1.38E+06	3.45E+05	1.16E+06	4.82E+05	4.65E+05	2.33E+06	2.32E+06	2.30E+06	1.47E+06	1.27E+06	1.64E+06
PE(32:2)	PE	687.4839	1.92E+07	7.92E+06	1.47E+07	8.92E+06	9.19E+06	2.78E+07	2.68E+07	2.82E+07	2.11E+07	1.91E+07	2.20E+07
PE(32:4)	PE	683.4526	1.39E+06	4.27E+05	1.19E+06	5.19E+05	5.52E+05	2.14E+06	2.10E+06	2.22E+06	1.44E+06	1.31E+06	1.55E+06
PE(34:2)	PE	715.5152	6.10E+05	3.18E+05	4.57E+05	3.59E+05	3.67E+05	9.28E+05	8.33E+05	9.00E+05	5.97E+05	5.61E+05	6.22E+05
PE(36:7)	PE	733.4683	1.15E+07	8.50E+06	9.20E+06	1.03E+07	1.02E+07	1.10E+07	1.20E+07	1.16E+07	1.32E+07	1.25E+07	1.33E+07
PE(38:7)	PE	761.4996	1.07E+07	1.67E+07	8.84E+06	1.63E+07	1.69E+07	8.48E+06	8.57E+06	9.19E+06	7.82E+06	8.00E+06	7.92E+06
PE(38:8)	PE	759.4839	7.23E+05	4.65E+05	6.84E+05	3.13E+05	3.19E+05	9.31E+05	9.19E+05	9.52E+05	7.31E+05	7.38E+05	7.29E+05
PE(38:9)	PE	757.4683	4.90E+06	5.04E+06	4.18E+06	5.71E+06	5.81E+06	4.64E+06	4.83E+06	5.14E+06	4.90E+06	4.72E+06	4.87E+06
PE(44:12)	PE	835.5152	8.33E+05	1.56E+06	6.84E+05	1.68E+06	1.92E+06	4.07E+05	3.85E+05	3.91E+05	3.64E+05	3.67E+05	3.72E+05
PG(14:0_20:5)	PG	740.4628	3.87E+07	3.59E+07	3.66E+07	3.44E+07	3.27E+07	4.62E+07	5.01E+07	5.17E+07	3.60E+07	3.20E+07	3.71E+07
PG(15:0_16:1)	PG	706.4785	1.45E+06	1.11E+06	9.84E+05	1.45E+06	1.72E+06	1.82E+06	1.75E+06	1.82E+06	1.25E+06	1.00E+06	1.30E+06
PG(16:0_16:1)	PG	720.4941	7.41E+07	1.02E+08	6.21E+07	1.07E+08	1.12E+08	6.41E+07	6.36E+07	6.65E+07	5.88E+07	5.51E+07	5.95E+07
PG(16:0_20:5)	PG	768.4941	6.92E+07	1.26E+08	7.34E+07	1.27E+08	1.44E+08	3.92E+07	4.00E+07	3.85E+07	5.13E+07	5.24E+07	4.86E+07
PG(16:1_14:0)	PG	692.4628	2.41E+07	1.16E+07	1.92E+07	1.59E+07	1.86E+07	3.13E+07	3.16E+07	3.33E+07	2.41E+07	2.02E+07	2.53E+07
PG(16:1_16:1)	PG	718.4785	1.00E+07	6.42E+06	7.07E+06	7.43E+06	8.29E+06	1.25E+07	1.24E+07	1.30E+07	1.07E+07	9.16E+06	1.07E+07
PG(16:1_20:5)	PG	766.4785	7.91E+07	9.04E+07	9.35E+07	8.89E+07	9.57E+07	8.41E+07	8.49E+07	8.70E+07	7.54E+07	6.48E+07	7.28E+07
PG(18:1_18:1)	PG	774.5411	4.70E+06	3.28E+06	3.58E+06	3.73E+06	2.96E+06	7.69E+06	6.95E+06	6.77E+06	3.78E+06	3.28E+06	3.77E+06
PG(18:1_18:2)	PG	772.5254	1.41E+06	1.60E+06	1.03E+06	1.48E+06	1.37E+06	1.93E+06	1.84E+06	1.80E+06	1.16E+06	9.58E+05	1.11E+06
PG(18:1_20:5)	PG	794.5098	2.31E+06	4.43E+06	2.59E+06	4.61E+06	5.15E+06	1.39E+06	1.39E+06	1.29E+06	1.70E+06	1.64E+06	1.58E+06
PG(28:0)	PG	666.4472	3.19E+06	1.66E+06	6.92E+06	1.91E+06	2.13E+06	4.41E+06	4.48E+06	4.85E+06	2.95E+06	2.39E+06	3.10E+06
PG(30:0)	PG	694.4785	2.06E+06	3.14E+06	1.73E+06	2.80E+06	2.73E+06	1.90E+06	1.89E+06	2.07E+06	1.58E+06	1.51E+06	1.55E+06
PG(32:0)	PG	722.5098	9.14E+05	2.51E+06	6.47E+05	1.53E+06	1.38E+06	5.63E+05	5.52E+05	5.36E+05	6.56E+05	6.89E+05	6.06E+05
PG(33:1)	PG	734.5098	3.88E+05	3.33E+05	2.60E+05	4.36E+05	5.34E+05	4.69E+05	4.42E+05	4.90E+05	3.27E+05	2.74E+05	3.42E+05
PG(34:2)	PG	746.5098	4.20E+06	6.30E+06	3.44E+06	6.37E+06	6.75E+06	3.97E+06	3.86E+06	4.07E+06	3.38E+06	3.04E+06	3.35E+06
PG(40:10)	PG	814.4785	1.32E+06	9.63E+05	1.66E+06	1.04E+06	1.01E+06	1.38E+06	1.40E+06	1.61E+06	1.24E+06	1.20E+06	1.26E+06
PI(15:0_14:0)	PI	768.4789	4.43E+08	4.30E+08	3.22E+08	4.37E+08	4.43E+08	4.71E+08	4.57E+08	4.29E+08	4.29E+08	4.28E+08	4.46E+08
PI(15:0_16:1)	PI	794.4945	1.13E+08	4.71E+07	9.25E+07	8.52E+07	1.01E+08	1.27E+08	1.19E+08	1.35E+08	1.17E+08	1.09E+08	1.23E+08
PI(39:1)	PI	906.6197	1.34E+06	8.03E+05	1.87E+06	7.31E+05	6.08E+05	2.24E+06	2.04E+06	2.11E+06	1.06E+06	1.01E+06	1.13E+06
PI(41:2)	PI	932.6354	1.20E+07	1.29E+07	1.35E+07	1.37E+07	1.09E+07	1.24E+07	1.30E+07	1.22E+07	1.03E+07	1.13E+07	1.05E+07
TG(10:0_14:0_20:4)	TG	742.6111	3.64E+07	5.31E+07	3.31E+07	2.50E+07	1.85E+07	4.34E+07	4.32E+07	4.18E+07	3.92E+07	3.76E+07	3.04E+07
TG(14:0_10:2_22:6)	TG	762.5798	5.37E+07	6.72E+07	4.57E+07	3.47E+07	3.04E+07	5.60E+07	5.87E+07	5.84E+07	6.46E+07	6.23E+07	4.79E+07
TG(14:0_10:3_22:4)	TG	764.5955	2.06E+07	5.29E+07	1.70E+07	2.89E+07	2.85E+07	1.52E+07	1.51E+07	1.53E+07	2.01E+07	1.76E+07	1.40E+07
TG(14:0_12:4_22:6)	TG	786.5798	8.91E+06	1.39E+07	8.33E+06	1.02E+07	8.88E+06	7.53E+06	7.55E+06	7.31E+06	8.54E+06	7.71E+06	6.74E+06
TG(14:0e_18:4_18:4)	TG	804.6632	3.58E+05	5.66E+05	2.48E+05	6.02E+05	4.50E+05	3.57E+05	3.29E+05	3.14E+05	3.27E+05	3.05E+05	2.60E+05
TG(15:0_14:0_16:0)	TG	764.6894	1.08E+07	1.17E+07	9.00E+06	1.22E+07	1.11E+07	1.12E+07	1.12E+07	1.07E+07	1.13E+07	1.07E+07	9.80E+06
TG(15:0_14:0_16:1)	TG	762.6737	5.54E+06	8.29E+06	4.64E+06	6.58E+06	4.97E+06	6.28E+06	5.74E+06	5.30E+06	5.82E+06	4.82E+06	3.88E+06
TG(15:0_14:0_18:3)	TG	786.6737	6.63E+06	1.14E+07	5.66E+06	1.03E+07	6.74E+06	7.04E+06	6.48E+06	5.81E+06	5.90E+06	5.54E+06	4.69E+06
TG(15:0_14:3_16:0)	TG	758.6424	1.59E+06	2.99E+06	1.28E+06	2.02E+06	1.43E+06	1.71E+06	1.54E+06	1.42E+06	1.42E+06	1.21E+06	1.07E+06
TG(15:0_16:0_16:0)	TG	792.7207	1.62E+07	1.57E+07	1.40E+07	1.71E+07	1.59E+07	1.62E+07	1.65E+07	1.53E+07	1.66E+07	1.55E+07	1.48E+07

TG(15:0_16:0_16:1)	TG	790.705	8.27E+06	1.18E+07	6.44E+06	9.31E+06	7.46E+06	9.12E+06	8.26E+06	6.84E+06	9.45E+06	7.56E+06	6.22E+06
TG(15:0_16:1_16:1)	TG	788.6894	1.21E+07	2.00E+07	9.28E+06	1.67E+07	1.31E+07	1.14E+07	1.06E+07	1.01E+07	1.05E+07	9.67E+06	7.76E+06
TG(15:0_16:1_20:5)	TG	836.6894	1.78E+07	3.13E+07	1.52E+07	1.88E+07	1.38E+07	2.09E+07	1.93E+07	1.96E+07	1.44E+07	1.53E+07	1.28E+07
TG(15:0_20:5_20:5)	TG	884.6894	7.29E+06	9.23E+06	6.22E+06	4.82E+06	3.75E+06	1.06E+07	9.84E+06	1.00E+07	6.38E+06	6.68E+06	5.74E+06
TG(16:0_11:3_12:4)	TG	666.4859	4.67E+05	4.12E+05	4.57E+05	2.21E+05	3.31E+05	1.11E+06	4.80E+05	6.58E+05	3.14E+05	3.00E+05	2.98E+05
TG(16:0_14:0_16:0)	TG	778.705	4.62E+06	3.97E+06	3.90E+06	4.58E+06	4.21E+06	4.88E+06	4.90E+06	4.46E+06	4.83E+06	4.37E+06	4.62E+06
TG(16:0_16:1_14:0)	TG	776.6894	9.94E+07	1.55E+08	7.14E+07	8.43E+07	7.25E+07	1.08E+08	9.75E+07	8.27E+07	9.54E+07	8.61E+07	8.35E+07
TG(16:0_16:1_16:0)	TG	804.7207	8.72E+07	1.16E+08	7.79E+07	6.21E+07	5.98E+07	9.28E+07	8.43E+07	7.39E+07	9.04E+07	8.10E+07	7.36E+07
TG(16:0_16:1_17:1)	TG	816.7207	9.39E+06	1.31E+07	8.20E+06	1.13E+07	8.97E+06	1.04E+07	9.83E+06	9.01E+06	1.06E+07	8.83E+06	7.28E+06
TG(16:0_16:1_20:4)	TG	852.7207	9.89E+07	1.09E+08	9.75E+07	5.14E+07	4.27E+07	1.10E+08	1.07E+08	1.09E+08	1.31E+08	1.25E+08	1.13E+08
TG(16:0_16:1_20:5)	TG	850.705	3.01E+08	6.87E+08	2.50E+08	3.23E+08	2.39E+08	2.62E+08	2.47E+08	2.40E+08	2.67E+08	2.99E+08	2.33E+08
TG(16:0_16:1_23:1)	TG	900.8146	9.24E+05	1.37E+06	8.06E+05	1.27E+06	1.10E+06	9.95E+05	8.91E+05	9.14E+05	1.02E+06	8.96E+05	7.68E+05
TG(16:0_17:0_18:1)	TG	846.7676	3.29E+06	3.73E+06	2.97E+06	3.71E+06	3.21E+06	3.44E+06	3.35E+06	3.07E+06	4.32E+06	3.52E+06	2.96E+06
TG(16:0_18:1_18:3)	TG	854.7363	1.58E+06	2.11E+06	1.64E+06	1.39E+06	1.23E+06	1.61E+06	1.55E+06	1.56E+06	1.97E+06	1.85E+06	1.48E+06
TG(16:0_18:3_20:5)	TG	874.705	1.41E+07	2.05E+07	1.18E+07	1.46E+07	1.20E+07	1.47E+07	1.37E+07	1.47E+07	1.17E+07	1.24E+07	1.09E+07
TG(16:0_20:4_20:5)	TG	900.7207	4.71E+06	1.04E+07	4.26E+06	3.67E+06	3.19E+06	4.40E+06	4.18E+06	4.35E+06	4.41E+06	4.96E+06	3.97E+06
TG(16:0_20:5_24:0)	TG	964.8459	1.59E+06	7.09E+05	1.37E+06	2.96E+05	3.48E+05	2.34E+06	2.23E+06	2.34E+06	1.93E+06	1.93E+06	1.78E+06
TG(16:0_22:6_22:6)	TG	950.7363	9.87E+06	9.44E+06	9.03E+06	4.73E+06	4.53E+06	1.34E+07	1.28E+07	1.27E+07	1.22E+07	1.24E+07	1.13E+07
TG(16:1_10:2_22:6)	TG	788.5955	9.76E+07	1.40E+08	8.59E+07	9.83E+07	7.52E+07	9.17E+07	9.51E+07	9.22E+07	1.12E+08	1.12E+08	8.65E+07
TG(16:1_12:4_22:6)	TG	812.5955	5.94E+07	7.41E+07	5.83E+07	5.54E+07	4.70E+07	4.60E+07	4.76E+07	4.72E+07	5.86E+07	5.84E+07	4.85E+07
TG(16:1_13:0_22:6)	TG	834.6737	1.16E+07	1.54E+07	1.10E+07	1.14E+07	7.85E+06	1.39E+07	1.28E+07	1.26E+07	9.77E+06	9.77E+06	8.30E+06
TG(16:1_14:0_14:0)	TG	748.6581	5.87E+07	8.76E+07	4.76E+07	6.02E+07	4.68E+07	6.77E+07	6.07E+07	6.19E+07	5.14E+07	5.16E+07	4.35E+07
TG(16:1_14:0_14:1)	TG	746.6424	3.17E+07	3.93E+07	2.67E+07	2.87E+07	1.91E+07	3.79E+07	3.62E+07	3.58E+07	3.27E+07	3.05E+07	2.61E+07
TG(16:1_14:0_14:2)	TG	744.6268	1.54E+07	3.13E+07	1.49E+07	1.61E+07	1.26E+07	1.65E+07	1.57E+07	1.48E+07	1.38E+07	1.16E+07	1.08E+07
TG(16:1_14:0_16:1)	TG	774.6737	2.57E+08	4.23E+08	2.01E+08	3.56E+08	2.56E+08	2.37E+08	2.18E+08	2.15E+08	2.14E+08	2.26E+08	1.87E+08
TG(16:1_14:1_16:1)	TG	772.6581	1.39E+08	2.04E+08	1.16E+08	1.51E+08	1.07E+08	1.41E+08	1.39E+08	1.35E+08	1.44E+08	1.41E+08	1.20E+08
TG(16:1_14:1_20:5)	TG	820.6581	2.03E+08	2.97E+08	1.72E+08	1.65E+08	1.15E+08	2.25E+08	2.22E+08	2.20E+08	2.13E+08	2.23E+08	1.77E+08
TG(16:1_16:1_16:0)	TG	802.705	2.21E+08	5.34E+08	1.70E+08	3.10E+08	2.25E+08	1.70E+08	1.56E+08	1.54E+08	1.90E+08	2.03E+08	1.57E+08
