Application Note

Lipidomics/Clinical Research

Agilent

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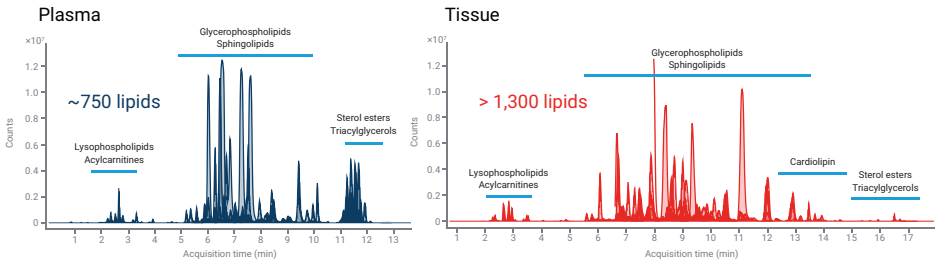
LC/MS dMRM Method Refinement Expands Targeted Lipidomics Studies from Plasma to Cells and Tissues



Authors

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Abstract

Liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS) with multiple reaction monitoring (MRM) allows measurement of hundreds of different lipid species of biological importance. Advances in LC/MS/MS technologies now enable scientists to map an increasingly broad range of lipids, including isomeric and isobaric species. This application note describes the expansion of existing LC/MS/MS plasma lipidomics methodology to other tissues such as brain tissue, which are known to contain substantially more varieties of lipid species and classes. To address the expanded set of lipid species and potential for isobaric and isotopic interreferences, the modified method extends the chromatographic gradient and adds and adjusts the MRM transitions monitored. The resulting LC/MS/MS method applies an impressive 940 MRM transitions to cover more than 1,300 molecular lipid species in brain tissue.

Introduction

Lipids play a central role in cellular structure and function across all biological tissues. Advances in the technologies used to study the lipidome enable scientists to map an increasingly broad range of lipids, including isomeric and isobaric species. Techniques such as liquid chromatography coupled with tandem mass spectrometry (LC/MS/MS) and multiple reaction monitoring (MRM) allow measurement of hundreds of different lipid species quickly and with a high degree of specificity. Ongoing improvements to chromatographic separations are adding even more detail to lipidomic studies.

The authors of this application note previously reported comprehensive LC/MS/MS methodology for detailed analysis of the plasma lipidome.[1,2] The method was subsequently shown to demonstrate strong precision and transferability in an interlaboratory study.[3] The methodology leverages analysis of pooled samples to annotate components prior to the analyses of individual study samples. Because that approach was developed for plasma, analysis of tissues and other cell types like brain tissue would benefit from method refinement.

By weight, brain tissue is mostly comprised of lipids which play diverse and important roles in neuron structure, signalling, and overall neurobiology. Notably, the brain lipidome consists of substantially more varieties of lipid species and classes than those reported in plasma. Compared to plasma lipidomics, the diversity and tissue dependency of glycerophospholipid acyl combinations found in brain and other tissues necessitates characterization of more lipid species, which in turn requires chromatography adjustments and the inclusion of additional transitions in the MRM method. Here, an extended gradient is applied to enhance separation and coverage of the longer glycerophospholipids present in brain tissues. Still, the potential for isobaric and isotopic interference from various species remains a challenge that is difficult to solve using a unit-resolution mass spectrometer. To address this problem, the method applies identification and exclusion of isotopic species to help select the best chromatographic peaks for integration. The targeted LC/MS/MS lipidomics methodology presented here now extends the analysis to brain tissue with more than 1,300 lipid species across 53 classes.

This application note also recommends strategies to further optimize a tissue-specific method for consistent results, including defining sample glycerophospholipids pools, identifying isomeric glycerophospholipid subclasses that share similar or identical masses and fragmentation patterns, characterizing glycerophospholipids, and assessing and extending method dynamic range. Employing these strategies provides valuable knowledge for the laboratory and ideally should be performed as part of every major tissue study.

Experimental

The experimental methodology is derived from application note 5994-3747EN.[1] Near-identical internal standards and preparation steps were used, with the other steps adjusted for tissue lipidomics.

Internal standard mix preparation

The internal standard mixture was prepared in house from commercially available sources (Table 1), but premade mixtures such as the SPLASH LIPIDOMIX Mass Spec Standard (Avanti, #330707) are also suitable. The internal standards used are largely derived from human plasma and serum, making it a challenge to obtain absolute quantification of each lipid species reported. However, the resulting relative quantification allows comparisons between samples that are analyzed using the same approach in the same study. Inclusion of external calibrant samples (e.g. NIST SRM 1950 for plasma and pooled tissues/cells for other studies) enables more consistent alignment between studies.

Quality control samples

Central to any lipidomic analysis are quality control samples that are used to monitor systematic study issues. These samples are needed to align the data generated and compensate for instrumental drift and variation (both within and between different batches), and to detect more serious errors within the data.

Pooled tissue quality control: Use of plasma quality control samples has been described[1], however, different control samples are required for different matrices to properly assess variance across the sample extraction process and analytical run. A tissue-specific pooled QC (PQC) is created by combining small aliquots from the biological replicates in the study. For studies where samples are measured in different batches, the PQC is necessary to harmonize measurements between runs. Typically, homogenates are aliquoted in the appropriate concentration and volume into Eppendorf tubes that can be used for the extraction.

Table 1. Internal standard information.

Name	MW	Stock Solution (µM)	Concentration in Mix (µM)	Final pmol added per sample (10 µL)	Solvent	Supplier (*Present in Avanti Mix)[1,2]
AC 16:0 d3	439.09	100	1	10	$CHCl_3$:MeOH (1:1)	Larodan (#71-1746-5)
CE 18:0 d6	659.16	2,000	100	1,000	$CHCl_3$:MeOH (1:1)	CDN isotopes (#D-5823)
Cer d18:1;O2/18:0 d7	572.99	200	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#860677P)
Cholic Acid d4	412.61	200	5	50	$CHCl_3$:MeOH (1:1)	Cayman (#20849)
Cholesterol d7	393.69	20,000	1,000	10,000	$CHCl_3$:MeOH (1:1)	Avanti (#700041P)*
DG 15:0_18:1 d7	587.97	800	20	200	$CHCl_3$:MeOH (1:1)	Avanti (#791647)*
Cer 18:0;O2/8:0	427.71	200	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#860626P)
FFA 18:1 d9	291.52	3,000	20	200	$CHCl_3$:MeOH (1:1)	Avanti (#861809)
Hex2Cer 18:1;O2/15:0 d7	855.21	400	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti (#330727)
Hex3Cer 18:1;O2/17:0	1038.35	100	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Matreya LLC (#1523)
HexCer 18:1;O2/15:0 d7	693.06	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#330729)
LPC 18:1 d7	528.71	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#791643)*
LPE 18:1 d7	486.63	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#791644)*
LPI 13:0	547.57	200	2	20	$CHCl_3$:MeOH (1:1)	Avanti (#850101)
PA 15:0_18:1 d7	689.93	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#791642)*
PC 15:0_18:1 d7	753.09	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#791637)*
PC P-18:0/18:1 d9	781.19	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#852475)*
PE 15:0_18:1 d7	711.01	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#791638)*
PE P-18:0/18:1 d9	739.11	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#852474)*
PG 15:0_18:1 d7	764.01	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#791640)*
PI 15:0_18:1 d7	847.12	400	5	50	$CHCl_3$:MeOH (1:1)	Avanti (#791641)*
PS 15:0_18:1 d7	777.00	400	5	50	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti (#791639)*
SPBP 18:1 d7	386.52	400	4	40	$CHCl_3$:MeOH:H_2O (1:1:0.2)	Avanti (#860659)
SHexCer 18:1;O2/12:0	741.03	200	1	10	$CHCl_3$:MeOH (1:1)	Avanti (#860573P)
SM 18:1;O2/15:0 d9	698.06	800	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#860686)
SPB 17:1;O2	285.47	400	2	20	$CHCl_3$:MeOH (1:1)	Avanti (#860640P)
TG 15:0_18:1_15:0 d7	812.35	400	10	100	$CHCl_3$:MeOH (1:1)	Avanti (#791648)*

[1] The specific CE and SM standards listed are not in the Avanti SPLASH LIPIDOMIX, but an equivalent standard is present.
[2] The plasmalogen standards are only available in the SPLASH LIPIDOMIX II mix.
MW = Molecular weight

Technical quality control: The use of technical quality controls (TQCs) to measure instrumental variance over time in large cohort studies has also been described.[1] Here, the TQCs were thawed and injected every 40 samples, and at the start and end of every batch. Similar technical controls can be pre-generated for batches of tissue samples if required, but small sample sets may not require TQCs.

Blank samples: The blank samples should align with the study samples. Typically, tissue homogenization is conducted in buffered solutions (e.g. phosphate-buffered saline). The same solutions should be used to generate the blank and extracted samples concurrently with the biological samples and the PQCs.

Porcine Brain Total Lipid Extract (Avanti, #131101C): This commercially available extract is readily accessible and contains many of the brain-specific lipids present in humans. Use of the extract enables retention-time adjustment during acquisition method setup and assessment of instrument performance. For user reference, annotated chromatograms for this extract are available at https://metabolomics.baker.edu.au/method/lipids. The sample was prepared in chloroform at 25 mg/mL diluted 1:100 in 1:1:0.1 butanol/methanol/water to yield approximately 250 µg/mL.

NIST SRM 1950: While the NIST SRM 1950 plasma sample is less relevant to tissue and cell lipidomics than plasma, it nonetheless provides an additional assessment of instrument performance and reference point. The lipid extraction procedure for NIST SRM 1950 is described in application note 5994-3747EN.[1]

Lipid extraction

In general, the authors observe good recovery of lipids from brain tissue homogenates using a single-phase butanol:methanol extraction as previously described for plasma.[3] Brain tissues were pre-homogenized using a Qiagen Tissue Lyser II (Cat number: 85300) with a Tissue Lyser Adapter Set 2 × 24 (cat. no. 6998) and stainless-steel beads (Qiagen, 5 mm cat. no. 69989). The homogenate was then probe sonicated. Following sonication, 10 µL of tissue homogenate (approximately 20 µg of protein) was transferred to a 1.5 mL Eppendorf tube using polypropylene positive displacement pipettes. In cases where samples required concentration/lyophilization, they were reconstituted in 10 µL of dH_2O. The 10 µL of sample was mixed with 100 µL extraction solvent of butanol:methanol (1:1) with 10 mM ammonium formate and the reconstituted mixture of internal standards (Table 3). Each sample was then vortexed for 5 seconds and subsequently bath-sonicated for 1 hour at 21 to 25 °C. Samples were then centrifuged (13,000 × g, 10 minutes, 20 °C), and the supernatant transferred into 1.5 mL glass sample vials (part number 5190-9590) with 200 µL glass inserts (part number 5183-2085). Samples were capped with PTFE/S caps (part number 5185-5820) and stored at –80 °C until immediately prior to analysis, whereupon they were thawed to room temperature (1 hour), bath-sonicated for 15 minutes, briefly vortexed, and then loaded into the instrument's autosampler.

Several approaches are available to isolate lipids from tissue homogenates, including the Folch[5], Matyash[6], and Bligh-Dyer[7] extraction methods, which have been routinely used in numerous laboratories. These approaches can be applied instead of single-phase extractions if desired, but with the disadvantage that several lipid classes, including the gangliosides, may partially solubilize in the aqueous phases or adhere onto the glass. Samples extracted using those methods would need to be reconstituted into a suitable solvent composition (e.g. 1:1:0.1 butanol/methanol/water) to prevent sample-solvent effects, such as breakthrough and loss of resolution of chromatographic peaks for the early-eluting, more polar lipid species.

LC/MS/MS instrumentation and methods

Extracted samples were separated using an Agilent 1290 Infinity II LC system with the:

- Agilent 1290 Infinity II Multisampler (G7167B)
- Agilent 1290 Infinity II High Speed (binary) Pump (G7120A)
- Agilent 1290 Infinity II Multicolumn Thermostat (G7116B)[1]

The chromatographic method is fully compatible with the Agilent 1290 Infinity III LC system and equivalent results are expected using both systems. The LC system was coupled to an Agilent 6495C triple quadrupole LC/MS (LC/TQ) system with an Agilent Jet Stream technology ion source. Lipid extracts (1 µL, equivalent to ~ 0.5 µg of protein) were injected and separated using a 20-minute gradient with the first minute diverted to waste. The 20-minute gradient provides better separation and broader coverage of glycerophospholipids and sphingolipids by reducing the number of concurrent transitions in the middle of the run. The chromatographic conditions are listed in Table 2.

Table 2. Chromatographic conditions.

Parameter	Agilent 1290 Infinity II/III LC
Analytical Column	Agilent ZORBAX Eclipse Plus C18, 1.8 µm, 100 × 2.1 mm column (p/n 959758-902)
Inline Filter	Agilent InfinityLab Quick Change inline filters, 0.2 µm (p/n 5067-1610)
Column Temperature	45 °C
Injection Volume	1–5 µL, sample-dependent
Autosampler Temperature	17 °C
Needle Wash	Wash vial, 3 s (BUME)/Flushport 50:50 A/B
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
Flow Rate	0.4 mL/min
Gradient Program	Time %B 0 15 2.5 50 2.6 57 12 70 12.5 80 15.4 90 15.5 100 16.5 100 17 15 20 15
Stop Time	20 min
Post Time	None
Segments	0 To waste 1 To MS 18.5 To waste

LC/MS/MS analysis was conducted using dynamic multiple reaction monitoring (dMRM) mode as shown in Figure 1. The dMRM mode allows the instrument to acquire MRM data only during specific retention time windows, reducing the number of concurrent ion transitions monitored. Mass spectrometer instrument and ion source parameters are provided in Table 3. The method can also be implemented on the 6495D LC/TQ instrument.

Dynamic multiple reaction monitoring method setup

To measure the large number of lipid species in a tissue lipidome, the specific retention time window in which each compound elutes must be defined so the LC/TQ instrument only scans for a given lipid species at specific points across the total run time. This retention time window varies for the different MRM transitions and is largely dependent on differences in peak widths. For the brain-specific method, the authors optimized the dMRM windows for each lipid class targeted. Using dMRM improves the instrument duty cycle and extends the average dwell time per compound.

Table 3. Mass spectrometer instrument and ion source parameters.

Parameter	Agilent 6495C LC/TQ
Ion Source	Agilent Jet Stream ion source
Polarity	Positive and Negative Switching
Gas Temperature	200 °C
Drying Gas (Nitrogen)	17 L/min
Nebulizer Gas	20 psi
Sheath Gas	280 °C
Sheath Gas Flow	10 L/min
Capillary Voltage	3,500 V (+), −2,500 V (−)
Nozzle Voltage	1,000 V (+), −1,000 V (−)
iFunnel High/low pressure RF	210/160 V (+), 210/160 V (−)
Scan Type	Dynamic MRM (dMRM)
Q1/Q2 Resolution	Unit (0.7 amu)
Delta EMV	100 V (+), 0 V (−)
Cell Acceleration Voltage	4–5 V
Cycle Time	700 ms
Time Filter Width	0.05 min
Total number of MRMs	940

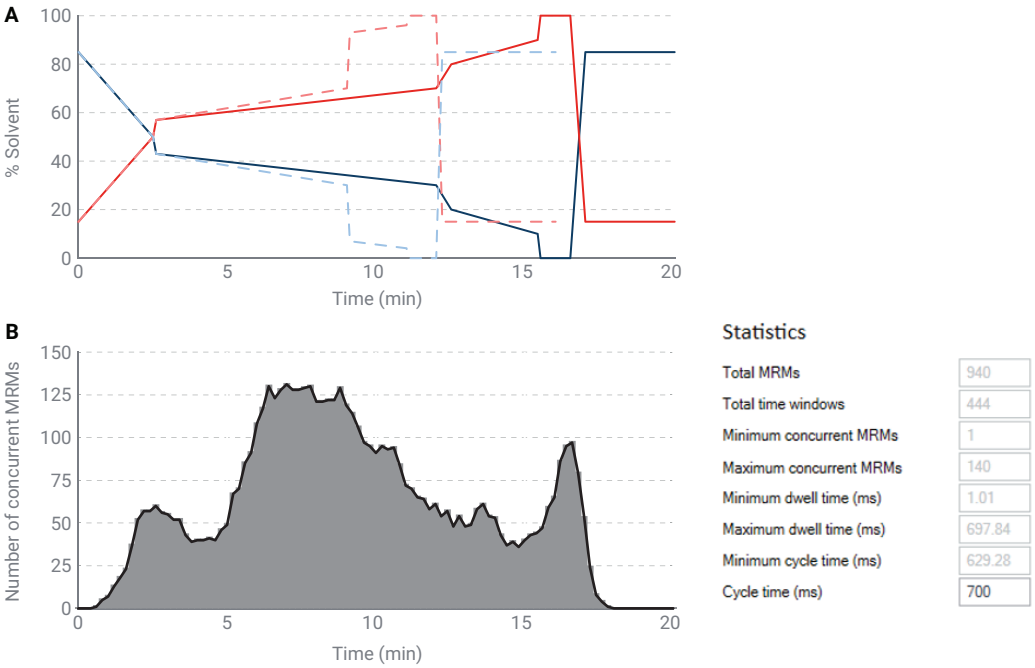

Figure 1. (A) Extended LC gradient and final dMRM Method. Due to the increased number of concurrent transitions in the middle of the run, the chromatographic method was extended to 20 minutes, enabling better separation and broader coverage of glycerophospholipids and sphingolipids. Solvent A (blue), solvent B (red), plasma-lipid gradient (dashed line), extended brain-lipid gradient (solid line). (B) is a dMRM summary plot showing the concurrent MRMs versus retention times and dMRM statistics.

The dMRM method was optimized using Agilent MassHunter Acquisition software for LC/MS, which aligns the MRM scan for each compound of interest with the compound's known retention time. The transitions monitored per lipid species along with all the other dMRM parameters are provided in Table A1 (Appendix). Positive ionization mode was used for most of the lipid classes. The method has a 700 ms cycle time, allowing for 940 MRM transitions to monitor more than 1,300 lipid species and isomers.

Because many factors can dramatically impact the retention time of each compound depending on the analytical setup, initial application of the method requires retention time calibration. Setting the retention time windows to a larger value (or performing unscheduled scans) is recommended to calibrate the method. The appropriate retention time windows are easily generated using the "split method" function of the Dynamic MRM viewer in the MassHunter Method Editor. Several notable lipid classes, including ceramides, heoxylceramides, and gangliosides can shift extensively between setups using the chromatographic conditions presented.

Each dMRM transition can correspond to one or more lipid species. The integration parameters used are available online (https://metabolomics.baker.edu.au/). For a more detailed, step-by-step description of the quantitation strategy and Quant method that covers > 1,300 lipids, request supporting documentation from Agilent.

Results and discussion

Extension of chromatographic method

To address the higher proportion and diversity of glycerophospholipids, including the various, more nonpolar compounds like triglycerides or cholesteryl esters that are present in human tissues compared to plasma and serum, the LC gradient was adjusted to extend the phospholipid section of the chromatogram (Figure 1). The extended gradient enhanced separation and coverage of the longer glycerophospholipids present in the tissues (Figures 2 and 3).

Structural annotation

Structural annotation of lipid species based on mass, fragmentation, and chromatography has been reported.[2] In general, single or even multiple MRM transitions often do not provide sufficient structural information for a given lipid species, particularly glycerophospholipids. There are many ways to handle this, each with limitations. The authors used a series of offline experiments conducted on a representative pooled brain sample to provide additional identification of the lipid structures at specific retention times. The following strategy provides a framework to follow for other users to create tissue-specific methods for their laboratory.

Glycerophospholipids pool definition: Major mammalian glycerophospholipids including phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylinositol (PI), phosphatidylserine (PS), phosphatidylglycerol (PG) and phosphatidic acid (PA) were considered for the study. Additional lipid subclasses of interest included plasmanyl (e.g. PE O) and plasmenyl (e.g. PE P) derivatives with a fatty alcohol or enol alcohol in the *sn1* position. To systematically identify the lipid species in any given sample, a series of MRM methods, each containing a large list of MRM parameters covering the lipid classes with all major feasible acyl sum compositions (i.e. 20 to 50 carbons, 0 to 12 double bonds), was used to define the detectable glycerophospholipids. The list of MRM transitions was built using the class-specific fragmentation characteristics (e.g. neutral losses and headgroup fragments) shown in Table 4. Defining the glycerophospholipids pool for consideration is essential for tissue samples not previously profiled, because their lipid diversity can vary dramatically (Figure 2).

