Supporting Information

Least Absolute Shrinkage and Selection Operator-based Prediction of Collision Cross Section Values for Ion Mobility Mass Spectrometric Analysis of Lipids

Jian-Ying Wang[a,b,c#], Ying-Hao Yin[a#], Jia-Yi Zheng[a], Li-Fang Liu[a*], Zhong-Ping Yao[b,c*], Gui-Zhong Xin[a*]

[a]State Key Laboratory of Natural Medicines, Department of Chinese Medicines Analysis, School of Traditional Chinese Pharmacy, China Pharmaceutical University, No. 24 Tongjia Lane, Nanjing, China.

[b]State Key Laboratory of Chinese Medicine and Molecular Pharmacology (Incubation) and Shenzhen Key Laboratory of Food Biological Safety Control, Shenzhen Research Institute of Hong Kong Polytechnic University, Shenzhen 518057, China.

[c]State Key Laboratory of Chemical Biology and Drug Discovery, Food Safety and Technology Research Centre and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong SAR, China.

[#]These authors contributed equally to this work.

***Corresponding author:**

Li-Fang Liu

State Key Laboratory of Natural Medicines, Department of Chinese Medicines Analysis, China Pharmaceutical University, No. 24 Tongjia Lane, Nanjing, China

E-mail address: liulifang69@126.com (L.F. Liu)

Gui-Zhong Xin
Department of Chinese Medicines Analysis, School of Traditional Chinese Pharmacy, China Pharmaceutical University, No. 24 Tongjia Lane, Nanjing, China
Tel: +86 13813884764; email address: xinguizhong1984@126.com

Zhong-Ping Yao
Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong
Tel: +852 2358 7332; fax: +852 2358 1559, email address: zhongping.yao@polyu.edu.hk

Contents:

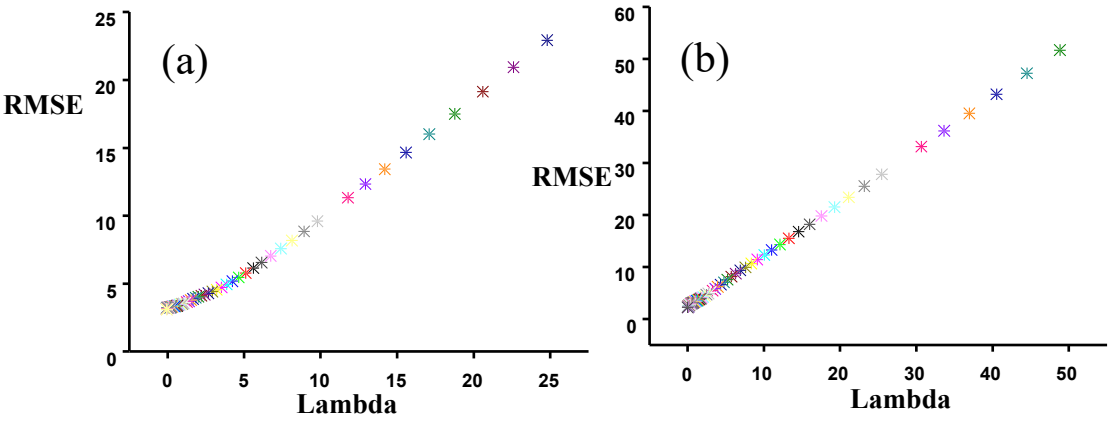

Figure S1. The relationship between Lambda and RMSE during model development in positive (a) and negative (b) ion modes

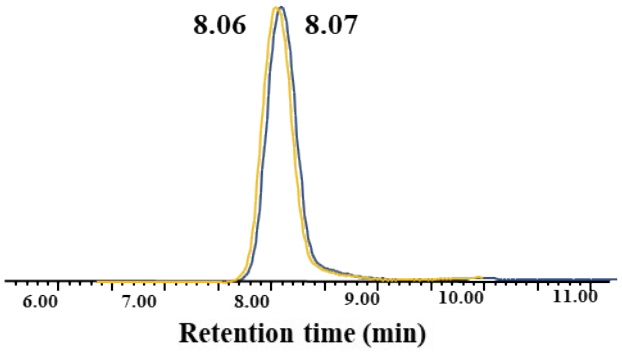

Figure S2. Chromatograms of sn-2 positional lipid isomers: 1,2-linolein-3-olein /1,3-linolein-2-olein.

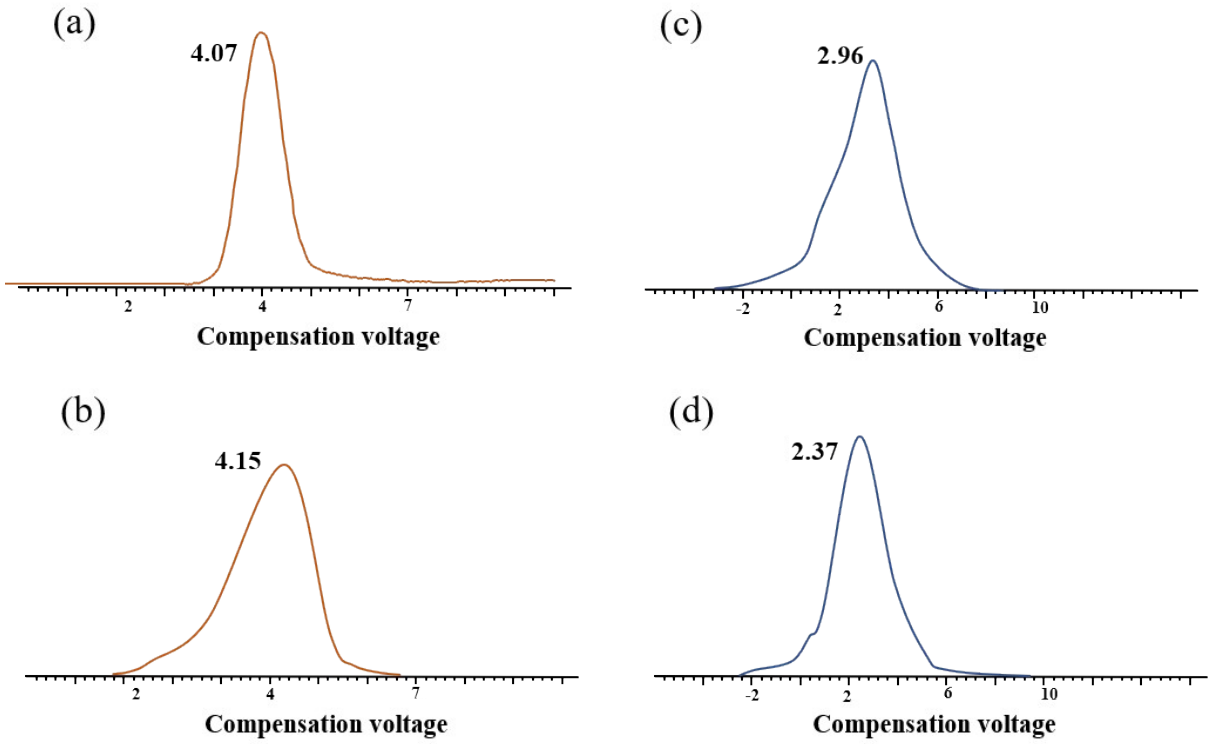

Figure S3. Total ionograms resulting from DMS-based analysis of lipid isomer including sn-positional isomers PC (16:0/14:0) / PC (14:0/16:0) (a,b) and C=C positional isomers PC (18:1△6-*cis*) / PC (18:1△9-*cis*) (c,d).