TG(16:1_16:1_16:1)	TG	800.6894	3.57E+08	6.68E+08	3.01E+08	6.35E+08	4.17E+08	2.68E+08	2.47E+08	2.42E+08	2.75E+08	2.93E+08	2.40E+08
TG(16:1_16:1_17:1)	TG	814.705	5.74E+06	9.25E+06	4.74E+06	7.94E+06	5.91E+06	6.31E+06	6.03E+06	5.76E+06	5.54E+06	4.92E+06	4.26E+06
TG(16:1_16:1_18:2)	TG	826.705	8.78E+07	1.91E+08	8.86E+07	9.55E+07	7.05E+07	7.18E+07	7.19E+07	7.02E+07	1.04E+08	1.16E+08	8.50E+07
TG(16:1_16:1_18:3)	TG	824.6894	2.20E+08	4.78E+08	2.20E+08	2.34E+08	1.69E+08	1.97E+08	1.85E+08	1.95E+08	2.06E+08	2.30E+08	1.76E+08
TG(16:1_16:1_20:5)	TG	848.6894	8.55E+08	1.40E+09	7.85E+08	1.11E+09	7.82E+08	7.60E+08	7.37E+08	7.37E+08	7.05E+08	7.83E+08	6.56E+08
TG(16:1_16:1_23:1)	TG	898.7989	8.44E+05	1.15E+06	6.42E+05	1.22E+06	1.05E+06	7.95E+05	7.56E+05	6.79E+05	7.46E+05	6.91E+05	5.74E+05
TG(16:1_16:1_24:0)	TG	914.8302	6.05E+06	1.68E+07	5.36E+06	9.36E+06	8.33E+06	6.53E+06	5.65E+06	7.21E+06	6.97E+06	7.24E+06	6.35E+06
TG(16:1_16:1_24:1)	TG	912.8146	1.07E+07	1.95E+07	8.91E+06	1.38E+07	1.24E+07	1.06E+07	9.63E+06	9.58E+06	8.15E+06	8.63E+06	7.72E+06
TG(16:1_16:1_24:2)	TG	910.7989	7.98E+06	1.38E+07	7.06E+06	7.64E+06	6.73E+06	8.51E+06	8.23E+06	8.41E+06	8.04E+06	8.41E+06	7.14E+06
TG(16:1_17:0_20:5)	TG	864.7207	2.89E+06	5.44E+06	2.64E+06	2.70E+06	2.11E+06	3.51E+06	3.28E+06	3.19E+06	2.43E+06	2.59E+06	2.18E+06
TG(16:1_18:1_16:1)	TG	828.7207	4.37E+07	8.34E+07	4.08E+07	5.68E+07	4.45E+07	4.36E+07	3.95E+07	4.03E+07	4.36E+07	4.32E+07	3.55E+07
TG(16:1_18:1_20:5)	TG	876.7207	5.45E+07	9.38E+07	4.82E+07	4.35E+07	3.33E+07	6.62E+07	5.92E+07	6.17E+07	4.70E+07	5.04E+07	4.15E+07
TG(16:1_18:3_20:5)	TG	872.6894	3.22E+07	4.70E+07	2.82E+07	2.54E+07	2.19E+07	2.42E+07	2.31E+07	2.25E+07	2.91E+07	3.32E+07	2.56E+07

TG(16:1_20:4_20:5)	TG	898.705	2.52E+07	2.57E+07	2.18E+07	1.60E+07	1.46E+07	2.78E+07	2.70E+07	2.75E+07	2.69E+07	2.91E+07	2.53E+07
TG(16:1_20:5_20:5)	TG	896.6894	7.97E+08	9.16E+08	7.18E+08	5.27E+08	4.38E+08	9.96E+08	9.30E+08	9.37E+08	7.33E+08	7.82E+08	6.71E+08
TG(16:1_20:5_22:1)	TG	932.7833	3.17E+06	4.92E+06	2.69E+06	2.70E+06	2.20E+06	3.73E+06	3.62E+06	3.69E+06	2.81E+06	3.08E+06	2.64E+06
TG(16:1_20:5_22:6)	TG	922.705	9.47E+07	1.28E+08	8.22E+07	7.76E+07	5.97E+07	1.28E+08	1.17E+08	1.18E+08	7.91E+07	8.18E+07	7.21E+07
TG(16:1_20:5_24:0)	TG	962.8302	6.24E+06	1.12E+07	5.18E+06	4.26E+06	4.16E+06	7.26E+06	6.86E+06	7.80E+06	5.08E+06	5.86E+06	5.35E+06
TG(16:1_20:5_24:1)	TG	960.8146	1.83E+07	2.62E+07	1.50E+07	1.33E+07	1.33E+07	2.22E+07	2.15E+07	1.87E+07	1.31E+07	1.36E+07	1.48E+07
TG(16:1_22:6_22:6)	TG	948.7207	1.48E+07	1.72E+07	1.56E+07	1.55E+07	1.57E+07	1.76E+07	1.67E+07	1.82E+07	1.22E+07	1.11E+07	1.21E+07
TG(16:1_24:1_14:0)	TG	886.7989	1.13E+07	1.49E+07	9.64E+06	1.17E+07	1.12E+07	1.28E+07	1.14E+07	1.10E+07	1.05E+07	1.01E+07	8.57E+06
TG(17:0_18:1_18:1)	TG	872.7833	1.34E+06	1.33E+06	1.15E+06	1.56E+06	1.30E+06	1.41E+06	1.34E+06	1.15E+06	1.57E+06	1.30E+06	1.09E+06
TG(18:0_16:0_16:0)	TG	834.7676	1.17E+07	1.24E+07	1.06E+07	1.30E+07	1.14E+07	1.21E+07	1.16E+07	1.12E+07	1.23E+07	1.18E+07	1.12E+07
TG(18:0_16:0_18:0)	TG	862.7989	4.66E+06	5.83E+06	3.97E+06	6.10E+06	5.14E+06	5.26E+06	4.72E+06	4.71E+06	4.88E+06	4.74E+06	4.51E+06
TG(18:0_16:0_18:3)	TG	856.752	1.59E+06	1.56E+06	1.51E+06	1.74E+06	1.30E+06	1.61E+06	1.64E+06	1.52E+06	1.68E+06	1.57E+06	1.59E+06
TG(18:0_16:1_16:1)	TG	830.7363	4.00E+06	6.73E+06	3.38E+06	3.68E+06	3.17E+06	3.90E+06	3.71E+06	3.50E+06	3.72E+06	3.68E+06	3.06E+06
TG(18:0_16:1_20:5)	TG	878.7363	1.97E+07	4.85E+07	1.60E+07	1.46E+07	1.17E+07	2.10E+07	1.91E+07	1.93E+07	1.89E+07	2.10E+07	1.62E+07
TG(18:0_17:0_18:1)	TG	874.7989	7.90E+05	8.98E+05	7.00E+05	9.73E+05	7.72E+05	8.51E+05	8.07E+05	7.12E+05	9.69E+05	7.86E+05	6.71E+05
TG(18:0_20:5_20:5)	TG	926.7363	3.85E+06	5.07E+06	3.28E+06	1.77E+06	1.66E+06	5.51E+06	5.03E+06	5.51E+06	3.87E+06	4.24E+06	3.44E+06
TG(18:1_18:1_20:5)	TG	904.752	4.56E+06	7.25E+06	4.08E+06	3.49E+06	2.98E+06	5.63E+06	5.29E+06	5.23E+06	4.34E+06	4.68E+06	3.79E+06
TG(18:1_18:1_22:1)	TG	940.8459	2.07E+06	3.79E+06	1.83E+06	2.92E+06	2.49E+06	2.31E+06	2.04E+06	2.34E+06	2.14E+06	2.22E+06	1.89E+06
TG(18:1_18:2_20:5)	TG	902.7363	5.22E+06	8.80E+06	4.53E+06	4.22E+06	3.66E+06	6.40E+06	5.93E+06	6.27E+06	4.84E+06	5.17E+06	4.21E+06
TG(18:1_20:5_20:5)	TG	924.7207	6.75E+07	8.72E+07	6.29E+07	5.12E+07	4.20E+07	8.22E+07	7.68E+07	7.85E+07	6.69E+07	7.08E+07	6.01E+07
TG(18:3_20:5_20:5)	TG	920.6894	2.66E+07	2.84E+07	3.36E+07	1.98E+07	1.55E+07	2.92E+07	2.95E+07	3.12E+07	2.78E+07	3.13E+07	2.67E+07
TG(18:3_22:6_22:6)	TG	972.7207	2.48E+06	1.69E+06	2.28E+06	9.98E+05	1.12E+06	2.91E+06	2.94E+06	3.05E+06	3.14E+06	2.96E+06	2.97E+06
TG(18:4_12:0_18:4)	TG	790.6111	1.83E+08	3.18E+08	1.53E+08	1.65E+08	1.35E+08	1.48E+08	1.50E+08	1.45E+08	1.83E+08	1.93E+08	1.47E+08
TG(18:4_12:4_22:6)	TG	834.5798	7.95E+06	2.05E+07	7.78E+06	1.18E+07	9.64E+06	6.06E+06	6.05E+06	6.22E+06	8.06E+06	8.40E+06	5.87E+06
TG(18:4_13:0_16:1)	TG	782.6424	7.40E+06	1.43E+07	6.36E+06	9.77E+06	6.54E+06	7.46E+06	7.00E+06	6.65E+06	6.24E+06	6.19E+06	4.88E+06
TG(18:4_14:0_14:0)	TG	770.6424	1.74E+08	3.29E+08	1.55E+08	1.72E+08	1.36E+08	1.56E+08	1.53E+08	1.50E+08	1.70E+08	1.69E+08	1.37E+08
TG(18:4_14:0_14:1)	TG	768.6268	1.64E+08	2.54E+08	1.46E+08	1.64E+08	1.22E+08	1.66E+08	1.67E+08	1.47E+08	1.68E+08	1.71E+08	1.34E+08
TG(18:4_14:0_15:0)	TG	784.6581	8.08E+06	1.79E+07	6.64E+06	1.08E+07	7.66E+06	7.51E+06	6.97E+06	6.45E+06	6.63E+06	6.90E+06	5.48E+06
TG(18:4_14:0_16:0)	TG	798.6737	2.73E+08	5.42E+08	2.19E+08	3.16E+08	2.28E+08	2.26E+08	2.22E+08	2.13E+08	2.79E+08	2.93E+08	2.30E+08
TG(18:4_14:0_16:1)	TG	796.6581	3.77E+08	7.55E+08	3.25E+08	4.61E+08	3.75E+08	2.77E+08	2.65E+08	2.61E+08	3.06E+08	3.25E+08	2.52E+08
TG(18:4_14:0_18:4)	TG	818.6424	1.97E+08	4.83E+08	1.70E+08	2.21E+08	1.66E+08	1.53E+08	1.50E+08	1.34E+08	1.73E+08	1.80E+08	1.41E+08
TG(18:4_14:1_14:1)	TG	766.6111	4.77E+07	6.31E+07	4.09E+07	3.74E+07	2.98E+07	5.21E+07	5.35E+07	5.14E+07	5.64E+07	5.32E+07	4.15E+07
TG(18:4_14:1_16:1)	TG	794.6424	2.28E+08	3.98E+08	1.97E+08	2.59E+08	1.99E+08	1.98E+08	1.98E+08	1.88E+08	2.33E+08	2.46E+08	1.87E+08
TG(18:4_14:1_17:1)	TG	808.6581	7.20E+06	1.29E+07	5.97E+06	8.98E+06	5.68E+06	8.00E+06	7.31E+06	6.87E+06	5.94E+06	5.97E+06	4.82E+06
TG(18:4_14:1_18:4)	TG	816.6268	2.52E+08	3.91E+08	2.09E+08	1.81E+08	1.40E+08	2.49E+08	2.50E+08	2.26E+08	2.59E+08	2.76E+08	2.03E+08
TG(18:4_14:1_20:5)	TG	842.6424	3.42E+08	4.64E+08	2.74E+08	2.64E+08	2.12E+08	3.48E+08	3.48E+08	3.06E+08	3.46E+08	3.44E+08	3.03E+08
TG(18:4_14:2_16:1)	TG	792.6268	1.12E+08	2.23E+08	9.47E+07	1.20E+08	9.51E+07	9.54E+07	9.60E+07	9.15E+07	1.14E+08	1.12E+08	8.66E+07
TG(18:4_14:2_18:4)	TG	814.6111	2.70E+07	4.27E+07	2.37E+07	2.17E+07	1.70E+07	2.61E+07	2.65E+07	2.56E+07	3.10E+07	3.22E+07	2.35E+07
TG(18:4_14:2_20:5)	TG	840.6268	7.35E+07	8.34E+07	6.29E+07	4.88E+07	4.14E+07	7.63E+07	7.97E+07	7.12E+07	8.94E+07	8.69E+07	7.01E+07
TG(18:4_14:4_18:4)	TG	810.5798	3.25E+07	4.65E+07	2.66E+07	2.60E+07	2.05E+07	2.52E+07	2.68E+07	2.69E+07	4.12E+07	4.55E+07	3.20E+07
TG(18:4_15:0_16:1)	TG	810.6737	8.77E+06	1.98E+07	7.68E+06	1.26E+07	8.38E+06	8.64E+06	7.97E+06	7.62E+06	6.44E+06	6.96E+06	5.56E+06

TG(18:4_15:0_18:4)	TG	832.6581	7.47E+06	1.69E+07	7.39E+06	9.12E+06	6.44E+06	7.54E+06	7.47E+06	6.87E+06	6.60E+06	7.33E+06	5.69E+06
TG(18:4_15:0_20:5)	TG	858.6737	4.79E+06	6.81E+06	4.44E+06	4.86E+06	3.50E+06	5.12E+06	4.87E+06	5.01E+06	3.96E+06	4.10E+06	3.67E+06
TG(18:4_16:0_18:4)	TG	846.6737	2.89E+08	4.60E+08	2.42E+08	2.52E+08	1.79E+08	2.99E+08	2.98E+08	2.92E+08	3.03E+08	3.20E+08	2.56E+08
TG(18:4_16:1_16:1)	TG	822.6737	6.21E+08	1.15E+09	5.45E+08	7.38E+08	5.29E+08	5.55E+08	5.28E+08	5.27E+08	5.03E+08	5.68E+08	4.50E+08
TG(18:4_16:1_17:0)	TG	838.705	3.19E+06	5.61E+06	2.83E+06	2.30E+06	1.75E+06	4.06E+06	3.92E+06	3.75E+06	3.38E+06	3.48E+06	2.99E+06
TG(18:4_16:1_18:4)	TG	844.6581	4.47E+08	9.60E+08	3.89E+08	4.46E+08	3.23E+08	3.55E+08	3.49E+08	3.42E+08	4.08E+08	4.48E+08	3.33E+08
TG(18:4_16:1_20:5)	TG	870.6737	4.54E+08	9.35E+08	4.02E+08	4.75E+08	3.20E+08	4.26E+08	4.11E+08	3.95E+08	3.84E+08	4.36E+08	3.53E+08
TG(18:4_16:1_22:0)	TG	908.7833	1.57E+06	2.15E+06	1.57E+06	1.63E+06	1.47E+06	1.62E+06	1.55E+06	1.57E+06	1.44E+06	1.39E+06	1.24E+06
TG(18:4_16:1_24:0)	TG	936.8146	8.12E+05	2.20E+06	7.28E+05	1.21E+06	1.09E+06	8.51E+05	7.34E+05	1.16E+06	1.11E+06	1.18E+06	9.60E+05
TG(18:4_16:1_24:1)	TG	934.7989	6.19E+06	1.38E+07	5.65E+06	5.75E+06	5.05E+06	6.69E+06	6.34E+06	6.33E+06	4.70E+06	5.39E+06	4.69E+06
TG(18:4_18:3_20:5)	TG	894.6737	3.00E+07	4.33E+07	3.22E+07	2.48E+07	2.16E+07	2.36E+07	2.30E+07	2.23E+07	2.81E+07	3.21E+07	2.51E+07
TG(18:4_18:4_18:4)	TG	866.6424	3.91E+07	1.24E+08	3.52E+07	4.83E+07	3.71E+07	2.88E+07	2.67E+07	2.69E+07	2.96E+07	3.29E+07	2.35E+07
