Application Note

Metabolomics/
Clinical Research

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A Comprehensive, Curated, High-Throughput Method for the Detailed Analysis of the Plasma Lipidome

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Abstract

The use of advanced lipidomic techniques such as liquid chromatography/tandem mass spectrometry (LC/MS/MS) to study the human lipidome at the population level has enabled researchers to probe the relationships between disease states and lipid metabolism. Such studies necessarily involve large sample numbers from population cohorts. Capturing a comprehensive picture of the lipidome requires the analysis of several hundred different lipid species, and thus a balance between depth of coverage and sample throughput. This application note describes a targeted LC/TQ-based method for the determination of 763 different human lipid species using a 10 µL volume of plasma. The total analysis time was 16 minutes per sample using a single column, reduced to 13 minutes when running a dual column system. Also discussed are considerations for sample preparation and lipid extraction, quality control strategies, internal standard formulation, instrument conditions, and data processing.

Introduction

Lipids are complex biological molecules with a diverse range of properties and functions. They comprise the primary component of cellular membranes and adipose tissue, and serve as the major energy storage molecule in mammalian systems. They also play an integral role in cell-signaling pathways. Consequently, an increased understanding of lipid biology is of great interest to a broad range of scientific fields, from agriculture to medicine.

Lipidomics is the study of the lipidome: the entire complement of lipids within a given biological system, such as a cell, tissue, or volume of plasma. Its ultimate goal is to obtain a global view of the lipid species present, their metabolism, and associated biology. In recent years, advances in lipidomic technology have enabled us to map the broad range of lipids, including isomeric and isobaric species, present within the lipidome. In particular, techniques such as liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS), and multiple reaction monitoring (MRM), now allow users to measure hundreds of different lipid species within a short timeframe and with a high degree of specificity. The improved sensitivity of newer instruments facilitates the determination of these compounds at minute concentrations within biological materials. Improvements to chromatographic separation provide further synergistic improvements to the ability to map the lipidome in ever increasing detail.

Perhaps the most exciting application of these advanced lipidomic techniques is in the study of the human lipidome at the population level, which reveals associations between lipid species, metabolic pathways, and disease status. Such studies are conducted using human plasma, where lipid species are largely present within lipoprotein particles (Figure 1), and samples are drawn from large population and clinical research studies containing many thousands of participants.[1,2] With such a large number of samples, a balance must be struck between depth of coverage, resolution of the collected mass spectrometry data, and sample throughput.

With these considerations in mind, this application note details a method to determine the concentration of 763 different lipid species from 44 lipid classes within a 10 µL sample of plasma, or an equivalent amount of cell or tissue homogenate. Analysis is conducted via a tandem quadrupole mass spectrometer (MS/MS), subsequent to separation by reversed-phase liquid chromatography. The lipid species/class ionization and fragmentation details together with the internal standards used are detailed in Table 1. The total analysis time is 16 minutes per sample for a single column method, or a 13-minute run time for a dual column system. This method uses Agilent LC/MS/MS instrumentation, integrated with the Agilent MassHunter software package, which allows rapid data processing.

While the reported methods were developed primarily for the analysis of high-throughput, large-cohort-study plasma samples, this protocol can easily be adapted to suit a variety of biological matrices. The LC separation and MS/MS parameters could also be tuned according to the level of structural resolution required, or the separation protocol modified to suit throughput requirements.

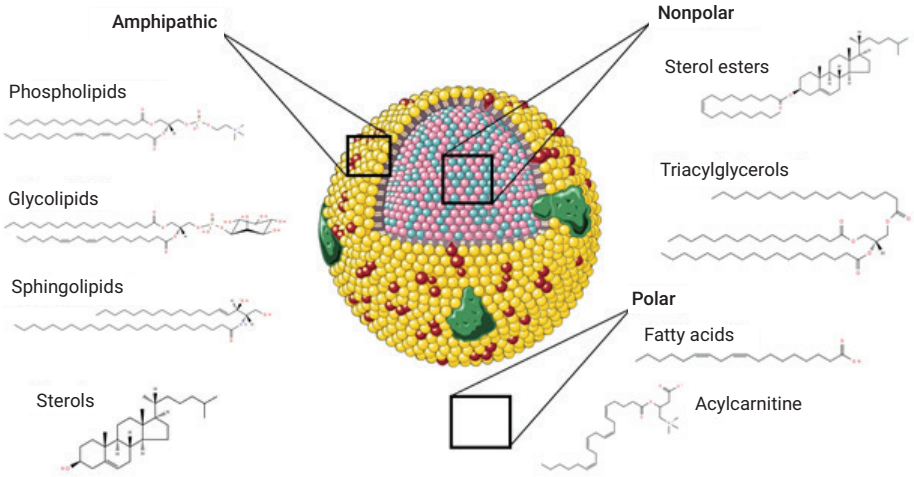

Figure 1. Diagram of lipid classes common in human plasma. Lipids are small amphiphilic molecules that comprise multiple classes and subclasses. In human plasma, the majority of these lipids are found in lipoprotein particles that circulate the periphery.

Table 1. Lipid class ionization and fragmentation details.

Lipid Class/Subclass	Parent Ion	Fragmentation[1]	No. of Lipid Species	Internal Standard	Internal Standard (pmol)/Sample
Sphingosine (Sph)	$[M + H]^+$	NL, 18.0 Da	2	Sph(d17:1)	20
Sphingosine-1-phosphate (S1P)	$[M + H]^+$	sphingoid base specific	4	S1P(18:1) d7	40
Dihydroceramide (dhCer)	$[M + H]^+$	sphingoid base specific	6	dhCer(d18:0/8:0)	50
Ceramide (Cer(d))	$[M + H]^+$	sphingoid base specific	41	Cer(d18:1-d7/18:0)	50
Deoxyceramide (Cer(m))	$[M + H]^+$	sphingoid base specific	11	Cer(d18:1-d7/18:0)	50
Ceramide-1-phosphate (C1P)	$[M + H]^+$	sphingoid base specific	1	Cer(d18:1-d7/18:0)	50
Monohexosylceramide (HexCer)	$[M + H]^+$	sphingoid base specific	13	HexCer(d18:1/15:0) d7	50
Dihexosylceramide (Hex2Cer)	$[M + H]^+$	sphingoid base specific	9	Hex2Cer(d18:1/15:0) d7	50
Trihexosylcermide (Hex3Cer)	$[M + H]^+$	sphingoid base specific	5	Hex3Cer(d18:1/17:0)	50
GM3 ganglioside (GM3)	$[M + H]^+$	sphingoid base specific	6	Hex3Cer(d18:1/17:0)	50
Sulfatide (SHexCer)	$[M + H]^+$	PI, *m/z* 264.3	5	SHexCer(d18:1/12:0)	10
Sphingomyelin (SM)	$[M + H]^+$	PI, *m/z* 184.1	45	SM(d18:1/15:0) d9	100
Phosphatidic acid (PA)	$[M + H]^+$	NL, 115.0 Da	4	PA(15:0_18:1) d7	50
Phosphatidylcholine (PC)	$[M + H]^+$	PI, *m/z* 184.1	70	PC(15:0_18:1) d7	100
Alkylphosphatidylcholine (PC(O))	$[M + H]^+$	PI, *m/z* 184.1	23	PC(15:0_18:1) d7	100
Alkenylphosphatidylcholine (plasmalogen) (PC(P))	$[M + H]^+$	PI, *m/z* 184.1	28	PC(P-18:0/18:1) d9	100
Lysophosphatidylcholine (LPC)	$[M + H]^+$	PI, *m/z* 184.1 and *m/z* 104.1	61	LPC(18:1) d7	100
Lysoalkylphosphatidylcholine (lysoplatelet activating factor) (LPC(O))	$[M + H]^+$	PI, *m/z* 104.1	10	LPC(18:1) d7	100
Lysoalkenylphosphatidylcholine (plasmalogen) (LPC(P))	$[M + H]^+$	PI, *m/z* 104.1	6	LPC(18:1) d7	100
Phosphatidylethanolamine (PE)	$[M + H]^+$	NL, 141.0 Da	32	PE(15:0_18:1) d7	100
Alkylphosphatidylethanolamine (PE(O))	$[M + H]^+$	NL, 141.0 Da	15	PE(15:0_18:1) d7	100
Alkenylphosphatidylethanolamine (plasmalogen) (PE(P))	$[M + H]^+$	Acyl chain specific	48	PE(P-18:0/18:1) d9	100
Lysophosphatidylethanolamine (LPE)	$[M + H]^+$	NL, 141.0 Da	12	LPE(18:1) d7	100
Lysoalkenylphosphatidylethanolamine (plasmalogen) (LPE(P))	$[M + H]^+$	NL, 171.9 Da	4	LPE(18:1) d7	100
Phosphatidylinositol (PI)	$[M + NH_4]^+$	NL, 277.0 Da	25	PI(15:0_18:1) d7	50
Phosphatidylinositol monophosphate (PIP1)	$[M + NH_4]^+$	NL, 357.0 Da	1	PI(15:0_18:1) d7	50
Lysophosphatidylinositol (LPI)	$[M + NH_4]^+$	NL, 277.0 Da	7	LPI(13:0)	20
Phosphatidylserine (PS)	$[M + H]^+$	NL, 185.0 Da	4	PS(15:0_18:1) d7	50
Phosphatidylglycerol (PG)	$[M + NH_4]^+$	NL, 189.0 Da	4	PG(15:0_18:1) d7	50
Cholesteryl ester (CE)	$[M + NH_4]^+$	PI, *m/z* 369.3	27	CE(18:0) d6	1,000
Free cholesterol (COH)	$[M + NH_4]^+$ Insource Fragment	PI, *m/z* 161.2	1	COH(d7)	10,000
Dehydrocholesterol ester (DE)	$[M + NH_4]^+$	PI, *m/z* 367.4	4	CE(18:0) d6	1,000
Methyl-cholesteryl ester (methyl-CE)	$[M + NH_4]^+$	PI, *m/z* 383.3	4	CE(18:0) d6	1,000
Methyl-dehydrocholesteryl ester (methyl-DE)	$[M + NH_4]^+$	PI, *m/z* 381.4	2	CE(18:0) d6	1,000
Dimethyl-cholesteryl ester (dimethyl-CE)	$[M + NH_4]^+$	PI, *m/z* 396.6	3	CE(18:0) d6	1,000
Free fatty acid (FFA)	[M - H]-	SIM	16	FFA(18:1) d9	200
Acylcarnitine (AC)	$[M + H]^+$	PI, *m/z* 85.1	28	AC(16:0) d3	10
Hydroxylated acylcarnitine (AC-OH)	$[M + H]^+$	PI, *m/z* 85.1	8	AC(16:0) d3	10
Bile acid (BA)	$[M + NH_4]^+$	Species dependent	2	Cholic acid d4	50
Diacylglycerol (DG)	$[M + NH_4]^+$	NL, fatty acid	24	DG(15:0_18:1) d7	200
Triacylglycerol (neutral loss, for associations) (TG [NL])	$[M + NH_4]^+$	NL, fatty acid	77	TG(15:0_18:1-d7_15:0)	100
Alkyldiacylglycerol (neutral loss, for associations) (TG(O) [NL])	$[M + NH_4]^+$	NL, fatty acid	19	TG(15:0_18:1-d7_15:0)	100
Ubiquinone	$[M + NH_4]^+$	PI, *m/z* 197.0	1	Hex3Cer(d18:1/17:0)	50
Oxidised lipids (OxSpecies)	Species dependent [+O]	Species dependent	6	Species dependent	–

[1] NL = neutral loss, PI = precursor ion

Experimental

Chemicals

Ammonium formate was purchased from Sigma-Aldrich (St. Louis, MO, USA). Methanol (LC), 1-butanol (LC), water (LC/MS Grade), acetonitrile, and 2-propanol (hypergrade for LC/MS, LiChrosolv) were purchased from Supelco (Bellefonte, PA, USA). NIST1950 QC material was purchased from National Institute of Standards and Technology (Los Angeles, CA, USA). All internal standards were purchased from Avanti Polar Lipids (Alabaster, AL, USA) except for acylcarnitine 16:0 d3 (Larodan AB, Solna, Sweden), cholesteryl ester 18:0 d6 (CDN Isotopes, Quebec, Canada), C18:1 d9 fatty acid (Sigma-Aldrich, St. Louis, MI, USA) and trihexosylceramide 17:0 (Matreya LLC, State College, PA, USA).

Preparation of internal standard mixture

To determine the relative concentrations of each lipid species under analysis, internal standards were added to each sample, consisting of stable-isotope-labeled and nonphysiological species. A mixture of internal standards were prepared in-house from commercially available sources (Table 2), but premade mixtures such as the SPLASH LIPIDOMIX Mass Spec Standard (Avanti) are also suitable. If an alternate internal standard preparation is to be used, the retention times of each additional standard compound will need to be generated and used to update both the instrument and data processing method files.

Individual internal standards were all stored at –80 °C as received from the supplier. To prepare the mixture, standards were thawed to room

Table 2. Internal standard information.

Name	Molecular Weight	Stock Solution (µM)	Concentration in Std Mix (µM)	pmol/Sample (10 µL)	Solvent	Supplier	Cat No.	Present in Avanti SPLASH LIPIDOMIX[1,2,3]
AC(16:0) d3	439.09	100	1	10	$CHCl_3$:MeOH (1:1)	Larodan	71-1746-5	No
CE(18:0) d6	659.16	2,000	100	1,000	$CHCl_3$:MeOH (1:1)	CDN isotopes	D-5823	No
Cer(d18:1-d7/18:0)	572.99	200	5	50	$CHCl_3$:MeOH (1:1)	Avanti	860677P	No
Cholic acid d4	412.61	200	5	50	$CHCl_3$:MeOH (1:1)	Cayman	20849	No
COH(d7)	393.69	20,000	1,000	10,000	$CHCl_3$:MeOH (1:1)	Avanti	700041P	Yes
DG(15:0_18:1) d7	587.97	800	20	200	$CHCl_3$:MeOH (1:1)	Avanti	791647	Yes
dhCer(d18:0/8:0)	427.71	200	5	50	$CHCl_3$:MeOH (1:1)	Avanti	860626P	No
FFA(18:1) d9	291.52	3,000	20	200	$CHCl_3$:MeOH (1:1)	Avanti	861809	No
Hex2Cer(d18:1/15:0) d7	855.21	400	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti	330727	No
Hex3Cer(d18:1/17:0)	1038.35	100	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Matreya LLC	1523	No
HexCer(d18:1/15:0) d7	693.06	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti	330729	No
LPC(18:1) d7	528.71	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	791643	Yes
LPE(18:1) d7	486.63	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	791644	Yes
LPI(13:0)	547.57	200	2	20	$CHCl_3$:MeOH (1:1)	Avanti	850101	No
PA(15:0_18:1) d7	689.93	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti	791642	Yes
PC(15:0_18:1) d7	753.09	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	791637	Yes
PC(P-18:0/18:1) d9	781.19	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	852475	Yes
PE(15:0_18:1) d7	711.01	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	791638	Yes
PE(P-18:0/18:1) d9	739.11	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	852474	Yes
PG(15:0_18:1) d7	764.01	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti	791640	Yes
PI(15:0_18:1) d7	847.12	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti	791641	Yes
PS(15:0_18:1) d7	777.00	400	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti	791639	Yes
S1P(18:1) d7	386.52	400	4	40	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti	860659	No
SHexCer(d18:1/12:0)	741.03	200	1	10	$CHCl_3$:MeOH (1:1)	Avanti	860573P	No
SM(d18:1/15:0) d9	698.06	800	10	100	$CHCl_3$:MeOH (1:1)	Avanti	860686	No
Sph(d17:1)	285.47	400	2	20	$CHCl_3$:MeOH (1:1)	Avanti	860640P	No
TG(15:0_18:1-d7_15:0)	812.35	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti	791648	Yes

[1] The specific CE and SM standards listed here are not in the Avanti SPLASH LIPIDOMIX but an equivalent standard is present.

[2] The plasmalogen standards are only available in the SPLASH II Lipidomix mix. Cholesterol (COH), PA, and PG standards are only available in SPLASH I LIPIDOMIX.

[3] Not all standards available in the SPLASH LIPIDOMIX are included at the same concentration shown in column 3.

temperature and then reconstituted in 1:1 chloroform:methanol to the prescribed stock solution concentration listed in column 3 of Table 2. The resulting stock solutions were then combined to yield a single mixture of all internal standards, at the final concentrations listed in column 4 of Table 2. This internal standard mixture was sonicated in a bath sonicator for 15 minutes to ensure complete mixing and then aliquoted into single use aliquots to be stored at –80 °C.

Preparation of extraction solvent

To prepare the solvent used to extract lipids from samples of plasma, preprepared aliquots of internal standard mixture were thawed to room temperature (1 hour), bath-sonicated for 15 minutes, then vortexed. The required volume of internal standard mixture (10 µL per sample to be extracted) was then dried down under vacuum and reconstituted in a tenfold volume of 1:1 butanol:methanol containing 10mM ammonium formate and bath-sonicated again for 15 minutes. For example, if 100 samples were to be extracted, then 1 mL of internal standard mix would be dried down and reconstituted in 10 mL of 1:1 butanol:methanol containing 10 mM ammonium formate.

Sample worklist, randomization, and inclusion of quality control samples

Prior to the extraction or analysis of samples, a sample worklist was generated, which specifies the order in which subject and control samples are handled. Samples remain in this order, first as they are extracted and then as they are introduced into the LC/MS/MS for analysis. To achieve this, all subject samples were initially randomized, to minimize the influence of extraction bias across the dataset. In the case of sample groups or time points with statistical relevance, these were kept paired, while factors such as collection order were randomized.

Subsequently, a number of different quality control samples were then introduced into the worklist. PQCs, NIST1950 QCs, and blank samples were extracted alongside subject samples using the same procedure, while TQCs were drawn from previously extracted and pooled plasma. These samples are required to align the resulting data and compensate for instrumental drift and variation (both within and between different batches), as well as detect more serious errors within the data. The composition and role of each quality control type is summarized below, along with the procedure for interspersing them within the sample worklist.

Plasma quality control (PQC)

PQC samples consisted of plasma collected from healthy volunteers (n = 8 to 20), pooled together, and dispensed into single-use aliquots, to be stored at –80 °C. To test for any variation introduced from the extraction process, PQC samples were included every 15 samples (with a minimum of 10 PQC samples per batch). The %CV of these samples enabled monitoring of the error introduced through pipetting and handling, and also alignment of batches where large numbers of samples dictate that multiple extraction batches are required.

Technical quality control (TQC)

TQC samples were prepared separately by extracting aliquots of the same plasma used for the PQCs, then pooling the extracts to remove extraction variability. These TQC samples then allow the specific monitoring of the instrument variability and performance (resolution, retention time drift, etc.) as the extraction variability has been removed. These samples were included every 15 biological samples with a minimum of 10 per batch.

NIST1950 quality control (NIST1950 QC)

NIST1950 is a commercially available, standardized source of plasma. The addition of NIST1950 quality control samples allows the accurate alignment not only of different sets of samples within the laboratory but also the alignment of different sample sets from other laboratories also using the NIST1950 QC. To avoid multiple freeze/thaw cycles, the NIST1950 QC sample was thawed and aliquoted (10 µL) into Eppendorf extraction tubes in a single process. NIST1950 QC samples were included every 30 samples with a minimum of eight samples across any batch.

Blank samples

Consisting of 10 µL of milliQ water, blank samples were included to monitor background signal, and were extracted at the same time as the biological samples and PQCs. They were included every 30 samples, with a minimum of five blank samples across any batch.

Lipid extraction of human plasma

To prevent fouling of the instrument due to the high concentrations of salt and protein, all plasma samples were extracted into solvent, such that the compounds of interest were transferred into solution, while salts and proteins could be pelleted and discarded.[3]

Lipid extractions were performed in 1.5 mL microcentrifuge tubes using polypropylene positive displacement pipettes. Ten microliters of plasma were mixed with 100 µL of extraction solvent, consisting of butanol:methanol (1:1) with 10 mM ammonium formate and the reconstituted mixture of internal standards (Table 2). Each sample was then vortexed for 5 seconds and subsequently bath-sonicated for 1 hour, with the temperature maintained at 21 to 25 °C. Samples were then centrifuged (13,000 xg, 10 minutes, 20 °C), and the

supernatant transferred into 1.5 mL glass sample vials (5190-9062) with 200 µL glass inserts (5183-2085). Samples should be capped using PTFE/S caps (5185-5820). Samples were stored at –80 °C until immediately before analysis, whereupon they were thawed to room temperature (1 hour), bath-sonicated for 15 minutes, briefly vortexed, and loaded into the instrument's autosampler.

If high-throughput analysis is required, samples can be extracted in 96-well plates on a Bravo platform using application note 5991-5724.[4]

Instrumentation and LC/MS/MS method

Extracted plasma samples were separated using an Agilent 1290 Infinity/Infinity II LC system, including:

- Agilent 1290 Infinity Autosampler (G4226A) **Note:** Alternatively, a 1290 Infinity II Multisampler (G7167B) can be used with minimal impact on retention times.
- Agilent 1290 Infinity II High-Speed (binary) Pump(s) (G7120A, two pumps are used for dual column setup)
- Agilent 1290 Infinity II Multicolumn Thermostat (G7116B), equipped with an Agilent InfinityLab Quick Change 2-position/10-port valve head (for dual-column setup, part number 5067-4240)

The plumbing requirements for single- and dual-column setups are depicted in Figure 2 and Table 5.

The LC system was coupled to an Agilent 6495C triple quadrupole LC/MS with an Agilent Jet Stream technology ionization source.

Lipid extracts (1 µL, equivalent to 0.1 µL plasma) were injected and separated using a 16-minute gradient, the conditions of which are detailed in Table 3, with the first 0.8 minutes diverted to waste. Alternatively a dual-column setup can be used to reduce analysis time with a 13-minute gradient

Table 3. Chromatographic conditions for single-column setup.

Parameter	Agilent 1290 Infinity/Infinity II LC
Analytical Column	Agilent ZORBAX Eclipse Plus C18, 100 × 2.1 mm, 1.8 µm (p/n 959758-902)
Inline Filter	Agilent 1290 Infinity II inline filter, 0.3 µm (p/n 5067-6189)
Column Temperature	45 °C
Injection Volume	1 µL (equivalent to 0.1 µL plasma)
Autosampler Temperature	20 °C
Needle Wash	Wash vial, 3 s, 1:1 butanol:methanol *Alternatively, flush port, 10 s, 1:1 mobile phase A/B can be used
Mobile Phase	A) 10 mM ammonium formate, 5 µM Agilent deactivator additive (p/n 5191-3940) in 5:3:2 water:acetonitrile:2-propanol B) 10 mM ammonium formate in 1:9:90 water:acetonitrile:2-propanol *DO NOT add deactivator additive to mobile phase B
Flow Rate	0.4 mL/min
Gradient Program	Time %B 0 15 2.5 50 2.6 57 9 70 9.1 93 11 96 11.1 100 12 100 12.2 15 16 15
Stop Time	16 min
Post Time	None

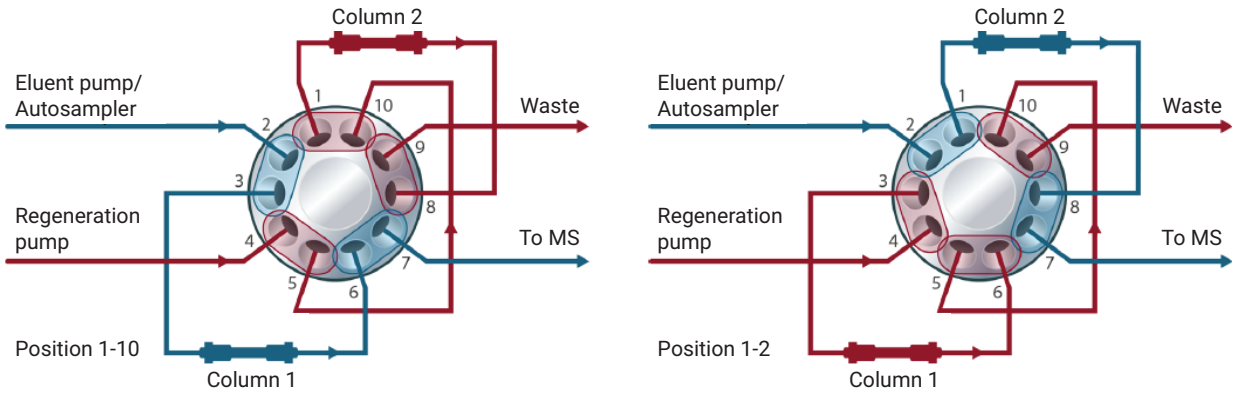

Figure 2. Dual-column setup. Example of switching valve plumbing to allow alternate column generation.

program detailed in Table 4. LC/MS/MS analysis was conducted via dynamic multiple reaction monitoring (dMRM). MS instrument parameters and source conditions are provided in Table 6. The development and further details of this methodology are available in a previously published article.[1]

Table 4. Chromatographic conditions for dual-column setup.

Parameter	Agilent 1290 Infinity/Infinity II LC	
Analytical Columns	2 × Agilent ZORBAX Eclipse Plus C18, 100 × 2.1 mm, 1.8 µm (p/n 959758-902)	
Inline Filters	2 × Agilent 1290 Infinity II inline filter, 0.3 µm (p/n 5067-6189)	
Column Temperature	45 °C	
Injection Volume	1 µL (equivalent to 0.1 µL plasma)	
Autosampler Temperature	20 °C	
Needle Wash	Wash vial, 3 s, 1:1 butanol:methanol *Alternatively, flush port, 10 s, 1:1 mobile phase A/B can be used	
Mobile Phase	A) 10 mM ammonium formate, 5 µM Agilent deactivator additive (p/n 5191-3940) in 5:3:2 water:acetonitrile:2-propanol B) 10 mM ammonium formate in 1:9:90 water:acetonitrile:2-propanol *DO NOT add deactivator additive to mobile phase B	
Flow Rates	0.4 mL/min	
Gradient Program	**Pump A (G7120A)** Time %B 0 15 2.5 50 2.6 57 9 70 9.1 93 11 96 11.1 100 12 100 12.2 15 12.9 15	**Pump B (G7120A)** Time %B 0 15 1 15 2 100 6 100 7 15 12.9 15
Stop Time	13 min	
Post-TIme	None	
MCT Valve Position	Use current, Increase valve position after run	

Table 5. LC tubing details for single column setup.

Location	Part Description	Part Number[1]
Binary Pump Mixer	V35 Jet Weaver mixer	G7120-68135
Tubing from Pump to Autosampler	Capillary, stainless steel, 0.17 mm id, 600 mm	G1312-67305
Needle	Needle assembly, 0.12 mm	G4226-87201
Needle Seat	Needle seat, 0.12 mm id	G4226-87012
Metering Capillary	Capillary stainless steel 0.17 × 160 mm S/SL ps/ps	G4226-60301
Sample Loop Assembly	20 µL loop assembly	G4226-60310
Autosampler to MCT	Capillary SST 0.12 × 500 mm long socket	5500-1157
Heat Exchanger	Standard flow heat exchanger, 1.6 µL	G7116-60015
Connection to Inline Filter	Quick Connect assembly ST 0.12 × 105 mm	5067-5957
Fittings For Heat Exchanger Entry/Exit	Quick Turn LC fitting	5067-5966
PEEK Tubing to MS	PEEK tubing, 0.13 mm id, 700 mm	0890-1915

[1] Part numbers are specific for LC configuration described here. If using an Agilent 1290 Infinity II Multisampler, some part numbers will differ.

Dynamic multiple reaction monitoring setup

A critical aspect of this methodology is the use of dynamic multiple reaction monitoring (dMRM) within the mass spectrometer. For the instrument to measure the large number of lipid species in the extended lipidome, the specific retention time window within which each compound elutes must be defined, such that the instrument only scans for a given lipid species at specific points across the total sample run time. This retention time window varies for different MRMs and is dependent largely on differences in peak width. This approach improves the instrument duty cycle and extends the average dwell time per compound (Figure 3).

A dMRM method was prepared using Agilent Masshunter Acquisition software, in which the MRM scan for each compound of interest was approximately aligned with the compound's known retention time. The retention times are provided in Table A1 (see Appendix). Collision energies and MRM transitions were optimized with a representative standard for each lipid class to provide maximum response. AJS source parameters were optimized using Agilent Source Optimizer software to balance sensitivity across all classes. A cycle time of 650 ms was chosen to maintain an adequate number of points across the peak for reliable quantitation. This study leveraged 665 transitions to monitor 763 human lipid species and isomers. With 665 transitions, the busiest section resulted in 115 transitions with an average dwell time below 5 ms. The 6495C LC/TQ

Table 6. MS instrument parameters.

