

Table S1. Detailed compound lists are provided

Name	Pattern	Class	FC	Pvalue	VIP	Up.Down
Acylcarnitine (2)						
AcCa(4:0)	pos	AcCa	2.962465756	0.012986475	1.665564387	up
AcCa(5:0)	pos	AcCa	2.165067771	0.03778202	1.183005361	up
N-Neurocerebroside (2)						
AEA(13:0)	pos	AEA	1.967444501	0.045759614	1.009934168	up
AEA(16:0)	pos	AEA	2.021085818	0.021908506	1.357393374	up
Biotinylated phosphatidylethanolamine (2)						
BiotinylPE (29:6)	neg	BiotinylPE	2.093762068	0.01954635	2.228902039	up
BiotinylPE (31:7)	neg	BiotinylPE	2.153262033	0.038153356	2.206834682	up
Dimethylphosphatidic acid (14)						
BisMePA(18:2/18:3)	pos	BisMePA	4.58249455	0.011810116	1.416778065	up
BisMePA(18:3/12:0)	pos	BisMePA	7.792648181	0.00013889	2.335732554	up
BisMePA(18:3/12:0)	pos	BisMePA	2.28621153	0.014295069	1.079267932	up
BisMePA(18:4/16:1)	pos	BisMePA	6.706283577	0.000175211	2.292041788	up
BisMePA(18:4/18:1)	pos	BisMePA	6.520776992	0.03314346	1.73542951	up
BisMePA(32:5)	pos	BisMePA	4.506516995	0.001671292	1.535457091	up
BisMePA(33:3)	pos	BisMePA	3.583616271	0.004747103	1.113750966	up
BisMePA(34:6)	pos	BisMePA	12.99711043	6.62892E-05	2.741937782	up
BisMePA(34:6)	pos	BisMePA	2.542127199	0.012293714	1.255293521	up
BisMePA(36:7)	pos	BisMePA	11.78573808	1.59096E-05	2.261698009	up
BisMePA(36:7)	pos	BisMePA	2.702825646	0.006282125	1.118679927	up
BisMePA(36:8)	pos	BisMePA	8.205354086	0.001143836	1.932803739	up
BisMePA(38:7)	pos	BisMePA	5.103107561	0.000763017	2.410239152	up
BisMePA(10:0/16:2)	pos	BisMePA	0.339428057	0.042596879	1.060351669	down
Ceramide (20)						

Cer(d12:0/18:0)	pos	Cer	2.678799908	0.01356081 3	1.54230460 8	up
Cer(d12:0/20:0)	pos	Cer	2.625931833	0.03465795 4	1.37073615 3	up
Cer(d12:0/22:0)	pos	Cer	3.404264623	0.00154102 6	1.46550848 7	up
Cer(d16:1/22:3)	pos	Cer	7.837667643	0.03002888 9	1.93977639 8	up
Cer(d16:1/22:3)	pos	Cer	3.447911503	0.00167945 6	1.90692671 8	up
Cer(d18:1/21:3)	pos	Cer	2.50047173	0.00916264 3	1.44213888	up
Cer(d18:2/23:0)	pos	Cer	2.323634753	0.00986195 5	1.03963821 6	up
Cer(d19:1/18:0)	pos	Cer	2.378752262	0.00278204 6	1.46021532 4	up
Cer(d19:1/23:3)	pos	Cer	3.217841159	0.01162089 3	1.53886240 4	up
Cer(d20:1/23:3)	pos	Cer	2.395576752	0.02520333	1.16947650 6	up
Cer(m18:0/16:0)	pos	Cer	1.796879453	0.02105100 5	1.14160448 5	up
Cer(m18:0/22:0)	pos	Cer	3.152987257	0.01319144 1	1.85259862	up
Cer(m34:2)	pos	Cer	2.304509705	0.02987518 1	1.55841051 9	up
Cer(t20:1/23:2)	pos	Cer	2.333107634	0.03170711 2	1.10795808 6	up
Cer(d18:0/16:0)	neg	Cer	1.645633094	0.02877622 6	1.64490527	up
Cer(d18:2/20:0)	neg	Cer	1.492007128	0.03152035 8	1.68355421 1	up
Cer(d18:2/22:0)	neg	Cer	1.522147961	0.03886727 3	1.34669746 3	up
Cer(d18:2/24:1)	neg	Cer	1.427799608	0.03068805 8	1.51674509 6	up
Cer(d19:1/24:1)	neg	Cer	1.984110783	0.01006871 8	1.01670260 6	up
Cer(d19:1/24:1)	neg	Cer	1.677219442	0.01489313 8	1.11727509 7	up
Phosphatidylcholine (1)						
CerP(d40:1)	neg	CerP	1.954265946	0.01250797 8	2.11270208	up
Cardiolipin (8)						
CL(22:1CHO/18:0/22:5 /22:5)	neg	CL	2.531936871	0.03571633 3	1.61642724 8	up
CL(27:3/16:0/16:0/18:0)	neg	CL	5.487842301	0.00012237 9	3.1092887	up
CL(27:3/16:0/16:0/18:0)	neg	CL	2.279968493	0.00398902 9	2.58751175	up
CL(42:5CHO/16:0/18:1)	neg	CL	2.224117558	0.00433094 7	1.55955836 1	up
CL(18:2/18:2/18:2/18:2)	neg	CL	0.461231468	0.02661532	2.56138559 3	down
CL(24:2/18:1/18:2/18:2)	neg	CL	0.24761229	0.04851174 5	2.25576438 5	down