Table S1. Information of lipid standards used for the validation

Lipid standard	*m/z*	Ions
Glycerol triheptadecanoate	866.8171	$[M+NH_4]^+$
TG(18:0/15:0/18:0)	866.8171	$[M+NH_4]^+$
TG(18:1(9Z)/16:0/18:1(9Z))	876.8015	$[M+NH_4]^+$
TG(18:1(9Z)/18:1(9Z)/16:0)	876.8015	$[M+NH_4]^+$
PE(16:0/16:0)	692.5225	$[M+H]^+$
PC(17:0/17:0)	762.6007	$[M+H]^+$
PC(17:0/0:0)	510.3554	$[M+H]^+$
POP TG(16:0/18:1(9Z)/16:0)	850.7858	$[M+NH_4]^+$
PPO TG(16:0/16:0/18:1(9Z))	850.7858	$[M+NH_4]^+$
1,2-linolein-3-olein	898.7950	$[M+NH_4]^+$
1,3-linolein-2-olein	898.7950	$[M+NH_4]^+$
oleic acid	281.3450	$[M+H]^+$
elaidic acid	281.3450	$[M+H]^+$
linoleic acid	279.3210	$[M+H]^+$
linoelaidic acid	279.3210	$[M+H]^+$
DHA	329.3680	$[M+H]^+$
DHA	329.3680	$[M+H]^+$
w-3AA	303.3380	$[M+H]^+$
w-6 AA	303.3380	$[M+H]^+$

Table S2. Molecular descriptors in positive ion mode

No.	MD	No.	MD	No.	MD	No.	MD
1	nSmallRings [a]	14	nAtomLAC [a]	27	C3SP3 [a]	40	Dipole.X [b]
2	tpsaEfficiency [a]	15	nAtomP [a]	28	bpol [a]	41	Dipole.Y [b]
3	Zagreb [a]	16	khs.dsCH [a]	29	BCUTw.1l [a]	42	Dipole.Z [b]
4	XLogP [a]	17	khs.dssC [a]	30	BCUTc.1l [a]	43	Dreiding.energy [b]
5	WTPT.2 [a]	18	khs.sNH2 [a]	31	BCUTp.1h [a]	44	MMFF94.energy [b]
6	WTPT.3 [a]	19	khs.ssNH [a]	32	nBase [a]	45	Minimal.projection.area [b]
7	WTPT.5 [a]	20	khs.ssssN [a]	33	ATSc4 [a]	46	Maximal.projection.area [b]
8	LipinskiFailures [a]	21	khs.sOH [a]	34	ATSc5 [a]	47	Minimal.projection.radius [b]
9	topoShape [a]	22	khs.dO [a]	35	nAtom [a]	48	Maximal.projection.radius [b]
10	MDEC.11 [a]	23	HybRatio [a]	36	ALogP [a]	49	Length.perpendicular.to.the.max.area [b]
11	MDEC.12 [a]	24	VPC.4 [a]	37	nAcid [a]	50	Length.perpendicular.to.the.min.area [b]
12	MDEC.22 [a]	25	SC.3 [a]	38	*m/z*	51	van.der.Waals.volume [b]
13	MDEC.23 [a]	26	C1SP3 [a]	39	Dipole [b]	52	Van.der.Waals.surface.area 3D [b]

[a] Calculation by R package rcdk; [b] Calculation by ChemAxon software. More detailed information of these molecular descriptors is provided below:

1 nSmallRings: The number of small rings from size 3 to 9

2. tpsaEfficiency: Polar surface area expressed as a ratio to molecular size

3. Zagreb: Sum of the squares of atom degree over all heavy atoms

4. XLogP: Prediction of logP based on the atom-type method

5. WTPT.2: Molecular ID / number of atoms

6. WTPT.3: Sum of path lengths starting from heteroatoms

7. WTPT.5: Sum of path lengths starting from nitrogens

8. LipinskiFailures: Number failures of the Lipinski's Rule Of 5

9. topoShape: A measure of the anisotropy in a molecule

10. MDEC.11: Molecular distance edge between all primary carbons

11. MDEC.12: Molecular distance edge between all primary and secondary carbons

12. MDEC.13: Molecular distance edge between all primary and tertiary carbons

13. MDEC.22: Molecular distance edge between all secondary carbons

14. MDEC.23: Molecular distance edge between all secondary and tertiary carbons

15. nAtomLAC: Number of atoms in the longest aliphatic chain

16. nAtomP: Number of atoms in the largest pi system

17. khs.dsCH: Count of atom-type E-State: =CH-

18. khs.dssC: Count of atom-type E-State: =C<

19. khs.sNH2: Count of atom-type E-State: -NH2

20. khs.ssNH: Count of atom-type E-State: -NH-

21. khs.ssssN: Count of atom-type E-State: -N<

22.. khs.sOH: Count of atom-type E-State: -OH

23. khs.dO: Count of atom-type E-State: =O

24. HybRatio: Fraction of sp3 carbons to sp2 carbons

25. VPC.4: Valence path cluster, orders 4
26. SC.3: Simple cluster, orders 3
27. C1SP3: Singly bound carbon bound to one other carbon
28. bpol: Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens)
29. BCUTw.1l: nhigh lowest atom weighted BCUTS
30. BCUTc.1l: nhigh lowest partial charge
31. BCUTp.1h: nlow highest polarizability:
32. nBase: Basic group count descriptor
33. ATSc4: AutocorrelationCharge using partial charges
34. ATSc5: AutocorrelationCharge using partial charges
35. nAtom: Number of atoms
36. ALogP: Ghose-Crippen LogKow
37. nAcid: Acidic group count descriptor
38: *m/z*: Mass to charge ratio
39. Dipole: Dipole moment
40. Dipole X: Dipole moments of the molecule oriented along x axis
41. Dipole Y: Dipole moments of the molecule oriented along y axis
42. Dipole Z: Dipole moments of the molecule oriented along z axis
43. Dreiding energy: The energy related to the 3D structure (conformation) of the molecule using dreiding force field
44. MMFF94 energy: The energy of the 3D structure (conformation) of the molecule using MMFF94 force field
45. Minimal projection area: The minimum of projection areas of the conformer, based on the van der Waals radius (in Å2
46. Maximal projection area: The maximum of projection areas of the conformer, based on the van der Waals radius (in Å2)
47. Minimal projection radius: The radius for the minimal projection area of the conformer (in Å)
48. Maximal projection radius: The radius for the maximal projection area of the conformer (in Å)
49. Length perpendicular to the max area: The maximal extension of the conformer perpendicular to the maximal projection area (in Å)
50. Length perpendicular to the min area: The minimal extension of the conformer perpendicular to the maximal projection area (in Å)
51. van der Waals volume: The van der Waals volume of the conformer (in Å3)
52. Van der Waals surface area 3D: The van der Waals surface of the molecule (in Å2)

