

McLean Group Collision Cross Section Database

MALDI Generated Data

Biomolecular Class	Name (parent name if fragmented)	species	m/z (Da)	Ω ($\text{\AA}^2$)	σ (# of measurements)
Lipids ¹					
lipid	PE 34:2	$[\text{M}+\text{H}]^+$	716.5	206.9	2.0(29)
lipid	PE 34:1	$[\text{M}+\text{H}]^+$	718.5	205.8	4.3(29)
lipid	SM (36:1)	$[\text{M}+\text{H}]^+$	731.6	221.1	2.0(33)
lipid	PE 34:2	$[\text{M}+\text{Na}]^+$	738.5	213.5	2.1(29)
lipid	PE 34:1	$[\text{M}+\text{Na}]^+$	740.5	214.7	1.5(29)
lipid	SM (36:1)	$[\text{M}+\text{Na}]^+$	753.6	221.3	2.6(33)
lipid	PC 34:2	$[\text{M}+\text{H}]^+$	758.6	217.4	3.2(33)
lipid	SM (38:1)	$[\text{M}+\text{H}]^+$	759.7	229.8	3.4(33)
lipid	PC 34:1	$[\text{M}+\text{H}]^+$	760.6	219.1	2.7(33)
lipid	PE 36:4	$[\text{M}+\text{Na}]^+$	762.5	214.4	1.6(29)
lipid	PE 36:2	$[\text{M}+\text{Na}]^+$	766.5	220.9	2.7(29)
lipid	PE 36:1	$[\text{M}+\text{Na}]^+$	768.6	221.7	4.8(29)
lipid	PC 34:2	$[\text{M}+\text{Na}]^+$	780.6	218.9	2.8(33)
lipid	SM (38:1)	$[\text{M}+\text{Na}]^+$	781.6	231.3	2.5(33)
lipid	PC 34:1	$[\text{M}+\text{Na}]^+$	782.6	221.7	3.2(33)
lipid	PC 36:2	$[\text{M}+\text{H}]^+$	786.6	222.6	2.2(33)
lipid	SM (40:1)	$[\text{M}+\text{H}]^+$	787.7	232.2	5.0(33)
lipid	PE 38:5	$[\text{M}+\text{Na}]^+$	788.5	220.6	5.2(29)
lipid	PC 36:1	$[\text{M}+\text{H}]^+$	788.6	227.4	4.3(33)
lipid	PE 38:4	$[\text{M}+\text{Na}]^+$	790.5	228.1	3.6(29)
lipid	CB (40:1)	$[\text{M}+\text{Na}]^+$	806.6	232.9	2.4(33)
lipid	PC 36:2	$[\text{M}+\text{Na}]^+$	808.6	226.7	4.6(33)
lipid	CB (39:1)h	$[\text{M}+\text{Na}]^+$	808.6	236.6	2.9(33)
lipid	PS 36:2	$[\text{M}+\text{Na}]^+$	810.5	217.1	5.5(29)
lipid	PC 36:1	$[\text{M}+\text{Na}]^+$	810.6	228.1	2.0(33)

lipid	PS 36:1	[M+Na] ⁺	812.5	222.6	2.4(29)
lipid	SM (42:2)	[M+H] ⁺	813.7	241.8	2.5(33)
lipid	SM (42:1)	[M+H] ⁺	815.7	242.1	6.3(33)
lipid	CB (40:2)h	[M+Na] ⁺	820.6	236.2	5.6(33)
lipid	CB (40:1)h	[M+Na] ⁺	822.6	234.6	5.3(33)
lipid	CB (42:6)	[M+Na] ⁺	824.6	237.9	1.9(33)
lipid	CB (42:2)	[M+Na] ⁺	832.7	238.8	1.7(33)
lipid	PS 38:4	[M+Na] ⁺	834.5	225.5	2.1(29)
lipid	CB (42:1)	[M+Na] ⁺	834.7	239.3	2.6(33)
lipid	SM (42:2)	[M+Na] ⁺	835.7	239.4	2.8(33)
lipid	CB (41:1)h	[M+Na] ⁺	836.7	240.2	3.4(33)
lipid	SM (42:1)	[M+Na] ⁺	837.7	239.3	4.7(33)
lipid	PS 38:1	[M+Na] ⁺	840.6	222.6	5.5(29)
lipid	CB (42:3)h	[M+Na] ⁺	846.6	238.8	2.2(33)
lipid	CB (42:2)h	[M+Na] ⁺	848.7	240.3	2.7(33)
lipid	CB (44:7)	[M+Na] ⁺	850.6	242.8	1.9(33)
lipid	CB (44:6)	[M+Na] ⁺	852.6	243.3	3.7(33)
lipid	PS 40:6	[M+Na] ⁺	858.5	231.9	2.8(29)
lipid	CB (44:2)	[M+Na] ⁺	860.7	245.9	5.2(33)
lipid	CB (44:1)	[M+Na] ⁺	862.7	244.3	5.5(33)
lipid	CB (44:8)h	[M+Na] ⁺	864.6	245.2	2.9(33)
lipid	CB (44:7)h	[M+Na] ⁺	866.6	252.2	5.1(33)
lipid	SM (44:1)	[M+Na] ⁺	866.7	247.9	4.3(33)
lipid	CB (44:2)h	[M+Na] ⁺	876.7	246.7	3.7(33)
lipid	PS 42:9	[M+Na] ⁺	880.5	238	1.7(29)
lipid	PS 42:8	[M+Na] ⁺	882.5	230.8	3.0(29)
lipid	PC 42:1	[M+Na] ⁺	894.7	238.2	2.3(33)
lipid	PC 42:0	[M+Na] ⁺	896.7	246.3	2.1(33)

Footnotes on table nomenclature:

1. Lipid nomenclature :

Glycerophospholipids:

Ex. PC X:Y

PC, PE, PS = abbreviated names phosphatidylcholine, phosphatidylethanolamine, phosphatidylserine.

X = total number of carbons in fatty acid chains

Y = total number of double bonds in fatty acid chains

Sphingolipids:

Ex. SM (x:y)

SM, CB = abbreviated names sphingomyelin, cerebroside

x = total number of carbons in the amide linked fatty acid of the ceramide plus eighteen carbons from the sphingosine backbone

y = total number of double bonds, one trans double bond in the sphingosine backbone plus the number of double bonds in the amide linked fatty acid of the ceramide

() = used to distinguish sphingolipid from glycerophospholipid nomenclature in the table

Hydroxylation on Cerebrosides:

Ex. CB (x:y)h

h = denotes hydroxylation on the number two carbon (from carbonyl) of the amide linked fatty acid.