Supplementary Table S5: Overview metabolic profiling and MS/MS fragmentation

Rank	mz_Rt pair	Ion mode	mz (median	RT	HMDB/ Chempub ID	Name	Class/Function	Formula	Exact Mass	Delta (mass- exact mass)	MS/MS	Ratio	p.value
	Frontal Cortex												
1	645.5/1323	+	645.53833	1323.0	LMSP03020039	PE-Cer(d14:2(4E,6E)/19:0) PE-Cer(d15:2(4E,6E)/18:0)	Ceramide phosphoethanolamines [SP0302]	C35H70N2O6P	644.4893	6.465E-05	ID	0.64	0.000
2	342.3/1378	+	342.31627	1378.2	-	not identified	-	-	-	-		0.61	0.004
3	426.4/681	+	426.36226	681.1	HMDB06464 HMDB05065	Elaidic carnitine Oleoylcarnitine	Acyl Carnitine Acyl Carnitine	C25H47NO4 C25H47NO4	425.3505	4.5E-03	ID	0.59	0.010
4	232.2/270	+	232.16595	269.9	HMDB02013	Butyrylcarnitine	Acyl Carnitine	C10H21N3O3	231.147	4.4E-03	ID	0.33	0.013
5	448.3/667	+	448.34585	666.6	74380333 123060515	N-docosanoyl taurine N-stearoyl tyrosine	N-acyl amine N-acyl amine	C24H49NO4S C27H45NO4	447.3382 447.3349	4.0E-04 3.7E-03	NP	0.70	0.013
6	765.6/1179	+	765.59871	1178.7	123064881	PG(O-20:0/16:0)/PG(O-16:0/20:0)	Glycerophosphoglycerol	C42H85O9P	764.5931	1.6E-03	ID	0.69	0.022
7	238.9/26	+	238.9299	26.0	-	not identified	-	-	-	-	-	0.57	0.022
8	171.2/647.1	+	171.2	647.1	-	not identified	-	-	-	-	-	3.69	0.028
9	510.6/565	+	541.6	565.0	-	not identified	-	-	-	-	-	2.13	0.028
10	367.1/609	+	367.07582	609.4	8439	Salicin 6-phosphate	Glycoside phosphate	C13H19O10P	366.0716	3.0E-03	NP	1.44	0.035
11	650.4/1019	+	650.43472	1019.1	135642574	PC(16:0/9:0(CHO))	Phophatidylcholine	C33H64NO9P	649.4319	4.5E-03	NP	0.71	0.035
12	299.2/619	+	299.2	619.0	-	not identified	-	-	-	-	-	1.59	0.035
13	530.5/1146	+	530.53018	1145.5	-	Water loss from #16 (548.5, 1146sec)	-	-	-	-	ID	0.58	0.035
14	130/25	+	130.03074	25.3	HMDB33561	2-Acetyl-4,5-dihydrothiazole	-	C5H7NOS	129.0248	1.4E-03	NP	0.70	0.043
15	184.1/1095	+	184.08643	1094.6	HMDB33141	Fragment of a phosphatidylcholine	-	C11H9N3	183.0796	5.0E-04	ID	1.33	0.043
16	548.5/1146	+	548.54009	1145.7	-	not identified	-	-	-	-	-	0.64	0.043
17	550.6/1035	+	550.62811	1035.2	LMSP00000005	Cer(m18:1(4E)/18:0)	Ceramide/Sphingolipid	C36H71NO2	549.5485	0.00013	ID	0.55	0.043
18	618.5/1252	+	618.51154	1252.4	-	not identified	-	-	-	-	-	0.58	0.043
19	631.6/1302	+	631.6175	1301.7	LMSP03020003	PE-Cer(d14:1(4E)/18:1(9Z))/PE-Cer(d14:2(4E,6E)/18:0)/PE-Cer(d16:2(4E,6E)/16:0)	Ceramide phosphoethanolamines	C34H67N2O6P	630.4737	0.00022	ID	0.68	0.043
20	252.1/526	+	252.1362	526.0	HMDB00101	Deoxyadenosine	Purine Nucleosides and Analogues	C10H13N5O3	251.101	0.00412	NP	2.62	0.043
21	643.5/1269	+	643.5198	1269.0	HMDB07312	DG(18:3(9Z,12Z,15Z)/20:2(11Z,14Z)/0:0)[iso2] (several)	Diacylglycerol	C41H70O5	642.5223	9.8E-03	NP	0.60	0.043

Rank	mz_Rt pair	Ion mode	mz (median	RT	HMDB/ Chempub ID	Name	Class/Function	Formula	Exact Mass	Delta (mass exact mass)	MS/MS	Ratio	p.value
	Hippocampus												