Table S3. Molecular descriptors in negative ion mode

No.	MD	No.	MD	No.	MD	No.	MD
1	nSmallRings [a]	17	MDEO.22 [a]	33	VPC.4 [a]	49	m.z
2	nRings5 [a]	18	nAtomLAC [a]	34	SC.3 [a]	50	Dipole [b]
3	tpsaEfficiency [a]	19	nAtomP [a]	35	SC.4 [a]	51	DipoleX [b]
4	Zagreb [a]	20	nAtomLC [a]	36	C1SP3 [a]	52	DipoleY [b]
5	XLogP [a]	21	khs.ssCH2 [a]	37	bpol [a]	53	DipoleZ [b]
6	WTPT.2 [a]	22	khs.dsCH [a]	38	BCUTw.1l [a]	54	Dreiding energy [b]
7	WTPT.3 [a]	23	khs.dssC [a]	39	BCUTc.1l [a]	55	MMFF94energy [b]
8	WTPT.5 [a]	24	khs.sNH2 [a]	40	BCUTp.1h [a]	56	Minimal projection area. [b]
9	LipinskiFailures [a]	25	khs.ssNH [a]	41	nBase [a]	57	Maximal projection area [b]
10	nRotB [a]	26	khs.dO [a]	42	ATSm1 [a]	58	Minimal projection radius [b]
11	topoShape [a]	27	khs.ddssS [a]	43	ATSc3 [a]	59	Maximal projection radius [b]
12	MDEC.11 [a]	28	Kier3 [a]	44	ATSc4 [a]	60	Length perpendicular to the max area [b]
13	MDEC.12 [a]	29	nHBAcc [a]	45	ATSc5 [a]	61	Length perpendicular to the min area [b]
14	MDEC.13 [a]	30	FMF [a]	46	nAtom [a]	62	Vander Waals volume [b]
15	MDEC.22 [a]	31	VP.0 [a]	47	ALogP [a]	63	Vander Waals surface area.3D. [b]
16	MDEC.23 [a]	32	SPC.4 [a]	48	nAcid [a]		

[a] Calculation by R package rcdk; [b] Calculation by ChemAxon software. The detailed information of these molecular descriptors is summarized below:

1 nSmallRings: The number of small rings from size 3 to 9

2. nRings5: Individual breakdown of 5 membered rings

3. tpsaEfficiency: Polar surface area expressed as a ratio to molecular size

4. Zagreb: Sum of the squares of atom degree over all heavy atoms

5. XLogP: Prediction of logP based on the atom-type method

6. WTPT.2: Molecular ID / number of atoms

7. WTPT.3: Sum of path lengths starting from heteroatoms

8. WTPT.5: Sum of path lengths starting from nitrogens

9. LipinskiFailures: Number failures of the Lipinski's Rule Of 5

10. nRotB: Number of rotatable bonds, excluding terminal bonds

11. topoShape: A measure of the anisotropy in a molecule

12. MDEC.11: Molecular distance edge between all primary carbons

13. MDEC.12: Molecular distance edge between all primary and secondary carbons

14. MDEC.13: Molecular distance edge between all primary and tertiary carbons

15. MDEC.22: Molecular distance edge between all secondary carbons

16. MDEC.23: Molecular distance edge between all secondary and tertiary carbons

17. MDEO.22: Molecular distance edge between all secondary oxygens

18. nAtomLAC: Number of atoms in the longest aliphatic chain

19. nAtomP: Number of atoms in the largest pi system

20. nAtomLC: Number of atoms in the largest chain

21. khs.ssCH2: Count of atom-type E-State: -CH2-
22. khs.dsCH: Count of atom-type E-State: =CH-
23. khs.dssC: Count of atom-type E-State: =C<
24. khs.sNH2: Count of atom-type E-State: -NH2
25. khs.ssNH: Count of atom-type E-State: -NH2
26. khs.dO: Count of atom-type E-State: =O
27. khs.ddssS: Count of atom-type E-State: >S==
28. Kier3: Calculation of Kier and Hall kappa molecular shape indices
29. nHBAcc: Number of hydrogen bond acceptors
30. FMF: Ratio of heavy atoms in the framework to the total number of heavy atoms in the molecule.
31. VP.0: Valence path, orders 0
32. SPC.4: Simple path cluster, orders 4
33. VPC.4: Valence path cluster, orders 4
34. SC.3: Simple cluster, orders 3
35. SC.4: Simple cluster, orders 4
36. C1SP3: Singly bound carbon bound to one other carbon
37. bpol: Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens)
38. BCUTw.1l: nhigh lowest atom weighted BCUTS
39. BCUTc.1l: nhigh lowest partial charge
40. BCUTp.1h: nlow highest polarizability
41. nBase: Basic group count descriptor
42. ATSm1: Autocorrelation Mass descriptor, weighted by scaled atomic mass
43. ATSc3: Autocorrelation Charge using partial charges
44. ATSc4: Autocorrelation Charge using partial charges
45. ATSc5: Autocorrelation Charge using partial charges
46. nAtom: Number of atoms
47. ALogP: Ghose-Crippen LogKow
48. nAcid: Acidic group count descriptor
49. *m/z*: Mass to charge ratio
50. Dipole: Dipole moment
52. Dipole.X: Dipole moments of the molecule oriented along x axis
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56. Minimal projection area: the minimum of projection areas of the conformer, based on the van der Waals radius (in Å2
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58. Minimal projection radius: calculates the radius for the minimal projection area of the conformer (in Å)
59. Maximal projection radius: calculates the radius for the maximal projection area of the conformer (in Å)

60. Length perpendicular to the max area: The maximal extension of the conformer perpendicular to the maximal projection area (in Å)
61. Length.perpendicular.to.the.min.area: The minimal extension of the conformer perpendicular to the maximal projection area (in Å)
62. van der Waals volume: The van der Waals volume of the conformer (in Å3)
63. Van der Waals surface area 3D: The van der Waals surface of the molecule (in Å2)