CL(45:9CHO/19:0/18:1)	neg	CL	0.283592078	0.00048776 2	2.24438003 1	down
CL(69:14CHO/17:0)	neg	CL	0.264197501	0.00048850 5	1.31309804 6	down
Cyclic phospholipid acid (2)						
cPA(16:1)	neg	cPA	2.121037436	0.01700648	1.4888677	up
cPA(18:0)	neg	cPA	1.644464471	0.03048158 7	2.06781556 6	up
Diacylglycerol (60)						
DG(10:0/12:0)	pos	DG	2.132541364	0.02647388 1	1.08274598 9	up
DG(10:0/16:1)	pos	DG	2.403765724	0.02153619 4	1.30415957 1	up
DG(10:0/27:7)	pos	DG	1.891609687	0.02257079 2	1.27151088 4	up
DG(12:0/14:0)	pos	DG	2.667202689	0.01494665 5	1.01366476 5	up
DG(12:0/18:1)	pos	DG	2.472981575	0.04391604 8	1.36995945 3	up
DG(12:0/18:2)	pos	DG	2.721089752	0.01219964 9	1.24568426 2	up
DG(12:0/20:5)	pos	DG	2.872243169	0.01073854 3	1.249278	up
DG(14:0/16:1)	pos	DG	2.604885115	0.01431944 4	1.48871356 6	up
DG(14:0/18:1)	pos	DG	2.576537476	0.01126527 3	1.53320910 9	up
DG(14:0/18:2)	pos	DG	3.684711805	0.02224809 1	1.55507622 8	up
DG(14:0/18:2)	pos	DG	3.866118264	0.00344662 5	2.17122381 6	up
DG(14:0/20:5)	pos	DG	2.59012525	0.01166977 7	1.3780319	up
DG(15:2/17:0)	pos	DG	2.485009079	0.02215066 4	1.05194828 3	up
DG(16:0)	pos	DG	2.834762395	0.00625984 7	1.67925907 8	up
DG(16:0/14:2)	pos	DG	2.290378351	0.01822721 3	1.37987942 2	up
DG(16:0/16:3)	pos	DG	1.928517346	0.03141536 5	1.02347620 7	up
DG(16:0/18:0)	pos	DG	1.977506644	0.00897536	1.10275886 4	up
DG(16:0/18:2)	pos	DG	2.166201604	0.01540288 4	1.19480233 9	up
DG(16:0/18:4)	pos	DG	2.071998178	0.01819542 3	1.29023176 8	up
DG(16:0/20:3)	pos	DG	1.997805425	0.00925574 6	1.09182261 8	up
DG(16:0/20:4)	pos	DG	2.203980172	0.01131294	1.36046058	up
DG(16:0/24:6)	pos	DG	2.792847915	0.03297480 9	1.18129861 8	up
DG(16:1/16:0)	pos	DG	3.647387991	0.00429124 8	2.44916502	up
DG(16:1/16:0)	pos	DG	2.143166636	0.02368553	1.64934345 9	up