Parameter	Agilent 6495C Triple Quadrupole LC/MS
Ion Source	Agilent Jet Stream
Polarity	Positive and Negative Switching
Gas Temperature	150 °C
Drying Gas (Nitrogen)	17 L/min
Nebulizer Gas	20 psi
Sheath Gas	200 °C
Sheath Gas Flow	10 L/min
Capillary Voltage	3,500 V (+), −3,000 V (−)
Nozzle Voltage	1,000 V (+), −1,500 V (−)
iFunnel High/Low Pressure RF	200/110 V (+), 150/60 V (−)
Scan Type	Dynamic MRM (dMRM)
Q1/Q2 Resolution	Unit (0.7 amu)
Delta EMV	100 V (+), 0 V (−)
Cell Acceleration Voltage	4 to 5 V
Cycle Time	650 ms
Time Filter Width	0.07 min
Total Number of MRMs	665 (positive: 646, negative: 19)

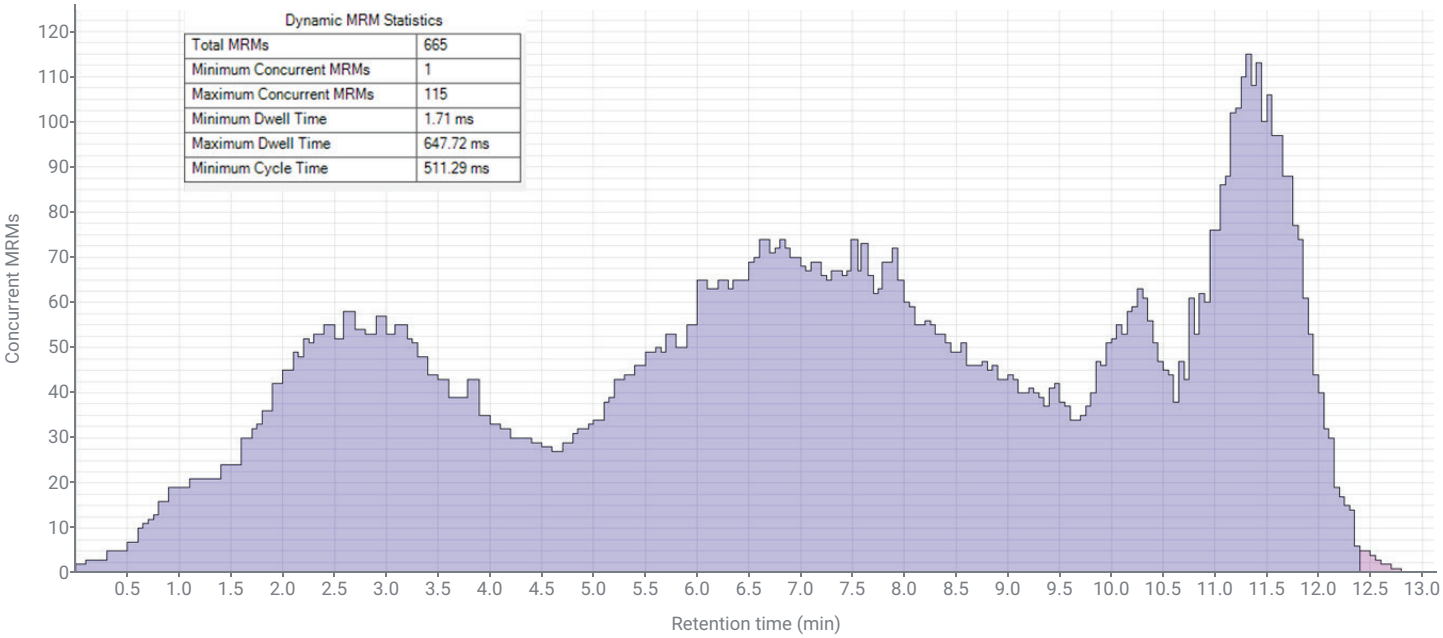

Figure 3. Concurrent MRMs versus retention times. Summary plot of the dMRM showing the concurrent MRMs at each retention time as well as the dMRM statistics showing the dwell time and concurrent MRM details.

was able to maintain excellent precision across these compounds even with these low dwell times (see Results and discussion).

Lipid nomenclature and structural elucidation in plasma

The lipid naming convention used throughout this document follows the guidelines established by the Lipid Maps Consortium and the shorthand notation subsequently published by Liebisch *et al*.[5-7] Phospholipids typically contain two fatty acid chains, and in the absence of detailed characterization, are expressed as the sum composition of carbon atoms and double bonds (i.e., PC(38:4)).

However, where an acyl chain composition has been determined, the naming convention indicates this (i.e., PC(38:4) is changed to PC(18:0_20:4)). This is also extended into other lipid classes and subclasses. Where the positions of the fatty acids on the glycerol backbone are known, this becomes PC(18:0/20:4) with the 18:0 in the sn-1 position and the 20:4 in the sn-2 position. Species that are separated chromatographically, but remain incompletely characterized, were labeled with an (a) or (b), for example PC(P-17:0/20:4) (a) and PC(P-17:0/20:4) (b), where (a) and (b) represent the elution order.

Structural annotation of the lipid species based on mass, fragmentation, and chromatography for this method have been previously reported.[1] In general, single, and even multiple MRM transitions often do not provide sufficient structural information for a given lipid species, particularly glycerophospholipids. There are many approaches to handle this, each with different limitations. This method leverages offline experiments to provide additional identification of the lipid structures at specific retention times, and is conducted on a representative pooled plasma sample rather than each individual sample in a cohort study. Details of such experiments are reported in Reference 1, and some examples are provided:

Phospholipid characterization: PC(36:2), measured by the transition 786.6 → 184.1, elutes as two peaks, which were labeled as PC(36:2) (a) and (b) based on retention time. Additional experiments using an orthogonal transition for the PC class, monitoring either in negative mode as a formate adduct, or positive using a sodium adduct, results in products specific to the fatty acids. Here, the (a) peak is predominately PC(18:1/18:1), whereas the second larger (b) peak is PC(18:0_18:2). This can be conducted on all glycerophospholipid and sphingomyelin species.

Synthetic standards: Several lipid isomers differed based on either the position of the double bond (for example, a phospholipid with a 22:5 fatty acid exists in plasma as either an omega-3 or omega-6 isoform). While many approaches are available to identify these using different fragmentation conditions, We opted to synthesize standards with the two isoforms, which were run on the chromatography for identification. Similarly, monomethyl-branched lipids (i.e., methylhexadecanoic acid) that are isomeric with conventional species (heptadecanoic acid) can be identified using techniques such as EID instead of CID, or based on elution time. The synthesis of standards helped characterize the retention time differences between branched and straight acyl chain isoforms when run alongside a plasma sample.

Plasmalogens: As PC(O) and PC(P) species are isomeric, a simple approach to rapidly confirm plasmalogen species is to treat the lipid extracts with HCl fumes, which selectively hydrolyzes species with the vinyl-ether bond (plasmalogens). Running two sequential samples, where one is hydrolyzed, confirms the identity of these species.

Isotopic overlap: Many of the chromatographic peaks observed can arise from isotopic species, as carbon exists as ^{13}C with a natural abundance of approximately 1.1% (i.e., the +2 isotope of PC(36:2) can be observed in the PC(36:1) transition, although typically this will be at a different retention time). This is particularly problematic with phosphatidylcholine and sphingomyelin species, owing to their large dynamic range. These can be readily identified and excluded by overlaying the transition, in the above example, 788.6 → 184.1 with 788.6 →185.1. The isotope mass increase is only possible in the product ion, if the precursor ion is an isotope. LC peaks that exist in both transitions (isotopes) can then be excluded.

Together, these approaches form the basis of the structural annotations and identification in this methodology. These experiments were conducted with pooled plasma samples (but more common reference plasma such as the NIST1950 plasma is also suitable). These annotations are then used when analyzing plasma samples. In instances where a new matrix is used (for example, brain tissue), this process should be repeated, owing to the different isomeric composition, relative abundances, and new species/classes not seen in plasma. Further, the method presented here focuses on plasma; further development of profiles specific for other tissues (i.e., brain) will further enhance such studies.

Considerations for sample handling and system configuration

While the final configuration and process is dependent on the user, the following considerations result in a more robust platform.

Sample freeze-thaw and temperature of the autosampler: The solubility of lipids at different temperatures can add variation to the analysis if not adequately controlled for. The lipid extraction results in a 1:10 dilution of plasma lipids into a 1:1:0.2 butanol:methanol:water mixture. When thawing out samples stored at –80 °C, samples were thawed at room temperature over an hour, bath-sonicated for 15 minutes, vortexed, and rested at room temperature for 2 hours prior to injection. This ensures that lipids reach an equilibrium prior to injection. Improper thawing can result in changes to lipid concentration over time, particularly in the less polar compounds (triglycerides and cholesteryl esters).

Divert valve: One key aspect in running larger sets of samples without sensitivity loss is diverting the first 0.8 minutes of the run, containing residual salts and polar compounds, into waste rather than the mass spectrometer. This is dependent on the column volume of the LC setup and needs to be adjusted as necessary.

In-line frits: To maintain column longevity and avoid blockages, an inline filter with 0.3 µm frit (part number 5067-6189) can prevent any precipitates from building up in the system.

Single/dual column configuration: Typically for smaller sets of samples, a single column is sufficient, resulting in an analysis time of approximately 16 minutes per sample. However, if throughput needs to be improved, a dual column setup enables re-equilibration of one column while analyzing a sample on a second column, resulting in an analysis time of 13 minutes per sample. A diagram of the dual column setup is shown in Figure 2 along with chromatography conditions for the two columns in Table 4.

Peak integration and data processing

The following is a brief summary of the data processing protocols used for the experiments detailed here. For a more detailed, step-by-step description of this method, request supporting documentation from Agilent.

The chromatographic data are first imported into Agilent MassHunter Quantitative Analysis (for QQQ) Ver. 10.0 or above, and a new Batch File containing each sample to be processed is created. A method file containing all relevant MRM transitions is then generated using the **New method from acquired MRM data** function, and a concentration is entered for each transition flagged as an ISTD (Table 4). By default, the peak selection is carried out by the agile2 integrator, however, where there were multiple peaks within the integration window, Spectrum Summation was used, which allows the user to manually select integration bounds. The website (https://metabolomics.baker.edu.au/method/lipids) contains annotated chromatograms for all lipid species, and can be used as guidance to determine the appropriate peak to integrate in cases of closely eluting isomers/isobars. An example of this annotation is provided in Figure 4. Where a single MRM transition has multiple peaks to be integrated, the transition can be duplicated and renamed in the method editor to allow for separate integration.

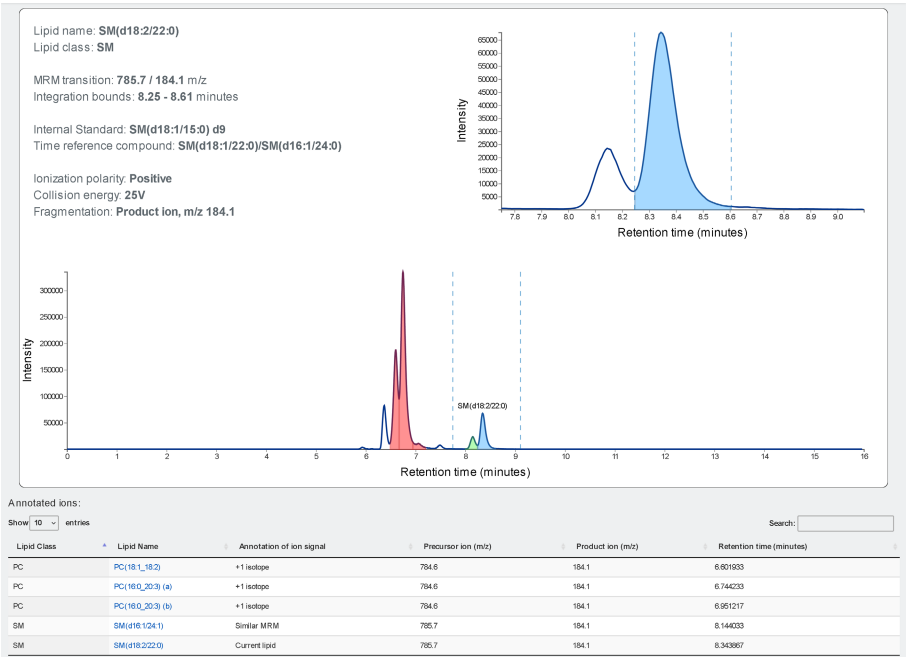

Figure 4. Example from website that references internal libraries of appropriate peaks to integrate in human plasma.

After application of the Method File to the Batch File, the **Compounds-at-a-Glance** function can be used to visually inspect a selection of samples and confirm the correct integration bounds have been selected. For larger batches where retention times may shift due to column performance or solvent differences, Spectrum Summation will fail, as the integration bounds are fixed. See Figure 5 as an example of this issue. This can be overcome by using Time Referencing, which automatically moves the defined integration bounds used for Spectrum Summation for each MRM according to specified reference peaks (Figure 5). For more detailed instructions on using Time Referencing as well as guides on batch alignment for larger cohorts, request supporting documentation from Agilent.

To calculate concentrations within MassHunter Quantitative Analysis (in sample sets not using Time Referencing), an ISTD compound is defined for each transition (Table A2). Once the method is applied and the batch file analysed, the Final Conc. value is automatically generated for all samples.

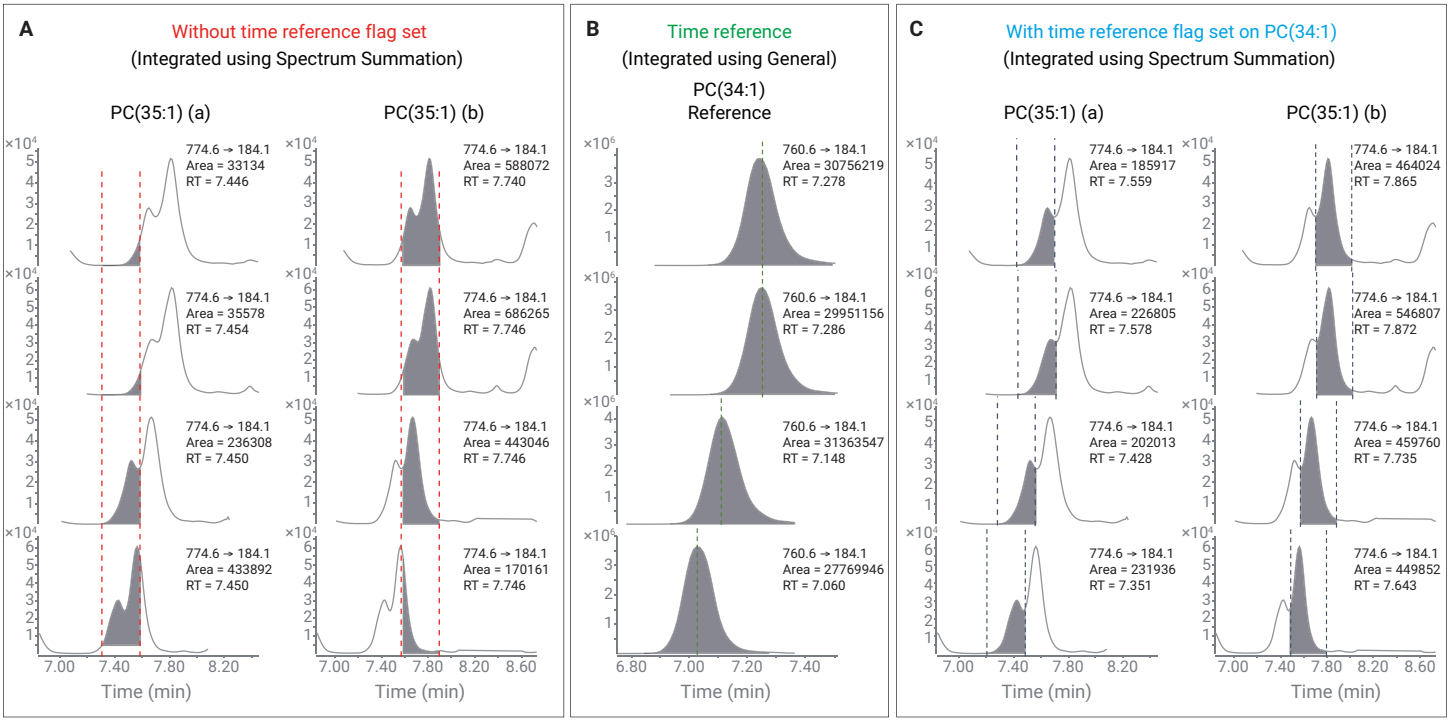

Figure 5. Use of time reference compounds to align difficult-to-integrate peaks. (A) Two isomers of PC(35:1) are integrated separately, but retention time drift results in poor integration using spectrum summation. (B) PC(34:1) is a good reference compound, owing to its high abundance and clean, symmetrical peak. (C) Integration of PC(35:1) after enabling time references and using PC(34:1) as the reference compound to correct for retention time drift.

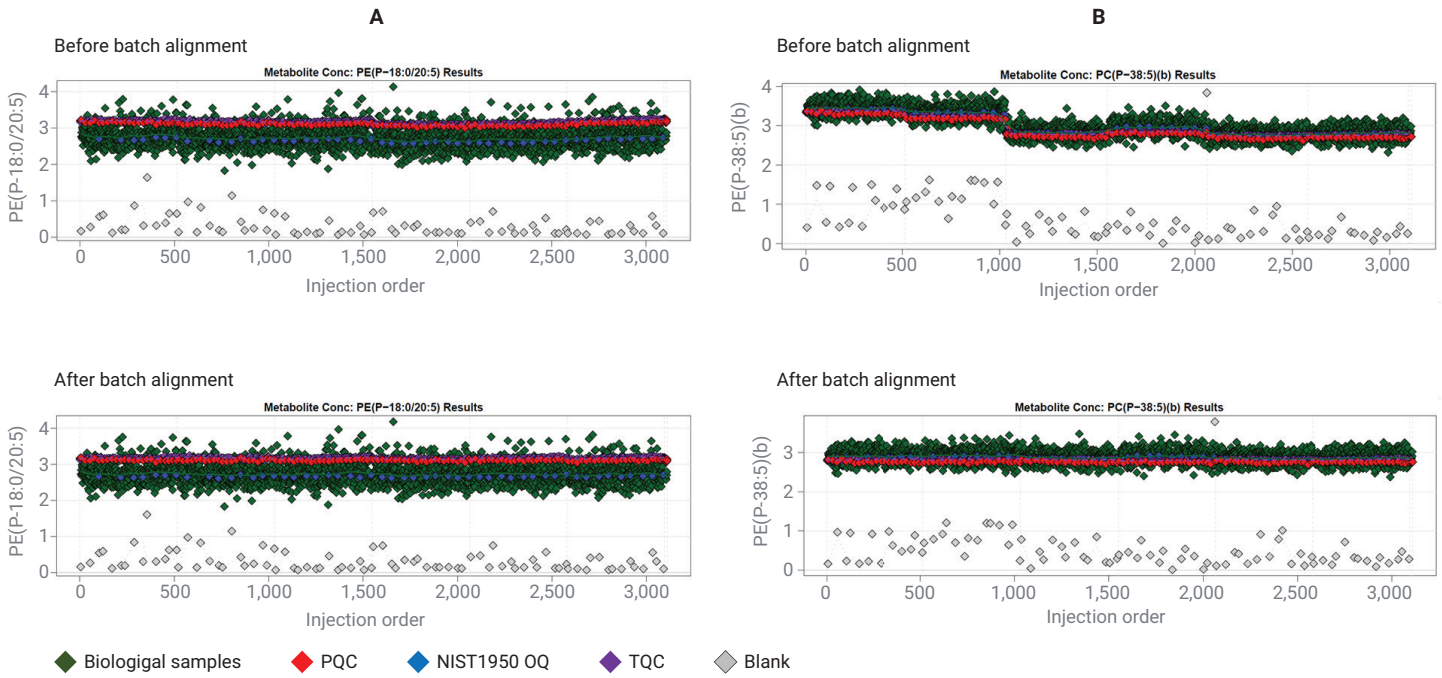

Figure 6. Example of batch alignment performed using the PQC sample across multiple batches. (A) An example of a lipid that maintains very little variability between batches with no increase or change in variability post alignment. (B) An example of a lipid with significant variability across different batches, and the improvement postalignment. All panels show six batches with a total of 2,500 biological samples (X-axis) and the lipid abundance on the log2 scale (Y-axis).

Results and discussion

To determine the reproducibility of the methodology, 50 TQCs were sequentially injected (see Figure 7 for an example chromatogram) and the %CVs of both peak area and lipid concentration were calculated. The mean and median %CVs for raw peak area were 5.1% and 4.1%, respectively, across 763 individual species. Upon calculating each lipid concentration, the mean and median %CVs were 5.6% and 4.0%, respectively. The individual %CVs for each individual lipid species are listed in Table A2. Background, often derived from solvents and plasticizers introduced both during the extraction and LC analysis, should be considered for these lipids. Table A2 shows background level for each lipid species as a percentage of the signal present in the NIST1950 QC sample. For 585 species, the background is

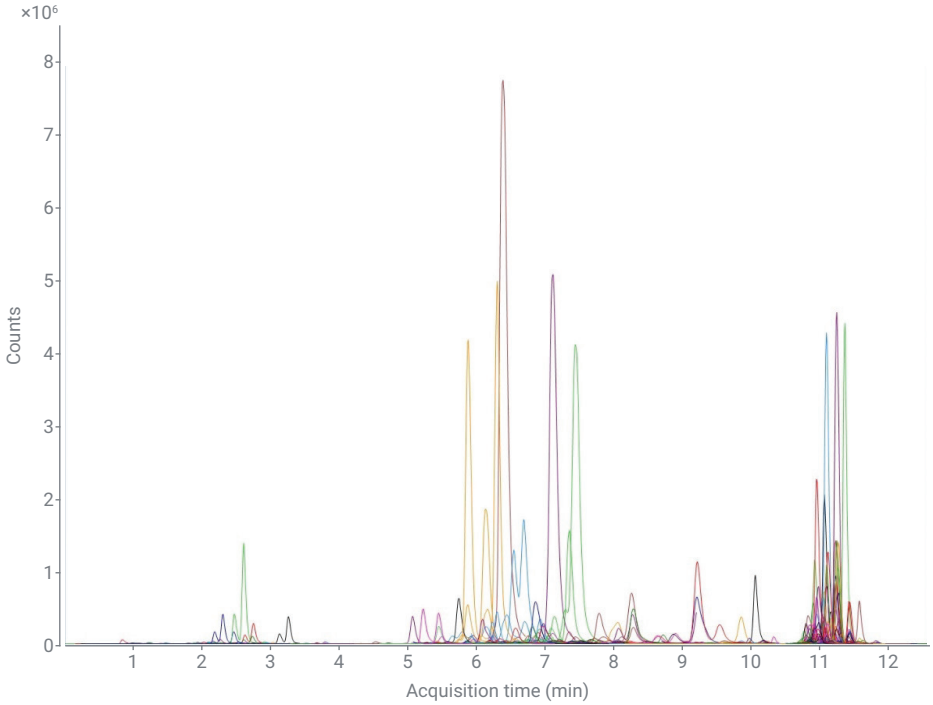

Figure 7. Overlaid MRM chromatograms of lipids measured in this method.

<1.0%, while only 28 species show a background >20.0%. Particular attention should be paid to free fatty acids and diacylglycerols with saturated fatty acid chains and some very low abundance lipid species.

The robustness of this methodology was further demonstrated by running a cohort of 2,500 plasma samples. This run was spread across six batches, each containing 417 samples, nine NIST1950 QCs, 23 PQCs, 14 blanks, and 25 TQCs. A summary of the %CVs of lipid concentrations from a single representative batch and across all aligned batches is presented in Table 7. For each quality control sample, a histogram CV% plot is presented in Figure 8 to highlight the number of lipids that fall within a CV threshold. Approximately 600 lipids had a CV less than 10% in quality control samples. A principle component analysis was then performed across all QCs and samples (Figure 9) to highlight the biological variance of the lipids relative to quality control samples.

This application note details a robust and highly curated LC/MS/MS-based protocol for the determination of over 750 different lipid species within a plasma sample or equivalent. The short run time, high reproducibility of the data, as well as the ability to align data across multiple batches, or even between different labs, enables large lipidomic datasets to be assembled. Such data are vital when seeking to define associations between lipid species and disease outcome to better understand disease pathogenesis.

Table 7. %CVs of each QC types from both within an individual batch as well as across multiple batches.

	NIST 1950 QC		PQC		TQC	
	Mean	Median	Mean	Median	Mean	Median
Single Batch (417 Samples)	9.7	7.7	7.9	6.6	7.0	5.6
All Batches (2,500 Samples)	9.7	7.7	8.9	7.4	8.6	7.0

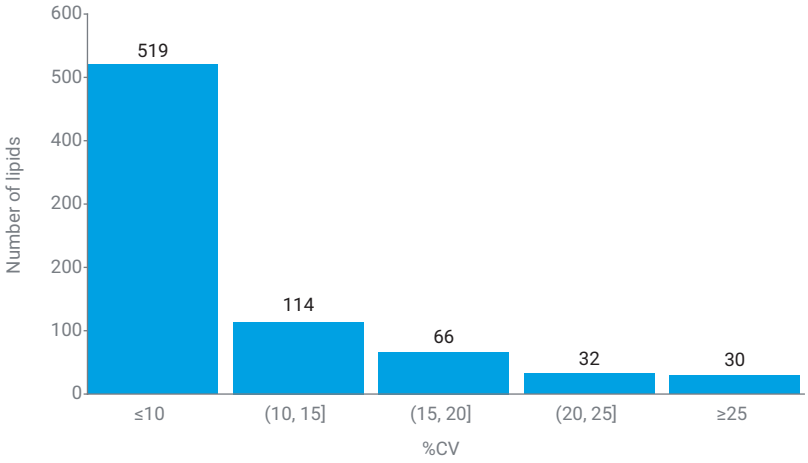

Figure 8. Histogram of coefficient of variation of lipids from various QC samples measured over a single batch.

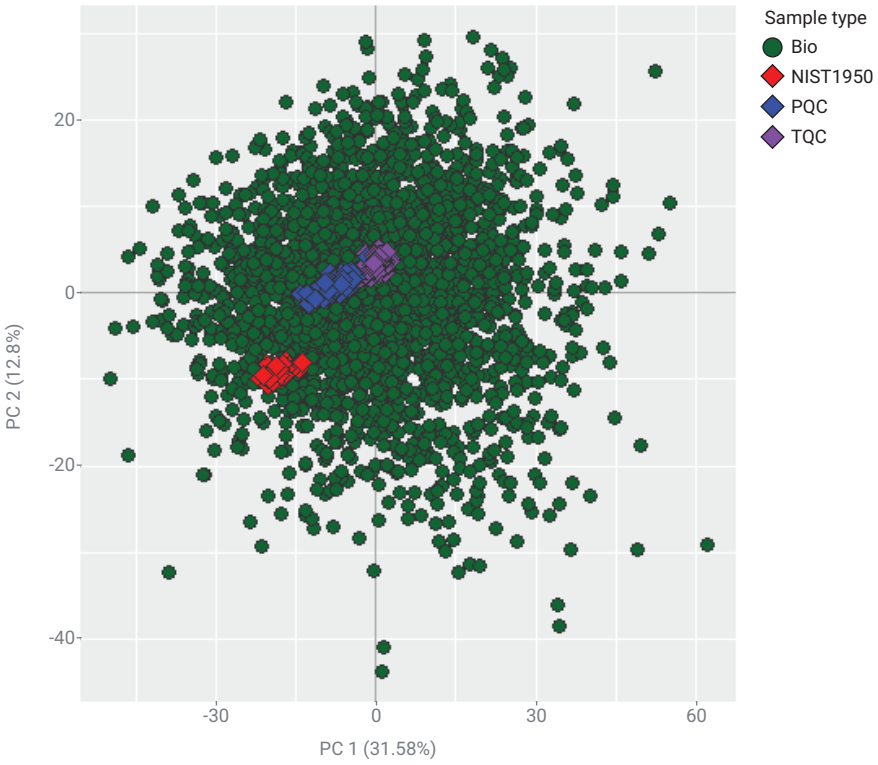

Figure 9. PCA of the lipidomic results from a batch of 2,500 biological samples and all associated QC samples.