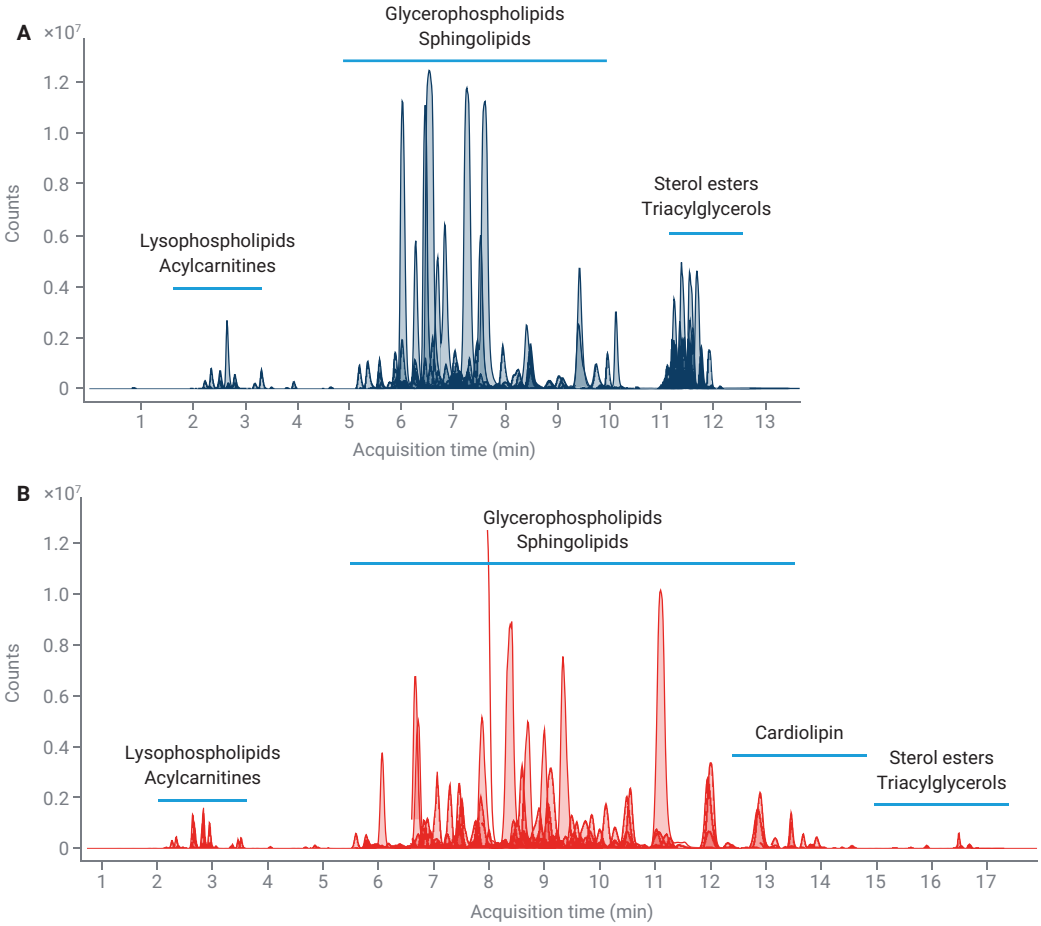

Figure 2. Representative dMRM chromatograms. (A) Pooled plasma sample (blue) analyzed using a shorter plasma-lipid chromatographic gradient[1], and (B) a pooled brain homogenate run using the extended gradient (red).

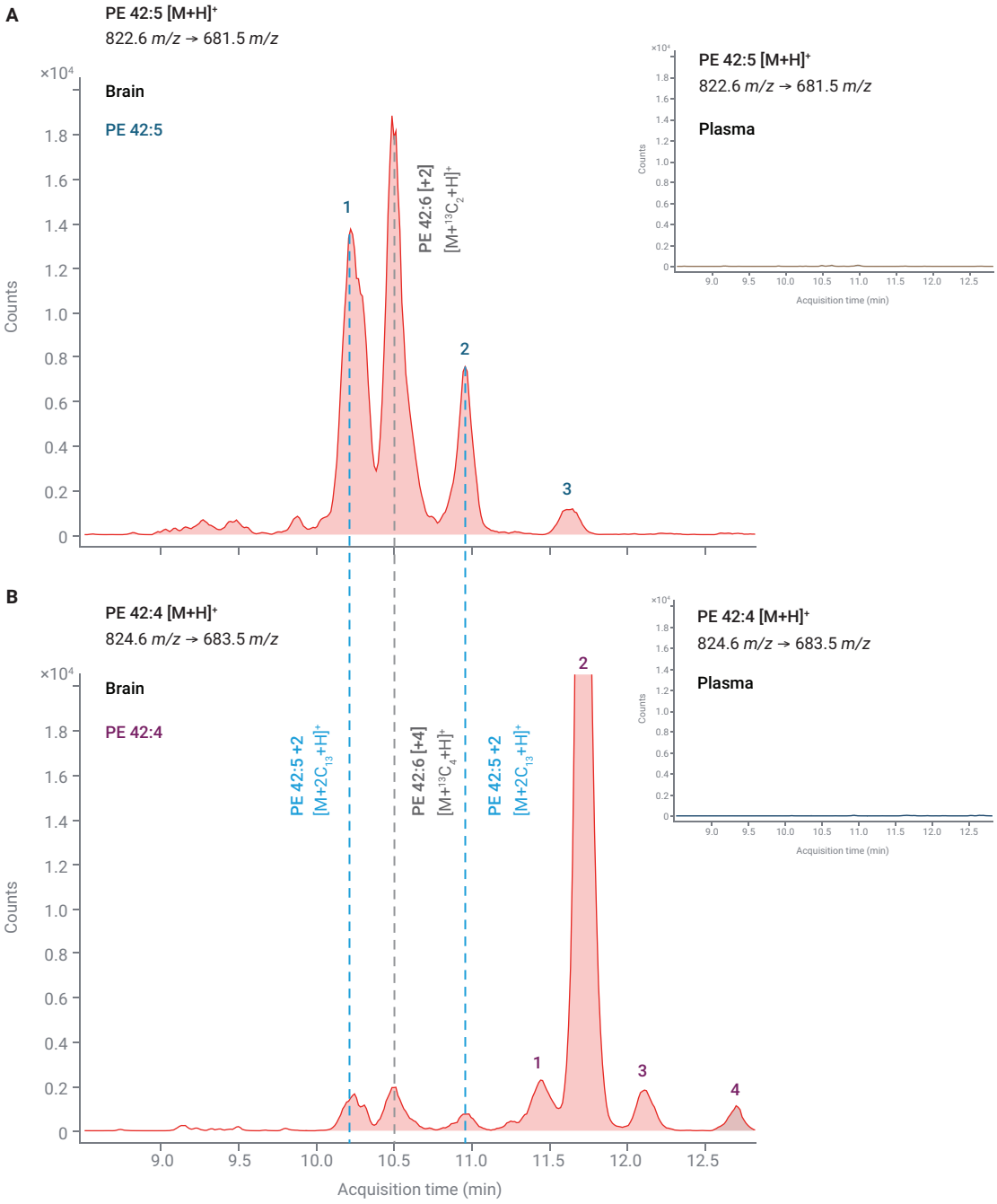

Figure 3. Increased lipid diversity in mammalian tissues in comparison to plasma and serum. Lipid diversity is greater in brain samples than in plasma. In brain, the PE 42:5 (A), which exists in high abundance, results in three distinct isomers that overlap with isotopic species arising from PE 42:4 (B). In plasma (insets), these lipids exist in negligible quantities. The multiple peaks (labeled 1–4) correspond to lipid isomers of the PE species.

Table 4. Lipid class ionization and fragmentation information used to define the detectable glycerophospholipids pools.

Lipid Class/Subclass	Abbreviation	Parent Ion	Fragmentation[1]	Internal Standard	Internal Standard (pmol)/Sample
Sphingosine	Sph	$[M + H]^+$	NL, 18.0 Da	SPB 17:1;O2 [IS]	20
Sphingosine-1-phosphate	S1P	$[M + H]^+$	sphingoid base specific	SPBP 18:1;O2 [D7]	40
Dihydroceramide	dhCer	$[M + H]^+$	sphingoid base specific	Cer 18:0;O2/8:0 [IS]	50
Ceramide	Cer	$[M + H]^+$	sphingoid base specific	Cer 18:1;O2 [D7]/18:0	50
Deoxyceramide	deoxyCer	$[M + H]^+$	sphingoid base specific	Cer 18:1;O2 [D7]/18:0	50
Ceramide-1-phosphate	C1P	$[M + H]^+$	sphingoid base specific	Cer 18:1;O2 [D7]/18:0	50
Monohexosylceramide	HexCer	$[M + H]^+$	sphingoid base specific	HexCer 18:1;O2 [D7]/15:0	50
Dihexosylceramide	Hex2Cer	$[M + H]^+$	sphingoid base specific	Hex2Cer 18:1;O2 [D7]/15:0	50
Trihexosylcermide	Hex3Cer	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GM3 ganglioside	GM3	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GM3 ganglioside	GM3	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GM1 ganglioside	GM1	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GD3 ganglioside	GD3	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GD2 ganglioside	GD2	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GD1 ganglioside	GD1	$[M + H]^+$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
GT1 ganglioside	GT1	$[M + 2H]^{2+}$	sphingoid base specific	Hex3Cer 18:1;O2/17:0 [IS]	50
Sulfatide	SHexCer	$[M + H]^+$	PI, *m/z* 264.3	SHexCer 18:1;O2/12:0 [IS]	10
Sphingomyelin	SM	$[M + H]^+$	PI, *m/z* 184.1	SM [D9] 18:1;O2/15:0	100
Phosphatidic acid	PA	$[M + H]^+$	NL, 115.0 Da	PA 15:0_18:1 [D7]	50
Alkylphosphatidic acid	PA O	$[M + H]^+$	NL, 115.0 Da	PA 15:0_18:1 [D7]	50
Phosphatidylcholine	PC	$[M + H]^+$	PI, *m/z* 184.1	PC 15:0_18:1 [D7]	100
Alkylphosphatidylcholine	PC O	$[M + H]^+$	PI, *m/z* 184.1	PC 15:0_18:1 [D7]	100
Alkenylphosphatidylcholine	PC P	$[M + H]^+$	PI, *m/z* 184.1	PC P-18:0/18:1 [D9]	100
Oxidized Phosphatidylcholine	oxPC	$[M + H]^+$	PI, *m/z* 184.1	PC 15:0_18:1 [D7]	100
Oxidized Alkylphosphatidylcholine	oxPC O	$[M + H]^+$	PI, *m/z* 184.1	PC 15:0_18:1 [D7]	100
Lysophosphatidylcholine	LPC	$[M + H]^+$	PI, *m/z* 184.1 and *m/z* 104.1	LPC 18:1 [D7]	100
Lysoalkylphosphatidylcholine	LPC O	$[M + H]^+$	PI, *m/z* 104.1	LPC 18:1 [D7]	100
Lysoalkenylphosphatidylcholine	LPC P	$[M + H]^+$	PI, *m/z* 104.1	LPC 18:1 [D7]	100
Phosphatidylethanolamine	PE	$[M + H]^+$	NL, 141.0 Da	PE 15:0_18:1 [D7]	100
Alkylphosphatidylethanolamine	PE O	$[M + H]^+$	NL, 141.0 Da	PE 15:0_18:1 [D7]	100
Alkenylphosphatidylethanolamine	PE P	$[M + H]^+$	Acyl chain specific	PE P-18:0/18:1 [D9]	100
Oxidized Phosphatidylethanolamine	oxPE	$[M + H]^+$	NL, 141.0 Da	PE 15:0_18:1 [D7]	100
Lysophosphatidylethanolamine	LPE	$[M + H]^+$	NL, 141.0 Da	LPE 18:1 [D7]	100
Lysoalkylphosphatidylethanolamine	LPE O	$[M + H]^+$	NL, 141.0 Da	LPE 18:1 [D7]	100
Lysoalkenylphosphatidylethanolamine	LPE P	$[M + H]^+$	NL, 171.9 Da	LPE 18:1 [D7]	100
Phosphatidylinositol	PI	$[M + NH_4]^+$	NL, 277.0 Da	PI 15:0_18:1 [D7]	50
Phosphatidylinositol monophosphate	PIP1	$[M + NH_4]^+$	NL, 357.0 Da	PI 15:0_18:1 [D7]	50
Lysophosphatidylinositol	LPI	$[M + NH_4]^+$	NL, 277.0 Da	LPI 13:0 [IS]	20
Phosphatidylserine	PS	$[M + H]^+$	NL, 185.0 Da	PS 15:0_18:1 [D7]	50
Phosphatidylglycerol	PG	$[M + NH_4]^+$	NL, 189.0 Da	PG 15:0_18:1 [D7]	50
Cholesteryl ester	CE	$[M + NH_4]^+$	PI, *m/z* 369.3	CE 18:0 [D6]	1,000
Free Cholesterol	COH	$[M + NH_4]^+$ In-source fragment	PI, *m/z* 161.2	COH [D7]	10,000
Free fatty acid	FFA	$[M - H]^-$	SIM	FFA 18:1 [D9]	200
Acylcarnitine	AC	$[M + H]^+$	PI, *m/z* 85.1	AC 16:0 [D3]	10

Lipid Class/Subclass	Abbreviation	Parent Ion	Fragmentation[1]	Internal Standard	Internal Standard (pmol)/Sample
Hydroxylated Acylcarnitine	AC;O	$[M + H]^+$	PI, *m/z* 85.1	AC 16:0 [D3]	10
Bismonoacylglycerophosphate	BMP	$[M + H]^+$	Species-dependent	BMP 14:0_14:0 [IS]	50
Diacylglycerol	DG	$[M + NH_4]^+$	NL, fatty acid	DG 15:0_18:1 [D7]	200
Alkylacylglycerol	DG O	$[M + NH_4]^+$	NL, alkyl chain	DG 15:0_18:1 [D7]	200
Triacylglycerol	TG [NL]	$[M + NH_4]^+$	NL, fatty acid	TG 15:0_15:0_18:1 [D7]	100
Alkyldiacylglycerol	TG O [NL]	$[M + NH_4]^+$	NL, fatty acid	TG 15:0_15:0_18:1 [D7]	100
Alkenyldiacylglycerol	TG P [NL]	$[M + NH_4]^+$	NL, alkenyl specific	TG 15:0_15:0_18:1 [D7]	100
Caridolipin	CL	$[M + NH_4]^+$	Phosphatdic acid	CL 14:0_14:0_14:0_14:0 [IS]	50
Coenzyme Q10	CoQ10	$[M + NH_4]^+$	PI, *m/z* 197.0	Hex3Cer 18:1;O2/17:0 [IS]	50

[1]NL = neutral loss, PI = precursor ion, SIM = single ion monitoring.

Overcoming glycerophospholipid isotopic and isobaric overlap: Because carbon exists as ^{13}C with a natural abundance of approximately 1.1%, many of the chromatographic peaks observed can arise from isotopic species. For unit resolution mass analyses, these isotopic species can make it difficult to identify the correct chromatographic peak for integration. This effect is particularly problematic for phosphatidylcholine and sphingomyelin species, owing to their large concentration ranges across tissue types. As an example, the multiple ^{13}C isotopes of PC 36:2 and single ^{13}C isotope of SM 40:1;O2 can be observed in the PC 36:1 transition at a different retention time.

To expedite identification of potential isotopic peaks using a tandem quadrupole mass spectrometer, preceding mass transitions (e.g. 811.5 *m/z* → 184.1 with 812.5 *m/z* → 184.1) can be overlayed to determine the peaks attributable to isotopic interference which can subsequently be excluded (Figure 4). This capability can be accessed and visualized with "Compounds at A Glance" feature in Agilent MassHunter Quantitative Analysis software. The isotopic peak identification experiments were conducted using pooled tissue homogenates, to determine species that exist within the samples. An example is available at https://metabolomics.baker.edu.au.

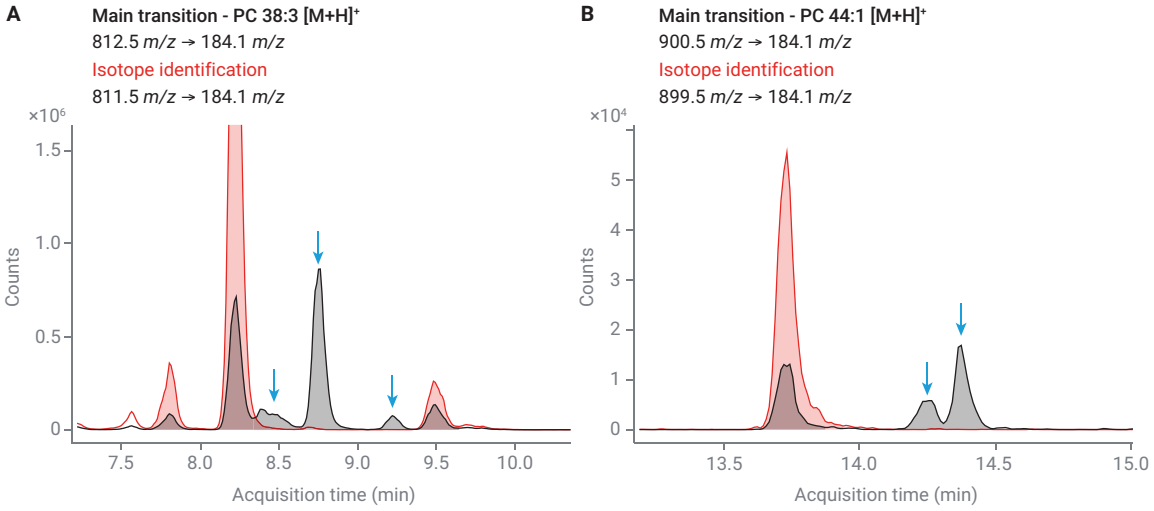

Figure 4. Identification of monoisotopic lipid species using mass offsets for each MRM transition along with chromatography. Extracted ion chromatograms (EICs) of (A) PC 38:3 (812.5 *m/z* → 184.1 *m/z*), black trace, and its preceding mass, 811.5 *m/z* → 184.1 *m/z*, red trace. (B) PC 44:1 (900.5 *m/z* → 184.1 *m/z*), black trace, and its preceding mass, 899.5 *m/z* → 184.1 *m/z*, red trace. Overlaying transitions with the preceding mass enables rapid identification of potential isotopic interferences that are common in lipidomic studies. Blue arrows denote peaks that are chosen as potential lipid isomers of interest for integration.

Alkenyl-glycerophospholipid (Plasmalogen) identification: With unit resolution analysis, many glycerophospholipid subclasses (e.g. phosphatidylcholine PC 33:2, alkylphosphatidylcholine PC O-34:2 and Alkenylphosphatidylcholine PC P-34:1) share similar or identical masses and fragmentation patterns under the experimental conditions presented. Notably, alkyl and alkenyl phosphatidylcholines are isomeric, and share the identical elemental composition. To facilitate rapid identification of plasmenyl species in tissue, a paired analysis with HCl hydrolysis can be conducted. This process involves using a matched lyophilized lipid extract, where one extract is exposed to HCl fumes 15 minutes before it is reconstituted into extraction solvent for injection. The paired samples are then overlayed in MassHunter Quantitative Analysis software for identification and annotation (Figure 5). The results obtained for each lipid are available at https://metabolomics.baker.edu.au.

Glycerophospholipid characterization: Glycerophospholipid characterization was similar to that previously described.[1] PC 36:2, measured using the transition 786.6 *m/z* → 184.1, can elute as two or more peaks which are labelled PC 36:2 [a] and [b] based on retention time. Additional experiments using an orthogonal MRM transition for the PC class, monitoring either in negative ion mode for the formate adduct or in positive ion mode for sodium or lithium adducts, yields product ions specific to the target fatty acids. These approaches have been described for the major lipid classes.[8,9,10] Table 5 lists the adducts and fragments for acyl annotation of lipid classes used for the characterization. Notably, the phosphatidylcholine species (PC, PC O, and PC P) and sphingomyelin (SM) were characterized using the formation of alkali adducts (sodium or lithium). Enhancement of alkali adduct formation was done by post-column infusion of sodium acetate (10 mM in 8:2 water:IPA) or lithium acetate (10 mM in 8:2 water:IPA) at 25 µL/minute. Systematic characterization can be conducted by collision induced dissociation (CID) of the specific precursor ions corresponding to the alkali adduct of the lipids using the LC/TQ instrument, or alternatively, a

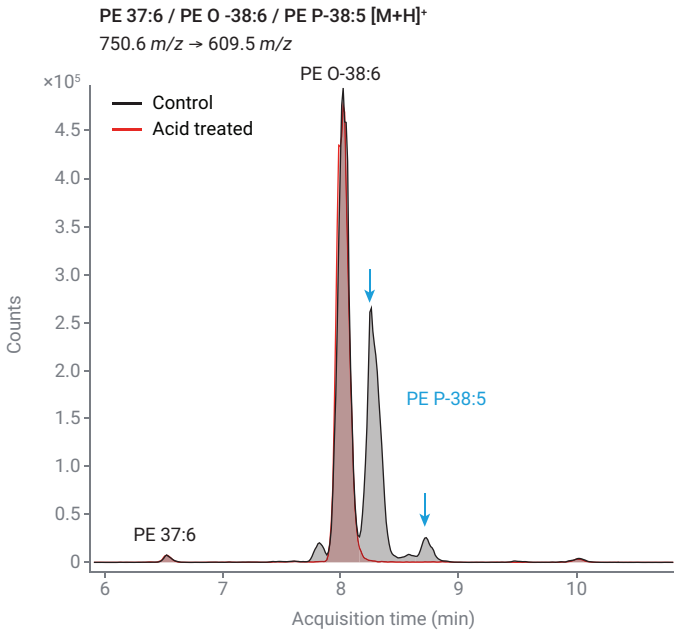

Figure 5. Using acid hydrolysis to characterise ether lipid isomers. Overlaid MRM chromatograms for matched extracts with (red) and without (black) exposure to HCl. Peaks corresponding to the plasmenyl (PE P) species are heavily hydrolysed after HCl exposure, suggesting that PE O-38:6 is the correct lipid annotation for the dominant peak at 8 minutes.

