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**Harmonizing Lipidomics: NIST Interlaboratory Comparison Exercise for Lipidomics using Standard Reference Material 1950 – Metabolites in Frozen Human Plasma**

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**Running Title**: Interlaboratory comparison exercise for lipidomics using SRM 1950

**Abbreviations:** bile acids (BA), ceramides (CER), certified reference material (CRM), cholesteryl esters (CE), coefficient of dispersion (COD), diacylglycerols (DAG), free fatty acids (FFA), free cholesterol (FC), hexosylceramide (HexCer), hydroxyeicosatetraenoic acid (HETE), LIPID Metabolites and Pathways Strategy (LIPID MAPS), lysophosphatidylcholines (LPC), lysophosphatidylethanolamines (LPE), mass spectrometry (MS), median of means (MEDM), National Institute of Standards and Technology (NIST), phosphatidylcholines (PC), phosphatidylethanolamines (PE), phosphatidylglycerols (PG), phosphatidylinositols (PI), phosphatidylserines (PS), Standard Reference Material (SRM), triacylglycerols (TAG)

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**Abstract**

As the lipidomics field continues to advance, self-evaluation within the community is critical. Here, we performed an interlaboratory comparison exercise for lipidomics using Standard Reference Material (SRM) 1950 – Metabolites in Frozen Human Plasma, a commercially available reference material. The interlaboratory study comprised 31 diverse laboratories, resulting in the measurement of 1527 unique lipids. Consensus location estimates and associated uncertainties were determined for 339 lipids measured at the sum composition level by five or more participating laboratories. These evaluated lipids detected in SRM 1950 serve as community-wide benchmarks for intra- and inter-laboratory quality control and method validation. The consensus locations were also compared to a previous examination of SRM 1950 by the LIPID MAPS consortium. While the central theme of the interlaboratory study was to provide values to help harmonize lipid measurement across the community, it was also initiated to stimulate a discussion regarding areas in need of improvement.

INTRODUCTION

The relationship between lipids and human health has been explored as early as the 1900s, where lipids were noted as important nutritional factors (1, 2) and were frequently altered from homeostatic concentrations in pathophysiological conditions (3-5). Throughout the century, lipids have been increasingly used to evaluate human health. However, it was not until the early 2000s, with the advent of mass spectrometric (MS) approaches (6), that the potential of lipid research can be realized. With the increased capacity to interrogate the lipidome, the number and types of human health applications employing lipid analysis has steadily risen (7-10). Over this period of rapid advancement, the lipidomics community, with leading endeavors from LIPID Metabolites and Pathways Strategy (LIPID MAPS), has pursued efforts to characterize several lipidomes, improve quantitative measurements, and delineate the complicated milieu of lipid interactions and pathways (11, 12). In 2010, LIPID MAPS formed a consortium to define the constituents of the mammalian lipidome using the National Institute of Standards and Technology (NIST) Standard Reference Material (SRM) 1950 – Metabolites in Frozen Human Plasma (13). The resulting lipidome was earmarked at 588 lipid species. This concerted effort was achieved piecemeal via contributions predominantly employing triple quadrupole MS technology for targeted lipid class measurements.

Within the past five years, advances in chromatography and the advent of high-resolution mass spectrometry (HRMS) have resulted in the measurement of a greater spectrum of lipids within the lipidome using a single platform (14-16). With this enhanced coverage of the lipidome, there is an increased probability of characterizing lipid pathways perturbed by disease. This is supported by the dramatic increase in potential biomarker discovery applications in lipidomics using untargeted platforms (17, 18). However, as the lipidomics field expands from targeted to untargeted assays across a diverse range of workflows and platforms, it is important for the lipidomics community to monitor and improve measurement activities.

The same inherent qualities that lend to the maturation of lipidomics and its widespread use as an approach to examine human health – namely the vast complexity in lipid structure, function, and abundance and their ubiquitous existence at membrane, cellular, tissue, and systemic levels (19, 20) – also imbue a variety of measurement challenges. Despite these challenges, lipidomic studies continue to emerge at an increased rate and with a push toward precision medicine (21-23). However, a substantial roadblock in the progression of translating lipidomics from the bench to routine clinical settings is the lack of standardization or harmonization within the lipidomics community (24). Without standardization, the assessment of data quality independent of time, place, and procedure is difficult (25, 26). As the field of lipidomics continues to progress, it will be critical to be able to control, minimize, or at the very least, understand intra- and inter-laboratory variability to ensure confidence in the discovery of real biological differences (27, 28). Several excellent lipidomics reviews (14, 29-31) conclude that the differences in methodology within the lipidomics community are extensive. This variation in lipidomics methodology has a direct impact on the resultant lipid profiles observed, affecting the number, type, and quantity of lipids observed (27, 28, 32). To date, the exact impact of this methodological diversity on community-wide lipid measurement and agreement is unknown.

Interlaboratory studies, where participants are instructed to perform a specific analysis on a homogenous and stable reference material followed by an evaluation and comparison of data at both an intra- and inter-laboratory level, are exercises well suited to critically evaluate the agreement of measurement within the lipidomics community and highlight areas of concern. NIST and others have coordinated Interlaboratory studies across disciplines for a wide variety of analytes, including omics-based profiles (33-40). For the latter, specifically for proteomics and metabolomics, interlaboratory studies have been presented with the theme of addressing the lack of agreement within the community by highlighting the need to develop standards, guidelines, and protocols, and to identify ways to evaluate lab performance, quality control, and dissemination (40-43). The paucity of commercially available reference materials for lipidomics, as well as the lack of a reason to extend quality control practices beyond the intra-laboratory level have limited the ability to benchmark data within the lipidomics community. The use of SRM 1950 as a control material for small molecule-based omics studies has been supported by a recent white paper on metabolomics-enabled precision medicine (44), where it is recommended that this certified reference material (CRM) be used as a material to aid in standardization and quality assessment across time and laboratories, at least until new reference materials are created. NIST produced this commercially available homogeneous material to aid in standardizing clinical measurements; other reports have noted its potential as a metabolomics reference material (45-48). We propose that SRM 1950 has equal value as a quality control sample for lipidomics and thus would be a suitable material for an interlaboratory comparison exercise.

Since 2014, NIST has been conducting an interlaboratory comparison exercise for lipidomics using SRM 1950. To provide a true cross-section of the lipidomics community, 31 national and international laboratories, composed of both global and targeted lipidomic methodologies spanning across academia, industry, and core facilities have participated. In addition to surveying differences in lipid methodology, the interlaboratory study was designed to highlight 1) the extent of agreement present in current lipidomic measurement within the community, 2) consensus locations with associated uncertainties for lipids present in SRM 1950, and 3) the challenges present in current lipid measurement. Reference results have been established for 339 lipids present in SRM 1950that can be used by laboratories to assess whether their data agree with the lipidomics community. These consensus locations are compared to the concentration values noted from the LIPID MAPS consortium (13).

MATERIALS AND METHODS

**Standard Reference Material (SRM) 1950**

A vial of SRM 1950 – Metabolites in Frozen Human Plasma was shipped on dry ice to participating laboratories. In collaboration with the National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK), NIST developed SRM 1950 in 2006 as a “normal” human plasma reference material. A full description of this material is provided in its Certificate of Analysis (COA, [www.nist.gov/srm](http://www.nist.gov/srm)). In brief, this plasma material was constructed from 100 fasted individuals in the age range of 40 to 50 years who represented the average composition of the US population, as defined by race, sex, and health (extreme health cohorts were excluded) (49). Due to these factors and its commercial availability, this material was selected for use in the interlaboratory lipidomics comparison exercise.

**Overview of Exercise**

Participants in the exercise were provided a data submission template that contained several tabs focused on obtaining basic laboratory and method information: sample preparation, sample introduction and chromatography, mass spectrometric approach, and data processing. Unless the participant declined to disclose details, information was obtained on sample chain of custody, extraction methodology, internal standard selection, chromatographic methods, mass spectrometer type, scanning approach employed (global and/or targeted), and the data handling/software utilized. For the analysis of SRM 1950, each laboratory was asked to employ the analytical procedures traditionally used in their laboratories and to report lipids identified and quantified (in triplicate) at nmol/mL plasma concentration levels. Laboratories were informed that all information, which could be used to link laboratories to their submitted data, would be excluded in resulting publications.

The template, which also listed potential target lipid species, is reproduced in NIST Internal Report (IR) XXXX (50).

**Organization of Submitted Data**

Each participating laboratory submitted an Excel workbook that contained lipid identifications and the respective triplicate concentration measurements (nmol/mL). Upon receipt of data, the mean and standard deviation were calculated for lipids with three replicates and non-zero concentration. Submitted data entries (lipid species name, *m/z* reported, and the adduct utilized) were compared to LipidPioneer (51) for accuracy and consistency. Submission errors found in lipid species assignment, mass assignment, and/or adduct reported were edited and subsequently verified by the laboratory. Laboratories reported lipids by fatty acyl constituents and/or by the sum composition (total carbons : total double bonds, C:DB). All entries were converted to sum composition for comparison across all laboratories. To accomplish this, concentrations for isomer lipid species per replicate were summed and the three replicate sums were used to calculate the mean and standard deviation. As an example, each replicate concentration of PC(16:1/18:1) and PC(16:0/18:2) were summed and reported as PC(34:2). Lipid isomers were included in the summation if they were reported by at least two laboratories.

**Calculation of Final Consensus Locations and Uncertainties**

The concept of calculating a consensus value and its associated uncertainty for measurements from multiple laboratories has been well studied and there are many approaches available to address this challenge (52). We considered several methods for estimating the consensus location and associated uncertainty for each submitted lipid species. The consensus approach employed for this exercise was the median of means (MEDM) method (53). The MEDM consensus value is simply the median of laboratory means. An associated standard uncertainty for the MEDM consensus value, *u*, is √(π/2*m*)×1.483×MAD, where *m* and MAD denote the number of laboratories and the median absolute deviation of the laboratory means, respectively (53). Analogous to the sample coefficient of variation, the sample coefficient of dispersion (COD) (54), expressed as a percentage, was calculated as 100\**u*/MEDM for each lipid species. These COD values were used to facilitate evaluation of the quality or "usefulness" of the consensus estimates. For evaluation purposes, the MEDM were deemed acceptable for quality control activities if they had a COD value less than 40 %.

The data in this study contained several extreme outliers (laboratory mean lipid concentrations). These outliers violated the normality assumptions made by more statistically efficient consensus estimation methods, such as Vangel-Rukhin (VR, (55, 56)) and DerSimonian-Laird (DSL, (57)). The presence of these outliers resulted in unrepresentative consensus values for these two methods. However, the MEDM method generated reasonable and representative consensus locations without requiring the omission of outlier laboratories from the analysis.

MEDM location estimates (nmol/mL) are only reported for lipids that were measured by at least five laboratories. NIST IR XXXX (50) details the consensus estimates and uncertainties in both tabular and graphical formats.

**Final Consensus Location Comparison**

The final consensus location estimates and the associated uncertainties determined in this study were compared to the lipid concentrations noted previously in the analysis of SRM 1950 conducted by the LIPID MAPS consortium (13) using predominantly triple quadrupole technology for targeted lipid class measurements. A percent change was calculated for lipids in SRM 1950, comparing the MEDM calculated in this study to the previously published values of the LIPID MAPS consortium. The values obtained from the LIPID MAPS consortium were set as the reference values in the percent change calculation. The final MEDM lipid species were summed by class to reflect those lipids that were common to the LIPID MAPS consortium.

RESULTS AND DISSCUSSION

**Construction of the Interlaboratory Comparison Exercise**

Lipid measurements were obtained from a diverse collection of laboratories that represent the current cross-section of lipid measurement within the community. Invitations were sent to 100 potential participants, spanning laboratories with differing levels of experience, publication history, and lipid methodology. Of these, 31 laboratories submitted lipidomic data with one laboratory submitting two lipidomic data sets from different MS platforms. The participants consisted of 55 % U.S / 45 % international-based, 52 % global / 48 % targeted profiling, and 78 % academic / 22 % commercial laboratories. Global profiling laboratories are here defined as those laboratories reporting at least three or more lipid categories within a data submission; targeted profiling as reporting values for lipids in less than three categories. Lipid categories were classified as fatty acyls (FA), glycerolipids (GL), glycerophospholipids (GP), sphingolipids (SP), and sterols (ST) (58, 59).

**Interlaboratory Breakdown of the SRM 1950 Plasma Lipidome**

Since the inception of lipidomics, there have been numerous reports aimed at ascertaining the composition of the human plasma lipidome. Based on the degree of lipid identification (sum composition vs individual isomers), it has been reported that anywhere between 150 and 700 lipids could be present within the human plasma lipidome (13, 60-67). As lipidomic techniques advance, it is possible that many more lipids will be identified. The LIPID MAPS report on SRM 1950 in 2011, for example, employing targeted class-specific analyses, noted 588 lipid species. At the sum composition level, 1527 unique lipid identifications were reported in the current study. This value should be viewed conservatively as it includes the sum of several isomeric lipid species. A breakdown of the lipid species reported, by lipid class and sub-class, can be found in NIST IR XXXX (50). The 1527 lipid species represent five lipid categories: FA (*n* = 177), GL (*n* = 317), GP (*n* = 679), SP (*n* = 236), and ST (*n* = 118).

Due to a high incidence of over-reporting observed within the study, lipid species were included in the final MEDM analysis only if reported by at least five laboratories (e.g., 745 lipids identified at the sum composition level were reported by only one laboratory). In total, there were 339 lipids that were reported by ≥ 5 laboratories: FA (*n* = 14), GL (*n* = 83), GP (*n* = 150), SP (*n* = 58), and ST (*n* = 34). A dissection of the number of lipids by class for those lipids with MEDM values is shown in Fig. 1A. The final calculated MEDM with CODs ≤ 40 % (*n* = 254), represent the most probable interval for which the true concentration value resides in SRM 1950, especially after factoring in the diverse methodologies employed by participating laboratories. Breakdowns of these consensus estimates organized by lipid category are presented for FA (Table 1), GL (Table 2), GP (Table 3), SP (Table 4), and ST (Table 5). The top five lipid classes using (COD ≤ 40 % criterion are: TAG (*n* = 42), PC (*n* = 53), SM (*n* = 30), PE (*n* = 29), and LPC (*n* = 25). All major lipid classes are represented (Fig. 2.) We endorse these consensus locations for use in quality control.

There were 97 lipids with COD ≤ 20 %, representing several lipid classes including: BA (*n* = 6), CE (*n* = 2), CER (*n* = 6), DAG (*n* = 1), eicosanoids (*n* = 1), free cholesterol, FFA (*n* = 2), LPC (*n* = 13), PC (*n =*30), PE (*n* = 12), PI (*n* = 12), SM (*n* = 6), and TAG (*n* = 5). This data suggests that the community measures phospholipids more consistently (specifically LPC, PC, PE and PI species) relative to other lipid classes. Approximately, 52 %, 48 %, 34 % and 80 % of the LPC, PC, PE, and PI species, respectively, were measured with a COD ≤ 20 %.