One limitation of this method remains the incomplete separation of some isomeric species, which is necessarily limited by run-time constraints. Note, however, that these limitations can be addressed with orthogonal experiments, use of various adducts or ionization modes, or expanding the chromatographic run. In return, the user must compromise with regard to analysis time and specificity.

The ability of LC/MS/MS to acquire quantitative lipidomics data remains a contentious topic within the field. Indeed, multiple factors have influence over the quantitative accuracy of the data, most notably matrix effects, differential suppression, and the different ionization efficiencies of various lipid species. For absolute quantitation, the difference in isotopic distribution between standards and the analyte of interest must also be corrected. For these reasons, this method is termed *relative quantification*, where the values obtained are comparable between samples, but not necessarily the absolute concentration in the sample. It can be rationalized that, in most instances, a study would aim to identify either associations (i.e., lipids metabolites that change with age) or fold differences between groups (healthy versus diabetic). In these types of analysis, the absolute quantitation provides no additional value over what was obtained here. In instances where alignment between studies is required (something that would be benefited by absolute quantitation), alignment using a reference material described here, such as the NIST SRM 1950, would overcome this issue.

This protocol covers a broad range of lipid metabolites, and it is not feasible to supply an internal standard for each compound. Therefore, a single internal standard for most lipid classes was used. Despite these restrictions, the method achieved good reproducibility and precision with regard to the relative quantitation of each lipid compound. Indeed, for most studies, the goal is determining the relative differences in lipid concentration between samples, or identifying associations between lipid species and participant characteristics or clinical outcomes in population studies. In such cases, absolute quantitation of lipid species serves little purpose beyond aligning results between different platforms.

In cases where alignment of the data between studies or labs is necessary, Agilent makes use of the NIST SRM 1950 plasma QC sample typically included in all the experiments. This sample can easily be obtained from several vendors and enables a common reference point for all lipids measured. Standardization and alignment is thus possible using the NIST QC samples as long as the lipid measurements fall within the linear dynamic range of the instrument.

This protocol can easily be adapted to suit other biological samples. However, given the potential differences between tissue lipidomes, it is recommended that tissue-specific annotations be undertaken for new tissue types, using the approaches described above. In the absence of a tissue-specific annotation, it is recommended that the annotations be reverted to sum composition level (for example, PC(36:2) (a) and (b)) when examining other matrices. Tissue-specific annotations may incorporate tissue-specific lipids such as cardiolipins, a lipid exclusively found in the mitochondria, not present in plasma or in the described method. Additional adaptations can also be made to the chromatography, particularly in the case of smaller studies where high throughput is not needed, as a longer and more shallow gradient would further improve lipid separation (including isomeric and isobaric species), enabling potentially more lipid isomers to be resolved, reducing signal suppression from coeluting species and further improving dwell times per transition.

References

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Appendix

Table A1. Agilent MassHunter Acquisition details for all dMRM transitions.[1]

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
1	AcylCarn	AC(10:0)	FALSE	316.3	Unit	85.1	Unit	0.9	0.6	166	30	5	Positive
2	AcylCarn	AC(12:0)	FALSE	344.3	Unit	85.1	Unit	1.2	0.6	166	30	5	Positive
3	AcylCarn	AC(12:1)	FALSE	342.3	Unit	85.1	Unit	1.0	0.6	166	30	5	Positive
4	AcylCarn	AC(13:0)	FALSE	358.3	Unit	85.1	Unit	1.4	0.6	166	30	5	Positive
5	AcylCarn	AC(14:0)	FALSE	372.3	Unit	85.1	Unit	1.8	0.6	166	30	5	Positive
6	AcylCarn	AC(14:0)-OH	FALSE	388.3	Unit	85.1	Unit	1.4	0.6	166	30	5	Positive
7	AcylCarn	AC(14:1)	FALSE	370.3	Unit	85.1	Unit	1.5	0.6	166	30	5	Positive
8	AcylCarn	AC(14:1)-OH	FALSE	386.3	Unit	85.1	Unit	1.1	0.6	166	30	5	Positive
9	AcylCarn	AC(14:2)	FALSE	368.3	Unit	85.1	Unit	1.2	0.6	166	30	5	Positive
10	AcylCarn	AC(15:0) (a\b)	FALSE	386.3	Unit	85.1	Unit	2.1	1	166	30	5	Positive
11	AcylCarn	AC(16:0)	FALSE	400.4	Unit	85.1	Unit	2.5	0.6	166	30	5	Positive
12	AcylCarn	AC(16:0)-OH	FALSE	416.4	Unit	85.1	Unit	2.0	0.6	166	30	5	Positive
13	AcylCarn	AcylCarnitine 16:0 d3 (IS)	TRUE	403.4	Unit	85.1	Unit	2.5	0.6	166	30	5	Positive
14	AcylCarn	AC(16:1)	FALSE	398.3	Unit	85.1	Unit	2.0	0.6	166	30	5	Positive
15	AcylCarn	AC(16:1)-OH	FALSE	414.3	Unit	85.1	Unit	1.6	0.6	166	30	5	Positive
16	AcylCarn	AC(17:0) (a\b)	FALSE	414.4	Unit	85.1	Unit	2.8	0.6	166	30	5	Positive
17	AcylCarn	AC(18:0)	FALSE	428.4	Unit	85.1	Unit	3.2	0.6	166	30	5	Positive
18	AcylCarn	AC(18:0)-OH	FALSE	444.4	Unit	85.1	Unit	2.7	0.6	166	30	5	Positive
19	AcylCarn	AC(18:1)	FALSE	426.4	Unit	85.1	Unit	2.7	0.6	166	30	5	Positive
20	AcylCarn	AC(18:1)-OH	FALSE	442.4	Unit	85.1	Unit	2.2	0.6	166	30	5	Positive
21	AcylCarn	AC(18:2)	FALSE	424.3	Unit	85.1	Unit	2.2	0.6	166	30	5	Positive
22	AcylCarn	AC(18:3)	FALSE	422.3	Unit	85.1	Unit	1.9	0.6	166	30	5	Positive
23	AcylCarn	AC(20:3) (a\b)	FALSE	450.3	Unit	85.1	Unit	2.5	0.6	166	30	5	Positive
24	AcylCarn	AC(20:3)-OH	FALSE	466.3	Unit	85.1	Unit	2.1	0.6	166	30	5	Positive
25	AcylCarn	AC(20:4)	FALSE	448.3	Unit	85.1	Unit	2.2	0.6	166	30	5	Positive
26	AcylCarn	AC(20:5)	FALSE	446.3	Unit	85.1	Unit	1.8	0.6	166	30	5	Positive
27	AcylCarn	AC(22:5)	FALSE	474.3	Unit	85.1	Unit	2.3	0.6	166	30	5	Positive
28	AcylCarn	AC(22:5)-OH	FALSE	490.3	Unit	85.1	Unit	2.0	0.6	166	30	5	Positive
29	AcylCarn	AC(22:6)	FALSE	472.3	Unit	85.1	Unit	2.2	0.6	166	30	5	Positive
30	AcylCarn	AC(24:0)	FALSE	512.3	Unit	85.1	Unit	5.0	0.6	166	30	5	Positive
31	AcylCarn	AC(24:1) (a\b)	FALSE	510.3	Unit	85.1	Unit	4.4	0.6	166	30	5	Positive
32	AcylCarn	AC(26:0)	FALSE	540.3	Unit	85.1	Unit	5.9	0.6	166	30	5	Positive
33	AcylCarn	AC(26:1)	FALSE	538.3	Unit	85.1	Unit	5.0	0.6	166	30	5	Positive
34	CE	CE(14:0)	FALSE	614.6	Unit	369.3	Unit	11.6	0.4	166	10	5	Positive
35	CE	CE(15:0)	FALSE	628.6	Unit	369.3	Unit	11.7	0.4	166	10	5	Positive
36	CE	CE(16:0)	FALSE	642.6	Unit	369.3	Unit	11.8	0.4	166	10	5	Positive
37	CE	CE(16:1)	FALSE	640.6	Unit	369.3	Unit	11.6	0.4	166	10	5	Positive
38	CE	CE(16:2)	FALSE	638.6	Unit	369.3	Unit	11.4	0.4	166	10	5	Positive
39	CE	CE(17:0)	FALSE	656.6	Unit	369.3	Unit	11.9	0.4	166	10	5	Positive
40	CE	CE(17:1)	FALSE	654.6	Unit	369.3	Unit	11.7	0.4	166	10	5	Positive
41	CE	CE(18:0)	FALSE	670.7	Unit	369.3	Unit	12.1	0.4	166	10	5	Positive
42	CE	CE 18:0-d6 (IS)	TRUE	676.7	Unit	375.3	Unit	12.0	0.4	166	10	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
43	CE	CE(18:1)	FALSE	668.6	Unit	369.3	Unit	11.8	0.4	166	10	5	Positive
44	CE	CE(18:2)	FALSE	666.6	Unit	369.3	Unit	11.6	0.4	166	10	5	Positive
45	oxLipid	CE(18:2) [+OH]	FALSE	682.6	Unit	369.3	Unit	10.9	0.6	166	10	5	Positive
46	CE	CE(18:3)	FALSE	664.6	Unit	369.3	Unit	11.4	0.4	166	10	5	Positive
47	CE	CE(20:0)	FALSE	698.7	Unit	369.3	Unit	12.2	0.6	166	10	5	Positive
48	CE	CE(20:1)	FALSE	696.7	Unit	369.3	Unit	12.0	0.4	166	10	5	Positive
49	CE	CE(20:2)	FALSE	694.7	Unit	369.3	Unit	11.8	0.4	166	10	5	Positive
50	CE	CE(20:3)	FALSE	692.6	Unit	369.3	Unit	11.7	0.4	166	10	5	Positive
51	CE	CE(20:4)	FALSE	690.6	Unit	369.3	Unit	11.5	0.4	166	10	5	Positive
52	oxLipid	CE(20:4) [+OH]	FALSE	706.6	Unit	369.3	Unit	10.9	0.6	166	10	5	Positive
53	CE	CE(20:5)	FALSE	688.6	Unit	369.3	Unit	11.3	0.4	166	10	5	Positive
54	CE	CE(22:0)	FALSE	726.7	Unit	369.3	Unit	12.4	0.6	166	10	5	Positive
55	CE	CE(22:1)	FALSE	724.7	Unit	369.3	Unit	12.2	0.4	166	10	5	Positive
56	CE	CE(22:4)	FALSE	718.7	Unit	369.3	Unit	11.7	0.4	166	10	5	Positive
57	CE	CE(22:5)	FALSE	716.6	Unit	369.3	Unit	11.5	1	166	10	5	Positive
58	CE	CE(22:6)	FALSE	714.6	Unit	369.3	Unit	11.4	0.4	166	10	5	Positive
59	CE	CE(24:0)	FALSE	754.7	Unit	369.3	Unit	12.6	0.4	166	10	5	Positive
60	CE	CE(24:1)	FALSE	752.7	Unit	369.3	Unit	12.4	0.4	166	10	5	Positive
61	CE	CE(24:4)	FALSE	746.7	Unit	369.3	Unit	11.9	0.4	166	10	5	Positive
62	CE	CE(24:5)	FALSE	744.7	Unit	369.3	Unit	11.7	0.4	166	10	5	Positive
63	CE	CE(24:6)	FALSE	742.7	Unit	369.3	Unit	11.5	0.4	166	10	5	Positive
64	Cer1P	Cer1P(d18:1/16:0)	FALSE	618.424	Unit	264.3	Unit	5.5	0.6	166	29	4	Positive
65	Cer	Cer(d16:1/16:0)	FALSE	510.6	Unit	236.3	Unit	6.7	0.5	166	25	5	Positive
66	Cer	Cer(d16:1/18:0)	FALSE	538.6	Unit	236.3	Unit	7.8	0.5	166	25	5	Positive
67	Cer	Cer(d16:1/20:0)	FALSE	566.6	Unit	236.3	Unit	9.1	0.5	166	25	5	Positive
68	Cer	Cer(d16:1/22:0)	FALSE	594.6	Unit	236.3	Unit	10.1	0.5	166	25	5	Positive
69	Cer	Cer(d16:1/23:0)	FALSE	608.6	Unit	236.3	Unit	10.2	0.5	166	25	5	Positive
70	Cer	Cer(d16:1/24:0)	FALSE	622.6	Unit	236.3	Unit	10.3	0.5	166	25	5	Positive
71	Cer	Cer(d16:1/24:1)	FALSE	620.6	Unit	236.3	Unit	10.1	0.5	166	25	5	Positive
72	Cer	Cer(d17:1/16:0)	FALSE	524.6	Unit	250.3	Unit	7.2	0.5	166	25	5	Positive
73	Cer	Cer(d17:1/18:0)	FALSE	552.6	Unit	250.3	Unit	8.4	0.5	166	25	5	Positive
74	Cer	Cer(d17:1/20:0)	FALSE	580.6	Unit	250.3	Unit	9.7	0.5	166	25	5	Positive
75	Cer	Cer(d17:1/22:0)	FALSE	608.6	Unit	250.3	Unit	10.2	0.5	166	25	5	Positive
76	Cer	Cer(d17:1/23:0)	FALSE	622.6	Unit	250.3	Unit	10.3	0.5	166	25	5	Positive
77	Cer	Cer(d17:1/24:0)	FALSE	636.6	Unit	250.3	Unit	10.4	0.5	166	25	5	Positive
78	Cer	Cer(d17:1/24:1)	FALSE	634.6	Unit	250.3	Unit	10.2	0.5	166	25	5	Positive
79	Cer	Cer(d18:1/16:0)	FALSE	538.5	Unit	264.3	Unit	7.8	0.7	166	25	5	Positive
80	Cer	Cer(d18:1/18:0)	FALSE	566.6	Unit	264.3	Unit	9.0	0.7	166	25	5	Positive
81	Cer	Cer(d18:1/20:0)	FALSE	594.6	Unit	264.3	Unit	10.1	0.7	166	25	5	Positive
82	Cer	Cer(d18:1/21:0)	FALSE	608.6	Unit	264.3	Unit	10.2	0.7	166	25	5	Positive
83	Cer	Cer(d18:1/22:0)	FALSE	622.6	Unit	264.3	Unit	10.3	0.7	166	25	5	Positive
84	Cer	Cer(d18:1/23:0)	FALSE	636.6	Unit	264.3	Unit	10.4	0.7	166	25	5	Positive
85	Cer	Cer(d18:1/24:0)	FALSE	650.6	Unit	264.3	Unit	10.5	0.7	166	25	5	Positive
86	Cer	Cer(d18:1/24:1)	FALSE	648.6	Unit	264.3	Unit	10.3	0.7	166	25	5	Positive
87	Cer	Cer(d18:1/26:0)	FALSE	678.6	Unit	264.3	Unit	10.7	0.7	166	25	5	Positive
88	Cer	Cer(d18:1-d7/18:0) (IS)	TRUE	573.6	Unit	271.4	Unit	9.0	1	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
89	Cer	Cer(d18:2/16:0)	FALSE	536.5	Unit	262.3	Unit	6.9	0.7	166	25	5	Positive
90	Cer	Cer(d18:2/18:0)	FALSE	564.6	Unit	262.3	Unit	8.1	0.7	166	25	5	Positive
91	Cer	Cer(d18:2/20:0)	FALSE	592.6	Unit	262.3	Unit	9.3	0.5	166	25	5	Positive
92	Cer	Cer(d18:2/22:0)	FALSE	620.6	Unit	262.3	Unit	10.1	0.5	166	25	5	Positive
93	Cer	Cer(d18:2/23:0)	FALSE	634.6	Unit	262.3	Unit	10.2	0.5	166	25	5	Positive
94	Cer	Cer(d18:2/24:0)	FALSE	648.6	Unit	262.3	Unit	10.4	0.5	166	25	5	Positive
95	Cer	Cer(d18:2/24:1)	FALSE	646.6	Unit	262.3	Unit	10.1	0.5	166	25	5	Positive
96	Cer	Cer(d18:2/26:0)	FALSE	676.6	Unit	262.3	Unit	10.5	0.5	166	25	5	Positive
97	Cer	Cer(d19:1/18:0)	FALSE	580.6	Unit	278.3	Unit	9.4	0.5	166	25	5	Positive
98	Cer	Cer(d19:1/20:0)	FALSE	608.6	Unit	278.3	Unit	10.1	0.5	166	25	5	Positive
99	Cer	Cer(d19:1/22:0)	FALSE	636.6	Unit	278.3	Unit	10.4	0.5	166	25	5	Positive
100	Cer	Cer(d19:1/23:0)	FALSE	650.6	Unit	278.3	Unit	10.5	0.5	166	25	5	Positive
101	Cer	Cer(d19:1/24:0)	FALSE	664.6	Unit	278.3	Unit	10.5	0.5	166	25	5	Positive
102	Cer	Cer(d19:1/24:1)	FALSE	662.6	Unit	278.3	Unit	10.4	0.5	166	25	5	Positive
103	Cer	Cer(d20:1/22:0)	FALSE	650.6	Unit	292.3	Unit	10.5	0.5	166	25	5	Positive
104	Cer	Cer(d20:1/23:0)	FALSE	664.6	Unit	292.3	Unit	10.6	0.5	166	25	5	Positive
105	Cer	Cer(d20:1/24:0)	FALSE	678.6	Unit	292.3	Unit	10.7	0.5	166	25	5	Positive
106	Cer	Cer(d20:1/24:1)	FALSE	676.6	Unit	292.3	Unit	10.5	0.5	166	25	5	Positive
107	m18:0	Cer(m18:0/20:0)	FALSE	580.6	Unit	268.4	Unit	10.3	0.6	166	35	5	Positive
108	m18:0	Cer(m18:0/22:0)	FALSE	608.6	Unit	268.4	Unit	10.5	0.6	166	35	5	Positive
109	m18:0	Cer(m18:0/23:0)	FALSE	622.6	Unit	268.4	Unit	10.6	0.6	166	35	5	Positive
110	m18:0	Cer(m18:0/24:0)	FALSE	636.6	Unit	268.4	Unit	10.7	0.6	166	35	5	Positive
111	m18:0	Cer(m18:0/24:1)	FALSE	634.6	Unit	268.4	Unit	10.5	0.6	166	35	5	Positive
112	m18:1	Cer(m18:1/18:0)	FALSE	550.6	Unit	266.4	Unit	9.3	0.6	166	35	5	Positive
113	m18:1	Cer(m18:1/20:0)	FALSE	578.6	Unit	266.4	Unit	10.1	0.6	166	35	5	Positive
114	m18:1	Cer(m18:1/22:0)	FALSE	606.6	Unit	266.4	Unit	10.3	0.6	166	35	5	Positive
115	m18:1	Cer(m18:1/23:0)	FALSE	620.6	Unit	266.4	Unit	10.4	0.6	166	35	5	Positive
116	m18:1	Cer(m18:1/24:0)	FALSE	634.6	Unit	266.4	Unit	10.5	0.6	166	35	5	Positive
117	m18:1	Cer(m18:1/24:1)	FALSE	632.6	Unit	266.4	Unit	10.4	0.6	166	35	5	Positive
118	Bile Acids	CA	FALSE	426.3	Unit	355.3	Unit	1.0	2	166	19	4	Positive
119	Bile Acids	Cholic Acid d4 (IS)	TRUE	430.3	Unit	359.3	Unit	1.0	1	166	19	4	Positive
120	COH	COH	FALSE	369.4	Unit	161.2	Unit	6.4	0.6	166	19	5	Positive
121	COH	COH-d7 (IS)	TRUE	376.4	Unit	161.2	Unit	6.4	0.6	166	19	5	Positive
122	DE	DE(16:0)	FALSE	640.6	Unit	367.4	Unit	11.6	0.6	166	10	4	Positive
123	DE	DE(18:1)	FALSE	666.6	Unit	367.4	Unit	11.6	0.6	166	10	4	Positive
124	DE	DE(18:1) ester d6 (IS)	TRUE	672.6	Unit	373.4	Unit	11.6	0.6	166	10	4	Positive
125	DE	DE(18:2)	FALSE	664.6	Unit	367.4	Unit	11.4	0.6	166	10	4	Positive
126	DE	DE(20:4)	FALSE	688.6	Unit	367.4	Unit	11.3	0.6	166	10	4	Positive
127	Bile Acids	dxCA	FALSE	410.3	Unit	357.3	Unit	1.6	2	166	15	5	Positive
128	DG	DG(15:0 18:1) d7 (IS)	TRUE	605.5	Unit	299.5	Unit	9.6	1	166	25	4	Positive
129	DG	DG(14:0_16:0)	FALSE	558.5	Unit	313.3	Unit	8.8	1.4	166	25	5	Positive
130	DG	DG(16:0_16:0)	FALSE	586.5	Unit	313.2	Unit	10.1	1.4	166	25	5	Positive
131	DG	DG(16:0_16:1)	FALSE	584.5	Unit	313.2	Unit	9.1	1.4	166	25	5	Positive
132	DG	DG(14:0_18:2)	FALSE	582.5	Unit	285.2	Unit	8.1	1.4	166	25	5	Positive
133	DG	DG(16:0_18:1)	FALSE	612.6	Unit	313.3	Unit	10.0	1.4	166	25	5	Positive
134	DG	DG(16:1_18:1)	FALSE	610.5	Unit	339.2	Unit	9.3	1.4	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
135	DG	DG(16:0_18:2)	FALSE	610.5	Unit	313.2	Unit	9.4	1.4	166	25	5	Positive
136	DG	DG(18:0_18:1)	FALSE	640.6	Unit	341.3	Unit	10.2	1.4	166	25	5	Positive
137	DG	DG(18:1_18:1)	FALSE	638.6	Unit	339.3	Unit	10.1	1.4	166	25	5	Positive
138	DG	DG(18:0_18:2)	FALSE	638.6	Unit	341.3	Unit	10.1	1.4	166	25	5	Positive
139	DG	DG(18:1_18:2)	FALSE	636.6	Unit	339.3	Unit	9.6	1.4	166	25	5	Positive
140	DG	DG(18:2_18:2)	FALSE	634.5	Unit	337.2	Unit	8.7	1.4	166	25	5	Positive
141	DG	DG(18:1_18:3)	FALSE	634.5	Unit	339.2	Unit	8.8	1.4	166	25	5	Positive
142	DG	DG(16:0_20:4)	FALSE	634.5	Unit	313.2	Unit	9.2	1.4	166	25	5	Positive
143	DG	DG(18:1_20:3)	FALSE	662.6	Unit	339.3	Unit	10.0	1.4	166	25	5	Positive
144	DG	DG(18:0_20:4)	FALSE	662.6	Unit	341.3	Unit	10.1	1.4	166	25	5	Positive
145	DG	DG(18:1_20:4)	FALSE	660.6	Unit	339.3	Unit	9.4	1.4	166	25	5	Positive
146	DG	DG(16:0_22:5)	FALSE	660.6	Unit	313.3	Unit	9.3	1.4	166	25	5	Positive
147	DG	DG(18:2_20:4)	FALSE	658.5	Unit	337.2	Unit	8.5	1.4	166	25	5	Positive
148	DG	DG(16:0_22:6)	FALSE	658.5	Unit	313.2	Unit	8.9	1.4	166	25	5	Positive
149	DG	DG(18:1_20:5)	FALSE	658.6	Unit	339.3	Unit	8.6	1.4	166	25	5	Positive
150	DG	DG(18:1_22:5)	FALSE	686.6	Unit	339.3	Unit	9.8	1.6	166	25	5	Positive
151	DG	DG(18:1_22:6)	FALSE	684.6	Unit	339.3	Unit	9.1	1.4	166	25	5	Positive
152	DG	DG(18:2_22:6)	FALSE	682.6	Unit	337.3	Unit	8.2	1.4	166	25	5	Positive
153	dhCer	dhCer(d18:0/16:0)	FALSE	540.5	Unit	284.3	Unit	8.3	0.6	166	27	4	Positive
154	dhCer	dhCer(d18:0/18:0)	FALSE	568.6	Unit	284.3	Unit	9.8	0.8	166	27	4	Positive
155	dhCer	dhCer(d18:0/20:0)	FALSE	596.6	Unit	284.3	Unit	10.2	0.8	166	27	4	Positive
156	dhCer	dhCer(d18:0/22:0)	FALSE	624.6	Unit	284.3	Unit	10.4	0.8	166	27	4	Positive
157	dhCer	dhCer(d18:0/24:0)	FALSE	652.7	Unit	284.3	Unit	10.6	0.8	166	27	4	Positive
158	dhCer	dhCer(d18:0/24:1)	FALSE	650.6	Unit	284.3	Unit	10.4	0.8	166	27	4	Positive
159	dhCer	dhCer 8:0 (IS)	TRUE	428.4	Unit	284.3	Unit	4.6	0.8	166	27	4	Positive
160	dimethyl-CE	dimethyl-CE(18:1)	FALSE	696.6	Unit	397.3	Unit	12.0	0.4	166	10	4	Positive
161	dimethyl-CE	dimethyl-CE(18:2)	FALSE	694.6	Unit	397.3	Unit	11.8	0.4	166	10	4	Positive
162	dimethyl-CE	dimethyl-CE(20:4)	FALSE	718.6	Unit	397.3	Unit	11.7	0.4	166	10	4	Positive
163	FFA	FA(14:0)	FALSE	227.2	Unit	227.2	Unit	3.1	2	166	0	4	Negative
164	FFA	FA(16:0)	FALSE	255.2	Unit	255.2	Unit	3.8	2	166	0	4	Negative
165	FFA	FA(16:1)	FALSE	253.2	Unit	253.2	Unit	3.3	2	166	0	4	Negative
166	FFA	FA(17:0)	FALSE	269.3	Unit	269.2	Unit	4.1	2	166	0	4	Negative
167	FFA	FA(17:1)	FALSE	267.2	Unit	267.2	Unit	3.6	2	166	0	4	Negative
168	FFA	FA(18:0)	FALSE	283.3	Unit	283.3	Unit	4.4	2	166	0	4	Negative
169	FFA	FA(18:1)	FALSE	281.3	Unit	281.2	Unit	3.9	2	166	0	4	Negative
170	FFA	FA(18:1) d9 (IS)	TRUE	290.3	Unit	290.2	Unit	3.9	2	166	0	4	Negative
171	FFA	FA(18:2)	FALSE	279.2	Unit	279.2	Unit	3.5	2	166	0	4	Negative
172	FFA	FA(18:3)	FALSE	277.2	Unit	277.2	Unit	3.1	2	166	0	4	Negative
173	FFA	FA(20:2)	FALSE	307.3	Unit	307.3	Unit	4.1	2	166	0	4	Negative
174	FFA	FA(20:3)	FALSE	305.3	Unit	305.2	Unit	3.8	2	166	0	4	Negative
175	FFA	FA(20:4)	FALSE	303.2	Unit	303.2	Unit	3.4	2	166	0	4	Negative
176	FFA	FA(20:4) d11 (IS)	TRUE	314.2	Unit	314.2	Unit	3.4	1	166	0	4	Negative
177	FFA	FA(20:5)	FALSE	301.2	Unit	301.2	Unit	3.0	2	166	0	4	Negative
178	FFA	FA(22:4)	FALSE	331.3	Unit	331.3	Unit	3.9	2	166	0	4	Negative
179	FFA	FA(22:5)	FALSE	329.3	Unit	329.2	Unit	3.6	2	166	0	4	Negative
180	FFA	FA(22:6) d5 (IS)	TRUE	332.2	Unit	332.2	Unit	3.2	1	166	0	4	Negative