DG(16:1/16:1)	pos	DG	2.674597709	0.01156200 9	1.38213522	up
DG(16:1/18:4)	pos	DG	3.060637343	0.04818330 7	1.26011695 2	up
DG(16:1/18:4)	pos	DG	3.335883952	0.00485841 2	1.89502159 5	up
DG(16:1/22:5)	pos	DG	2.670252462	0.01055566 2	1.37608241 1	up
DG(16:3/16:1)	pos	DG	8.035886123	0.00223913 3	2.27793968 5	up
DG(16:3/16:1)	pos	DG	2.319852045	0.01138764 3	1.33005456 1	up
DG(17:1/20:0)	pos	DG	2.460422726	0.01958785 1	1.45829871 4	up
DG(17:2/15:1)	pos	DG	1.81757411	0.01072042 1	1.38817934 5	up
DG(17:2/15:2)	pos	DG	2.519748296	0.02388144 6	1.65543803 1	up
DG(17:2/15:2)	pos	DG	2.072882468	0.04371625 1	1.30552626 3	up
DG(17:2/20:4)	pos	DG	2.019416383	0.01176544 6	1.04735244 3	up
DG(17:2/23:6)	pos	DG	2.101437702	0.03708283 6	1.83513115 4	up
DG(18:1/20:1)	pos	DG	1.8036264	0.02889554 6	1.12718913 8	up
DG(18:1/22:6)	pos	DG	2.245410948	0.03469429 5	1.21155979 2	up
DG(18:2/20:4)	pos	DG	3.3310092	0.00250181 9	1.26790668 7	up
DG(18:4/12:0)	pos	DG	2.137646124	0.02890470 2	1.18697650 6	up
DG(18:4/15:2)	pos	DG	2.179797865	0.03047347 7	1.17461075 7	up
DG(18:4/18:0)	pos	DG	2.217240229	0.01580044 7	1.76079182 9	up
DG(23:6/13:0)	pos	DG	2.91245194	0.00496755 9	1.90025521 3	up
DG(24:6/16:0)	pos	DG	2.843560126	0.03222262 9	1.18815252 9	up
DG(26:4)	pos	DG	2.962871251	0.00218995 4	1.93981344 7	up
DG(26:4)	pos	DG	2.070358606	0.02653381 4	1.26563505 4	up
DG(28:7)	pos	DG	1.946147906	0.04593858 9	1.08035474 4	up
DG(4:0/16:1)	pos	DG	2.36228156	0.01939314 9	1.14168400 8	up
DG(5:0/6:0)	pos	DG	3.665224054	0.01150446 2	1.73395799 8	up
DG(8:0/18:4)	pos	DG	2.490650393	0.01908134 5	1.38983751 4	up
DG(13:0/15:0)	pos	DG	0.295533957	0.03213861 9	2.02161734 7	down
DG(13:0/18:1)	pos	DG	0.363099503	0.02226124 2	1.63359259 5	down
DG(17:0/18:0)	pos	DG	0.43106993	0.01113500 5	1.52737672 7	down

DG(18:0/20:2)	pos	DG	0.287469679	0.04020836 5	1.94567595 3	down
DG(18:0/22:5)	pos	DG	0.48267265	0.04708072 6	1.30766409 7	down
DG(18:2/20:0)	pos	DG	0.498446422	0.03534135 3	1.13110276 7	down
DG(19:2)	pos	DG	0.411137023	0.02235431 5	1.97065073 7	down
DG(19:3/18:0)	pos	DG	0.429481641	0.01050117 2	1.53405951 8	down
DG(20:0/18:1)	pos	DG	0.245836376	0.02459109 4	1.51794424 1	down
DG(20:0/20:4)	pos	DG	0.242754935	0.02309392 8	1.37166268 4	down
Fatty acid (6)						
FA(16:1)	neg	FA	2.009898791	0.03498646 8	1.40777042 5	up
FA(17:0)+COOH:(s)	neg	FA	1.838903577	0.04540895	1.35254690 7	up
FA(22:1)+OX:(s)	neg	FA	3.030519385	0.02366880 4	2.47365507 7	up
FA(14:0)+COOH:(s)	neg	FA	0.15979913	0.03927441 4	2.02071707	down
FA(14:0)+COOH:(s)	neg	FA	0.110115338	0.04397599 2	2.39073837 2	down
FA(27:3)	neg	FA	0.429912253	0.02246805 6	2.25385918 1	down
Ganglioside GM3 (1)						
GM3(d36:1)	neg	GM3	2.800701893	0.00329557 6	1.54364295 2	up
Monosaccharide ceramide (5)						
Hex1Cer(d18:1/24:1)	pos	Hex1Cer	3.320316523	0.00097501 9	1.72483983 2	up
Hex1Cer(d19:1/22:0)	pos	Hex1Cer	8.539822658	0.01974864 6	1.03102097	up
Hex1Cer(d19:0/18:1)	neg	Hex1Cer	1.93935237	0.03395090 4	1.56617259	up
Hex1Cer(t18:1/18:1)	neg	Hex1Cer	2.242756976	0.00902501 9	1.69024652 4	up
Hex1Cer(d18:2/24:0)	neg	Hex1Cer	0.183959332	0.00590320 6	2.01291990 6	down
Trihexosyl-ceramide (4)						
Hex3Cer(d18:1/16:0)	pos	Hex3Cer	4.062920634	0.01118092 7	1.44498446 1	up
Hex3Cer(d18:1/16:0)	pos	Hex3Cer	2.71020805	0.04192949 8	1.08276526 9	up
Hex3Cer(d18:1/22:0)	pos	Hex3Cer	4.861768749	0.00364675	1.72268313 5	up
Hex3Cer(d18:1/22:0)	pos	Hex3Cer	2.914864765	0.01733947 1	1.34393708	up
Hemolytic phosphatidic acid (3)						
LBPA(14:0/16:1)	neg	LBPA	5.924818473	0.02069012 4	1.74469993 7	up