TG(18:4_20:5_20:5)	TG	918.6737	1.43E+08	2.53E+08	1.05E+08	9.30E+07	8.60E+07	1.43E+08	1.29E+08	1.20E+08	1.27E+08	1.42E+08	1.05E+08
TG(18:4_20:5_22:0)	TG	956.7833	3.26E+06	6.93E+06	2.74E+06	2.54E+06	2.59E+06	3.67E+06	3.61E+06	3.82E+06	2.83E+06	3.23E+06	2.75E+06
TG(18:4_20:5_24:1)	TG	982.7989	2.91E+06	6.96E+06	2.35E+06	2.19E+06	2.17E+06	3.20E+06	3.03E+06	3.14E+06	2.27E+06	2.88E+06	2.30E+06
TG(19:1_16:1_20:5)	TG	890.7363	5.29E+06	6.77E+06	4.55E+06	3.47E+06	2.81E+06	7.95E+06	7.75E+06	7.35E+06	4.28E+06	4.27E+06	4.45E+06
TG(19:1_18:4_20:5)	TG	912.7207	1.43E+06	1.61E+06	1.21E+06	9.76E+05	8.29E+05	1.96E+06	2.01E+06	1.95E+06	1.18E+06	1.19E+06	1.30E+06
TG(19:1_20:5_20:5)	TG	938.7363	5.31E+05	3.24E+05	4.37E+05	1.75E+05	1.82E+05	9.15E+05	8.63E+05	8.61E+05	4.11E+05	3.94E+05	4.71E+05
TG(20:5_12:2_20:5)	TG	838.6111	6.39E+07	9.75E+07	7.01E+07	6.12E+07	5.26E+07	4.97E+07	5.12E+07	5.08E+07	5.80E+07	5.96E+07	4.52E+07
TG(20:5_12:3_20:5)	TG	836.5955	1.13E+08	8.99E+07	8.75E+07	5.83E+07	4.75E+07	1.31E+08	1.35E+08	1.35E+08	1.48E+08	1.55E+08	1.17E+08
TG(20:5_12:4_22:6)	TG	860.5955	3.66E+07	5.16E+07	3.79E+07	3.58E+07	2.74E+07	2.63E+07	2.74E+07	2.66E+07	3.04E+07	3.20E+07	2.61E+07
TG(20:5_14:1_20:5)	TG	868.6581	8.99E+07	1.31E+08	7.75E+07	5.91E+07	4.32E+07	1.05E+08	1.02E+08	1.03E+08	9.67E+07	1.03E+08	7.93E+07
TG(20:5_14:2_21:1)	TG	888.7207	1.56E+06	1.92E+06	1.31E+06	1.06E+06	8.47E+05	2.42E+06	2.38E+06	2.41E+06	1.35E+06	1.35E+06	1.34E+06
TG(20:5_14:3_20:5)	TG	864.6268	7.95E+07	1.60E+08	6.53E+07	5.93E+07	5.05E+07	7.01E+07	6.92E+07	6.04E+07	8.62E+07	8.82E+07	6.71E+07
TG(20:5_14:3_22:6)	TG	890.6424	4.63E+07	3.99E+07	4.31E+07	2.57E+07	2.06E+07	5.23E+07	5.32E+07	5.20E+07	5.43E+07	5.73E+07	4.80E+07
TG(20:5_14:4_20:5)	TG	862.6111	2.74E+07	2.80E+07	2.44E+07	1.94E+07	1.64E+07	2.71E+07	2.87E+07	2.78E+07	3.41E+07	3.46E+07	2.79E+07
TG(20:5_14:4_22:6)	TG	888.6268	1.37E+07	3.15E+07	1.40E+07	1.53E+07	1.16E+07	1.05E+07	1.01E+07	1.03E+07	1.12E+07	1.27E+07	9.46E+06
TG(20:5_17:1_20:5)	TG	910.705	2.56E+06	3.02E+06	2.21E+06	1.67E+06	1.38E+06	4.07E+06	3.70E+06	3.87E+06	2.12E+06	2.19E+06	1.93E+06
TG(20:5_20:4_20:5)	TG	946.705	1.14E+07	9.02E+06	1.00E+07	5.31E+06	4.86E+06	1.70E+07	1.54E+07	1.51E+07	1.07E+07	1.13E+07	9.82E+06
TG(20:5_20:5_20:5)	TG	944.6894	1.24E+08	1.02E+08	9.01E+07	5.38E+07	4.51E+07	2.10E+08	1.79E+08	1.71E+08	1.19E+08	1.10E+08	1.02E+08
TG(20:5_20:5_22:6)	TG	970.705	3.91E+07	3.61E+07	3.17E+07	2.02E+07	1.76E+07	6.62E+07	5.44E+07	4.81E+07	3.22E+07	3.14E+07	2.89E+07
TG(20:5_20:5_24:1)	TG	1008.8146	3.57E+06	3.48E+06	3.04E+06	1.44E+06	1.55E+06	5.50E+06	5.28E+06	5.59E+06	2.93E+06	3.46E+06	3.17E+06
TG(20:5_22:6_22:6)	TG	996.7207	2.12E+07	1.36E+07	1.87E+07	9.75E+06	1.06E+07	2.81E+07	2.41E+07	2.76E+07	1.26E+07	1.23E+07	1.25E+07
TG(22:0_18:2_18:2)	TG	938.8302	2.29E+06	3.94E+06	2.05E+06	2.05E+06	1.68E+06	2.55E+06	2.35E+06	2.48E+06	2.58E+06	2.67E+06	2.28E+06
TG(22:6_14:3_22:6)	TG	916.6581	2.38E+07	2.04E+07	2.08E+07	1.16E+07	9.78E+06	3.52E+07	3.16E+07	3.17E+07	2.51E+07	2.52E+07	2.08E+07
TG(22:6_22:6_22:6)	TG	1022.7363	9.51E+05	6.85E+05	8.81E+05	6.41E+05	7.39E+05	1.90E+06	1.47E+06	1.71E+06	7.90E+05	7.07E+05	7.58E+05
TG(24:0_18:3_20:5)	TG	986.8302	3.36E+05	1.64E+05	2.88E+05	5.97E+04	7.16E+04	4.60E+05	4.63E+05	4.88E+05	4.22E+05	4.11E+05	4.08E+05
TG(24:1_12:1_20:4)	TG	906.7676	8.54E+06	1.69E+07	7.30E+06	7.21E+06	6.39E+06	9.89E+06	9.46E+06	9.39E+06	7.71E+06	8.42E+06	7.16E+06
TG(24:1_12:1_22:6)	TG	930.7676	1.25E+06	2.57E+06	1.19E+06	1.15E+06	1.12E+06	1.16E+06	1.16E+06	1.20E+06	1.18E+06	1.26E+06	1.11E+06
TG(26:1_16:1_20:5)	TG	988.8459	9.98E+05	1.26E+06	7.10E+05	6.16E+05	6.73E+05	1.48E+06	1.29E+06	1.37E+06	7.71E+05	8.46E+05	7.54E+05
TG(60:8)	TG	958.7989	5.36E+06	6.57E+06	4.57E+06	3.19E+06	3.20E+06	6.99E+06	6.97E+06	6.97E+06	4.77E+06	5.10E+06	4.79E+06

Job Name	Radiatus_smart
Sample	
c-1	Radiatu TV_TM_210304_Rs_3.raw
c-2	Radiatu TV_TM_210304_Rs_2.raw
c-3	Radiatu TV_TM_210304_Rs_1.raw
s1-1	Radiatu TV_TM_210304_R1_3.raw
s1-2	Radiatu TV_TM_210304_R1_2.raw
s1-3	Radiatu TV_TM_210304_R1_1.raw
s10-1	Radiatu TV_TM_210304_ID_05.raw
s10-2	Radiatu TV_TM_210304_ID_04.raw
s10-3	Radiatu TV_TM_210304_ID_03.raw
s10-4	Radiatu TV_TM_210304_ID_02.raw
s10-5	Radiatu TV_TM_210304_ID_01.raw
s2-1	Radiatu TV_TM_210304_R2_3.raw
s2-2	Radiatu TV_TM_210304_R2_2.raw
s2-3	Radiatu TV_TM_210304_R2_1.raw
s3-1	Radiatu TV_TM_210304_R3_3.raw
s3-2	Radiatu TV_TM_210304_R3_2.raw
s3-3	Radiatu TV_TM_210304_R3_1.raw
s4-1	Radiatu TV_TM_210304_B1_3.raw
s4-2	Radiatu TV_TM_210304_B1_2.raw
s4-3	Radiatu TV_TM_210304_B1_1.raw
s5-1	Radiatu TV_TM_210304_B2_3.raw
s5-2	Radiatu TV_TM_210304_B2_2.raw
s5-3	Radiatu TV_TM_210304_B2_1.raw
s6-1	Radiatu TV_TM_210304_B3_3.raw
s6-2	Radiatu TV_TM_210304_B3_2.raw
s6-3	Radiatu TV_TM_210304_B3_1.raw
s7-1	Radiatu TV_TM_210304_W1_3.raw
s7-2	Radiatu TV_TM_210304_W1_2.raw
s7-3	Radiatu TV_TM_210304_W1_1.raw
s8-1	Radiatu TV_TM_210304_W2_3.raw
s8-2	Radiatu TV_TM_210304_W2_2.raw
s8-3	Radiatu TV_TM_210304_W2_1.raw
s9-1	Radiatu TV_TM_210304_W3_3.raw
s9-2	Radiatu TV_TM_210304_W3_2.raw
s9-3	Radiatu TV_TM_210304_W3_1.raw

Result

LipidMolec	Class	Calc Mass	MainArea[c]	MainArea[s1]	MainArea[s10	MainArea[s2]	MainArea[s3]	MainArea[s4]	MainArea[s5]	MainArea[s6]	MainArea[s7]	MainArea[s8]	MainArea[s9]
DG(14:0_14:0)	DG	512.4441	1.01E+06	8.33E+05	1.05E+06	6.15E+05	7.84E+05	1.56E+06	1.23E+06	1.06E+06	1.05E+06	1.01E+06	1.17E+06
DG(14:0_14:0)	DG	512.4441	3.25E+05	1.95E+05	3.42E+05	1.63E+05	2.12E+05	4.66E+05	3.70E+05	3.59E+05	3.38E+05	4.11E+05	4.11E+05
DG(14:0_14:0)	DG	512.4441	1.58E+06	9.18E+05	1.64E+06	7.65E+05	1.06E+06	2.34E+06	1.81E+06	1.98E+06	1.46E+06	2.00E+06	2.26E+06
DG(14:0_20:5)	DG	586.4597	4.18E+06	2.36E+06	4.01E+06	1.45E+06	2.26E+06	6.77E+06	4.84E+06	4.17E+06	2.79E+06	5.10E+06	8.59E+06
DG(15:0_16:1)	DG	552.4754	5.50E+05	4.85E+05	5.78E+05	3.97E+05	5.49E+05	7.93E+05	6.45E+05	6.02E+05	4.81E+05	5.00E+05	5.87E+05
DG(16:0_14:0)	DG	540.4754	4.84E+05	5.14E+05	5.52E+05	4.36E+05	4.51E+05	4.94E+05	4.74E+05	4.22E+05	4.40E+05	5.80E+05	6.37E+05
DG(16:0_16:0)	DG	568.5067	1.29E+05	1.62E+05	1.26E+05	1.38E+05	1.33E+05	9.41E+04	1.12E+05	9.51E+04	1.06E+05	1.49E+05	1.57E+05
DG(16:0_16:1)	DG	566.491	1.39E+07	1.02E+07	1.31E+07	8.57E+06	1.08E+07	2.52E+07	1.78E+07	1.65E+07	9.01E+06	9.19E+06	1.33E+07
DG(16:0_16:1)	DG	566.491	2.57E+07	1.95E+07	2.42E+07	1.67E+07	2.17E+07	4.42E+07	3.31E+07	2.95E+07	1.87E+07	1.88E+07	2.66E+07
DG(16:0_18:2)	DG	592.5067	1.05E+06	6.68E+05	1.04E+06	5.37E+05	6.40E+05	1.68E+06	1.10E+06	1.02E+06	6.59E+05	1.17E+06	2.23E+06
DG(16:0_20:5)	DG	614.491	1.30E+06	9.09E+05	1.20E+06	8.30E+05	9.48E+05	1.63E+06	1.63E+06	1.46E+06	9.87E+05	1.55E+06	1.97E+06
DG(16:0_20:5)	DG	614.491	5.18E+06	3.13E+06	5.09E+06	1.97E+06	2.87E+06	7.45E+06	5.52E+06	5.07E+06	3.69E+06	6.36E+06	1.18E+07
DG(16:0_22:6)	DG	640.5067	2.72E+06	1.44E+06	2.58E+06	8.31E+05	1.15E+06	4.56E+06	2.92E+06	2.62E+06	1.84E+06	3.29E+06	5.89E+06
DG(16:1_14:0)	DG	538.4597	3.18E+07	2.16E+07	3.33E+07	1.68E+07	2.43E+07	5.63E+07	4.20E+07	4.12E+07	2.90E+07	3.05E+07	3.49E+07
DG(16:1_14:0)	DG	538.4597	2.67E+06	1.53E+06	2.87E+06	1.18E+06	1.63E+06	6.45E+06	4.01E+06	2.91E+06	1.84E+06	2.01E+06	3.00E+06
DG(16:1_16:1)	DG	564.4754	1.47E+07	1.52E+07	1.47E+07	1.30E+07	1.47E+07	2.37E+07	1.73E+07	1.62E+07	1.04E+07	1.04E+07	1.51E+07
DG(16:1_16:1)	DG	564.4754	1.20E+07	1.37E+07	1.18E+07	1.22E+07	1.37E+07	1.65E+07	1.22E+07	1.25E+07	6.52E+06	8.68E+06	1.42E+07
DG(16:1_18:2)	DG	590.491	5.21E+05	3.49E+05	5.75E+05	2.43E+05	2.74E+05	7.46E+05	5.13E+05	4.74E+05	3.54E+05	6.72E+05	1.17E+06
DG(16:1_20:5)	DG	612.4754	1.14E+07	1.17E+07	1.05E+07	1.11E+07	1.15E+07	1.46E+07	1.26E+07	9.95E+06	8.21E+06	1.08E+07	1.31E+07
DG(16:1_20:5)	DG	612.4754	1.24E+07	1.01E+07	1.25E+07	6.62E+06	8.84E+06	1.74E+07	1.34E+07	1.28E+07	7.97E+06	1.40E+07	2.28E+07
DG(16:1_22:6)	DG	638.491	5.57E+06	3.95E+06	5.80E+06	2.45E+06	3.07E+06	8.43E+06	5.92E+06	5.05E+06	3.73E+06	7.10E+06	1.12E+07
DG(18:4_20:5)	DG	634.4597	1.46E+06	1.05E+06	1.50E+06	8.51E+05	1.03E+06	2.39E+06	1.84E+06	1.61E+06	1.03E+06	1.32E+06	1.67E+06
DG(18:4_20:5)	DG	634.4597	1.47E+06	2.45E+06	1.53E+06	7.19E+05	7.79E+05	2.54E+06	1.54E+06	1.37E+06	6.92E+05	1.51E+06	1.98E+06
DG(20:5_14:1)	DG	584.4441	6.40E+07	1.73E+07	6.20E+07	1.55E+07	1.40E+07	1.63E+08	1.41E+08	9.78E+07	5.25E+07	6.41E+07	5.19E+07
DG(20:5_20:4)	DG	662.491	2.65E+06	9.01E+05	2.67E+06	5.63E+05	8.65E+05	4.78E+06	3.11E+06	2.30E+06	1.84E+06	3.97E+06	6.27E+06
DG(20:5_20:5)	DG	660.4754	4.98E+06	4.75E+06	5.20E+06	2.11E+06	2.72E+06	8.98E+06	5.99E+06	4.58E+06	2.65E+06	5.75E+06	7.85E+06