Table 5. Adducts and fragments for acyl annotation of lipid classes.

Lipid Class/Subclass	Abbreviation	Additional Annotation Ion	Annotation Fragmentation	Source
Sphingomyelin	SM	$[M+Na]^+$ or $[M+Li]^+$	sphingoid base specific	doi.org/10.1016/S1044-0305(99)00150-6
Phosphatidic acid	PA	$[M-H]^-$	fatty acyl ion	
Alkylphosphatidic acid	PA O	$[M-H]^-$	fatty acyl ion	
Phosphatidylcholine	PC	$[M+Na]^+$ or $[M+Li]^+$	*sn1* or *sn2* acyl loss	doi.org/10.1016/S1044-0305(03)00064-3
Alkylphosphatidylcholine	PC O	$[M+Na]^+$ or $[M+Li]^+$	*sn2* acyl loss	doi.org/10.1016/S1044-0305(03)00064-3
Alkenylphosphatidylcholine	PC P	$[M+Na]^+$ or $[M+Li]^+$	*sn2* acyl loss	doi.org/10.1016/S1044-0305(03)00064-3
Phosphatidylethanolamine	PE	$[M-H]^-$	fatty acyl ion	
Alkylphosphatidylethanolamine	PE O	$[M-H]^-$	fatty acyl ion	
Phosphatidylinositol	PI	$[M-H]^-$	fatty acyl ion	
Phosphatidylinositol monophosphate	PIP1	$[M-H]^-$	fatty acyl ion	
Phosphatidylserine	PS	$[M-H]^-$	fatty acyl ion	
Phosphatidylglycerol	PG	$[M-H]^-$	fatty acyl ion	
Bismonoacylglycerophosphate	BMP	[M-H]-	fatty acyl ion	

liquid chromatography/quadrupole time-of-flight (LC/Q-TOF) instrument. Many other lipids readily ionize in negative ion mode, resulting in product ions specific to the acyl composition. Using this approach, the authors annotated lipid isomers and isobars by aligning chromatographic peaks by their elution time to the main analytical run. The authors also annotated porcine brain (Avanti, 131101C), the NIST SRM 1950, and brain tissue homogenates. These annotations are available online at (https://metabolomics.baker.edu.au/). In all of these experiments the authors mapped the acyl-chain-specific product ions using an Agilent Revident high-resolution LC/Q-TOF instrument operated in Quadrupole Resolved All Ions (Q-RAI) mode, a type of data-independent acquisition (DIA), in which the quadrupole isolates a wide *m/z* window before ions enter the collision cell, with one or more collision energies associated with each window. Using a 20-Da window size helped reduce the occurrence of interfering acyl chain fragments from outside the isolation window (Figure 6).

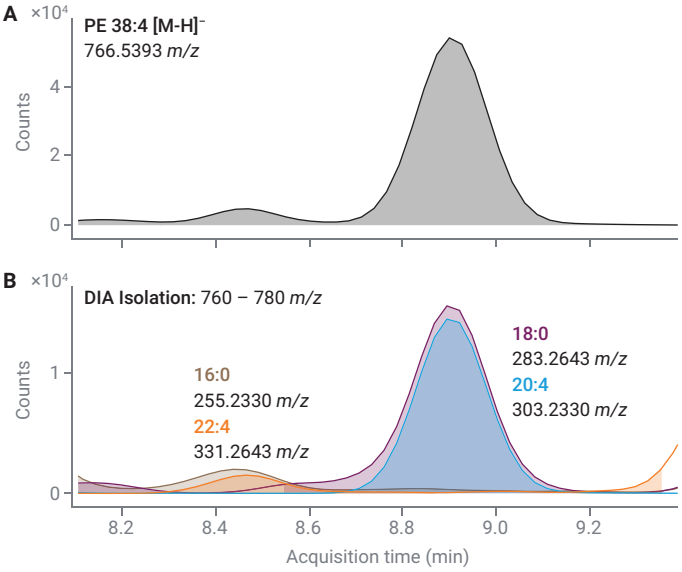

Figure 6. Characterization of phospholipid structures using LC/Q-TOF data independent acquisition. Overlaid EICs for the [M-H]- precursor and predicted acyl-chain fragments corresponding to PE 38:4 are shown.

dMRM performance

Once structural annotation was completed, the LC/TQ dMRM method was finalized and assessed. The densest section of the chromatographic run included 140 transitions, where the shortest dwell time was 1.01 ms. The 6495C LC/TQ maintained excellent precision across the compounds associated with those transitions, even at the relatively short dwell times. The same dMRM method can be used on the 6495D LC/TQ. The enhanced performance of the 6495D LC/TQ allows for even more concurrent MRM transitions while maintaining a minimum cycle time of 0.5 ms, potentially enabling laboratories to target substantially more than 1,300 lipids in a single run.

Lipid nomenclature

The lipid naming convention used throughout the results and discussion follows the guidelines established by the Lipid Maps Consortium and the shorthand notation published by Liebisch *et al.*[6,7,8] 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 (e.g. PC 38:4).

However, where an acyl chain composition has been determined, the naming convention indicates this composition such that an isoform of PC 38:4 is annotated as PC 18:0_20:4. This convention is also extended to other lipid classes and subclasses. When the positions of the fatty acids on the glycerol backbone are known, the convention becomes PC 18:0/20:4 with the 18:0 in the *sn1* position and the 20:4 in the *sn2* position. Species which are separated chromatographically but remain incompletely characterised were labelled 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] represents the elution order.

Assessing and extending linear dynamic range

Initial scouting experiments indicated whether the lipids measured are within their typical linear signal range based on representative samples. Lipid concentrations in tissues, particularly brain, can span several orders of magnitude, even within the same class. To assess linear range, serial injections ranging from 0.2 µL to 5 µL of a pooled sample were analyzed and the peak area over injection volume was examined. The ratio of analyte area to its internal standard can also be used. Injection or extraction volumes can then be adjusted to best suit the linear range for the lipids of interest.

In instances where specific lipid classes (glycerophospholipids, sphingolipids) hit the upper linear dynamic range at low volumes, adjusting the MRM transition to monitor the +2 isotope (e.g. for PC 34:2, 760.5 → 186.1 instead of 758.5 → 184.1) can improve upper signal linearity if detector saturation is the cause. This approach has been described previously.[11] In these instances, the internal standard would need to be measured as the +2 isotope transition as well. Depending on the lipid fragmentation, monitoring the isotope can have a varying degree of signal change. For PC, there are a limited number of carbons on the head group (5/42). Therefore, when using the transition

760.5 → 186.1, the proportional signal observed is based on the probability of two carbon isotopes on PC 34:2, specifically on the phosphocholine head group only. The result is an approximate 100-fold reduction in detector signal. There are many instances where this approach does not benefit linearity, notably with sterols and neutral lipids, which in large concentrations would limit ionization efficiency and potentially saturate the ion source rather than the detector.

Method extension to cell lines and other tissues

Next to plasma lipidomics, lipid profiles from cell lines are of widespread research interest. The brain-tissue-specific method presented encompasses a broader range of transitions and thus could potentially be directly applied to other types of cell lines. Cellular lipid profiles exhibit a high degree of phospholipid heterogeneity and complexity, and in this respect the brain-tissue-optimized method offers benefits compared to the plasma-based lipid method.[1] In the authors' experience, the lipid species annotations generally hold true across different matrices at matched elution times. However, there may be cases where the structural annotations of lipid species made based on brain tissue are inaccurate when extended to cellular lipids. It is the responsibility of the laboratory to confirm the identity of lipids species by orthogonal means when significant differences in lipid profiles influencing biological conclusions are observed. Additionally, there may be cell-line specific lipids that are absent from (not covered by) the brain method that would be missed if it were applied to other tissues. When this is a concern, the method can be fine-tuned to other matrices of interest using the curation strategies presented here.

Conclusion

This application note highlights the considerations and strategies used to modify previously reported plasma lipidomics methodology[1] for use in profiling brain lipids. The resulting LC/TQ method applied an impressive 940 MRM transitions to cover more than 1,300 molecular lipid species. Using monophasic lipid extraction, extended LC separation, and dMRM method optimization, a broad range of lipid species and classes were covered, offering the potential for further extension of the method to additional tissue types and cell lines.

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Appendix

Table A1. Transitions monitored per lipid species and dMRM parameters.