Table S4 Identification results for untargeted lipidomics of obese zebrafish*

NO.	*m/z*	*Matched m/z*	Exp CCS (Å²)	Pre CCS (Å²)	ΔCCS (Å²)	Lipid candidate
1	279.2323	279.2330	186.5	182.7	3.8	9E,11E-Octadecadienoic acid
2	407.2940	407.2956	141.2	143.2	2	18Z-heptacosenoic acid
				141.6	0.4	20Z-heptacosenoic acid
3	526.2902	526.2928	224.6	223.5	1.1	LysoPE (0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
				224.9	0.3	LysoPE (22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)
4	623.5688	623.5609	276.9	276.3	0.6	DG (16:0/20:1/0:0)
5	762.6010	762.6007	301.7	304.3	2.5	PC (18:0/16:0)
6	784.5817	784.5851	304.4	300.9	3.5	PC (16:1(9Z)/20:2(11Z,14Z))
				301.0	3.4	PC (20:2(11Z,14Z)/16:1(9Z))
7	790.6892	790.6919	312.5	310.0	2.5	TG (14:1(9Z)/14:1(9Z)/18:1(9Z))
				309.5	3	TG (18:1(9Z)/14:1(9Z)/14:1(9Z))
				310.6	1.9	TG (14:0/14:0/18:3(6Z,9Z,12Z))
				309.5	3	TG (14:0/18:3(6Z,9Z,12Z)/14:0)
				310.4	2.1	TG (18:3(6Z,9Z,12Z)/14:0/14:0)
				309.7	2.8	TG (14:1(9Z)/14:1(9Z)/18:1(11Z))
				310.7	1.8	TG (14:1(9Z)/18:1(11Z)/14:1(9Z))
				311.6	0.9	TG (14:1(9Z)/18:1(9Z)/14:1(9Z))
8	792.7058	792.7076	312.5	305.9	6.6	TG (16:1(9Z)/16:1(9Z)/14:0)
				305.3	7.2	TG (16:1(9Z)/14:0/16:1(9Z))
				306.1	6.4	TG (14:0/16:1(9Z)/16:1(9Z))
9	794.7217	794.7232	315.1	309.5	5.6	TG (14:0/14:0/18:1(9Z))
				311.0	4.1	TG (14:0/18:1(9Z)/14:0)
				309.5	5.6	TG (18:1(9Z)/14:0/14:0)
				311.2	3.9	TG (14:0/18:1(11Z)/14:0)
10	806.7206	806.7232	316.9	312.0	4.9	TG (16:1(9Z)/16:1(9Z)/15:0)
				312.2	4.7	TG (15:0/16:1(9Z)/16:1(9Z))
11	816.7054	816.7076	316.0	315.0	1	TG (14:0/14:0/20:4(5Z,8Z,11Z,14Z))
				317.0	1	TG (14:0/20:4(5Z,8Z,11Z,14Z)/14:0)
				314.7	1.3	TG (14:0/14:0/20:4(8Z,11Z,14Z,17Z))
				316.9	0.9	TG (14:0/20:4(8Z,11Z,14Z,17Z)/14:0)
				315.3	0.7	TG (20:4(5Z,8Z,11Z,14Z)/14:0/14:0)
12	818.7222	818.7232	317.8	315.0	2.8	TG (14:0/14:0/20:3(8Z,11Z,14Z))
				317.5	0.3	TG (14:0/20:3(8Z,11Z,14Z)/14:0)
				314.7	3.1	TG (20:3(8Z,11Z,14Z)/14:0/14:0)
				315.0	2.8	TG (14:0/14:0/20:3(5Z,8Z,11Z))
				318.0	0.2	TG (14:0/20:3(5Z,8Z,11Z)/14:0)
13	820.7391	820.7389	320.4	315.0	5.4	TG (14:1(9Z)/14:1(9Z)/20:0)
				314.0	6.4	TG (20:0/14:1(9Z)/14:1(9Z))
				317.2	3.2	TG (14:1(9Z)/20:0/14:1(9Z))
14	832.5851	832.5851	305.3	301.6	3.7	PC (22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))

				304.1	1.2	PC (18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
15	836.7706	836.7702	325.5	321.7	3.8	TG (14:0/20:1(11Z)/15:0)
				319.9	5.6	TG (15:0/14:0/20:1(11Z))
				319.4	6.1	TG (20:1(11Z)/14:0/15:0)
				322.3	3.2	TG (15:0/20:1(11Z)/14:0)
16	842.7221	842.7232	319.5	321.1	1.6	TG (16:1(9Z)/16:1(9Z)/18:3(6Z,9Z,12Z))
				316.7	2.8	TG (16:1(9Z)/18:3(6Z,9Z,12Z)/16:1(9Z))
				320.7	1.2	TG (18:3(6Z,9Z,12Z)/16:1(9Z)/16:1(9Z))
				321.3	1.8	TG (16:1(9Z)/16:1(9Z)/18:3(9Z,12Z,15Z))
				316.9	2.6	TG (16:1(9Z)/18:3(9Z,12Z,15Z)/16:1(9Z))
				320.8	1.3	TG (18:3(9Z,12Z,15Z)/16:1(9Z)/16:1(9Z))
17	848.7715	848.7702	326.4	323.6	2.8	TG (14:1(9Z)/22:0/14:1(9Z))
				323.9	2.5	TG (22:0/14:1(9Z)/14:1(9Z))
				325.0	1.4	TG (14:1(9Z)/14:1(9Z)/22:0)
18	849.6943	849.6943	323.8	322.1	1.7	PG (O-20:0/22:0)
19	854.7204	854.7232	323.8	321.9	1.9	TG (18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)/15:0)
				323.2	0.6	TG (18:3(6Z,9Z,12Z)/15:0/18:3(6Z,9Z,12Z))
				322.0	1.8	TG (15:0/18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))
				321.9	1.9	TG (18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z)/15:0)
				322.1	1.7	TG (15:0/18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))
				321.6	2.2	TG (15:0/18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))
				322.0	1.8	TG (15:0/18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))
				323.5	0.3	TG (18:3(9Z,12Z,15Z)/15:0/18:3(9Z,12Z,15Z))
				323.5	0.3	TG (18:3(6Z,9Z,12Z)/15:0/18:3(9Z,12Z,15Z))
20	866.8167	866.8171	327.2	328.5	1.3	TG (18:0/15:0/18:0)
				329.3	2.1	TG (15:0/18:0/18:0)
				328.2	1	Glycerol triheptadecanoate
				328.0	0.8	TG (18:0/18:0/15:0)
21	868.7381	868.7389	325.5	325.2	0.3	TG (16:1(9Z)/16:1(9Z)/20:4(5Z,8Z,11Z,14Z))
				325.2	0.3	TG (16:1(9Z)/20:4(5Z,8Z,11Z,14Z)/16:1(9Z))
				324.9	0.6	TG (16:1(9Z)/16:1(9Z)/20:4(8Z,11Z,14Z,17Z))
				323.7	1.8	TG (16:1(9Z)/20:4(8Z,11Z,14Z,17Z)/16:1(9Z))
				325.6	0.1	TG (20:4(5Z,8Z,11Z,14Z)/16:1(9Z)/16:1(9Z))
22	870.7527	870.7545	325.5	325.2	0.3	TG (16:1(9Z)/16:1(9Z)/20:3(8Z,11Z,14Z))
				324.4	1.1	TG (16:1(9Z)/20:3(8Z,11Z,14Z)/16:1(9Z))
				325.0	0.5	TG (20:3(8Z,11Z,14Z)/16:1(9Z)/16:1(9Z))
				325.0	0.5	TG (16:1(9Z)/16:1(9Z)/20:3(5Z,8Z,11Z))
				325.6	0.1	TG (16:1(9Z)/20:3(5Z,8Z,11Z)/16:1(9Z))