There were 85 lipids with MEDM estimates associated with COD > 40 % (supplemental Tables S1 to S5 for lipid categories FA, GL, GP, SP, and ST, respectively) in 13 lipid classes: CE (*n* = 4), CER (*n* = 7), FFA (*n* = 6), DAG (*n* = 19), HexCer (*n* = 1), LPE (*n* = 2), PC (*n* = 10), PE (*n* = 6), PG (*n* = 2), PI (*n* = 2), PS (*n* = 1), SM (*n* = 8), and TAG (*n* = 17). The classes with the greatest percentage of lipids with COD > 40 % were CER (40 %), DAG (79 %), FFA (54 %), and TAG (28 %). These findings lend greater insight into the lipids and lipid classes most affected by measurement diversity and emphasize a need to improve measurement uniformity. The lipids with COD > 40 % should not be used for quality control; rather, we suggest that these lipids and lipid classes represent challenges requiring improvement in lipid measurement.

By lipid class, the largest overall lipid concentration using the lipids having MEDM values was attributed to CE (47 %), PC (18 %), cholesterol (12 %), TAG (9 %), and SM (5 %), as shown in Fig. 1B. The lipid category with the fewest MEDM values was the fatty acyls, which comprised FFA (*n* = 11) and eicosanoids (*n* = 3), as shown in Table 1. As part of this exercise, SRM 1950 was sent to nine targeted laboratories for eicosanoid measurement. However, only six laboratories provided eicosanoid concentrations (two laboratories were not able to measure any eicosanoids in SRM 1950). In total, 143 eicosanoids were measured by at least one laboratory; however, only three (5-HETE, 12-HETE, and 15-HETE) were measured by at least five laboratories.

Table 2 lists the MEDM estimates for two lipid classes of the GL category: DAG (*n* = 24) and TAG (*n* = 59). Table 3 lists the estimates for the numerous lipids of several classes in the GP category, including LPC (*n* = 25), LPE (*n* = 8), PC (*n* = 63), PE (*n* = 35), PG (*n* = 3), PI (*n* = 15), and PS (*n* = 1). Table 4 lists the estimates for three classes in the SP category, including ceramides (*n* = 15), hexosyl ceramides (*n* = 5), and sphingomyelins (*n* = 38). Table 5 lists the estimates for the ST category, including cholesteryl esters (*n* = 19), bile acids (*n* = 14), and free cholesterol. These ST lipids represent about 59% of the total lipid concentration of SRM 1950 (See Figure 1B).

Additional “tentative” consensus location values for those lipids with only three to four laboratories reporting (*n* = 192) are listed in supplemental Table S6 to expand the lipidome coverage for SRM 1950. These values are calculated using the DSL estimator, which is more reliable than the MEDM with small numbers of normally distributed data (53,58). For inclusion as a “tentative” location, we set the criteria at having a DSL-based COD ≤ 40 % and the percent difference between the DSL and MEDM estimates ≤ 20 %. There were 62 lipids that fit this criterion (supplemental Table S6), largely represented by eicosanoids (*n* = 20) and TAG (*n* = 7). One lipid with a “tentative” value was total cholesterol, which has a certified concentration of (3917 ± 85) nmol/mL. The DSL estimate for total cholesterol was (3980 ± 24) nmol/mL.

**Usefulness of Final Consensus Values**

Certified reference materials are widely employed to assess measurement methodologies. For example, a laboratory can have confidence that the process or method employed provided a quality measurement if their measured value agrees with the certified value within the combined uncertainties of the measured and certified values. Moreover, CRMs can also be used to evaluate different sources of variability (e.g., sample preparation, instrumental data acquisition, and analysis), determine the long-term robustness of measurement processes, and validate methods (68). SRM 1950 is a CRM produced by NIST. While the consensus values generated for SRM 1950 in this interlaboratory study are not certified, the values are a cross-section of measurements obtained within the lipidomics community using a CRM with which researchers can assess measurement methodology (e.g., quantitation performance). The calculated consensus locations provide the lipidomics community the opportunity to extend quality control activities beyond the typical practices performed internally using *in-house* materials. On a wider scale, SRM 1950 has 339 robustly measured lipids (by sum composition), which can help benchmark lipid measurement within the community. A new automated lipid validation tool, LipidQC, has been introduced (69), which allows users to rapidly compare their experimental SRM 1950 lipid concentrations to the consensus estimates generated from this interlaboratory exercise. Use of SRM 1950 for quality control can now be a first step toward community-wide harmonization, which is a vital component in uncovering the full potential of lipidomics in clinical science.

**Comparison of Consensus Locations to LIPID MAPS Consortium Concentrations**

The calculated consensus values were compared to the lipid concentrations noted in a report by Quehenberger et al. where lipids were investigated in SRM 1950 by several members of the LIPID MAPS consortium using targeted (class-specific) methods (13). In total, the LIPID MAPS report found 588 lipids in SRM 1950 from several lipid classes. A comparison of those lipid species to those reported in the interlaboratory exercise (by five or more laboratories) resulted in 226 overlapping lipid species.

A comparison of these overlapping species, organized by lipid class, is shown in supplemental Tables S7 to S16. The individual MEDM and LIPID MAPS study values were also summed by lipid class and the results (derived values in supplemental Table S17) were compared in Figs. 3A (high concentration lipids) and 3B (low concentration lipids). The sum of the 226 lipids in common from the LIPID MAPS study (8438 ± 106, nmol/mL) was much higher than that of the same lipid species determined in this exercise (6218 ± 475, nmol/mL). As s shown in Figs. 3A and 3B, this difference was driven mostly by PC, PE, and TAG species. The main contributors to the difference between the two studies were phospholipids and to a lesser extent non-polar lipids. This coincided with a large percent change in the interlaboratory consensus estimates relative to the LIPID MAPS measurements, with percent changes: LPC (48 %), LPE (‑80 %), PC (‑56 %), PE (-83 %), PI (58 %), and TAG (‑54 %). Reporting at the sum composition level might contribute to these differences as the isomer lipids contributing to the sums may not be the same. Overall, the total lipid content for common lipids showed that the LIPID MAPS sum was 30 % larger than the summed composition of common lipids that were determined in this exercise, signifying a difference in measurement effects between studies.

**Future of Lipidomic Quantitation**

To date, no clear community-wide consensus exists for the best approach to quantify lipids. Quantitation, using lipidomic approaches, is a polarizing subject within the community, with both methodological and philosophical differences to consider. The community has limited agreement on the definition of current quantitation approaches (absolute, semi-, and relative) and determination of the essential guidelines to perform each approach. Furthermore, the discussion of quantitation becomes more convoluted when assessing strategies for both targeted and global profiling approaches because neither has been explicitly studied. There is a quantitation tradeoff between these two approaches. Generally, targeted approaches employ calibration curves and appropriate standards, which improve quantitation, while global approaches typically provide more lipid identifications in a single analysis. Even in targeted studies for lipidomics, appropriate standards are often not available and single point calibration is commonly used. The lipidomics community is implementing relative quantitation experiments to increase accuracy in untargeted studies, with a focus on monitoring lipid species changes between sample groups rather than determining the exact concentration of lipids (70-72). Laboratories generally employ semi-quantitative approaches to provide concentrations for lipid species; however, several assumptions are generally made using this approach (29, 72-74).

One major impediment to uniform quantitation within the community is the lack of suitable internal standards. To date, several different types of internal standards have been employed (odd-chained, deuterated, or 13C-labeled), but each has limitations. Ideally, multiple internal standards should be employed for all types and classes of lipids to improve quantitation. However, the availability of lipids that can serve as internal standards is limited. In this study, the specific internal standards utilized largely influenced the reported final lipid concentration. For example, if a laboratory quantified a lipid class with an internal standard from a different class, often the concentration values were quite different from those obtained from laboratories using standards from the appropriate lipid class. We found that several odd-chain lipids, often used by laboratories as exogenous internal standards, were used endogenously by participating laboratories in this exercise (e.g., CE 17:0, *n* = 6; LPC 17:0, *n* = 6; SM d35:1, *n* = 9; and TAG 51:3 *n* = 5).

Comparing the consensus values from this exercise (using a variety of quantitation mass spectrometry platforms: triple quadrupole, quadrupole time-of-flight, and orbitrap) to the concentration values obtained using the targeted triple quadrupole platforms, we found that the targeted approaches generally had significantly higher calculated concentration values. As the community begins to develop and establish guidelines for quality assurance and quality control, discussions need to include acceptable practices for quantitation across the varying platforms present within the lipidomics community.

CONCLUSION

The purpose of this lipidomics interlaboratory comparison exercise was to identify the metrological questions and/or gaps that exist in current lipidomics measurement. To determine the principal areas of need, the interlaboratory exercise was initiated using a commercially available CRM, SRM 1950. This interlaboratory study provides an initial outlook into the variance associated with current lipid methodologies. The robustly measured SRM 1950 consensus estimates can be used for community-wide quality control and quality assessment. These values were compared to those previously reported by LIPID MAPS. From a community perspective, the exercise also provided valuable insight into the potential strengths and weaknesses of current lipidomic measurement. Future reports from this interlaboratory study will focus on the influence that the laboratory-provided methodological information had on the resultant trends in the collective data. We currently intend to provide a supplemental survey to direct future measurement efforts regarding lipidomics measurement.

DISCLAIMER

Certain commercial equipment, instruments, or materials are identified in this paper to specify adequately the experimental procedures. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology; nor does it imply that the materials or equipment identified are necessarily the best for the purpose. Furthermore, the content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institute of Standards and Technology, the U.S. National Institutes of Health, or of any of the participating organizations.

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Table 1. Final consensus location estimates for fatty acyl (FA) lipids measured in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | Number of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| FFA 16:0 | 5 | nmol/mL | 43 | 13 | 31 |
| FFA 18:3 | 6 | nmol/mL | 2.9 | 0.62 | 21 |
| FFA 20:4 | 7 | nmol/mL | 4.7 | 1.5 | 31 |
| FFA 20:5 | 7 | nmol/mL | 0.42 | 0.056 | 13 |
| FFA 22:6 | 8 | nmol/mL | 1.5 | 0.17 | 11 |
|  |  |  |  |  |  |
| 12-HETE | 5 | pmol/mL | 6.8 | 1.5 | 23 |
| 15-HETE | 5 | pmol/mL | 2.4 | 0.64 | 27 |
| 5-HETE | 5 | pmol/mL | 10 | 1.3 | 13 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values ≤ 40 %. The abbreviations identify free fatty acids (FFA) and hydroxyeicosatetraenoic acids (HETEs).

Table 2. Final consensus location estimates for glycerolipids (GL) measured in SRM 1950

| Lipid | Number of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| --- | --- | --- | --- | --- | --- |
| DAG 30:0 | 7 | nmol/mL | 0.83 | 0.17 | 20 |
| DAG 34:1 | 16 | nmol/mL | 6.1 | 2.4 | 40 |
| DAG 36:2 | 16 | nmol/mL | 6.2 | 2.2 | 36 |
| DAG 36:3 | 15 | nmol/mL | 8.4 | 3.3 | 39 |
| DAG 36:4 | 12 | nmol/mL | 2.8 | 1.0 | 38 |
|  |  |  |  |  |  |
| TAG 46:2 | 8 | nmol/mL | 3.6 | 1.3 | 37 |
| TAG 48:0 | 10 | nmol/mL | 4.5 | 1.2 | 26 |
| TAG 48:1 | 16 | nmol/mL | 13 | 3.2 | 24 |
| TAG 48:2 | 15 | nmol/mL | 16 | 2.8 | 18 |
| TAG 48:4 | 5 | nmol/mL | 1.3 | 0.23 | 18 |
| TAG 49:1 | 9 | nmol/mL | 2.0 | 0.42 | 21 |
| TAG 49:2 | 6 | nmol/mL | 1.8 | 0.56 | 31 |
| TAG 50:0 | 11 | nmol/mL | 3.8 | 0.83 | 22 |
| TAG 50:1 | 14 | nmol/mL | 38 | 10.0 | 26 |
| TAG 50:2 | 15 | nmol/mL | 47 | 12 | 26 |
| TAG 50:3 | 16 | nmol/mL | 23 | 6.6 | 29 |
| TAG 50:4 | 15 | nmol/mL | 8.7 | 2.9 | 34 |
| TAG 50:5 | 7 | nmol/mL | 1.6 | 0.64 | 40 |
| TAG 51:1 | 7 | nmol/mL | 1.8 | 0.48 | 27 |
| TAG 51:2 | 8 | nmol/mL | 4.8 | 1.1 | 22 |
| TAG 51:3 | 5 | nmol/mL | 4.8 | 1.9 | 39 |
| TAG 52:1 | 11 | nmol/mL | 14 | 2.9 | 20 |
| TAG 52:2 | 16 | nmol/mL | 44 | 14 | 33 |
| TAG 52:3 | 16 | nmol/mL | 100 | 29 | 28 |
| TAG 52:4 | 15 | nmol/mL | 48 | 17 | 35 |
| TAG 52:5 | 13 | nmol/mL | 15 | 5.7 | 39 |
| TAG 52:6 | 8 | nmol/mL | 4.0 | 1.4 | 35 |
| TAG 52:7 | 5 | nmol/mL | 0.39 | 0.13 | 33 |
| TAG 53:2 | 9 | nmol/mL | 1.9 | 0.41 | 21 |
| TAG 53:3 | 6 | nmol/mL | 3.7 | 1.1 | 29 |
| TAG 53:4 | 6 | nmol/mL | 2.4 | 0.76 | 32 |
| TAG 54:1 | 10 | nmol/mL | 3.2 | 0.91 | 29 |
| TAG 54:2 | 13 | nmol/mL | 8.2 | 2.6 | 31 |
| TAG 54:3 | 15 | nmol/mL | 26 | 9.8 | 37 |
| TAG 54:4 | 15 | nmol/mL | 36 | 13 | 35 |
| TAG 54:5 | 15 | nmol/mL | 27 | 11 | 38 |
| TAG 54:6 | 16 | nmol/mL | 14 | 5.1 | 37 |
| TAG 54:7 | 7 | nmol/mL | 5.6 | 1.5 | 26 |
| TAG 56:2 | 5 | nmol/mL | 0.69 | 0.23 | 33 |
| TAG 56:3 | 6 | nmol/mL | 1.4 | 0.14 | 10 |
| TAG 56:4 | 10 | nmol/mL | 2.0 | 0.56 | 28 |
| TAG 56:5 | 12 | nmol/mL | 4.1 | 1.4 | 33 |
| TAG 56:7 | 8 | nmol/mL | 13 | 2.7 | 20 |
| TAG 56:9 | 5 | nmol/mL | 0.71 | 0.27 | 38 |
| TAG 58:7 | 5 | nmol/mL | 2.0 | 0.64 | 32 |
| TAG 58:8 | 9 | nmol/mL | 0.68 | 0.21 | 31 |
| TAG 58:9 | 6 | nmol/mL | 1.2 | 0.27 | 22 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values ≤ 40 %. The abbreviations identify diacylglycerols (DAG) and triacylglycerols (TAG).