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta RT	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
AC	AC 12:0	FALSE	344.30	Unit	85.10	1.26	1	166	30	5	Positive
AC	AC 12:1	FALSE	342.30	Unit	85.10	1.03	0.6	166	30	5	Positive
AC	AC 13:0 [a/b]	FALSE	358.30	Unit	85.10	1.44	0.8	166	30	5	Positive
AC	AC 14:0	FALSE	372.30	Unit	85.10	1.87	1	166	30	5	Positive
AC	AC 14:0;O	FALSE	388.30	Unit	85.10	1.40	0.8	166	30	5	Positive
AC	AC 14:1	FALSE	370.30	Unit	85.10	1.52	1.2	166	30	5	Positive
AC	AC 14:1;O	FALSE	386.30	Unit	85.10	1.19	0.8	166	30	5	Positive
AC	AC 14:2	FALSE	368.30	Unit	85.10	1.19	1	166	30	5	Positive
AC	AC 16:0	FALSE	400.40	Unit	85.10	2.56	1	166	30	5	Positive
AC	AC 16:0 [D3]	FALSE	403.40	Unit	85.10	2.56	1	166	30	5	Positive
AC	AC 16:0;O	FALSE	416.40	Unit	85.10	2.03	0.6	166	30	5	Positive
AC	AC 16:1	FALSE	398.30	Unit	85.10	2.09	0.8	166	30	5	Positive
AC	AC 16:1;O	FALSE	414.30	Unit	85.10	1.67	0.8	166	30	5	Positive
AC	AC 17:0 [a/b/c]	FALSE	414.40	Unit	85.10	2.96	1	166	30	5	Positive
AC	AC 18:0	FALSE	428.40	Unit	85.10	3.24	0.8	166	30	5	Positive
AC	AC 18:0;O	FALSE	444.40	Unit	85.10	2.72	0.6	166	30	5	Positive
AC	AC 18:1	FALSE	426.40	Unit	85.10	2.74	0.8	166	30	5	Positive
AC	AC 18:1;O	FALSE	442.40	Unit	85.10	2.24	0.8	166	30	5	Positive
AC	AC 18:2	FALSE	424.30	Unit	85.10	2.28	0.8	166	30	5	Positive
AC	AC 20:3 [a/b]	FALSE	450.30	Unit	85.10	2.52	1	166	30	5	Positive
AC	AC 20:3;O	FALSE	466.30	Unit	85.10	2.12	0.8	166	30	5	Positive
AC	AC 20:4	FALSE	448.30	Unit	85.10	2.27	0.8	166	30	5	Positive
AC	AC 22:5	FALSE	474.30	Unit	85.10	1.92	0.8	166	30	5	Positive
AC	AC 22:6	FALSE	472.30	Unit	85.10	2.18	0.8	166	30	5	Positive
AC	AC 24:0	FALSE	512.30	Unit	85.10	5.17	0.8	166	30	5	Positive
AC	AC 24:1	FALSE	510.30	Unit	85.10	4.42	0.8	166	30	5	Positive
BMP	BMP 14:0 14:0 (IS)	FALSE	684.50	Unit	285.20	4.61	1.6	166	20	5	Positive
BMP	BMP 16:0 16:0	FALSE	740.54	Unit	313.27	7.32	1	166	20	5	Positive
BMP	BMP 16:0 18:0	FALSE	768.58	Unit	313.27	8.29	1	166	20	5	Positive
BMP	BMP 16:0 18:1	FALSE	766.56	Unit	313.27	7.40	1	166	20	5	Positive
BMP	BMP 16:1 18:1	FALSE	764.54	Unit	311.26	7.05	1	166	20	5	Positive
BMP	BMP 18:0 18:1	FALSE	794.59	Unit	339.29	8.53	1	166	20	5	Positive
BMP	BMP 18:1 18:1	FALSE	792.60	Unit	339.30	6.15	2	166	20	5	Positive
BMP	BMP 18:1 18:2	FALSE	790.56	Unit	337.27	5.55	1	166	20	5	Positive
BMP	BMP 18:1 22:6	FALSE	838.56	Unit	339.29	5.33	1	166	20	5	Positive
BMP	BMP 18:2 22:6	FALSE	836.54	Unit	337.27	4.80	1	166	20	5	Positive
BMP	BMP 20:4 22:6	FALSE	860.54	Unit	361.27	4.76	1	166	20	5	Positive
BMP	BMP 22:5 22:6	FALSE	886.56	Unit	385.27	5.06	2	166	20	5	Positive
BMP	BMP 22:6 22:6	FALSE	884.54	Unit	385.27	4.64	2	166	20	5	Positive
CE	CE 16:0	FALSE	642.60	Unit	369.30	16.81	0.6	166	10	5	Positive
CE	CE 16:1	FALSE	640.60	Unit	369.30	16.60	0.6	166	10	5	Positive
CE	CE 17:0	FALSE	656.60	Unit	369.30	16.91	0.6	166	10	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
CE	CE 17:1	FALSE	654.60	Unit	369.30	16.70	0.6	166	10	5	Positive
CE	CE 18:0	FALSE	670.70	Unit	369.30	17.05	0.6	166	10	5	Positive
CE	CE 18:0-d6 [IS]	FALSE	676.60	Unit	375.30	17.05	0.6	166	10	5	Positive
CE	CE 18:1	FALSE	668.60	Unit	369.30	16.82	0.6	166	10	5	Positive
CE	CE 18:2	FALSE	666.60	Unit	369.30	16.65	0.6	166	10	5	Positive
CE	CE 18:3	FALSE	664.60	Unit	369.30	16.47	0.6	166	10	5	Positive
CE	CE 20:1	FALSE	696.70	Unit	369.30	17.02	0.6	166	10	5	Positive
CE	CE 20:2	FALSE	694.70	Unit	369.30	16.85	0.6	166	10	5	Positive
CE	CE 20:3	FALSE	692.60	Unit	369.30	16.68	0.6	166	10	5	Positive
CE	CE 20:4	FALSE	690.60	Unit	369.30	16.54	0.6	166	10	5	Positive
CE	CE 20:5	FALSE	688.60	Unit	369.30	16.35	0.6	166	10	5	Positive
CE	CE 22:4	FALSE	718.70	Unit	369.30	16.72	0.6	166	10	5	Positive
CE	CE 22:5	FALSE	716.60	Unit	369.30	16.62	0.6	166	10	5	Positive
CE	CE 22:6	FALSE	714.60	Unit	369.30	16.46	0.6	166	10	5	Positive
oxCE	CE 22:6;O	FALSE	730.60	Unit	369.30	14.86	1	166	10	5	Positive
CE	CE 24:4	FALSE	746.70	Unit	369.30	16.90	0.6	166	10	5	Positive
CE	CE 24:5	FALSE	744.70	Unit	369.30	16.76	0.6	166	10	5	Positive
Cer	Cer 16:1;O2/20:0	FALSE	566.60	Unit	236.30	10.48	1	166	35	5	Positive
Cer	Cer 16:1;O2/22:0	FALSE	594.60	Unit	236.30	12.30	1	166	35	5	Positive
Cer	Cer 16:1;O2/23:0	FALSE	608.60	Unit	236.30	13.19	1	166	35	5	Positive
Cer	Cer 16:1;O2/24:0	FALSE	622.60	Unit	236.30	13.64	1	166	35	5	Positive
Cer	Cer 16:1;O2/24:1	FALSE	620.60	Unit	236.30	12.37	1	166	35	5	Positive
Cer	Cer 17:1;O2/16:0	FALSE	524.60	Unit	250.30	8.00	1	166	35	5	Positive
Cer	Cer 17:1;O2/18:0 [a/b]	FALSE	552.60	Unit	250.30	9.58	1.2	166	35	5	Positive
Cer	Cer 17:1;O2/20:0	FALSE	580.60	Unit	250.30	11.33	1	166	35	5	Positive
Cer	Cer 17:1;O2/23:0	FALSE	622.60	Unit	250.30	13.60	1	166	35	5	Positive
Cer	Cer 17:1;O2/24:0	FALSE	636.60	Unit	250.30	13.98	1	166	35	5	Positive
Cer	Cer 17:1;O2/24:1 [a/b]	FALSE	634.60	Unit	250.30	13.16	1	166	35	5	Positive
DeoxyCer	Cer 18:0;O/18:0	FALSE	552.60	Unit	268.40	12.24	1	166	35	5	Positive
DeoxyCer	Cer 18:0;O/20:0	FALSE	580.60	Unit	268.40	13.59	0.6	166	35	5	Positive
DeoxyCer	Cer 18:0;O/22:0	FALSE	608.60	Unit	268.40	14.31	0.6	166	35	5	Positive
DeoxyCer	Cer 18:0;O/23:0	FALSE	622.60	Unit	268.40	14.64	0.6	166	35	5	Positive
DeoxyCer	Cer 18:0;O/24:0	FALSE	636.60	Unit	268.40	14.93	0.6	166	35	5	Positive
DeoxyCer	Cer 18:0;O/24:1	FALSE	634.60	Unit	268.40	14.34	0.6	166	35	5	Positive
dhCer	Cer 18:0;O2/16:0 [a/b]	FALSE	540.50	Unit	284.30	9.30	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/18:0 [a/b]	FALSE	568.60	Unit	284.30	11.04	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/20:0 [a/b]	FALSE	596.60	Unit	284.30	12.88	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/22:0 [a/b]	FALSE	624.60	Unit	284.30	13.85	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/24:0 [a/b]	FALSE	652.70	Unit	284.30	14.53	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/24:1 [a/b]	FALSE	650.60	Unit	284.30	13.86	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/26:0 [a/b]	FALSE	680.70	Unit	284.30	15.14	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/26:1 [a/b]	FALSE	678.60	Unit	284.30	14.51	1.2	166	35	4	Positive
dhCer	Cer 18:0;O2/8:0 [IS]	FALSE	428.60	Unit	284.30	4.79	1.2	166	35	4	Positive
DeoxyCer	Cer 18:1;O/18:0 [a/b]	FALSE	550.60	Unit	266.40	10.80	1.2	166	35	5	Positive
DeoxyCer	Cer 18:1;O/20:0 [a/b]	FALSE	578.60	Unit	266.40	12.60	1.2	166	35	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
DeoxyCer	Cer 18:1;O/22:0 [a/b]	FALSE	606.60	Unit	266.40	13.75	1.2	166	35	5	Positive
DeoxyCer	Cer 18:1;O/23:0 [a/b]	FALSE	620.60	Unit	266.40	14.10	1.2	166	35	5	Positive
DeoxyCer	Cer 18:1;O/24:0 [a/b]	FALSE	634.60	Unit	266.40	14.44	1.2	166	35	5	Positive
DeoxyCer	Cer 18:1;O/24:1 [a/b]	FALSE	632.60	Unit	266.40	13.58	1.2	166	35	5	Positive
Cer	Cer 18:1;O2 [d7]/18:0	FALSE	573.60	Unit	271.40	10.32	1.5	166	25	5	Positive
Cer	Cer 18:1;O2/14:0	FALSE	510.50	Unit	264.30	7.28	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/16:0	FALSE	538.50	Unit	264.30	8.70	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/18:0	FALSE	566.60	Unit	264.30	10.38	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/19:0	FALSE	580.60	Unit	264.30	11.25	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/20:0	FALSE	594.60	Unit	264.30	12.17	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/21:0	FALSE	608.60	Unit	264.30	13.08	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/22:0	FALSE	622.60	Unit	264.30	13.57	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/23:0	FALSE	636.60	Unit	264.30	13.95	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/24:0	FALSE	650.60	Unit	264.30	14.28	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/24:1	FALSE	648.60	Unit	264.30	13.58	0.8	166	25	5	Positive
Cer	Cer 18:1;O2/26:0	FALSE	678.60	Unit	264.30	12.09	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/14:0	FALSE	508.50	Unit	262.30	6.30	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/16:0	FALSE	536.50	Unit	262.30	7.57	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/18:0	FALSE	564.60	Unit	262.30	9.06	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/20:0	FALSE	592.60	Unit	262.30	10.76	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/21:0	FALSE	606.60	Unit	262.30	11.68	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/22:0	FALSE	620.60	Unit	262.30	12.65	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/23:0	FALSE	634.60	Unit	262.30	13.38	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/24:0	FALSE	648.60	Unit	262.30	13.76	0.8	166	25	5	Positive
Cer	Cer 18:2;O2/24:1	FALSE	646.60	Unit	262.30	12.71	0.8	166	25	5	Positive
Cer	Cer 19:1;O2/18:0 [a/b]	FALSE	580.60	Unit	278.30	11.23	1	166	25	5	Positive
Cer	Cer 19:1;O2/20:0	FALSE	608.60	Unit	278.30	13.07	1	166	25	5	Positive
Cer	Cer 19:1;O2/24:1	FALSE	662.60	Unit	278.30	13.93	1.2	166	25	5	Positive
Cer	Cer 20:1;O2/18:0	FALSE	594.60	Unit	292.30	12.15	0.8	166	25	5	Positive
Cer	Cer 20:1;O2/22:0	FALSE	650.60	Unit	292.30	14.25	0.8	166	25	5	Positive
Cer	Cer 20:1;O2/23:0	FALSE	664.60	Unit	292.30	14.57	0.8	166	25	5	Positive
Cer	Cer 20:1;O2/24:0	FALSE	678.60	Unit	292.30	14.87	0.8	166	25	5	Positive
Cer	Cer 20:1;O2/24:1	FALSE	676.60	Unit	292.30	14.26	0.8	166	25	5	Positive
CL	CL 14:0_14:0_14:0_14:0 [IS]	FALSE	1258.10	Unit	495.50	13.96	0.8	166	35	4	Positive
CL	CL 68:2 [PI-34:1]	FALSE	1423.01	Unit	577.50	15.71	0.8	166	35	4	Positive
CL	CL 70:3 [PI-34:1]	FALSE	1449.01	Unit	577.50	15.76	0.8	166	35	4	Positive
CL	CL 70:4 [PI-34:1]	FALSE	1447.01	Unit	577.50	15.48	0.8	166	35	4	Positive
CL	CL 70:4 [PI-36:2]	FALSE	1447.01	Unit	603.50	15.46	0.8	166	35	4	Positive
CL	CL 70:5 [PI-36:3]	FALSE	1445.01	Unit	601.50	15.17	0.8	166	35	4	Positive
CL	CL 72:4 [PI-36:2]	FALSE	1475.01	Unit	603.50	15.81	0.8	166	35	4	Positive
CL	CL 72:4 [PI-36:3]	FALSE	1475.01	Unit	601.50	15.81	0.8	166	35	4	Positive
CL	CL 72:5 [PI-34:1] [a/b]	FALSE	1473.01	Unit	577.50	15.77	1.5	166	35	4	Positive
CL	CL 72:5 [PI-36:2]	FALSE	1473.01	Unit	603.50	15.53	0.8	166	35	4	Positive
CL	CL 72:5 [PI-36:3]	FALSE	1473.01	Unit	601.50	15.53	0.8	166	35	4	Positive
CL	CL 72:5 [PI-38:4]	FALSE	1473.01	Unit	627.50	15.77	0.8	166	35	4	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
CL	CL 72:6 [PI-34:1]	FALSE	1471.01	Unit	577.50	15.45	0.8	166	35	4	Positive
CL	CL 72:6 [PI-36:2] [a/b]	FALSE	1471.01	Unit	603.50	15.27	1	166	35	4	Positive
CL	CL 72:6 [PI-36:3]	FALSE	1471.01	Unit	601.50	15.25	1	166	35	4	Positive
CL	CL 72:6 [PI-36:4] [a/b]	FALSE	1471.01	Unit	599.50	15.27	1.5	166	35	4	Positive
CL	CL 72:6 [PI-38:4] [a/b]	FALSE	1471.01	Unit	627.50	15.28	1	166	35	4	Positive
CL	CL 72:7 [PI-34:1] [a/b]	FALSE	1469.01	Unit	577.50	15.17	1.5	166	35	4	Positive
CL	CL 72:7 [PI-36:2]	FALSE	1469.01	Unit	603.50	15.14	1	166	35	4	Positive
CL	CL 72:7 [PI-36:3] [a/b]	FALSE	1469.01	Unit	601.50	14.97	1	166	35	4	Positive
CL	CL 72:7 [PI-36:4] [a/b]	FALSE	1469.01	Unit	599.50	14.97	1.5	166	35	4	Positive
CL	CL 72:7 [PI-38:4] [a/b]	FALSE	1469.01	Unit	627.50	14.97	1	166	35	4	Positive
CL	CL 72:8 [PI-36:3]	FALSE	1467.01	Unit	601.50	14.84	1	166	35	4	Positive
CL	CL 72:8 [PI-36:4] [a/b/c]	FALSE	1467.01	Unit	599.50	14.68	1	166	35	4	Positive
CL	CL 74:6 [PI-38:4] [a/b]	FALSE	1499.01	Unit	627.50	15.63	1	166	35	4	Positive
CL	CL 74:7 [PI-36:3] [a/b]	FALSE	1497.01	Unit	601.50	15.35	1	166	35	4	Positive
CL	CL 74:7 [PI-38:4] [a/b]	FALSE	1497.01	Unit	627.50	15.37	1	166	35	4	Positive
CL	CL 74:8 [PI-34:1]	FALSE	1495.01	Unit	577.50	15.34	1	166	35	4	Positive
CL	CL 74:8 [PI-36:4] [a/b]	FALSE	1495.01	Unit	599.50	15.30	1	166	35	4	Positive
CL	CL 74:8 [PI-40:7]	FALSE	1495.01	Unit	649.50	15.34	1	166	35	4	Positive
CL	CL 74:9 [PI-36:3]	FALSE	1493.01	Unit	601.50	14.93	1	166	35	4	Positive
CL	CL 74:9 [PI-36:4] [a/b]	FALSE	1493.01	Unit	599.50	14.94	1	166	35	4	Positive
CL	CL 74:9 [PI-40:7]	FALSE	1493.01	Unit	649.50	15.03	1	166	35	4	Positive
CL	CL 76:10 [PI-38:4] [a/b]	FALSE	1519.01	Unit	627.50	15.03	1	166	35	4	Positive
CL	CL 76:10 [PI-40:7]	FALSE	1519.01	Unit	649.50	15.12	1	166	35	4	Positive
CL	CL 76:11 [PI-40:7] [a/b]	FALSE	1517.01	Unit	649.50	14.83	1	166	35	4	Positive
CL	CL 76:8 [PI-38:4] [a/b]	FALSE	1523.01	Unit	627.50	15.47	1	166	35	4	Positive
CL	CL 76:9 [PI-38:4] [a/b]	FALSE	1521.01	Unit	627.50	15.32	1	166	35	4	Positive
CL	CL 76:9 [PI-40:7]	FALSE	1521.01	Unit	649.50	15.38	1	166	35	4	Positive
COH	COH	FALSE	369.40	Unit	161.20	7.06	0.8	166	20	5	Positive
COH	COH [D7]	FALSE	376.40	Unit	161.20	6.90	0.8	166	20	5	Positive
DG	DG 15:0_18:1 [D7]	FALSE	605.50	Unit	299.50	11.11	1	166	25	4	Positive
DG	DG 16:0_16:1	FALSE	584.50	Unit	313.20	10.32	1	166	25	5	Positive
DG	DG 16:0_18:1	FALSE	612.60	Unit	313.30	12.08	1	166	25	5	Positive
DG	DG 16:0_18:2	FALSE	610.50	Unit	313.20	10.80	1	166	25	5	Positive
DG	DG 16:0_20:4	FALSE	634.50	Unit	313.20	10.61	1	166	25	5	Positive
DG	DG 16:0_22:5	FALSE	660.60	Unit	313.30	11.30	2	166	25	5	Positive
DG	DG 16:0_22:6	FALSE	658.50	Unit	313.20	10.24	1	166	25	5	Positive
DG	DG 16:1_18:1	FALSE	610.50	Unit	339.20	10.60	2	166	25	5	Positive
DG	DG 18:0_18:1	FALSE	640.60	Unit	341.30	13.50	0.8	166	25	5	Positive
DG	DG 18:0_18:2	FALSE	638.60	Unit	341.30	12.60	1	166	25	5	Positive
DG	DG 18:0_20:4	FALSE	662.60	Unit	341.30	12.42	1	166	25	5	Positive
DG	DG 18:1_18:1	FALSE	638.60	Unit	339.30	12.32	1	166	25	5	Positive
DG	DG 18:1_18:2	FALSE	636.60	Unit	339.30	11.05	1	166	25	5	Positive
DG	DG 18:1_20:4	FALSE	660.60	Unit	339.30	10.83	1	166	25	5	Positive
DG	DG 18:2_18:2	FALSE	634.50	Unit	337.20	9.83	1	166	25	5	Positive
DG	DG 18:2_20:4	FALSE	658.50	Unit	337.20	9.65	0.8	166	25	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
DG O	DG O-16:0_16:0	FALSE	572.50	Unit	313.20	13.65	0.8	166	25	4	Positive
DG O	DG O-16:0_18:1	FALSE	598.50	Unit	339.20	13.62	0.8	166	25	4	Positive
DG O	DG O-16:0_22:6	FALSE	644.50	Unit	385.20	11.86	0.8	166	25	4	Positive
DG O	DG O-18:0_20:4	FALSE	648.50	Unit	361.20	13.76	0.8	166	25	4	Positive
DG O	DG O-18:1_16:0	FALSE	598.50	Unit	313.20	13.56	0.8	166	25	4	Positive
DG O	DG O-18:1_20:4	FALSE	646.50	Unit	361.20	13.63	0.8	166	25	4	Positive
DG O	DG O-18:1_22:6	FALSE	670.50	Unit	385.20	13.39	0.8	166	25	4	Positive
FFA	FFA 18:0	FALSE	283.30	Unit	283.30	4.57	0.7	166	0	4	Negative
FFA	FFA 18:1	FALSE	281.30	Unit	281.20	3.97	0.7	166	0	4	Negative
FFA	FFA 18:1-d9 [IS]	FALSE	290.30	Unit	290.20	3.94	0.7	166	0	4	Negative
FFA	FFA 18:2	FALSE	279.20	Unit	279.20	3.53	0.7	166	0	4	Negative
FFA	FFA 20:2	FALSE	307.30	Unit	307.30	4.18	0.7	166	0	4	Negative
FFA	FFA 20:3 [a/b]	FALSE	305.30	Unit	305.20	3.74	0.7	166	0	4	Negative
FFA	FFA 20:4	FALSE	303.20	Unit	303.20	3.45	0.7	166	0	4	Negative
FFA	FFA 20:4-d11 [IS]	FALSE	314.20	Unit	314.20	3.44	0.7	166	0	4	Negative
FFA	FFA 20:5	FALSE	301.20	Unit	301.20	2.73	0.7	166	0	4	Negative
FFA	FFA 22:4	FALSE	331.30	Unit	331.30	3.96	0.7	166	0	4	Negative
FFA	FFA 22:5 [a/b]	FALSE	329.30	Unit	329.20	3.68	1	166	0	4	Negative
FFA	FFA 22:6	FALSE	327.20	Unit	327.20	3.30	0.7	166	0	4	Negative
FFA	FFA 22:6-d5 [IS]	FALSE	332.20	Unit	332.20	3.29	0.7	166	0	4	Negative
GD1	GD1 18:1;O2/18:0	FALSE	1837.98	Unit	264.30	4.81	1	166	63	4	Positive
GD1	GD1 18:1;O2/20:0	FALSE	1865.98	Unit	264.30	5.54	1	166	63	4	Positive
GD1	GD1 20:1;O2/18:0	FALSE	1865.98	Unit	292.30	5.67	1	166	63	4	Positive
GD1	GD1 20:1;O2/20:0	FALSE	1893.98	Unit	292.30	6.67	1	166	63	4	Positive
GD2	GD2 18:1;O2/18:0	FALSE	1675.93	Unit	264.30	4.80	1	166	63	4	Positive
GD2	GD2 20:1;O2/18:0	FALSE	1703.93	Unit	292.30	5.30	1	166	63	4	Positive
GD2	GD2 18:1;O2/20:0	FALSE	1703.93	Unit	264.30	5.30	1	166	63	4	Positive
GD2	GD2 20:1;O2/20:0	FALSE	1731.93	Unit	292.30	6.00	1	166	63	4	Positive
GD3	GD3 18:1;O2/18:0	FALSE	1472.85	Unit	264.30	5.10	1	166	63	4	Positive
GD3	GD3 18:1;O2/20:0	FALSE	1500.85	Unit	264.30	6.00	1	166	63	4	Positive
GD3	GD3 20:1;O2/18:0	FALSE	1500.85	Unit	292.30	6.00	1	166	63	4	Positive
GD3	GD3 20:1;O2/20:0	FALSE	1528.85	Unit	292.30	6.80	1	166	63	4	Positive
GM1	GM1 18:1;O2/18:0	FALSE	1546.88	Unit	264.30	5.58	1	166	63	4	Positive
GM1	GM1 20:1;O2/18:0	FALSE	1574.92	Unit	292.30	6.51	1	166	63	4	Positive
GM2	GM2 18:1;O2/18:0	FALSE	1384.83	Unit	264.30	5.78	1	166	63	4	Positive
GM2	GM2 18:1;O2/20:0	FALSE	1412.83	Unit	264.30	6.77	1	166	63	4	Positive
GM2	GM2 20:1;O2/18:0	FALSE	1412.83	Unit	292.30	6.74	1	166	63	4	Positive
GM2	GM2 20:1;O2/20:0	FALSE	1440.83	Unit	292.30	7.91	1	166	63	4	Positive
GM3	GM3 18:1;O2/16:0	FALSE	1153.70	Unit	264.30	4.41	1	166	63	5	Positive
GM3	GM3 18:1;O2/18:0	FALSE	1181.80	Unit	264.30	5.95	1	166	63	5	Positive
GM3	GM3 18:1;O2/20:0	FALSE	1209.80	Unit	264.30	7.00	1	166	63	5	Positive
GM3	GM3 18:1;O2/22:0	FALSE	1237.80	Unit	264.30	8.21	1	166	63	5	Positive
GM3	GM3 18:1;O2/24:0	FALSE	1265.80	Unit	264.30	9.65	1	166	63	5	Positive
GM3	GM3 18:1;O2/24:1	FALSE	1263.80	Unit	264.30	8.19	1	166	63	5	Positive
GM3	GM3 20:1;O2/18:0	FALSE	1209.80	Unit	292.30	6.50	1	166	63	5	Positive
GM3	GM3 20:1;O2/20:0	FALSE	1237.80	Unit	292.30	7.80	1	166	63	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
GT1	GT1 18:1;O2/18:0 [a/b]	FALSE	1065.04	Unit	264.30	4.41	0.8	166	63	4	Positive
GT1	GT1 18:1;O2/20:0 [a/b]	FALSE	1079.05	Unit	264.30	5.03	0.8	166	63	4	Positive
GT1	GT1 20:1;O2/18:0 [a/b]	FALSE	1079.04	Unit	292.30	5.00	0.8	166	63	4	Positive
GT1	GT1 20:1;O2/20:0 [a/b]	FALSE	1093.05	Unit	292.30	5.78	0.8	166	63	4	Positive