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
181	FFA	FA(22:6)	FALSE	327.2	Unit	327.2	Unit	3.3	2	166	0	4	Negative
182	GM3	GM3(d18:1/16:0)	FALSE	1153.7	Unit	264.3	Unit	4.9	1	166	61	5	Positive
183	GM3	GM3(d18:1/18:0)	FALSE	1181.8	Unit	264.3	Unit	5.6	1	166	61	5	Positive
184	GM3	GM3(d18:1/20:0)	FALSE	1209.8	Unit	264.3	Unit	6.5	1	166	61	5	Positive
185	GM3	GM3(d18:1/22:0)	FALSE	1237.8	Unit	264.3	Unit	7.5	1	166	61	5	Positive
186	GM3	GM3(d18:1/24:0)	FALSE	1265.8	Unit	264.3	Unit	8.5	1	166	61	5	Positive
187	GM3	GM3(d18:1/24:1)	FALSE	1263.8	Unit	264.3	Unit	7.5	1	166	61	5	Positive
188	HexCer	HexCer(d16:1/18:0)	FALSE	700.6	Unit	236.3	Unit	6.6	0.5	166	35	5	Positive
189	HexCer	HexCer(d16:1/20:0)	FALSE	728.6	Unit	236.3	Unit	7.7	0.5	166	35	5	Positive
190	HexCer	HexCer(d16:1/22:0)	FALSE	756.7	Unit	236.3	Unit	8.9	0.5	166	35	5	Positive
191	HexCer	HexCer(d16:1/24:0)	FALSE	784.7	Unit	236.3	Unit	10.0	0.5	166	35	5	Positive
192	HexCer	HexCer(d18:1/16:0)	FALSE	700.6	Unit	264.3	Unit	6.6	0.6	166	35	5	Positive
193	HexCer	HexCer(d18:1/18:0)	FALSE	728.6	Unit	264.3	Unit	7.6	0.6	166	35	5	Positive
194	HexCer	HexCer(d18:1/20:0)	FALSE	756.6	Unit	264.3	Unit	8.8	0.6	166	35	5	Positive
195	HexCer	HexCer(d18:1/22:0)	FALSE	784.7	Unit	264.3	Unit	10.0	0.6	166	35	5	Positive
196	HexCer	HexCer(d18:1/24:0)	FALSE	812.7	Unit	264.3	Unit	10.2	0.6	166	35	5	Positive
197	HexCer	HexCer(d18:1/24:1)	FALSE	810.7	Unit	264.3	Unit	10.0	0.6	166	35	5	Positive
198	HexCer	HexCer(d18:2/20:0)	FALSE	754.6	Unit	262.3	Unit	7.9	0.5	166	35	5	Positive
199	HexCer	HexCer(d18:2/22:0)	FALSE	782.7	Unit	262.3	Unit	9.0	0.5	166	35	5	Positive
200	HexCer	HexCer(d18:2/24:0)	FALSE	810.7	Unit	262.3	Unit	10.1	0.5	166	35	5	Positive
201	Hex2Cer	Hex2Cer(d16:1/16:0)	FALSE	834.6	Unit	236.3	Unit	5.2	0.5	166	49	5	Positive
202	Hex2Cer	Hex2Cer(d16:1/24:1)	FALSE	944.7	Unit	236.3	Unit	8.2	0.5	166	49	5	Positive
203	Hex2Cer	Hex2Cer(d18:1/15:0) d7 (IS)	TRUE	855.6	Unit	271.3	Unit	5.6	1	166	49	5	Positive
204	Hex2Cer	Hex2Cer(d18:1/16:0)	FALSE	862.6	Unit	264.3	Unit	6.1	0.6	166	49	5	Positive
205	Hex2Cer	Hex2Cer(d18:1/20:0)	FALSE	918.7	Unit	264.3	Unit	8.1	0.6	166	49	5	Positive
206	Hex2Cer	Hex2Cer(d18:1/22:0)	FALSE	946.7	Unit	264.3	Unit	9.3	0.6	166	49	5	Positive
207	Hex2Cer	Hex2Cer(d18:1/24:0)	FALSE	974.8	Unit	264.3	Unit	10.1	0.6	166	49	5	Positive
208	Hex2Cer	Hex2Cer(d18:1/24:1)	FALSE	972.7	Unit	264.3	Unit	9.3	0.6	166	49	5	Positive
209	Hex2Cer	Hex2Cer(d18:2/16:0)	FALSE	860.6	Unit	262.3	Unit	5.4	0.5	166	49	5	Positive
210	Hex2Cer	Hex2Cer(d18:2/24:1)	FALSE	970.7	Unit	262.3	Unit	8.4	0.5	166	49	5	Positive
211	Hex3Cer	Hex3Cer(d18:1/16:0)	FALSE	1024.7	Unit	264.3	Unit	5.7	0.5	166	61	5	Positive
212	Hex3Cer	Hex3Cer(d18:1/17:0) (IS)	TRUE	1038.7	Unit	264.3	Unit	6.2	0.5	166	61	5	Positive
213	Hex3Cer	Hex3Cer(d18:1/18:0)	FALSE	1052.7	Unit	264.3	Unit	6.6	0.5	166	61	5	Positive
214	Hex3Cer	Hex3Cer(d18:1/22:0)	FALSE	1108.8	Unit	264.3	Unit	8.8	0.5	166	61	5	Positive
215	Hex3Cer	Hex3Cer(d18:1/24:0)	FALSE	1136.8	Unit	264.3	Unit	10.0	0.7	166	61	5	Positive
216	Hex3Cer	Hex3Cer(d18:1/24:1)	FALSE	1134.8	Unit	264.3	Unit	8.8	0.5	166	61	5	Positive
217	Hex2Cer	HexCer(d18:1/15:0) d7 (IS)	TRUE	693.6	Unit	271.3	Unit	6.1	1	166	35	5	Positive
218	LPC	LPC(14:0) (a\b)	FALSE	468.3	Unit	184.1	Unit	1.9	1	166	21	5	Positive
219	LPC	LPC(15:0) (a\b)	FALSE	482.3	Unit	184.1	Unit	2.3	1	166	21	5	Positive
220	LPC	LPC(16:0) (a\b)	FALSE	496.3	Unit	184.1	Unit	2.6	1	166	21	5	Positive
221	LPC	LPC(16:1) (a\b)	FALSE	494.3	Unit	184.1	Unit	2.1	1	166	21	5	Positive
222	LPC	LPC(17:0) [sn1]	FALSE	510.4	Unit	184.1	Unit	2.9	1	166	21	5	Positive
223	LPC	LPC(17:1) (a\b\c)	FALSE	508.4	Unit	184.1	Unit	2.5	1	166	21	5	Positive
224	LPC	LPC(18:0) (a\b)	FALSE	524.4	Unit	184.1	Unit	3.3	1	166	21	5	Positive
225	LPC	LPC(18:1) (a\b)	FALSE	522.4	Unit	184.1	Unit	2.8	1	166	21	5	Positive
226	LPC	LPC(18:1) d7 (IS)	TRUE	529.4	Unit	184.1	Unit	2.8	1	166	21	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
227	LPC	LPC(18:2) (a\b)	FALSE	520.3	Unit	184.1	Unit	2.3	1	166	21	5	Positive
228	oxLipid	LPC(18:2) [+OH]	FALSE	536.3	Unit	184.1	Unit	1.0	1	166	21	5	Positive
229	LPC	LPC(18:3) (a\b\c)	FALSE	518.3	Unit	184.1	Unit	2.0	1	166	21	5	Positive
230	LPC (104)	LPC 18:3(104)	FALSE	518.3	Unit	104.1	Unit	2.0	0.8	166	21	5	Positive
231	LPC	LPC(19:0) (a\b\c)	FALSE	538.4	Unit	184.1	Unit	3.5	1	166	21	5	Positive
232	LPC	LPC(19:1) (a\b\c)	FALSE	536.4	Unit	184.1	Unit	3.1	1	166	21	5	Positive
233	LPC	LPC(20:0) (a\b)	FALSE	552.4	Unit	184.1	Unit	3.8	1	166	21	5	Positive
234	LPC	LPC(20:1) (a\b)	FALSE	550.4	Unit	184.1	Unit	3.4	1	166	21	5	Positive
235	LPC	LPC(20:2) (a\b)	FALSE	548.4	Unit	184.1	Unit	2.9	1	166	21	5	Positive
236	LPC	LPC(20:3) (a\b)	FALSE	546.4	Unit	184.1	Unit	2.6	1	166	21	5	Positive
237	LPC (104)	LPC 20:3(104)	FALSE	546.4	Unit	104.1	Unit	2.6	1	166	21	5	Positive
238	LPC	LPC(20:4) (a\b)	FALSE	544.3	Unit	184.1	Unit	2.3	1	166	21	5	Positive
239	oxLipid	LPC(20:4) [+OH]	FALSE	560.3	Unit	184.1	Unit	1.4	1.5	166	21	5	Positive
240	LPC	LPC(20:5) (a\b)	FALSE	542.3	Unit	184.1	Unit	1.9	1	166	21	5	Positive
241	LPC	LPC(22:0) (a\b)	FALSE	580.4	Unit	184.1	Unit	4.4	1	166	21	5	Positive
242	LPC	LPC(22:1) (a\b)	FALSE	578.4	Unit	184.1	Unit	3.9	1	166	21	5	Positive
243	LPC	LPC(22:4) (a\b)	FALSE	572.4	Unit	184.1	Unit	2.8	1	166	21	5	Positive
244	LPC (104)	LPC 22:5(104)	FALSE	570.4	Unit	104.1	Unit	2.5	1.5	166	21	5	Positive
245	LPC	LPC(22:5) (a\b\c)	FALSE	570.4	Unit	184.1	Unit	2.5	1	166	21	5	Positive
246	LPC	LPC(22:6) (a\b)	FALSE	568.3	Unit	184.1	Unit	2.2	1	166	21	5	Positive
247	oxLipid	LPC(22:6) [+OH]	FALSE	584.3	Unit	184.1	Unit	1.5	1.5	166	21	5	Positive
248	LPC	LPC(24:0) (a\b)	FALSE	608.5	Unit	184.1	Unit	5.1	1	166	21	5	Positive
249	LPC	LPC(26:0) (a\b)	FALSE	636.5	Unit	184.1	Unit	5.9	1	166	21	5	Positive
250	LPCO	LPC(O-16:0)	FALSE	482.4	Unit	104.1	Unit	3.0	3	166	23	5	Positive
251	LPCO	LPC(O-18:0)	FALSE	510.4	Unit	104.1	Unit	3.6	3	166	23	5	Positive
252	LPCO	LPC(O-18:1)	FALSE	508.4	Unit	104.1	Unit	3.1	3	166	23	5	Positive
253	LPCO	LPC(O-20:0)	FALSE	538.4	Unit	104.1	Unit	4.1	3	166	23	5	Positive
254	LPCO	LPC(O-20:1)	FALSE	536.4	Unit	104.1	Unit	3.7	3	166	23	5	Positive
255	LPCO	LPC(O-22:0)	FALSE	566.5	Unit	104.1	Unit	4.8	2	166	23	5	Positive
256	LPCO	LPC(O-22:1)	FALSE	564.4	Unit	104.1	Unit	4.2	2	166	23	5	Positive
257	LPCO	LPC(O-24:0)	FALSE	594.5	Unit	104.1	Unit	5.6	1	166	23	5	Positive
258	LPCO	LPC(O-24:1)	FALSE	592.5	Unit	104.1	Unit	4.8	2	166	23	5	Positive
259	LPCO	LPC(O-24:2)	FALSE	590.5	Unit	104.1	Unit	4.3	2	166	23	5	Positive
260	LPCP	LPC(P-16:0)	FALSE	480.3	Unit	104.1	Unit	3.0	0.6	166	25	5	Positive
261	LPCP	LPC(P-17:0) (a\b)	FALSE	494.3	Unit	104.1	Unit	3.3	1	166	25	5	Positive
262	LPCP	LPC(P-18:0)	FALSE	508.3	Unit	104.1	Unit	3.6	0.6	166	25	5	Positive
263	LPCP	LPC(P-18:1)	FALSE	506.3	Unit	104.1	Unit	3.1	0.6	166	25	5	Positive
264	LPCP	LPC(P-20:0)	FALSE	536.3	Unit	104.1	Unit	4.1	0.6	166	25	5	Positive
265	LPE	LPE(16:0) (a\b)	FALSE	454.3	Unit	313.3	Unit	2.7	1	166	17	5	Positive
266	LPE	LPE(17:0) (a\b)	FALSE	468.3	Unit	327.3	Unit	3.1	1	166	17	5	Positive
267	LPE	LPE(18:0) (a\b)	FALSE	482.3	Unit	341.3	Unit	3.4	1	166	17	5	Positive
268	LPE	LPE(18:1) (a\b)	FALSE	480.3	Unit	339.3	Unit	2.9	1	166	17	5	Positive
269	LPE	LPE(18:1) d7 (IS)	TRUE	487.3	Unit	346.3	Unit	2.9	1	166	17	5	Positive
270	LPE	LPE(18:2) (a\b)	FALSE	478.3	Unit	337.3	Unit	2.4	1	166	17	5	Positive
271	LPE	LPE(20:4) (a\b)	FALSE	502.3	Unit	361.3	Unit	2.4	1	166	17	5	Positive
272	LPE	LPE(22:6) (a\b)	FALSE	526.3	Unit	385.3	Unit	2.3	1	166	17	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
273	LPEP	LPE(P-16:0)	FALSE	438.3	Unit	266.4	Unit	3.1	1	166	19	5	Positive
274	LPEP	LPE(P-18:0)	FALSE	466.3	Unit	294.4	Unit	3.7	1	166	19	5	Positive
275	LPEP	LPE(P-18:1)	FALSE	464.3	Unit	292.4	Unit	3.3	1	166	19	5	Positive
276	LPEP	LPE(P-20:0)	FALSE	494.3	Unit	322.4	Unit	4.2	1	166	19	5	Positive
277	LPI	LPI 13:0 (IS)	TRUE	548.3	Unit	271.3	Unit	1.3	1	166	21	5	Positive
278	LPI	LPI(18:0)	FALSE	618.3	Unit	341.3	Unit	2.9	1	166	21	5	Positive
279	LPI	LPI(18:1) (a\b)	FALSE	616.3	Unit	339.3	Unit	2.4	1	166	21	5	Positive
280	LPI	LPI(18:2) (a\b)	FALSE	614.3	Unit	337.3	Unit	1.9	1	166	21	5	Positive
281	LPI	LPI(20:4) (a\b)	FALSE	638.3	Unit	361.3	Unit	1.9	1	166	21	5	Positive
282	Methyl-CE	methyl-CE(18:0)	FALSE	684.6	Unit	383.3	Unit	12.2	0.4	166	10	4	Positive
283	Methyl-CE	methyl-CE(18:1)	FALSE	682.6	Unit	383.3	Unit	11.9	0.4	166	10	4	Positive
284	Methyl-CE	methyl-CE(18:2)	FALSE	680.6	Unit	383.3	Unit	11.7	0.4	166	10	4	Positive
285	Methyl-CE	methyl-CE(20:4)	FALSE	704.6	Unit	383.3	Unit	11.6	0.4	166	10	4	Positive
286	mDE	methyl-DE(18:1)	FALSE	680.6	Unit	381.4	Unit	11.7	0.6	166	10	4	Positive
287	mDE	methyl-DE(18:2)	FALSE	678.6	Unit	381.4	Unit	11.5	0.6	166	10	4	Positive
288	MG	MG(18:1) d7 (IS)	TRUE	364.2	Unit	272.2	Unit	3.7	1	166	11	4	Positive
289	PA	PA(15:0_18:1) d7 (IS)	TRUE	685.6	Unit	570.6	Unit	6.2	2	166	13	4	Positive
290	PA	PA(34:1)	FALSE	692.6	Unit	577.6	Unit	6.7	2	166	13	4	Positive
291	PA	PA(36:2)	FALSE	718.6	Unit	603.6	Unit	7.0	2	166	13	4	Positive
292	PA	PA(36:3)	FALSE	716.6	Unit	601.6	Unit	6.4	2	166	13	4	Positive
293	PA	PA(36:4)	FALSE	714.6	Unit	599.6	Unit	5.7	2	166	13	4	Positive
294	PC	PC(28:0)	FALSE	678.5	Unit	184.1	Unit	5.2	0.8	166	25	5	Positive
295	PC	PC(14:0_16:0)	FALSE	706.5	Unit	184.1	Unit	6.0	0.8	166	25	5	Positive
296	PC	PC(31:0) (a\b)	FALSE	720.6	Unit	184.1	Unit	6.4	0.8	166	25	5	Positive
297	PC	PC(31:1)	FALSE	718.5	Unit	184.1	Unit	5.8	0.6	166	25	5	Positive
298	PC	PC(16:0_16:0)	FALSE	734.6	Unit	184.1	Unit	7.0	0.6	166	25	5	Positive
299	PC	PC(32:1)	FALSE	732.6	Unit	184.1	Unit	6.2	0.6	166	25	5	Positive
300	PC	PC(32:2)	FALSE	730.5	Unit	184.1	Unit	5.6	0.6	166	25	5	Positive
301	PC	PC(33:0) (a\b)	FALSE	748.6	Unit	184.1	Unit	7.5	1.2	166	25	5	Positive
302	PC	PC(33:1)	FALSE	746.6	Unit	184.1	Unit	6.7	0.6	166	25	5	Positive
303	PC	PC(33:2)	FALSE	744.6	Unit	184.1	Unit	6.0	0.6	166	25	5	Positive
304	PC	PC(16:0_18:0)	FALSE	762.6	Unit	184.1	Unit	8.1	0.6	166	25	5	Positive
305	PC	PC(16:0_18:1)	FALSE	760.6	Unit	184.1	Unit	7.2	0.6	166	25	5	Positive
306	PC	PC(16:0_18:2)	FALSE	758.6	Unit	184.1	Unit	6.5	0.6	166	25	5	Positive
307	oxLipid	PC(34:2) [+OH]	FALSE	774.6	Unit	184.1	Unit	4.8	1	166	25	5	Positive
308	PC	PC(34:3) (a\b\c)	FALSE	756.6	Unit	184.1	Unit	5.9	1.2	166	25	5	Positive
309	PC	PC(14:0_20:4)	FALSE	754.5	Unit	184.1	Unit	5.5	0.6	166	25	5	Positive
310	PC	PC(34:5)	FALSE	752.5	Unit	184.1	Unit	5.1	0.6	166	25	5	Positive
311	PC	PC(35:1) (a\b)	FALSE	774.6	Unit	184.1	Unit	7.7	1.2	166	25	5	Positive
312	PC	PC(35:2) (a\b)	FALSE	772.6	Unit	184.1	Unit	6.9	1.2	166	25	5	Positive
313	PC	PC(35:3) (a\b\c)	FALSE	770.6	Unit	184.1	Unit	6.3	3	166	25	5	Positive
314	PC	PC(15:0_20:4)	FALSE	768.6	Unit	184.1	Unit	6.0	0.6	166	25	5	Positive
315	PC	PC(35:5)	FALSE	766.5	Unit	184.1	Unit	5.4	0.6	166	25	5	Positive
316	PC	PC(18:0_18:1)	FALSE	788.6	Unit	184.1	Unit	8.3	0.8	166	25	5	Positive
317	PC	PC(36:2) (a\b)	FALSE	786.6	Unit	184.1	Unit	7.5	1	166	25	5	Positive
318	PC	PC(36:3) (a\b\c)	FALSE	784.6	Unit	184.1	Unit	6.8	1.2	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
319	PC	PC(36:4) (a\b)	FALSE	782.6	Unit	184.1	Unit	6.3	1.6	166	25	5	Positive
320	oxLipid	PC(36:4) [+OH]	FALSE	798.6	Unit	184.1	Unit	5.4	2	166	25	5	Positive
321	PC	PC(36:5) (a\b)	FALSE	780.6	Unit	184.1	Unit	5.8	1	166	25	5	Positive
322	PC	PC(36:6) (a\b)	FALSE	778.5	Unit	184.1	Unit	5.3	0.6	166	25	5	Positive
323	PC	PC(37:4) (a\b)	FALSE	796.6	Unit	184.1	Unit	6.9	1.2	166	25	5	Positive
324	PC	PC(15:0_22:6)	FALSE	792.6	Unit	184.1	Unit	5.8	0.6	166	25	5	Positive
325	PC	PC(38:2)	FALSE	814.6	Unit	184.1	Unit	8.6	1.4	166	25	5	Positive
326	PC	PC(18:0_20:3)	FALSE	812.6	Unit	184.1	Unit	7.9	1.4	166	25	5	Positive
327	PC	PC(38:4) (a\b\c)	FALSE	810.6	Unit	184.1	Unit	7.3	1.6	166	25	5	Positive
328	PC	PC(38:5) (a\b)	FALSE	808.6	Unit	184.1	Unit	6.7	1	166	25	5	Positive
329	PC	PC(38:6) (a\b)	FALSE	806.6	Unit	184.1	Unit	6.1	1.2	166	25	5	Positive
330	oxLipid	PC(38:6) [+OH]	FALSE	822.6	Unit	184.1	Unit	5.3	2	166	25	5	Positive
331	PC	PC(38:7) (a\b\c)	FALSE	804.6	Unit	184.1	Unit	5.6	1	166	25	5	Positive
332	PC	PC(39:5) (a\b)	FALSE	822.6	Unit	184.1	Unit	6.8	1.2	166	25	5	Positive
333	PC	PC(39:6) (a\b)	FALSE	820.6	Unit	184.1	Unit	6.7	1	166	25	5	Positive
334	PC	PC(40:4) (a\b)	FALSE	838.6	Unit	184.1	Unit	8.4	1.2	166	25	5	Positive
335	PC	PC(40:5) (a\b)	FALSE	836.6	Unit	184.1	Unit	7.8	1.2	166	25	5	Positive
336	PC	PC(18:0_22:6)	FALSE	834.6	Unit	184.1	Unit	7.3	0.6	166	25	5	Positive
337	PC	PC(40:7) (a\b\c)	FALSE	832.6	Unit	184.1	Unit	6.4	1	166	25	5	Positive
338	PC	PC(40:8)	FALSE	830.6	Unit	184.1	Unit	5.8	0.8	166	25	5	Positive
339	PC	PC(15:0_18:1) d7 (IS)	TRUE	753.6	Unit	184.1	Unit	6.7	0.7	166	25	5	Positive
340	PC (O)	PC(O-16:0/16:0)	FALSE	720.6	Unit	184.1	Unit	7.7	0.8	166	25	5	Positive
341	PC (O)	PC(O-32:1)	FALSE	718.5	Unit	184.1	Unit	7.2	0.8	166	25	5	Positive
342	PC (O)	PC(O-32:2)	FALSE	716.6	Unit	184.1	Unit	6.3	0.8	166	25	5	Positive
343	PC (O)	PC(O-34:1)	FALSE	746.6	Unit	184.1	Unit	7.9	0.8	166	25	5	Positive
344	PC (O)	PC(O-34:2)	FALSE	744.6	Unit	184.1	Unit	7.2	1	166	25	5	Positive
345	PC (O)	PC(O-34:4)	FALSE	740.6	Unit	184.1	Unit	6.1	0.8	166	25	5	Positive
346	PC (O)	PC(O-35:4)	FALSE	754.5	Unit	184.1	Unit	6.7	0.8	166	25	5	Positive
347	PC (O)	PC(O-36:0)	FALSE	776.6	Unit	184.1	Unit	10.0	0.8	166	25	5	Positive
348	PC (O)	PC(O-18:0/18:1)	FALSE	774.6	Unit	184.1	Unit	9.1	0.8	166	25	5	Positive
349	PC (O)	PC(O-36:2) (a\b)	FALSE	772.6	Unit	184.1	Unit	8.2	1.2	166	25	5	Positive
350	PC (O)	PC(O-36:3) (a\b)	FALSE	770.6	Unit	184.1	Unit	7.4	1.2	166	25	5	Positive
351	PC (O)	PC(O-16:0/20:4)	FALSE	768.6	Unit	184.1	Unit	7.1	0.8	166	25	5	Positive
352	PC (O)	PC(O-36:5)	FALSE	766.5	Unit	184.1	Unit	6.4	0.8	166	25	5	Positive
353	PC (O)	PC(O-18:0/20:4)	FALSE	796.6	Unit	184.1	Unit	8.2	0.8	166	25	5	Positive
354	PC (O)	PC(O-38:5)	FALSE	794.6	Unit	184.1	Unit	7.2	0.8	166	25	5	Positive
355	PC (O)	PC(O-16:0/22:6)	FALSE	792.6	Unit	184.1	Unit	6.9	0.8	166	25	5	Positive
356	PC (O)	PC(O-40:5)	FALSE	822.6	Unit	184.1	Unit	8.3	0.8	166	25	5	Positive
357	PC (O)	PC(O-18:0/22:6)	FALSE	820.6	Unit	184.1	Unit	8.0	1	166	25	5	Positive
358	PC (O)	PC(O-40:7)	FALSE	818.6	Unit	184.1	Unit	7.0	1	166	25	5	Positive
359	PC (P)	PC(P-18:0/18:1) d9 (IS)	TRUE	781.6	Unit	184.1	Unit	8.9	1	166	25	5	Positive
360	PC (P)	PC(P-16:0/14:0)	FALSE	690.4	Unit	184.1	Unit	6.6	0.8	166	25	5	Positive
361	PC (P)	PC(P-16:0/16:0)	FALSE	718.5	Unit	184.1	Unit	7.6	0.8	166	25	5	Positive
362	PC (P)	PC(P-16:0/16:1)	FALSE	716.6	Unit	184.1	Unit	6.8	0.8	166	25	5	Positive
363	PC (P)	PC(P-16:0/18:0)	FALSE	746.6	Unit	184.1	Unit	8.8	0.8	166	25	5	Positive
364	PC (P)	PC(P-16:0/18:1)	FALSE	744.6	Unit	184.1	Unit	7.8	0.8	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
365	PC (P)	PC(P-16:0/18:2)	FALSE	742.5	Unit	184.1	Unit	7.0	0.8	166	25	5	Positive
366	PC (P)	PC(P-16:0/18:3)	FALSE	740.6	Unit	184.1	Unit	6.4	0.8	166	25	5	Positive
367	PC (P)	PC(P-35:2) (a\b)	FALSE	756.6	Unit	184.1	Unit	7.5	1.5	166	25	5	Positive
368	PC (P)	PC(P-15:0/20:4) (a\b)	FALSE	752.6	Unit	184.1	Unit	6.3	1	166	25	5	Positive
369	PC (P)	PC(P-36:2) (a\b)	FALSE	770.6	Unit	184.1	Unit	8.1	1	166	25	5	Positive
370	PC (P)	PC(P-36:3)	FALSE	768.5	Unit	184.1	Unit	7.3	1	166	25	5	Positive
371	PC (P)	PC(P-16:0/20:4)	FALSE	766.5	Unit	184.1	Unit	6.9	0.8	166	25	5	Positive
372	PC (P)	PC(P-16:0/20:5)	FALSE	764.6	Unit	184.1	Unit	6.3	0.8	166	25	5	Positive
373	PC (P)	PC(P-37:4) (a\b)	FALSE	780.5	Unit	184.1	Unit	7.4	1	166	25	5	Positive
374	PC (P)	PC(P-18:0/20:4)	FALSE	794.6	Unit	184.1	Unit	8.0	0.8	166	25	5	Positive
375	PC (P)	PC(P-38:5) (a\b)	FALSE	792.6	Unit	184.1	Unit	7.2	1.2	166	25	5	Positive
376	PC (P)	PC(P-16:0/22:6)	FALSE	790.6	Unit	184.1	Unit	6.7	0.8	166	25	5	Positive
377	PC (P)	PC(P-20:0/20:4)	FALSE	822.6	Unit	184.1	Unit	9.2	0.8	166	25	5	Positive
378	PC (P)	PC(P-18:0/22:5)	FALSE	820.6	Unit	184.1	Unit	8.1	1	166	25	5	Positive
379	PC (P)	PC(P-18:0/22:6)	FALSE	818.6	Unit	184.1	Unit	7.8	0.8	166	25	5	Positive
380	PC (P)	PC(P-18:1/22:6)	FALSE	816.6	Unit	184.1	Unit	6.8	0.8	166	25	5	Positive
381	PE	PE(16:0_16:0)	FALSE	692.5	Unit	551.5	Unit	7.4	0.6	166	19	5	Positive
382	PE	PE(16:0_16:1)	FALSE	690.5	Unit	549.5	Unit	6.6	0.6	166	19	5	Positive
383	PE	PE(16:0_18:1)	FALSE	718.5	Unit	577.5	Unit	7.6	0.6	166	19	5	Positive
384	PE	PE(16:0_18:2)	FALSE	716.5	Unit	575.5	Unit	6.8	0.6	166	19	5	Positive
385	PE	PE(34:3) (a\b\c)	FALSE	714.5	Unit	573.5	Unit	6.2	1	166	19	5	Positive
386	PE	PE(35:1) (a\b)	FALSE	732.6	Unit	591.5	Unit	8.0	1	166	19	5	Positive
387	PE	PE(35:2) (a\b)	FALSE	730.5	Unit	589.5	Unit	7.3	1	166	19	5	Positive
388	PE	PE(18:0_18:1)	FALSE	746.6	Unit	605.6	Unit	8.8	0.6	166	19	5	Positive
389	PE	PE(36:2) (a\b)	FALSE	744.6	Unit	603.5	Unit	7.9	1	166	19	5	Positive
390	PE	PE(36:3) (a\b)	FALSE	742.5	Unit	601.5	Unit	7.1	0.6	166	19	5	Positive
391	PE	PE(16:0_20:4)	FALSE	740.5	Unit	599.5	Unit	6.8	0.6	166	19	5	Positive
392	PE	PE(36:5) (a\b)	FALSE	738.5	Unit	597.5	Unit	6.1	1	166	19	5	Positive
393	PE	PE(37:4) (a\b)	FALSE	754.6	Unit	613.5	Unit	7.2	1	166	19	5	Positive
394	PE	PE(18:0_20:3) (a\b)	FALSE	770.6	Unit	629.6	Unit	8.5	1.2	166	19	5	Positive
395	PE	PE(18:0_20:4)	FALSE	768.6	Unit	627.5	Unit	7.9	0.6	166	19	5	Positive
396	PE	PE(38:5) (a\b)	FALSE	766.5	Unit	625.5	Unit	7.1	1	166	19	5	Positive
397	PE	PE(16:0_22:6)	FALSE	764.5	Unit	623.5	Unit	6.6	0.6	166	19	5	Positive
398	PE	PE(39:6) (a\b)	FALSE	778.5	Unit	637.5	Unit	7.0	1	166	19	5	Positive
399	PE	PE(40:4) (a\b)	FALSE	796.6	Unit	655.6	Unit	8.9	1	166	19	5	Positive
400	PE	PE(18:0_22:5) (a\b)	FALSE	794.6	Unit	653.6	Unit	8.2	1.4	166	19	5	Positive
401	PE	PE(18:0_22:6)	FALSE	792.6	Unit	651.5	Unit	7.6	0.6	166	19	5	Positive
402	PE	PE(18:1_22:6) (a\b)	FALSE	790.5	Unit	649.5	Unit	6.8	0.6	166	19	5	Positive
403	PE	PE(15:0_18:1) d7 (IS)	TRUE	711.6	Unit	570.5	Unit	7.0	1	166	19	5	Positive
404	PE (O)	PE(O-34:1)	FALSE	704.6	Unit	563.5	Unit	8.3	0.8	166	19	5	Positive
405	PE (O)	PE(O-16:0/18:2)	FALSE	702.5	Unit	561.5	Unit	7.6	0.8	166	19	5	Positive
406	PE (O)	PE(O-36:3) (a\b)	FALSE	728.6	Unit	587.5	Unit	7.8	1	166	19	5	Positive
407	PE (O)	PE(O-16:0/20:4)	FALSE	726.5	Unit	585.5	Unit	7.5	0.8	166	19	5	Positive
408	PE (O)	PE(O-36:5)	FALSE	724.5	Unit	583.5	Unit	6.8	0.8	166	19	5	Positive
409	PE (O)	PE(O-38:4) (a\b)	FALSE	754.6	Unit	613.6	Unit	8.5	1.2	166	19	5	Positive
410	PE (O)	PE(O-38:5) (a\b)	FALSE	752.6	Unit	611.5	Unit	7.8	1.2	166	19	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
411	PE (O)	PE(O-16:0/22:6)	FALSE	750.6	Unit	609.5	Unit	7.3	1.2	166	19	5	Positive
412	PE (O)	PE(O-18:0/22:5)	FALSE	780.6	Unit	639.6	Unit	8.7	0.8	166	19	5	Positive
413	PE (O)	PE(O-18:0/22:6)	FALSE	778.5	Unit	637.5	Unit	8.2	0.8	166	19	5	Positive
414	PE (O)	PE(O-18:1/22:6)	FALSE	776.6	Unit	635.5	Unit	7.4	0.8	166	19	5	Positive
415	PE (P)	PE(P-15:0/22:6)	FALSE	734.5	Unit	385.3	Unit	6.5	1	166	19	5	Positive
416	PE (P)	PE(P-16:0/18:1)	FALSE	702.5	Unit	339.3	Unit	8.3	0.6	166	19	5	Positive
417	PE (P)	PE(P-16:0/18:2)	FALSE	700.5	Unit	337.3	Unit	7.4	0.6	166	19	5	Positive
418	PE (P)	PE(P-16:0/20:3) (a\b)	FALSE	726.5	Unit	363.3	Unit	7.8	0.6	166	19	5	Positive
419	PE (P)	PE(P-16:0/20:4)	FALSE	724.5	Unit	361.3	Unit	7.3	0.6	166	19	5	Positive
420	PE (P)	PE(P-16:0/20:5)	FALSE	722.5	Unit	359.3	Unit	6.7	0.6	166	19	5	Positive
421	PE (P)	PE(P-16:0/22:4)	FALSE	752.6	Unit	389.3	Unit	8.2	0.6	166	19	5	Positive
422	PE (P)	PE(P-16:0/22:5) (a\b)	FALSE	750.5	Unit	387.3	Unit	7.6	1.4	166	19	5	Positive
423	PE (P)	PE(P-16:0/22:6)	FALSE	748.5	Unit	385.3	Unit	7.1	0.6	166	19	5	Positive
424	PE (P)	PE(P-17:0/20:4) (a\b)	FALSE	738.6	Unit	361.3	Unit	7.8	1	166	19	5	Positive
425	PE (P)	PE(P-17:0/22:6) (a\b)	FALSE	762.6	Unit	385.3	Unit	7.6	1	166	19	5	Positive
426	PE (P)	PE(P-18:0/18:1)	FALSE	730.6	Unit	339.3	Unit	9.5	0.6	166	19	5	Positive
427	PE (P)	PE(P-18:0/18:1) d9 (IS)	TRUE	739.5	Unit	348.3	Unit	9.4	1	166	19	5	Positive
428	PE (P)	PE(P-18:0/18:2)	FALSE	728.6	Unit	337.3	Unit	8.6	0.6	166	19	5	Positive
429	PE (P)	PE(P-18:0/18:3)	FALSE	726.5	Unit	335.3	Unit	7.9	1	166	19	5	Positive
430	PE (P)	PE(P-18:0/20:3) (a\b)	FALSE	754.5	Unit	363.3	Unit	9.0	0.6	166	19	5	Positive
431	PE (P)	PE(P-18:0/20:4)	FALSE	752.6	Unit	361.3	Unit	8.5	0.6	166	19	5	Positive
432	PE (P)	PE(P-18:0/20:5)	FALSE	750.5	Unit	359.3	Unit	7.8	0.6	166	19	5	Positive
433	PE (P)	PE(P-18:0/22:4)	FALSE	780.6	Unit	389.3	Unit	9.4	0.6	166	19	5	Positive
434	PE (P)	PE(P-18:0/22:5) (a\b)	FALSE	778.5	Unit	387.3	Unit	8.8	1.4	166	19	5	Positive
435	PE (P)	PE(P-18:0/22:6)	FALSE	776.6	Unit	385.3	Unit	8.2	0.6	166	19	5	Positive
436	PE (P)	PE(P-18:1/18:1) (a\b)	FALSE	728.6	Unit	339.3	Unit	8.5	0.6	166	19	5	Positive
437	PE (P)	PE(P-18:1/18:2) (a\b)	FALSE	726.5	Unit	337.3	Unit	7.7	0.6	166	19	5	Positive
438	PE (P)	PE(P-18:1/20:3) (a\b)	FALSE	752.5	Unit	363.3	Unit	8.0	0.6	166	19	5	Positive
439	PE (P)	PE(P-18:1/20:4) (a\b)	FALSE	750.5	Unit	361.3	Unit	7.6	0.6	166	19	5	Positive
440	PE (P)	PE(P-18:1/20:5) (a\b)	FALSE	748.5	Unit	359.3	Unit	6.9	0.6	166	19	5	Positive
441	PE (P)	PE(P-18:1/22:4)	FALSE	778.5	Unit	389.3	Unit	8.4	0.6	166	19	5	Positive
442	PE (P)	PE(P-18:1/22:5) (a\b)	FALSE	776.6	Unit	387.3	Unit	7.8	1.4	166	19	5	Positive
443	PE (P)	PE(P-18:1/22:6) (a\b)	FALSE	774.5	Unit	385.3	Unit	7.3	1	166	19	5	Positive
444	PE (P)	PE(P-19:0/20:4) (a\b)	FALSE	766.6	Unit	361.3	Unit	9.0	1	166	19	5	Positive
445	PE (P)	PE(P-20:0/18:1)	FALSE	758.6	Unit	339.3	Unit	10.1	0.6	166	19	5	Positive
446	PE (P)	PE(P-20:0/18:2)	FALSE	756.6	Unit	337.3	Unit	9.9	0.6	166	19	5	Positive
447	PE (P)	PE(P-20:0/20:4)	FALSE	780.6	Unit	361.3	Unit	9.7	0.6	166	19	5	Positive
448	PE (P)	PE(P-20:0/22:6)	FALSE	804.6	Unit	385.3	Unit	9.5	0.6	166	19	5	Positive
449	PE (P)	PE(P-20:1/20:4)	FALSE	778.5	Unit	361.3	Unit	8.6	0.6	166	19	5	Positive
450	PE (P)	PE(P-20:1/22:6)	FALSE	802.6	Unit	385.3	Unit	8.3	0.6	166	19	5	Positive
451	PG	PG(34:1)	FALSE	766.6	Unit	577.5	Unit	6.0	0.6	166	17	5	Positive
452	PG	PG(36:1)	FALSE	794.6	Unit	605.6	Unit	7.1	0.6	166	17	5	Positive
453	PG	PG(36:2)	FALSE	792.6	Unit	603.5	Unit	6.5	0.6	166	17	5	Positive
454	PG	PG(15:0_18:1) d7 (IS)	TRUE	759.6	Unit	570.6	Unit	5.9	1	166	17	5	Positive
455	PI	PI(15:0_18:1) d7 (IS)	FALSE	847.6	Unit	570.6	Unit	5.6	1.5	166	17	5	Positive
456	PI	PI(16:0/16:0)	FALSE	828.6	Unit	551.6	Unit	5.9	0.8	166	17	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
457	PI	PI(16:0_16:1)	FALSE	826.5	Unit	549.5	Unit	5.3	0.8	166	17	5	Positive
458	PI	PI(34:0)	FALSE	856.6	Unit	579.6	Unit	6.8	0.8	166	17	5	Positive
459	PI	PI(34:1)	FALSE	854.6	Unit	577.6	Unit	6.0	0.8	166	17	5	Positive
460	PI	PI(15-MHDA_18:1)/PI(17:0_18:1)	FALSE	868.6	Unit	591.6	Unit	6.5	0.8	166	17	5	Positive
461	PI	PI(15-MHDA_18:2)/PI(17:0_18:2)	FALSE	866.6	Unit	589.6	Unit	5.9	0.8	166	17	5	Positive
462	PI	PI(18:0_18:1)	FALSE	882.6	Unit	605.6	Unit	7.0	0.8	166	17	5	Positive
463	PI	PI(36:2)	FALSE	880.6	Unit	603.6	Unit	6.3	3	166	17	5	Positive
464	PI	PI(36:3) (a\b)	FALSE	878.6	Unit	601.6	Unit	5.7	1	166	17	5	Positive
465	PI	PI(16:0_20:4)	FALSE	876.6	Unit	599.6	Unit	5.4	0.8	166	17	5	Positive
466	PI	PI(37:4)	FALSE	890.6	Unit	613.6	Unit	5.8	1	166	17	5	Positive
467	PI	PI(37:6)	FALSE	886.6	Unit	609.6	Unit	5.7	1	166	17	5	Positive
468	PI	PI(18:0_20:2)	FALSE	908.6	Unit	631.6	Unit	7.2	0.8	166	17	5	Positive
469	PI	PI(18:0_20:3) (a\b)	FALSE	906.6	Unit	629.6	Unit	6.8	1	166	17	5	Positive
470	PI	PI(18:0_20:4)	FALSE	904.6	Unit	627.6	Unit	6.3	0.8	166	17	5	Positive
471	PI	PI(38:5) (a\b)	FALSE	902.6	Unit	625.6	Unit	5.6	1	166	17	5	Positive
472	PI	PI(38:6)	FALSE	900.6	Unit	623.6	Unit	5.3	0.8	166	17	5	Positive
473	PI	PI(40:4) (a\b)	FALSE	932.6	Unit	655.6	Unit	7.1	0.8	166	17	5	Positive
474	PI	PI(18:0_22:5) (a\b)	FALSE	930.6	Unit	653.6	Unit	6.5	1	166	17	5	Positive
475	PI	PI(18:0_22:6)	FALSE	928.6	Unit	651.6	Unit	6.1	0.8	166	17	5	Positive
476	PIP	PIP1(38:4)	FALSE	984.7	Unit	627.7	Unit	5.3	2	166	20	4	Positive
477	PS	PS(36:1)	FALSE	790.6	Unit	605.6	Unit	7.1	1	166	23	5	Positive
478	PS	PS(36:2)	FALSE	788.5	Unit	603.5	Unit	6.4	1	166	23	5	Positive
479	PS	PS(38:4)	FALSE	812.5	Unit	627.5	Unit	6.3	1	166	23	5	Positive
480	PS	PS(40:5)	FALSE	838.6	Unit	653.6	Unit	6.4	1	166	23	5	Positive
481	PS	PS(15:0_18:1) d7 (IS)	TRUE	755.5	Unit	570.5	Unit	5.7	1	166	23	4	Positive
482	S1P	S1P(d16:1)	FALSE	352.2	Unit	236.3	Unit	1.5	3	166	12	4	Positive
483	S1P	S1P(d18:0)	FALSE	382.2	Unit	284.3	Unit	2.3	3	166	12	4	Positive
484	S1P	S1P(d18:1)	FALSE	380.2	Unit	264.3	Unit	2.1	3	166	12	4	Positive
485	S1P	S1P(d18:1) d7 (IS)	TRUE	387.2	Unit	271.3	Unit	2.1	1	166	12	4	Positive
486	S1P	S1P(d18:2)	FALSE	378.2	Unit	262.3	Unit	1.6	3	166	12	4	Positive
487	SM	SM(d17:1/14:0)	FALSE	661.5	Unit	184.1	Unit	4.8	0.6	166	29	5	Positive
488	SM	SM(d18:0/14:0)	FALSE	677.6	Unit	184.1	Unit	5.5	0.6	166	29	5	Positive
489	SM	SM(d18:1/14:0)/SM(d16:1/16:0)	FALSE	675.5	Unit	184.1	Unit	5.2	0.6	166	29	5	Positive
490	SM	SM(d18:2/14:0)	FALSE	673.5	Unit	184.1	Unit	4.7	0.6	166	29	5	Positive
491	SM	SM(d17:1/16:0)	FALSE	689.6	Unit	184.1	Unit	5.6	0.6	166	29	5	Positive
492	SM	SM(d18:0/16:0)	FALSE	705.6	Unit	184.1	Unit	6.4	0.6	166	29	5	Positive
493	SM	SM(d18:1/16:0)	FALSE	703.6	Unit	184.1	Unit	6.0	0.6	166	29	5	Positive
494	SM	SM(d18:2/16:0)	FALSE	701.6	Unit	184.1	Unit	5.4	0.6	166	29	5	Positive
495	SM	SM(34:3)	FALSE	699.5	Unit	184.1	Unit	4.9	0.6	166	29	5	Positive
496	SM	SM(35:1) (a\b)	FALSE	717.6	Unit	184.1	Unit	6.4	0.6	166	29	5	Positive
497	SM	SM(35:2) (a\b)	FALSE	715.6	Unit	184.1	Unit	5.9	1	166	29	5	Positive
498	SM	SM(d18:1/18:0)/SM(d16:1/20:0)	FALSE	731.6	Unit	184.1	Unit	7.0	0.6	166	29	5	Positive
499	SM	SM(d18:2/18:0)	FALSE	729.6	Unit	184.1	Unit	6.2	0.6	166	29	5	Positive
500	SM	SM(d18:2/18:1)	FALSE	727.6	Unit	184.1	Unit	5.6	0.6	166	29	5	Positive
501	SM	SM(37:1)	FALSE	745.6	Unit	184.1	Unit	7.6	1	166	29	5	Positive
502	SM	SM(37:2)	FALSE	743.5	Unit	184.1	Unit	6.7	0.6	166	29	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
503	SM	SM(d18:1/20:0)/SM(d16:1/22:0)	FALSE	759.6	Unit	184.1	Unit	8.2	0.6	166	29	5	Positive
504	SM	SM(d18:2/20:0)	FALSE	757.6	Unit	184.1	Unit	7.3	0.6	166	29	5	Positive
505	SM	SM(38:3) (a\b)	FALSE	755.6	Unit	184.1	Unit	6.5	1	166	29	5	Positive
506	SM	SM(d16:1/23:0)/SM(d17:1/22:0)	FALSE	773.7	Unit	184.1	Unit	8.8	0.6	166	29	5	Positive
507	SM	SM(d18:0/22:0)	FALSE	789.7	Unit	184.1	Unit	9.8	0.6	166	29	5	Positive
508	SM	SM(d18:1/22:0)/SM(d16:1/24:0)	FALSE	787.7	Unit	184.1	Unit	9.4	0.6	166	29	5	Positive
509	SM	SM(40:2) (a\b)	FALSE	785.7	Unit	184.1	Unit	8.3	1.4	166	29	5	Positive
510	SM	SM(40:3) (a\b)	FALSE	783.6	Unit	184.1	Unit	7.5	1.2	166	29	5	Positive
511	SM	SM(41:0)	FALSE	803.7	Unit	184.1	Unit	10.1	0.8	166	29	5	Positive
512	SM	SM(41:1) (a\b)	FALSE	801.7	Unit	184.1	Unit	9.9	1	166	29	5	Positive
513	SM	SM(41:2) (a\b)	FALSE	799.7	Unit	184.1	Unit	8.9	1.4	166	29	5	Positive
514	SM	SM(d18:1/24:0)	FALSE	815.7	Unit	184.1	Unit	10.1	0.6	166	29	5	Positive
515	SM	SM(42:2) (a\b)	FALSE	813.7	Unit	184.1	Unit	9.5	1.4	166	29	5	Positive
516	SM	SM(43:1)	FALSE	829.7	Unit	184.1	Unit	10.2	0.8	166	29	5	Positive
517	SM	SM(43:2) (a\b\c)	FALSE	827.7	Unit	184.1	Unit	9.9	1.4	166	29	5	Positive
518	SM	SM(44:1)	FALSE	843.6	Unit	184.1	Unit	10.3	1	166	29	5	Positive
519	SM	SM(44:2)	FALSE	841.6	Unit	184.1	Unit	10.1	1	166	29	5	Positive
520	SM	SM(44:3)	FALSE	839.6	Unit	184.1	Unit	9.6	2	166	29	5	Positive
521	SM	SM(d18:1/15:0) d9 (IS)	TRUE	698.6	Unit	193.1	Unit	5.6	1	166	29	5	Positive
522	SPN	Sph(d17:1) (IS)	FALSE	286.3	Unit	268.3	Unit	1.8	3	166	10	4	Positive
523	SPN	Sph(d18:1)	FALSE	300.3	Unit	282.3	Unit	2.4	3	166	10	4	Positive
524	SPN	Sph(d18:2)	FALSE	298.3	Unit	280.3	Unit	1.8	3	166	10	4	Positive
525	Sulfatides	SHexCer(d18:1/12:0) (IS)	TRUE	724.8	Unit	264.3	Unit	4.1	0.6	166	56	5	Positive
526	Sulfatides	SHexCer(d18:1/16:0(OH))	FALSE	796.8	Unit	264.3	Unit	5.0	0.6	166	56	5	Positive
527	Sulfatides	SHexCer(d18:1/16:0)	FALSE	780.8	Unit	264.3	Unit	5.2	0.6	166	56	5	Positive
528	Sulfatides	SHexCer(d18:1/24:0(OH))	FALSE	908.8	Unit	264.3	Unit	8.6	0.6	166	56	5	Positive
529	Sulfatides	SHexCer(d18:1/24:1(OH))	FALSE	906.8	Unit	264.3	Unit	7.5	0.8	166	56	5	Positive
530	Sulfatides	SHexCer(d18:1/24:1)	FALSE	890.8	Unit	264.3	Unit	7.7	0.6	166	56	5	Positive
531	TG	TG(48:0) [NL-16:0]	FALSE	824.8	Unit	551.5	Unit	11.4	0.7	166	25	5	Positive
532	TG	TG(48:0) [NL-18:0]	FALSE	824.8	Unit	523.5	Unit	11.4	0.7	166	25	5	Positive
533	TG	TG(48:1) [NL-16:1]	FALSE	822.8	Unit	551.5	Unit	11.3	0.7	166	25	5	Positive
534	TG	TG(48:1) [NL-18:1]	FALSE	822.8	Unit	523.5	Unit	11.3	0.7	166	25	5	Positive
535	TG	TG(48:1) [NL-18:1] d7 (IS)	TRUE	829.8	Unit	523.5	Unit	11.3	1	166	25	5	Positive
536	TG	TG(48:2) [NL-14:0]	FALSE	820.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
537	TG	TG(48:2) [NL-14:1]	FALSE	820.8	Unit	577.5	Unit	11.1	0.7	166	25	5	Positive
538	TG	TG(48:2) [NL-16:1]	FALSE	820.8	Unit	549.5	Unit	11.1	0.7	166	25	5	Positive
539	TG	TG(48:2) [NL-18:2]	FALSE	820.8	Unit	523.5	Unit	11.1	0.7	166	25	5	Positive
540	TG	TG(48:3) [NL-14:0]	FALSE	818.8	Unit	573.5	Unit	11.0	0.7	166	25	5	Positive
541	TG	TG(48:3) [NL-16:1]	FALSE	818.8	Unit	547.5	Unit	11.0	0.7	166	25	5	Positive
542	TG	TG(48:3) [NL-18:3]	FALSE	818.8	Unit	523.5	Unit	11.0	0.7	166	25	5	Positive
543	TG	TG(49:1) [NL-16:1]	FALSE	836.8	Unit	565.5	Unit	11.4	0.7	166	25	5	Positive
544	TG	TG(49:1) [NL-17:1]	FALSE	836.8	Unit	551.5	Unit	11.4	0.7	166	25	5	Positive
545	TG	TG(50:0) [NL-18:0]	FALSE	852.8	Unit	551.5	Unit	11.6	0.7	166	25	5	Positive
546	TG	TG(50:1) [NL-14:0]	FALSE	850.8	Unit	605.5	Unit	11.5	0.7	166	25	5	Positive
547	TG	TG(50:1) [NL-16:0]	FALSE	850.8	Unit	577.5	Unit	11.5	0.7	166	25	5	Positive
548	TG	TG(50:1) [NL-18:1]	FALSE	850.8	Unit	551.5	Unit	11.5	0.7	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
549	TG	TG(50:2) [NL-14:0]	FALSE	848.8	Unit	603.5	Unit	11.3	0.7	166	25	5	Positive
550	TG	TG(50:2) [NL-16:1]	FALSE	848.8	Unit	577.5	Unit	11.3	0.7	166	25	5	Positive
551	TG	TG(50:2) [NL-18:1]	FALSE	848.8	Unit	549.5	Unit	11.3	0.7	166	25	5	Positive
552	TG	TG(50:2) [NL-18:2]	FALSE	848.8	Unit	551.5	Unit	11.3	0.7	166	25	5	Positive
553	TG	TG(50:3) [NL-14:0]	FALSE	846.8	Unit	601.5	Unit	11.1	0.7	166	25	5	Positive
554	TG	TG(50:3) [NL-14:1]	FALSE	846.8	Unit	603.5	Unit	11.1	0.7	166	25	5	Positive
555	TG	TG(50:3) [NL-16:1]	FALSE	846.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
556	TG	TG(50:3) [NL-18:2]	FALSE	846.8	Unit	549.5	Unit	11.1	0.7	166	25	5	Positive
557	TG	TG(50:3) [NL-18:3]	FALSE	846.8	Unit	551.5	Unit	11.2	0.7	166	25	5	Positive
558	TG	TG(50:4) [NL-14:0]	FALSE	844.8	Unit	599.5	Unit	11.0	0.7	166	25	5	Positive
559	TG	TG(50:4) [NL-18:3]	FALSE	844.8	Unit	549.5	Unit	11.0	0.7	166	25	5	Positive
560	TG	TG(50:4) [NL-20:4]	FALSE	844.8	Unit	523.5	Unit	11.1	0.7	166	25	5	Positive
561	TG	TG(51:0) [NL-16:0]	FALSE	866.7	Unit	593.4	Unit	11.7	0.7	166	25	5	Positive
562	TG	TG(51:1) [NL-17:0]	FALSE	864.8	Unit	577.5	Unit	11.5	0.7	166	25	5	Positive
563	TG	TG(51:2) [NL-15:0]	FALSE	862.8	Unit	603.5	Unit	11.4	0.7	166	25	5	Positive
564	TG	TG(51:2) [NL-17:0]	FALSE	862.8	Unit	575.5	Unit	11.4	0.7	166	25	5	Positive
565	TG	TG(51:2) [NL-17:1]	FALSE	862.8	Unit	577.5	Unit	11.4	0.7	166	25	5	Positive
566	TG	TG(52:1) [NL-18:0]	FALSE	878.8	Unit	577.5	Unit	11.7	0.7	166	25	5	Positive
567	TG	TG(52:1) [NL-18:1]	FALSE	878.8	Unit	579.5	Unit	11.7	0.7	166	25	5	Positive
568	TG	TG(52:2) [NL-16:0]	FALSE	876.8	Unit	603.5	Unit	11.5	0.7	166	25	5	Positive
569	TG	TG(52:2) [NL-18:2]	FALSE	876.8	Unit	579.5	Unit	11.5	0.7	166	25	5	Positive
570	TG	TG(52:3) [NL-16:1]	FALSE	874.8	Unit	603.5	Unit	11.3	0.7	166	25	5	Positive
571	TG	TG(52:3) [NL-18:2]	FALSE	874.8	Unit	577.5	Unit	11.3	0.7	166	25	5	Positive
572	TG	TG(52:4) [NL-16:1]	FALSE	872.8	Unit	601.5	Unit	11.2	0.7	166	25	5	Positive
573	TG	TG(52:4) [NL-18:2]	FALSE	872.8	Unit	575.5	Unit	11.2	0.7	166	25	5	Positive
574	TG	TG(52:4) [NL-18:3]	FALSE	872.8	Unit	577.5	Unit	11.2	0.7	166	25	5	Positive
575	TG	TG(52:5) [NL-18:3]	FALSE	870.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
576	TG	TG(52:5) [NL-20:4]	FALSE	870.8	Unit	549.5	Unit	11.1	0.7	166	25	5	Positive
577	TG	TG(52:5) [NL-20:5]	FALSE	870.8	Unit	551.5	Unit	11.1	0.7	166	25	5	Positive
578	TG	TG(53:2) [NL-17:1]	FALSE	890.8	Unit	605.5	Unit	11.6	0.7	166	25	5	Positive
579	TG	TG(53:2) [NL-18:1]	FALSE	890.8	Unit	591.5	Unit	11.5	0.7	166	25	5	Positive
580	TG	TG(54:0) [NL-18:0]	FALSE	908.8	Unit	607.5	Unit	12.0	0.7	166	25	5	Positive
581	TG	TG(54:1) [NL-18:1]	FALSE	906.8	Unit	607.5	Unit	11.9	0.7	166	25	5	Positive
582	TG	TG(54:2) [NL-18:0]	FALSE	904.8	Unit	603.5	Unit	11.7	0.7	166	25	5	Positive
583	TG	TG(54:2) [NL-20:1]	FALSE	904.8	Unit	577.5	Unit	11.7	0.7	166	25	5	Positive
584	TG	TG(54:3) [NL-18:1]	FALSE	902.8	Unit	603.5	Unit	11.5	0.7	166	25	5	Positive
585	TG	TG(54:3) [NL-18:2]	FALSE	902.8	Unit	605.5	Unit	11.5	0.7	166	25	5	Positive
586	TG	TG(54:4) [NL-18:2]	FALSE	900.8	Unit	603.5	Unit	11.3	0.7	166	25	5	Positive
587	TG	TG(54:4) [NL-20:3]	FALSE	900.8	Unit	577.5	Unit	11.4	0.7	166	25	5	Positive
588	TG	TG(54:5) [NL-18:3]	FALSE	898.8	Unit	603.5	Unit	11.2	0.7	166	25	5	Positive
589	TG	TG(54:5) [NL-20:4]	FALSE	898.8	Unit	577.5	Unit	11.3	0.7	166	25	5	Positive
590	TG	TG(54:6) [NL-18:3]	FALSE	896.8	Unit	601.5	Unit	11.1	0.7	166	25	5	Positive
591	TG	TG(54:6) [NL-20:4]	FALSE	896.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
592	TG	TG(54:6) [NL-20:5]	FALSE	896.8	Unit	577.5	Unit	11.1	0.7	166	25	5	Positive
593	TG	TG(54:6) [NL-22:6]	FALSE	896.8	Unit	551.5	Unit	11.2	0.7	166	25	5	Positive
594	TG	TG(54:7) [NL-20:5]	FALSE	894.8	Unit	575.5	Unit	11.0	0.7	166	25	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
595	TG	TG(54:7) [NL-22:6]	FALSE	894.8	Unit	549.5	Unit	11.0	0.7	166	25	5	Positive
596	TG	TG(56:6) [NL-20:4]	FALSE	924.8	Unit	603.5	Unit	11.3	0.7	166	25	5	Positive
597	TG	TG(56:6) [NL-22:5]	FALSE	924.8	Unit	577.5	Unit	11.3	0.7	166	25	5	Positive
598	TG	TG(56:7) [NL-20:4]	FALSE	922.8	Unit	601.5	Unit	11.1	0.7	166	25	5	Positive
599	TG	TG(56:7) [NL-20:5]	FALSE	922.8	Unit	603.5	Unit	11.1	0.7	166	25	5	Positive
600	TG	TG(56:7) [NL-22:5]	FALSE	922.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
601	TG	TG(56:7) [NL-22:6]	FALSE	922.8	Unit	577.5	Unit	11.2	0.7	166	25	5	Positive
602	TG	TG(56:8) [NL-20:4]	FALSE	920.8	Unit	599.5	Unit	11.0	0.7	166	25	5	Positive
603	TG	TG(56:8) [NL-20:5]	FALSE	920.8	Unit	601.5	Unit	11.0	0.7	166	25	5	Positive
604	TG	TG(56:8) [NL-22:6]	FALSE	920.8	Unit	575.5	Unit	11.1	0.7	166	25	5	Positive
605	TG	TG(56:9) [NL-22:6]	FALSE	918.8	Unit	573.5	Unit	10.9	0.7	166	25	5	Positive
606	TG	TG(58:10) [NL-22:6]	FALSE	944.9	Unit	599.5	Unit	11.0	0.7	166	25	5	Positive
607	TG	TG(58:8) [NL-22:6]	FALSE	948.8	Unit	603.5	Unit	11.2	0.7	166	25	5	Positive
608	TG	TG(58:9) [NL-22:6]	FALSE	946.9	Unit	601.5	Unit	11.1	0.7	166	25	5	Positive
609	TG SIM	TG(48:0) [SIM]	FALSE	824.8	Unit	824.8	Unit	11.4	0.7	166	0	5	Positive
610	TG SIM	TG(48:1) [SIM]	FALSE	822.8	Unit	822.8	Unit	11.3	0.7	166	0	5	Positive
611	TG SIM	TG(48:2) [SIM]	FALSE	820.8	Unit	820.8	Unit	11.1	0.7	166	0	5	Positive
612	TG SIM	TG(48:3) [SIM]	FALSE	818.8	Unit	818.8	Unit	11.0	0.7	166	0	5	Positive
613	TG SIM	TG(49:1) [SIM]	FALSE	836.8	Unit	836.8	Unit	11.4	0.7	166	0	5	Positive
614	TG SIM	TG(50:0) [SIM]	FALSE	852.8	Unit	852.8	Unit	11.6	0.7	166	0	5	Positive
615	TG SIM	TG(50:1) [SIM]	FALSE	850.8	Unit	850.8	Unit	11.5	0.7	166	0	5	Positive
616	TG SIM	TG(50:2) [SIM]	FALSE	848.8	Unit	848.8	Unit	11.3	0.7	166	0	5	Positive
617	TG SIM	TG(50:3) [SIM]	FALSE	846.8	Unit	846.8	Unit	11.1	0.7	166	0	5	Positive
618	TG SIM	TG(50:4) [SIM]	FALSE	844.8	Unit	844.8	Unit	11.0	0.7	166	0	5	Positive
619	TG SIM	TG(51:0) [SIM]	FALSE	866.7	Unit	866.7	Unit	11.7	0.7	166	0	5	Positive
620	TG SIM	TG(51:1) [SIM]	FALSE	864.8	Unit	864.8	Unit	11.5	0.7	166	0	5	Positive
621	TG SIM	TG(51:2) [SIM]	FALSE	862.8	Unit	862.8	Unit	11.4	0.7	166	0	5	Positive
622	TG SIM	TG(52:1) [SIM]	FALSE	878.8	Unit	878.8	Unit	11.7	0.7	166	0	5	Positive
623	TG SIM	TG(52:2) [SIM]	FALSE	876.8	Unit	876.8	Unit	11.5	0.7	166	0	5	Positive
624	TG SIM	TG(52:3) [SIM]	FALSE	874.8	Unit	874.8	Unit	11.3	0.7	166	0	5	Positive
625	TG SIM	TG(52:4) [SIM]	FALSE	872.8	Unit	872.8	Unit	11.2	0.7	166	0	5	Positive
626	TG SIM	TG(52:5) [SIM]	FALSE	870.8	Unit	870.8	Unit	11.0	0.7	166	0	5	Positive
627	TG SIM	TG(53:2) [SIM]	FALSE	890.8	Unit	890.8	Unit	11.5	0.7	166	0	5	Positive
628	TG SIM	TG(54:0) [SIM]	FALSE	908.8	Unit	908.8	Unit	12.0	0.7	166	0	5	Positive
629	TG SIM	TG(54:1) [SIM]	FALSE	906.8	Unit	906.8	Unit	11.9	0.7	166	0	5	Positive
630	TG SIM	TG(54:2) [SIM]	FALSE	904.8	Unit	904.8	Unit	11.7	0.7	166	0	5	Positive
631	TG SIM	TG(54:3) [SIM]	FALSE	902.8	Unit	902.8	Unit	11.5	0.7	166	0	5	Positive
632	TG SIM	TG(54:4) [SIM]	FALSE	900.8	Unit	900.8	Unit	11.3	0.7	166	0	5	Positive
633	TG SIM	TG(54:5) [SIM]	FALSE	898.8	Unit	898.8	Unit	11.2	0.7	166	0	5	Positive
634	TG SIM	TG(54:6) [SIM]	FALSE	896.8	Unit	896.8	Unit	11.1	0.7	166	0	5	Positive
635	TG SIM	TG(54:7) [SIM]	FALSE	894.8	Unit	894.8	Unit	11.0	0.7	166	0	5	Positive
636	TG SIM	TG(56:6) [SIM]	FALSE	924.8	Unit	924.8	Unit	11.3	0.7	166	0	5	Positive
637	TG SIM	TG(56:7) [SIM]	FALSE	922.8	Unit	922.8	Unit	11.2	0.7	166	0	5	Positive
638	TG SIM	TG(56:8) [SIM]	FALSE	920.8	Unit	920.8	Unit	11.1	0.7	166	0	5	Positive
639	TG SIM	TG(56:9) [SIM]	FALSE	918.8	Unit	918.8	Unit	10.9	0.7	166	0	5	Positive
640	TG SIM	TG(58:10) [SIM]	FALSE	944.9	Unit	944.9	Unit	11.0	0.7	166	0	5	Positive