Table S5 Training dataset for positive ion mode[1-2,4-6]

Lipid ion	*m/z*	CCS value (Å^2)	Instrument
(3'-sulfo)Galbeta-Cer(d18:1/24:0)	892.6547	309.1	TWIMS
(3'-sulfo)Galbeta-Cer(d18:1/24:1)	890.6391	307.4	TWIMS
Cer(18:1/16:0)	538.5199	253.6	TWIMS
Cer(d18:0/16:0)	540.5350	261.0	TWIMS
Cer(d18:0/18:0)	568.5660	263.1	TWIMS
Cer(d18:0/18:1)	566.5520	261.3	TWIMS
Cer(d18:0/20:0)	596.5980	277.0	TWIMS
Cer(d18:0/22:0)	624.6230	274.1	TWIMS
Cer(d18:0/22:0)	624.6290	284.0	TWIMS
Cer(d18:0/24:0)	652.6600	293.0	TWIMS
Cer(d18:0/24:1)	650.6450	279.1	TWIMS
Cer(d18:0/26:0)	680.6920	299.0	TWIMS
Cer(d18:0/26:1)	678.6760	297.0	TWIMS
Cer(d18:1/14:0)	492.4780	251.0	TWIMS
Cer(d18:1/16:0)	520.5090	258.0	TWIMS
Cer(d18:1/18:0)	566.5520	261.2	TWIMS
Cer(d18:1/18:0)	548.5400	266.0	TWIMS
Cer(d18:1/18:0)	566.5512	261.6	TWIMS
Cer(d18:1/18:0)	588.5332	268.6	TWIMS
Cer(d18:1/18:1(9Z))	564.5350	257.6	TWIMS
Cer(d18:1/18:1)	564.5350	257.6	TWIMS
Cer(d18:1/20:0)	594.5820	266.5	TWIMS
Cer(d18:1/20:0)	576.5710	273.0	TWIMS
Cer(d18:1/22:0)	622.6130	271.8	TWIMS
Cer(d18:1/22:0)	604.6030	279.0	TWIMS
Cer(d18:1/22:0)	622.6138	272.3	TWIMS
Cer(d18:1/23:0)	636.6294	275.6	TWIMS
Cer(d18:1/23:0)	658.6114	281.6	TWIMS
Cer(d18:1/24:0)	650.6450	279.1	TWIMS
Cer(d18:1/24:0)	632.6340	287	TWIMS
Cer(d18:1/24:0)	650.6451	279.3	TWIMS
Cer(d18:1/24:1)	648.6300	276.8	TWIMS
Cer(d18:1/24:1)	630.6180	285.0	TWIMS
Cer(d18:1/25:0)	664.6607	282.0	TWIMS
Cer(d18:1/26:0)	678.6720	284.4	TWIMS
Cer(d18:1/26:0)	660.6650	295.0	TWIMS
Cer(d18:1/26:1)	676.6600	282.4	TWIMS
Cer(d18:1/26:1)	658.6500	293.0	TWIMS
Cer(d18:2/23:0)	634.6138	273.5	TWIMS
Cer(d18:2/23:0)	656.5958	273.8	TWIMS
Cer(d18:2/23:0)	656.5958	273.8	TWIMS
DG(16:0/16:0)	551.5030	256.3	TWIMS
DG(16:0/18:0)	614.5740	276.0	TWIMS

DG(16:0/18:1(11Z)/0:0)	612.5567	261.1	TWIMS
DG(16:0/18:1(9Z)/0:0)	612.5550	271.0	TWIMS
DG(16:0/18:2)	610.5360	268.0	TWIMS
DG(16:1/18:1)	610.5370	264.0	TWIMS
DG(18:1(9Z)/18:1(9Z)/0:0)	638.5710	273.0	TWIMS
DG(18:1/18:1)	603.5430	263.5	TWIMS
DG(18:1/18:2)	636.5330	269.0	TWIMS
DG(18:2(9Z,12Z)/16:0/ 0:0)	615.4951	260.5	TWIMS
DG(18:2(9Z,12Z)/18:2 (9Z,12Z))	639.4950	261.5	TWIMS
DG(18:2/18:2)	599.5080	255.9	TWIMS
GlcCer(d18:1/18:0)	750.5860	282.2	TWIMS
GlcCer(d18:1/18:0)	728.6040	282.6	TWIMS
GlcCer(d18:1/18:0)	728.6040	284.1	TWIMS
GlcCer(d18:1/18:1)	726.5880	281.8	TWIMS
GlcCer(d18:1/20:0)	756.6350	287.8	TWIMS
GlcCer(d18:1/22:0)	784.6650	293.2	TWIMS
GlcCer(d18:1/22:0)	784.6650	293.2	TWIMS
GlcCer(d18:1/22:0)	806.6560	294.3	TWIMS
GlcCer(d18:1/24:0)	812.6960	299.7	TWIMS
GlcCer(d18:1/24:0)	834.6760	299.1	TWIMS
GlcCer(d18:1/24:1)	810.6830	298.2	TWIMS
GlcCer(d18:1/24:1)	832.6660	297.3	TWIMS
GlcCer(d18:1/26:1)	838.7090	304.5	TWIMS
GlcCer(d18:1/26:1)	860.6940	304.7	TWIMS
HexCer(d18:1/12:0)	644.5100	277.0	TWIMS
HexCer(d18:1/16:0)	700.5720	284.0	TWIMS
HexCer(d18:1/18:0)	728.6040	286.0	TWIMS
HexCer(d18:1/20:0)	756.6350	291.0	TWIMS
HexCer(d18:1/23:0)	798.6820	296.0	TWIMS
HexCer(d18:1/24:1)	810.6820	301.0	TWIMS
HexCer(d18:1/26:0)	840.7290	309.0	TWIMS
HexCer(d18:1/26:1)	838.7130	307.0	TWIMS
HexCer(d18:1/h20:0)	772.6300	293.0	TWIMS
HexCerd18:1/24:0	812.6970	304.0	TWIMS
LPC(14:0)	468.3090	220.8	TWIMS
LPC(16:0)	496.3400	228.5	TWIMS
LPC(20:2)	548.3710	250.0	TWIMS
LPC(20:3)	546.3550	249.0	TWIMS
LPC(20:4)	544.3400	242.0	TWIMS
LPC(O-16:0)	482.3610	234.0	TWIMS
LPC(O-18:0)	510.3920	241.0	TWIMS
LPC(P-16:0)	480.3450	230.0	TWIMS
LPC(P-18:0)	508.3760	232.0	TWIMS
LPC18:1	522.3550	240.0	TWIMS