Table 3. Final consensus location estimates for glycerophospholipids (GP) measured in SRM 1950

| Lipid | Number of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| --- | --- | --- | --- | --- | --- |
| LPC 14:0 | 16 | nmol/mL | 1.0 | 0.20 | 19 |
| LPC 15:0 | 9 | nmol/mL | 0.52 | 0.11 | 22 |
| LPC 16:0 | 20 | nmol/mL | 73 | 11 | 15 |
| LPC O-16:0 | 10 | nmol/mL | 0.55 | 0.16 | 29 |
| LPC P-16:0 | 8 | nmol/mL | 0.46 | 0.13 | 27 |
| LPC 16:1 | 19 | nmol/mL | 2.4 | 0.35 | 15 |
| LPC 17:0 | 6 | nmol/mL | 1.4 | 0.24 | 18 |
| LPC 17:1 | 6 | nmol/mL | 0.25 | 0.071 | 29 |
| LPC 18:0 | 20 | nmol/mL | 27 | 3.3 | 12 |
| LPC O-18:0 | 6 | nmol/mL | 0.16 | 0.058 | 36 |
| LPC 18:1 | 19 | nmol/mL | 18 | 2.3 | 13 |
| LPC 18:2 | 19 | nmol/mL | 22 | 2.9 | 13 |
| LPC 18:3 | 18 | nmol/mL | 0.44 | 0.13 | 30 |
| LPC 20:0 | 7 | nmol/mL | 0.10 | 0.034 | 34 |
| LPC 20:1 | 13 | nmol/mL | 0.19 | 0.024 | 12 |
| LPC 20:2 | 9 | nmol/mL | 0.23 | 0.044 | 19 |
| LPC 20:3 | 18 | nmol/mL | 1.8 | 0.26 | 15 |
| LPC 20:4 | 20 | nmol/mL | 6.0 | 0.60 | 10 |
| LPC 20:5 | 15 | nmol/mL | 0.33 | 0.092 | 28 |
| LPC 22:0 | 5 | nmol/mL | 0.025 | 0.0017 | 7 |
| LPC 22:1 | 5 | nmol/mL | 0.013 | 0.0046 | 36 |
| LPC 22:4 | 8 | nmol/mL | 0.12 | 0.041 | 33 |
| LPC 22:5 | 12 | nmol/mL | 0.43 | 0.13 | 30 |
| LPC 22:6 | 17 | nmol/mL | 0.77 | 0.14 | 18 |
| LPC 24:0 | 5 | nmol/mL | 0.046 | 0.015 | 33 |
|  |  |  |  |  |  |
| LPE 16:0 | 14 | nmol/mL | 0.91 | 0.27 | 29 |
| LPE 18:0 | 15 | nmol/mL | 1.6 | 0.55 | 34 |
| LPE 18:1 | 14 | nmol/mL | 1.4 | 0.47 | 35 |
| LPE 18:2 | 16 | nmol/mL | 1.9 | 0.56 | 30 |
| LPE 20:4 | 14 | nmol/mL | 1.1 | 0.41 | 37 |
| LPE 22:6 | 12 | nmol/mL | 0.52 | 0.18 | 34 |
|  |  |  |  |  |  |
| PC 30:0 | 11 | nmol/mL | 1.6 | 0.32 | 20 |
| PC O-30:0/29:0 | 7 | nmol/mL | 0.072 | 0.026 | 36 |
| PC O-30:1/P-30:0 | 7 | nmol/mL | 0.047 | 0.0096 | 20 |
| PC 32:0 | 18 | nmol/mL | 7.2 | 1.0 | 14 |
| PC O-32:0/31:0 | 11 | nmol/mL | 1.5 | 0.41 | 28 |
| PC 32:1 | 18 | nmol/mL | 13 | 1.9 | 15 |
| PC O-32:1/P-32:0/31:1 | 11 | nmol/mL | 1.6 | 0.24 | 14 |
| PC O-32:2/P-32:1/31:2 | 8 | nmol/mL | 0.34 | 0.093 | 28 |
| PC 32:3 | 8 | nmol/mL | 0.42 | 0.14 | 34 |
| PC P-33:1/32:2 | 16 | nmol/mL | 2.6 | 0.37 | 14 |
| PC 34:0 | 12 | nmol/mL | 2.1 | 0.37 | 18 |
| PC O-34:0/33:0 | 10 | nmol/mL | 0.76 | 0.17 | 22 |
| PC 34:1 | 19 | nmol/mL | 120 | 21 | 17 |
| PC O-34:1/P-34:0/33:1 | 17 | nmol/mL | 4.9 | 0.86 | 17 |
| PC O-34:2/P-34:1/33:2 | 17 | nmol/mL | 5.2 | 1.3 | 25 |
| PC O-34:3/P-34:2/33:3 | 12 | nmol/mL | 4.7 | 0.88 | 19 |
| PC P-35:1/34:2 | 18 | nmol/mL | 240 | 47 | 19 |
| PC P-35:2/34:3 | 18 | nmol/mL | 12 | 1.7 | 14 |
| PC O-35:4/34:4 | 9 | nmol/mL | 1.0 | 0.25 | 24 |
| PC 34:5 | 5 | nmol/mL | 0.034 | 0.0045 | 13 |
| PC 36:1 | 17 | nmol/mL | 26 | 4.6 | 17 |
| PC O-36:1/P-36:0/35:1 | 16 | nmol/mL | 3.5 | 0.99 | 28 |
| PC 36:2 | 18 | nmol/mL | 140 | 25 | 17 |
| PC O-36:2/P-36:1/35:2 | 17 | nmol/mL | 7.4 | 1.7 | 22 |
| PC 36:3 | 17 | nmol/mL | 100 | 14 | 14 |
| PC O-36:3/P-36:2/35:3 | 12 | nmol/mL | 3.7 | 0.82 | 22 |
| PC 36:4 | 19 | nmol/mL | 150 | 28 | 19 |
| PC O-36:4/P-36:3/35:4 | 17 | nmol/mL | 12 | 1.4 | 12 |
| PC 36:5 | 16 | nmol/mL | 11 | 1.8 | 17 |
| PC O-36:5/P-36:4/35:5 | 11 | nmol/mL | 6.9 | 1.6 | 23 |
| PC P-36:5/35:6 | 5 | nmol/mL | 0.30 | 0.094 | 31 |
| PC 36:6 | 8 | nmol/mL | 0.28 | 0.088 | 32 |
| PC 38:2 | 15 | nmol/mL | 2.3 | 0.20 | 9 |
| PC O-38:2/37:2 | 6 | nmol/mL | 0.98 | 0.32 | 32 |
| PC 38:3 | 14 | nmol/mL | 26 | 5.2 | 20 |
| PC O-38:3/P-38:2/37:3 | 14 | nmol/mL | 1.5 | 0.51 | 34 |
| PC 38:4 | 18 | nmol/mL | 84 | 14 | 17 |
| PC O-38:4/P-38:3/37:4 | 12 | nmol/mL | 7.4 | 2.0 | 27 |
| PC 38:5 | 18 | nmol/mL | 42 | 7.9 | 19 |
| PC O-38:5/P-38:4/37:5 | 16 | nmol/mL | 11 | 1.6 | 14 |
| PC 38:6 | 18 | nmol/mL | 41 | 4.4 | 11 |
| PC O-38:6/P-38:5/37:6 | 12 | nmol/mL | 3.6 | 1.0 | 29 |
| PC P-38:6/36:0 | 10 | nmol/mL | 1.2 | 0.39 | 33 |
| PC 40:4 | 18 | nmol/mL | 2.9 | 0.37 | 13 |
| PC O-40:2/P-40:1 | 5 | nmol/mL | 0.069 | 0.021 | 30 |
| PC O-40:4/P-40:3/39:4 | 8 | nmol/mL | 0.95 | 0.38 | 40 |
| PC 40:5 | 18 | nmol/mL | 6.7 | 1.1 | 16 |
| PC O-40:5/P-40:4/39:5 | 12 | nmol/mL | 1.7 | 0.45 | 27 |
| PC 40:6 | 17 | nmol/mL | 14 | 2.6 | 19 |
| PC 40:7 | 16 | nmol/mL | 3.5 | 0.76 | 21 |
| PC O-40:7/P-40:6/39:7 | 9 | nmol/mL | 1.1 | 0.23 | 20 |
| PC 40:8 | 14 | nmol/mL | 0.73 | 0.20 | 28 |
| PC O-42:5/P-42:4 | 7 | nmol/mL | 0.79 | 0.12 | 15 |
|  |  |  |  |  |  |
| PE 32:1 | 6 | nmol/mL | 0.34 | 0.12 | 36 |
| PE 34:1 | 14 | nmol/mL | 1.2 | 0.17 | 14 |
| PE 34:2 | 16 | nmol/mL | 2.2 | 0.26 | 12 |
| PE O-34:2/P-34:1 | 11 | nmol/mL | 0.78 | 0.17 | 22 |
| PE O-34:3/P-34:2 | 11 | nmol/mL | 1.5 | 0.41 | 27 |
| PE 36:0 | 11 | nmol/mL | 0.28 | 0.10 | 36 |
| PE 36:1 | 14 | nmol/mL | 1.3 | 0.26 | 20 |
| PE 36:2 | 16 | nmol/mL | 6.7 | 0.79 | 12 |
| PE O-36:2/P-36:1/35:2 | 12 | nmol/mL | 0.93 | 0.22 | 23 |
| PE 36:3 | 16 | nmol/mL | 2.4 | 0.38 | 16 |
| PE O-36:3/P-36:2/35:3 | 15 | nmol/mL | 3.2 | 0.76 | 24 |
| PE 36:4 | 16 | nmol/mL | 3.1 | 0.39 | 13 |
| PE O-36:4/P-36:3 | 14 | nmol/mL | 1.6 | 0.29 | 18 |
| PE O-36:5/P-36:4 | 15 | nmol/mL | 4.9 | 1.9 | 38 |
| PE 38:3 | 14 | nmol/mL | 0.95 | 0.20 | 21 |
| PE 38:4 | 16 | nmol/mL | 8.1 | 1.2 | 15 |
| PE O-38:4/P-38:3/37:4 | 9 | nmol/mL | 0.94 | 0.18 | 19 |
| PE 38:5 | 12 | nmol/mL | 2.7 | 0.47 | 17 |
| PE O-38:5/P-38:4 | 17 | nmol/mL | 5.8 | 1.9 | 33 |
| PE 38:6 | 15 | nmol/mL | 3.2 | 0.59 | 19 |
| PE O-38:6/P-38:5 | 16 | nmol/mL | 4.9 | 1.2 | 25 |
| PE O-38:7/P-38:6 | 8 | nmol/mL | 3.5 | 0.98 | 28 |
| PE 40:4 | 10 | nmol/mL | 0.26 | 0.082 | 31 |
| PE 40:5 | 12 | nmol/mL | 0.73 | 0.23 | 31 |
| PE O-40:5/P-40:4/39:5 | 12 | nmol/mL | 0.73 | 0.13 | 17 |
| PE 40:6 | 14 | nmol/mL | 1.8 | 0.36 | 20 |
| PE O-40:6/P-40:5/39:6 | 14 | nmol/mL | 1.3 | 0.31 | 23 |
| PE 40:7 | 11 | nmol/mL | 0.77 | 0.26 | 33 |
| PE O-40:7/P-40:6/39:7 | 14 | nmol/mL | 2.5 | 0.72 | 29 |
|  |  |  |  |  |  |
| PI 32:1 | 10 | nmol/mL | 0.56 | 0.11 | 19 |
| PI 34:1 | 14 | nmol/mL | 2.4 | 0.42 | 17 |
| PI 34:2 | 14 | nmol/mL | 2.8 | 0.38 | 14 |
| PI 36:1 | 13 | nmol/mL | 2.1 | 0.59 | 28 |
| PI 36:2 | 15 | nmol/mL | 7.7 | 0.93 | 12 |
| PI 36:3 | 14 | nmol/mL | 2.2 | 0.29 | 14 |
| PI 36:4 | 14 | nmol/mL | 3.0 | 0.48 | 16 |
| PI 38:3 | 14 | nmol/mL | 3.4 | 0.54 | 16 |
| PI 38:4 | 17 | nmol/mL | 19 | 2.2 | 11 |
| PI 38:5 | 15 | nmol/mL | 2.5 | 0.44 | 18 |
| PI 38:6 | 10 | nmol/mL | 0.32 | 0.031 | 10 |
| PI 40:4 | 7 | nmol/mL | 0.30 | 0.042 | 14 |
| PI 40:6 | 12 | nmol/mL | 0.84 | 0.16 | 19 |
|  |  |  |  |  |  |
| PG 36:2 | 6 | nmol/mL | 0.67 | 0.24 | 36 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values ≤ 40 %. The abbreviations identify lysophosphatidylcholines (LPC), lysophosphatidylethanolamines (LPE), phosphatidylcholines (PC), phosphatidylethanolamines (PE), phosphatidylglycerols (PG), and phosphatidylinositols (PI). For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a “/”.