Cmpnd No.	Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Ret Time (min)	Delta RT	Frag.	Collision Energy	Cell Accelerator Voltage	Polarity
641	TG SIM	TG(O-50:1) [SIM]	FALSE	836.8	Unit	836.8	Unit	11.8	0.7	166	0	5	Positive
642	TG SIM	TG(O-50:2) [SIM]	FALSE	834.8	Unit	834.8	Unit	11.6	0.7	166	0	5	Positive
643	TG SIM	TG(O-52:1) [SIM]	FALSE	864.8	Unit	864.8	Unit	12.0	0.7	166	0	5	Positive
644	TG SIM	TG(O-52:2) [SIM]	FALSE	862.8	Unit	862.8	Unit	11.8	0.7	166	0	5	Positive
645	TG SIM	TG(O-54:2) [SIM]	FALSE	890.8	Unit	890.8	Unit	12.0	0.7	166	0	5	Positive
646	TG (O)	TG(O-50:1) [NL-15:0]	FALSE	836.8	Unit	577.5	Unit	11.8	0.7	166	25	5	Positive
647	TG (O)	TG(O-50:1) [NL-16:0]	FALSE	836.8	Unit	563.5	Unit	11.8	0.7	166	25	5	Positive
648	TG (O)	TG(O-50:1) [NL-17:1]	FALSE	836.8	Unit	551.5	Unit	11.8	0.7	166	25	5	Positive
649	TG (O)	TG(O-50:1) [NL-18:1]	FALSE	836.8	Unit	537.5	Unit	11.8	0.7	166	25	5	Positive
650	TG (O)	TG(O-50:2) [NL-16:1]	FALSE	834.8	Unit	563.5	Unit	11.6	0.7	166	25	5	Positive
651	TG (O)	TG(O-50:2) [NL-18:1]	FALSE	834.8	Unit	535.5	Unit	11.6	0.7	166	25	5	Positive
652	TG (O)	TG(O-50:2) [NL-18:2]	FALSE	834.8	Unit	537.5	Unit	11.6	0.7	166	25	5	Positive
653	TG (O)	TG(O-52:0) [NL-16:0]	FALSE	866.8	Unit	593.5	Unit	12.2	0.7	166	25	5	Positive
654	TG (O)	TG(O-52:1) [NL-16:0]	FALSE	864.8	Unit	591.5	Unit	12.0	0.7	166	25	5	Positive
655	TG (O)	TG(O-52:1) [NL-18:1]	FALSE	864.8	Unit	565.5	Unit	12.0	0.7	166	25	5	Positive
656	TG (O)	TG(O-52:2) [NL-16:0]	FALSE	862.8	Unit	589.5	Unit	11.8	0.7	166	25	5	Positive
657	TG (O)	TG(O-52:2) [NL-17:1]	FALSE	862.8	Unit	577.5	Unit	11.8	0.7	166	25	5	Positive
658	TG (O)	TG(O-52:2) [NL-18:1]	FALSE	862.8	Unit	563.5	Unit	11.8	0.7	166	25	5	Positive
659	TG (O)	TG(O-54:2) [NL-17:1]	FALSE	890.8	Unit	605.5	Unit	12.0	0.7	166	25	5	Positive
660	TG (O)	TG(O-54:2) [NL-18:1]	FALSE	890.8	Unit	591.5	Unit	12.0	0.7	166	25	5	Positive
661	TG (O)	TG(O-54:3) [NL-17:1]	FALSE	888.8	Unit	603.5	Unit	11.8	0.7	166	25	5	Positive
662	TG (O)	TG(O-54:3) [NL-18:1]	FALSE	888.8	Unit	589.5	Unit	11.8	0.7	166	25	5	Positive
663	TG (O)	TG(O-54:4) [NL-17:1]	FALSE	886.8	Unit	601.5	Unit	11.6	0.7	166	25	5	Positive
664	TG (O)	TG(O-54:4) [NL-18:2]	FALSE	886.8	Unit	589.5	Unit	11.6	0.7	166	25	5	Positive
665	Ubiquinone	Ubiquinone	FALSE	880.7	Unit	197	Unit	11.0	0.4	166	17	5	Positive