DG(20:5_22:5)	DG	688.5067	2.31E+06	6.41E+05	2.33E+06	3.99E+05	6.30E+05	3.64E+06	2.58E+06	1.88E+06	1.81E+06	3.45E+06	5.97E+06
DG(20:5_22:6)	DG	686.491	6.37E+06	4.04E+06	6.53E+06	2.40E+06	3.16E+06	1.18E+07	8.23E+06	6.53E+06	3.61E+06	7.80E+06	1.13E+07
DG(22:5_22:6)	DG	714.5223	3.39E+06	9.86E+05	3.38E+06	5.95E+05	1.00E+06	5.49E+06	3.70E+06	2.66E+06	3.08E+06	5.02E+06	8.53E+06
DG(22:6_22:6)	DG	712.5067	3.79E+06	2.66E+06	3.92E+06	1.48E+06	1.91E+06	6.49E+06	4.65E+06	3.56E+06	2.50E+06	4.80E+06	6.64E+06
DG(30:2e)	DG	522.4648	2.88E+07	1.98E+07	2.78E+07	1.54E+07	2.35E+07	4.68E+07	3.50E+07	3.86E+07	2.62E+07	2.68E+07	3.25E+07
DG(30:2e)	DG	522.4648	3.21E+06	2.83E+06	2.51E+06	2.88E+06	3.14E+06	5.19E+06	3.18E+06	3.91E+06	1.44E+06	2.04E+06	3.64E+06
DG(32:2e)	DG	550.4961	6.73E+06	6.54E+06	6.12E+06	5.43E+06	7.74E+06	9.97E+06	6.98E+06	7.31E+06	5.30E+06	5.17E+06	7.84E+06
DG(32:2e)	DG	550.4961	1.39E+06	1.29E+06	1.00E+06	1.40E+06	1.49E+06	2.22E+06	1.36E+06	1.66E+06	6.18E+05	7.90E+05	1.38E+06
DG(32:3e)	DG	548.4805	1.55E+08	1.47E+08	1.46E+08	1.16E+08	1.60E+08	2.44E+08	1.81E+08	2.05E+08	1.21E+08	1.13E+08	1.43E+08
DG(32:3e)	DG	548.4805	1.13E+07	1.16E+07	9.30E+06	1.26E+07	1.29E+07	1.76E+07	1.11E+07	1.40E+07	4.65E+06	6.03E+06	1.12E+07
DG(34:4)	DG	588.4754	1.15E+06	6.40E+05	1.19E+06	4.05E+05	5.60E+05	1.84E+06	1.17E+06	1.12E+06	7.81E+05	1.43E+06	2.66E+06
DG(34:5)	DG	586.4597	3.94E+06	2.93E+06	3.74E+06	2.65E+06	3.24E+06	6.64E+06	4.82E+06	4.39E+06	2.96E+06	3.65E+06	4.83E+06
DG(36:4e)	DG	602.5274	3.09E+06	3.57E+06	2.98E+06	1.91E+06	1.48E+06	4.92E+06	3.05E+06	3.10E+06	2.02E+06	5.99E+06	2.55E+06
DG(40:8)	DG	664.5067	1.44E+06	3.84E+05	1.35E+06	2.04E+05	3.16E+05	2.52E+06	1.50E+06	1.06E+06	9.56E+05	2.07E+06	3.68E+06

LPC(14:0)	LPC	467.3012	4.76E+07	3.20E+07	4.93E+07	1.99E+07	2.58E+07	8.67E+07	7.78E+07	8.58E+07	4.17E+07	4.08E+07	3.25E+07
LPC(16:0)	LPC	495.3325	2.75E+07	1.62E+07	2.90E+07	1.11E+07	1.49E+07	4.97E+07	4.82E+07	4.91E+07	2.27E+07	2.33E+07	2.30E+07
LPC(16:1)	LPC	493.3168	4.00E+08	5.37E+08	4.19E+08	3.94E+08	4.22E+08	5.54E+08	4.64E+08	5.32E+08	3.11E+08	2.61E+08	2.18E+08
LPC(18:0)	LPC	523.3638	5.87E+05	5.33E+05	5.75E+05	2.93E+05	5.13E+05	8.87E+05	8.72E+05	8.78E+05	5.11E+05	5.07E+05	5.55E+05
LPC(18:1)	LPC	521.3481	6.07E+07	4.21E+07	5.95E+07	3.23E+07	4.59E+07	1.10E+08	7.72E+07	9.43E+07	6.84E+07	4.93E+07	3.83E+07
LPC(18:2)	LPC	519.3325	1.79E+08	1.40E+08	1.90E+08	9.80E+07	1.17E+08	3.12E+08	2.47E+08	2.95E+08	1.70E+08	1.64E+08	1.50E+08
LPC(18:3)	LPC	517.3168	9.50E+07	9.31E+07	9.70E+07	6.53E+07	7.78E+07	1.72E+08	1.26E+08	1.43E+08	7.81E+07	7.10E+07	5.58E+07
LPC(18:4)	LPC	515.3012	1.22E+08	1.26E+08	1.34E+08	9.52E+07	1.08E+08	2.01E+08	1.68E+08	1.88E+08	8.93E+07	8.57E+07	6.04E+07
LPC(20:2)	LPC	547.3638	6.22E+05	6.66E+05	6.64E+05	4.89E+05	5.23E+05	7.77E+05	7.28E+05	7.70E+05	5.65E+05	7.46E+05	5.29E+05
LPC(20:3)	LPC	545.3481	2.16E+07	1.21E+07	2.19E+07	8.61E+06	1.30E+07	3.90E+07	2.96E+07	3.01E+07	2.41E+07	2.22E+07	1.68E+07
LPC(20:4)	LPC	543.3325	2.07E+08	1.13E+08	2.00E+08	7.47E+07	1.15E+08	3.89E+08	3.11E+08	3.30E+08	2.05E+08	1.90E+08	1.81E+08
LPC(20:5)	LPC	541.3168	4.97E+08	4.02E+08	5.07E+08	2.88E+08	3.72E+08	1.04E+09	8.48E+08	8.64E+08	3.21E+08	3.02E+08	2.56E+08
LPC(22:4)	LPC	571.3638	3.91E+06	2.52E+06	3.83E+06	1.71E+06	2.66E+06	6.85E+06	5.53E+06	5.69E+06	4.24E+06	3.63E+06	3.43E+06
LPC(22:5)	LPC	569.3481	5.35E+07	3.55E+07	5.39E+07	2.42E+07	3.37E+07	8.81E+07	7.75E+07	8.06E+07	5.75E+07	4.96E+07	5.01E+07
LPC(22:6)	LPC	567.3325	4.83E+08	4.29E+08	5.19E+08	2.91E+08	3.45E+08	8.67E+08	7.66E+08	8.37E+08	3.23E+08	3.02E+08	2.48E+08
LPE(16:1)	LPE	451.2699	4.03E+05	3.58E+05	4.58E+05	3.09E+05	2.87E+05	6.08E+05	5.79E+05	7.52E+05	3.07E+05	3.62E+05	2.54E+05
LPE(22:5)	LPE	527.3012	1.83E+06	8.76E+05	2.07E+06	7.32E+05	1.12E+06	2.89E+06	2.45E+06	3.30E+06	1.91E+06	1.86E+06	2.04E+06
LPE(22:6)	LPE	525.2855	4.30E+07	3.70E+07	4.61E+07	3.45E+07	4.23E+07	7.13E+07	5.69E+07	7.76E+07	3.02E+07	3.17E+07	2.85E+07
LPG(14:0)	LPG	456.2488	6.11E+05	3.28E+05	5.52E+05	2.19E+05	2.87E+05	1.11E+06	9.19E+05	9.64E+05	5.60E+05	5.50E+05	6.27E+05
LPG(16:0)	LPG	484.2801	2.86E+06	3.24E+06	3.88E+06	1.87E+06	2.78E+06	3.13E+06	2.87E+06	2.63E+06	3.45E+06	3.10E+06	3.44E+06
LPG(16:1)	LPG	482.2645	4.16E+06	3.68E+06	4.11E+06	2.91E+06	2.88E+06	6.87E+06	6.24E+06	6.02E+06	3.58E+06	2.95E+06	3.84E+06
MG(14:0)	MG	302.2457	2.11E+06	1.38E+06	2.92E+06	1.10E+06	1.80E+06	1.89E+06	1.56E+06	1.97E+06	1.97E+06	2.85E+06	4.69E+06
MG(16:0)	MG	330.277	1.15E+06	1.12E+06	1.61E+06	9.18E+05	1.16E+06	7.90E+05	8.73E+05	1.13E+06	8.36E+05	1.42E+06	2.08E+06
MGDG(14:0_14:0)	MGDG	674.4969	3.72E+06	2.32E+06	3.93E+06	1.92E+06	2.47E+06	5.72E+06	4.31E+06	4.30E+06	3.90E+06	4.83E+06	4.75E+06
MGDG(14:0_14:1)	MGDG	672.4812	1.30E+06	9.69E+05	1.53E+06	7.56E+05	1.09E+06	2.79E+06	1.71E+06	1.58E+06	1.16E+06	1.20E+06	1.41E+06
MGDG(14:0_16:3)	MGDG	696.4812	6.55E+07	7.29E+07	5.50E+07	6.05E+07	8.49E+07	7.30E+07	5.03E+07	4.40E+07	4.69E+07	6.26E+07	8.25E+07
MGDG(14:0_16:4)	MGDG	694.4656	4.43E+07	3.59E+07	4.56E+07	2.22E+07	2.10E+07	7.10E+07	6.01E+07	6.07E+07	4.61E+07	4.91E+07	5.59E+07
MGDG(15:0_16:3)	MGDG	710.4969	9.97E+05	1.37E+06	9.94E+05	1.12E+06	1.35E+06	1.19E+06	8.59E+05	7.81E+05	6.81E+05	7.40E+05	9.97E+05
MGDG(16:0_14:0)	MGDG	702.5282	6.60E+06	6.91E+06	7.19E+06	5.95E+06	6.19E+06	6.73E+06	6.54E+06	5.84E+06	6.14E+06	8.07E+06	8.71E+06
MGDG(16:0_16:0)	MGDG	730.5595	2.05E+06	2.63E+06	2.09E+06	2.17E+06	2.16E+06	1.70E+06	1.86E+06	1.62E+06	1.72E+06	2.39E+06	2.41E+06
MGDG(16:0_16:1)	MGDG	728.5438	1.59E+08	1.14E+08	1.42E+08	9.62E+07	1.23E+08	2.62E+08	1.94E+08	1.72E+08	1.02E+08	1.03E+08	1.51E+08
MGDG(16:0_18:3)	MGDG	752.5438	3.34E+06	3.52E+06	3.57E+06	3.21E+06	3.40E+06	5.06E+06	3.69E+06	3.69E+06	2.17E+06	2.66E+06	3.94E+06
MGDG(16:0_20:4)	MGDG	778.5595	7.94E+05	5.98E+05	8.31E+05	5.11E+05	5.83E+05	8.86E+05	8.87E+05	8.51E+05	6.85E+05	1.06E+06	1.25E+06
MGDG(16:0_20:5)	MGDG	776.5438	1.51E+07	1.04E+07	1.49E+07	9.42E+06	1.10E+07	1.99E+07	1.95E+07	1.80E+07	1.12E+07	1.76E+07	2.21E+07
MGDG(16:1_14:0)	MGDG	700.5126	2.88E+08	1.99E+08	2.67E+08	1.64E+08	2.21E+08	4.32E+08	3.46E+08	3.10E+08	2.52E+08	2.58E+08	2.96E+08
MGDG(16:1_14:1)	MGDG	698.4969	2.63E+07	1.76E+07	2.35E+07	1.45E+07	2.19E+07	4.47E+07	3.30E+07	3.33E+07	2.43E+07	2.61E+07	2.75E+07
MGDG(16:1_15:0)	MGDG	714.5282	4.82E+06	4.28E+06	5.18E+06	3.46E+06	4.78E+06	7.43E+06	5.90E+06	5.63E+06	4.23E+06	4.43E+06	5.15E+06
MGDG(16:1_15:1)	MGDG	712.5126	8.65E+05	7.03E+05	9.02E+05	5.75E+05	7.41E+05	1.35E+06	1.04E+06	9.37E+05	7.97E+05	8.71E+05	1.01E+06
MGDG(16:1_16:1)	MGDG	726.5282	1.49E+08	1.48E+08	1.45E+08	1.31E+08	1.45E+08	2.29E+08	1.74E+08	1.66E+08	1.04E+08	1.07E+08	1.50E+08
MGDG(16:1_16:2)	MGDG	724.5126	8.16E+07	1.11E+08	7.47E+07	9.75E+07	1.06E+08	1.03E+08	7.91E+07	7.72E+07	5.12E+07	5.08E+07	7.53E+07
MGDG(16:1_16:3)	MGDG	722.4969	1.74E+08	2.66E+08	1.98E+08	2.49E+08	2.47E+08	1.73E+08	1.38E+08	1.28E+08	1.13E+08	1.20E+08	1.57E+08
MGDG(16:1_16:4)	MGDG	720.4812	1.46E+08	1.75E+08	1.55E+08	1.75E+08	1.86E+08	1.73E+08	1.45E+08	1.40E+08	1.18E+08	1.21E+08	1.43E+08

MGDG(16:1_18:0)	MGDG	756.5752	7.86E+05	6.29E+05	7.30E+05	5.30E+05	7.09E+05	1.28E+06	9.27E+05	7.79E+05	4.51E+05	5.25E+05	7.59E+05
MGDG(16:1_18:1)	MGDG	754.5595	4.75E+06	3.83E+06	4.32E+06	3.21E+06	3.64E+06	7.20E+06	5.55E+06	4.97E+06	2.91E+06	3.26E+06	5.18E+06
MGDG(16:1_18:4)	MGDG	748.5126	4.31E+07	2.91E+07	3.73E+07	2.49E+07	3.31E+07	8.45E+07	5.53E+07	5.66E+07	2.79E+07	3.49E+07	5.17E+07
MGDG(16:1_20:2)	MGDG	780.5752	4.46E+05	2.70E+05	4.70E+05	2.06E+05	2.50E+05	6.05E+05	4.64E+05	4.09E+05	4.54E+05	5.31E+05	8.60E+05
MGDG(16:1_22:6)	MGDG	800.5438	1.11E+06	8.07E+05	1.25E+06	6.96E+05	6.77E+05	1.41E+06	1.38E+06	1.23E+06	8.91E+05	1.34E+06	2.01E+06
MGDG(18:1_16:3)	MGDG	750.5282	5.85E+06	7.34E+06	6.06E+06	6.75E+06	7.11E+06	6.74E+06	5.18E+06	4.77E+06	4.03E+06	4.85E+06	6.37E+06
MGDG(18:3_16:3)	MGDG	746.4969	6.55E+06	1.45E+07	1.70E+07	1.16E+07	1.13E+07	8.08E+06	7.07E+06	5.27E+06	5.54E+06	5.87E+06	4.99E+06
MGDG(18:3_16:3)	MGDG	746.4969	5.59E+06	9.18E+06	6.11E+06	7.57E+06	7.60E+06	6.01E+06	4.36E+06	4.09E+06	3.68E+06	3.81E+06	5.64E+06
MGDG(18:3_20:5)	MGDG	798.5282	3.36E+06	3.21E+06	5.52E+06	2.52E+06	2.97E+06	5.08E+06	3.77E+06	3.10E+06	3.00E+06	3.72E+06	5.72E+06
MGDG(18:4_16:3)	MGDG	744.4812	3.26E+07	4.52E+07	2.86E+07	3.41E+07	3.86E+07	3.51E+07	2.99E+07	2.59E+07	2.59E+07	2.80E+07	2.57E+07
MGDG(18:4_16:4)	MGDG	742.4656	5.30E+06	5.56E+06	6.25E+06	3.26E+06	3.51E+06	8.41E+06	7.02E+06	5.54E+06	5.45E+06	5.87E+06	4.69E+06
MGDG(18:4_18:4)	MGDG	770.4969	4.17E+07	2.68E+07	3.66E+07	2.38E+07	3.10E+07	7.73E+07	5.18E+07	5.26E+07	2.64E+07	3.36E+07	4.73E+07