LBPA(16:1/16:1)	neg	LBPA	1.66778087	0.02189226 9	1.44574494 9	up
LBPA(18:1/18:2)	neg	LBPA	0.163657179	0.02260570 3	3.31966239 1	down
Lysophosphatidic acid (2)						
LPA(16:1)	neg	LPA	1.599961296	0.04237944 8	1.44176906	up
LPA(18:3)	neg	LPA	0.391179675	0.03884571 5	1.39980357 3	down
Lyso- phosphatidylcholine (7)						
LPC(16:2)	pos	LPC	2.37317487	0.04647016	1.56077664 5	up
LPC(16:2)	pos	LPC	2.393115122	0.00959186 6	1.86288160 1	up
LPC(28:1)	pos	LPC	3.07518209	0.00779954 3	1.70931412 2	up
LPC(28:2)	pos	LPC	2.231404389	0.04679153 3	1.26919199 7	up
LPC(15:0)	neg	LPC	0.452380609	0.02381015 2	2.13985776 5	down
LPC(17:0)	neg	LPC	0.442884942	0.01534781 4	2.55652191 7	down
LPC(17:0)	neg	LPC	0.453571134	0.02529279 4	1.78837830 7	down
Lipopolysaccharide (1)						
LPG(18:1)	neg	LPG	0.006400797	0.03974450 3	2.55309833 5	down
Hemolytic phosphatidylinositol (1)						
LPI(16:1)	neg	LPI	2.288250696	0.03512620 2	1.36162313 9	up
Lipopolysaccharide (2)						
LPS(20:0)	pos	LPS	2.954181318	0.04547945 1	1.03456244 7	up
LPS(16:1)	neg	LPS	1.828475638	0.03289134 9	1.50766729 3	up
Methylphosphatidylcholine (6)						
MePC(32:4)	pos	MePC	3.64432363	0.01950950 8	1.56204338 2	up
MePC(39:10)	pos	MePC	6.10302001	0.00010793 4	2.88806972 1	up
MePC(39:10)	pos	MePC	3.301540675	0.00169569 1	2.25774914 4	up
MePC(41:11)	pos	MePC	4.364163416	2.15192E-05	1.26755474 2	up
MePC(46:14)	pos	MePC	3.417429144	0.00319434 3	2.19880699 6	up
MePC(46:14)	pos	MePC	1.863034026	0.03731898 9	1.63439531 6	up
Monogalactosyl diacylglycerol (5)						