[1] The number of transitions here is lower than the final list of lipid species as some transitions allow for the monitoring of multiple peaks that are separated upon integration.

Table A2. Suggested reference compounds for each lipid species as well as response factors and %CV values.

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
AC(10:0)	316.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	7.2	<1
AC(12:0)	344.3 → 85.1	AC(12:0) [reference]	AC(16:0) d3	1	2.7	<1
AC(12:1)	342.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	5.4	<1
AC(13:0)	358.3 → 85.1	AC(12:0) [reference]	AC(16:0) d3	1	1.8	1.16
AC(14:0)	372.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	1.7	2.02
AC(14:0)-OH	388.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	4.0	1.38
AC(14:1)	370.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	2.6	<1
AC(14:1)-OH	386.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	5.9	<1
AC(14:2)	368.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	3.1	<1
AC(15:0) (a)	386.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	6.2	2.06
AC(15:0) (b)	386.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	10.3	12.37
AC(16:0)	400.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	1.6	<1
AC(16:0)-OH	416.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	7.9	3.41
AC(16:1)	398.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	2.5	1.29
AC(16:1)-OH	414.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	6.1	6.41
AC(17:0) (a)	414.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	6.7	7.62
AC(17:0) (b)	414.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	6.2	8.87

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
AC(18:0)	428.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	2.8	<1
AC(18:0)-OH	444.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	11.9	8.3
AC(18:1)	426.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	1.9	<1
AC(18:1)-OH	442.4 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	7.9	1.29
AC(18:2)	424.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	2.4	<1
AC(18:3)	422.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	4.6	7.71
AC(20:3) (a)	450.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	8.0	6.11
AC(20:3) (b)	450.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	17.1	23.07
AC(20:3)-OH	466.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	11.4	<1
AC(20:4)	448.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	14.1	7.47
AC(20:5)	446.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	8.2	2.97
AC(22:5)	474.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	17.9	<1
AC(22:5)-OH	490.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	7.9	1.24
AC(22:6)	472.3 → 85.1	AcylCarnitine 16:0 d3 (IS) [reference]	AC(16:0) d3	1	16.8	24.67
AC(24:0)	512.3 → 85.1	AC(24:0) [reference]	AC(16:0) d3	1	3.0	<1
AC(24:1) (a)	510.3 → 85.1	AC(24:0) [reference]	AC(16:0) d3	1	5.9	2.21
AC(24:1) (b)	510.3 → 85.1	AC(24:0) [reference]	AC(16:0) d3	1	9.8	6.96
AC(26:0)	540.3 → 85.1	AC(24:0) [reference]	AC(16:0) d3	1	3.3	<1
AC(26:1)	538.3 → 85.1	AC(24:0) [reference]	AC(16:0) d3	1	3.7	<1
CA	426.3 → 355.3	Cholic Acid d4 (IS) [reference]	Cholic acid d4	1	5.4	10
CE(14:0)	614.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	4.3	18.4	<1
CE(15:0)	628.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	2.4	12.0	1.03
CE(16:0)	642.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1.7	2.3	<1
CE(16:1)	640.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	10.4	<1
CE(16:2)	638.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.5	9.8	<1
CE(17:0)	656.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1.3	4.9	<1
CE(17:1)	654.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.7	7.5	<1
CE(18:0)	670.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1.1	2.0	<1
CE(18:1)	668.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.6	3.1	<1
CE(18:2)	666.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.3	4.5	<1
CE(18:2) [+OH]	682.6 → 369.3	CE(18:3) [reference]	CE(18:0) d6	1	9.4	<1
CE(18:3)	664.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.3	7.9	<1
CE(20:0)	698.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1.1	12.9	6.67
CE(20:1)	696.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.4	5.1	3.45
CE(20:2)	694.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	2.8	<1
CE(20:3)	692.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	2.9	<1
CE(20:4)	690.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	4.1	<1
CE(20:4) [+OH]	706.6 → 369.3	CE(20:5) [reference]	CE(18:0) d6	1	10.9	<1
CE(20:5)	688.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	3.7	<1
CE(22:0)	726.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.6	14.8	8.7
CE(22:1)	724.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.3	17.0	3.71
CE(22:4)	718.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	4.4	<1
CE(22:5)	716.6 → 369.3	CE(22:6) [reference]	CE(18:0) d6	0.2	4.3	<1
CE(22:6)	714.6 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.2	6.1	<1
CE(24:0)	754.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.5	18.7	16.71
CE(24:1)	752.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.3	16.6	6.78
CE(24:4)	746.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.1	8.4	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
CE(24:5)	744.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.1	8.1	<1
CE(24:6)	742.7 → 369.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	0.1	13.7	<1
Cer(d16:1/16:0)	510.6 → 236.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	12.6	1.31
Cer(d16:1/18:0)	538.6 → 236.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	7.5	3.53
Cer(d16:1/20:0)	566.6 → 236.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	4.2	2.12
Cer(d16:1/22:0)	594.6 → 236.3	Cer(d16:1/22:0) [reference]	Cer(d18:1-d7/18:0)	1	14.3	1.33
Cer(d16:1/23:0)	608.6 → 236.3	Cer(d16:1/23:0) [reference]	Cer(d18:1-d7/18:0)	1	14.1	1.7
Cer(d16:1/24:0)	622.6 → 236.3	Cer(d16:1/24:0) [reference]	Cer(d18:1-d7/18:0)	1	15.3	1.2
Cer(d16:1/24:1)	620.6 → 236.3	Cer(d16:1/24:1) [reference]	Cer(d18:1-d7/18:0)	1	14.2	<1
Cer(d17:1/16:0)	524.6 → 250.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	12.9	7.44
Cer(d17:1/18:0)	552.6 → 250.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	11.1	28.25
Cer(d17:1/20:0)	580.6 → 250.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	8.4	8.01
Cer(d17:1/22:0)	608.6 → 250.3	Cer(d17:1/22:0) [reference]	Cer(d18:1-d7/18:0)	1	13.5	2.66
Cer(d17:1/23:0)	622.6 → 250.3	Cer(d17:1/23:0) [reference]	Cer(d18:1-d7/18:0)	1	16.2	2.04
Cer(d17:1/24:0)	636.6 → 250.3	Cer(d17:1/24:0) [reference]	Cer(d18:1-d7/18:0)	1	14.5	2.13
Cer(d17:1/24:1)	634.6 → 250.3	Cer(d17:1/24:1) [reference]	Cer(d18:1-d7/18:0)	1	14.2	<1
Cer(d18:1/16:0)	538.5 → 264.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	3.9	<1
Cer(d18:1/18:0)	566.6 → 264.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	3.1	1.11
Cer(d18:1/20:0)	594.6 → 264.3	Cer(d18:1/21:0) [reference]	Cer(d18:1-d7/18:0)	1	13.7	3.03
Cer(d18:1/21:0)	608.6 → 264.3	Cer(d18:1/21:0) [reference]	Cer(d18:1-d7/18:0)	1	14.2	2.95
Cer(d18:1/22:0)	622.6 → 264.3	Cer(d18:1/22:0) [reference]	Cer(d18:1-d7/18:0)	1	13.5	<1
Cer(d18:1/23:0)	636.6 → 264.3	Cer(d18:1/23:0) [reference]	Cer(d18:1-d7/18:0)	1	13.4	<1
Cer(d18:1/24:0)	650.6 → 264.3	Cer(d18:1/24:0) [reference]	Cer(d18:1-d7/18:0)	1	15.9	<1
Cer(d18:1/24:1)	648.6 → 264.3	Cer(d18:1/24:1) [reference]	Cer(d18:1-d7/18:0)	1	13.5	<1
Cer(d18:1/26:0)	678.6 → 264.3	Cer(d18:1/26:0) [reference]	Cer(d18:1-d7/18:0)	1	17.3	13.36
Cer(d18:2/16:0)	536.5 → 262.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	9.9	1.09
Cer(d18:2/18:0)	564.6 → 262.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	7.2	<1
Cer(d18:2/20:0)	592.6 → 262.3	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	7.4	<1
Cer(d18:2/22:0)	620.6 → 262.3	Cer(d18:2/22:0) [reference]	Cer(d18:1-d7/18:0)	1	14.5	<1
Cer(d18:2/23:0)	634.6 → 262.3	Cer(d18:2/23:0) [reference]	Cer(d18:1-d7/18:0)	1	14.4	<1
Cer(d18:2/24:0)	648.6 → 262.3	Cer(d18:2/24:0) [reference]	Cer(d18:1-d7/18:0)	1	16.0	<1
Cer(d18:2/24:1)	646.6 → 262.3	Cer(d18:2/24:1) [reference]	Cer(d18:1-d7/18:0)	1	14.4	<1
Cer(d18:2/26:0)	676.6 → 262.3	Cer(d18:2/24:0) [reference]	Cer(d18:1-d7/18:0)	1	18.2	2.79
Cer(d19:1/18:0)	580.6 → 278.3	Cer(d19:1/20:0) [reference]	Cer(d18:1-d7/18:0)	1	13.5	4.15
Cer(d19:1/20:0)	608.6 → 278.3	Cer(d19:1/20:0) [reference]	Cer(d18:1-d7/18:0)	1	16.3	13.82
Cer(d19:1/22:0)	636.6 → 278.3	Cer(d19:1/22:0) [reference]	Cer(d18:1-d7/18:0)	1	15.2	<1
Cer(d19:1/23:0)	650.6 → 278.3	Cer(d19:1/23:0) [reference]	Cer(d18:1-d7/18:0)	1	15.4	<1
Cer(d19:1/24:0)	664.6 → 278.3	Cer(d19:1/24:0) [reference]	Cer(d18:1-d7/18:0)	1	16.0	<1
Cer(d19:1/24:1)	662.6 → 278.3	Cer(d19:1/24:1) [reference]	Cer(d18:1-d7/18:0)	1	14.8	<1
Cer(d20:1/22:0)	650.6 → 292.3	Cer(d20:1/22:0) [reference]	Cer(d18:1-d7/18:0)	1	17.1	8.75
Cer(d20:1/23:0)	664.6 → 292.3	Cer(d20:1/23:0) [reference]	Cer(d18:1-d7/18:0)	1	17.0	5.41
Cer(d20:1/24:0)	678.6 → 292.3	Cer(d20:1/24:0) [reference]	Cer(d18:1-d7/18:0)	1	16.6	5.37
Cer(d20:1/24:1)	676.6 → 292.3	Cer(d20:1/24:1) [reference]	Cer(d18:1-d7/18:0)	1	16.4	1.26
Cer(m18:0/20:0)	580.6 → 268.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	14.2	3
Cer(m18:0/22:0)	608.6 → 268.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	15.3	<1
Cer(m18:0/23:0)	622.6 → 268.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	14.8	1.08
Cer(m18:0/24:0)	636.6 → 268.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	15.7	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
Cer(m18:0/24:1)	634.6 → 268.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	15.2	1.36
Cer(m18:1/18:0)	550.6 → 266.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	14.2	<1
Cer(m18:1/20:0)	578.6 → 266.4	Cer(m18:1/20:0) [reference]	Cer(d18:1-d7/18:0)	1	14.6	<1
Cer(m18:1/22:0)	606.6 → 266.4	Cer(m18:1/20:0) [reference]	Cer(d18:1-d7/18:0)	1	14.4	<1
Cer(m18:1/23:0)	620.6 → 266.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	13.2	<1
Cer(m18:1/24:0)	634.6 → 266.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	15.3	<1
Cer(m18:1/24:1)	632.6 → 266.4	Cer(d18:1-d7/18:0) (IS) [reference]	Cer(d18:1-d7/18:0)	1	14.4	<1
Cer1P(d18:1/16:0)	618.4 → 264.3	Cer1P(d18:1/16:0) [reference]	Cer(d18:1-d7/18:0)	1	16.6	<1
COH	369.4 → 161.2	COH-d7 (IS) [reference]	COH(d7)	1	7.9	<1
DE(16:0)	640.6 → 367.4	DE(18:1) ester d6 (IS) [reference]	CE(18:0) d6	1	16.7	1.74
DE(18:1)	666.6 → 367.4	DE(18:1) ester d6 (IS) [reference]	CE(18:0) d6	1	6.8	<1
DE(18:2)	664.6 → 367.4	DE(18:1) ester d6 (IS) [reference]	CE(18:0) d6	1	7.7	<1
DE(20:4)	688.6 → 367.4	DE(18:1) ester d6 (IS) [reference]	CE(18:0) d6	1	7.8	<1
DG(14:0_16:0)	558.5 → 313.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	3.3	28.6
DG(14:0_18:2)	582.5 → 285.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	7.8	1.94
DG(16:0_16:0)	586.5 → 313.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	0.5	4.5	16.01
DG(16:0_16:1)	584.5 → 313.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	2.9	10.96
DG(16:0_18:1)	612.6 → 313.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	4.2	2.83
DG(16:0_18:2)	610.5 → 313.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	4.8	<1
DG(16:0_20:4)	634.5 → 313.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	4.1	6.05
DG(16:0_22:5)	660.6 → 313.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	7.7	7.88
DG(16:0_22:6)	658.5 → 313.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	7.2	4.45
DG(16:1_18:1)	610.5 → 339.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	2.7	3.86
DG(18:0_18:1)	640.6 → 341.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	3.6	5.13
DG(18:0_18:2)	638.6 → 341.3	DG(18:0_18:2) [reference]	DG(15:0_18:1) d7	1	4.3	1.73
DG(18:0_20:4)	662.6 → 341.3	DG(18:0_20:4) [reference]	DG(15:0_18:1) d7	1	8.7	1.64
DG(18:1_18:1)	638.6 → 339.3	DG(18:0_18:2) [reference]	DG(15:0_18:1) d7	1	3.4	1.2
DG(18:1_18:2)	636.6 → 339.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	2.4	<1
DG(18:1_18:3)	634.5 → 339.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	4.0	<1
DG(18:1_20:3)	662.6 → 339.3	DG(18:0_20:4) [reference]	DG(15:0_18:1) d7	1	4.7	1.22
DG(18:1_20:4)	660.6 → 339.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	2.6	<1
DG(18:1_20:5)	658.6 → 339.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	3.5	2.71
DG(18:1_22:5)	686.6 → 339.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	5.1	3.15
DG(18:1_22:6)	684.6 → 339.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	3.6	1.27
DG(18:2_18:2)	634.5 → 337.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	0.5	3.0	<1
DG(18:2_20:4)	658.5 → 337.2	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	3.9	<1
DG(18:2_22:6)	682.6 → 337.3	DG(15:0 18:1) d7 (IS) [reference]	DG(15:0_18:1) d7	1	4.8	<1
dhCer(d18:0/16:0)	540.5 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	11.8	32.71
dhCer(d18:0/18:0)	568.6 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	9.4	23.82
dhCer(d18:0/20:0)	596.6 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	14.6	16.64
dhCer(d18:0/22:0)	624.6 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	15.4	1.67
dhCer(d18:0/24:0)	652.7 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	16.1	2.87
dhCer(d18:0/24:1)	650.6 → 284.3	dhCer(d18:0/8:0) [reference]	dhCer(d18:0/8:0)	1	14.3	<1
dimethyl-CE(18:1)	696.6 → 397.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	6.0	<1
dimethyl-CE(18:2)	694.6 → 397.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	2.6	<1
dimethyl-CE(20:4)	718.6 → 397.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	5.0	<1
dxCA	410.3 → 357.3	Cholic Acid d4 (IS) [reference]	Cholic acid d4	1	4.7	8.07