Hex2Cer	Hex2Cer 18:1;O2 [D7]/15:0	FALSE	855.60	Unit	271.30	5.95	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/16:0	FALSE	862.60	Unit	264.30	6.50	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/18:0	FALSE	890.70	Unit	264.30	7.74	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/20:0 [a/b]	FALSE	918.70	Unit	264.30	9.20	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/22:0	FALSE	946.70	Unit	264.30	10.79	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/24:0	FALSE	974.80	Unit	264.30	12.57	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:1;O2/24:1	FALSE	972.70	Unit	264.30	10.80	0.8	166	49	5	Positive
Hex2Cer	Hex2Cer 18:2;O2/24:1	FALSE	970.70	Unit	262.30	9.60	0.8	166	49	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/17:0 [IS]	FALSE	1038.70	Unit	264.30	6.64	0.8	166	63	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/18:0	FALSE	1052.70	Unit	264.30	7.24	0.8	166	63	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/20:0	FALSE	1080.70	Unit	264.30	8.60	0.8	166	63	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/22:0	FALSE	1108.80	Unit	264.30	10.13	0.8	166	63	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/24:0	FALSE	1136.80	Unit	264.30	11.80	0.8	166	63	5	Positive
Hex3Cer	Hex3Cer 18:1;O2/24:1 [a/b]	FALSE	1134.80	Unit	264.30	10.38	0.8	166	63	5	Positive
Hex-Cer	Hex-Cer 16:1;O2/18:0	FALSE	700.60	Unit	236.30	7.14	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 16:1;O2/20:0	FALSE	728.60	Unit	236.30	8.53	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 16:1;O2/22:0	FALSE	756.70	Unit	236.30	10.17	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 16:1;O2/24:0	FALSE	784.70	Unit	236.30	11.35	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2 [D7]/15:0	FALSE	693.60	Unit	271.30	6.51	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/16:0 [a/b]	FALSE	700.60	Unit	264.30	7.07	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/18:0 [a/b]	FALSE	728.60	Unit	264.30	8.45	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/20:0	FALSE	756.60	Unit	264.30	10.03	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/22:0	FALSE	784.70	Unit	264.30	11.56	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/24:0 [a/b]	FALSE	812.70	Unit	264.30	13.34	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:1;O2/24:1 [a/b]	FALSE	810.70	Unit	264.30	11.79	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:2;O2/18:0 [a/b]	FALSE	726.60	Unit	262.30	7.38	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:2;O2/20:0 [a/b]	FALSE	754.60	Unit	262.30	8.81	0.8	166	35	5	Positive
Hex-Cer	Hex-Cer 18:2;O2/22:0 [a/b]	FALSE	782.70	Unit	262.30	10.44	1.2	166	35	5	Positive
Hex-Cer	Hex-Cer 18:2;O2/24:0 [a/b]	FALSE	810.70	Unit	262.30	12.20	1.2	166	35	5	Positive
LPC	LPC 14:0 [a/b]	FALSE	468.30	Unit	184.10	1.94	1.2	166	20	5	Positive
LPC	LPC 15:0 [a/b]	FALSE	482.30	Unit	184.10	2.43	1.2	166	20	5	Positive
LPC	LPC 16:0 [a/b]	FALSE	496.30	Unit	184.10	2.78	1.2	166	20	5	Positive
LPC	LPC 16:1	FALSE	494.30	Unit	184.10	2.21	1.2	166	20	5	Positive
LPC	LPC 17:0 [a/b/c]	FALSE	510.40	Unit	184.10	3.12	1.2	166	20	5	Positive
LPC	LPC 17:1 [a/b]	FALSE	508.40	Unit	184.10	2.47	1.2	166	20	5	Positive
LPC	LPC 18:0 [a/b]	FALSE	524.40	Unit	184.10	3.43	1.2	166	20	5	Positive
LPC	LPC 18:1 [a/b]	FALSE	522.40	Unit	184.10	2.80	1.2	166	20	5	Positive
LPC	LPC 18:1 [D7]	FALSE	529.40	Unit	184.10	2.91	1.2	166	20	5	Positive
LPC	LPC 18:2 [a/b]	FALSE	520.30	Unit	184.10	2.34	1.2	166	20	5	Positive
LPC	LPC 18:3	FALSE	518.30	Unit	184.10	2.01	1.2	166	20	5	Positive
LPC	LPC 19:0 [a/b]	FALSE	538.40	Unit	184.10	3.69	1.2	166	20	5	Positive
LPC	LPC 19:1 [a/b/c]	FALSE	536.40	Unit	184.10	3.09	1.2	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
LPC	LPC 20:0 [a/b]	FALSE	552.40	Unit	184.10	3.95	1.2	166	20	5	Positive
LPC	LPC 20:1 [a/b]	FALSE	550.40	Unit	184.10	3.49	1.2	166	20	5	Positive
LPC	LPC 20:2 [a/b]	FALSE	548.40	Unit	184.10	2.97	1.2	166	20	5	Positive
LPC	LPC 20:3 [104]	FALSE	546.40	Unit	104.10	2.70	1.2	166	20	5	Positive
LPC	LPC 20:3 [a/b]	FALSE	546.40	Unit	184.10	2.59	1.2	166	20	5	Positive
LPC	LPC 20:4 [a/b]	FALSE	544.30	Unit	184.10	2.32	1.2	166	20	5	Positive
LPC	LPC 20:4;O	FALSE	560.30	Unit	184.10	1.62	1.2	166	20	5	Positive
LPC	LPC 20:5 [a/b]	FALSE	542.30	Unit	184.10	1.92	1.2	166	20	5	Positive
LPC	LPC 22:1 [a/b]	FALSE	578.40	Unit	184.10	4.00	1.2	166	20	5	Positive
LPC	LPC 22:4 [a/b]	FALSE	572.40	Unit	184.10	2.84	1.2	166	20	5	Positive
LPC	LPC 22:5 [104]	FALSE	570.40	Unit	104.10	2.75	1.5	166	20	5	Positive
LPC	LPC 22:5 [a/b]	FALSE	570.40	Unit	184.10	2.64	1.5	166	20	5	Positive
LPC	LPC 22:6 [a/b]	FALSE	568.30	Unit	184.10	2.25	1.2	166	20	5	Positive
oxLPC	LPC 22:6;O	FALSE	584.30	Unit	184.10	1.71	1.2	166	20	5	Positive
LPC	LPC 24:0 [a/b]	FALSE	608.50	Unit	184.10	5.45	1.2	166	20	5	Positive
LPC	LPC 26:0 [a/b]	FALSE	636.50	Unit	184.10	6.53	1.2	166	20	5	Positive
LPC O	LPC O-16:0	FALSE	482.40	Unit	104.10	2.43	1.4	166	25	5	Positive
LPC O	LPC O-18:0	FALSE	510.40	Unit	104.10	3.12	1.4	166	25	5	Positive
LPC O	LPC O-18:1 | LPC P-18:0	FALSE	508.40	Unit	104.10	3.64	2	166	25	5	Positive
LPC O	LPC O-20:0	FALSE	538.40	Unit	104.10	4.30	2	166	25	5	Positive
LPC O	LPC O-20:1	FALSE	536.40	Unit	104.10	3.80	2	166	25	5	Positive
LPC O	LPC O-22:0	FALSE	566.50	Unit	104.10	5.01	0.7	166	25	5	Positive
LPC O	LPC O-24:0	FALSE	594.50	Unit	104.10	5.97	0.7	166	25	5	Positive
LPC O	LPC O-24:1 [a/b]	FALSE	592.50	Unit	104.10	5.02	0.8	166	25	5	Positive
LPC P	LPC P-16:0	FALSE	480.30	Unit	104.10	3.06	1	166	25	5	Positive
LPC P	LPC P-18:1	FALSE	506.30	Unit	104.10	3.17	1	166	25	5	Positive
LPE	LPE 16:0 [a/b]	FALSE	454.30	Unit	313.30	2.90	1	166	20	5	Positive
LPE	LPE 17:0 [a/b/c] | LPE O-18:0	FALSE	468.30	Unit	327.30	3.24	2	166	20	5	Positive
LPE	LPE 18:0 [a/b]	FALSE	482.30	Unit	341.30	3.52	1	166	20	5	Positive
LPE	LPE 18:1 [a/b]	FALSE	480.30	Unit	339.30	2.93	1	166	20	5	Positive
LPE	LPE 18:1 [D7]	FALSE	487.30	Unit	346.30	3.02	1	166	20	5	Positive
LPE	LPE 18:2 [a/b/c]	FALSE	478.30	Unit	337.30	2.46	1	166	20	5	Positive
LPE	LPE 20:4 [a/b]	FALSE	502.30	Unit	361.30	2.44	1	166	20	5	Positive
LPE	LPE 22:4 [a/b]	FALSE	530.30	Unit	389.30	2.96	1	166	20	5	Positive
LPE	LPE 22:6 [a/b]	FALSE	526.30	Unit	385.30	2.37	1	166	20	5	Positive
LPE P	LPE P-16:0	FALSE	438.30	Unit	266.40	3.20	0.7	166	20	5	Positive
LPE P	LPE P-18:0	FALSE	466.30	Unit	294.40	3.76	0.7	166	20	5	Positive
LPE P	LPE P-18:1	FALSE	464.30	Unit	292.40	3.32	0.7	166	20	5	Positive
LPE P	LPE P-20:0	FALSE	494.30	Unit	322.40	4.36	0.7	166	20	5	Positive
LPI	LPI 13:0 [IS]	FALSE	548.30	Unit	271.30	1.38	1	166	20	5	Positive
LPI	LPI 18:1 [a/b]	FALSE	616.30	Unit	339.30	2.48	1	166	20	5	Positive
LPI	LPI 20:4 [a/b]	FALSE	638.30	Unit	361.30	1.92	1	166	20	5	Positive
LPS	LPS 18:1 [a/b]	FALSE	524.50	Unit	339.50	2.37	1	166	25	4	Positive
LPS	LPS 22:4 [a/b]	FALSE	574.50	Unit	389.50	2.41	1	166	25	4	Positive
LPS	LPS 22:6 [a/b]	FALSE	570.50	Unit	385.50	1.85	1	166	25	4	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PA | PA O	PA 15:0/18:1 [D7]	FALSE	685.60	Unit	570.60	6.66	2	166	20	4	Positive
PA | PA O	PA 32:1	FALSE	664.60	Unit	549.60	6.20	1	166	20	4	Positive
PA | PA O	PA 34:1	FALSE	692.60	Unit	577.60	7.30	1	166	20	4	Positive
PA | PA O	PA 34:2	FALSE	690.60	Unit	575.60	6.49	1	166	20	4	Positive
PA | PA O	PA 36:1	FALSE	720.60	Unit	605.60	8.67	1	166	20	4	Positive
PA | PA O	PA 36:2 [a/b]	FALSE	718.60	Unit	603.60	7.51	1	166	20	4	Positive
PA | PA O	PA 36:3 [a/b]	FALSE	716.60	Unit	601.60	6.78	1	166	20	4	Positive
PA | PA O	PA 36:4	FALSE	714.60	Unit	599.60	6.44	1	166	20	4	Positive
PA | PA O	PA 37:1 | PA-O 38:1	FALSE	734.60	Unit	619.60	10.75	4	166	20	4	Positive
PA | PA O	PA 37:2 | PA-O 38:2	FALSE	732.60	Unit	617.60	9.85	4	166	20	4	Positive
PA | PA O	PA 37:4	FALSE	728.60	Unit	613.60	7.20	1	166	20	4	Positive
PA | PA O	PA 38:1	FALSE	748.60	Unit	633.60	10.10	1	166	20	4	Positive
PA | PA O	PA 38:2 [a/b]	FALSE	746.60	Unit	631.60	9.20	1	166	20	4	Positive
PA | PA O	PA 38:3 [a/b]	FALSE	744.60	Unit	629.60	8.11	2	166	20	4	Positive
PA | PA O	PA 38:4 [a/b/c]	FALSE	742.60	Unit	627.60	7.61	2	166	20	4	Positive
PA | PA O	PA 38:6	FALSE	738.60	Unit	623.60	6.21	1	166	20	4	Positive
PA | PA O	PA 42:0	FALSE	806.60	Unit	691.60	14.10	1	166	20	4	Positive
PA | PA O	PA 42:1	FALSE	804.60	Unit	689.60	13.30	1	166	20	4	Positive
PA | PA O	PA 42:2	FALSE	802.60	Unit	687.60	12.03	1	166	20	4	Positive
PA | PA O	PA 42:4	FALSE	798.60	Unit	683.60	9.77	1	166	20	4	Positive
PA | PA O	PA 43:1	FALSE	818.60	Unit	703.60	13.70	1	166	20	4	Positive
PA | PA O	PA 44:1	FALSE	832.60	Unit	717.60	14.06	1	166	20	4	Positive
PA | PA O	PA 44:2	FALSE	830.60	Unit	715.60	13.41	1	166	20	4	Positive
PA | PA O	PA 46:2	FALSE	858.60	Unit	743.60	14.15	1	166	20	4	Positive
PA | PA O	PA-O 38:4	FALSE	728.60	Unit	613.60	8.60	1	166	20	4	Positive
PC | PC O | PC P	PC 15:0/18:1 [D7]	FALSE	753.60	Unit	184.10	7.31	1	166	35	5	Positive
PC | PC O | PC P	PC 15:0/18:1 [D7] [+2]	FALSE	755.60	Unit	186.10	7.31	1	166	35	5	Positive
oxPC	PC 21:1;O	FALSE	594.37	Unit	184.10	2.78	3	166	35	4	Positive
oxPC	PC 21:1;O2	FALSE	610.36	Unit	184.10	3.37	3	166	35	4	Positive
oxPC	PC 22:2;O	FALSE	606.37	Unit	184.10	2.89	3.5	166	35	4	Positive
oxPC	PC 22:2;O2	FALSE	622.36	Unit	184.10	3.41	3.5	166	35	4	Positive
oxPC	PC 23:2;O	FALSE	620.38	Unit	184.10	2.89	3.5	166	35	4	Positive
oxPC	PC 23:2;O2	FALSE	636.38	Unit	184.10	2.98	3	166	35	4	Positive
oxPC	PC 23:2;O3	FALSE	652.37	Unit	184.10	2.48	4	166	35	4	Positive
oxPC	PC 23:3;O2	FALSE	634.36	Unit	184.10	3.43	3	166	35	4	Positive
oxPC	PC 23:3;O3 | PC 24:2;O2 | PC 25:1;O	FALSE	650.36	Unit	184.10	3.26	3	166	35	4	Positive
oxPC	PC 24:2;O3 | PC 25:1;O2	FALSE	666.39	Unit	184.10	3.19	3	166	35	4	Positive
PC | PC O | PC P	PC 30:0	FALSE	706.50	Unit	184.10	6.52	1	166	35	5	Positive
PC | PC O | PC P	PC 30:1	FALSE	704.50	Unit	184.10	5.81	1	166	35	5	Positive
PC | PC O | PC P	PC 31:1 [a/b/c]	FALSE	718.50	Unit	184.10	6.50	1	166	35	5	Positive
PC | PC O | PC P	PC 32:0	FALSE	734.50	Unit	184.10	8.18	1	166	35	5	Positive
PC | PC O | PC P	PC 32:1 [a/b]	FALSE	732.50	Unit	184.10	7.00	1	166	35	5	Positive
PC | PC O | PC P	PC 32:2 [a/b]	FALSE	730.50	Unit	184.10	6.10	1	166	35	5	Positive
PC | PC O | PC P	PC 33:0 [a/b]	FALSE	748.50	Unit	184.10	8.50	1.5	166	35	5	Positive
PC | PC O | PC P	PC 33:1	FALSE	746.50	Unit	184.10	7.50	1	166	35	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PC | PC O | PC P	PC O-34:1	FALSE	746.50	Unit	184.10	9.00	1	166	35	5	Positive
PC | PC O | PC P	PC P-34:0	FALSE	746.50	Unit	184.10	10.30	1	166	35	5	Positive
PC | PC O | PC P	PC 33:2	FALSE	744.50	Unit	184.10	6.50	1	166	35	5	Positive
PC | PC O | PC P	PC O-34:2 [a/b/c]	FALSE	744.50	Unit	184.10	8.00	1	166	35	5	Positive
PC | PC O | PC P	PC P-34:1	FALSE	744.50	Unit	184.10	8.90	1.5	166	35	5	Positive
PC | PC O | PC P	PC 34:0 {+2]	FALSE	764.50	Unit	186.10	9.00	1	166	35	5	Positive
PC | PC O | PC P	PC 34:1 [+2]	FALSE	762.50	Unit	186.10	7.93	1.2	166	35	5	Positive
PC | PC O | PC P	PC 34:2 [+2]	FALSE	760.50	Unit	186.10	7.10	1.2	166	35	5	Positive
PC | PC O | PC P	PC 34:2;O2	FALSE	790.50	Unit	184.10	4.02	2.5	166	35	5	Positive
PC | PC O | PC P	PC 34:3	FALSE	756.50	Unit	184.10	6.56	1.5	166	35	5	Positive
PC | PC O | PC P	PC 35:1	FALSE	774.50	Unit	184.10	8.65	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-36:1 [a/b/c]	FALSE	774.50	Unit	184.10	10.70	1.2	166	35	5	Positive
PC | PC O | PC P	PC 35:2	FALSE	772.50	Unit	184.10	7.75	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-36:2 [a/b]	FALSE	772.50	Unit	184.10	9.25	1.2	166	35	5	Positive
PC | PC O | PC P	PC P-36:1	FALSE	772.50	Unit	184.10	10.50	1	166	35	5	Positive
PC | PC O | PC P	PC 35:3 [a/b]	FALSE	770.50	Unit	184.10	6.50	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-36:3 [a/b]	FALSE	770.50	Unit	184.10	8.25	1.2	166	35	5	Positive
PC | PC O | PC P	PC P-36:2	FALSE	770.50	Unit	184.10	9.10	1.1	166	35	5	Positive
PC | PC O | PC P	PC 35:4	FALSE	768.50	Unit	184.10	6.40	1	166	35	5	Positive
PC | PC O | PC P	PC O-36:4 | PC P-36:3	FALSE	768.50	Unit	184.10	8.00	2	166	35	5	Positive
PC | PC O | PC P	PC 36:1 [+2]	FALSE	790.50	Unit	186.10	9.36	1	166	35	5	Positive
PC | PC O | PC P	PC 36:2 [a/b]	FALSE	786.50	Unit	184.10	8.30	1	166	35	5	Positive
PC | PC O | PC P	PC 36:3 [a/b/c] [+2]	FALSE	786.50	Unit	186.10	7.20	2	166	35	5	Positive
PC | PC O | PC P	PC 36:4 [a/b/c] [+2]	FALSE	784.50	Unit	186.10	6.70	2	166	35	5	Positive
PC | PC O | PC P	PC 36:4;O	FALSE	798.50	Unit	184.10	4.90	2	166	35	5	Positive
PC | PC O | PC P	PC 36:4;O2	FALSE	814.50	Unit	184.10	4.00	4	166	35	5	Positive
PC | PC O | PC P	PC 38:2 [a/b/c]	FALSE	814.50	Unit	184.10	8.75	1	166	35	5	Positive
PC | PC O | PC P	PC 36:5 [a/b]	FALSE	780.50	Unit	184.10	6.30	2	166	35	5	Positive
PC | PC O | PC P	PC 36:6	FALSE	778.50	Unit	184.10	5.77	1	166	35	5	Positive
PC | PC O | PC P	PC 37:2	FALSE	800.50	Unit	184.10	9.00	1	166	35	5	Positive
PC | PC O | PC P	PC O-38:2	FALSE	800.50	Unit	184.10	10.50	1	166	35	5	Positive
PC | PC O | PC P	PC P-38:1	FALSE	800.50	Unit	184.10	11.80	1	166	35	5	Positive
PC | PC O | PC P	PC 37:5	FALSE	794.50	Unit	184.10	6.50	1	166	35	5	Positive
PC | PC O | PC P	PC O-38:5 | PC P-38:4 [a/b]	FALSE	794.50	Unit	184.10	8.50	2	166	35	5	Positive
PC | PC O | PC P	PC 37:6	FALSE	792.50	Unit	184.10	6.20	1	166	35	5	Positive
PC | PC O | PC P	PC O-38:6	FALSE	792.50	Unit	184.10	7.79	2	166	35	5	Positive
PC | PC O | PC P	PC 38:3 [a/b/c]	FALSE	812.50	Unit	184.10	8.80	3	166	35	5	Positive
PC | PC O | PC P	PC 38:4 [a/b] [+2]	FALSE	812.50	Unit	186.10	7.90	2	166	35	5	Positive
PC | PC O | PC P	PC 38:5 [a/b] [+2]	FALSE	810.50	Unit	186.10	7.20	2	166	35	5	Positive
PC | PC O | PC P	PC 38:6 [a/b] [+2]	FALSE	808.50	Unit	186.10	6.60	1.2	166	35	5	Positive
PC | PC O | PC P	PC 38:6;O2	FALSE	838.50	Unit	184.10	6.00	3	166	35	5	Positive
PC | PC O | PC P	PC 38:6;O4	FALSE	902.50	Unit	184.10	5.00	3	166	35	5	Positive
PC | PC O | PC P	PC 38:7 [a/b]	FALSE	804.50	Unit	184.10	6.00	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-39:7	FALSE	804.50	Unit	184.10	7.70	1.2	166	35	5	Positive
PC | PC O | PC P	PC 39:4	FALSE	824.50	Unit	184.10	8.50	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-40:4 [a/b] | PC P-40:3	FALSE	824.50	Unit	184.10	10.50	2	166	35	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PC | PC O | PC P	PC 39:6 [a/b/c]	FALSE	820.50	Unit	184.10	7.30	2	166	35	5	Positive
PC | PC O | PC P	PC O-40:6 [a/b]	FALSE	820.50	Unit	184.10	9.00	2	166	35	5	Positive
PC | PC O | PC P	PC 39:7 [a/b]	FALSE	818.50	Unit	184.10	6.30	1	166	35	5	Positive
PC | PC O | PC P	PC O-40:7 [a/b/c]	FALSE	818.50	Unit	184.10	8.20	1.5	166	35	5	Positive
PC | PC O | PC P	PC 40:4 [a/b]	FALSE	838.50	Unit	184.10	9.20	2	166	35	5	Positive
PC | PC O | PC P	PC 40:5 [a/b]	FALSE	836.50	Unit	184.10	8.70	2	166	35	5	Positive
PC | PC O | PC P	PC 40:6 [+2]	FALSE	836.50	Unit	186.10	7.80	2	166	35	5	Positive
PC | PC O | PC P	PC 40:7	FALSE	832.50	Unit	184.10	6.70	1.2	166	35	5	Positive
PC | PC O | PC P	PC 40:8	FALSE	830.50	Unit	184.10	6.00	2	166	35	5	Positive
PC | PC O | PC P	PC 42:0	FALSE	874.50	Unit	184.10	14.30	1	166	35	5	Positive
PC | PC O | PC P	PC 42:1 [a/b]	FALSE	872.50	Unit	184.10	13.70	1	166	35	5	Positive
PC | PC O | PC P	PC 42:4 [a/b/c]	FALSE	866.50	Unit	184.10	10.50	2	166	35	5	Positive
PC | PC O | PC P	PC 42:6 [a/b/c]	FALSE	862.50	Unit	184.10	9.00	2.5	166	35	5	Positive
PC | PC O | PC P	PC 42:8 [a/b]	FALSE	858.50	Unit	184.10	6.80	2	166	35	5	Positive
PC | PC O | PC P	PC 43:0	FALSE	888.50	Unit	184.10	14.49	1	166	35	5	Positive
PC | PC O | PC P	PC 44:0	FALSE	902.50	Unit	184.10	14.75	1	166	35	5	Positive
PC | PC O | PC P	PC 44:1 [a/b]	FALSE	900.50	Unit	184.10	14.46	1	166	35	5	Positive
PC | PC O | PC P	PC 44:2	FALSE	898.50	Unit	184.10	13.85	1	166	35	5	Positive
PC | PC O | PC P	PC 44:3	FALSE	896.50	Unit	184.10	13.24	2	166	35	5	Positive
PC | PC O | PC P	PC 44:4 [a/b] | PC O-45:4	FALSE	894.50	Unit	184.10	12.50	3	166	35	5	Positive
PC | PC O | PC P	PC 44:5	FALSE	892.50	Unit	186.10	11.50	2	166	35	5	Positive
PC | PC O | PC P	PC 44:6	FALSE	892.50	Unit	186.10	10.00	2	166	35	5	Positive
PC | PC O | PC P	PC 45:1 [a/b] | PC O-46:1	FALSE	914.50	Unit	184.10	14.70	2	166	35	5	Positive
PC | PC O | PC P	PC 45:2 | PC O-46:2	FALSE	912.50	Unit	184.10	14.30	2	166	35	5	Positive
PC | PC O | PC P	PC 46:1 [a/b]	FALSE	928.50	Unit	184.10	15.00	2	166	35	5	Positive
PC | PC O | PC P	PC 46:2	FALSE	926.50	Unit	184.10	14.30	2	166	35	5	Positive
PC | PC O | PC P	PC 46:3	FALSE	924.50	Unit	184.10	14.00	2	166	35	5	Positive
PC | PC O | PC P	PC 46:4 [a/b/c]	FALSE	922.50	Unit	184.10	13.75	2	166	35	5	Positive
PC | PC O | PC P	PC 46:5	FALSE	920.50	Unit	184.10	13.20	2	166	35	5	Positive
PC | PC O | PC P	PC O-32:1 [a/b/c]	FALSE	718.50	Unit	184.10	7.75	1.2	166	35	5	Positive
PC | PC O | PC P	PC O-34:0	FALSE	748.50	Unit	184.10	10.50	1	166	35	5	Positive
PC | PC O | PC P	PC O-36:5 | PC P-36:4	FALSE	766.50	Unit	184.10	7.02	3	166	35	5	Positive
PC | PC O | PC P	PC O-38:4 [a/b] | PC P-38:3	FALSE	796.50	Unit	184.10	9.00	2	166	35	5	Positive
PC | PC O | PC P	PC O-38:4;O2	FALSE	828.50	Unit	184.10	5.00	4	166	35	5	Positive
PC | PC O | PC P	PC O-38:7 [a/b]	FALSE	790.50	Unit	184.10	7.20	2	166	35	5	Positive
PC | PC O | PC P	PC O-40:8	FALSE	816.50	Unit	184.10	7.10	2	166	35	5	Positive
PC | PC O | PC P	PC O-44:5	FALSE	878.50	Unit	184.10	12.85	2	166	35	5	Positive
PC | PC O | PC P	PC P-18:0/18:1 [D9]	FALSE	781.60	Unit	184.10	10.11	1.5	166	35	5	Positive
PC | PC O | PC P	PC P-32:0	FALSE	718.50	Unit	184.10	8.60	0.8	166	35	5	Positive
PC | PC O | PC P	PC P-32:1	FALSE	716.50	Unit	184.10	6.90	2	166	35	5	Positive
PC | PC O | PC P	PC P-40:4 [a/b/c]	FALSE	822.50	Unit	184.10	10.00	2	166	35	5	Positive