LPE(18:0)	482.3230	220.8	TWIMS
LPE(20:5)	498.2630	219.0	TWIMS
LPE(20:5)	498.2630	219.0	TWIMS
LPE(O-16:0)	438.2980	209.0	TWIMS
LPE(P-16:0)	460.2780	214.7	TWIMS
LPE(P-16:0)	454.2920	213.4	TWIMS
LPE(P-16:0)	476.2740	218.8	TWIMS
LPE(P-18:0)	488.3090	222.0	TWIMS
LPE(P-18:0)	476.2740	218.8	TWIMS
LPE(P-18:0)	504.3060	224.8	TWIMS
LPC(20:4(8Z,11Z,14Z,17Z))	544.3400	232.4	TWIMS
PA(16:0/18:1(9Z))	675.4965	271.0	TWIMS
PA(16:0/18:2(9Z,12Z))	673.4808	267.5	TWIMS
PA(18:0/18:1(9Z))	720.5544	277.7	TWIMS
PA(18:0/18:2(9Z,12Z))	723.4941	274.0	TWIMS
PC(10:0/10:0)	566.380	245.4	TWIMS
PC(12:0/12:0)	622.4400	258.4	TWIMS
PC(14:0/14:0)	678.5100	276.4	TWIMS
PC(15:0/0:0)	482.3246	225.0	TWIMS
PC(16:0/18:1(9E))	760.5856	287.1	TWIMS
PC(16:0/18:2(9Z,12Z))	758.5700	285.2	TWIMS
PC(16:0/18:2(9Z,12Z))	780.5520	289.4	TWIMS
PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	828.5520	293.3	TWIMS
PC(18:0/0:0)	524.3716	237.9	TWIMS
PC(18:0/0:0)	546.3536	240.8	TWIMS
PC(18:0/18:1(9Z))	788.6169	293.9	TWIMS
PC(18:0/18:1(9Z))	810.5989	297.1	TWIMS
PC(18:0/18:2(9Z,12Z))	786.6013	291.3	TWIMS
PC(18:0/18:2(9Z,12Z))	808.5833	295.1	TWIMS
PC(18:0/20:4(5Z,8Z,11Z,14Z))	832.5833	298.5	TWIMS
PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	834.6013	296.2	TWIMS
PC(20:0/0:0)	552.4029	243.9	TWIMS
PC(6:0/6:0)	454.2600	213.3	TWIMS
PC(8:0/8:0)	510.3200	230.6	TWIMS
PC(O-16:0/18:2(9Z,12Z))	744.5907	286.0	TWIMS
PE(10:0/10:0)	524.3300	233.0	TWIMS
PE(12:0/12:0)	580.4000	246.7	TWIMS
PE(14:0/14:0)	636.4600	259.2	TWIMS
PE(16:0/18:1(9Z))	718.5387	274.7	TWIMS
PE(16:0/18:1(9Z))	740.5207	281.2	TWIMS
PE(16:0/18:2(9Z,12Z))	716.5230	272.7	TWIMS
PE(16:0/18:2(9Z,12Z))	738.5050	277.6	TWIMS
PE(16:0/20:4(5Z,8Z,11Z,14Z))	762.5050	281.2	TWIMS
PE(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	786.5050	283.6	TWIMS

PE(17:0/0:0)	468.3090	217.1	TWIMS
PE(18:0/18:1(9Z))	746.5700	281.3	TWIMS
PE(18:0/18:1(9Z))	768.5520	287.5	TWIMS
PE(18:0/18:2(9Z,12Z))	744.5543	279.3	TWIMS
PE(18:0/18:2(9Z,12Z))	766.5363	284.6	TWIMS
PE(18:0/20:4(5Z,8Z,11Z,14Z))	768.5543	282.9	TWIMS
PE(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	792.5543	284.5	TWIMS
PE(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	814.5363	290.3	TWIMS
PE(6:0/6:0)	412.2100	202.1	TWIMS
PE(8:0/8:0)	468.2700	220.0	TWIMS
PE(8:0/8:0)	468.2700	217.9	TWIMS
PE(O-16:0/0:0)	438.2980	209.0	TWIMS
PE(P-16:0/18:2(9Z,12Z))	700.5281	270.0	TWIMS
PE(P-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	748.5281	278.0	TWIMS
PE(P-18:0/20:5(5Z,8Z,11Z,14Z,17Z))	750.5437	280.2	TWIMS
PG(16:0/18:2(9Z,12Z))	747.5176	283.3	TWIMS
PG(16:0/18:2(9Z,12Z))	764.5442	284.9	TWIMS
PG(16:1(9Z)/22:4(7Z,10Z,13Z,16Z))	819.5152	288.8	TWIMS
PG(18:0/18:1(9Z))	777.5645	292.0	TWIMS
PG(18:0/18:1(9Z))	799.5465	287.5	TWIMS
PG(18:0/18:1(9Z))	794.5911	292.5	TWIMS
PG(18:0/18:2(9Z,12Z))	775.5489	288.9	TWIMS
PG(18:0/20:4(5Z,8Z,11Z,14Z))	816.5755	294.5	TWIMS
PG(18:1(9Z)/18:1(9Z))	797.5309	286.0	TWIMS
PG(18:1(9Z)/18:2(9Z,12Z))	773.5332	285.4	TWIMS
PG(18:1(9Z)/18:2(9Z,12Z))	790.5598	286.5	TWIMS
PG(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	797.5332	292.1	TWIMS
PG(18:1(9Z)/22:4(7Z,10Z,13Z,16Z))	847.5465	295.2	TWIMS
PG(18:1(9Z)/22:4(7Z,10Z,13Z,16Z))	842.5911	298.9	TWIMS
PG(18:2(9Z,12Z)/18:2(9Z,12Z))	788.5442	283.4	TWIMS
PG(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	795.5176	289.3	TWIMS
PG(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	817.4996	286.0	TWIMS
PG(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	812.5442	290.2	TWIMS
PG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	840.5755	296.6	TWIMS
PG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))	845.5309	292.4	TWIMS
PI(16:0/18:1(9Z))	837.5493	294.9	TWIMS
PI(16:0/18:1(9Z))	859.5313	292.4	TWIMS
PI(16:0/18:1(9Z))	854.5759	295.8	TWIMS
PI(16:1(9Z)/18:1(9Z))	835.5336	291.6	TWIMS
PI(16:1(9Z)/18:1(9Z))	852.5602	292.9	TWIMS
PI(17:0/20:4(5Z,8Z,11Z,14Z))	873.5493	298.9	TWIMS
PI(17:0/20:4(5Z,8Z,11Z,14Z))	895.5313	297.6	TWIMS
PI(17:0/20:4(5Z,8Z,11Z,14Z))	890.5759	300.2	TWIMS
PI(17:2(9Z,12Z)/18:0)	866.5759	295.6	TWIMS