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
FA(14:0)	227.2 → 227.2	FA(22:6) d5 (IS) [reference]	FFA(18:1) d9	1	6.2	67.45
FA(16:0)	255.2 → 255.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	2.0	23.4
FA(16:1)	253.2 → 253.2	FA(20:4) d11 (IS) [reference]	FFA(18:1) d9	1	4.8	14.87
FA(17:0)	269.2 → 269.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	3.6	79.9
FA(17:1)	267.2 → 267.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	2.8	70.54
FA(18:0)	283.3 → 283.3	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	4.5	94.5
FA(18:1)	281.2 → 281.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	1.6	2.23
FA(18:2)	279.2 → 279.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	3.1	10.48
FA(18:3)	277.2 → 277.2	FA(22:6) d5 (IS) [reference]	FFA(18:1) d9	1	3.8	9.42
FA(20:2)	307.3 → 307.3	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	6.7	73.72
FA(20:3)	305.2 → 305.2	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	3.9	76.41
FA(20:4)	303.2 → 303.2	FA(20:4) d11 (IS) [reference]	FFA(18:1) d9	1	5.1	14.41
FA(20:5)	301.2 → 301.2	FA(22:6) d5 (IS) [reference]	FFA(18:1) d9	1	7.3	26.16
FA(22:4)	331.3 → 331.3	FA(18:1) d9 (IS) [reference]	FFA(18:1) d9	1	4.5	34.32
FA(22:5)	329.2 → 329.2	FA(20:4) d11 (IS) [reference]	FFA(18:1) d9	1	7.8	43.67
FA(22:6)	327.2 → 327.2	FA(22:6) d5 (IS) [reference]	FFA(18:1) d9	1	4.6	26.58
GM3(d18:1/16:0)	1153.7 → 264.3	GM3(d18:1/16:0) [reference]	Hex3Cer(d18:1/17:0)	1	4.2	<1
GM3(d18:1/18:0)	1181.8 → 264.3	GM3(d18:1/16:0) [reference]	Hex3Cer(d18:1/17:0)	1	4.4	<1
GM3(d18:1/20:0)	1209.8 → 264.3	GM3(d18:1/16:0) [reference]	Hex3Cer(d18:1/17:0)	1	7.4	<1
GM3(d18:1/22:0)	1237.8 → 264.3	GM3(d18:1/22:0) [reference]	Hex3Cer(d18:1/17:0)	1	5.6	<1
GM3(d18:1/24:0)	1265.8 → 264.3	GM3(d18:1/24:0) [reference]	Hex3Cer(d18:1/17:0)	1	4.9	<1
GM3(d18:1/24:1)	1263.8 → 264.3	GM3(d18:1/22:0) [reference]	Hex3Cer(d18:1/17:0)	1	5.1	<1
Hex2Cer(d16:1/16:0)	834.6 → 236.3	Hex2Cer(d18:1/15:0) d7 (IS) [reference]	Hex2Cer(d18:1/15:0) d7	1	4.2	<1
Hex2Cer(d16:1/24:1)	944.7 → 236.3	Hex2Cer(d16:1/24:1) [reference]	Hex2Cer(d18:1/15:0) d7	1	8.6	<1
Hex2Cer(d18:1/16:0)	862.6 → 264.3	Hex2Cer(d18:1/16:0) [reference]	Hex2Cer(d18:1/15:0) d7	1	2.4	<1
Hex2Cer(d18:1/20:0)	918.7 → 264.3	Hex2Cer(d18:1/22:0) [reference]	Hex2Cer(d18:1/15:0) d7	1	9.0	<1
Hex2Cer(d18:1/22:0)	946.7 → 264.3	Hex2Cer(d18:1/22:0) [reference]	Hex2Cer(d18:1/15:0) d7	1	3.8	<1
Hex2Cer(d18:1/24:0)	974.8 → 264.3	Hex2Cer(d18:1/24:0) [reference]	Hex2Cer(d18:1/15:0) d7	1	4.4	<1
Hex2Cer(d18:1/24:1)	972.7 → 264.3	Hex2Cer(d18:1/24:1) [reference]	Hex2Cer(d18:1/15:0) d7	1	2.6	<1
Hex2Cer(d18:2/16:0)	860.6 → 262.3	Hex2Cer(d18:1/15:0) d7 (IS) [reference]	Hex2Cer(d18:1/15:0) d7	1	4.6	<1
Hex2Cer(d18:2/24:1)	970.7 → 262.3	Hex2Cer(d18:2/24:1) [reference]	Hex2Cer(d18:1/15:0) d7	1	4.7	<1
Hex3Cer(d18:1/16:0)	1024.7 → 264.3	Hex3Cer(d18:1/17:0) (IS) [reference]	Hex3Cer(d18:1/17:0)	1	4.4	<1
Hex3Cer(d18:1/18:0)	1052.7 → 264.3	Hex3Cer(d18:1/17:0) (IS) [reference]	Hex3Cer(d18:1/17:0)	1	11.2	1.58
Hex3Cer(d18:1/22:0)	1108.8 → 264.3	Hex3Cer(d18:1/17:0) (IS) [reference]	Hex3Cer(d18:1/17:0)	1	5.3	<1
Hex3Cer(d18:1/24:0)	1136.8 → 264.3	Hex3Cer(d18:1/17:0) (IS) [reference]	Hex3Cer(d18:1/17:0)	1	5.3	<1
Hex3Cer(d18:1/24:1)	1134.8 → 264.3	Hex3Cer(d18:1/17:0) (IS) [reference]	Hex3Cer(d18:1/17:0)	1	5.1	<1
HexCer(d16:1/18:0)	700.6 → 236.3	HexCer(d16:1/20:0) [reference]	HexCer(d18:1/15:0) d7	1	16.7	3.78
HexCer(d16:1/20:0)	728.6 → 236.3	HexCer(d16:1/20:0) [reference]	HexCer(d18:1/15:0) d7	1	9.8	2.88
HexCer(d16:1/22:0)	756.7 → 236.3	HexCer(d16:1/24:0) [reference]	HexCer(d18:1/15:0) d7	1	6.8	<1
HexCer(d16:1/24:0)	784.7 → 236.3	HexCer(d16:1/24:0) [reference]	HexCer(d18:1/15:0) d7	1	6.2	<1
HexCer(d18:1/16:0)	700.6 → 264.3	HexCer(d18:1/16:0) [reference]	HexCer(d18:1/15:0) d7	1	8.6	<1
HexCer(d18:1/18:0)	728.6 → 264.3	HexCer(d18:1/18:0) [reference]	HexCer(d18:1/15:0) d7	1	6.9	<1
HexCer(d18:1/20:0)	756.6 → 264.3	HexCer(d18:1/20:0) [reference]	HexCer(d18:1/15:0) d7	1	7.2	<1
HexCer(d18:1/22:0)	784.7 → 264.3	HexCer(d18:1/22:0) [reference]	HexCer(d18:1/15:0) d7	1	2.5	<1
HexCer(d18:1/24:0)	812.7 → 264.3	HexCer(d18:1/24:0) [reference]	HexCer(d18:1/15:0) d7	1	3.5	<1
HexCer(d18:1/24:1)	810.7 → 264.3	HexCer(d18:1/24:1) [reference]	HexCer(d18:1/15:0) d7	1	2.6	<1
HexCer(d18:2/20:0)	754.6 → 262.3	HexCer(d18:2/20:0) [reference]	HexCer(d18:1/15:0) d7	1	13.0	1.36

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
HexCer(d18:2/22:0)	782.7 → 262.3	HexCer(d18:2/20:0) [reference]	HexCer(d18:1/15:0) d7	1	7.1	<1
HexCer(d18:2/24:0)	810.7 → 262.3	HexCer(d18:2/24:0) [reference]	HexCer(d18:1/15:0) d7	1	4.2	<1
LPC(14:0) [sn1]	468.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	2.0	<1
LPC(14:0) [sn2]	468.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.5	<1
LPC(15:0) [sn1]	482.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	1.9	17.68
LPC(15:0) [sn2]	482.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.7	<1
LPC(15-MHDA) [sn1] / LPC(17:0) [sn2]	510.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.1	<1
LPC(15-MHDA) [sn1] [104_sn1]	510.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	3.0	<1
LPC(15-MHDA) [sn2]	510.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	3.7	<1
LPC(16:0) [sn1]	496.3 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	1.8	<1
LPC(16:0) [sn2]	496.3 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.1	<1
LPC(16:1) [sn1]	494.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	1.5	<1
LPC(16:1) [sn2]	494.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.4	<1
LPC(17:0) [sn1]	510.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.1	<1
LPC(17:1) (a) [sn1] [104_sn1]	508.4 → 104.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.3	<1
LPC(17:1) [sn1] (a) / LPC(17:1) [sn2] (b)	508.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	2.3	<1
LPC(17:1) [sn1] (b)	508.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.8	2.07
LPC(17:1) [sn2] (a)	508.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.6	<1
LPC(18:0) [sn1]	524.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	2.0	<1
LPC(18:0) [sn2]	524.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	2.8	<1
LPC(18:1) [sn1]	522.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	1.5	<1
LPC(18:1) [sn2]	522.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	1.9	<1
LPC(18:2) [+OH]	536.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	8.8	4.8
LPC(18:2) [sn1]	520.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	1.7	<1
LPC(18:2) [sn2]	520.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.6	<1
LPC(18:3) (a) [sn1] [104_sn1]	518.3 → 104.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.8	<1
LPC(18:3) [sn1] (a)/LPC(18:3) [sn2] (b)	518.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.4	<1
LPC(18:3) [sn1] (b)	518.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.7	<1
LPC(18:3) [sn2] (a)	518.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.3	<1
LPC(19:0) (a) [sn1] [104_sn1]	538.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	5.9	<1
LPC(19:0) [sn1] (a) / LPC(19:0) [sn2] (b)	538.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.3	1.21
LPC(19:0) [sn1] (b)	538.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	3.9	<1
LPC(19:0) [sn2] (a)	538.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	6.9	6.16
LPC(19:1) (a)	536.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	10.0	4.92
LPC(19:1) (b)	536.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.4	2.96
LPC(19:1) (c)	536.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	9.0	28.49
LPC(20:0) [sn1]	552.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.5	<1
LPC(20:0) [sn2]	552.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.8	2.53
LPC(20:1) [sn1]	550.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.1	<1
LPC(20:1) [sn2]	550.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.1	1
LPC(20:2) [sn1]	548.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	2.8	<1
LPC(20:2) [sn2]	548.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.1	<1
LPC(20:3) [sn1]	546.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.4	<1
LPC(20:3) [sn2]	546.4 → 184.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	3.3	<1
LPC(20:4) [+OH]	560.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	15.4	25.83
LPC(20:4) [sn1]	544.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.3	<1
LPC(20:4) [sn2]	544.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.0	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
LPC(20:5) [sn1]	542.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.3	<1
LPC(20:5) [sn2]	542.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.6	<1
LPC(22:0) [sn1]	580.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	8.0	<1
LPC(22:0) [sn2]	580.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	8.6	<1
LPC(22:1) [sn1]	578.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.8	3.53
LPC(22:1) [sn2]	578.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	8.3	15.86
LPC(22:4) [sn1]	572.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.7	<1
LPC(22:4) [sn2]	572.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.5	<1
LPC(22:5) (n3) [sn1] [104_sn1]	570.4 → 104.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.3	<1
LPC(22:5) [sn1] (n3)/LPC(22:5) [sn2] (n6)	570.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.0	<1
LPC(22:5) [sn1] (n6)	570.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.8	<1
LPC(22:5) [sn2] (n3)	570.4 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	4.0	<1
LPC(22:6) [sn1]	568.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	3.8	<1
LPC(22:6) [sn2]	568.3 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	5.0	<1
LPC(22:6) [+OH]	584.3 -> 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	38.1	53.47
LPC(24:0) [sn1]	608.5 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	6.9	<1
LPC(24:0) [sn2]	608.5 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	8.0	<1
LPC(26:0) [sn1]	636.5 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	6.4	43.83
LPC(26:0) [sn2]	636.5 → 184.1	LPC(18:1) d7 (IS) [reference]	LPC(18:1) d7	1	7.3	51.49
LPC(O-16:0)	482.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.1	<1
LPC(O-18:0)	510.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	3.5	<1
LPC(O-18:1)	508.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.4	<1
LPC(O-20:0)	538.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	6.3	<1
LPC(O-20:1)	536.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.3	<1
LPC(O-22:0)	566.5 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	5.8	<1
LPC(O-22:1)	564.4 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	7.1	<1
LPC(O-24:0)	594.5 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	4.4	<1
LPC(O-24:1)	592.5 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	5.6	1.54
LPC(O-24:2)	590.5 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	7.9	<1
LPC(P-16:0)	480.3 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	2.2	<1
LPC(P-17:0) (a)	494.3 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	5.3	3.84
LPC(P-17:0) (b)	494.3 → 104.1	LPC(O-16:0) [reference]	LPC(18:1) d7	1	6.7	8.79
LPC(P-18:0)	508.3 → 104.1	LPC(P-18:0) [reference]	LPC(18:1) d7	1	5.1	<1
LPC(P-18:1)	506.3 → 104.1	LPC(P-18:1) [reference]	LPC(18:1) d7	1	4.6	<1
LPC(P-20:0)	536.3 → 104.1	LPC(P-18:1) [reference]	LPC(18:1) d7	1	11.3	<1
LPE(16:0) [sn1]	454.3 → 313.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.5	<1
LPE(16:0) [sn2]	454.3 → 313.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.1	<1
LPE(17:0)	468.3 -> 327.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	22.8	7.3
LPE(18:0) [sn1]	482.3 → 341.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	3.6	<1
LPE(18:0) [sn2]	482.3 → 341.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.3	<1
LPE(18:1) [sn1]	480.3 → 339.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.0	<1
LPE(18:1) [sn2]	480.3 → 339.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.6	<1
LPE(18:2) [sn1]	478.3 → 337.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	3.9	<1
LPE(18:2) [sn2]	478.3 → 337.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.0	<1
LPE(20:4) [sn1]	502.3 → 361.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.3	<1
LPE(20:4) [sn2]	502.3 → 361.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	6.1	<1
LPE(22:6) [sn1]	526.3 → 385.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	5.0	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
LPE(22:6) [sn2]	526.3 → 385.3	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	7.3	<1
LPE(P-16:0)	438.3 → 266.4	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	11.2	<1
LPE(P-18:0)	466.3 → 294.4	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	9.6	<1
LPE(P-18:1)	464.3 → 292.4	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	15.8	<1
LPE(P-20:0)	494.3 → 322.4	LPE(18:1) d7 (IS) [reference]	LPE(18:1) d7	1	21.6	21.11
LPI(18:0)	618.3 → 341.3	LPI(18:0) [reference]	LPI(13:0)	1	18.7	2.56
LPI(18:1) [sn1]	616.3 → 339.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	10.8	<1
LPI(18:1) [sn2]	616.3 → 339.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	25.4	<1
LPI(18:2) [sn1]	614.3 → 337.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	10.6	<1
LPI(18:2) [sn2]	614.3 → 337.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	10.6	3.74
LPI(20:4) [sn1]	638.3 → 361.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	12.4	<1
LPI(20:4) [sn2]	638.3 → 361.3	LPI 13:0 (IS) [reference]	LPI(13:0)	1	11.9	<1
methyl-CE(18:0)	684.6 → 383.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	14.6	4.15
methyl-CE(18:1)	682.6 → 383.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	4.3	<1
methyl-CE(18:2)	680.6 → 383.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	2.9	<1
methyl-CE(20:4)	704.6 → 383.3	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	4.1	<1
methyl-DE(18:1)	680.6 → 381.4	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	9.7	<1
methyl-DE(18:2)	678.6 → 381.4	CE 18:0-d6 (IS) [reference]	CE(18:0) d6	1	6.2	<1
PA(34:1)	692.6 → 577.6	PA(15:0_18:1) d7 (IS) [reference]	PA(15:0_18:1) d7	1	11.1	<1
PA(36:2)	718.6 → 603.6	PA(15:0_18:1) d7 (IS) [reference]	PA(15:0_18:1) d7	1	13.2	5.97
PA(36:3)	716.6 → 601.6	PA(15:0_18:1) d7 (IS) [reference]	PA(15:0_18:1) d7	1	13.7	6.68
PA(36:4)	714.6 → 599.6	PA(15:0_18:1) d7 (IS) [reference]	PA(15:0_18:1) d7	1	15.5	10.42
PC(14:0_16:0)	706.5 → 184.1	PC(14:0_16:0) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(14:0_20:4)	754.5 → 184.1	PC(14:0_20:4) [reference]	PC(15:0_18:1) d7	1	2.3	<1
PC(14:0_22:6)	778.5 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.7	<1
PC(15:0_20:3)	770.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	3.7	<1
PC(15:0_20:4)	768.6 → 184.1	PC(15:0_20:4) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(15:0_22:6)	792.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(15-MHDA_18:1)	774.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(15-MHDA_18:2)	772.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.1	<1
PC(15-MHDA_20:4)	796.6 → 184.1	PC(16:0_18:2) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(15-MHDA_22:6)	820.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.1	<1
PC(16:0_16:0)	734.6 → 184.1	PC(16:0_16:0) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(16:0_18:0)	762.6 → 184.1	PC(18:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(16:0_18:1)	760.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	3.2	<1
PC(16:0_18:2)	758.6 → 184.1	PC(16:0_18:2) [reference]	PC(15:0_18:1) d7	1	5.5	<1
PC(16:0_18:3) (a)	756.6 → 184.1	PC(32:2) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(16:0_18:3) (b)	756.6 → 184.1	PC(32:2) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(16:0_20:3) (a)	784.6 → 184.1	PC(33:1) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(16:0_20:3) (b)	784.6 → 184.1	PC(33:1) [reference]	PC(15:0_18:1) d7	1	3.0	<1
PC(16:0_20:4)	782.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	4.0	<1
PC(16:0_20:5)	780.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.5	<1
PC(16:0_22:6)	806.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(16:1_18:2)	756.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	2.9	<1
PC(16:1_20:4)	780.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.9	<1
PC(16:1_22:6)	804.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.5	<1
PC(17:0_18:1)	774.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.4	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
PC(17:0_18:2)	772.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.6	<1
PC(17:0_20:4)	796.6 → 184.1	PC(16:0_18:2) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(17:0_22:6)	820.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(17:1_18:2)	770.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	2.3	<1
PC(18:0_18:1)	788.6 → 184.1	PC(18:0_18:1) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(18:0_18:2)	786.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	3.3	<1
PC(18:0_20:3)	812.6 → 184.1	PC(18:0_18:1) [reference]	PC(15:0_18:1) d7	1	1.8	<1
PC(18:0_20:4)	810.6 → 184.1	PC(18:0_20:4) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(18:0_22:4)	838.6 → 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(18:0_22:5) (n3)/PC(20:1_20:4)	836.6 → 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	1.8	<1
PC(18:0_22:5) (n6)	836.6 → 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	2.1	<1
PC(18:0_22:6)	834.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(18:1_18:1)	786.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	3.3	<1
PC(18:1_18:2)	784.6 → 184.1	PC(33:1) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(18:1_20:3)	810.6 → 184.1	PC(18:0_20:4) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(18:1_22:6) (a)	832.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(18:1_22:6) (b)	832.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	3.9	<1
PC(18:2_18:2)	782.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	3.7	<1
PC(18:2_20:5)	804.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(20:0_20:4)	838.6 → 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	3.1	<1
PC(28:0)	678.5 → 184.1	PC(28:0) [reference]	PC(15:0_18:1) d7	1	3.5	<1
PC(31:0) (a)	720.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(31:0) (b)	720.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.9	<1
PC(31:1)	718.5 → 184.1	PC(14:0_16:0) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(32:1)	732.6 → 184.1	PC(16:0_16:0) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(32:2)	730.5 → 184.1	PC(32:2) [reference]	PC(15:0_18:1) d7	1	1.8	<1
PC(33:0) (a)	748.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	1.7	<1
PC(33:0) (b)	748.6 → 184.1	PC(16:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.6	<1
PC(33:1)	746.6 → 184.1	PC(33:1) [reference]	PC(15:0_18:1) d7	1	1.7	<1
PC(33:2)	744.6 → 184.1	PC(33:2) [reference]	PC(15:0_18:1) d7	1	2.8	<1
PC(34:2) [+OH]	774.6 -> 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	50.5	<1
PC(34:5)	752.5 → 184.1	PC(34:5) [reference]	PC(15:0_18:1) d7	1	3.6	<1
PC(35:5)	766.5 → 184.1	PC(15:0_20:4) [reference]	PC(15:0_18:1) d7	1	3.1	<1
PC(36:4) [+OH]	798.6 → 184.1	PC(15:0_18:1) d7 (IS) [reference]	PC(15:0_18:1) d7	1	4.2	<1
PC(36:6) (a)	778.5 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	3.0	<1
PC(38:2)	814.6 → 184.1	PC(18:0_18:1) [reference]	PC(15:0_18:1) d7	1	2.4	2.16
PC(38:4) (b)	810.6 → 184.1	PC(18:0_20:4) [reference]	PC(15:0_18:1) d7	1	1.8	<1
PC(38:5) (a)	808.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.2	<1
PC(38:5) (b)	808.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.8	<1
PC(38:6) (a)	806.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.4	<1
PC(38:6) [+OH]	822.6 → 184.1	PC(18:0_20:4) [reference]	PC(15:0_18:1) d7	1	4.3	<1
PC(38:7) (c)	804.6 → 184.1	PC(15:0_22:6) [reference]	PC(15:0_18:1) d7	1	3.3	<1
PC(39:5) (a)	822.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	3.1	<1
PC(39:5) (b)	822.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(40:7) (a)	832.6 → 184.1	PC(18:0_22:6) [reference]	PC(15:0_18:1) d7	1	2.7	<1
PC(40:8)	830.6 → 184.1	PC(16:0_18:2) [reference]	PC(15:0_18:1) d7	1	2.5	<1
PC(42:10)	854.5 → 184.1	PC(34:5) [reference]	PC(15:0_18:1) d7	1	3.0	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
PC(O-16:0/16:0)	720.6 → 184.1	PC(O-16:0/16:0) [reference]	PC(15:0_18:1) d7	1	2.7	<1
PC(O-16:0/20:3)	770.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	2.1	<1
PC(O-16:0/20:4)	768.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(O-16:0/22:6)	792.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(O-18:0/18:1)	774.6 → 184.1	PC(O-36:0) [reference]	PC(15:0_18:1) d7	1	4.6	<1
PC(O-18:0/18:2)	772.6 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	2.3	<1
PC(O-18:0/20:4)	796.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(O-18:0/22:6)	820.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	2.6	<1
PC(O-18:1/18:1)	772.6 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	2.6	<1
PC(O-18:1/18:2)	770.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	1.6	<1
PC(O-32:1)	718.5 → 184.1	PC(O-16:0/16:0) [reference]	PC(15:0_18:1) d7	1	2.8	<1
PC(O-32:2)	716.6 → 184.1	PC(16:0_18:2) [reference]	PC(15:0_18:1) d7	1	2.5	1.55
PC(O-34:1)	746.6 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	2.0	<1
PC(O-34:2)	744.6 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	1.7	<1
PC(O-34:4)	740.6 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	2.8	2.57
PC(O-35:4)	754.5 → 184.1	PC(O-34:1) [reference]	PC(15:0_18:1) d7	1	1.9	93.31
PC(O-36:0)	776.6 → 184.1	PC(O-36:0) [reference]	PC(15:0_18:1) d7	1	3.7	<1
PC(O-36:5)	766.5 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(O-38:5)	794.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	1.9	<1
PC(O-40:5)	822.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	2.1	<1
PC(O-40:7)	818.6 → 184.1	PC(O-38:5) [reference]	PC(15:0_18:1) d7	1	2.4	<1
PC(P-15:0/20:4) (a)	752.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	4.5	2.73
PC(P-15:0/20:4) (b)	752.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	4.9	7.07
PC(P-16:0/14:0)	690.4 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	4.0	<1
PC(P-16:0/16:0)	718.5 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	3.3	<1
PC(P-16:0/16:1)	716.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	2.6	<1
PC(P-16:0/18:0)	746.6 → 184.1	PC(P-18:0/18:1) d9 (IS) [reference]	PC(P-18:0/18:1) d9	1	2.7	3.56
PC(P-16:0/18:1)	744.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	1.2	<1
PC(P-16:0/18:2)	742.5 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	3.4	<1
PC(P-16:0/18:3)	740.6 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	3.1	1.53
PC(P-16:0/20:4)	766.5 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	2.4	<1
PC(P-16:0/20:5)	764.6 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	3.3	<1
PC(P-16:0/22:6)	790.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	3.5	<1
PC(P-17:0/20:4) (a)	780.5 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	3.2	<1
PC(P-17:0/20:4) (b)	780.5 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	3.8	<1
PC(P-18:0/18:2)	770.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	1.4	<1
PC(P-18:0/20:4)	794.6 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	1.4	<1
PC(P-18:0/22:5)	820.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	1.8	<1
PC(P-18:0/22:6)	818.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	2.9	<1
PC(P-18:1/18:1)	770.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	2.1	<1
PC(P-18:1/22:6)	816.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	5.8	1.18
PC(P-20:0/20:4)	822.6 → 184.1	PC(P-18:0/18:1) d9 (IS) [reference]	PC(P-18:0/18:1) d9	1	2.6	1.89
PC(P-35:2) (a)	756.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	2.9	<1
PC(P-35:2) (b)	756.6 → 184.1	PC(P-16:0/18:1) [reference]	PC(P-18:0/18:1) d9	1	3.0	<1
PC(P-36:3)	768.5 → 184.1	PC(P-16:0/20:4) [reference]	PC(P-18:0/18:1) d9	1	2.1	<1
PC(P-38:5) (a)	792.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	3.1	<1
PC(P-38:5) (b)	792.6 → 184.1	PC(P-16:0/22:6) [reference]	PC(P-18:0/18:1) d9	1	2.2	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
PE(15-MHDA_18:1)	732.6 → 591.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	12.8	17.5
PE(15-MHDA_18:2)	730.5 → 589.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	9.1	<1
PE(15-MHDA_20:4)	754.6 → 613.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	11.1	<1
PE(15-MHDA_22:6)	778.5 → 637.5	PE(16:0_22:6) [reference]	PE(15:0_18:1) d7	1	9.4	<1
PE(16:0_16:0)	692.5 → 551.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	17.5	<1
PE(16:0_16:1)	690.5 → 549.5	PE(16:0_16:1) [reference]	PE(15:0_18:1) d7	1	8.9	<1
PE(16:0_18:1)	718.5 → 577.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	2.5	<1
PE(16:0_18:2)	716.5 → 575.5	PE(16:0_18:2) [reference]	PE(15:0_18:1) d7	1	2.5	<1
PE(16:0_18:3) (a)	714.5 → 573.5	PE(16:0_18:2) [reference]	PE(15:0_18:1) d7	1	7.0	1.14
PE(16:0_18:3) (b)	714.5 → 573.5	PE(16:0_18:2) [reference]	PE(15:0_18:1) d7	1	6.9	<1
PE(16:0_20:3)	742.5 → 601.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	2.7	<1
PE(16:0_20:4)	740.5 → 599.5	PE(18:0_20:4) [reference]	PE(15:0_18:1) d7	1	1.5	<1
PE(16:0_20:5)	738.5 → 597.5	PE(16:0_16:1) [reference]	PE(15:0_18:1) d7	1	4.3	<1
PE(16:0_22:6)	764.5 → 623.5	PE(16:0_22:6) [reference]	PE(15:0_18:1) d7	1	5.8	<1
PE(16:1_18:2)	714.5 → 573.5	PE(16:0_18:2) [reference]	PE(15:0_18:1) d7	1	10.5	<1
PE(16:1_20:4)	738.5 → 597.5	PE(16:0_16:1) [reference]	PE(15:0_18:1) d7	1	7.3	<1
PE(17:0_18:1)	732.6 → 591.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	11.0	<1
PE(17:0_18:2)	730.5 → 589.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	8.0	1.13
PE(17:0_20:4)	754.6 → 613.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	5.0	<1
PE(17:0_22:6)	778.5 → 637.5	PE(16:0_22:6) [reference]	PE(15:0_18:1) d7	1	9.1	2.42
PE(18:0_18:1)	746.6 → 605.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	2.0	<1
PE(18:0_18:2)	744.6 → 603.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	1.5	<1
PE(18:0_20:3) (a)	770.6 → 629.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	2.3	<1
PE(18:0_20:3) (b)	770.6 → 629.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	4.3	<1
PE(18:0_20:4)	768.6 → 627.5	PE(18:0_20:4) [reference]	PE(15:0_18:1) d7	1	1.4	<1
PE(18:0_22:4)	796.6 → 655.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	4.5	<1
PE(18:0_22:5) (n3)	794.6 → 653.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	2.5	<1
PE(18:0_22:5) (n6)	794.6 → 653.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	3.8	<1
PE(18:0_22:6)	792.6 → 651.5	PE(18:0_22:6) [reference]	PE(15:0_18:1) d7	1	2.9	<1
PE(18:1_18:1)	744.6 → 603.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	5.8	<1
PE(18:1_18:2)	742.5 → 601.5	PE(16:0_18:1) [reference]	PE(15:0_18:1) d7	1	3.0	<1
PE(18:1_22:6) (a)	790.5 → 649.5	PE(18:0_22:6) [reference]	PE(15:0_18:1) d7	1	4.2	1.05
PE(18:1_22:6) (b)	790.5 → 649.5	PE(18:0_22:6) [reference]	PE(15:0_18:1) d7	1	7.9	1.59
PE(20:0_20:4)	796.6 → 655.6	PE(18:0_18:1) [reference]	PE(15:0_18:1) d7	1	7.8	<1
PE(38:5) (a)	766.5 → 625.5	PE(18:0_20:4) [reference]	PE(15:0_18:1) d7	1	3.2	<1
PE(38:5) (b)	766.5 → 625.5	PE(18:0_20:4) [reference]	PE(15:0_18:1) d7	1	2.7	<1
PE(O-16:0/18:2)	702.5 → 561.5	PE(O-34:1) [reference]	PE(15:0_18:1) d7	1	4.6	<1
PE(O-16:0/20:3)	728.6 → 587.5	PE(18:0_22:6) [reference]	PE(15:0_18:1) d7	1	6.9	<1
PE(O-16:0/20:4)	726.5 → 585.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	2.5	<1
PE(O-16:0/22:4)	754.6 → 613.6	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	5.1	8.97
PE(O-16:0/22:6)	750.6 → 609.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	2.5	<1
PE(O-18:0/20:4)	754.6 → 613.6	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	2.7	<1
PE(O-18:0/22:5)	780.6 → 639.6	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	5.1	<1
PE(O-18:0/22:6)	778.5 → 637.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	3.1	<1
PE(O-18:1/18:2)	728.6 → 587.5	PE(18:0_22:6) [reference]	PE(15:0_18:1) d7	1	4.5	<1
PE(O-18:1/22:6)	776.6 → 635.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	2.9	<1
PE(O-34:1)	704.6 → 563.5	PE(O-34:1) [reference]	PE(15:0_18:1) d7	1	3.1	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
PE(O-36:5)	724.5 → 583.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	6.5	1.71
PE(O-38:5) (a)	752.6 → 611.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	3.0	<1
PE(O-38:5) (b)	752.6 → 611.5	PE(P-18:0/20:4) [reference]	PE(15:0_18:1) d7	1	4.7	1.69
PE(P-15:0/22:6)	734.5 → 385.3	PE(P-16:0/18:2) [reference]	PE(P-18:0/18:1) d9	1	12.0	<1
PE(P-16:0/18:1)	702.5 → 339.3	PE(P-16:0/18:2) [reference]	PE(P-18:0/18:1) d9	1	2.8	<1
PE(P-16:0/18:2)	700.5 → 337.3	PE(P-16:0/18:2) [reference]	PE(P-18:0/18:1) d9	1	2.1	<1
PE(P-16:0/20:3) (a)	726.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.9	<1
PE(P-16:0/20:3) (b)	726.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	8.0	1.32
PE(P-16:0/20:4)	724.5 → 361.3	PE(P-16:0/18:2) [reference]	PE(P-18:0/18:1) d9	1	3.0	<1
PE(P-16:0/20:5)	722.5 → 359.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.2	<1
PE(P-16:0/22:4)	752.6 → 389.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.2	<1
PE(P-16:0/22:5) (n3)	750.5 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.6	<1
PE(P-16:0/22:5) (n6)	750.5 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	6.2	<1
PE(P-16:0/22:6)	748.5 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.5	<1
PE(P-17:0/20:4) (a)	738.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.7	<1
PE(P-17:0/20:4) (b)	738.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.2	<1
PE(P-17:0/22:6) (a)	762.6 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.9	<1
PE(P-17:0/22:6) (b)	762.6 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.9	<1
PE(P-18:0/18:1)	730.6 → 339.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.9	<1
PE(P-18:0/18:2)	728.6 → 337.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.1	<1
PE(P-18:0/18:3)	726.5 → 335.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	12.7	<1
PE(P-18:0/20:3) (a)	754.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.6	<1
PE(P-18:0/20:3) (b)	754.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	6.8	<1
PE(P-18:0/20:4)	752.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	1.4	<1
PE(P-18:0/20:5)	750.5 → 359.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.8	<1
PE(P-18:0/22:4)	780.6 → 389.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.9	<1
PE(P-18:0/22:5) (n3)	778.5 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.2	<1
PE(P-18:0/22:5) (n6)	778.5 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	6.7	1.39
PE(P-18:0/22:6)	776.6 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.0	<1
PE(P-18:1/18:1) (a)	728.6 → 339.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.0	<1
PE(P-18:1/18:1) (b)	728.6 → 339.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	6.2	<1
PE(P-18:1/18:2) (a)	726.5 → 337.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.0	<1
PE(P-18:1/18:2) (b)	726.5 → 337.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.5	<1
PE(P-18:1/20:3) (a)	752.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	6.1	<1
PE(P-18:1/20:3) (b)	752.5 → 363.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	9.5	<1
PE(P-18:1/20:4) (a)	750.5 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	2.4	<1
PE(P-18:1/20:4) (b)	750.5 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.0	<1
PE(P-18:1/20:5) (a)	748.5 → 359.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.1	<1
PE(P-18:1/20:5) (b)	748.5 → 359.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	7.7	<1
PE(P-18:1/22:4)	778.5 → 389.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	9.4	<1
PE(P-18:1/22:5) (a)	776.6 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.4	2.73
PE(P-18:1/22:5) (b)	776.6 → 387.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	8.9	<1
PE(P-18:1/22:6) (a)	774.5 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	1.9	<1
PE(P-18:1/22:6) (b)	774.5 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.1	<1
PE(P-19:0/20:4) (a)	766.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	12.3	1.51
PE(P-19:0/20:4) (b)	766.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	9.2	<1
PE(P-20:0/18:1)	758.6 → 339.3	PE(P-18:0/18:1) d9 (IS) [reference]	PE(P-18:0/18:1) d9	1	6.7	3.32