MGDG(18:4_20:5)	MGDG	796.5126	1.34E+07	9.67E+06	1.31E+07	7.42E+06	1.04E+07	2.48E+07	1.68E+07	1.25E+07	9.99E+06	1.34E+07	1.82E+07
MGDG(20:4_16:2)	MGDG	774.5282	9.66E+07	9.86E+07	1.17E+08	9.56E+07	1.01E+08	1.35E+08	1.13E+08	9.13E+07	6.88E+07	9.31E+07	1.12E+08
MGDG(20:4_20:5)	MGDG	824.5438	8.85E+05	5.60E+05	1.03E+06	5.31E+05	5.22E+05	1.11E+06	1.13E+06	8.68E+05	7.21E+05	9.69E+05	1.73E+06
MGDG(20:5_15:2)	MGDG	758.4969	1.98E+06	2.21E+06	1.48E+06	1.45E+06	2.06E+06	3.09E+06	2.37E+06	1.97E+06	1.50E+06	1.72E+06	1.69E+06
MGDG(20:5_16:2)	MGDG	772.5126	1.82E+08	1.86E+08	1.48E+08	1.69E+08	2.06E+08	2.12E+08	1.86E+08	1.39E+08	1.49E+08	1.76E+08	1.90E+08
MGDG(20:5_16:3)	MGDG	770.4969	3.95E+08	4.15E+08	3.76E+08	3.84E+08	4.03E+08	4.74E+08	4.32E+08	3.77E+08	3.37E+08	3.70E+08	3.61E+08
MGDG(20:5_16:4)	MGDG	768.4812	3.86E+08	1.95E+08	3.66E+08	1.67E+08	1.70E+08	5.60E+08	5.36E+08	4.62E+08	3.53E+08	3.87E+08	3.52E+08
MGDG(20:5_17:3)	MGDG	784.5126	6.24E+05	5.19E+05	6.61E+05	4.10E+05	5.30E+05	9.69E+05	8.21E+05	5.44E+05	5.34E+05	6.99E+05	8.08E+05
MGDG(20:5_20:5)	MGDG	822.5282	5.85E+06	5.07E+06	5.72E+06	5.42E+06	5.25E+06	7.27E+06	7.74E+06	5.55E+06	3.50E+06	4.53E+06	9.21E+06
MGDG(22:6_16:4)	MGDG	794.4969	7.30E+06	2.96E+06	5.65E+06	1.93E+06	2.24E+06	8.02E+06	7.50E+06	8.52E+06	6.08E+06	9.49E+06	1.82E+07
MGDG(22:6_20:5)	MGDG	848.5438	2.09E+06	1.25E+06	1.91E+06	1.11E+06	1.18E+06	3.77E+06	3.54E+06	2.88E+06	1.71E+06	2.36E+06	2.15E+06
MGDG(22:6_22:6)	MGDG	874.5595	5.78E+05	5.47E+05	6.62E+05	4.46E+05	4.46E+05	8.47E+05	7.04E+05	6.54E+05	5.18E+05	6.51E+05	6.21E+05
MGDG(32:5)	MGDG	720.4812	5.34E+07	4.38E+07	5.00E+07	3.68E+07	5.02E+07	7.73E+07	5.94E+07	5.94E+07	4.61E+07	4.82E+07	5.38E+07
MGDG(38:9)	MGDG	796.5126	9.59E+07	9.92E+07	1.23E+08	9.55E+07	1.00E+08	1.35E+08	1.13E+08	9.12E+07	7.06E+07	9.29E+07	1.11E+08
PC(10:0_20:3)	PC	699.4839	2.05E+06	2.79E+06	2.60E+06	2.68E+06	2.87E+06	3.56E+06	2.17E+06	1.95E+06	1.44E+06	1.43E+06	8.65E+05
PC(10:1e_10:4)	PC	541.3168	4.99E+08	4.04E+08	5.18E+08	2.90E+08	3.74E+08	1.05E+09	8.51E+08	8.67E+08	3.23E+08	3.04E+08	2.57E+08
PC(14:0_14:0)	PC	677.4996	3.15E+07	1.52E+07	3.15E+07	1.29E+07	2.14E+07	6.85E+07	4.48E+07	4.28E+07	2.86E+07	3.50E+07	2.90E+07
PC(14:0_20:4)	PC	753.5309	5.08E+07	3.75E+07	4.46E+07	3.55E+07	3.90E+07	1.04E+08	6.66E+07	6.46E+07	4.00E+07	4.50E+07	4.12E+07
PC(14:0_20:5)	PC	751.5152	9.12E+07	6.54E+07	8.73E+07	6.01E+07	7.33E+07	1.94E+08	1.36E+08	1.16E+08	5.78E+07	6.84E+07	6.08E+07
PC(14:1e)	PC	465.2855	1.53E+06	1.06E+06	1.65E+06	6.80E+05	7.92E+05	2.83E+06	2.50E+06	2.72E+06	1.59E+06	1.45E+06	8.49E+05
PC(16:0_14:0)	PC	705.5309	1.47E+07	6.69E+06	1.38E+07	5.41E+06	7.80E+06	2.92E+07	2.22E+07	2.17E+07	1.14E+07	1.43E+07	1.69E+07
PC(16:0_16:1)	PC	731.5465	7.26E+07	5.21E+07	6.79E+07	4.99E+07	5.78E+07	1.45E+08	1.04E+08	1.07E+08	5.16E+07	5.20E+07	5.17E+07
PC(16:0_18:1)	PC	759.5778	8.12E+06	4.18E+06	8.17E+06	3.59E+06	4.78E+06	1.86E+07	1.20E+07	1.38E+07	6.20E+06	6.43E+06	6.42E+06
PC(16:0_18:2)	PC	757.5622	3.15E+07	2.11E+07	3.09E+07	1.98E+07	2.22E+07	6.38E+07	4.26E+07	4.60E+07	2.58E+07	2.58E+07	2.50E+07
PC(16:1_14:0)	PC	703.5152	9.26E+07	7.98E+07	7.85E+07	7.35E+07	8.25E+07	1.76E+08	1.21E+08	1.19E+08	7.38E+07	7.51E+07	6.35E+07
PC(16:1_14:3)	PC	697.4683	1.04E+06	8.23E+05	1.08E+06	6.63E+05	6.32E+05	2.26E+06	1.52E+06	1.57E+06	7.76E+05	9.03E+05	4.87E+05
PC(16:1_16:1)	PC	729.5309	1.29E+08	1.70E+08	1.22E+08	1.56E+08	1.48E+08	2.05E+08	1.41E+08	1.40E+08	8.81E+07	8.91E+07	8.36E+07
PC(16:1_18:2)	PC	755.5465	4.28E+07	3.45E+07	3.83E+07	3.32E+07	3.22E+07	8.25E+07	5.31E+07	5.51E+07	3.50E+07	3.86E+07	3.44E+07
PC(16:1_20:3)	PC	781.5622	1.84E+07	7.95E+06	1.77E+07	6.89E+06	8.83E+06	4.22E+07	2.92E+07	2.68E+07	1.45E+07	1.69E+07	1.90E+07
PC(16:1_20:4)	PC	779.5465	8.69E+07	5.27E+07	8.82E+07	4.60E+07	5.56E+07	1.86E+08	1.35E+08	1.20E+08	6.54E+07	7.29E+07	7.58E+07

PC(16:1_20:5)	PC	777.5309	2.54E+08	2.71E+08	2.39E+08	2.66E+08	2.82E+08	4.61E+08	3.24E+08	2.63E+08	1.61E+08	1.79E+08	1.69E+08
PC(18:1_14:2)	PC	727.5152	4.91E+07	7.82E+07	4.96E+07	7.17E+07	7.08E+07	6.78E+07	4.71E+07	4.29E+07	3.36E+07	3.17E+07	2.54E+07
PC(18:1_18:1)	PC	785.5935	8.90E+06	9.12E+06	8.89E+06	5.51E+06	4.13E+06	1.61E+07	1.02E+07	9.41E+06	5.86E+06	1.52E+07	7.22E+06
PC(18:1_20:5)	PC	805.5622	6.99E+07	4.10E+07	6.58E+07	3.65E+07	4.24E+07	1.66E+08	1.09E+08	1.04E+08	5.01E+07	5.34E+07	5.51E+07
PC(18:2_14:2)	PC	725.4996	1.61E+07	2.01E+07	1.71E+07	1.79E+07	1.99E+07	3.27E+07	2.13E+07	2.00E+07	1.06E+07	1.17E+07	7.86E+06
PC(18:2e_18:2)	PC	767.5829	6.72E+06	1.51E+07	6.36E+06	1.50E+07	1.17E+07	3.30E+06	3.26E+06	4.06E+06	2.95E+06	3.59E+06	3.37E+06
PC(18:3_20:5)	PC	801.5309	4.73E+07	3.37E+07	4.31E+07	3.34E+07	3.85E+07	1.09E+08	6.98E+07	5.85E+07	2.86E+07	3.50E+07	3.31E+07
PC(18:4_20:5)	PC	799.5152	3.57E+07	2.85E+07	2.55E+07	1.89E+07	2.33E+07	9.59E+07	6.05E+07	4.52E+07	1.64E+07	2.41E+07	2.10E+07
PC(18:5e)	PC	513.2855	1.13E+07	1.32E+07	1.19E+07	1.02E+07	1.06E+07	1.79E+07	1.57E+07	1.70E+07	9.51E+06	7.11E+06	4.89E+06
PC(19:2e)	PC	533.3481	4.49E+05	4.64E+05	4.73E+05	3.30E+05	4.28E+05	6.18E+05	5.57E+05	5.46E+05	4.80E+05	5.13E+05	3.17E+05
PC(19:3e)	PC	531.3325	8.14E+05	1.11E+06	7.83E+05	7.32E+05	9.64E+05	9.73E+05	1.01E+06	9.20E+05	7.02E+05	6.30E+05	4.91E+05
PC(19:4e)	PC	529.3168	1.78E+06	1.70E+06	1.77E+06	1.18E+06	1.53E+06	2.90E+06	2.59E+06	2.59E+06	1.64E+06	1.45E+06	1.02E+06
PC(20:1e_22:6)	PC	845.6298	2.78E+06	3.74E+06	2.71E+06	3.52E+06	2.65E+06	3.22E+06	3.20E+06	3.82E+06	1.81E+06	1.69E+06	2.27E+06
PC(20:2e_16:1)	PC	769.5985	1.74E+06	2.13E+06	1.71E+06	1.86E+06	1.84E+06	1.96E+06	1.82E+06	1.85E+06	1.12E+06	1.38E+06	1.27E+06
PC(20:4_14:2)	PC	749.4996	9.36E+06	1.29E+07	9.07E+06	1.23E+07	1.19E+07	1.42E+07	1.03E+07	9.15E+06	6.34E+06	6.33E+06	4.13E+06
PC(20:4_20:4)	PC	829.5622	2.23E+07	9.13E+06	2.23E+07	9.03E+06	1.10E+07	5.07E+07	3.37E+07	2.66E+07	1.87E+07	2.42E+07	2.47E+07
PC(20:4e_16:1)	PC	765.5672	8.05E+06	9.37E+06	7.79E+06	9.20E+06	7.42E+06	8.10E+06	8.83E+06	9.84E+06	6.21E+06	8.50E+06	7.32E+06
PC(20:5_18:2)	PC	803.5465	1.23E+08	1.06E+08	1.12E+08	1.03E+08	9.83E+07	2.38E+08	1.67E+08	1.50E+08	8.17E+07	9.74E+07	9.57E+07
PC(20:5_20:4)	PC	827.5465	6.71E+07	3.17E+07	6.90E+07	3.15E+07	4.16E+07	1.59E+08	1.07E+08	7.56E+07	4.72E+07	6.17E+07	6.96E+07
PC(20:5_20:5)	PC	825.5309	1.71E+08	1.39E+08	1.60E+08	1.26E+08	1.51E+08	4.14E+08	2.81E+08	1.97E+08	7.68E+07	1.07E+08	1.10E+08
PC(20:5_22:5)	PC	853.5622	2.86E+07	1.20E+07	2.67E+07	1.20E+07	1.46E+07	6.70E+07	4.61E+07	3.64E+07	2.27E+07	2.77E+07	3.18E+07
PC(20:5_22:6)	PC	851.5465	9.65E+07	6.61E+07	8.11E+07	7.03E+07	7.35E+07	2.19E+08	1.56E+08	1.17E+08	4.64E+07	6.37E+07	6.65E+07
PC(21:5e)	PC	555.3325	1.27E+07	1.32E+07	1.36E+07	1.06E+07	8.98E+06	1.84E+07	1.73E+07	1.93E+07	1.13E+07	1.08E+07	8.47E+06
PC(22:5_13:0)	PC	765.5309	5.82E+06	5.28E+06	6.20E+06	4.58E+06	5.29E+06	1.06E+07	7.60E+06	6.70E+06	4.64E+06	5.27E+06	6.41E+06
PC(22:5_22:6)	PC	879.5778	3.81E+06	2.11E+06	3.87E+06	1.76E+06	1.98E+06	7.05E+06	5.98E+06	5.31E+06	3.64E+06	3.81E+06	3.77E+06
PC(22:6_14:1)	PC	775.5152	4.62E+07	6.02E+07	4.11E+07	5.82E+07	6.55E+07	7.96E+07	5.47E+07	4.10E+07	2.56E+07	2.51E+07	2.10E+07
PC(22:6_14:1)	PC	775.5152	6.36E+06	4.23E+06	5.42E+06	3.89E+06	4.67E+06	1.38E+07	8.89E+06	8.49E+06	4.92E+06	5.35E+06	5.11E+06
PC(22:6_22:6)	PC	877.5622	1.01E+07	8.69E+06	7.35E+06	7.77E+06	7.01E+06	2.10E+07	1.59E+07	1.44E+07	5.33E+06	6.69E+06	5.53E+06
PC(23:5e)	PC	583.3638	1.13E+06	1.13E+06	1.18E+06	8.90E+05	8.57E+05	1.28E+06	1.28E+06	1.32E+06	1.29E+06	1.22E+06	1.08E+06
PC(24:5e)	PC	597.3794	3.20E+05	2.13E+05	3.54E+05	1.51E+05	1.75E+05	5.18E+05	4.74E+05	5.44E+05	3.52E+05	2.82E+05	3.04E+05
PC(28:1)	PC	675.4839	5.58E+05	4.35E+05	5.44E+05	3.78E+05	4.56E+05	1.17E+06	8.06E+05	6.84E+05	4.81E+05	5.31E+05	2.80E+05
PC(29:0)	PC	691.5152	9.40E+05	5.13E+05	9.58E+05	4.35E+05	6.24E+05	1.54E+06	1.20E+06	1.18E+06	9.80E+05	1.15E+06	1.18E+06
PC(29:5)	PC	681.437	1.08E+06	1.30E+06	1.17E+06	1.25E+06	1.81E+06	8.83E+05	5.43E+05	4.83E+05	1.49E+06	1.08E+06	7.60E+05
PC(30:2)	PC	701.4996	2.34E+07	2.34E+07	2.18E+07	1.98E+07	2.59E+07	4.52E+07	3.05E+07	2.79E+07	1.76E+07	1.63E+07	1.25E+07
PC(31:1)	PC	717.5309	2.49E+07	1.89E+07	2.00E+07	1.32E+07	1.99E+07	4.81E+07	3.82E+07	2.97E+07	2.15E+07	2.22E+07	2.84E+07
PC(31:2)	PC	715.5152	4.53E+05	3.35E+05	4.05E+05	2.98E+05	3.77E+05	9.74E+05	5.71E+05	5.23E+05	3.79E+05	4.06E+05	2.99E+05
PC(31:7)	PC	705.437	5.24E+05	4.77E+05	6.20E+05	4.31E+05	7.02E+05	8.76E+05	5.44E+05	4.16E+05	6.55E+05	5.46E+05	4.34E+05
PC(32:0)	PC	733.5622	3.88E+06	2.17E+06	3.80E+06	1.78E+06	2.43E+06	6.85E+06	5.72E+06	5.88E+06	2.75E+06	3.48E+06	5.11E+06