Table 4. Final consensus location estimates for sphingolipids (SP) measured in SRM 1950

| Lipid | Number of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| --- | --- | --- | --- | --- | --- |
| HexCer d34:1 | 6 | nmol/mL | 0.86 | 0.21 | 25 |
| HexCer d36:1 | 5 | nmol/mL | 0.13 | 0.043 | 34 |
| HexCer d40:1 | 5 | nmol/mL | 2.4 | 0.68 | 28 |
| HexCer d42:1 | 6 | nmol/mL | 2.7 | 0.73 | 27 |
| CER d34:1 | 17 | nmol/mL | 0.28 | 0.044 | 16 |
| CER d36:1 | 14 | nmol/mL | 0.12 | 0.021 | 17 |
| CER d38:1 | 16 | nmol/mL | 0.11 | 0.021 | 20 |
| CER d40:1 | 18 | nmol/mL | 0.65 | 0.12 | 18 |
| CER d40:2 | 6 | nmol/mL | 0.15 | 0.021 | 14 |
| CER d41:1 | 7 | nmol/mL | 0.67 | 0.27 | 40 |
| CER d42:1 | 19 | nmol/mL | 1.9 | 0.47 | 24 |
| CER d42:2 | 19 | nmol/mL | 0.82 | 0.10 | 12 |
|  |  |  |  |  |  |
| SM d31:1 | 5 | nmol/mL | 0.19 | 0.049 | 25 |
| SM d32:1 | 14 | nmol/mL | 8.4 | 1.4 | 17 |
| SM d32:2 | 10 | nmol/mL | 0.66 | 0.24 | 36 |
| SM d33:1 | 14 | nmol/mL | 4.7 | 0.64 | 14 |
| SM d34:0 | 14 | nmol/mL | 5.8 | 1.3 | 22 |
| SM d34:1 | 21 | nmol/mL | 100 | 15 | 15 |
| SM d34:2 | 17 | nmol/mL | 16 | 2.2 | 14 |
| SM d35:1 | 9 | nmol/mL | 2.5 | 0.58 | 23 |
| SM d35:2 | 6 | nmol/mL | 0.52 | 0.21 | 39 |
| SM d36:0 | 11 | nmol/mL | 2.0 | 0.49 | 24 |
| SM d36:1 | 22 | nmol/mL | 20 | 3.7 | 18 |
| SM d36:2 | 22 | nmol/mL | 9.6 | 1.5 | 16 |
| SM d36:3 | 13 | nmol/mL | 1.3 | 0.41 | 31 |
| SM d37:1 | 11 | nmol/mL | 1.0 | 0.23 | 23 |
| SM d38:1 | 17 | nmol/mL | 11 | 3.1 | 27 |
| SM d38:2 | 17 | nmol/mL | 5.2 | 1.3 | 25 |
| SM d38:3 | 8 | nmol/mL | 0.61 | 0.24 | 39 |
| SM d39:1 | 14 | nmol/mL | 3.6 | 1.0 | 29 |
| SM d39:2 | 9 | nmol/mL | 0.61 | 0.16 | 26 |
| SM d40:1 | 17 | nmol/mL | 20 | 5.1 | 25 |
| SM d40:2 | 15 | nmol/mL | 12 | 2.8 | 24 |
| SM d40:3 | 8 | nmol/mL | 2.2 | 0.79 | 37 |
| SM d41:1 | 14 | nmol/mL | 7.7 | 2.1 | 27 |
| SM d41:2 | 14 | nmol/mL | 5.8 | 1.4 | 24 |
| SM d41:3 | 7 | nmol/mL | 0.77 | 0.30 | 39 |
| SM d42:1 | 21 | nmol/mL | 20 | 5.4 | 28 |
| SM d42:2 | 18 | nmol/mL | 44 | 11 | 25 |
| SM d42:3 | 12 | nmol/mL | 17 | 4.7 | 27 |
| SM d43:2 | 10 | nmol/mL | 1.0 | 0.29 | 29 |
| SM d44:2 | 9 | nmol/mL | 0.40 | 0.13 | 32 |

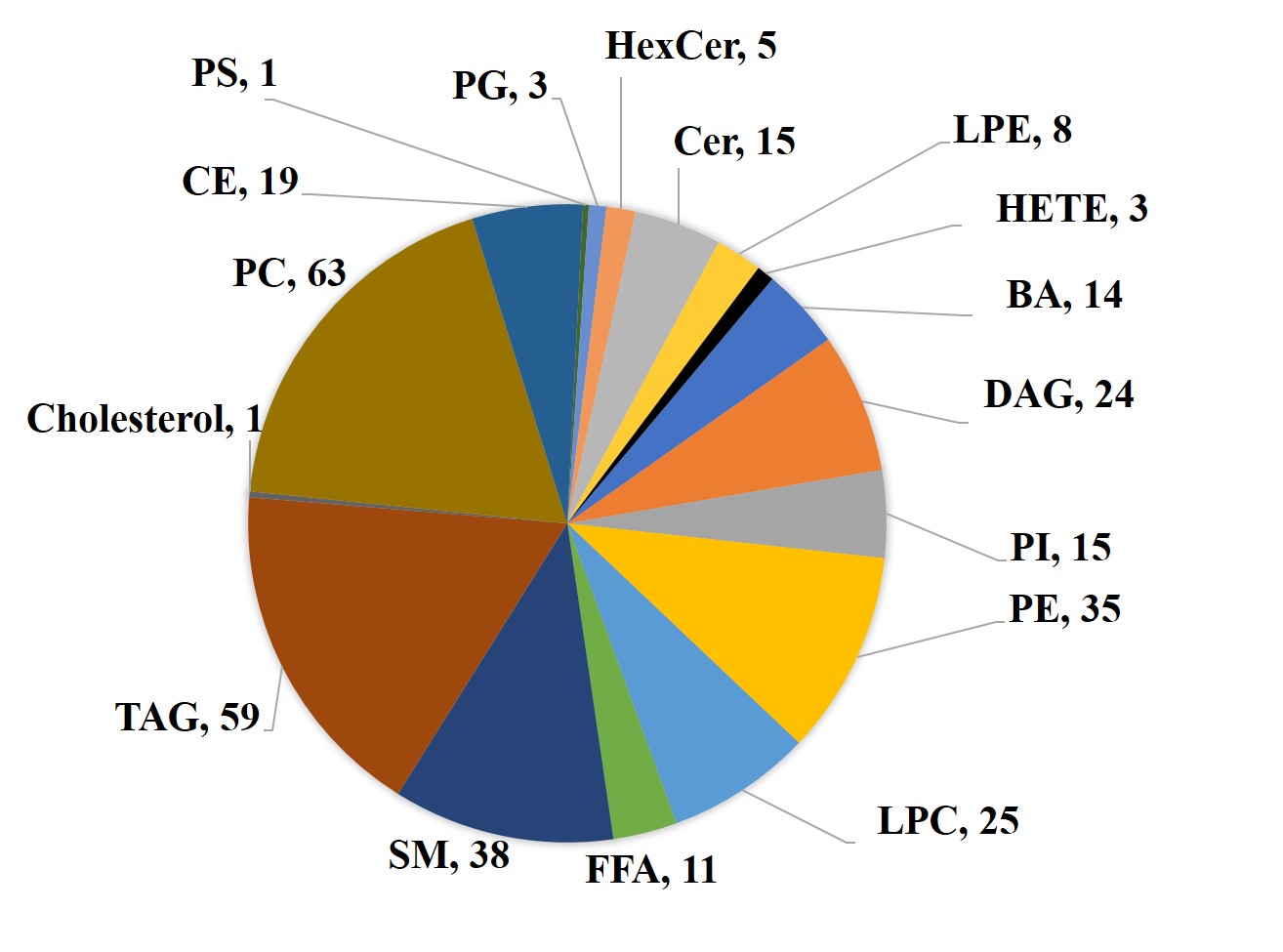
MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values ≤ 40 %. The abbreviations identify hexosylceramides (HexCer), ceramides (CER), and sphingomyelins (SM).

Table 5. Final consensus location estimates for sterol (ST) lipids measured in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| CE 14:0 | 7 | nmol/mL | 16 | 6.0 | 37 |
| CE 15:0 | 6 | nmol/mL | 5.3 | 1.8 | 34 |
| CE 16:0 | 13 | nmol/mL | 210 | 58 | 28 |
| CE 16:1 | 11 | nmol/mL | 100 | 27 | 27 |
| CE 16:2 | 5 | nmol/mL | 1.9 | 0.46 | 25 |
| CE 17:1 | 9 | nmol/mL | 8.2 | 1.0 | 13 |
| CE 18:0 | 7 | nmol/mL | 15 | 3.7 | 25 |
| CE 18:1 | 14 | nmol/mL | 450 | 110 | 25 |
| CE 18:2 | 14 | nmol/mL | 1,700 | 430 | 26 |
| CE 18:3 | 13 | nmol/mL | 84 | 24 | 28 |
| CE 20:3 | 13 | nmol/mL | 35 | 12 | 35 |
| CE 20:4 | 14 | nmol/mL | 350 | 58 | 17 |
| CE 20:5 | 12 | nmol/mL | 38 | 8.6 | 23 |
| CE 22:5 | 6 | nmol/mL | 4.1 | 1.6 | 39 |
| CE 22:6 | 11 | nmol/mL | 37 | 9.5 | 26 |
|  |  |  |  |  |  |
| Cholesterol | 8 | nmol/mL | 770 | 110 | 14 |
|  |  |  |  |  |  |
| CDCA | 7 | nmol/mL | 0.30 | 0.11 | 38 |
| CA | 9 | nmol/mL | 0.12 | 0.034 | 28 |
| DCA | 9 | nmol/mL | 0.35 | 0.083 | 24 |
| GCDCA | 8 | nmol/mL | 1.1 | 0.18 | 17 |
| GDCA | 7 | nmol/mL | 0.43 | 0.069 | 16 |
| GLCA | 6 | nmol/mL | 0.025 | 0.0018 | 7 |
| GUDCA | 6 | nmol/mL | 0.15 | 0.024 | 16 |
| GCA | 6 | nmol/mL | 0.24 | 0.069 | 29 |
| LCA | 8 | nmol/mL | 0.014 | 0.0036 | 26 |
| TCDCA | 9 | nmol/mL | 0.084 | 0.0050 | 6 |
| TCA | 9 | nmol/mL | 0.026 | 0.0056 | 22 |
| TDCA | 8 | nmol/mL | 0.040 | 0.0064 | 16 |
| TLCA | 5 | nmol/mL | 0.0027 | 0.00069 | 26 |
| UDCA | 8 | nmol/mL | 0.11 | 0.024 | 22 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values ≤ 40 %. The abbreviations identify chenodeoxycholic acid (CDCA), cholic acid (CA), cholesteryl ester (CE), deoxycholic acid (DCA), glycochenodeoxycholic acid (GCDCA), glycodeoxycholic acid (GCDA), glycolithocholic acid (GLCA), glycoursodeoxycholic acid (GUDCA), glyocholic acid (GCA), lithocholic acid (LCA), taurochenodeoxycholic acid (TCDCA), taurocholic acid (TCA), taurodeoxycholic acid (TDCA), taurolithocholic acid (TLCA), ursodeoxycholic acid (UDCA).

**A**



**B**

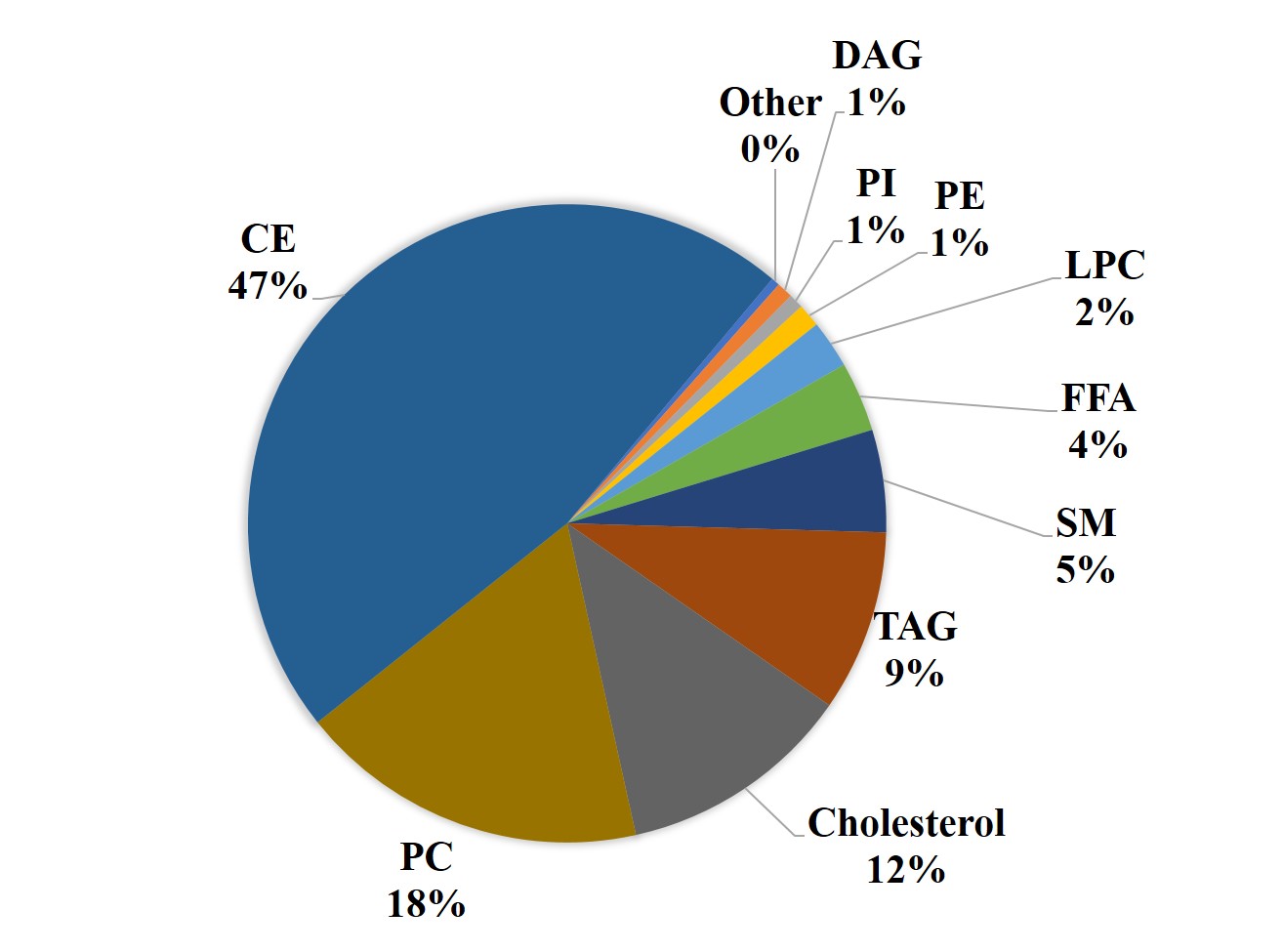


Figure 1: Lipid class composition of SRM 1950. A) Number of lipid species (*n* = 339). B) Concentration. Only lipid species that were measured by at least five participating laboratories are included.