PE | PE O	PE 15:0/18:1 [D7]	FALSE	711.60	Unit	570.50	7.69	2	166	20	5	Positive
PE | PE O	PE 15:0/18:1 [D7] [+2]	FALSE	713.60	Unit	570.50	7.68	2	166	20	5	Positive
oxPE	PE 22:2;O2	FALSE	580.32	Unit	439.32	3.88	2	166	20	4	Positive
oxPE	PE 23:2;O2	FALSE	594.33	Unit	453.33	3.90	2	166	20	4	Positive
oxPE	PE 25:1;O2	FALSE	624.38	Unit	483.38	3.85	2	166	20	4	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PE | PE O	PE 30:0	FALSE	664.50	Unit	523.50	6.86	1.2	166	20	5	Positive
PE | PE O	PE 32:0	FALSE	692.50	Unit	551.50	8.22	1.2	166	20	5	Positive
PE | PE O	PE 32:1 [a/b]	FALSE	690.50	Unit	549.50	7.29	2	166	20	5	Positive
PE | PE O	PE 33:1 | PE O-34:1	FALSE	704.50	Unit	563.50	9.38	2	166	20	5	Positive
PE | PE O	PE 33:2	FALSE	702.50	Unit	561.50	8.45	1	166	20	5	Positive
PE | PE O	PE 34:0	FALSE	720.50	Unit	579.50	9.77	1	166	20	5	Positive
PE | PE O	PE 34:1	FALSE	718.50	Unit	577.50	8.50	1	166	20	5	Positive
PE | PE O	PE 34:2	FALSE	716.50	Unit	575.50	7.36	2	166	20	5	Positive
PE | PE O	PE 34:3 [a/b/c/d/e]	FALSE	714.50	Unit	573.50	6.93	2	166	20	5	Positive
PE | PE O	PE 35:1 [a/b] | PE O-36:1	FALSE	732.50	Unit	591.50	10.31	4	166	20	5	Positive
PE | PE O	PE 35:2 | PE O-36:2 [a/b]	FALSE	730.50	Unit	589.50	9.09	3	166	20	5	Positive
PE | PE O	PE 35:4 | PE O-36:4	FALSE	726.50	Unit	585.50	8.56	1	166	20	5	Positive
PE | PE O	PE 36:0	FALSE	748.50	Unit	607.50	11.43	1	166	20	5	Positive
PE | PE O	PE 36:1 [+2]	FALSE	748.50	Unit	605.50	9.86	1.5	166	20	5	Positive
PE | PE O	PE 36:2 [a/b] [+2]	FALSE	746.50	Unit	603.50	8.69	1.5	166	20	5	Positive
PE | PE O	PE 36:3 [a/b/c]	FALSE	742.50	Unit	601.50	7.83	2	166	20	5	Positive
PE | PE O	PE 36:4 [a/b] [+2]	FALSE	742.50	Unit	599.50	7.37	1.5	166	20	5	Positive
PE | PE O	PE 36:5 [a/b]	FALSE	738.50	Unit	597.50	6.61	2	166	20	5	Positive
PE | PE O	PE 36:6	FALSE	736.50	Unit	595.50	6.06	1.5	166	20	5	Positive
PE | PE O	PE 37:2 | PE O-38:2	FALSE	758.50	Unit	617.50	11.79	3	166	20	5	Positive
PE | PE O	PE 37:4	FALSE	754.50	Unit	613.50	8.00	0.8	166	20	5	Positive
PE | PE O	PE O-38:4 [a/b]	FALSE	754.50	Unit	613.50	9.50	1.6	166	20	5	Positive
PE | PE O	PE 37:5	FALSE	752.50	Unit	611.50	6.80	1	166	20	5	Positive
PE | PE O	PE O-38:5 [a/b]	FALSE	752.50	Unit	611.50	8.50	1.4	166	20	5	Positive
PE | PE O	PE 37:6	FALSE	750.50	Unit	609.50	6.50	0.8	166	20	5	Positive
PE | PE O	PE O-38:6	FALSE	750.50	Unit	609.50	8.00	1	166	20	5	Positive
PE | PE O	PE 38:1 [a/b]	FALSE	774.50	Unit	633.50	11.65	1.2	166	20	5	Positive
PE | PE O	PE 38:2 [a/b]	FALSE	772.50	Unit	631.50	10.16	2	166	20	5	Positive
PE | PE O	PE 38:3 [a/b]	FALSE	770.50	Unit	629.50	9.40	2	166	20	5	Positive
PE | PE O	PE 38:4 [a/b/c]	FALSE	768.50	Unit	627.50	8.50	2	166	20	5	Positive
PE | PE O	PE 38:5 [a/b]	FALSE	766.50	Unit	625.50	7.78	2	166	20	5	Positive
PE | PE O	PE 38:6 [a/b/c]	FALSE	764.50	Unit	623.50	7.13	1	166	20	5	Positive
PE | PE O	PE 38:7 [a/b/c/d/e]	FALSE	762.50	Unit	621.50	6.28	2.4	166	20	5	Positive
PE | PE O	PE 39:4	FALSE	782.50	Unit	641.50	9.10	1	166	20	5	Positive
PE | PE O	PE O-40:4	FALSE	782.50	Unit	641.50	11.00	1	166	20	5	Positive
PE | PE O	PE 39:5 [a/b]	FALSE	780.50	Unit	639.50	8.40	1	166	20	5	Positive
PE | PE O	PE O-40:5 [a/b]	FALSE	780.50	Unit	639.50	10.30	1.2	166	20	5	Positive
PE | PE O	PE 39:6	FALSE	778.50	Unit	637.50	7.80	1	166	20	5	Positive
PE | PE O	PE O-40:6	FALSE	778.50	Unit	637.50	9.50	1	166	20	5	Positive
PE | PE O	PE 40:1 [a/b]	FALSE	802.50	Unit	661.50	13.22	2	166	20	5	Positive
PE | PE O	PE 40:2 [a/b]	FALSE	800.50	Unit	659.50	12.04	2	166	20	5	Positive
PE | PE O	PE 40:3 [a/b]	FALSE	798.50	Unit	657.50	10.91	2	166	20	5	Positive
PE | PE O	PE 40:4 [a/b/c]	FALSE	796.50	Unit	655.50	9.90	1.6	166	20	5	Positive
PE | PE O	PE 40:5 [a/b]	FALSE	794.50	Unit	653.50	9.24	1.6	166	20	5	Positive
PE | PE O	PE 40:6 [a/b]	FALSE	792.50	Unit	651.50	8.51	1	166	20	5	Positive
PE | PE O	PE 40:7 [a/b/c/d]	FALSE	790.50	Unit	649.50	7.45	1.6	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PE | PE O	PE 40:8 [a/b/c]	FALSE	788.50	Unit	647.50	6.74	1.6	166	20	5	Positive
PE | PE O	PE 42:10 [a/b]	FALSE	812.50	Unit	671.50	6.35	1	166	20	5	Positive
PE | PE O	PE 42:2 [a/b]	FALSE	828.50	Unit	687.50	13.31	2	166	20	5	Positive
PE | PE O	PE 42:3 [a/b]	FALSE	826.50	Unit	685.50	12.25	2	166	20	5	Positive
PE | PE O	PE 42:4 [a/b/c/d]	FALSE	824.50	Unit	683.50	11.70	3	166	20	5	Positive
PE | PE O	PE 42:5 [a/b/c]	FALSE	822.50	Unit	681.50	10.70	3	166	20	5	Positive
PE | PE O	PE 42:6 [a/b/c/d/e/f]	FALSE	820.50	Unit	679.50	9.75	4	166	20	5	Positive
PE | PE O	PE 42:7 [a/b/c/d/e]	FALSE	818.50	Unit	677.50	8.42	2	166	20	5	Positive
PE | PE O	PE 42:8 [a/b]	FALSE	816.50	Unit	675.50	7.55	2	166	20	5	Positive
PE | PE O	PE 42:9 [a/b/c]	FALSE	814.50	Unit	673.50	6.78	1.6	166	20	5	Positive
PE | PE O	PE 42:9 [d]	FALSE	814.50	Unit	673.50	8.40	1	166	20	5	Positive
PE | PE O	PE 44:10 [a/b]	FALSE	840.50	Unit	699.50	7.20	1.6	166	20	5	Positive
PE | PE O	PE 44:11 [a/b]	FALSE	838.50	Unit	697.50	6.81	1	166	20	5	Positive
PE | PE O	PE 44:12	FALSE	836.50	Unit	695.50	6.15	1	166	20	5	Positive
PE | PE O	PE 44:2	FALSE	856.50	Unit	715.50	14.09	1	166	20	5	Positive
PE | PE O	PE 44:8 [a/b]	FALSE	844.50	Unit	703.50	8.75	2.4	166	20	5	Positive
PE | PE O	PE 46:10 [a/b]	FALSE	868.50	Unit	727.50	8.46	1	166	20	5	Positive
PE | PE O	PE 46:11 [a/b/c]	FALSE	866.50	Unit	725.50	7.66	1	166	20	5	Positive
PE | PE O	PE 46:12	FALSE	864.50	Unit	723.50	6.85	1	166	20	5	Positive
PE | PE O	PE 46:5 [a/b]	FALSE	878.50	Unit	737.50	13.55	1	166	20	5	Positive
PE | PE O	PE 46:7	FALSE	874.50	Unit	733.50	11.61	1	166	20	5	Positive
PE | PE O	PE O-32:1	FALSE	676.50	Unit	535.50	7.99	1.2	166	20	5	Positive
PE | PE O	PE O-34:0	FALSE	706.50	Unit	565.50	10.75	1.2	166	20	5	Positive
PE | PE O	PE O-36:5	FALSE	724.50	Unit	583.50	7.39	1	166	20	5	Positive
PE | PE O	PE O-36:6	FALSE	722.50	Unit	581.50	6.69	1	166	20	5	Positive
PE | PE O	PE O-42:4 [a/b]	FALSE	810.50	Unit	669.50	12.29	2	166	20	5	Positive
PE | PE O	PE O-42:6 [a/b]	FALSE	806.50	Unit	665.50	9.19	1.5	166	20	5	Positive
PE P	PE P-16:0/16:0	FALSE	676.50	Unit	313.30	8.98	1	166	20	5	Positive
PE P	PE P-16:0/16:1 [a/b/c]	FALSE	674.50	Unit	311.30	7.83	2	166	20	5	Positive
PE P	PE P-16:0/18:0	FALSE	704.50	Unit	341.30	10.58	1	166	20	5	Positive
PE P	PE P-16:0/18:1	FALSE	702.50	Unit	339.30	9.24	2	166	20	5	Positive
PE P	PE P-16:0/18:2 [a/b]	FALSE	700.50	Unit	337.30	8.22	2	166	20	5	Positive
PE P	PE P-16:0/19:1	FALSE	716.50	Unit	353.30	9.93	2	166	20	5	Positive
PE P	PE P-16:0/20:0	FALSE	732.50	Unit	369.30	12.31	1	166	20	5	Positive
PE P	PE P-16:0/20:1 [a/b]	FALSE	730.50	Unit	367.30	10.74	2	166	20	5	Positive
PE P	PE P-16:0/20:2 [a/b]	FALSE	728.50	Unit	365.30	9.68	2	166	20	5	Positive
PE P	PE P-16:0/20:3 [a/b/c]	FALSE	726.50	Unit	363.30	8.61	2	166	20	5	Positive
PE P	PE P-16:0/20:4	FALSE	724.50	Unit	361.30	8.06	1	166	20	5	Positive
PE P	PE P-16:0/20:5	FALSE	722.50	Unit	359.30	7.22	1	166	20	5	Positive
PE P	PE P-16:0/21:1 [a/b]	FALSE	744.50	Unit	381.30	11.52	1	166	20	5	Positive
PE P	PE P-16:0/21:2	FALSE	742.50	Unit	379.30	10.39	1	166	20	5	Positive
PE P	PE P-16:0/21:3 [a/b]	FALSE	740.50	Unit	377.30	9.46	1	166	20	5	Positive
PE P	PE P-16:0/21:4	FALSE	738.50	Unit	375.30	8.51	1	166	20	5	Positive
PE P	PE P-16:0/22:1	FALSE	758.50	Unit	395.30	12.36	1.5	166	20	5	Positive
PE P	PE P-16:0/22:2	FALSE	756.50	Unit	393.30	11.13	2	166	20	5	Positive
PE P	PE P-16:0/22:3 [a/b]	FALSE	754.50	Unit	391.30	9.92	1.5	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PE P	PE P-16:0/22:4	FALSE	752.50	Unit	389.30	9.11	1	166	20	5	Positive
PE P	PE P-16:0/22:5 [a/b]	FALSE	750.50	Unit	387.30	8.68	2	166	20	5	Positive
PE P	PE P-16:0/22:6	FALSE	748.50	Unit	385.30	7.77	0.8	166	20	5	Positive
PE P	PE P-16:0/22:7	FALSE	746.50	Unit	383.30	7.03	0.8	166	20	5	Positive
PE P	PE P-16:0/23:1	FALSE	772.50	Unit	409.30	13.20	1	166	20	5	Positive
PE P	PE P-16:0/23:2 [a/b]	FALSE	770.50	Unit	407.30	11.87	1	166	20	5	Positive
PE P	PE P-16:0/23:3	FALSE	768.50	Unit	405.30	10.76	1	166	20	5	Positive
PE P	PE P-16:0/24:1	FALSE	786.50	Unit	423.30	13.62	1	166	20	5	Positive
PE P	PE P-16:0/24:2	FALSE	784.50	Unit	421.30	12.71	1	166	20	5	Positive
PE P	PE P-16:0/24:3 [a/b]	FALSE	782.50	Unit	419.30	11.59	1	166	20	5	Positive
PE P	PE P-16:0/24:4	FALSE	780.50	Unit	417.30	10.37	1	166	20	5	Positive
PE P	PE P-16:0/24:5 [a/b]	FALSE	778.50	Unit	415.30	9.37	2	166	20	5	Positive
PE P	PE P-16:0/24:6 [a/b]	FALSE	776.50	Unit	413.30	8.69	2	166	20	5	Positive
PE P	PE P-16:1/20:4	FALSE	722.50	Unit	361.30	7.32	2	166	20	5	Positive
PE P	PE P-16:1/22:4	FALSE	750.50	Unit	389.30	8.25	2	166	20	5	Positive
PE P	PE P-16:1/22:6	FALSE	746.50	Unit	385.30	7.05	1	166	20	5	Positive
PE P	PE P-17:0/20:3 [a/b/c/d]	FALSE	740.50	Unit	363.30	9.58	3	166	20	5	Positive
PE P	PE P-17:0/20:4 [a/b]	FALSE	738.50	Unit	361.30	8.56	2	166	20	5	Positive
PE P	PE P-17:0/22:2 [a/b]	FALSE	770.50	Unit	393.30	11.95	2	166	20	5	Positive
PE P	PE P-17:0/22:3 [a/b]	FALSE	768.50	Unit	391.30	10.79	2	166	20	5	Positive
PE P	PE P-17:0/22:4 [a/b]	FALSE	766.50	Unit	389.30	9.73	2	166	20	5	Positive
PE P	PE P-17:0/22:5 [a/b/c/d]	FALSE	764.50	Unit	387.30	9.17	3	166	20	5	Positive
PE P	PE P-17:0/22:6 [a/b]	FALSE	762.50	Unit	385.30	8.34	2	166	20	5	Positive
PE P	PE P-17:0/24:4 [a/b]	FALSE	794.50	Unit	417.30	11.58	1	166	20	5	Positive
PE P	PE P-17:0/24:5	FALSE	792.50	Unit	415.30	10.44	1	166	20	5	Positive
PE P	PE P-17:0/24:6	FALSE	790.50	Unit	413.30	9.42	1	166	20	5	Positive
PE P	PE P-18:0/14:0	FALSE	676.50	Unit	285.30	9.03	1	166	20	5	Positive
PE P	PE P-18:0/16:0	FALSE	704.50	Unit	313.30	10.58	1	166	20	5	Positive
PE P	PE P-18:0/16:1 [a/b/c]	FALSE	702.50	Unit	311.30	9.30	2	166	20	5	Positive
PE P	PE P-18:0/16:2	FALSE	700.50	Unit	309.30	8.90	1	166	20	5	Positive
PE P	PE P-18:0/17:0	FALSE	718.50	Unit	327.30	10.99	1	166	20	5	Positive
PE P	PE P-18:0/17:1	FALSE	716.50	Unit	325.30	10.07	1	166	20	5	Positive
PE P	PE P-18:0/18:1	FALSE	730.50	Unit	339.30	10.86	1	166	20	5	Positive
PE P	PE P-18:0/18:1 [D9]	FALSE	739.50	Unit	348.30	10.77	1	166	20	5	Positive
PE P	PE P-18:0/18:2	FALSE	728.50	Unit	337.30	9.71	1	166	20	5	Positive
PE P	PE P-18:0/18:3	FALSE	726.50	Unit	335.30	9.14	1	166	20	5	Positive
PE P	PE P-18:0/20:1 [a/b]	FALSE	758.50	Unit	367.30	12.40	1.5	166	20	5	Positive
PE P	PE P-18:0/20:2 [a/b]	FALSE	756.50	Unit	365.30	11.32	1.5	166	20	5	Positive
PE P	PE P-18:0/20:3 [a/b]	FALSE	754.50	Unit	363.30	10.39	1.5	166	20	5	Positive
PE P	PE P-18:0/20:4	FALSE	752.50	Unit	361.30	9.55	1	166	20	5	Positive
PE P	PE P-18:0/20:5	FALSE	750.50	Unit	359.30	8.62	1	166	20	5	Positive
PE P	PE P-18:0/21:1	FALSE	772.50	Unit	381.30	13.18	1	166	20	5	Positive
PE P	PE P-18:0/21:2	FALSE	770.50	Unit	379.30	12.00	1	166	20	5	Positive
PE P	PE P-18:0/21:3	FALSE	768.50	Unit	377.30	11.09	1	166	20	5	Positive
PE P	PE P-18:0/22:1	FALSE	786.50	Unit	395.30	13.64	1	166	20	5	Positive
PE P	PE P-18:0/22:2	FALSE	784.50	Unit	393.30	12.86	1	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PE P	PE P-18:0/22:3 [a/b]	FALSE	782.50	Unit	391.30	11.65	2	166	20	5	Positive
PE P	PE P-18:0/22:4	FALSE	780.50	Unit	389.30	10.70	1	166	20	5	Positive
PE P	PE P-18:0/22:5 [a/b]	FALSE	778.50	Unit	387.30	9.80	2	166	20	5	Positive
PE P	PE P-18:0/22:6	FALSE	776.50	Unit	385.30	9.22	1.2	166	20	5	Positive
PE P	PE P-18:0/22:7	FALSE	774.50	Unit	383.30	8.40	1	166	20	5	Positive
PE P	PE P-18:0/24:1	FALSE	814.50	Unit	423.30	14.27	1	166	20	5	Positive
PE P	PE P-18:0/24:2	FALSE	812.50	Unit	421.30	13.75	1	166	20	5	Positive
PE P	PE P-18:0/24:3	FALSE	810.50	Unit	419.30	13.22	1	166	20	5	Positive
PE P	PE P-18:0/24:4	FALSE	808.50	Unit	417.30	12.03	1	166	20	5	Positive
PE P	PE P-18:0/24:5 [a/b]	FALSE	806.50	Unit	415.30	11.29	1	166	20	5	Positive
PE P	PE P-18:0/24:6	FALSE	804.50	Unit	413.30	10.24	1	166	20	5	Positive
PE P	PE P-18:1/18:0	FALSE	730.50	Unit	341.30	10.75	1	166	20	5	Positive
PE P	PE P-18:1/18:1	FALSE	728.50	Unit	339.30	9.43	1	166	20	5	Positive
PE P	PE P-18:1/18:2	FALSE	726.50	Unit	337.30	8.39	2	166	20	5	Positive
PE P	PE P-18:1/20:1	FALSE	756.50	Unit	367.30	10.91	2	166	20	5	Positive
PE P	PE P-18:1/20:2	FALSE	754.50	Unit	365.30	9.88	2	166	20	5	Positive
PE P	PE P-18:1/20:3 [a/b]	FALSE	752.50	Unit	363.30	8.81	2	166	20	5	Positive
PE P	PE P-18:1/20:4 [a/b]	FALSE	750.50	Unit	361.30	8.25	1.2	166	20	5	Positive
PE P	PE P-18:1/20:5	FALSE	748.50	Unit	359.30	7.36	1	166	20	5	Positive
PE P	PE P-18:1/21:1	FALSE	770.50	Unit	381.30	11.69	1.2	166	20	5	Positive
PE P	PE P-18:1/21:2	FALSE	768.50	Unit	379.30	10.56	2	166	20	5	Positive
PE P	PE P-18:1/21:3	FALSE	766.50	Unit	377.30	9.62	1	166	20	5	Positive
PE P	PE P-18:1/22:1 [a/b]	FALSE	784.50	Unit	395.30	12.56	2	166	20	5	Positive
PE P	PE P-18:1/22:2	FALSE	782.50	Unit	393.30	11.31	1	166	20	5	Positive
PE P	PE P-18:1/22:3 [a/b/c]	FALSE	780.50	Unit	391.30	10.75	1	166	20	5	Positive
PE P	PE P-18:1/22:4 [a/b]	FALSE	778.50	Unit	389.30	9.29	1	166	20	5	Positive
PE P	PE P-18:1/22:5 [a/b/c/d]	FALSE	776.50	Unit	387.30	8.83	2	166	20	5	Positive
PE P	PE P-18:1/22:6 [a/b]	FALSE	774.50	Unit	385.30	7.97	2	166	20	5	Positive
PE P	PE P-18:1/22:7	FALSE	772.50	Unit	383.30	7.19	1	166	20	5	Positive
PE P	PE P-18:1/23:1	FALSE	798.50	Unit	409.30	13.31	1	166	20	5	Positive
PE P	PE P-18:1/23:2	FALSE	796.50	Unit	407.30	12.01	1	166	20	5	Positive
PE P	PE P-18:1/24:1	FALSE	812.50	Unit	423.30	13.71	1	166	20	5	Positive
PE P	PE P-18:1/24:2	FALSE	810.50	Unit	421.30	12.88	1	166	20	5	Positive
PE P	PE P-18:1/24:3	FALSE	808.50	Unit	419.30	11.77	2	166	20	5	Positive
PE P	PE P-18:1/24:4 [a/b]	FALSE	806.50	Unit	417.30	10.57	2	166	20	5	Positive
PE P	PE P-18:1/24:5 [a/b]	FALSE	804.50	Unit	415.30	9.83	2	166	20	5	Positive
PE P	PE P-18:1/24:6	FALSE	802.50	Unit	413.30	8.85	2	166	20	5	Positive
PE P	PE P-18:2/16:0	FALSE	700.50	Unit	313.30	8.19	2	166	20	5	Positive
PE P	PE P-18:2/20:1	FALSE	754.50	Unit	367.30	9.81	2	166	20	5	Positive
PE P	PE P-18:2/20:2	FALSE	752.50	Unit	365.30	8.69	2	166	20	5	Positive
PE P	PE P-18:2/20:3	FALSE	750.50	Unit	363.30	8.20	2	166	20	5	Positive
PE P	PE P-18:2/20:4	FALSE	748.50	Unit	361.30	7.30	2	166	20	5	Positive
PE P	PE P-18:2/22:2 [a/b]	FALSE	780.50	Unit	393.30	10.22	3	166	20	5	Positive
PE P	PE P-18:2/22:4 [a/b]	FALSE	776.50	Unit	389.30	8.50	2	166	20	5	Positive
PE P	PE P-18:2/22:6	FALSE	772.50	Unit	385.30	7.04	2	166	20	5	Positive
PE P	PE P-19:0/20:4	FALSE	766.50	Unit	361.30	7.56	1	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PE P	PE P-19:0/22:4 [a/b]	FALSE	794.50	Unit	389.30	11.55	1	166	20	5	Positive
PE P	PE P-19:0/22:6 [a/b]	FALSE	790.50	Unit	385.30	10.01	2	166	20	5	Positive
PE P	PE P-19:1/20:4	FALSE	764.50	Unit	361.30	8.95	1	166	20	5	Positive
PE P	PE P-19:1/22:4	FALSE	792.50	Unit	389.30	10.06	1	166	20	5	Positive
PE P	PE P-19:1/22:6	FALSE	788.50	Unit	385.30	8.65	1	166	20	5	Positive
PE P	PE P-20:0/20:4	FALSE	780.50	Unit	361.30	11.19	1	166	20	5	Positive
PE P	PE P-20:0/22:4	FALSE	808.50	Unit	389.30	12.43	1	166	20	5	Positive
PE P	PE P-20:0/22:6	FALSE	804.50	Unit	385.30	10.85	1	166	20	5	Positive
PE P	PE P-20:1/16:0	FALSE	730.50	Unit	313.30	10.69	1	166	20	5	Positive
PE P	PE P-20:1/18:0	FALSE	758.50	Unit	341.30	12.40	1	166	20	5	Positive
PE P	PE P-20:1/18:1	FALSE	756.50	Unit	339.30	10.96	1	166	20	5	Positive
PE P	PE P-20:1/20:1	FALSE	784.50	Unit	367.30	12.52	1	166	20	5	Positive
PE P	PE P-20:1/20:2	FALSE	782.50	Unit	365.30	11.41	1	166	20	5	Positive
PE P	PE P-20:1/20:3 [a/b]	FALSE	780.50	Unit	363.30	10.27	1	166	20	5	Positive
PE P	PE P-20:1/20:4 [a/b]	FALSE	778.50	Unit	361.30	9.67	1.5	166	20	5	Positive
PE P	PE P-20:1/22:2	FALSE	810.50	Unit	393.30	12.88	1	166	20	5	Positive
PE P	PE P-20:1/22:3	FALSE	808.50	Unit	391.30	11.55	2	166	20	5	Positive
PE P	PE P-20:1/22:4	FALSE	806.50	Unit	389.30	10.80	1	166	20	5	Positive
PE P	PE P-20:1/22:6 [a/b]	FALSE	802.50	Unit	385.30	9.34	1	166	20	5	Positive
PG	PG 15:0_18:1 [D7]	FALSE	759.60	Unit	570.60	6.18	1.5	166	20	4	Positive
PG	PG 32:0	FALSE	740.60	Unit	551.50	6.54	0.7	166	20	4	Positive
PG	PG 32:1	FALSE	738.60	Unit	549.50	5.70	0.7	166	20	4	Positive
PG	PG 33:0	FALSE	754.60	Unit	565.50	7.17	0.7	166	20	4	Positive
PG	PG 33:1	FALSE	752.60	Unit	563.50	6.23	0.7	166	20	4	Positive
PG	PG 34:0	FALSE	768.60	Unit	579.50	7.81	0.7	166	20	4	Positive
PG	PG 34:1	FALSE	766.60	Unit	577.50	6.70	0.7	166	20	4	Positive
PG	PG 34:2	FALSE	764.60	Unit	575.50	5.89	1	166	20	4	Positive
PG	PG 35:1	FALSE	780.60	Unit	591.50	7.33	0.7	166	20	4	Positive
PG	PG 36:1	FALSE	794.60	Unit	605.50	7.98	1	166	20	4	Positive
PG	PG 36:2	FALSE	792.60	Unit	603.50	6.94	2	166	20	4	Positive
PG	PG 36:3	FALSE	790.60	Unit	601.50	6.16	1.5	166	20	4	Positive
PG	PG 36:4 [a/b]	FALSE	788.60	Unit	599.50	5.92	2	166	20	4	Positive
PG	PG 36:5	FALSE	786.60	Unit	597.50	5.30	1	166	20	4	Positive
PG	PG 38:3	FALSE	818.60	Unit	629.50	7.32	2	166	20	4	Positive
PG	PG 38:4	FALSE	816.60	Unit	627.50	6.49	2	166	20	4	Positive
PG	PG 38:5	FALSE	814.60	Unit	625.50	6.05	2	166	20	4	Positive
PG	PG 38:6 [a/b]	FALSE	812.60	Unit	623.50	5.46	1.5	166	20	4	Positive
PG	PG 40:4 [a/b]	FALSE	844.60	Unit	655.50	8.06	1.5	166	20	4	Positive
PG	PG 40:6 [a/b/c]	FALSE	840.60	Unit	651.50	6.88	1	166	20	4	Positive
PG	PG 40:8	FALSE	836.60	Unit	647.50	5.34	1	166	20	4	Positive
PI | PI O	PI 15:0_18:1 [D7]	FALSE	847.60	Unit	570.60	5.89	1.5	166	20	5	Positive
PI | PI O	PI 32:0	FALSE	828.60	Unit	551.60	6.22	1	166	20	5	Positive
PI | PI O	PI 32:1	FALSE	826.60	Unit	549.60	5.50	1	166	20	5	Positive
PI | PI O	PI 33:0	FALSE	842.60	Unit	565.60	6.77	1	166	20	5	Positive
