

Supplementary table 3: Conditions for tandem mass spectrometry analysis of lipid species.

Lipid class/subclass	Parent Ion	Fragmentation*	Internal standard	Internal standard (pmol)	Collision Energy (V)
Sphingosine	[M+H] ⁺	NL, 18.0 Da	Sph(d17:1)	50	8
Sphingosine-1-phosphate	[M+H] ⁺	Sphingoid specific [^]	Sph(d17:1)	50	11-16
Dihydroceramide	[M+H] ⁺	Sphingoid specific [^]	dhCer(d18:0/8:0)	50	31
Ceramide	[M+H] ⁺	Sphingoid specific [^]	Cer(d18:1/17:0)	100	23-29
Monohexosylceramide	[M+H] ⁺	Sphingoid specific [^]	HexCer (d18:1/16:0) d3	50	33
Dihexosylceramide	[M+H] ⁺	Sphingoid specific [^]	Hex2Cer(d18:1/16:0) d3	50	53
Trihexosylceramide	[M+H] ⁺	PI, m/z 264.3	Hex3Cer(d18:1/17:0)	50	57
GM3 ganglioside	[M+H] ⁺	Sphingoid specific [^]	Hex3Cer(d18:1/17:0)	50	57
GM1 ganglioside	[M+2H] ²⁺	PI, m/z 366.2	Hex3Cer(d18:1/17:0)	50	9
Sulfatide	[M+H] ⁺	PI, m/z 264.3	Sulfatide(d18:1/12:0)	50	56
Ceramide-1-phosphate	[M+H] ⁺	PI, m/z 264.3	Cer(d18:1/17:0)	50	29
Sphingomyelin	[M+H] ⁺	PI, m/z 184.1	SM(d18:1/12:0)	200	25
Phosphatidylcholine	[M+H] ⁺	PI, m/z 184.1	PC(13:0/13:0)	100	21
Alkylphosphatidylcholine	[M+H] ⁺	PI, m/z 184.1	PC(13:0/13:0)	100	21
Alkenylphosphatidylcholine	[M+H] ⁺	PI, m/z 184.1	PC(13:0/13:0)	100	21
Lysophosphatidylcholine	[M+H] ⁺	PI, m/z 184.1 & m/z 104.1	LPC(13:0)	100	21
Lysoalkylphosphatidylcholine	[M+H] ⁺	PI, m/z 104.1	LPC(13:0)	100	21
Lysoalkenylphosphatidylcholine	[M+H] ⁺	PI, m/z 104.1	LPC(13:0)	100	21
Phosphatidylethanolamine	[M+H] ⁺	NL, 141.0 Da	PE(17:0/17:0)	100	17
Alkylphosphatidylethanolamine	[M+H] ⁺	NL, 141.0 Da	PE(17:0/17:0)	100	17
Alkenylphosphatidylethanolamine	[M+H] ⁺	Acyl specific	PE(17:0/17:0)	100	17
Lysophosphatidylethanolamine	[M+H] ⁺	NL, 141.0 Da	PE(17:0/17:0)	100	17
Lysoalkenylphosphatidylethanolamine	[M+H] ⁺	NL, 171.9 Da	PE(17:0/17:0)	100	19
Phosphatidylinositol	[M+NH ₄] ⁺	NL, 277.0 Da	PE(17:0/17:0)	100	17
Lysophosphatidylinositol	[M+NH ₄] ⁺	NL, 277.0 Da	LPI(13:0)	100	17
Phosphatidylserine	[M+H] ⁺	NL, 185.0 Da	PS(17:0/17:0)	100	25
Phosphatidylglycerol	[M+NH ₄] ⁺	NL, 189.0 Da	PG(17:0/17:0)	100	21
Free cholesterol	[M+NH ₄] ⁺	PI, m/z 369.3	COH d7	10000	23
Cholesteryl ester	[M+NH ₄] ⁺	PI, m/z 369.3	CE(18:0) d6	1000	10
Other sterol ester derivative	[M+NH ₄] ⁺	PI, m/z 367.3	CE(18:0) d6	1000	12
Acylcarnitines	[M+H] ⁺	PI, m/z 85.1	LPC(13:0)	100	30
Diacylglycerol	[M+NH ₄] ⁺	NL, fatty acid	DG(15:0/15:0)	200	21
Triacylglycerol	[M+NH ₄] ⁺	NL, fatty acid	TG(17:0/17:0/17:0)	100	21
Alkyltriacylglycerol	[M+NH ₄] ⁺	NL, fatty acid	TG(17:0/17:0/17:0)	100	21
Ubiquinone	[M+NH ₄] ⁺	PI, m/z 197.0	Hex3Cer(d18:1/17:0)	50	17

* PI, product ion; NL, neutral loss [^] d18:1 base, 264.3. d18:2 base, 262.3, d16:1 base, 236.1, d17:1 base, 250.3, d20:1 base, 292.3, d20:2 base, 290.3.