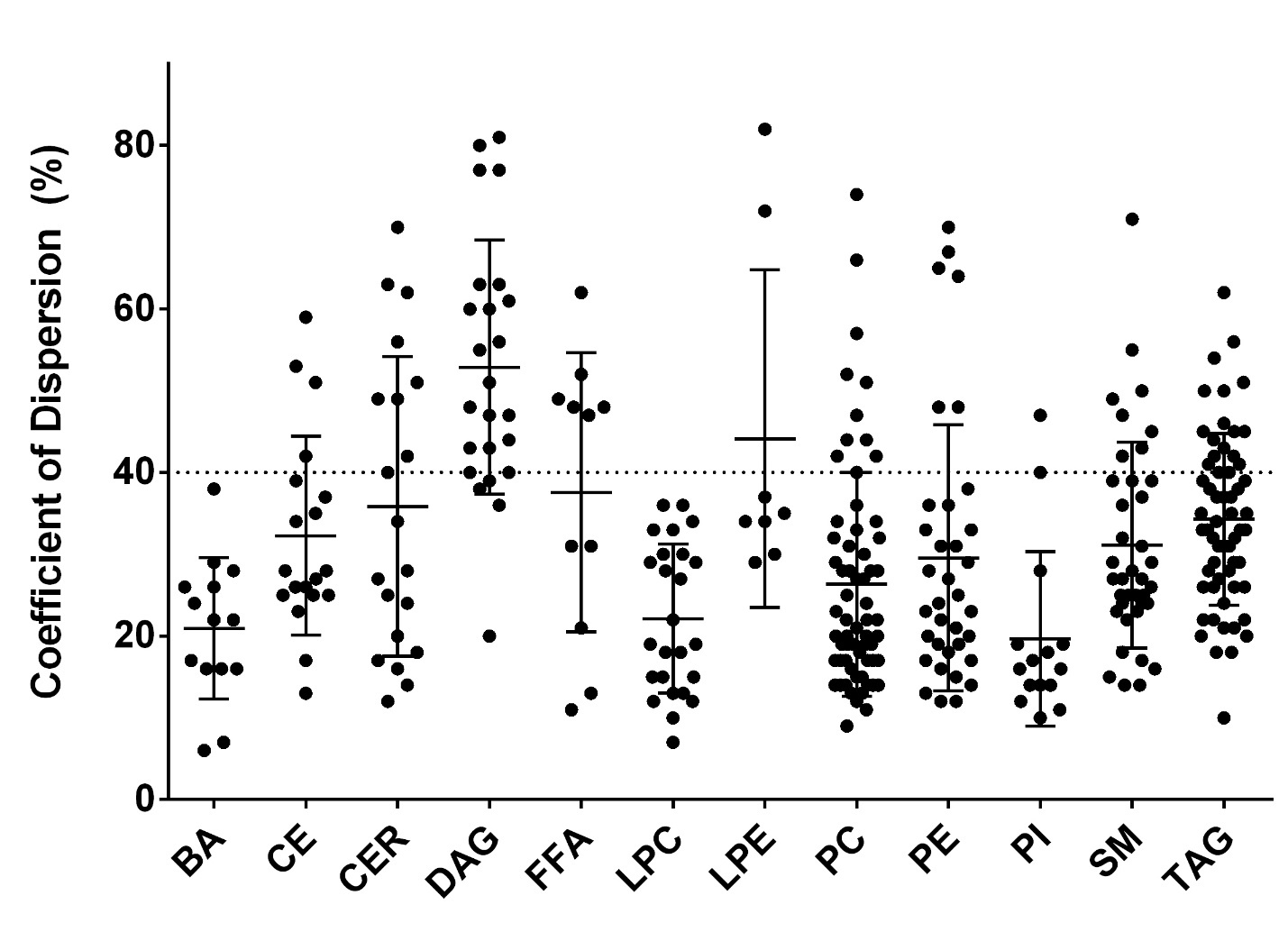
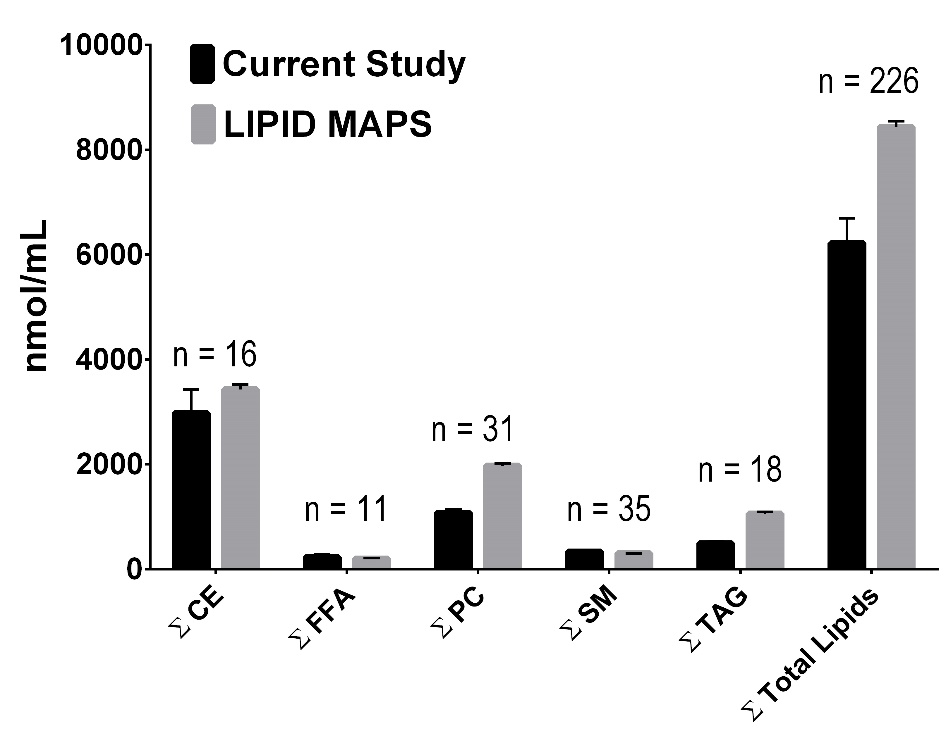
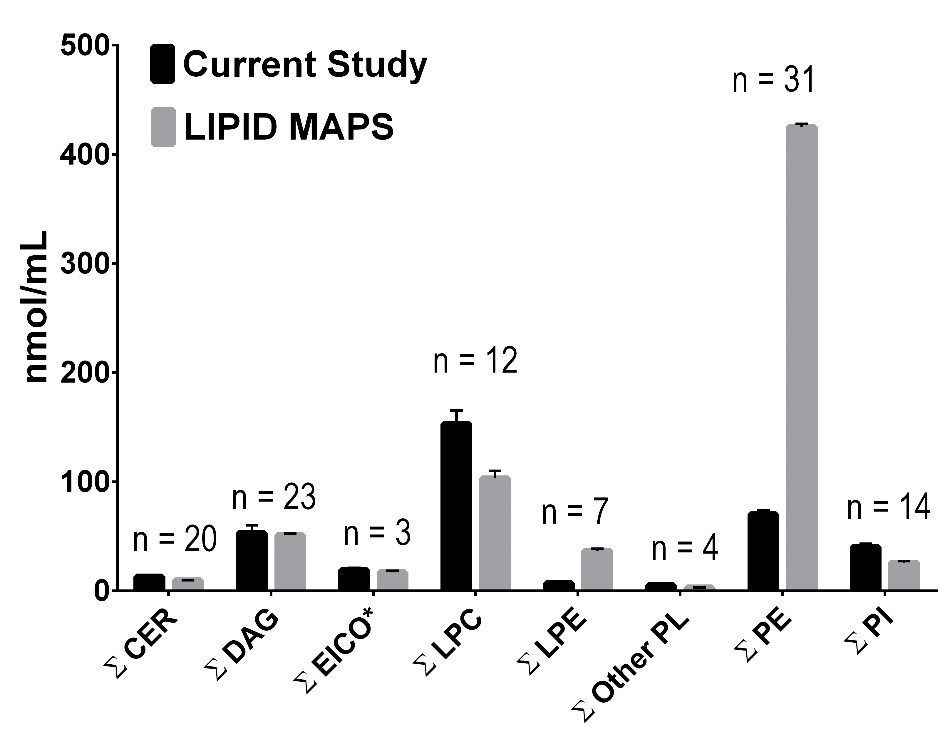


Fig. 2. Coefficient of dispersion (COD, in %) for the MEDM lipids (n ≥ 5 laboratories reporting) organized by lipid class. The COD was calculated by dividing the standard uncertainty by the final MEDM. CODs not shown in the figure are free cholesterol, eicosanoids, phosphatidylglycerols, and phosphatidylserines.



**A**



**B**

Fig. 3A Sum of MEDM values (in nmol/mL plasma) for the most and least concentrated lipid classes compared to the sum of concentrations provided by the LIPID MAPS consortium (A and B, respectively). The comparisons entail summing only the lipids measured in common between the compared data sets, with the total number of lipids fitting this criterion (per class and total) provided above each bar graph. Other PL represents the sum of PG and PS species. The error bars associated with the values standard uncertainties on the location estimates. Further information on this comparison is included in Supplementary Material.

Supplemental Information

Journal of Lipid Research: Full Article

**Harmonizing Lipidomics: NIST Interlaboratory Comparison Exercise for Lipidomics using Standard Reference Material 1950 – Metabolites in Frozen Human Plasma**

John A. Bowden, Alan Heckert, Candice Z. Ulmer, Christina M. Jones, Jeremy P. Koelmel, et al.

Tables S1 – S5: Consensus location and uncertainty estimates for lipids measured in SRM 1950 with COD > 40 %, organized by lipid class: FA, GL, GP, SP, and ST, respectively.

Table. S6: Consensus location and uncertainty estimates (DSL and MEDM) for lipids reported by only three or four laboratories.

Table S7 – S16: Percent differences between lipid consensus MEDM locations, organized by lipid class, to concentrations previously reported in the LIPID MAPS consortium study

Table S17: Percent difference between summed interlaboratory consensus location estimates to summed concentrations derived from concentrations reported by the LIPID MAPS consortium

Table S1. Consensus location and uncertainty estimates for fatty acyl (FA) lipids measured in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| FFA 16:1 | 6 | nmol/mL | 6.1 | 2.9 | 48 |
| FFA 18:0 | 5 | nmol/mL | 15 | 9.0 | 62 |
| FFA 18:1 | 6 | nmol/mL | 110 | 53 | 48 |
| FFA 18:2 | 6 | nmol/mL | 44 | 22 | 49 |
| FFA 20:3 | 5 | nmol/mL | 1.3 | 0.62 | 47 |
| FFA 22:5 | 5 | nmol/mL | 1.1 | 0.56 | 52 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values > 40 %. The abbreviation identifies free fatty acids (FFA).

Table S2. Consensus location and uncertainty estimates for glycerolipids (GL) measured in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| DAG 32:0 | 11 | nmol/mL | 2.6 | 1.2 | 44 |
| DAG 32:1 | 10 | nmol/mL | 1.2 | 0.62 | 51 |
| DAG 32:2 | 11 | nmol/mL | 0.62 | 0.29 | 48 |
| DAG 34:0 | 10 | nmol/mL | 6.5 | 3.6 | 56 |
| DAG 34:2 | 14 | nmol/mL | 4.4 | 1.9 | 43 |
| DAG 34:3 | 7 | nmol/mL | 0.31 | 0.20 | 63 |
| DAG 36:0 | 9 | nmol/mL | 1.6 | 0.98 | 60 |
| DAG 36:1 | 12 | nmol/mL | 2.6 | 1.1 | 43 |
| DAG 36:5 | 6 | nmol/mL | 0.89 | 0.54 | 61 |
| DAG 38:0 | 7 | nmol/mL | 0.24 | 0.13 | 55 |
| DAG 38:1 | 5 | nmol/mL | 0.51 | 0.39 | 77 |
| DAG 38:2 | 5 | nmol/mL | 1.5 | 1.2 | 81 |
| DAG 38:3 | 5 | nmol/mL | 1.3 | 1.0 | 80 |
| DAG 38:4 | 11 | nmol/mL | 0.95 | 0.38 | 40 |
| DAG 38:5 | 11 | nmol/mL | 1.8 | 0.82 | 47 |
| DAG 38:6 | 9 | nmol/mL | 0.77 | 0.37 | 47 |
| DAG 40:5 | 5 | nmol/mL | 0.084 | 0.053 | 63 |
| DAG 40:6 | 6 | nmol/mL | 0.28 | 0.17 | 60 |
| DAG 40:7 | 5 | nmol/mL | 0.89 | 0.68 | 77 |
|  |  |  |  |  |  |
| TAG 42:0 | 5 | nmol/mL | 0.38 | 0.19 | 50 |
| TAG 42:1 | 5 | nmol/mL | 0.37 | 0.17 | 45 |
| TAG 42:2 | 6 | nmol/mL | 0.16 | 0.064 | 41 |
| TAG 44:0 | 5 | nmol/mL | 1.2 | 0.73 | 62 |
| TAG 44:1 | 7 | nmol/mL | 1.7 | 0.84 | 50 |
| TAG 44:2 | 6 | nmol/mL | 0.90 | 0.40 | 45 |
| TAG 46:0 | 6 | nmol/mL | 2.8 | 1.6 | 56 |
| TAG 46:1 | 8 | nmol/mL | 5.7 | 2.6 | 46 |
| TAG 46:3 | 5 | nmol/mL | 0.76 | 0.34 | 45 |
| TAG 48:3 | 11 | nmol/mL | 3.3 | 1.3 | 41 |
| TAG 51:4 | 6 | nmol/mL | 1.4 | 0.62 | 43 |
| TAG 52:0 | 8 | nmol/mL | 3.4 | 1.8 | 54 |
| TAG 53:5 | 6 | nmol/mL | 0.84 | 0.37 | 44 |
| TAG 54:0 | 9 | nmol/mL | 2.4 | 1.3 | 51 |
| TAG 56:6 | 15 | nmol/mL | 6.4 | 2.7 | 42 |
| TAG 56:8 | 11 | nmol/mL | 3.3 | 1.3 | 40 |
| TAG 58:6 | 5 | nmol/mL | 1.6 | 0.68 | 42 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values > 40 %. The abbreviations identify diacylglycerols (DAG) and triacylglycerols (TAG).

Table S3. Consensus location and uncertainty estimates for glycerophospholipids (GP) in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| LPE 20:3 | 5 | nmol/mL | 0.52 | 0.38 | 72 |
| LPE 22:1 | 5 | nmol/mL | 0.036 | 0.030 | 82 |
| PC 30:1 | 5 | nmol/mL | 0.76 | 0.43 | 57 |
| PC O-34:4/P-34:3 | 6 | nmol/mL | 0.12 | 0.079 | 66 |
| PC O-36:0/35:0 | 5 | nmol/mL | 0.72 | 0.53 | 74 |
| PC 38:0 | 6 | nmol/mL | 2.0 | 0.85 | 42 |
| PC 38:1 | 6 | nmol/mL | 0.37 | 0.17 | 47 |
| PC 38:7 | 8 | nmol/mL | 0.79 | 0.35 | 44 |
| PC 40:2 | 8 | nmol/mL | 0.23 | 0.10 | 44 |
| PC 40:3 | 7 | nmol/mL | 0.27 | 0.14 | 51 |
| PC O-40:6/P-40:5/39:6 | 11 | nmol/mL | 1.8 | 0.74 | 42 |
| PC 42:6 | 5 | nmol/mL | 0.079 | 0.041 | 52 |
| PE 34:0 | 5 | nmol/mL | 1.6 | 1.1 | 65 |
| PE O-34:1/P-34:0 | 6 | nmol/mL | 0.46 | 0.22 | 48 |
| PE 36:5 | 11 | nmol/mL | 0.26 | 0.13 | 48 |
| PE O-36:6/P-36:5 | 7 | nmol/mL | 0.70 | 0.49 | 70 |
| PE 38:1 | 7 | nmol/mL | 2.6 | 1.7 | 67 |
| PE 38:2 | 7 | nmol/mL | 1.9 | 1.2 | 64 |
| PI 38:2 | 8 | nmol/mL | 0.34 | 0.16 | 47 |
| PI 40:5 | 8 | nmol/mL | 0.63 | 0.26 | 40 |
| PG 34:1 | 5 | nmol/mL | 1.3 | 0.60 | 45 |
| PG 36:1 | 5 | nmol/mL | 0.83 | 0.61 | 73 |
| PS 38:4 | 6 | nmol/mL | 2.2 | 1.6 | 74 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values > 40 %. The abbreviations identify lysophosphatidylethanolamines (LPE), phosphatidylcholines (PC), phosphatidylethanolamines (PE), phosphatidylglycerols (PG), phosphatidylinositols (PI), and phosphatidylserines (PS). For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a “/”.