PI(18:0/0:0)	601.3353	244.7	TWIMS
PI(18:0/18:1(9Z))	865.5806	301.6	TWIMS
PI(18:0/18:1(9Z))	887.5626	299.0	TWIMS
PI(18:0/18:1(9Z))	882.6072	302.2	TWIMS
PI(18:0/18:2(9Z,12Z))	863.5649	299.3	TWIMS
PI(18:0/18:2(9Z,12Z))	885.5469	297.6	TWIMS
PI(18:0/20:2(11Z,14Z))	891.5962	305.1	TWIMS
PI(18:0/20:2(11Z,14Z))	913.5782	303.2	TWIMS
PI(18:0/20:2(11Z,14Z))	908.6228	306.0	TWIMS
PI(18:0/20:3(8Z,11Z,14Z))	889.5806	304.2	TWIMS
PI(18:0/20:3(8Z,11Z,14Z))	911.5626	303.1	TWIMS
PI(18:0/20:3(8Z,11Z,14Z))	906.6072	306.0	TWIMS
PI(18:0/20:4(5Z,8Z,11Z,14Z))	887.5649	302.3	TWIMS
PI(18:0/20:4(5Z,8Z,11Z,14Z))	904.5915	304.0	TWIMS
PI(18:1(9Z)/18:2(9Z,12Z))	861.5493	296.4	TWIMS
PI(18:1(9Z)/18:2(9Z,12Z))	883.5313	295.5	TWIMS
PI(18:1(9Z)/18:2(9Z,12Z))	878.5759	297.4	TWIMS
PI(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	885.5493	299.9	TWIMS
PI(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	907.5313	298.7	TWIMS
PI(18:4(6Z,9Z,12Z,15Z)/18:0)	859.5336	296.5	TWIMS
PI(18:4(6Z,9Z,12Z,15Z)/18:0)	881.5156	294.5	TWIMS
PI(18:4(6Z,9Z,12Z,15Z)/18:0)	876.5602	297.3	TWIMS
PI(19:1(9Z)/18:2(9Z,12Z))	897.5469	298.9	TWIMS
PI(19:1(9Z)/18:2(9Z,12Z))	892.5915	301.4	TWIMS
PI(20:1(11Z)/20:3(8Z,11Z,14Z))	937.5782	307.1	TWIMS
PI(20:1(11Z)/20:4(5Z,8Z,11Z,14Z))	913.5806	307.1	TWIMS
PI(20:1(11Z)/20:4(5Z,8Z,11Z,14Z))	935.5626	305.8	TWIMS
PI(20:1(11Z)/20:4(5Z,8Z,11Z,14Z))	930.6072	308.6	TWIMS
PI(20:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))	928.5915	306.1	TWIMS
LPS(18:0/0:0)	526.3145	228.3	TWIMS
LPS(18:0/0:0)	548.2965	232.1	TWIMS
PS(18:1(9Z)/18:0)	790.5598	286.2	TWIMS
PS(18:1(9Z)/18:0)	812.5418	287.5	TWIMS
PS(18:1(9Z)/18:1(9Z))	788.5441	283.0	TWIMS
PS(18:1(9Z)/18:1(9Z))	810.5261	284.2	TWIMS
PS(18:1(9Z)/20:0)	818.5911	292.9	TWIMS
PS(18:1(9Z)/22:2(13Z,16Z))	842.5911	295.2	TWIMS
PS(18:4(6Z,9Z,12Z,15Z)/20:0)	834.5261	290.6	TWIMS
PS(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))	836.5441	289.6	TWIMS
PS(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))	858.5261	293.9	TWIMS
PS(22:4(7Z,10Z,13Z,16Z)/18:1(9Z))	838.5598	292.1	TWIMS
PS(22:4(7Z,10Z,13Z,16Z)/18:1(9Z))	860.5418	296.7	TWIMS
SM(d16:1/16:0)	675.5441	276.6	TWIMS
SM(d16:1/18:1)	701.5597	281.4	TWIMS

SM(d18:0/14:0)	677.5597	278.5	TWIMS
SM(d18:0/16:0)	705.5910	285.0	TWIMS
SM(d18:0/16:0)	727.5730	284.8	TWIMS
SM(d18:0/18:0)	733.6220	299.0	TWIMS
SM(d18:0/20:0)	761.6530	305.0	TWIMS
SM(d18:0/22:0)	789.6840	312.0	TWIMS
SM(d18:0/24:0)	817.7160	320.0	TWIMS
SM(d18:0/26:0)	845.7470	326.0	TWIMS
SM(d18:1/15:0)	689.5597	279.2	TWIMS
SM(d18:1/16:0)	703.5760	281.1	TWIMS
SM(d18:1/18:0)	753.5887	290.0	TWIMS
SM(d18:1/18:0)	731.6070	286.6	TWIMS
SM(d18:1/18:1)	729.5910	283.2	TWIMS
SM(d18:1/20:0)	759.6380	292.2	TWIMS
SM(d18:1/22:0)	787.6690	311.0	TWIMS
SM(d18:1/22:1)	785.6530	307.0	TWIMS
SM(d18:1/24:0)	815.6970	302.2	TWIMS
SM(d18:1/24:1)	813.6840	315.0	TWIMS
SM(d18:1/26:0)	843.7310	324.0	TWIMS
SM(d18:1/26:1)	841.7160	320.0	TWIMS
SM(d18:2/22:0)	785.6536	298.4	TWIMS
SM(d18:2/22:1)	783.6380	294.6	TWIMS
SM(d18:2/22:1)	813.6849	304.2	TWIMS
SM(d18:2/22:1)	835.6669	304.4	TWIMS
SM(d18:2/24:1)	811.6693	302.0	TWIMS
SM(d19:1/16:0)	717.5910	285.1	TWIMS
SM(d19:1/16:0)	739.5730	285.6	TWIMS
SM(d19:1/18:0)	745.6223	290.8	TWIMS
TG(12:0/12:0/16:0)	712.6455	285.0	TWIMS
TG(13:0/17:0/20:3(8Z,11Z,14Z))	846.7551	313.0	TWIMS
TG(14:1(9Z)/14:1(9Z)/18:1(9Z))	790.6925	297.1	TWIMS
TG(15:1(9Z)/15:1(9Z)/18:1(9Z))	818.7238	304.8	TWIMS
TG(16:1(9Z)/16:1(9Z)/18:2(9Z,12Z))	844.7394	309.5	TWIMS
TG(17:0/18:3(9Z,12Z,15Z)/19:0)	902.8177	326.5	TWIMS
TG(17:1(9Z)/17:1(9Z)/18:3(6Z,9Z,12Z))	870.7551	314.7	TWIMS

Table S6 Training dataset for negative ion mode[1-5]