PC(32:5)	PC	723.4839	2.85E+06	3.77E+06	2.47E+06	2.42E+06	2.50E+06	5.23E+06	3.49E+06	3.50E+06	1.87E+06	2.14E+06	1.16E+06
PC(33:1)	PC	745.5622	3.73E+07	2.59E+07	2.82E+07	2.24E+07	2.57E+07	6.89E+07	4.33E+07	3.01E+07	1.94E+07	1.92E+07	3.05E+07
PC(34:1e)	PC	745.5985	9.86E+05	1.46E+06	9.88E+05	1.45E+06	1.04E+06	8.45E+05	9.53E+05	1.29E+06	5.69E+05	8.63E+05	8.09E+05
PC(34:7)	PC	747.4839	4.57E+05	6.59E+05	4.37E+05	4.75E+05	5.74E+05	6.89E+05	4.79E+05	4.56E+05	3.27E+05	3.70E+05	1.53E+05

PC(36:2e)	PC	771.6142	2.35E+06	3.21E+06	1.90E+06	2.88E+06	2.25E+06	2.29E+06	2.50E+06	3.24E+06	1.57E+06	1.78E+06	2.00E+06
PC(36:3)	PC	783.5778	4.53E+06	4.23E+06	4.57E+06	2.63E+06	2.34E+06	9.25E+06	5.93E+06	5.70E+06	3.13E+06	5.37E+06	3.57E+06
PC(36:8)	PC	773.4996	5.17E+06	7.17E+06	4.68E+06	5.98E+06	6.72E+06	8.43E+06	5.82E+06	4.65E+06	3.02E+06	3.74E+06	2.29E+06
PC(36:9)	PC	771.4839	3.31E+06	5.13E+06	3.27E+06	2.19E+06	2.08E+06	7.14E+06	4.60E+06	4.12E+06	1.79E+06	2.26E+06	1.48E+06
PC(37:5)	PC	793.5622	5.47E+06	4.37E+06	4.17E+06	3.70E+06	4.18E+06	7.60E+06	7.17E+06	6.35E+06	4.39E+06	6.15E+06	6.97E+06
PC(37:6)	PC	791.5465	1.54E+07	1.57E+07	1.46E+07	1.46E+07	1.53E+07	2.11E+07	1.76E+07	1.53E+07	1.24E+07	1.42E+07	1.77E+07
PC(38:5)	PC	807.5778	8.99E+06	4.11E+06	9.11E+06	3.42E+06	4.40E+06	1.90E+07	1.31E+07	1.26E+07	8.48E+06	8.36E+06	9.16E+06
PC(40:10)	PC	825.5309	8.24E+06	8.47E+06	7.66E+06	8.06E+06	7.45E+06	1.57E+07	1.15E+07	1.07E+07	4.99E+06	5.56E+06	4.73E+06
PC(40:6)	PC	833.5935	6.64E+05	2.64E+05	6.39E+05	2.10E+05	2.70E+05	1.31E+06	8.79E+05	9.26E+05	8.84E+05	7.64E+05	6.45E+05
PC(40:6e)	PC	819.6142	3.08E+06	2.55E+06	2.55E+06	2.06E+06	1.88E+06	4.84E+06	4.21E+06	3.95E+06	1.92E+06	2.43E+06	3.82E+06
PC(40:7)	PC	831.5778	5.37E+06	3.25E+06	5.16E+06	2.81E+06	2.97E+06	1.04E+07	7.17E+06	6.75E+06	5.37E+06	6.06E+06	5.32E+06
PC(42:11)	PC	851.5465	2.32E+06	9.34E+05	2.41E+06	9.19E+05	1.14E+06	6.12E+06	3.68E+06	3.05E+06	1.88E+06	2.47E+06	2.41E+06
PC(42:9)	PC	855.5778	3.50E+06	1.02E+06	3.34E+06	9.03E+05	1.19E+06	6.60E+06	4.87E+06	3.78E+06	3.88E+06	4.23E+06	5.09E+06
PC(44:10)	PC	881.5935	4.52E+05	1.94E+05	4.30E+05	1.22E+05	1.48E+05	7.76E+05	6.18E+05	5.37E+05	5.78E+05	5.40E+05	6.80E+05
PE(16:0_16:1)	PE	689.4996	2.05E+06	2.09E+06	2.21E+06	1.62E+06	1.14E+06	3.49E+06	3.03E+06	3.57E+06	1.25E+06	1.77E+06	1.45E+06
PE(16:1_16:1)	PE	687.4839	1.47E+06	1.90E+06	1.56E+06	1.32E+06	7.55E+05	2.77E+06	2.33E+06	2.61E+06	6.64E+05	9.36E+05	7.19E+05
PE(18:1_18:2)	PE	741.5309	6.82E+05	5.83E+05	7.29E+05	4.93E+05	3.00E+05	1.55E+06	7.70E+05	9.30E+05	3.74E+05	1.16E+06	4.12E+05
PE(18:1_22:6)	PE	789.5309	1.26E+06	4.73E+05	1.08E+06	5.41E+05	6.85E+05	2.19E+06	1.58E+06	2.01E+06	9.55E+05	1.14E+06	1.32E+06
PE(20:2_22:6)	PE	815.5465	3.82E+06	1.92E+06	4.22E+06	1.90E+06	2.66E+06	6.80E+06	5.15E+06	6.49E+06	4.19E+06	4.59E+06	4.11E+06
PE(20:4_22:6)	PE	811.5152	1.42E+06	6.06E+05	1.39E+06	6.38E+05	9.18E+05	2.63E+06	1.95E+06	2.56E+06	1.16E+06	1.39E+06	1.52E+06
PE(20:5_18:2)	PE	761.4996	7.86E+05	1.12E+06	7.59E+05	7.90E+05	9.67E+05	1.06E+06	8.12E+05	1.02E+06	5.59E+05	6.66E+05	6.80E+05
PE(20:5_20:5)	PE	783.4839	1.18E+06	1.60E+06	1.08E+06	1.18E+06	1.45E+06	1.61E+06	1.24E+06	1.55E+06	8.67E+05	1.01E+06	9.91E+05
PE(20:5_22:6)	PE	809.4996	1.22E+07	9.53E+06	1.18E+07	1.16E+07	1.26E+07	2.30E+07	1.56E+07	1.99E+07	5.62E+06	7.74E+06	7.61E+06
PE(22:5_22:6)	PE	837.5309	5.20E+06	2.56E+06	5.50E+06	2.37E+06	3.57E+06	9.12E+06	6.94E+06	8.89E+06	5.12E+06	5.48E+06	5.44E+06
PE(22:6_22:6)	PE	835.5152	5.65E+06	4.80E+06	5.68E+06	5.21E+06	5.60E+06	9.84E+06	7.48E+06	1.03E+07	3.32E+06	4.38E+06	3.35E+06
PE(30:1)	PE	661.4683	8.87E+05	8.46E+05	9.04E+05	6.42E+05	4.76E+05	1.61E+06	1.09E+06	1.38E+06	5.18E+05	1.17E+06	6.61E+05
PE(33:2)	PE	701.4996	5.54E+05	4.75E+05	5.91E+05	3.72E+05	3.06E+05	8.97E+05	7.08E+05	1.07E+06	3.61E+05	5.19E+05	5.37E+05
PE(36:2)	PE	743.5465	6.77E+05	4.35E+05	6.60E+05	3.98E+05	2.52E+05	1.30E+06	7.86E+05	1.02E+06	4.12E+05	1.19E+06	5.11E+05
PE(44:10)	PE	839.5465	4.15E+05	1.01E+05	4.31E+05	8.24E+04	1.67E+05	6.71E+05	4.89E+05	6.25E+05	5.58E+05	5.12E+05	6.57E+05
PG(14:0_14:0)	PG	666.4472	2.64E+06	1.53E+06	3.21E+06	1.20E+06	1.76E+06	4.07E+06	3.31E+06	3.99E+06	2.94E+06	3.18E+06	2.87E+06
PG(16:0_14:0)	PG	694.4785	4.89E+06	3.54E+06	5.14E+06	2.76E+06	4.09E+06	7.46E+06	5.81E+06	6.42E+06	4.52E+06	4.57E+06	5.70E+06
PG(16:0_16:0)	PG	722.5098	1.49E+06	1.43E+06	1.28E+06	1.20E+06	1.71E+06	2.12E+06	1.52E+06	1.62E+06	1.17E+06	1.18E+06	1.75E+06
PG(16:0_16:1)	PG	720.4941	2.69E+07	2.31E+07	2.49E+07	1.90E+07	2.61E+07	3.75E+07	2.96E+07	3.39E+07	2.10E+07	1.89E+07	2.37E+07
PG(16:0_18:2)	PG	746.5098	4.38E+07	4.06E+07	4.15E+07	3.70E+07	4.62E+07	3.04E+07	3.31E+07	2.52E+07	5.13E+07	6.15E+07	5.51E+07
PG(16:0_20:4)	PG	770.5098	1.76E+06	1.10E+06	1.71E+06	7.66E+05	1.33E+06	1.26E+06	1.23E+06	1.07E+06	2.93E+06	3.14E+06	3.21E+06
PG(16:0_20:5)	PG	768.4941	8.99E+07	1.03E+08	9.78E+07	8.49E+07	1.16E+08	8.32E+07	7.29E+07	5.86E+07	1.00E+08	1.17E+08	1.16E+08
PG(16:1_14:0)	PG	692.4628	1.33E+07	1.27E+07	1.47E+07	9.50E+06	1.25E+07	1.92E+07	1.54E+07	1.74E+07	1.13E+07	1.11E+07	1.20E+07
PG(16:1_16:1)	PG	718.4785	6.69E+06	6.96E+06	4.83E+06	5.29E+06	6.49E+06	9.11E+06	7.71E+06	8.46E+06	3.68E+06	3.92E+06	5.13E+06
PG(16:1_18:1)	PG	746.5098	4.38E+07	4.07E+07	4.15E+07	3.70E+07	4.62E+07	3.05E+07	3.31E+07	2.52E+07	5.13E+07	6.15E+07	5.51E+07
PG(16:1_18:2)	PG	744.4941	2.39E+06	1.62E+06	2.48E+06	1.19E+06	1.48E+06	3.64E+06	2.84E+06	3.19E+06	2.15E+06	2.59E+06	3.07E+06
PG(16:1_20:5)	PG	766.4785	2.96E+07	1.91E+07	3.32E+07	1.49E+07	1.54E+07	5.71E+07	5.07E+07	5.39E+07	1.69E+07	2.03E+07	2.38E+07
PG(16:1_22:6)	PG	792.4941	9.83E+06	8.16E+06	1.04E+07	5.87E+06	7.42E+06	1.62E+07	1.34E+07	1.43E+07	7.12E+06	7.70E+06	1.01E+07

PG(18:1_18:1)	PG	774.5411	1.21E+06	1.49E+06	1.34E+06	9.05E+05	7.15E+05	1.75E+06	1.15E+06	1.17E+06	8.23E+05	2.13E+06	9.90E+05
PG(18:2_22:6)	PG	818.5098	9.50E+05	3.85E+05	8.89E+05	2.87E+05	4.67E+05	1.33E+06	1.04E+06	1.16E+06	6.75E+05	1.17E+06	2.14E+06
PG(18:4_16:1)	PG	740.4628	7.69E+07	6.45E+07	8.19E+07	5.01E+07	6.39E+07	1.22E+08	9.03E+07	8.08E+07	8.26E+07	8.31E+07	9.29E+07
PG(18:4_20:5)	PG	788.4628	5.54E+05	4.77E+05	5.74E+05	3.38E+05	4.86E+05	8.85E+05	6.80E+05	7.12E+05	3.78E+05	4.85E+05	5.74E+05
PG(20:4_22:6)	PG	842.5098	9.20E+05	3.55E+05	9.04E+05	2.57E+05	4.57E+05	1.41E+06	1.05E+06	1.02E+06	8.08E+05	1.13E+06	2.30E+06
PG(20:5_20:4)	PG	816.4941	6.91E+05	1.92E+05	7.71E+05	1.25E+05	2.86E+05	1.08E+06	7.80E+05	7.34E+05	5.44E+05	8.52E+05	1.73E+06
PG(20:5_20:5)	PG	814.4785	2.54E+07	2.09E+07	2.41E+07	1.40E+07	1.83E+07	3.14E+07	3.18E+07	2.79E+07	2.75E+07	3.27E+07	2.84E+07
PG(20:5_22:6)	PG	840.4941	2.44E+06	1.60E+06	2.43E+06	1.16E+06	1.80E+06	3.83E+06	3.11E+06	3.04E+06	1.56E+06	2.18E+06	3.56E+06
PG(22:6_22:6)	PG	866.5098	1.53E+06	1.03E+06	1.60E+06	7.14E+05	1.03E+06	2.43E+06	2.02E+06	2.10E+06	9.89E+05	1.49E+06	2.42E+06
PG(30:2)	PG	690.4472	5.21E+05	6.98E+05	6.08E+05	4.87E+05	6.53E+05	5.91E+05	5.77E+05	6.68E+05	4.54E+05	4.43E+05	3.86E+05
PG(31:1)	PG	706.4785	9.00E+05	1.36E+06	1.02E+06	1.18E+06	1.25E+06	1.04E+06	8.21E+05	8.29E+05	6.06E+05	6.21E+05	7.60E+05
PG(32:3)	PG	716.4628	5.51E+05	9.11E+05	6.59E+05	6.57E+05	7.53E+05	6.78E+05	5.74E+05	6.86E+05	3.44E+05	3.34E+05	3.20E+05
PG(32:3)	PG	716.4628	4.65E+06	3.19E+06	4.99E+06	2.54E+06	3.83E+06	6.82E+06	5.42E+06	6.05E+06	4.33E+06	4.38E+06	5.29E+06
PG(33:1)	PG	734.5098	1.86E+08	1.57E+08	1.78E+08	1.23E+08	1.52E+08	2.82E+08	2.30E+08	2.05E+08	1.89E+08	1.94E+08	2.12E+08
PG(37:1)	PG	790.5724	9.68E+05	1.02E+06	8.29E+05	9.65E+05	1.26E+06	1.64E+06	7.98E+05	6.86E+05	6.44E+05	5.72E+05	1.04E+06
PI(15:0_16:0)	PI	796.5102	9.67E+07	9.87E+07	1.18E+08	9.57E+07	1.01E+08	1.35E+08	1.13E+08	9.14E+07	6.89E+07	9.32E+07	1.12E+08
PI(16:0_14:0)	PI	782.4945	1.26E+06	1.97E+06	8.69E+05	1.53E+06	1.86E+06	1.32E+06	1.08E+06	8.06E+05	9.17E+05	1.01E+06	1.10E+06
PI(16:0_16:1)	PI	808.5102	5.68E+06	4.48E+06	7.61E+06	4.55E+06	4.60E+06	1.14E+07	7.93E+06	7.43E+06	3.86E+06	4.53E+06	4.27E+06
PI(16:1_14:0)	PI	780.4789	1.98E+06	2.21E+06	1.48E+06	1.45E+06	2.06E+06	3.09E+06	2.37E+06	1.98E+06	1.50E+06	1.72E+06	1.70E+06
PI(29:0)	PI	768.4789	1.41E+07	2.12E+07	2.36E+07	1.64E+07	1.70E+07	2.26E+07	1.74E+07	1.56E+07	9.80E+06	1.17E+07	1.28E+07
PI(38:2)	PI	890.5884	9.23E+06	9.69E+06	9.14E+06	9.16E+06	9.62E+06	1.67E+07	1.06E+07	1.03E+07	5.35E+06	5.71E+06	7.58E+06
PI(39:1)	PI	906.6197	8.61E+06	5.66E+06	9.67E+06	4.80E+06	6.21E+06	1.92E+07	1.22E+07	1.09E+07	6.20E+06	9.31E+06	1.01E+07
PI(41:1)	PI	934.651	1.13E+06	9.33E+05	1.18E+06	8.27E+05	9.92E+05	1.55E+06	1.17E+06	9.67E+05	1.03E+06	1.33E+06	1.62E+06