Table S4. Consensus location and uncertainty estimates for sphingolipids (SP) in SRM 1950

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | | Consensus Location | Standard Uncertainty | COD (%) |
| HexCer d42:2 | 6 | | nmol/mL | 1.1 | 0.59 | 51 |
| CER d32:1 | 8 | | nmol/mL | 0.051 | 0.021 | 42 |
| CER d34:0 | 5 | | nmol/mL | 0.045 | 0.031 | 70 |
| CER d36:2 | 7 | | nmol/mL | 0.026 | 0.014 | 56 |
| CER d42:0 | 6 | | nmol/mL | 0.28 | 0.18 | 63 |
| CER d42:3 | 5 | | nmol/mL | 0.23 | 0.14 | 62 |
| CER d44:1 | 7 | | nmol/mL | 0.063 | 0.031 | 49 |
| CER d44:2 | 7 | | nmol/mL | 0.044 | 0.022 | 49 |
| SM d32:0 | 9 | | nmol/mL | 0.47 | 0.22 | 47 |
| SM d37:2 | 5 | | nmol/mL | 0.21 | 0.10 | 50 |
| SM d38:0 | 8 | | nmol/mL | 0.92 | 0.51 | 55 |
| SM d40:0 | 10 | | nmol/mL | 1.5 | 0.65 | 43 |
| SM d42:4 | 8 | | nmol/mL | 4.2 | 1.8 | 42 |
| SM d43:1 | 9 | | nmol/mL | 0.62 | 0.28 | 45 |
| SM d44:1 | 9 | | nmol/mL | 0.25 | 0.12 | 49 |
| SM d44:3 | 5 | | nmol/mL | 0.27 | 0.19 | 71 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values > 40 %. The abbreviations identify hexosylceramides (HexCer), ceramides (CER), and sphingomyelins (SM).

Table S5. Consensus location and uncertainty estimates for sterol (ST) lipids in SRM 1950

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | Consensus Location | Standard Uncertainty | COD (%) |
| CE 17:0 | 6 | nmol/mL | 6.0 | 2.5 | 42 |
| CE 20:1 | 6 | nmol/mL | 1.3 | 0.66 | 51 |
| CE 20:2 | 9 | nmol/mL | 5.8 | 3.1 | 53 |
| CE 22:4 | 7 | nmol/mL | 1.2 | 0.70 | 59 |

MEDM consensus estimates shown were calculated for those lipids measured by at least five laboratories and had COD values > 40 %. The abbreviation identifies cholesteryl ester (CE).

Table S6. Consensus location and uncertainty estimates (DSL and MEDM) for lipids reported by only three or four laboratories.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | DSL Consensus Location | DSL Standard Uncertainty | MEDM Consensus Location | DSL COD (%) | Difference (%) |
| Taurolithocholic acid sulfate | 3 | nmol/mL | 0.088 | 0.018 | 0.10 | 21 | 15 |
| ω-Muricholic acid | 3 | nmol/mL | 0.0056 | 0.00013 | 0.0057 | 2 | 1 |
| CE 22:0 | 4 | nmol/mL | 0.35 | 0.034 | 0.36 | 10 | 2 |
| CE 24:0 | 3 | nmol/mL | 0.28 | 0.052 | 0.31 | 18 | 7 |
| CE 24:1 | 3 | nmol/mL | 0.15 | 0.014 | 0.15 | 9 | 1 |
| Total Cholesterol | 3 | nmol/mL | 4,000 | 24 | 4,000 | 1 | 0 |
| HexCer 38:1 | 3 | nmol/mL | 0.20 | 0.00015 | 0.20 | 0 | 0 |
| CER d16:0 | 3 | nmol/mL | 0.052 | 0.0075 | 0.056 | 14 | 9 |
| CER d20:0 | 3 | nmol/mL | 0.028 | 0.0076 | 0.030 | 28 | 8 |
| CER d24:0 | 3 | nmol/mL | 0.090 | 0.033 | 0.084 | 37 | 6 |
| CER d39:1 | 4 | nmol/mL | 0.093 | 0.016 | 0.11 | 18 | 15 |
| DHC 16:0 | 3 | nmol/mL | 5.3 | 0.67 | 5.5 | 13 | 4 |
| DHC 22:0 | 3 | nmol/mL | 0.26 | 0.046 | 0.29 | 18 | 12 |
| DHC 24:0 | 3 | nmol/mL | 0.40 | 0.050 | 0.33 | 12 | 20 |
| DHC 24:1 | 3 | nmol/mL | 0.97 | 0.14 | 1.1 | 15 | 13 |
| DAG 40:4 | 4 | nmol/mL | 0.91 | 0.34 | 0.83 | 38 | 10 |
| FFA 17:0 | 3 | nmol/mL | 1.7 | 0.23 | 1.7 | 14 | 1 |
| FFA 17:1 | 3 | nmol/mL | 0.86 | 0.15 | 0.86 | 18 | 0 |
| FFA 20:1 | 3 | nmol/mL | 1.8 | 0.17 | 1.6 | 9 | 9 |
| LPC O-18:1 | 3 | nmol/mL | 0.41 | 0.13 | 0.35 | 31 | 16 |
| LPC O-20:0 | 4 | nmol/mL | 0.023 | 0.0049 | 0.025 | 22 | 9 |
| LPC 24:1 | 3 | nmol/mL | 0.022 | 0.0071 | 0.023 | 33 | 4 |

Final consensus location estimates for lipids with only three to four laboratories reporting (in nmol/mL plasma). The final consensus estimate (highlighted in grey) and COD (%) were determined using the DSL estimation. The criteria for inclusion was that the DSL mean had to have a COD ≤ 40 % and a percent difference between the DSL and MEDM consensus estimates had to be ≤ 20 %. Abbreviations: cholesteryl ester (CE), hexosylceramide (HexCer), ceramide (CER), dihydroceramide (DHC), diacylglycerol (DAG), free fatty acids (FFA), and lysophosphatidylcholine (LPC).

Table S6. (cont…)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | DSL Consensus Location | DSL Standard Uncertainty | MEDM Consensus Location | DSL COD (%) | Percent Difference (%) |
| LPC 26:0 | 3 | nmol/mL | 0.015 | 0.0031 | 0.016 | 21 | 3 |
| PC 28:0 | 4 | nmol/mL | 0.16 | 0.025 | 0.15 | 15 | 5 |
| PC O-42:6/P-42:5 | 4 | nmol/mL | 0.46 | 0.14 | 0.55 | 29 | 18 |
| PC O-42:7 | 3 | nmol/mL | 0.067 | 0.0011 | 0.078 | 2 | 15 |
| PC O-44:5/P-44:4 | 3 | nmol/mL | 1.3 | 0.30 | 1.4 | 24 | 6 |
| PE 34:3 | 4 | nmol/mL | 0.14 | 0.020 | 0.15 | 14 | 8 |
| PE 35:1 | 4 | nmol/mL | 0.15 | 0.045 | 0.14 | 30 | 5 |
| PG 34:2 | 4 | nmol/mL | 0.55 | 0.22 | 0.45 | 40 | 19 |
| PG 36:3 | 4 | nmol/mL | 0.50 | 0.11 | 0.43 | 22 | 15 |
| PS 38:1 | 3 | nmol/mL | 0.23 | 0.046 | 0.25 | 20 | 9 |
| PS 38:2 | 3 | nmol/mL | 0.24 | 0.040 | 0.27 | 16 | 11 |
| SM d35:0 | 3 | nmol/mL | 0.044 | 0.0072 | 0.050 | 16 | 13 |
| SM d42:5 | 3 | nmol/mL | 0.36 | 0.021 | 0.37 | 6 | 4 |
| dhSph-1P | 3 | nmol/mL | 0.10 | 0.035 | 0.10 | 35 | 4 |
| Sph-1P | 3 | nmol/mL | 0.42 | 0.0076 | 0.41 | 2 | 2 |
| TAG 44:3 | 4 | nmol/mL | 0.18 | 0.0094 | 0.18 | 5 | 1 |
| TAG 47:2 | 3 | nmol/mL | 0.21 | 0.027 | 0.22 | 13 | 7 |
| TAG 49:0 | 3 | nmol/mL | 0.31 | 0.055 | 0.29 | 18 | 5 |
| TAG 54:8 | 4 | nmol/mL | 0.92 | 0.30 | 0.90 | 32 | 2 |
| TAG 55:3 | 3 | nmol/mL | 0.43 | 0.15 | 0.35 | 34 | 20 |
| TAG 58:11 | 3 | nmol/mL | 0.11 | 0.018 | 0.13 | 16 | 13 |
| TAG 58:3 | 3 | nmol/mL | 0.19 | 0.019 | 0.21 | 10 | 8 |

Final consensus location estimates for lipids with only three to four laboratories reporting (in nmol/mL plasma). The final consensus estimate (highlighted in grey) and COD (%) were determined using the DSL estimation. The criteria for inclusion was that the DSL mean had to have a COD ≤ 40 % and a percent difference between the DSL and MEDM consensus estimates had to be ≤ 20 %. Abbreviations: lysophosphatidylcholine (LPC), phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylglycerol (PG), phosphatidylserine (PS), sphingomyelin (SM), and triacylglycerol (TAG).

Table S6. (cont…)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | # of Labs | Units | DSL Consensus Location | DSL Standard Uncertainty | MEDM Consensus Location | DSL COD (%) | Percent Difference (%) |
| 11,12-DiHETrE | 3 | pmol/mL | 0.82 | 0.28 | 1.0 | 34 | 20 |
| 11-HDoHE | 3 | pmol/mL | 0.63 | 0.092 | 0.61 | 15 | 3 |
| 12(13)-DiHOME | 3 | pmol/mL | 5.1 | 0.38 | 5.0 | 7 | 3 |
| 12(13)-EpOME | 3 | pmol/mL | 6.9 | 2.0 | 7.8 | 28 | 12 |
| 12-HHTrE | 3 | pmol/mL | 0.23 | 0.053 | 0.27 | 23 | 18 |
| 13-HOTrE | 3 | pmol/mL | 0.54 | 0.056 | 0.56 | 10 | 4 |
| 14-HDoHE | 4 | pmol/mL | 1.3 | 0.11 | 1.3 | 8 | 2 |
| 17-HDoHE | 3 | pmol/mL | 0.82 | 0.036 | 0.84 | 4 | 2 |
| 18-HEPE | 3 | pmol/mL | 0.28 | 0.069 | 0.25 | 25 | 10 |
| 20-HETE | 3 | pmol/mL | 2.1 | 0.53 | 2.0 | 25 | 7 |
| 5,6-EET | 3 | pmol/mL | 0.82 | 0.28 | 1.0 | 34 | 20 |
| 5-HEPE | 4 | pmol/mL | 0.85 | 0.016 | 0.86 | 2 | 2 |
| 8-HETE | 4 | pmol/mL | 0.98 | 0.22 | 1.1 | 22 | 15 |
| 8-HETrE | 3 | pmol/mL | 0.38 | 0.093 | 0.46 | 24 | 19 |
| 9,10-DiHOME | 3 | pmol/mL | 6.7 | 0.44 | 7.0 | 7 | 5 |
| 9-HEPE | 4 | pmol/mL | 0.43 | 0.087 | 0.50 | 20 | 15 |
| 9-HETE | 4 | pmol/mL | 0.85 | 0.082 | 0.85 | 10 | 0 |
| 9-HODE | 3 | pmol/mL | 10 | 2.6 | 9.7 | 25 | 5 |
| 9-OxoODE (9-KODE) | 3 | pmol/mL | 7.3 | 1.3 | 6.8 | 18 | 7 |
| PGE2 | 4 | pmol/mL | 0.035 | 0.014 | 0.040 | 40 | 14 |

Final consensus location estimates for lipids with only three to four laboratories reporting (in pmol/mL plasma). The final consensus estimate (highlighted in grey) and COD (%) were determined using the DSL estimation. The criteria for inclusion was that the DSL mean had to have a COD ≤ 40 % and a percent difference between the DSL and MEDM consensus estimates had to be ≤ 20 %.

**Comparison of final consensus location estimates calculated in this exercise to the lipid concentrations reported in the LIPID MAPS consortium**

The comparison was made on an individual lipid species basis (comparing common species between both studies). With both the LIPID MAPS and this study, the standard uncertainties represent the expected “one standard deviation” uncertainty of the consensus value. The percent change between the final consensus location estimate of the interlaboratory exercise (CIL) and the LIPID MAPS value (CLM) was calculated using the following equation: percent change = ((CIL – CLM)/CLM)) x 100. The LIPID MAPS values for the DAGs listed here are a summation of the reported 1,2- and 1,3-DAG species, same with the FFA 18:3 and FFA 20:3 species. The associated derived uncertainty per summed lipid was calculated by squaring the listed uncertainty provided (variance for those two isomers added), summing the two variances, and taking the square root of the final summer variance.