Lipid ion	*m/z*	Experimental CCS value (Å^2)	Instrument
(9E,12E)-Octadecadienoicacid	279.2320	190.4	TWIMS
(9Z,12Z)-Octadecadienoic acid	279.2321	190.4	TWIMS
Cer(d18:1/18:0)	564.5360	249.7	TWIMS
Cer(d18:1/20:0)	592.5660	255.8	TWIMS
Cer(d18:1/22:0	620.5950	262.0	TWIMS
Cer(d18:1/24:0)	648.6240	268.0	TWIMS
Cer(d18:1/24:1)	646.6130	266.4	TWIMS
cis-FA(16:1)	254.2246	164.2	DTIMS
cis-FA(18:1)	282.2559	172.4	DTIMS
cis-FA(22:1)	338.3185	187.0	DTIMS
cis-FA(24:1)	366.3498	193.5	DTIMS
DG(18:2(9Z,12Z)/16:0)	615.4951	260.5	TWIMS
DG(18:2(9Z,12Z)/18:2 (9Z,12Z))	639.4950	261.5	TWIMS
FA(12:0)	200.1776	151.9	DTIMS
FA(14:0)	228.2089	158.2	DTIMS
FA(16:0)	256.2402	165.6	DTIMS
FA(17:0)	269.2480	174.0	TWIMS
FA(18:0)	284.2715	173.7	DTIMS
FA(18:2)	280.2402	171.3	DTIMS
FA(18:3)	278.2246	170.5	DTIMS
FA(20:0)	311.2950	187.0	TWIMS
FA(20:0)	312.3028	181.7	DTIMS
FA(22:0)	339.3260	191.0	TWIMS
FA(22:0)	340.3341	189.5	DTIMS
Hexyldecanoic acid	255.2320	187.2	TWIMS
LPE(16:0)	452.2780	212.0	TWIMS
LPE(16:0)	452.2770	206.0	TWIMS
LPE(18:0)	480.3100	219.0	TWIMS
LPE(18:0)	480.3090	212.9	TWIMS
LPE(20:0)	508.3410	225.0	TWIMS
LPE(20:1)	506.3260	224.0	TWIMS
LPE(20:2)	504.3100	222.0	TWIMS
LPE(20:5)	498.2630	219.0	TWIMS
LPE(22:6)	524.2780	223.0	TWIMS
LPE(O-16:0)	438.2980	209.0	TWIMS
LPE(P-16:0)	436.2830	211.0	TWIMS
LPE(P-16:0)	436.2840	204.7	TWIMS
LPE(P-18:0)	464.3140	217.0	TWIMS
LPE(P-18:0)	464.3140	211.4	TWIMS
MG(18:2(9Z,12Z))	377.2654	204.6	TWIMS
PA(16:0/18:1)	673.4850	266.0	TWIMS

PA(18:0/18:1)	701.5130	272.4	TWIMS
PA(18:1/18:1)	699.4990	270.0	TWIMS
PC(10:0/10:0	624.3900	260.1	TWIMS
PC(12:0/12:0	680.4500	272.4	TWIMS
PC(14:0/14:0	736.5100	282.9	TWIMS
PC(16:0/16:0	792.5800	294.2	TWIMS
PC(16:0/16:0)	768.5210	295.2	TWIMS
PC(16:0/16:1)	766.5180	294.0	TWIMS
PC(16:0/18:1)	794.5470	301.1	TWIMS
PC(16:1/18:1)	792.5310	298.8	TWIMS
PC(18:0/18:0	848.6400	305.1	TWIMS
PC(18:0/18:1)	822.5670	306.8	TWIMS
PC(18:1/18:2)	818.5450	304.0	TWIMS
PC(18:1/20:4)	842.5470	307.1	TWIMS
PC(18:2(9Z,12Z)/16:0)	758.5667	286.4	TWIMS
PC(20:0/20:0	904.7000	315.4	TWIMS
PC(22:0/22:0	960.7600	326.4	TWIMS
PC(8:0/8:0	568.3300	248.6	TWIMS
PE(10:0/10:0	522.3200	229.9	TWIMS
PE(12:0/12:0	578.3800	242.3	TWIMS
PE(15:0/15:0	662.4800	260.3	TWIMS
PE(16:0/16:0	690.5100	266.7	TWIMS
PE(16:0/16:1)	688.4950	266.2	TWIMS
PE(16:0/18:0)	718.5350	274.7	TWIMS
PE(16:0/18:1)	716.5240	273.8	TWIMS
PE(16:0/20:4)	738.5080	276.3	TWIMS
PE(16:0/22:6)	762.5100	281.3	TWIMS
PE(16:1/18:1)	714.5090	272.2	TWIMS
PE(17:0/17:0	718.5400	272.5	TWIMS
PE(18:0/20:4)	766.5380	283.1	TWIMS
PE(18:1/18:0)	744.5540	280.4	TWIMS
PE(18:1/18:1)	742.5400	279.2	TWIMS
PE(18:1/18:2)	740.5230	277.4	TWIMS
PE(18:1/20:4)	764.5130	281.5	TWIMS
PE(8:0/8:0)	466.2600	217.7	TWIMS
PE14:0/14:0	634.450	254.6	TWIMS
PI(16:1/18:1)	833.5170	292.5	TWIMS
PI(18:0/18:0)	865.580	303.8	TWIMS
PI(18:0/20:3)	887.5530	308.8	TWIMS
PI(18:0/20:4)	885.5390	307.5	TWIMS
PI(18:1/20:4)	883.5260	305.6	TWIMS
PS(16:1/18:0)	760.5140	285.4	TWIMS
PS(16:1/18:1)	758.5050	283.2	TWIMS
PS(18:0/18:1)	788.5360	291.5	TWIMS

PS(18:0/20:3)	812.5250	294.8	TWIMS
PS(18:0/20:4)	810.5290	294.2	TWIMS
PS(18:0/22:4)	838.5610	301.5	TWIMS
PS(18:0/22:6)	834.5290	298.6	TWIMS
PS(18:1/18:1)	786.5280	289.9	TWIMS
PS(18:1/18:2)	784.5160	287.8	TWIMS
PS(18:1/20:1)	814.5450	296.7	TWIMS
PS(18:1/20:4)	808.5140	292.3	TWIMS
PS(18:1/22:2)	840.5740	302.4	TWIMS
SM(d18:0/16:0)	739.5390	291.8	TWIMS
SM(d18:1/16:0)	737.5350	291.5	TWIMS
TG(15:0/18:2(9Z,12Z)/ 18;2(9Z,12Z))	858.7515	314.4	TWIMS
TG(16:0/18:1(9Z)/18:2 (9Z,12Z))	874.7837	318.2	TWIMS
TG(16:0/18:2(9Z,12Z)/ 16:0)	848.7678	314.5	TWIMS
TG(16:0/18:2(9Z,12Z)/ 18:2(9Z, 12Z))	872.7674	316.9	TWIMS
TG(18:0/18:1(11Z)/18:3(9Z,12Z,15Z))	900.7993	319.4	TWIMS
TG(18:1(9Z)/18:2(9Z,1 2Z)/18:2(9Z,12Z))	898.7837	320.7	TWIMS
TG(18:2(9Z,12Z)/18:2(9Z,12Z)/18:2(9Z,12Z))	896.7666	319.3	TWIMS
TG(18:2(9Z,12Z)/18:2(9Z,12Z)/20:1(11Z))	926.8141	326.7	TWIMS
TG(18:2(9Z,12Z)/18:2(9Z,12Z)/20:2(11Z,14Z))	924.7992	325.5	TWIMS
TG(22:1(11Z/18:2(9Z, 12Z)/18:2(9Z,12Z))	954.8455	332.5	TWIMS
trans-FA(16:1)	254.2246	165.1	DTIMS
trans-FA(18:1)	282.2559	173.3	DTIMS
trans-FA(22:1)	338.3185	187.6	DTIMS
trans-FA(24:1)	366.3498	193.9	DTIMS

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