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
PE(P-20:0/18:2)	756.6 → 337.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.7	<1
PE(P-20:0/20:4)	780.6 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.3	<1
PE(P-20:0/22:6)	804.6 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	4.0	<1
PE(P-20:1/20:4)	778.5 → 361.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	3.8	<1
PE(P-20:1/22:6)	802.6 → 385.3	PE(P-18:0/20:4) [reference]	PE(P-18:0/18:1) d9	1	5.5	<1
PG(34:1)	766.6 → 577.5	PG(15:0_18:1) d7 (IS) [reference]	PG(15:0_18:1) d7	1	12.2	<1
PG(36:1)	794.6 → 605.6	PG(15:0_18:1) d7 (IS) [reference]	PG(15:0_18:1) d7	1	10.9	<1
PG(36:2)	792.6 → 603.5	PG(15:0_18:1) d7 (IS) [reference]	PG(15:0_18:1) d7	1	12.2	<1
PI(38:5) (b)	902.6 → 625.6	PI(38:6) [reference]	PI(15:0_18:1) d7	1	4.0	<1
PI(15-MHDA_18:1)/PI(17:0_18:1)	868.6 → 591.6	PI(34:1) [reference]	PI(15:0_18:1) d7	1	7.3	<1
PI(15-MHDA_18:2)/PI(17:0_18:2)	866.6 → 589.6	PI(15-MHDA_18:2)/PI(17:0_18:2) [reference]	PI(15:0_18:1) d7	1	8.0	<1
PI(37:4)	890.6 → 613.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	6.4	<1
PI(16:0/16:0)	828.6 → 551.6	PI(34:1) [reference]	PI(15:0_18:1) d7	1	5.7	<1
PI(16:0_16:1)	826.5 → 549.5	PI(16:0_16:1) [reference]	PI(15:0_18:1) d7	1	3.8	<1
PI(16:0_20:3) (a)	878.6 → 601.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	4.7	<1
PI(16:0_20:3) (b)	878.6 → 601.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	5.3	<1
PI(16:0_20:4)	876.6 → 599.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	2.2	<1
PI(18:0_18:1)	882.6 → 605.6	PI(18:0_18:1) [reference]	PI(15:0_18:1) d7	1	2.5	<1
PI(18:0_20:2)	908.6 → 631.6	PI(18:0_20:4) [reference]	PI(15:0_18:1) d7	1	5.7	<1
PI(18:0_20:3) (a)	906.6 → 629.6	PI(18:0_20:4) [reference]	PI(15:0_18:1) d7	1	9.5	<1
PI(18:0_20:3) (b)	906.6 → 629.6	PI(18:0_20:4) [reference]	PI(15:0_18:1) d7	1	3.2	<1
PI(18:0_20:4)	904.6 → 627.6	PI(18:0_20:4) [reference]	PI(15:0_18:1) d7	1	3.7	<1
PI(18:0_22:4)	932.6 → 655.6	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	6.2	<1
PI(18:0_22:5) (n3)	930.6 → 653.6	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	13.4	<1
PI(18:0_22:5) (n6)	930.6 → 653.6	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	9.0	<1
PI(18:0_22:6)	928.6 → 651.6	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	3.3	<1
PI(18:1_18:2)	878.6 → 601.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	3.8	<1
PI(20:0_20:4)	932.6 → 655.6	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	9.2	<1
PI(34:0)	856.6 → 579.6	PI(18:0_18:1) [reference]	PI(15:0_18:1) d7	1	7.8	<1
PI(34:1)	854.6 → 577.6	PI(34:1) [reference]	PI(15:0_18:1) d7	1	2.3	<1
PI(36:2)	880.6 → 603.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	10.9	<1
PI(37:6)	886.6 → 609.6	PI(16:0_20:4) [reference]	PI(15:0_18:1) d7	1	11.7	<1
PI(38:5) (a)	902.6 → 625.6	PI(38:6) [reference]	PI(15:0_18:1) d7	1	3.7	<1
PI(38:6)	900.6 → 623.6	PI(38:6) [reference]	PI(15:0_18:1) d7	1	3.6	<1
PIP1(38:4)	984.7 → 627.7	PI(18:0_22:6) [reference]	PI(15:0_18:1) d7	1	7.0	1.52
PS(36:1)	790.6 → 605.6	PS(15:0_18:1) d7 (IS) [reference]	PS(15:0_18:1) d7	1	4.7	<1
PS(36:2)	788.5 → 603.5	PS(15:0_18:1) d7 (IS) [reference]	PS(15:0_18:1) d7	1	4.9	6.95
PS(38:4)	812.5 → 627.5	PS(15:0_18:1) d7 (IS) [reference]	PS(15:0_18:1) d7	1	11.9	<1
PS(40:5)	838.6 → 653.6	PS(15:0_18:1) d7 (IS) [reference]	PS(15:0_18:1) d7	1	6.8	16.53
S1P(d16:1)	352.2 → 236.3	S1P(d18:1) d7 (IS) [reference]	S1P(18:1) d7	1	6.9	4.6
S1P(d18:0)	382.2 → 284.3	S1P(d18:1) d7 (IS) [reference]	S1P(18:1) d7	1	14.7	<1
S1P(d18:1)	380.2 → 264.3	S1P(d18:1) d7 (IS) [reference]	S1P(18:1) d7	1	5.6	<1
S1P(d18:2)	378.2 → 262.3	S1P(d18:1) d7 (IS) [reference]	S1P(18:1) d7	1	5.1	<1
SHexCer(d18:1/16:0(OH))	796.8 → 264.3	SHexCer(d18:1/16:0) [reference]	SHexCer(d18:1/12:0)	1	6.2	<1
SHexCer(d18:1/16:0)	780.8 → 264.3	SHexCer(d18:1/16:0) [reference]	SHexCer(d18:1/12:0)	1	8.1	<1
SHexCer(d18:1/24:0(OH))	908.8 → 264.3	SHexCer(d18:1/24:1(OH)) [reference]	SHexCer(d18:1/12:0)	1	10.9	<1
SHexCer(d18:1/24:1(OH))	906.8 → 264.3	SHexCer(d18:1/24:1(OH)) [reference]	SHexCer(d18:1/12:0)	1	12.8	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
SHexCer(d18:1/24:1)	890.8 → 264.3	SHexCer(d18:1/24:1(OH)) [reference]	SHexCer(d18:1/12:0)	1	16.3	<1
SM(34:3)	699.5 → 184.1	SM(d18:2/14:0) [reference]	SM(d18:1/15:0) d9	1	4.4	<1
SM(35:2) (b)	715.6 → 184.1	SM(d17:1/16:0) [reference]	SM(d18:1/15:0) d9	1	5.0	<1
SM(37:1)	745.6 → 184.1	SM(d18:1/18:0)/SM(d16:1/20:0) [reference]	SM(d18:1/15:0) d9	1	1.8	<1
SM(37:2)	743.5 → 184.1	SM(d18:2/18:0) [reference]	SM(d18:1/15:0) d9	1	1.6	<1
SM(38:3) (a)	755.6 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	3.0	<1
SM(38:3) (b)	755.6 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	2.8	66.33
SM(40:3) (a)	783.6 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	2.2	<1
SM(40:3) (b)	783.6 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	2.0	<1
SM(40:4)	781.5 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	4.5	<1
SM(41:0)	803.7 → 184.1	SM(d18:1/24:0) [reference]	SM(d18:1/15:0) d9	1	3.3	<1
SM(41:1) (a)	801.7 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	5.3	<1
SM(43:1)	829.7 → 184.1	SM(43:1) [reference]	SM(d18:1/15:0) d9	1	2.5	<1
SM(43:2) (b)	827.7 → 184.1	SM(d19:1/24:1) [reference]	SM(d18:1/15:0) d9	1	2.5	<1
SM(43:2) (c)	827.7 → 184.1	SM(d19:1/24:1) [reference]	SM(d18:1/15:0) d9	1	2.3	<1
SM(44:1)	843.6 → 184.1	SM(44:2) [reference]	SM(d18:1/15:0) d9	1	4.5	<1
SM(44:2)	841.6 → 184.1	SM(44:2) [reference]	SM(d18:1/15:0) d9	1	2.8	<1
SM(44:3)	839.6 → 184.1	SM(44:2) [reference]	SM(d18:1/15:0) d9	1	4.2	<1
SM(d16:1/19:0)	717.6 → 184.1	SM(d18:2/18:0) [reference]	SM(d18:1/15:0) d9	1	4.0	<1
SM(d16:1/23:0)/SM(d17:1/22:0)	773.7 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	2.9	<1
SM(d16:1/24:1)	785.7 → 184.1	SM(d18:1/22:0)/SM(d16:1/24:0) [reference]	SM(d18:1/15:0) d9	1	2.0	<1
SM(d17:1/14:0)	661.5 → 184.1	SM(d18:1/15:0) d9 (IS) [reference]	SM(d18:1/15:0) d9	1	2.8	<1
SM(d17:1/16:0)	689.6 → 184.1	SM(d17:1/16:0) [reference]	SM(d18:1/15:0) d9	1	1.4	<1
SM(d17:1/24:1)	799.7 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	2.9	<1
SM(d18:0/14:0)	677.6 → 184.1	SM(d18:1/15:0) d9 (IS) [reference]	SM(d18:1/15:0) d9	1	4.4	<1
SM(d18:0/16:0)	705.6 → 184.1	SM(d18:1/16:0) [reference]	SM(d18:1/15:0) d9	1	4.2	<1
SM(d18:0/22:0)	789.7 → 184.1	SM(d18:1/22:0)/SM(d16:1/24:0) [reference]	SM(d18:1/15:0) d9	1	6.6	<1
SM(d18:1/14:0)/SM(d16:1/16:0)	675.5 → 184.1	SM(d18:1/15:0) d9 (IS) [reference]	SM(d18:1/15:0) d9	1	3.6	<1
SM(d18:1/16:0)	703.6 → 184.1	SM(d18:1/16:0) [reference]	SM(d18:1/15:0) d9	1	2.8	<1
SM(d18:1/17:0)/SM(d17:1/18:0)	717.6 → 184.1	SM(d18:2/18:0) [reference]	SM(d18:1/15:0) d9	1	3.0	<1
SM(d18:1/18:0)/SM(d16:1/20:0)	731.6 → 184.1	SM(d18:1/18:0)/SM(d16:1/20:0) [reference]	SM(d18:1/15:0) d9	1	2.1	<1
SM(d18:1/20:0)/SM(d16:1/22:0)	759.6 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	1.7	<1
SM(d18:1/22:0)/SM(d16:1/24:0)	787.7 → 184.1	SM(d18:1/22:0)/SM(d16:1/24:0) [reference]	SM(d18:1/15:0) d9	1	1.6	<1
SM(d18:1/23:0)/SM(d17:1/24:0)	801.7 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	1.3	<1
SM(d18:1/24:0)	815.7 → 184.1	SM(d18:1/24:0) [reference]	SM(d18:1/15:0) d9	1	4.0	<1
SM(d18:1/24:1)	813.7 → 184.1	SM(d18:1/24:1) [reference]	SM(d18:1/15:0) d9	1	1.7	<1
SM(d18:2/14:0)	673.5 → 184.1	SM(d18:2/14:0) [reference]	SM(d18:1/15:0) d9	1	5.6	<1
SM(d18:2/16:0)	701.6 → 184.1	SM(d18:2/16:0) [reference]	SM(d18:1/15:0) d9	1	2.8	<1
SM(d18:2/17:0)	715.6 → 184.1	SM(d17:1/16:0) [reference]	SM(d18:1/15:0) d9	1	2.9	<1
SM(d18:2/18:0)	729.6 → 184.1	SM(d18:2/18:0) [reference]	SM(d18:1/15:0) d9	1	1.9	<1
SM(d18:2/18:1)	727.6 → 184.1	SM(d18:2/16:0) [reference]	SM(d18:1/15:0) d9	1	2.2	<1
SM(d18:2/20:0)	757.6 → 184.1	SM(d18:2/20:0) [reference]	SM(d18:1/15:0) d9	1	2.0	<1
SM(d18:2/22:0)	785.7 → 184.1	SM(d18:1/22:0)/SM(d16:1/24:0) [reference]	SM(d18:1/15:0) d9	1	1.7	<1
SM(d18:2/23:0)	799.7 → 184.1	SM(d16:1/23:0)/SM(d17:1/22:0) [reference]	SM(d18:1/15:0) d9	1	2.7	<1
SM(d18:2/24:0)	813.7 → 184.1	SM(d18:1/24:1) [reference]	SM(d18:1/15:0) d9	1	4.1	<1
SM(d19:1/24:1)	827.7 → 184.1	SM(d19:1/24:1) [reference]	SM(d18:1/15:0) d9	1	4.2	<1
Sph(d18:1)	300.3 → 282.3	Sph(d17:1) [reference]	Sph(d17:1)	1	6.8	58.42

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
Sph(d18:2)	298.3 → 280.3	Sph(d17:1) [reference]	Sph(d17:1)	1	25.7	76.52
TG(48:0) [NL-16:0]	824.8 → 551.5	TG(48:0) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	1.25
TG(48:0) [NL-18:0]	824.8 → 523.5	TG(48:0) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	2.08
TG(48:0) [SIM]	824.8 → 824.8	TG(48:0) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	2.5	2.86
TG(48:1) [NL-16:1]	822.8 → 551.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	2.66
TG(48:1) [NL-18:1]	822.8 → 523.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(48:1) [SIM]	822.8 → 822.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.5	1.49
TG(48:2) [NL-14:0]	820.8 → 575.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(48:2) [NL-14:1]	820.8 → 577.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	1.14
TG(48:2) [NL-16:1]	820.8 → 549.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.7	4.14
TG(48:2) [NL-18:2]	820.8 → 523.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.7	<1
TG(48:2) [SIM]	820.8 → 820.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(48:3) [NL-14:0]	818.8 → 573.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(48:3) [NL-16:1]	818.8 → 547.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	5.58
TG(48:3) [NL-18:3]	818.8 → 523.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.6	<1
TG(48:3) [SIM]	818.8 → 818.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.8	4.47
TG(49:1) [NL-16:1]	836.8 → 565.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.9	14.31
TG(49:1) [NL-17:1]	836.8 → 551.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.8	<1
TG(49:1) [SIM]	836.8 → 836.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	13.44
TG(50:0) [NL-18:0]	852.8 → 551.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.8	<1
TG(50:0) [SIM]	852.8 → 852.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	1.84
TG(50:1) [NL-14:0]	850.8 → 605.5	TG(50:1) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	5.4	<1
TG(50:1) [NL-16:0]	850.8 → 577.5	TG(50:1) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	3.2	<1
TG(50:1) [NL-18:1]	850.8 → 551.5	TG(50:1) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	3.5	<1
TG(50:1) [SIM]	850.8 → 850.8	TG(50:1) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	3.5	<1
TG(50:2) [NL-14:0]	848.8 → 603.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(50:2) [NL-16:1]	848.8 → 577.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.6	<1
TG(50:2) [NL-18:1]	848.8 → 549.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(50:2) [NL-18:2]	848.8 → 551.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(50:2) [SIM]	848.8 → 848.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.6	<1
TG(50:3) [NL-14:0]	846.8 → 601.5	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	2.9	<1
TG(50:3) [NL-14:1]	846.8 → 603.5	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(50:3) [NL-16:1]	846.8 → 575.5	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	<1
TG(50:3) [NL-18:2]	846.8 → 549.5	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	<1
TG(50:3) [NL-18:3]	846.8 → 551.5	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	<1
TG(50:3) [SIM]	846.8 → 846.8	TG(50:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	2.5	<1
TG(50:4) [NL-14:0]	844.8 → 599.5	TG(50:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(50:4) [NL-18:3]	844.8 → 549.5	TG(50:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.2	<1
TG(50:4) [NL-20:4]	844.8 → 523.5	TG(50:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	4.2	<1
TG(50:4) [SIM]	844.8 → 844.8	TG(50:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.4	<1
TG(51:0) [NL-16:0]	866.7 → 593.4	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.2	<1
TG(51:0) [SIM]	866.7 → 866.7	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	9.6	<1
TG(51:1) [NL-17:0]	864.8 → 577.5	TG(51:1) [NL-17:0] [reference]	TG(15:0_18:1-d7_15:0)	1	5.6	<1
TG(51:1) [SIM]	864.8 → 864.8	TG(51:2) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.8	<1
TG(51:2) [NL-15:0]	862.8 → 603.5	TG(51:2) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	5.6	<1
TG(51:2) [NL-17:0]	862.8 → 575.5	TG(51:2) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	<1
TG(51:2) [NL-17:1]	862.8 → 577.5	TG(51:2) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
TG(51:2) [SIM]	862.8 → 862.8	TG(51:2) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	3.13
TG(52:1) [NL-18:0]	878.8 → 577.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.2	<1
TG(52:1) [NL-18:1]	878.8 → 579.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(52:1) [SIM]	878.8 → 878.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.5	<1
TG(52:2) [NL-16:0]	876.8 → 603.5	TG(52:2) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	4.8	<1
TG(52:2) [NL-18:2]	876.8 → 579.5	TG(52:2) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	2.8	<1
TG(52:2) [SIM]	876.8 → 876.8	TG(52:2) [NL-16:0] [reference]	TG(15:0_18:1-d7_15:0)	1	8.1	<1
TG(52:3) [NL-16:1]	874.8 → 603.5	TG(52:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	6.1	<1
TG(52:3) [NL-18:2]	874.8 → 577.5	TG(52:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(52:3) [SIM]	874.8 → 874.8	TG(52:3) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	8.1	<1
TG(52:4) [NL-16:1]	872.8 → 601.5	TG(52:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.2	<1
TG(52:4) [NL-18:2]	872.8 → 575.5	TG(52:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	<1
TG(52:4) [NL-18:3]	872.8 → 577.5	TG(52:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	<1
TG(52:4) [SIM]	872.8 → 872.8	TG(52:4) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	<1
TG(52:5) [NL-18:3]	870.8 → 575.5	TG(52:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.9	<1
TG(52:5) [NL-20:4]	870.8 → 549.5	TG(52:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(52:5) [NL-20:5]	870.8 → 551.5	TG(52:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(52:5) [SIM]	870.8 → 870.8	TG(52:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.7	<1
TG(53:2) [NL-17:1]	890.8 → 605.5	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	5.5	<1
TG(53:2) [NL-18:1]	890.8 → 591.5	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	<1
TG(53:2) [SIM]	890.8 → 890.8	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	<1
TG(54:0) [NL-18:0]	908.8 → 607.5	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	8.23
TG(54:0) [SIM]	908.8 → 908.8	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.0	4.98
TG(54:1) [NL-18:1]	906.8 → 607.5	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	<1
TG(54:1) [SIM]	906.8 → 906.8	TG(53:2) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	<1
TG(54:2) [NL-18:0]	904.8 → 603.5	TG(54:2) [NL-20:1] [reference]	TG(15:0_18:1-d7_15:0)	1	4.1	<1
TG(54:2) [NL-20:1]	904.8 → 577.5	TG(54:2) [NL-20:1] [reference]	TG(15:0_18:1-d7_15:0)	1	4.4	<1
TG(54:2) [SIM]	904.8 → 904.8	TG(54:2) [NL-20:1] [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(54:3) [NL-18:1]	902.8 → 603.5	TG(54:3) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.8	<1
TG(54:3) [NL-18:2]	902.8 → 605.5	TG(54:3) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	5.4	<1
TG(54:3) [SIM]	902.8 → 902.8	TG(54:3) [NL-18:1] [reference]	TG(15:0_18:1-d7_15:0)	1	2.7	<1
TG(54:4) [NL-18:2]	900.8 → 603.5	TG(54:4) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	4.3	<1
TG(54:4) [NL-20:3]	900.8 → 577.5	TG(54:4) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	<1
TG(54:4) [SIM]	900.8 → 900.8	TG(54:4) [NL-18:2] [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(54:5) [NL-18:3]	898.8 → 603.5	TG(54:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.6	<1
TG(54:5) [NL-20:4]	898.8 → 577.5	TG(54:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(54:5) [SIM]	898.8 → 898.8	TG(54:5) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	<1
TG(54:6) [NL-18:3]	896.8 → 601.5	TG(54:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(54:6) [NL-20:4]	896.8 → 575.5	TG(54:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(54:6) [NL-20:5]	896.8 → 577.5	TG(54:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.8	<1
TG(54:6) [NL-22:6]	896.8 → 551.5	TG(54:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	<1
TG(54:6) [SIM]	896.8 → 896.8	TG(54:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.2	<1
TG(54:7) [NL-20:5]	894.8 → 575.5	TG(54:7) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(54:7) [NL-22:6]	894.8 → 549.5	TG(54:7) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.5	<1
TG(54:7) [SIM]	894.8 → 894.8	TG(54:7) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	2.1	<1
TG(56:6) [NL-20:4]	924.8 → 603.5	TG(56:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	6.3	<1
TG(56:6) [NL-22:5]	924.8 → 577.5	TG(56:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.2	<1

Compound Name	Transition	Time Reference Compound	ISTD Compound	Response Factor	%CV[1]	% Background[2]
TG(56:6) [SIM]	924.8 → 924.8	TG(56:6) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.5	<1
TG(56:7) [NL-20:4]	922.8 → 601.5	TG(56:7) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	<1
TG(56:7) [NL-20:5]	922.8 → 603.5	TG(56:7) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	<1
TG(56:7) [NL-22:5]	922.8 → 575.5	TG(56:7) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	<1
TG(56:7) [NL-22:6]	922.8 → 577.5	TG(56:7) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	<1
TG(56:7) [SIM]	922.8 → 922.8	TG(56:7) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	2.2	<1
TG(56:8) [NL-20:4]	920.8 → 599.5	TG(56:8) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.2	<1
TG(56:8) [NL-20:5]	920.8 → 601.5	TG(56:8) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(56:8) [NL-22:6]	920.8 → 575.5	TG(56:8) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	2.4	<1
TG(56:8) [SIM]	920.8 → 920.8	TG(56:8) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	<1
TG(56:9) [NL-22:6]	918.8 → 573.5	TG(56:9) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	<1
TG(56:9) [SIM]	918.8 → 918.8	TG(56:9) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	2.6	57.34
TG(58:10) [NL-22:6]	944.9 → 599.5	TG(58:10) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(58:10) [SIM]	944.9 → 944.9	TG(58:10) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	2.2	<1
TG(58:8) [NL-22:6]	948.8 → 603.5	TG(58:8) [NL-22:6] [reference]	TG(15:0_18:1-d7_15:0)	1	3.8	<1
TG(58:9) [NL-22:6]	946.9 → 601.5	TG(58:9) [SIM] [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(O-50:1) [NL-15:0]	836.8 → 577.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	6.0	<1
TG(O-50:1) [NL-16:0]	836.8 → 563.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	<1
TG(O-50:1) [NL-17:1]	836.8 → 551.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	7.8	<1
TG(O-50:1) [NL-18:1]	836.8 → 537.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.9	<1
TG(O-50:1) [SIM]	836.8 → 836.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.6	<1
TG(O-50:2) [NL-16:1]	834.8 → 563.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	5.5	12.07
TG(O-50:2) [NL-18:1]	834.8 → 535.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.6	<1
TG(O-50:2) [NL-18:2]	834.8 → 537.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	7.0	<1
TG(O-50:2) [SIM]	834.8 → 834.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.1	35.14
TG(O-52:0) [NL-16:0]	866.8 → 593.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	8.3	2.04
TG(O-52:1) [NL-16:0]	864.8 → 591.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(O-52:1) [NL-18:1]	864.8 → 565.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.7	<1
TG(O-52:1) [SIM]	864.8 → 864.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	2.5	<1
TG(O-52:2) [NL-16:0]	862.8 → 589.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.5	<1
TG(O-52:2) [NL-17:1]	862.8 → 577.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	5.6	<1
TG(O-52:2) [NL-18:1]	862.8 → 563.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.7	<1
TG(O-52:2) [SIM]	862.8 → 862.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(O-54:2) [NL-17:1]	890.8 → 605.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.7	<1
TG(O-54:2) [NL-18:1]	890.8 → 591.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.0	<1
TG(O-54:2) [SIM]	890.8 → 890.8	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	3.3	<1
TG(O-54:3) [NL-17:1]	888.8 → 603.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	7.4	<1
TG(O-54:3) [NL-18:1]	888.8 → 589.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	4.0	<1
TG(O-54:4) [NL-17:1]	886.8 → 601.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	11.7	<1
TG(O-54:4) [NL-18:2]	886.8 → 589.5	TG(48:1) [NL-18:1] d7 (IS) [reference]	TG(15:0_18:1-d7_15:0)	1	5.6	<1
Ubiquinone	880.7 → 197.0	Ubiquinone [reference]	TG(15:0_18:1-d7_15:0)	1	2.3	<1

[1] %CV was calculated for each lipid species concentration from 50 sequentially injected TQCs.

[2] % Background is the median blank concentration as a percentage of the average NIST1950 concentration within the same LC/MS batch.

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