TG(10:0_14:0_20:4)	TG	742.6111	5.19E+06	3.19E+06	4.74E+06	2.03E+06	2.17E+06	1.19E+07	6.74E+06	8.05E+06	2.69E+06	3.71E+06	4.45E+06
TG(12:0e_10:1_10:3)	TG	560.4441	2.57E+07	4.51E+07	2.67E+07	4.12E+07	3.92E+07	2.42E+07	1.86E+07	1.71E+07	1.40E+07	1.54E+07	2.10E+07
TG(12:0e_10:2_10:3)	TG	558.4284	2.71E+07	3.34E+07	2.79E+07	2.99E+07	3.32E+07	3.65E+07	2.86E+07	2.66E+07	1.95E+07	2.11E+07	2.60E+07
TG(12:1e_10:1_10:1)	TG	562.4597	7.62E+06	1.05E+07	7.67E+06	9.55E+06	9.90E+06	9.46E+06	7.41E+06	7.16E+06	4.86E+06	4.89E+06	6.91E+06
TG(12:1e_10:3_10:3)	TG	554.3971	3.79E+06	4.45E+06	3.53E+06	2.43E+06	2.57E+06	5.31E+06	4.36E+06	3.48E+06	4.13E+06	4.33E+06	4.03E+06
TG(14:0_10:1_22:6)	TG	764.5955	3.09E+06	2.47E+06	2.91E+06	1.90E+06	1.83E+06	5.90E+06	3.44E+06	4.53E+06	1.73E+06	2.41E+06	2.57E+06
TG(14:0_14:0_14:0)	TG	722.6424	9.50E+06	7.05E+06	8.06E+06	6.50E+06	7.90E+06	1.53E+07	9.63E+06	1.12E+07	7.06E+06	9.95E+06	1.24E+07
TG(14:0_14:0_14:2)	TG	718.6111	9.11E+05	1.48E+06	8.74E+05	1.22E+06	9.38E+05	1.51E+06	8.35E+05	9.17E+05	5.18E+05	5.80E+05	5.63E+05
TG(14:0_14:1_16:1)	TG	746.6424	3.57E+07	3.65E+07	3.11E+07	3.43E+07	3.74E+07	6.47E+07	3.68E+07	4.35E+07	1.64E+07	2.22E+07	3.05E+07
TG(14:0_14:3_22:6)	TG	816.6268	5.19E+06	7.44E+06	4.42E+06	2.66E+06	2.43E+06	9.66E+06	5.97E+06	7.62E+06	2.32E+06	4.11E+06	4.40E+06
TG(14:0_18:3_20:5)	TG	846.6737	4.26E+07	5.42E+07	3.71E+07	4.43E+07	4.82E+07	7.08E+07	4.33E+07	5.48E+07	1.30E+07	2.64E+07	4.19E+07
TG(14:0_20:4_20:5)	TG	872.6894	2.30E+07	2.09E+07	2.03E+07	1.47E+07	1.66E+07	3.96E+07	2.37E+07	2.77E+07	8.18E+06	2.02E+07	3.82E+07
TG(14:0_20:5_14:0)	TG	796.6581	1.07E+08	1.21E+08	9.25E+07	1.14E+08	1.09E+08	1.94E+08	1.10E+08	1.40E+08	3.45E+07	5.92E+07	9.14E+07
TG(15:0_14:1_16:1)	TG	760.6581	4.83E+06	5.53E+06	4.35E+06	5.53E+06	5.49E+06	8.32E+06	4.82E+06	5.29E+06	2.57E+06	3.39E+06	4.01E+06
TG(15:0_16:0_18:1)	TG	818.7363	7.33E+06	8.51E+06	7.41E+06	9.67E+06	8.48E+06	1.06E+07	7.09E+06	7.12E+06	5.01E+06	5.82E+06	6.22E+06
TG(15:0_16:0_20:5)	TG	838.705	1.87E+06	1.95E+06	1.53E+06	1.48E+06	1.66E+06	3.18E+06	1.82E+06	2.29E+06	7.12E+05	1.36E+06	2.80E+06
TG(15:0_16:0_24:0)	TG	904.8459	1.32E+06	1.41E+06	1.08E+06	1.34E+06	1.33E+06	1.54E+06	1.38E+06	1.30E+06	1.30E+06	1.33E+06	1.27E+06
TG(15:0_16:1_16:0)	TG	790.705	1.80E+07	2.07E+07	1.59E+07	2.32E+07	2.33E+07	2.80E+07	1.72E+07	1.92E+07	8.98E+06	1.14E+07	1.63E+07
TG(15:0_16:1_20:5)	TG	836.6894	4.70E+06	4.93E+06	4.18E+06	4.20E+06	4.54E+06	7.53E+06	4.99E+06	5.96E+06	1.74E+06	3.56E+06	5.91E+06

TG(15:0_16:1_22:5)	TG	864.7207	1.37E+06	1.65E+06	1.22E+06	1.07E+06	1.05E+06	2.30E+06	1.21E+06	1.44E+06	5.39E+05	1.13E+06	1.91E+06
TG(15:0_16:1_24:0)	TG	902.8302	5.00E+05	5.98E+05	4.58E+05	5.56E+05	4.85E+05	6.78E+05	4.89E+05	4.26E+05	3.84E+05	4.57E+05	4.05E+05
TG(15:0_17:0_21:0)	TG	876.8146	1.33E+06	1.36E+06	1.17E+06	1.33E+06	1.32E+06	1.53E+06	1.35E+06	1.26E+06	1.28E+06	1.31E+06	1.25E+06
TG(16:0_12:0_13:0)	TG	708.6268	1.03E+06	1.07E+06	9.22E+05	1.01E+06	1.01E+06	1.15E+06	1.05E+06	1.02E+06	1.07E+06	1.08E+06	9.76E+05
TG(16:0_14:0_14:0)	TG	750.6737	2.97E+07	2.69E+07	2.74E+07	2.31E+07	2.66E+07	4.40E+07	2.89E+07	3.39E+07	1.96E+07	2.54E+07	3.72E+07
TG(16:0_14:0_20:5)	TG	824.6894	9.92E+07	8.05E+07	8.66E+07	7.44E+07	8.09E+07	1.72E+08	1.02E+08	1.27E+08	3.57E+07	7.05E+07	1.41E+08
TG(16:0_16:0_14:0)	TG	778.705	4.25E+07	3.89E+07	4.16E+07	3.86E+07	4.28E+07	6.06E+07	4.05E+07	4.57E+07	2.95E+07	3.56E+07	5.08E+07
TG(16:0_16:0_20:4)	TG	854.7363	1.72E+07	1.60E+07	1.61E+07	1.30E+07	1.28E+07	3.00E+07	1.65E+07	2.10E+07	7.59E+06	1.13E+07	2.70E+07
TG(16:0_16:0_22:5)	TG	880.752	8.44E+06	9.20E+06	8.26E+06	4.53E+06	4.35E+06	1.64E+07	7.40E+06	8.66E+06	4.67E+06	4.68E+06	1.81E+07
TG(16:0_16:1_16:0)	TG	804.7207	1.65E+08	1.67E+08	1.27E+08	1.86E+08	1.92E+08	2.73E+08	1.63E+08	2.03E+08	6.88E+07	8.85E+07	1.58E+08
TG(16:0_16:1_18:1)	TG	830.7363	3.44E+07	4.27E+07	2.85E+07	3.95E+07	3.70E+07	5.71E+07	3.05E+07	3.72E+07	1.40E+07	1.84E+07	3.55E+07
TG(16:0_16:1_20:4)	TG	852.7207	5.43E+07	4.29E+07	5.23E+07	3.37E+07	3.78E+07	9.92E+07	5.80E+07	7.44E+07	1.88E+07	3.83E+07	8.88E+07
TG(16:0_16:1_22:6)	TG	876.7207	3.71E+07	3.16E+07	3.16E+07	2.73E+07	2.89E+07	5.91E+07	4.05E+07	4.91E+07	1.41E+07	3.01E+07	5.53E+07
TG(16:0_16:1_24:0)	TG	916.8459	1.74E+06	2.37E+06	1.31E+06	2.07E+06	2.05E+06	2.91E+06	1.56E+06	1.48E+06	8.86E+05	9.98E+05	1.26E+06
TG(16:0_17:0_18:1)	TG	846.7676	2.86E+06	3.51E+06	2.83E+06	3.63E+06	2.84E+06	4.38E+06	2.64E+06	2.60E+06	2.04E+06	2.26E+06	2.28E+06
TG(16:0_17:1_18:1)	TG	844.752	4.32E+06	5.69E+06	4.25E+06	5.54E+06	4.43E+06	6.51E+06	4.03E+06	4.23E+06	2.86E+06	3.13E+06	3.66E+06
TG(16:0_18:1_16:0)	TG	832.752	2.01E+07	2.80E+07	2.12E+07	2.07E+07	2.02E+07	3.64E+07	1.85E+07	2.13E+07	1.06E+07	1.20E+07	1.78E+07
TG(16:0_18:1_18:1)	TG	858.7676	1.78E+07	2.87E+07	1.57E+07	1.30E+07	1.20E+07	3.72E+07	1.36E+07	1.37E+07	9.84E+06	9.16E+06	1.93E+07
TG(16:0_18:1_19:0)	TG	874.7989	8.66E+05	1.28E+06	8.36E+05	9.94E+05	7.29E+05	1.50E+06	7.50E+05	6.63E+05	6.19E+05	6.85E+05	6.44E+05
TG(16:0_18:1_22:5)	TG	906.7676	3.19E+06	5.49E+06	3.18E+06	1.36E+06	1.29E+06	7.55E+06	2.17E+06	2.36E+06	1.69E+06	1.39E+06	6.15E+06
TG(16:0_18:2_22:6)	TG	902.7363	7.12E+06	5.85E+06	7.00E+06	3.87E+06	4.07E+06	1.12E+07	6.85E+06	8.09E+06	3.46E+06	7.03E+06	1.55E+07
TG(16:0_18:3_16:1)	TG	826.705	6.43E+07	6.91E+07	6.23E+07	6.82E+07	6.62E+07	1.05E+08	6.21E+07	7.74E+07	2.23E+07	4.01E+07	8.22E+07
TG(16:0_20:1_18:1)	TG	886.7989	8.01E+06	1.48E+07	7.80E+06	6.15E+06	5.59E+06	1.77E+07	6.30E+06	6.01E+06	4.32E+06	4.08E+06	9.04E+06
TG(16:0_20:5_20:5)	TG	898.705	2.97E+07	2.10E+07	2.55E+07	1.40E+07	1.72E+07	5.13E+07	3.34E+07	3.63E+07	1.09E+07	2.80E+07	5.57E+07
TG(16:0_22:5_22:6)	TG	952.752	1.66E+06	9.77E+05	1.34E+06	6.78E+05	9.72E+05	2.40E+06	1.59E+06	1.77E+06	8.72E+05	1.68E+06	3.96E+06
TG(16:1_10:1_21:1)	TG	786.6737	8.30E+06	1.07E+07	6.96E+06	1.11E+07	1.11E+07	1.27E+07	7.38E+06	8.59E+06	3.04E+06	4.29E+06	6.43E+06
TG(16:1_10:2_22:6)	TG	788.5955	1.38E+06	4.56E+06	1.24E+06	6.50E+05	5.39E+05	2.65E+06	1.20E+06	1.68E+06	3.44E+05	6.50E+05	6.34E+05
TG(16:1_12:0_14:0)	TG	720.6268	3.47E+06	4.05E+06	3.07E+06	3.57E+06	3.21E+06	6.09E+06	3.52E+06	3.84E+06	1.91E+06	2.35E+06	2.85E+06
TG(16:1_14:0_14:0)	TG	748.6581	1.66E+08	1.47E+08	1.41E+08	1.38E+08	1.58E+08	2.76E+08	1.72E+08	2.01E+08	8.39E+07	1.20E+08	1.93E+08
TG(16:1_14:0_14:2)	TG	744.6268	1.14E+07	1.53E+07	1.04E+07	1.34E+07	1.45E+07	1.92E+07	1.00E+07	1.22E+07	4.97E+06	7.06E+06	9.43E+06
TG(16:1_14:0_15:0)	TG	762.6737	1.38E+07	1.38E+07	1.14E+07	1.39E+07	1.51E+07	2.23E+07	1.40E+07	1.45E+07	6.56E+06	9.02E+06	1.33E+07
TG(16:1_14:0_16:0)	TG	776.6894	3.44E+08	3.29E+08	2.75E+08	3.34E+08	3.53E+08	5.46E+08	3.41E+08	4.19E+08	1.58E+08	2.04E+08	3.78E+08
TG(16:1_14:0_16:1)	TG	774.6737	4.56E+08	4.88E+08	3.85E+08	4.86E+08	4.97E+08	7.26E+08	4.49E+08	5.36E+08	1.78E+08	2.51E+08	4.45E+08
TG(16:1_14:1_16:1)	TG	772.6581	1.67E+08	2.10E+08	1.49E+08	2.03E+08	2.07E+08	2.77E+08	1.62E+08	1.99E+08	6.21E+07	8.52E+07	1.33E+08
TG(16:1_14:1_20:5)	TG	820.6581	2.52E+07	2.95E+07	2.24E+07	2.23E+07	2.47E+07	4.45E+07	2.69E+07	3.39E+07	8.84E+06	1.69E+07	2.47E+07
TG(16:1_16:1_15:0)	TG	788.6894	2.27E+07	2.77E+07	1.88E+07	3.03E+07	2.93E+07	3.44E+07	2.04E+07	2.34E+07	8.23E+06	1.17E+07	1.81E+07
TG(16:1_16:1_16:0)	TG	802.705	4.88E+08	5.34E+08	4.32E+08	6.36E+08	6.00E+08	7.53E+08	4.36E+08	5.55E+08	1.38E+08	1.99E+08	4.26E+08
TG(16:1_16:1_16:1)	TG	800.6894	3.85E+08	4.74E+08	3.19E+08	5.24E+08	4.95E+08	5.85E+08	3.54E+08	4.42E+08	1.10E+08	1.63E+08	3.04E+08
TG(16:1_16:1_17:1)	TG	814.705	6.72E+06	8.20E+06	5.97E+06	8.55E+06	8.09E+06	1.01E+07	6.28E+06	7.03E+06	2.83E+06	3.98E+06	6.12E+06
TG(16:1_16:1_18:1)	TG	828.7207	5.11E+07	5.72E+07	4.57E+07	6.09E+07	5.52E+07	7.94E+07	4.55E+07	5.75E+07	1.68E+07	2.76E+07	5.97E+07
TG(16:1_16:1_20:4)	TG	850.705	1.45E+08	1.22E+08	1.21E+08	1.15E+08	1.27E+08	2.39E+08	1.61E+08	2.02E+08	5.05E+07	9.82E+07	1.93E+08
TG(16:1_16:1_20:5)	TG	848.6894	1.51E+08	1.51E+08	1.33E+08	1.34E+08	1.43E+08	2.50E+08	1.63E+08	2.05E+08	4.51E+07	9.90E+07	1.81E+08

TG(16:1_17:1_18:1)	TG	842.7363	3.56E+06	4.94E+06	3.43E+06	4.37E+06	3.73E+06	5.55E+06	3.44E+06	3.92E+06	2.00E+06	2.30E+06	3.04E+06
TG(16:1_18:1_18:1)	TG	856.752	1.46E+07	2.03E+07	1.40E+07	1.29E+07	1.19E+07	2.59E+07	1.32E+07	1.49E+07	8.22E+06	8.68E+06	1.98E+07
TG(16:1_18:1_20:4)	TG	878.7363	2.20E+07	2.18E+07	2.23E+07	1.45E+07	1.59E+07	3.90E+07	2.28E+07	2.71E+07	9.64E+06	1.61E+07	3.67E+07
TG(16:1_18:2_20:5)	TG	874.705	3.61E+07	3.30E+07	3.20E+07	2.86E+07	2.92E+07	5.55E+07	3.75E+07	4.58E+07	1.31E+07	3.11E+07	5.63E+07