Table S7. Percent difference between cholesteryl ester (CE) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | LIPID MAPS | |  |
| Lipid | Units | Consensus Location | Standard Uncertainty | Mean | Standard Uncertainty | Difference (%) |
| CE 14:0 | nmol/mL | 16 | 6.0 | 80 | 2 | -80 |
| CE 15:0 | nmol/mL | 5.3 | 1.8 | 30 | 1 | -82 |
| CE 16:0 | nmol/mL | 210 | 58 | 190 | 6 | 8 |
| CE 16:1 | nmol/mL | 100 | 27 | 111 | 4 | -8 |
| CE 16:2 | nmol/mL | 1.9 | 0.46 | 31 | 1 | -94 |
| CE 17:0 | nmol/mL | 6.0 | 2.5 | 32 | 1 | -81 |
| CE 17:1 | nmol/mL | 8.2 | 1.0 | 31 | 1 | -73 |
| CE 18:0 | nmol/mL | 15 | 3.7 | 59 | 3 | -74 |
| CE 18:1 | nmol/mL | 450 | 110 | 533 | 13 | -15 |
| CE 18:2 | nmol/mL | 1,700 | 430 | 1820 | 85 | -9 |
| CE 18:3 | nmol/mL | 84 | 24 | 147 | 8 | -43 |
| CE 20:1 | nmol/mL | 1.3 | 0.66 | 30 | 1 | -96 |
| CE 20:2 | nmol/mL | 5.8 | 3.1 | 34 | 2 | -83 |
| CE 20:3 | nmol/mL | 35 | 12 | 32 | 1 | 9 |
| CE 20:4 | nmol/mL | 350 | 58 | 237 | 13 | 46 |
| CE 22:6 | nmol/mL | 37 | 9.5 | 32 | 2 | 16 |
|  |  |  |  |  |  |  |
| Cholesterol | nmol/mL | 770 | 110 | 820 | 9 | -6 |

Table S8. Percent difference between ceramide (CER) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | | MEDM | | | | | LIPID MAPS | | | |  | |
| Lipid | Units | | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | | Difference  (%) | |
| HexCer d34:1 | | nmol/mL | | 0.86 | | 0.21 | 0.336 | | | 0.029 | 155 | |
| HexCer d36:1 | | nmol/mL | | 0.13 | | 0.043 | 0.0275 | | | 0.0037 | 362 | |
| HexCer d40:1 | | nmol/mL | | 2.4 | | 0.68 | 0.522 | | | 0.033 | 366 | |
| HexCer d42:1 | | nmol/mL | | 2.7 | | 0.73 | 0.409 | | | 0.028 | 555 | |
| HexCer d42:2 | | nmol/mL | | 1.1 | | 0.59 | 0.332 | | | 0.009 | 243 | |
| CER d32:1 | | nmol/mL | | 0.051 | | 0.021 | 0.012 | | | 0.001 | 328 | |
| *CER d34:0* | | nmol/mL | | 0.045 | | 0.031 | 0.261 | | | 0.0004 | -83 | |
| CER d34:1 | | nmol/mL | | 0.28 | | 0.044 | 0.331 | | | 0.029 | -16 | |
| CER d36:1 | | nmol/mL | | 0.12 | | 0.021 | 0.128 | | | 0.012 | -5 | |
| CER d36:2 | | nmol/mL | | 0.026 | | 0.014 | 0.022 | | | 0.001 | 16 | |
| CER d38:1 | | nmol/mL | | 0.11 | | 0.021 | 0.145 | | | 0.007 | -25 | |
| CER d40:1 | | nmol/mL | | 0.65 | | 0.12 | 1.22 | | | 0.046 | -46 | |
| *CER d40:2* | | nmol/mL | | 0.15 | | 0.021 | 0.2 | | | 0.009 | -28 | |
| CER d41:1 | | nmol/mL | | 0.67 | | 0.27 | 0.281 | | | 0.033 | 138 | |
| *CER d42:0* | | nmol/mL | | 0.28 | | 0.18 | 1.22 | | | 0.004 | -77 | |
| CER d42:1 | | nmol/mL | | 1.9 | | 0.47 | 3 | | | 0.107 | -36 | |
| CER d42:2 | | nmol/mL | | 0.82 | | 0.10 | 1 | | | 0.029 | -18 | |
| *CER d42:3* | | nmol/mL | | 0.23 | | 0.14 | 0.001 | | | 0.0001 | 22700 | |
| CER d44:1 | | nmol/mL | | 0.063 | | 0.031 | 0.061 | | | 0.0007 | 3 | |
| CER d44:2 | | nmol/mL | | 0.044 | | 0.022 | 0.036 | | | 0.002 | 23 | |

All ceramides are noted to contain a d18:1 backbone, unless italicized (indicating the presence of d18:0 or d18:2).

Table S9. Percent difference between diacylglycerol (DAG) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | | | | LIPID MAPS | | | |  | |
| Lipid | Units | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | | Difference (%) | |
| DAG 30:0 | nmol/mL | | 0.83 | | 0.17 | 0.823 | | | 0.21 | 1 | |
| DAG 32:0 | nmol/mL | | 2.6 | | 1.2 | 2.097 | | | 0.421 | 25 | |
| DAG 32:1 | nmol/mL | | 1.2 | | 0.62 | 1.481 | | | 0.145 | -18 | |
| DAG 32:2 | nmol/mL | | 0.62 | | 0.29 | 0.576 | | | 0.072 | 7 | |
| DAG 34:0 | nmol/mL | | 6.5 | | 3.6 | 2.41 | | | 0.541 | 168 | |
| DAG 34:1 | nmol/mL | | 6.1 | | 2.4 | 5.35 | | | 0.628 | 13 | |
| DAG 34:2 | nmol/mL | | 4.4 | | 1.9 | 3.98 | | | 0.376 | 10 | |
| DAG 34:3 | nmol/mL | | 0.31 | | 0.20 | 2.221 | | | 0.176 | -86 | |
| DAG 36:0 | nmol/mL | | 1.6 | | 0.98 | 1.459 | | | 0.2 | 12 | |
| DAG 36:1 | nmol/mL | | 2.6 | | 1.1 | 1.601 | | | 0.335 | 59 | |
| DAG 36:2 | nmol/mL | | 6.2 | | 2.2 | 5.42 | | | 0.56 | 14 | |
| DAG 36:3 | nmol/mL | | 8.4 | | 3.3 | 9.94 | | | 1.016 | -15 | |
| DAG 36:4 | nmol/mL | | 2.8 | | 1.0 | 6.7 | | | 0.665 | -59 | |
| DAG 36:5 | nmol/mL | | 0.89 | | 0.54 | 1.273 | | | 0.039 | -30 | |
| DAG 38:0 | nmol/mL | | 0.24 | | 0.13 | 0.043 | | | 0.021 | 458 | |
| DAG 38:1 | nmol/mL | | 0.51 | | 0.39 | 0.013 | | | 0.005 | 3831 | |
| DAG 38:2 | nmol/mL | | 1.5 | | 1.2 | 0.024 | | | 0.01 | 5983 | |
| DAG 38:3 | nmol/mL | | 1.3 | | 1.0 | 0.287 | | | 0.02 | 353 | |
| DAG 38:4 | nmol/mL | | 0.95 | | 0.38 | 0.976 | | | 0.111 | -3 | |
| DAG 38:5 | nmol/mL | | 1.8 | | 0.82 | 1.863 | | | 0.202 | -6 | |
| DAG 38:6 | nmol/mL | | 0.77 | | 0.37 | 1.536 | | | 0.095 | -50 | |
| DAG 40:6 | nmol/mL | | 0.28 | | 0.17 | 0.298 | | | 0.036 | -5 | |
| DAG 40:7 | nmol/mL | | 0.89 | | 0.68 | 0.428 | | | 0.07 | 108 | |

The LIPID MAPS values for the DAGs were a summation of the reported 1,2- and 1,3-DAG species.

Table S10. Percent difference between free fatty acid (FFA) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | | | | LIPID MAPS | | | |  | |
| Lipid | Units | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | | Difference (%) | |
| FFA 16:0 | nmol/mL | | 43 | | 13 | 63.8 | | | 0.4 | -33 | |
| FFA 16:1 | nmol/mL | | 6.1 | | 2.9 | 14.7 | | | 0.169 | -59 | |
| FFA 18:0 | nmol/mL | | 15 | | 9.0 | 22.1 | | | 0.035 | -34 | |
| FFA 18:1 | nmol/mL | | 110 | | 53 | 80.3 | | | 9.331 | 37 | |
| FFA 18:2 | nmol/mL | | 44 | | 22 | 15.2 | | | 0.437 | 191 | |
| FFA 18:3 | nmol/mL | | 2.9 | | 0.62 | 1.145 | | | 0.006 | 152 | |
| FFA 20:3 | nmol/mL | | 1.3 | | 0.62 | 0.978 | | | 0.021 | 35 | |
| FFA 20:4 | nmol/mL | | 4.7 | | 1.5 | 2.94 | | | 0.058 | 61 | |
| FFA 20:5 | nmol/mL | | 0.42 | | 0.056 | 0.435 | | | 0.01 | -3 | |
| FFA 22:5 | nmol/mL | | 1.1 | | 0.56 | 0.4 | | | 0.005 | 170 | |
| FFA 22:6 | nmol/mL | | 1.5 | | 0.17 | 0.99 | | | 0.009 | 55 | |
|  |  | |  | |  |  | | |  |  | |
| 12-HETE | pmol/mL | | 6.8 | | 1.5 | 4.22 | | | 0.292 | 61 | |
| 15-HETE | pmol/mL | | 2.4 | | 0.64 | 0.8 | | | 0.023 | 199 | |
| 5-HETE | pmol/mL | | 10 | | 1.3 | 11.9 | | | 1.4 | -14 | |

The LIPID MAPS values for the 18:3 FFA and 20:3 FFA were a summation of the reported species.

Table S11. Percent difference between lysophospholipid consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | | MEDM | | | | | LIPID MAPS | | |  | | |
| Lipid | Units | | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | Difference (%) | | |
| LPC 16:0 | | nmol/mL | | 73 | | 11 | 29.8 | | | 4.9 | | 145 |
| LPC O-16:0 | | nmol/mL | | 0.55 | | 0.16 | 0.491 | | | 0.089 | | 11 |
| LPC P-16:0 | | nmol/mL | | 0.46 | | 0.13 | 1.73 | | | 0.26 | | -74 |
| LPC 16:1 | | nmol/mL | | 2.4 | | 0.35 | 3.77 | | | 0.68 | | -37 |
| LPC 18:0 | | nmol/mL | | 27 | | 3.3 | 23.3 | | | 3.5 | | 15 |
| LPC O-18:0 | | nmol/mL | | 0.16 | | 0.058 | 0.911 | | | 0.149 | | -83 |
| LPC 18:1 | | nmol/mL | | 18 | | 2.3 | 14.8 | | | 2.3 | | 24 |
| LPC 18:2 | | nmol/mL | | 22 | | 2.9 | 16.9 | | | 2.2 | | 31 |
| LPC 20:3 | | nmol/mL | | 1.8 | | 0.26 | 3.26 | | | 0.43 | | -46 |
| LPC 20:4 | | nmol/mL | | 6.0 | | 0.60 | 5.73 | | | 0.73 | | 5 |
| LPC 22:5 | | nmol/mL | | 0.43 | | 0.13 | 1 | | | 0.11 | | -58 |
| LPC 22:6 | | nmol/mL | | 0.77 | | 0.14 | 1.57 | | | 0.18 | | -51 |
|  | |  | |  | |  |  | | |  | |  |
| LPE 16:0 | | nmol/mL | | 0.91 | | 0.27 | 3.45 | | | 0.42 | | -74 |
| LPE 18:0 | | nmol/mL | | 1.6 | | 0.55 | 7.41 | | | 0.76 | | -78 |
| LPE 18:1 | | nmol/mL | | 1.4 | | 0.47 | 6.44 | | | 0.71 | | -79 |
| LPE 18:2 | | nmol/mL | | 1.9 | | 0.56 | 7.85 | | | 1.06 | | -76 |
| LPE 20:4 | | nmol/mL | | 1.1 | | 0.41 | 7.32 | | | 0.75 | | -85 |
| LPE 22:1 | | nmol/mL | | 0.036 | | 0.030 | 0.311 | | | 0.099 | | -100 |
| LPE 22:6 | | nmol/mL | | 0.52 | | 0.18 | 3.86 | | | 0.44 | | -87 |

Table S12. Percent difference between phosphatidylcholine (PC) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | LIPID MAPS | |  |
| Lipid | Units | Consensus Location | Standard Uncertainty | Mean | Standard Uncertainty | Difference (%) |
| PC 30:1 | nmol/mL | 0.76 | 0.43 | 1.12 | 0.11 | -32 |
| PC 32:0 | nmol/mL | 7.2 | 1.0 | 11.4 | 0.6 | -37 |
| PC 32:1 | nmol/mL | 13 | 1.9 | 28.6 | 1.8 | -55 |
| PC P-33:1/**32:2** | nmol/mL | 2.6 | 0.37 | 9.8 | 0.45 | -73 |
| PC 34:0 | nmol/mL | 2.1 | 0.37 | 7.66 | 2.05 | -73 |
| PC 34:1 | nmol/mL | 120 | 21 | 89.3 | 8.1 | 33 |
| PC **O-34:1**/P-34:0/33:1 | nmol/mL | 4.9 | 0.86 | 2.8 | 0.13 | 75 |
| PC **O-34:2**/P-34:1/33:2 | nmol/mL | 5.2 | 1.3 | 3.99 | 0.21 | 30 |
| PC P-35:1/**34:2** | nmol/mL | 240 | 47 | 188 | 14 | 30 |
| PC P-35:2/**34:3** | nmol/mL | 12 | 1.7 | 13.8 | 1 | -12 |
| PC 36:1 | nmol/mL | 26 | 4.6 | 99.8 | 13 | -74 |
| PC **O-36:1/P-36:0**/35:1 | nmol/mL | 3.5 | 0.99 | 2.57 | 0.55 | 36 |
| PC 36:2 | nmol/mL | 140 | 25 | 254 | 18 | -44 |
| PC **O-36:2/P-36:1**/35:2 | nmol/mL | 7.4 | 1.7 | 6.25 | 0.55 | 19 |
| PC 36:3 | nmol/mL | 100 | 14 | 165 | 13 | -39 |
| PC 36:4 | nmol/mL | 150 | 28 | 172 | 11 | -14 |
| PC **O-36:4/P-36:3**/35:4 | nmol/mL | 12 | 1.4 | 29 | 1.5 | -60 |
| PC 36:5 | nmol/mL | 11 | 1.8 | 12.8 | 1.2 | -15 |
| PC 38:2 | nmol/mL | 2.3 | 0.20 | 37.6 | 5.7 | -94 |
| PC **O-38:3/P-38:2**/37:3 | nmol/mL | 1.5 | 0.51 | 11.6 | 0.9 | -87 |
| PC 38:4 | nmol/mL | 84 | 14 | 254 | 21 | -67 |
| PC 38:5 | nmol/mL | 42 | 7.9 | 86.3 | 9 | -51 |
| PC **O-38:5/P-38:4**/37:5 | nmol/mL | 11 | 1.6 | 49.9 | 2.8 | -77 |
| PC 38:6 | nmol/mL | 41 | 4.4 | 62.9 | 4.9 | -36 |
| PC P-38:6/**36:0** | nmol/mL | 1.2 | 0.39 | 7.95 | 1.51 | -85 |
| PC 40:2 | nmol/mL | 0.23 | 0.10 | 133 | 16 | -100 |
| PC 40:4 | nmol/mL | 2.9 | 0.37 | 36.7 | 5.5 | -92 |
| PC 40:5 | nmol/mL | 6.7 | 1.1 | 66.6 | 10.1 | -90 |
| PC 40:6 | nmol/mL | 14 | 2.6 | 79.4 | 10.3 | -82 |
| PC 40:7 | nmol/mL | 3.5 | 0.76 | 23.1 | 4.5 | -85 |
| PC 40:8 | nmol/mL | 0.73 | 0.20 | 27 | 2.5 | -97 |

Lipid identifications in bold indicate the reported isomer/lipid identification made by the LIPID MAPS consortium for that lipid, whereas the consensus mean identification reported in this report includes all the lipid reported for that lipid at the sum composition level.