PI | PI O	PI 33:1	FALSE	840.60	Unit	563.60	5.90	1	166	20	5	Positive
PI | PI O	PI 34:0	FALSE	856.60	Unit	579.60	7.32	1	166	20	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PI | PI O	PI 34:1	FALSE	854.60	Unit	577.60	6.38	1	166	20	5	Positive
PI | PI O	PI 34:2	FALSE	852.60	Unit	575.60	5.71	1	166	20	5	Positive
PI | PI O	PI 34:3	FALSE	850.60	Unit	573.60	5.89	1	166	20	5	Positive
PI | PI O	PI 35:1	FALSE	868.60	Unit	591.60	6.95	2	166	20	5	Positive
PI | PI O	PI 35:2 | PI-O 36:2	FALSE	866.60	Unit	589.60	6.06	2	166	20	5	Positive
PI | PI O	PI 36:0	FALSE	884.60	Unit	607.60	8.83	1	166	20	5	Positive
PI | PI O	PI 36:1	FALSE	882.60	Unit	605.60	7.60	1	166	20	5	Positive
PI | PI O	PI 36:2	FALSE	880.60	Unit	603.60	6.75	1	166	20	5	Positive
PI | PI O	PI 36:3 [a/b/c]	FALSE	878.60	Unit	601.60	6.10	2	166	20	5	Positive
PI | PI O	PI 36:4	FALSE	876.60	Unit	599.60	5.68	1	166	20	5	Positive
PI | PI O	PI 36:5	FALSE	874.60	Unit	597.60	5.17	1	166	20	5	Positive
PI | PI O	PI 37:2 | PI-O 38:2	FALSE	894.60	Unit	617.60	7.25	2	166	20	5	Positive
PI | PI O	PI 37:3	FALSE	892.60	Unit	615.60	6.82	2	166	20	5	Positive
PI | PI O	PI 37:4 | PI-O 38:4	FALSE	890.60	Unit	613.60	6.25	2.5	166	20	5	Positive
PI | PI O	PI 37:5 | PI-O 38:5	FALSE	888.60	Unit	611.60	5.69	2	166	20	5	Positive
PI | PI O	PI 38:2 [a/b]	FALSE	908.60	Unit	631.60	7.82	2	166	20	5	Positive
PI | PI O	PI 38:3 [a/b]	FALSE	906.60	Unit	629.60	7.29	2	166	20	5	Positive
PI | PI O	PI 38:4	FALSE	904.60	Unit	627.60	6.68	1	166	20	5	Positive
PI | PI O	PI 38:5	FALSE	902.60	Unit	625.60	5.83	1	166	20	5	Positive
PI | PI O	PI 38:6 [a/b]	FALSE	900.60	Unit	623.60	5.46	2	166	20	5	Positive
PI | PI O	PI 40:3 [a/b]	FALSE	934.60	Unit	657.60	8.37	2	166	20	5	Positive
PI | PI O	PI 40:4 [a/b]	FALSE	932.60	Unit	655.60	7.29	2	166	20	5	Positive
PI | PI O	PI 40:5 [a/b]	FALSE	930.60	Unit	653.60	6.92	2	166	20	5	Positive
PI | PI O	PI 40:6 [a/b]	FALSE	928.60	Unit	651.60	6.50	1	166	20	5	Positive
PI | PI O	PI 40:7 [a/b/c]	FALSE	926.60	Unit	649.60	5.66	2	166	20	5	Positive
PI | PI O	PI 40:8	FALSE	924.60	Unit	647.60	5.16	1	166	20	5	Positive
PI | PI O	PI O-36:4	FALSE	862.60	Unit	585.60	6.19	1	166	20	5	Positive
PIP1	PIP1 34:1	FALSE	917.52	Unit	577.52	5.49	1	166	20	4	Positive
PIP1	PIP1 38:4	FALSE	967.52	Unit	627.52	5.92	1	166	20	4	Positive
PS	PS 15:0/18:1-d7 [IS]	FALSE	755.50	Unit	570.50	5.98	1	166	20	4	Positive
PS | PS O	PS 32:0	FALSE	736.47	Unit	551.47	6.41	1	166	20	4	Positive
PS | PS O	PS 32:1	FALSE	734.47	Unit	549.47	5.63	1	166	20	4	Positive
PS | PS O	PS 33:1 | PS-O 34:1	FALSE	748.47	Unit	563.47	7.14	2	166	20	4	Positive
PS | PS O	PS 34:0	FALSE	764.47	Unit	579.47	7.48	1	166	20	4	Positive
PS | PS O	PS 34:1	FALSE	762.47	Unit	577.47	6.48	1	166	20	4	Positive
PS | PS O	PS 34:2	FALSE	760.47	Unit	575.47	5.83	2	166	20	4	Positive
PS | PS O	PS 36:1	FALSE	790.47	Unit	605.47	7.65	1.5	166	20	4	Positive
PS | PS O	PS 36:2 [a/b]	FALSE	788.47	Unit	603.47	6.67	2	166	20	4	Positive
PS | PS O	PS 36:3	FALSE	786.47	Unit	601.47	6.15	2	166	20	4	Positive
PS | PS O	PS 36:4	FALSE	784.47	Unit	599.47	5.76	1	166	20	4	Positive
PS | PS O	PS 38:1	FALSE	818.47	Unit	633.47	9.01	1	166	20	4	Positive
PS | PS O	PS 38:2 [a/b]	FALSE	816.47	Unit	631.47	8.01	2	166	20	4	Positive
PS | PS O	PS 38:3 [a/b/c]	FALSE	814.47	Unit	629.47	7.15	2	166	20	4	Positive
PS | PS O	PS 38:4 [a/b/c]	FALSE	812.47	Unit	627.47	6.74	2	166	20	4	Positive
PS | PS O	PS 38:5	FALSE	810.47	Unit	625.47	6.02	2	166	20	4	Positive
PS | PS O	PS 38:6	FALSE	808.47	Unit	623.47	5.60	1	166	20	4	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
PS | PS O	PS 39:1 [a/b]	FALSE	832.47	Unit	647.47	9.64	2	166	20	4	Positive
PS | PS O	PS 39:2 [a/b]	FALSE	830.47	Unit	645.47	8.49	2	166	20	4	Positive
PS | PS O	PS 39:3	FALSE	828.47	Unit	643.47	7.98	2	166	20	4	Positive
PS | PS O	PS 39:4 [a/b/c/d]	FALSE	826.47	Unit	641.47	7.20	2.4	166	20	4	Positive
PS | PS O	PS-O 40:4 [a/b]	FALSE	826.47	Unit	641.47	8.50	1.2	166	20	4	Positive
PS | PS O	PS 39:6	FALSE	822.47	Unit	637.47	6.00	1	166	20	4	Positive
PS | PS O	PS O 40:6	FALSE	822.47	Unit	637.47	7.20	1.2	166	20	4	Positive
PS | PS O	PS 40:1	FALSE	846.47	Unit	661.47	10.44	1.2	166	20	4	Positive
PS | PS O	PS 40:2	FALSE	844.47	Unit	659.47	9.02	1.2	166	20	4	Positive
PS | PS O	PS 40:3 [a/b/c]	FALSE	842.47	Unit	657.47	8.26	2	166	20	4	Positive
PS | PS O	PS 40:4	FALSE	840.47	Unit	655.47	7.43	2	166	20	4	Positive
PS | PS O	PS 40:5 [a/b]	FALSE	838.47	Unit	653.47	6.95	2	166	20	4	Positive
PS | PS O	PS 40:6	FALSE	836.47	Unit	651.47	6.54	1	166	20	4	Positive
PS | PS O	PS 40:7	FALSE	834.47	Unit	649.47	5.89	2	166	20	4	Positive
PS | PS O	PS 40:8	FALSE	832.47	Unit	647.47	5.20	1	166	20	4	Positive
PS | PS O	PS 41:2	FALSE	858.47	Unit	673.47	9.90	1	166	20	4	Positive
PS | PS O	PS 41:3 [a/b/c]	FALSE	856.47	Unit	671.47	9.00	4	166	20	4	Positive
PS | PS O	PS 41:4 [a/b/c]	FALSE	854.47	Unit	669.47	8.00	2	166	20	4	Positive
PS | PS O	PS 42:1 [a/b]	FALSE	874.47	Unit	689.47	12.31	1.5	166	20	4	Positive
PS | PS O	PS 42:10	FALSE	856.47	Unit	671.47	5.03	1	166	20	4	Positive
PS | PS O	PS 42:2	FALSE	872.47	Unit	687.47	10.63	1	166	20	4	Positive
PS | PS O	PS 42:3 [a/b]	FALSE	870.47	Unit	685.47	9.60	2	166	20	4	Positive
PS | PS O	PS 42:4 [a/b/c]	FALSE	868.47	Unit	683.47	8.66	2	166	20	4	Positive
PS | PS O	PS 42:8 [a/b]	FALSE	860.47	Unit	675.47	5.90	3	166	20	4	Positive
PS | PS O	PS 42:9 [a/b]	FALSE	858.47	Unit	673.47	6.57	3	166	20	4	Positive
PS | PS O	PS 44:2	FALSE	900.47	Unit	715.47	12.28	1	166	20	4	Positive
PS | PS O	PS 44:7	FALSE	890.47	Unit	705.47	7.82	2	166	20	4	Positive
PS | PS O	PS 46:10	FALSE	912.47	Unit	727.47	6.43	2	166	20	4	Positive
PS | PS O	PS 46:7	FALSE	918.47	Unit	733.47	9.19	1	166	20	4	Positive
PS | PS O	PS 46:8	FALSE	916.47	Unit	731.47	8.60	1	166	20	4	Positive
SHexCer	SHexCer 18:1;O2/12:0 [IS]	FALSE	724.80	Unit	264.30	4.14	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/16:0	FALSE	780.50	Unit	264.30	5.34	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/18:0	FALSE	808.80	Unit	264.30	6.27	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/18:0;O	FALSE	824.80	Unit	264.30	5.99	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/18:1	FALSE	806.80	Unit	264.30	4.70	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/20:0	FALSE	836.80	Unit	264.30	7.40	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/20:0;O	FALSE	852.80	Unit	264.30	7.11	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/22:0	FALSE	864.80	Unit	264.30	8.71	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/22:1	FALSE	862.80	Unit	264.30	7.45	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/23:0;O	FALSE	894.80	Unit	264.30	9.06	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/23:1	FALSE	876.80	Unit	264.30	8.08	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/24:0;O	FALSE	908.80	Unit	264.30	9.81	1	166	49	4	Positive
SHexCer	SHexCer 18:1;O2/24:1	FALSE	890.80	Unit	264.30	8.73	1	166	49	4	Positive
SHexCer	SHexCer 30:1;O2 [IS]	FALSE	724.50	Unit	626.40	4.14	1	166	20	4	Positive
SHexCer	SHexCer 34:1;O2	FALSE	780.50	Unit	682.40	5.40	1	166	20	4	Positive
SHexCer	SHexCer 36:1;O2	FALSE	808.50	Unit	710.40	6.29	1	166	20	4	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
SHexCer	SHexCer 36:1;O3	FALSE	824.50	Unit	726.40	6.02	1	166	20	4	Positive
SHexCer	SHexCer 38:1;O2	FALSE	836.80	Unit	738.80	7.38	1	166	20	4	Positive
SHexCer	SHexCer 38:1;O3	FALSE	852.50	Unit	754.40	7.14	1	166	20	4	Positive
SHexCer	SHexCer 40:1;O2	FALSE	864.80	Unit	766.70	8.71	1	166	20	4	Positive
SHexCer	SHexCer 40:2;O2	FALSE	862.80	Unit	764.40	7.45	1	166	20	4	Positive
SHexCer	SHexCer 41:1;O3	FALSE	894.80	Unit	796.70	9.06	1	166	20	4	Positive
SHexCer	SHexCer 41:2;O2	FALSE	876.80	Unit	778.70	8.07	1	166	20	4	Positive
SHexCer	SHexCer 42:1;O3	FALSE	908.80	Unit	810.70	9.80	1	166	20	4	Positive
SHexCer	SHexCer 42:2;O2	FALSE	890.80	Unit	792.70	8.73	1	166	20	4	Positive
SHexCer	SHexCer 44:1;O3	FALSE	936.50	Unit	838.40	10.23	1	166	20	4	Positive
SM	SM [D9] 18:1;O2/15:0	FALSE	698.60	Unit	193.10	5.99	1	166	35	5	Positive
SM	SM [D9] 18:1;O2/15:0 [+2]	FALSE	700.60	Unit	195.10	5.99	1	166	35	5	Positive
SM	SM 30:1;O2	FALSE	647.50	Unit	184.10	4.77	1	166	35	5	Positive
SM	SM 31:1;O2	FALSE	661.50	Unit	184.10	5.13	1	166	35	5	Positive
SM	SM 32:0;O2	FALSE	677.50	Unit	184.10	5.54	1	166	35	5	Positive
SM	SM 32:1;O2 [a/b]	FALSE	675.50	Unit	184.10	5.54	1	166	35	5	Positive
SM	SM 32:2;O2	FALSE	673.50	Unit	184.10	4.92	1	166	35	5	Positive
SM	SM 33:1;O2	FALSE	689.50	Unit	184.10	5.99	1	166	35	5	Positive
SM	SM 33:2;O2	FALSE	687.50	Unit	184.10	5.29	1	166	35	5	Positive
SM	SM 34:0;O2	FALSE	705.50	Unit	184.10	6.93	1	166	35	5	Positive
SM	SM 34:1;O2 [+2]	FALSE	705.50	Unit	186.10	6.52	1	166	35	5	Positive
SM	SM 34:2;O2	FALSE	701.50	Unit	184.10	5.71	1	166	35	5	Positive
SM	SM 35:1;O2	FALSE	717.50	Unit	184.10	7.08	1	166	35	5	Positive
SM	SM 35:2;O2	FALSE	715.50	Unit	184.10	6.24	1	166	35	5	Positive
SM	SM 36:0;O2	FALSE	733.50	Unit	184.10	8.15	1	166	35	5	Positive
SM	SM 36:1;O2 [+2]	FALSE	733.50	Unit	186.10	7.68	1	166	35	5	Positive
SM	SM 36:2;O2 [a/b] [+2]	FALSE	731.50	Unit	186.10	6.76	1	166	35	5	Positive
SM	SM 36:3;O2	FALSE	727.50	Unit	184.10	6.09	1	166	35	5	Positive
SM	SM 37:1;O2	FALSE	745.50	Unit	184.10	8.31	2	166	35	5	Positive
SM	SM 37:2;O2	FALSE	743.50	Unit	184.10	6.90	2	166	35	5	Positive
SM	SM 38:0;O2	FALSE	761.50	Unit	184.10	9.82	1	166	35	5	Positive
SM	SM 38:1;O2	FALSE	759.50	Unit	184.10	9.17	1	166	35	5	Positive
SM	SM 38:2;O2	FALSE	757.50	Unit	184.10	8.07	1	166	35	5	Positive
SM	SM 39:1;O2 [a/b]	FALSE	773.50	Unit	184.10	10.14	1	166	35	5	Positive
SM	SM 39:2;O2	FALSE	771.50	Unit	184.10	8.88	1	166	35	5	Positive
SM	SM 40:1;O2	FALSE	787.50	Unit	184.10	10.63	2	166	35	5	Positive
SM	SM 40:2;O2 [a/b]	FALSE	785.50	Unit	184.10	9.27	2	166	35	5	Positive
SM	SM 40:3;O2	FALSE	783.50	Unit	184.10	8.24	1	166	35	5	Positive
SM	SM 41:0;O2	FALSE	803.50	Unit	184.10	12.00	2	166	35	5	Positive
SM	SM 41:1;O2	FALSE	801.50	Unit	184.10	11.82	1	166	35	5	Positive
SM	SM 41:2;O2 [a/b]	FALSE	799.50	Unit	184.10	9.77	2	166	35	5	Positive
SM	SM 42:0;O2	FALSE	817.50	Unit	184.10	13.18	1	166	35	5	Positive
SM	SM 42:1;O2 [a/b/c]	FALSE	815.50	Unit	184.10	12.15	2	166	35	5	Positive
SM	SM 42:2;O2 [a/b]	FALSE	813.50	Unit	184.10	10.71	2	166	35	5	Positive
SM	SM 42:3;O2	FALSE	811.50	Unit	184.10	9.71	2	166	35	5	Positive
SM	SM 42:4;O2	FALSE	809.50	Unit	184.10	8.52	2	166	35	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
SM	SM 43:0;O2 [a/b]	FALSE	831.50	Unit	184.10	13.65	2	166	35	5	Positive
SM	SM 43:1;O2 [a/b]	FALSE	829.50	Unit	184.10	13.33	2	166	35	5	Positive
SM	SM 43:2;O2 [a/b]	FALSE	827.50	Unit	184.10	11.85	1	166	35	5	Positive
SM	SM 43:3;O2	FALSE	825.50	Unit	184.10	10.35	1	166	35	5	Positive
SM	SM 44:1;O2 [a/b]	FALSE	843.50	Unit	184.10	13.76	1	166	35	5	Positive
SM	SM 44:2;O2 [a/b]	FALSE	841.50	Unit	184.10	12.47	1	166	35	5	Positive
SM	SM 44:3;O2 [a/b]	FALSE	839.50	Unit	184.10	11.14	1	166	35	5	Positive
SM	SM 44:4;O2	FALSE	837.50	Unit	184.10	9.86	1	166	35	5	Positive
SM	SM 45:1;O2	FALSE	857.50	Unit	184.10	13.60	2	166	35	5	Positive
SM	SM 45:2;O2	FALSE	855.50	Unit	184.10	13.27	2	166	35	5	Positive
SM	SM 45:3;O2	FALSE	853.50	Unit	184.10	12.62	1	166	35	5	Positive
SM	SM 46:2;O2	FALSE	869.50	Unit	184.10	13.68	1	166	35	5	Positive
SM	SM 46:3;O2	FALSE	867.50	Unit	184.10	12.88	2	166	35	5	Positive
SM	SM 46:4;O2	FALSE	865.50	Unit	184.10	11.72	1	166	35	5	Positive
Sph	SPB 17:0;O2 [IS]	FALSE	288.30	Unit	270.30	2.26	1	166	10	4	Positive
Sph	SPB 17:1;O2 [IS]	FALSE	286.30	Unit	268.30	2.14	1	166	10	4	Positive
Sph	SPB 18:1;O2	FALSE	300.30	Unit	282.30	2.48	1	166	10	4	Positive
Sph	SPB 18:2;O2	FALSE	298.30	Unit	280.30	1.98	1	166	10	4	Positive
Sph	SPB 20:1;O2	FALSE	328.30	Unit	310.30	3.18	1	166	10	4	Positive
S1P	SPBP 17:1;O2	FALSE	366.20	Unit	250.30	1.90	1	166	12	4	Positive
S1P	SPBP 18:0;O2	FALSE	382.20	Unit	284.30	2.45	1	166	12	4	Positive
S1P	SPBP 18:1;O2	FALSE	380.20	Unit	264.30	2.23	1	166	12	4	Positive
S1P	SPBP 18:1;O2 [D7]	FALSE	387.20	Unit	271.30	2.22	1	166	12	4	Positive
S1P	SPBP 20:1;O2	FALSE	408.20	Unit	292.30	2.97	1	166	12	4	Positive
TG | TG O	TG 15:0_15:0_18:1 [D7]	FALSE	829.80	Unit	523.50	16.41	1	166	25	5	Positive
TG | TG O	TG 48:0 [NL-16:0]	FALSE	824.80	Unit	551.50	16.57	1	166	25	5	Positive
TG | TG O	TG 48:0 [NL-18:0]	FALSE	824.80	Unit	523.50	16.59	1	166	25	5	Positive
TG | TG O	TG 48:1 [NL-16:1]	FALSE	822.80	Unit	551.50	16.44	1	166	25	5	Positive
TG | TG O	TG 48:1 [NL-18:1]	FALSE	822.80	Unit	523.50	16.41	1	166	25	5	Positive
TG | TG O	TG 48:2 [NL-14:0]	FALSE	820.80	Unit	575.50	16.18	1	166	25	5	Positive
TG | TG O	TG 48:2 [NL-14:1]	FALSE	820.80	Unit	577.50	16.24	1	166	25	5	Positive
TG | TG O	TG 48:2 [NL-16:1]	FALSE	820.80	Unit	549.50	16.25	1	166	25	5	Positive
TG | TG O	TG 48:2 [NL-18:2]	FALSE	820.80	Unit	523.50	16.19	1	166	25	5	Positive
TG | TG O	TG 48:3 [NL-14:0]	FALSE	818.80	Unit	573.50	15.85	1	166	25	5	Positive
TG | TG O	TG 48:3 [NL-16:1]	FALSE	818.80	Unit	547.50	15.83	1	166	25	5	Positive
TG | TG O	TG 48:3 [NL-18:3]	FALSE	818.80	Unit	523.50	15.86	1	166	25	5	Positive
TG | TG O	TG 49:1 [NL-16:1]	FALSE	836.80	Unit	565.50	16.51	1	166	25	5	Positive
TG | TG O	TG 49:1 [NL-17:1] | TG O-50:1 [NL-17:1]	FALSE	836.80	Unit	551.50	16.51	1	166	25	5	Positive
TG | TG O	TG 50:0 [NL-18:0]	FALSE	852.80	Unit	551.50	16.73	1	166	25	5	Positive
TG | TG O	TG 50:1 [NL-14:0]	FALSE	850.80	Unit	605.50	16.59	1	166	25	5	Positive
TG | TG O	TG 50:1 [NL-16:0]	FALSE	850.80	Unit	577.50	16.59	1	166	25	5	Positive
TG | TG O	TG 50:1 [NL-18:1]	FALSE	850.80	Unit	551.50	16.59	1	166	25	5	Positive
TG | TG O	TG 50:2 [NL-14:0]	FALSE	848.80	Unit	603.50	16.44	1	166	25	5	Positive
TG | TG O	TG 50:2 [NL-16:1]	FALSE	848.80	Unit	577.50	16.44	1	166	25	5	Positive
TG | TG O	TG 50:2 [NL-18:1]	FALSE	848.80	Unit	549.50	16.44	1	166	25	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
TG | TG O	TG 50:2 [NL-18:2]	FALSE	848.80	Unit	551.50	16.45	1	166	25	5	Positive
TG | TG O	TG 50:3 [NL-14:0]	FALSE	846.80	Unit	601.50	16.23	1	166	25	5	Positive
TG | TG O	TG 50:3 [NL-14:1]	FALSE	846.80	Unit	603.50	16.29	1	166	25	5	Positive
TG | TG O	TG 50:3 [NL-16:1]	FALSE	846.80	Unit	575.50	16.25	1	166	25	5	Positive
TG | TG O	TG 50:3 [NL-18:2]	FALSE	846.80	Unit	549.50	16.23	1	166	25	5	Positive
TG | TG O	TG 50:3 [NL-18:3]	FALSE	846.80	Unit	551.50	16.29	1	166	25	5	Positive
TG | TG O	TG 50:4 [NL-14:0]	FALSE	844.80	Unit	599.50	15.88	1	166	25	5	Positive
TG | TG O	TG 50:4 [NL-20:4]	FALSE	844.80	Unit	523.50	16.09	1	166	25	5	Positive
TG | TG O	TG 51:0 [NL-16:0]	FALSE	866.70	Unit	593.40	16.81	1	166	25	5	Positive
TG | TG O	TG 51:1 [NL-17:0]	FALSE	864.80	Unit	577.50	16.66	1	166	25	5	Positive
TG | TG O	TG 51:2 [NL-15:0]	FALSE	862.80	Unit	603.50	16.53	1	166	25	5	Positive
TG | TG O	TG 51:2 [NL-17:0]	FALSE	862.80	Unit	575.50	16.53	1	166	25	5	Positive
TG | TG O	TG 51:2 [NL-17:1] | TG O-52:2 [NL-17:1]	FALSE	862.80	Unit	577.50	16.53	1	166	25	5	Positive
TG | TG O	TG 52:1 [NL-18:0]	FALSE	878.80	Unit	577.50	16.74	1	166	25	5	Positive
TG | TG O	TG 52:1 [NL-18:1]	FALSE	878.80	Unit	579.50	16.74	1	166	25	5	Positive
TG | TG O	TG 52:2 [NL-16:0]	FALSE	876.80	Unit	603.50	16.61	1	166	25	5	Positive
TG | TG O	TG 52:2 [NL-18:2]	FALSE	876.80	Unit	579.50	16.63	1	166	25	5	Positive
TG | TG O	TG 52:3 [NL-16:1]	FALSE	874.80	Unit	603.50	16.47	1	166	25	5	Positive
TG | TG O	TG 52:3 [NL-18:2]	FALSE	874.80	Unit	577.50	16.48	1	166	25	5	Positive
TG | TG O	TG 52:4 [NL-16:1]	FALSE	872.80	Unit	601.50	16.29	1	166	25	5	Positive
TG | TG O	TG 52:4 [NL-18:2]	FALSE	872.80	Unit	575.50	16.30	1	166	25	5	Positive
TG | TG O	TG 52:4 [NL-18:3]	FALSE	872.80	Unit	577.50	16.32	1	166	25	5	Positive
TG | TG O	TG 52:5 [NL-18:3]	FALSE	870.80	Unit	575.50	16.01	1	166	25	5	Positive
TG | TG O	TG 52:5 [NL-20:4]	FALSE	870.80	Unit	549.50	16.14	1	166	25	5	Positive
TG | TG O	TG 52:5 [NL-20:5]	FALSE	870.80	Unit	551.50	16.14	1	166	25	5	Positive
TG | TG O	TG 53:2 [NL-17:1] | TG O-54:2 [NL-17:1]	FALSE	890.80	Unit	605.50	16.68	1	166	25	5	Positive
TG | TG O	TG 53:2 [NL-18:1] | TG O-54:2 [NL-18:1]	FALSE	890.80	Unit	591.50	16.68	1	166	25	5	Positive
TG | TG O	TG 54:0 [NL-18:0]	FALSE	908.80	Unit	607.50	17.02	1	166	25	5	Positive
TG | TG O	TG 54:1 [NL-18:1]	FALSE	906.80	Unit	607.50	16.89	1	166	25	5	Positive
TG | TG O	TG 54:2 [NL-18:0]	FALSE	904.80	Unit	603.50	16.76	1	166	25	5	Positive
TG | TG O	TG 54:2 [NL-20:1]	FALSE	904.80	Unit	577.50	16.74	1	166	25	5	Positive
TG | TG O	TG 54:3 [NL-18:1]	FALSE	902.80	Unit	603.50	16.62	1	166	25	5	Positive
TG | TG O	TG 54:3 [NL-18:2]	FALSE	902.80	Unit	605.50	16.64	1	166	25	5	Positive
TG | TG O	TG 54:4 [NL-18:2]	FALSE	900.80	Unit	603.50	16.49	1	166	25	5	Positive
TG | TG O	TG 54:4 [NL-20:3]	FALSE	900.80	Unit	577.50	16.52	1	166	25	5	Positive
TG | TG O	TG 54:5 [NL-18:3]	FALSE	898.80	Unit	603.50	16.36	1	166	25	5	Positive
TG | TG O	TG 54:5 [NL-20:4]	FALSE	898.80	Unit	577.50	16.43	1	166	25	5	Positive
TG | TG O	TG 54:6 [NL-18:3]	FALSE	896.80	Unit	601.50	16.04	1	166	25	5	Positive
TG | TG O	TG 54:6 [NL-20:4]	FALSE	896.80	Unit	575.50	16.23	1	166	25	5	Positive
TG | TG O	TG 54:6 [NL-20:5]	FALSE	896.80	Unit	577.50	16.26	1	166	25	5	Positive
TG | TG O	TG 54:6 [NL-22:6]	FALSE	896.80	Unit	551.50	16.35	1	166	25	5	Positive
TG | TG O	TG 54:7 [NL-20:5]	FALSE	894.80	Unit	575.50	16.00	1	166	25	5	Positive
TG | TG O	TG 54:7 [NL-22:6]	FALSE	894.80	Unit	549.50	16.01	1	166	25	5	Positive
TG | TG O	TG 56:6 [NL-20:4]	FALSE	924.80	Unit	603.50	16.46	1	166	25	5	Positive