TG(16:1_20:1_22:1)	TG	940.8459	1.97E+06	3.39E+06	1.79E+06	1.96E+06	1.99E+06	3.82E+06	1.26E+06	1.28E+06	9.65E+05	6.74E+05	2.59E+06
TG(16:1_20:5_20:5)	TG	896.6894	3.92E+07	4.55E+07	3.42E+07	2.39E+07	2.82E+07	6.84E+07	4.46E+07	4.99E+07	1.25E+07	3.31E+07	5.45E+07
TG(16:1_22:5_22:6)	TG	950.7363	7.02E+06	5.89E+06	6.12E+06	3.87E+06	4.48E+06	1.08E+07	6.63E+06	7.43E+06	3.21E+06	7.30E+06	1.52E+07
TG(17:0_18:1_18:1)	TG	872.7833	1.15E+06	1.84E+06	9.98E+05	1.22E+06	8.50E+05	2.24E+06	8.89E+05	7.91E+05	7.43E+05	7.79E+05	9.95E+05
TG(18:0_16:0_18:1)	TG	860.7833	5.30E+06	9.09E+06	5.18E+06	4.90E+06	4.20E+06	1.08E+07	4.31E+06	4.47E+06	3.55E+06	3.57E+06	4.83E+06
TG(18:0_16:0_20:1)	TG	888.8146	2.76E+06	4.60E+06	2.81E+06	2.86E+06	2.63E+06	5.20E+06	2.39E+06	2.35E+06	1.60E+06	1.76E+06	2.22E+06
TG(18:1_17:1_18:1)	TG	870.7676	1.06E+06	1.64E+06	9.13E+05	1.13E+06	8.64E+05	1.91E+06	8.54E+05	7.88E+05	7.23E+05	7.33E+05	1.12E+06
TG(18:1_18:1_18:1)	TG	884.7833	1.43E+07	2.05E+07	1.21E+07	9.73E+06	8.75E+06	2.69E+07	1.22E+07	1.02E+07	9.44E+06	7.97E+06	2.18E+07
TG(18:1_18:1_18:2)	TG	882.7676	8.71E+06	8.66E+06	8.01E+06	6.12E+06	5.33E+06	1.37E+07	8.17E+06	7.57E+06	7.03E+06	5.30E+06	1.90E+07
TG(18:1_18:1_20:5)	TG	904.752	4.83E+06	6.60E+06	4.60E+06	2.38E+06	2.35E+06	1.01E+07	3.90E+06	4.28E+06	2.57E+06	2.95E+06	9.64E+06
TG(18:1_18:1_22:6)	TG	930.7676	1.39E+06	1.93E+06	1.24E+06	4.66E+05	4.30E+05	2.88E+06	9.06E+05	8.98E+05	9.48E+05	6.39E+05	3.42E+06
TG(18:1_18:2_22:1)	TG	938.8302	1.08E+06	1.43E+06	9.31E+05	1.03E+06	9.65E+05	1.48E+06	7.70E+05	6.84E+05	6.62E+05	3.90E+05	2.16E+06
TG(18:1_20:4_20:5)	TG	926.7363	1.06E+06	1.51E+06	9.51E+05	4.31E+05	3.95E+05	1.95E+06	7.64E+05	8.50E+05	6.65E+05	6.62E+05	2.44E+06
TG(18:4_14:0_14:0)	TG	770.6424	6.31E+07	7.53E+07	5.04E+07	6.69E+07	6.99E+07	1.06E+08	5.98E+07	7.14E+07	2.36E+07	3.42E+07	4.71E+07
TG(18:4_14:0_14:1)	TG	768.6268	2.86E+07	2.60E+07	2.61E+07	2.08E+07	2.08E+07	6.36E+07	3.51E+07	4.40E+07	1.16E+07	1.68E+07	2.06E+07
TG(18:4_14:0_14:2)	TG	766.6111	4.33E+06	5.29E+06	4.23E+06	4.88E+06	5.16E+06	6.02E+06	3.70E+06	4.55E+06	2.21E+06	2.98E+06	3.66E+06
TG(18:4_14:0_15:0)	TG	784.6581	4.57E+06	4.54E+06	4.28E+06	4.51E+06	4.55E+06	6.20E+06	4.40E+06	5.11E+06	2.33E+06	3.05E+06	4.69E+06
TG(18:4_14:0_16:0)	TG	798.6737	1.85E+08	2.51E+08	1.62E+08	2.51E+08	2.37E+08	2.91E+08	1.66E+08	2.13E+08	5.25E+07	8.09E+07	1.43E+08
TG(18:4_14:0_18:4)	TG	818.6424	1.11E+07	1.68E+07	1.10E+07	1.12E+07	1.19E+07	1.85E+07	1.01E+07	1.26E+07	4.19E+06	8.35E+06	1.05E+07
TG(18:4_14:0_20:5)	TG	844.6581	2.48E+07	3.42E+07	2.23E+07	2.21E+07	2.30E+07	4.35E+07	2.49E+07	3.11E+07	8.25E+06	1.69E+07	2.23E+07
TG(18:4_14:1_16:1)	TG	794.6424	2.71E+07	3.47E+07	2.48E+07	2.97E+07	2.71E+07	5.14E+07	2.91E+07	3.89E+07	8.58E+06	1.36E+07	1.76E+07
TG(18:4_14:1_20:5)	TG	842.6424	7.23E+06	1.16E+07	6.35E+06	5.01E+06	4.82E+06	1.24E+07	8.12E+06	1.08E+07	2.52E+06	4.73E+06	5.29E+06
TG(18:4_14:2_16:1)	TG	792.6268	6.97E+06	1.06E+07	6.20E+06	7.27E+06	6.70E+06	1.30E+07	6.89E+06	9.52E+06	2.25E+06	3.59E+06	4.22E+06
TG(18:4_14:2_18:4)	TG	814.6111	4.69E+06	6.98E+06	4.37E+06	5.41E+06	4.76E+06	7.34E+06	4.51E+06	6.38E+06	1.63E+06	2.51E+06	2.81E+06
TG(18:4_14:2_20:5)	TG	840.6268	6.73E+06	9.77E+06	6.46E+06	7.06E+06	7.05E+06	9.16E+06	5.76E+06	7.35E+06	2.72E+06	5.22E+06	6.41E+06
TG(18:4_14:4_16:0)	TG	790.6111	3.77E+06	8.27E+06	3.34E+06	2.55E+06	2.28E+06	7.25E+06	3.30E+06	4.42E+06	1.03E+06	1.98E+06	2.13E+06
TG(18:4_15:0_16:1)	TG	810.6737	6.85E+06	8.24E+06	6.23E+06	9.19E+06	8.86E+06	8.88E+06	5.98E+06	7.08E+06	2.70E+06	3.87E+06	6.05E+06
TG(18:4_16:0_22:5)	TG	900.7207	3.86E+06	3.78E+06	3.90E+06	2.25E+06	2.33E+06	6.40E+06	3.67E+06	4.36E+06	1.82E+06	2.77E+06	7.28E+06
TG(18:4_16:1_16:1)	TG	822.6737	1.30E+08	1.09E+08	1.15E+08	9.52E+07	1.03E+08	2.26E+08	1.51E+08	1.74E+08	4.85E+07	9.56E+07	1.74E+08
TG(18:4_16:1_20:5)	TG	870.6737	2.27E+07	2.71E+07	1.99E+07	1.31E+07	1.54E+07	4.22E+07	2.44E+07	2.68E+07	7.21E+06	1.89E+07	3.09E+07
TG(18:4_18:4_20:5)	TG	892.6581	1.17E+07	1.43E+07	1.05E+07	7.51E+06	8.29E+06	1.80E+07	1.15E+07	1.31E+07	4.02E+06	1.01E+07	1.57E+07
TG(18:4_20:4_20:5)	TG	920.6894	1.26E+07	9.52E+06	1.12E+07	6.53E+06	7.65E+06	1.77E+07	1.31E+07	1.47E+07	5.34E+06	1.27E+07	2.20E+07
TG(18:4_20:5_20:5)	TG	918.6737	1.66E+07	1.91E+07	1.62E+07	1.13E+07	1.23E+07	2.26E+07	1.72E+07	2.00E+07	5.97E+06	1.52E+07	2.28E+07
TG(19:1_14:0_16:1)	TG	816.7207	8.07E+06	9.80E+06	7.08E+06	1.07E+07	9.57E+06	1.18E+07	7.78E+06	8.45E+06	4.58E+06	5.44E+06	6.77E+06
TG(20:1_18:1_18:1)	TG	912.8146	4.12E+06	8.16E+06	3.57E+06	2.89E+06	2.68E+06	9.54E+06	2.57E+06	2.39E+06	1.85E+06	1.28E+06	5.48E+06
TG(20:1_18:1_18:2)	TG	910.7989	2.58E+06	3.03E+06	2.23E+06	1.74E+06	1.50E+06	4.12E+06	2.03E+06	1.77E+06	1.90E+06	1.14E+06	6.17E+06
TG(20:1_18:1_18:3)	TG	908.7833	1.57E+06	2.36E+06	1.40E+06	6.18E+05	4.85E+05	3.16E+06	9.51E+05	8.91E+05	1.00E+06	4.19E+05	4.35E+06
TG(20:1_18:1_22:6)	TG	958.7989	3.18E+05	7.27E+05	2.52E+05	8.93E+04	7.36E+04	9.71E+05	1.46E+05	1.22E+05	1.55E+05	6.51E+04	5.90E+05

TG(20:4e_16:1_16:1)	TG	836.7258	1.39E+06	1.62E+06	1.12E+06	1.73E+06	2.42E+06	6.59E+05	1.19E+06	7.26E+05	8.78E+05	2.16E+06	1.47E+06
TG(20:5_12:2_20:5)	TG	838.6111	1.51E+06	3.49E+06	1.33E+06	8.39E+05	8.22E+05	3.23E+06	1.10E+06	1.42E+06	3.75E+05	8.75E+05	1.04E+06
TG(20:5_12:3_20:5)	TG	836.5955	2.21E+06	1.03E+07	2.09E+06	1.04E+06	6.94E+05	3.37E+06	1.21E+06	1.64E+06	2.87E+05	6.64E+05	7.86E+05
TG(20:5_14:1_20:5)	TG	868.6581	3.36E+06	5.15E+06	3.08E+06	2.01E+06	2.05E+06	6.00E+06	3.57E+06	4.42E+06	1.19E+06	2.82E+06	3.80E+06
TG(20:5_14:1_22:6)	TG	894.6737	3.31E+06	5.38E+06	2.85E+06	2.45E+06	2.77E+06	4.67E+06	3.27E+06	4.01E+06	1.13E+06	2.72E+06	3.67E+06
TG(20:5_14:3_20:4)	TG	866.6424	1.41E+07	1.96E+07	1.30E+07	1.31E+07	1.31E+07	2.07E+07	1.32E+07	1.65E+07	5.03E+06	9.89E+06	1.28E+07
TG(20:5_14:3_20:5)	TG	864.6268	8.20E+06	1.25E+07	7.34E+06	5.53E+06	5.30E+06	1.41E+07	9.37E+06	1.23E+07	2.96E+06	5.59E+06	6.46E+06
TG(20:5_14:4_20:5)	TG	862.6111	1.24E+06	2.84E+06	1.15E+06	1.05E+06	9.91E+05	1.90E+06	1.03E+06	1.36E+06	4.29E+05	8.19E+05	8.14E+05
TG(20:5_18:2_20:5)	TG	922.705	2.37E+07	2.07E+07	1.95E+07	1.56E+07	1.71E+07	4.02E+07	2.75E+07	3.18E+07	8.52E+06	2.28E+07	3.57E+07
TG(20:5_18:2_22:6)	TG	948.7207	6.51E+06	5.60E+06	5.37E+06	4.19E+06	4.46E+06	9.70E+06	6.47E+06	7.24E+06	2.64E+06	7.09E+06	1.25E+07
TG(20:5_20:4_20:5)	TG	946.705	2.68E+06	1.86E+06	2.44E+06	1.12E+06	1.34E+06	3.28E+06	2.55E+06	2.66E+06	1.44E+06	3.13E+06	5.49E+06
TG(20:5_20:4_22:6)	TG	972.7207	3.59E+06	1.42E+06	3.02E+06	1.09E+06	1.38E+06	6.08E+06	4.41E+06	4.66E+06	1.65E+06	4.54E+06	7.50E+06
TG(20:5_20:5_20:5)	TG	944.6894	1.12E+07	9.46E+06	9.50E+06	7.59E+06	7.83E+06	1.54E+07	1.22E+07	1.40E+07	4.44E+06	1.13E+07	1.67E+07
TG(20:5_20:5_22:6)	TG	970.705	6.32E+06	6.51E+06	5.38E+06	3.21E+06	3.48E+06	1.23E+07	8.41E+06	9.58E+06	2.00E+06	6.22E+06	7.79E+06
TG(20:5_22:6_16:0)	TG	924.7207	2.15E+07	1.46E+07	1.89E+07	1.07E+07	1.23E+07	3.54E+07	2.46E+07	2.81E+07	9.28E+06	2.19E+07	4.08E+07
TG(20:5_22:6_22:6)	TG	996.7207	2.14E+06	2.43E+06	1.88E+06	1.29E+06	1.25E+06	3.19E+06	2.49E+06	2.79E+06	7.88E+05	2.26E+06	2.86E+06
TG(22:6_14:3_22:6)	TG	916.6581	1.77E+06	2.28E+06	1.62E+06	7.57E+05	6.47E+05	3.81E+06	2.46E+06	3.08E+06	6.35E+05	1.70E+06	1.49E+06
TG(25:0_15:0_16:0)	TG	918.8615	1.49E+06	1.59E+06	1.22E+06	1.48E+06	1.44E+06	1.71E+06	1.50E+06	1.44E+06	1.37E+06	1.44E+06	1.37E+06
TG(25:0_16:0_16:0)	TG	932.8772	9.48E+05	1.02E+06	7.76E+05	9.26E+05	9.30E+05	1.06E+06	9.68E+05	9.23E+05	8.98E+05	9.54E+05	8.77E+05
TG(25:1_14:0_16:1)	TG	900.8146	5.48E+05	9.79E+05	4.71E+05	6.07E+05	4.46E+05	1.16E+06	3.85E+05	3.51E+05	3.00E+05	3.37E+05	3.98E+05
TG(26:1_14:0_16:1)	TG	914.8302	3.98E+06	6.93E+06	3.90E+06	4.19E+06	4.43E+06	7.87E+06	2.94E+06	3.15E+06	1.67E+06	1.63E+06	3.62E+06
TG(26:1_14:1_18:3)	TG	936.8146	9.40E+05	1.73E+06	8.58E+05	1.08E+06	1.11E+06	1.56E+06	6.53E+05	7.71E+05	3.93E+05	3.91E+05	8.81E+05
TG(34:1)	TG	608.5016	3.13E+05	1.95E+05	3.19E+05	2.61E+05	3.15E+05	8.55E+05	4.02E+05	3.83E+05	1.30E+05	2.26E+05	1.80E+05
TG(34:2)	TG	606.4859	2.83E+05	2.15E+05	2.95E+05	2.95E+05	2.99E+05	6.84E+05	3.25E+05	3.05E+05	8.91E+04	1.57E+05	1.27E+05
TG(40:8)	TG	678.4859	2.19E+06	2.57E+06	2.28E+06	2.02E+06	2.34E+06	2.84E+06	2.39E+06	2.56E+06	1.87E+06	1.86E+06	2.14E+06
TG(40:9)	TG	676.4703	1.08E+06	1.71E+06	1.17E+06	1.19E+06	1.42E+06	1.23E+06	1.06E+06	1.12E+06	8.91E+05	7.65E+05	8.42E+05
TG(44:12)	TG	726.4859	4.62E+06	3.54E+06	4.57E+06	2.55E+06	3.67E+06	7.71E+06	6.67E+06	6.57E+06	3.37E+06	3.40E+06	4.61E+06
TG(58:11)	TG	924.7207	1.63E+06	1.26E+06	1.33E+06	9.17E+05	1.23E+06	2.49E+06	1.86E+06	1.60E+06	1.09E+06	1.10E+06	1.40E+06