Table S13. Percent difference between phosphatidylethanolamine (PE) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | |  | MEDM | | | | LIPID MAPS | | | |  | |
| Lipid | | Units | Consensus Location | | Standard Uncertainty | | Mean | | Standard Uncertainty | | Difference (%) | |
| PE 32:1 | nmol/mL | | | 0.34 | | 0.12 | | 0.904 | | 0.065 | | -63 | |
| PE 34:0 | nmol/mL | | | 1.6 | | 1.1 | | 0.801 | | 0.128 | | 103 | |
| PE 34:1 | nmol/mL | | | 1.2 | | 0.17 | | 5.95 | | 0.18 | | -79 | |
| PE 34:2 | nmol/mL | | | 2.2 | | 0.26 | | 12 | | 0.8 | | -82 | |
| PE O-34:2/**P-34:1** | nmol/mL | | | 0.78 | | 0.17 | | 3.93 | | 0.13 | | -80 | |
| PE O-34:3/**P-34:2** | nmol/mL | | | 1.5 | | 0.41 | | 7.32 | | 0.23 | | -79 | |
| PE 36:0 | nmol/mL | | | 0.28 | | 0.10 | | 14.1 | | 0.6 | | -98 | |
| PE 36:1 | nmol/mL | | | 1.3 | | 0.26 | | 8.21 | | 0.37 | | -85 | |
| PE 36:2 | nmol/mL | | | 6.7 | | 0.79 | | 29.5 | | 0.9 | | -77 | |
| PE **O-36:2/P-36:1**/35:2 | nmol/mL | | | 0.93 | | 0.22 | | 5.46 | | 0.18 | | -83 | |
| PE 36:3 | nmol/mL | | | 2.4 | | 0.38 | | 16 | | 0.5 | | -85 | |
| PE **O-36:3/P-36:2**/35:3 | nmol/mL | | | 3.2 | | 0.76 | | 13.7 | | 0.5 | | -77 | |
| PE 36:4 | nmol/mL | | | 3.1 | | 0.39 | | 22.9 | | 0.5 | | -86 | |
| PE O-36:4/P-36:3 | nmol/mL | | | 1.6 | | 0.29 | | 11.7 | | 0.3 | | -86 | |
| PE 36:5 | nmol/mL | | | 0.26 | | 0.13 | | 4.1 | | 0.2 | | -94 | |
| PE O-36:5/P-36:4 | nmol/mL | | | 4.9 | | 1.9 | | 19.6 | | 0.9 | | -75 | |
| PE 38:1 | nmol/mL | | | 2.6 | | 1.7 | | 10.3 | | 0.3 | | -75 | |
| PE 38:2 | nmol/mL | | | 1.9 | | 1.2 | | 0.763 | | 0.142 | | 144 | |
| PE 38:3 | nmol/mL | | | 0.95 | | 0.20 | | 6.83 | | 0.73 | | -86 | |
| PE 38:4 | nmol/mL | | | 8.1 | | 1.2 | | 48.1 | | 2 | | -83 | |
| PE 38:5 | nmol/mL | | | 2.7 | | 0.47 | | 20.9 | | 0.8 | | -87 | |
| PE O-38:5/P-38:4 | nmol/mL | | | 5.8 | | 1.9 | | 54.6 | | 0.3 | | -89 | |
| PE 38:6 | nmol/mL | | | 3.2 | | 0.59 | | 19.5 | | 0.7 | | -84 | |
| PE O-38:6/P-38:5 | nmol/mL | | | 4.9 | | 1.2 | | 32.7 | | 0.6 | | -85 | |
| PE 40:4 | nmol/mL | | | 0.26 | | 0.082 | | 2.34 | | 0.06 | | -89 | |
| PE 40:5 | nmol/mL | | | 0.73 | | 0.23 | | 4.84 | | 0.44 | | -85 | |
| PE **O-40:5**/P-40:4/39:5 | nmol/mL | | | 0.73 | | 0.13 | | 7.7 | | 0.25 | | -91 | |
| PE 40:6 | nmol/mL | | | 1.8 | | 0.36 | | 10 | | 0.5 | | -82 | |
| PE **O-40:6**/P-40:5/39:6 | nmol/mL | | | 1.3 | | 0.31 | | 11.5 | | 0.3 | | -89 | |
| PE 40:7 | nmol/mL | | | 0.77 | | 0.26 | | 2.57 | | 0.18 | | -70 | |
| PE **O-40:7**/P-40:6/39:7 | nmol/mL | | | 2.5 | | 0.72 | | 15.9 | | 0.4 | | -84 | |

Lipid identifications in bold indicate the reported isomer/lipid identification made by the LIPID MAPS consortium for that lipid, whereas the consensus mean identification reported in this report includes all the lipid reported for that lipid at the sum composition level.

Table S14. Percent difference between other phospholipid consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | | | | LIPID MAPS | | | |  |
| Lipid | Units | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | | Difference (%) |
| PG 34:1 | nmol/mL | | 1.3 | | 0.60 | 0.604 | | | 0.044 | 119 | |
| PG 36:1 | nmol/mL | | 0.83 | | 0.61 | 1.59 | | | 0.12 | -48 | |
| PG 36:2 | nmol/mL | | 0.67 | | 0.24 | 0.194 | | | 0.01 | 243 | |
|  |  | |  | |  |  | | |  |  | |
| PI 32:1 | nmol/mL | | 0.56 | | 0.11 | 0.746 | | | 0.165 | -25 | |
| PI 34:1 | nmol/mL | | 2.4 | | 0.42 | 1.78 | | | 0.14 | 37 | |
| PI 34:2 | nmol/mL | | 2.8 | | 0.38 | 2.64 | | | 1.3 | 4 | |
| PI 36:1 | nmol/mL | | 2.1 | | 0.59 | 1.77 | | | 0.14 | 20 | |
| PI 36:3 | nmol/mL | | 2.2 | | 0.29 | 1.17 | | | 0.06 | 84 | |
| PI 36:4 | nmol/mL | | 3.0 | | 0.48 | 1.27 | | | 0.08 | 135 | |
| PI 38:2 | nmol/mL | | 0.34 | | 0.16 | 0.189 | | | 0.059 | 81 | |
| PI 38:3 | nmol/mL | | 3.4 | | 0.54 | 1.83 | | | 0.14 | 84 | |
| PI 38:4 | nmol/mL | | 19 | | 2.2 | 11 | | | 0.7 | 74 | |
| PI 38:5 | nmol/mL | | 2.5 | | 0.44 | 1.28 | | | 0.14 | 95 | |
| PI 38:6 | nmol/mL | | 0.32 | | 0.031 | 0.498 | | | 0.13 | -35 | |
| PI 40:4 | nmol/mL | | 0.30 | | 0.042 | 0.451 | | | 0.03 | -33 | |
| PI 40:5 | nmol/mL | | 0.63 | | 0.26 | 0.475 | | | 0.046 | 33 | |
| PI 40:6 | nmol/mL | | 0.84 | | 0.16 | 0.54 | | | 0.053 | 56 | |
|  |  | |  | |  |  | | |  |  | |
| PS 38:4 | nmol/mL | | 2.2 | | 1.6 | 0.481 | | | 0.083 | 353 | |

Table S15. Percent difference between sphingomyelin (SM) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | | | LIPID MAPS | | | |  | |
| Lipid | Units | Consensus Location | | Standard Uncertainty | | Mean | | Standard Uncertainty | | Difference (%) | |
| SM d32:0 | nmol/mL | | 0.47 | | 0.22 | | 1 | | 0.01 | | -53 |
| SM d32:1 | nmol/mL | | 8.4 | | 1.4 | | 9.17 | | 0.18 | | -8 |
| SM d32:2 | nmol/mL | | 0.66 | | 0.24 | | 0.544 | | 0.016 | | 21 |
| SM d33:1 | nmol/mL | | 4.7 | | 0.64 | | 6.22 | | 0.12 | | -25 |
| SM d34:0 | nmol/mL | | 5.8 | | 1.3 | | 16.7 | | 0.2 | | -66 |
| SM d34:1 | nmol/mL | | 100 | | 15 | | 81 | | 0.9 | | 26 |
| SM d34:2 | nmol/mL | | 16 | | 2.2 | | 0.702 | | 0.021 | | 2136 |
| SM d35:1 | nmol/mL | | 2.5 | | 0.58 | | 3.75 | | 0.36 | | -34 |
| SM d36:0 | nmol/mL | | 2.0 | | 0.49 | | 4.11 | | 0.08 | | -51 |
| SM d36:1 | nmol/mL | | 20 | | 3.7 | | 16.2 | | 0.4 | | 25 |
| SM d36:2 | nmol/mL | | 9.6 | | 1.5 | | 10.8 | | 0.2 | | -11 |
| SM d36:3 | nmol/mL | | 1.3 | | 0.41 | | 1.05 | | 0.07 | | 26 |
| SM d37:1 | nmol/mL | | 1.0 | | 0.23 | | 0.902 | | 0.055 | | 12 |
| SM d38:0 | nmol/mL | | 0.92 | | 0.51 | | 2.78 | | 0.03 | | -67 |
| SM d38:1 | nmol/mL | | 11 | | 3.1 | | 9.98 | | 0.24 | | 14 |
| SM d38:2 | nmol/mL | | 5.2 | | 1.3 | | 6.6 | | 0.24 | | -21 |
| SM d38:3 | nmol/mL | | 0.61 | | 0.24 | | 0.511 | | 0.044 | | 20 |
| SM d39:1 | nmol/mL | | 3.6 | | 1.0 | | 4.34 | | 0.13 | | -17 |
| SM d39:2 | nmol/mL | | 0.61 | | 0.16 | | 0.894 | | 0.044 | | -32 |
| SM d40:0 | nmol/mL | | 1.5 | | 0.65 | | 3.32 | | 0.1 | | -55 |
| SM d40:1 | nmol/mL | | 20 | | 5.1 | | 15 | | 0.4 | | 33 |
| SM d40:2 | nmol/mL | | 12 | | 2.8 | | 15.7 | | 0.6 | | -24 |
| SM d40:3 | nmol/mL | | 2.2 | | 0.79 | | 1.47 | | 0.1 | | 47 |
| SM d41:1 | nmol/mL | | 7.7 | | 2.1 | | 7 | | 0.27 | | 9 |
| SM d41:2 | nmol/mL | | 5.8 | | 1.4 | | 5.85 | | 0.15 | | -1 |
| SM d41:3 | nmol/mL | | 0.77 | | 0.30 | | 0.672 | | 0.011 | | 15 |
| SM d42:1 | nmol/mL | | 20 | | 5.4 | | 12.5 | | 0.6 | | 58 |
| SM d42:2 | nmol/mL | | 44 | | 11 | | 33 | | 0.8 | | 33 |
| SM d42:3 | nmol/mL | | 17 | | 4.7 | | 21.2 | | 0.6 | | -18 |
| SM d42:4 | nmol/mL | | 4.2 | | 1.8 | | 3.67 | | 0.17 | | 14 |
| SM d43:1 | nmol/mL | | 0.62 | | 0.28 | | 1.3 | | 0.05 | | -52 |
| SM d43:2 | nmol/mL | | 1.0 | | 0.29 | | 1.73 | | 0.07 | | -40 |
| SM d44:1 | nmol/mL | | 0.25 | | 0.12 | | 0.216 | | 0.005 | | 14 |
| SM d44:2 | nmol/mL | | 0.40 | | 0.13 | | 0.276 | | 0.011 | | 45 |
| SM d44:3 | nmol/mL | | 0.27 | | 0.19 | | 0.468 | | 0.007 | | -42 |

Table S16. Percent difference between triacylglycerols (TAG) consensus locations and concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | MEDM | | | | | LIPID MAPS | | | |  | |
| Lipid | Units | Consensus Location | | Standard Uncertainty | | | Mean | Standard Uncertainty | | | Difference (%) | |
| TAG 48:1 | nmol/mL | | 13 | | 3.2 | 27 | | | 2.9 | -51 | |
| TAG 48:2 | nmol/mL | | 16 | | 2.8 | 20.2 | | | 4.1 | -22 | |
| TAG 50:0 | nmol/mL | | 3.8 | | 0.83 | 11.6 | | | 2.8 | -67 | |
| TAG 50:1 | nmol/mL | | 38 | | 10.0 | 63.6 | | | 1.8 | -40 | |
| TAG 50:2 | nmol/mL | | 47 | | 12 | 79.8 | | | 8.9 | -42 | |
| TAG 50:3 | nmol/mL | | 23 | | 6.6 | 57.1 | | | 5.5 | -60 | |
| TAG 50:4 | nmol/mL | | 8.7 | | 2.9 | 18.9 | | | 3.2 | -54 | |
| TAG 52:1 | nmol/mL | | 14 | | 2.9 | 29.6 | | | 1.9 | -52 | |
| TAG 52:2 | nmol/mL | | 44 | | 14 | 139.5 | | | 10 | -68 | |
| TAG 52:3 | nmol/mL | | 100 | | 29 | 214.8 | | | 22 | -52 | |
| TAG 52:4 | nmol/mL | | 48 | | 17 | 90.9 | | | 9.6 | -47 | |
| TAG 52:5 | nmol/mL | | 15 | | 5.7 | 32 | | | 1.4 | -54 | |
| TAG 54:2 | nmol/mL | | 8.2 | | 2.6 | 21.5 | | | 4.3 | -62 | |
| TAG 54:3 | nmol/mL | | 26 | | 9.8 | 69.1 | | | 9.5 | -62 | |
| TAG 54:4 | nmol/mL | | 36 | | 13 | 68.5 | | | 10.3 | -48 | |
| TAG 54:5 | nmol/mL | | 27 | | 11 | 53.6 | | | 6 | -49 | |
| TAG 54:6 | nmol/mL | | 14 | | 5.1 | 36.5 | | | 2.6 | -62 | |
| TAG 56:6 | nmol/mL | | 6.4 | | 2.7 | 23.5 | | | 2.6 | -73 | |

Table S17. Percent difference between summed interlaboratory consensus location estimates to summed concentrations derived from concentrations reported by the LIPID MAPS consortium

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Σ MEDM | | Σ LIPID MAPS | |  |
| Lipid Class | Number of Lipid Species | Units | Consensus Location | Standard Uncertainty | Mean | Standard Uncertainty | Difference (%) |
| CE | 16 | nmol/mL | 2981 | 450 | 3429 | 88 | -13 |
| CER/HexCer | 20 | nmol/mL | 13 | 1 | 9.54 | 0.14 | 33 |
| Cholesterol | 1 | nmol/mL | 767 | 111 | 820 | 9 | -6 |
| DAG | 23 | nmol/mL | 53 | 7 | 50.80 | 1.77 | 4 |
| EICO | 3 | pmol/mL | 19 | 2 | 16.92 | 1.43 | 15 |
| FFA | 11 | nmol/mL | 229 | 59 | 203 | 9 | 13 |
| LPC | 12 | nmol/mL | 153 | 12 | 103 | 7 | 48 |
| LPE | 7 | nmol/mL | 7 | 1 | 36.64 | 1.77 | -80 |
| Other PL | 4 | nmol/mL | 5 | 2 | 2.87 | 0.15 | 74 |
| PC | 31 | nmol/mL | 1074 | 68 | 1974 | 47 | -46 |
| PE | 31 | nmol/mL | 70 | 4 | 425 | 3 | -83 |
| PI | 14 | nmol/mL | 40 | 3 | 25.64 | 1.52 | 58 |
| SM | 35 | nmol/mL | 334 | 22 | 301 | 2 | 11 |
| TAG | 18 | nmol/mL | 491 | 46 | 1058 | 33 | -54 |
| Total Lipids | 226 | nmol/mL | 6218 | 475 | 8438 | 106 | -26 |

The summed uncertainty was calculated by using the variance for the sum (i.e., squaring all the uncertainty values), summing the variances per lipid class, and taking the square root of the value. Other PL includes PG (*n* = 3) and PS (*n* = 1) species.