Compound Group	Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	Ret Time (min)	Delta Ret Time	Fragmentor	Collision Energy	Cell Accelerator Voltage	Polarity
TG | TG O	TG 56:6 [NL-22:5]	FALSE	924.80	Unit	577.50	16.50	2	166	25	5	Positive
TG | TG O	TG 56:7 [NL-20:4]	FALSE	922.80	Unit	601.50	16.27	1	166	25	5	Positive
TG | TG O	TG 56:7 [NL-20:5]	FALSE	922.80	Unit	603.50	16.30	1	166	25	5	Positive
TG | TG O	TG 56:7 [NL-22:5]	FALSE	922.80	Unit	575.50	16.36	1	166	25	5	Positive
TG | TG O	TG 56:7 [NL-22:6]	FALSE	922.80	Unit	577.50	16.36	1	166	25	5	Positive
TG | TG O	TG 56:8 [NL-20:4]	FALSE	920.80	Unit	599.50	16.14	1	166	25	5	Positive
TG | TG O	TG 56:8 [NL-20:5]	FALSE	920.80	Unit	601.50	16.14	1	166	25	5	Positive
TG | TG O	TG 56:8 [NL-22:6]	FALSE	920.80	Unit	575.50	16.10	1	166	25	5	Positive
TG | TG O	TG 56:9 [NL-22:6]	FALSE	918.80	Unit	573.50	15.77	1	166	25	5	Positive
TG | TG O	TG 58:10 [NL-22:6]	FALSE	944.90	Unit	599.50	16.01	1	166	25	5	Positive
TG | TG O	TG 58:8 [NL-22:6]	FALSE	948.80	Unit	603.50	16.39	1	166	25	5	Positive
TG | TG O	TG 58:9 [NL-22:6]	FALSE	946.90	Unit	601.50	16.20	1	166	25	5	Positive
TG | TG O	TG O-50:1 [NL-15:0]	FALSE	836.80	Unit	577.50	16.72	1	166	25	5	Positive
TG | TG O	TG O-50:1 [NL-16:0]	FALSE	836.80	Unit	563.50	16.68	1	166	25	5	Positive
TG | TG O	TG O-50:1 [NL-18:1]	FALSE	836.80	Unit	537.50	16.69	1	166	25	5	Positive
TG | TG O	TG O-50:2 [NL-16:1]	FALSE	834.80	Unit	563.50	16.65	1	166	25	5	Positive
TG | TG O	TG O-50:2 [NL-18:1]	FALSE	834.80	Unit	535.50	16.84	1	166	25	5	Positive
TG | TG O	TG O-50:2 [NL-18:2]	FALSE	834.80	Unit	537.50	16.65	1	166	25	5	Positive
TG | TG O	TG O-50:3 [NL-18:2]	FALSE	832.80	Unit	535.50	16.24	1	166	25	5	Positive
TG | TG O	TG O-52:0 [NL-16:0]	FALSE	866.80	Unit	593.50	17.01	1	166	25	5	Positive
TG | TG O	TG O-52:1 [NL-16:0]	FALSE	864.80	Unit	591.50	17.12	1	166	25	5	Positive
TG | TG O	TG O-52:1 [NL-18:1]	FALSE	864.80	Unit	565.50	16.97	1	166	25	5	Positive
TG | TG O	TG O-52:2 [NL-16:0]	FALSE	862.80	Unit	589.50	16.76	1	166	25	5	Positive
TG | TG O	TG O-52:2 [NL-18:1]	FALSE	862.80	Unit	563.50	16.76	1	166	25	5	Positive
TG | TG O	TG O-54:3 [NL-17:1] | TG P-54:2 [NL-P-18:0]	FALSE	888.80	Unit	603.50	16.83	2	166	25	5	Positive
TG | TG O	TG O-54:3 [NL-18:1]	FALSE	888.80	Unit	589.50	16.78	1	166	25	5	Positive
TG | TG O	TG O-54:4 [NL-17:1] | TG P-54:3 [NL-P-18:0]	FALSE	886.80	Unit	601.50	16.69	2	166	25	5	Positive
TG | TG O	TG O-54:4 [NL-18:2]	FALSE	886.80	Unit	589.50	16.66	2	166	25	5	Positive
TG | TG O	TG O-54:8 [NL-17:1] | TG P-54:9 [NL-P-18:0]	FALSE	878.80	Unit	581.50	16.63	1	166	25	5	Positive
TG | TG O	TG O-54:8 [NL-18:2]	FALSE	870.80	Unit	573.50	16.00	2	166	25	5	Positive
CoQ10	Ubiquinol	FALSE	882.70	Unit	197.00	15.12	1	166	17	5	Positive
CoQ10	Ubiquinone	FALSE	880.70	Unit	197.00	15.80	1	166	17	5	Positive

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