1	382.3_619	+	382.301	619.1	4266008 24701448	Prostaglandin F2 alpha dimethyl amide 5,6-DiHETrE-EA (several)	Prostaglandin Endocannabinoid	C22H39NO4	381.2879	5.8E-03	NP	0.39	0.003
2	535.5_1310	+	535.469	1309.7	-	not identified	-	-	-	-	-	0.55	0.003
3	716.8_529	+	716.787	528.8	-	not identified	-	-	-	-	-	0.57	0.003
4	308.1_219	+	308.056	218.8	-	not identified	-	-	-	-	-	0.48	0.023
5	771.6_1472	+	771.633	1471.8	123068775	SM(d18:2/21:0)	Ceramide posphocholine	C44H87N2O6P	770.6302	4.5E-03	NP	0.57	0.023
					123067209	PA(O-20:0/22:2(13Z,16Z))	Glycerophosphate	C45H87O7P	770.6189	6.8E-03			
6	658.2_529	+	658.192	528.8	-	not identified	-	-	-	-	-	0.65	0.023
7	651.1_134	+	651.101	134.3	-	not identified	-	-	-	-	-	0.52	0.031
8	359.2_661	+	359.246	661.4	HMDB12983	Kinetensin 1-3	Peptide	C15H30N6O4	358.2329	5.9E-03	NP	0.56	0.031
9	799.7_1372	+	799.661	1371.8	123068785	SM(d17:1/24:1) or SM(d18:2/23:0)	Sphingomyelin	C46H91N2O6P	798.6615	7.8E-03	ID	1.72	0.031
10	626.5_1146	+	626.519	1146.3	-	not identified	-	-	-	-	-	0.58	0.031
11	360.3_662	+	661.535	360.3	-	S-palmitoyl-L-cysteine	Palmitoylated residue	C19H37NO3S	359.2494	5.7E-03	NP	0.59	0.031
12	550.4_1299	+	550.417	1299.4	-	not identified	-	-	-	-	-	0.62	0.031
13	140.1_1645	+	140.082	1644.9	207572	4-Amino-5-hydroxymethyl-2-methylpyrimidine	Thiamin metabolism	C6H9N3O	139.0746	1.7E-04	NP	0.35	0.042
					5035	L-Histidinal	Histidin metabolism	C6H9N3O					
14	390.3_1230	+	390.283	1230.0	-	not identified	-	-	-	-	-	0.63	0.042
15	545.3_725	+	545.343	724.5	-	PC (no database match, Isotope of 544.3 (PC 20:4))	-	-	-	-	T	0.67	0.042
16	882.6_1302	+	882.593	1302.0	123061384	PC(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z))	Phophatidylcholine	C52H84NO8P	881.5935	7.7E-03	NP	0.69	0.042
17	280.2_254	+	280.222	254.4	-	not identified	-	-	-	-	-	0.70	0.042
1	479.3_760	-	479.297	759.93	-	Phospholipid - ID cannot be confirmed	-	-	-	-	T	0.55	3E-05
2	853.6_1138	-	853.574	1138.4	-	not identified	-	-	-	-	-		0.007
3	218.1_300	-	218.103	299.67	149588	Pantothenic acid	Vitamine	C9H17NO5	219.1107	4.6E-05	NP	0.80	0.019
4	194.1_632	-	194.082	632.37	HMDB14903	Metyrosine	Tyrosine	C10H13NO3	195.0895	2.3E-04	NP	0.61	0.023
					HMDB29217	Tyrosine methylester	Tyrosine	C10H13NO3					
5	566.3_758	-	566.343	758	LMGP01050056	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	Glycerophosphocholine	C30H50NO7P	567.3325	3.196E-05	ID	1.30	0.023
6	567.3_758	-	567.348		-	Isotope of 566.3, 758 sec							
7	149_1534	-	149.004	1533.6	-	not identified	-	-	-	-	-		0.029
8	442.3_661	-	442.278	660.7	-	not identified	-	-	-	-	-		0.035
9	480.3_746	-	480.309	746.3	LMGP01060010	PC(O-16:0/0:0)	Phosphatidylcholine	C24H52NO6P	481.3532	-7.75E-05	ID	1.43	0.043
10	532.3_815	-	532.301	814.95	LMSP02010055	Cer(d14:2(4E,6E)/20:1(11Z))	N-acylsphingosines (ceramides)	C34H63NO3	533.4808	-0.000325	ID	0.70	0.043