MG(16:0)	pos	MG	2.759406122	0.00764783 5	1.62542937 1	up
MG(16:1)	pos	MG	3.233180547	0.04412490 3	1.52650149	up
MG(16:1)	pos	MG	4.165171084	0.00218080 9	2.32122900 6	up
MG(20:4)	pos	MG	1.985146418	0.02486743	1.26387833 4	up
MG(22:6)	pos	MG	2.153626007	0.01612036 7	1.31447832 4	up
Phosphatidic acid (17)						
PA(16:1)	pos	PA	12.46373157	0.01323192 3	1.76902782 2	up
PA(16:0/16:0)	neg	PA	1.587210937	0.03675626 7	1.11662349 6	up
PA(16:0/16:1)	neg	PA	2.974355124	0.02720493 6	1.35591594 9	up
PA(16:0/18:1)	neg	PA	1.927733874	0.04384276 9	1.16522995 3	up
PA(16:1/18:1)	neg	PA	7.81981789	1.05946E-05	1.45799447	up
PA(16:1/18:1)	neg	PA	3.029137778	0.00026871 1	1.21234399 4	up
PA(18:0/16:1)	neg	PA	2.982005663	0.00025543	1.45978798 3	up
PA(18:0/16:1)	neg	PA	1.671822782	0.01393875 3	1.05456867 5	up
PA(18:0/18:2)	neg	PA	1.930927767	0.01319286 5	2.07596074 5	up
PA(42:0)	neg	PA	1.80003251	0.02864889 4	1.01632047 1	up
PA(18:1/18:3)	neg	PA	0.452388958	0.01017835 6	1.35242061 7	down
PA(18:3/28:6)	neg	PA	0.336944249	0.00904002 8	1.63630495 1	down
PA(23:0/18:1)	neg	PA	0.418034584	0.00100488 2	1.93135236	down
PA(23:0/18:1)	neg	PA	0.676089078	0.03661803 1	1.03597267 2	down
PA(24:0/18:1)	neg	PA	0.63129021	0.00433153 9	1.12623510 6	down
PA(26:5/22:6)	neg	PA	0.672145145	0.03682367 1	1.43093519 7	down
PA(26:5/22:6)	neg	PA	0.509549127	0.00544777 8	2.45647962 5	down
Phosphatidylcholine (125)						
PC(14:0/15:2)	pos	PC	7.656217636	0.00104943 9	2.26506896 1	up
PC(14:0/15:2)	pos	PC	2.660875813	0.00806236 2	1.51116939 1	up
PC(15:0/19:4)	pos	PC	3.438828308	0.01532254	1.35668186 4	up
PC(15:2/22:6)	pos	PC	2.368732943	0.01542109 4	1.65998816 5	up

PC(16:0/18:2)	pos	PC	2.219758048	0.02464539 2	1.65654151 7	up
PC(16:1/18:1)	pos	PC	2.83444168	0.00654744 9	1.07905548 1	up
PC(16:1/19:2COOH)	pos	PC	3.378074412	0.00389447 1	1.31691937 4	up
PC(16:2/21:6)	pos	PC	2.608367808	0.04401882 8	1.48149181 8	up
PC(16:2/21:6)	pos	PC	1.948175385	0.03086685 2	1.24628422 6	up
PC(16:3/15:0)	pos	PC	2.299048633	0.01399129 7	1.57665862 9	up
PC(18:2/13:1)	pos	PC	6.222259786	0.00050832	1.69828186	up
PC(18:2/13:1)	pos	PC	2.481431884	0.00886037 4	1.08772053 7	up
PC(18:2/21:4COOH)	pos	PC	2.465086978	0.02656433 1	1.34359473 3	up
PC(18:4/15:2)	pos	PC	6.411442951	0.00027749	1.86893425 8	up
PC(18:4/15:2)	pos	PC	2.728170165	0.00507707 6	1.28177458 4	up
PC(18:4/18:1COOH)	pos	PC	2.577521139	0.01211948 7	2.02760525 6	up
PC(18:4/19:0COOH)	pos	PC	4.748579686	0.00090257 9	1.15109326 9	up
PC(18:4CHO)	pos	PC	2.410482286	0.04963763 7	1.41604608 2	up
PC(18:4COOH/18:0)	pos	PC	2.356223878	0.01499500 4	1.38247232 9	up
PC(20:5/14:0COOH)	pos	PC	3.702846257	0.03255464 7	2.38797341 7	up
PC(24:1/15:4COOH)	pos	PC	2.286035774	0.00491792 7	1.14864560 5	up
PC(31:2)	pos	PC	3.77385768	0.01411106	1.25081839 7	up
PC(32:1CHO)	pos	PC	4.482731382	0.00193242 7	1.87371686 3	up
PC(32:1CHO)	pos	PC	2.547402089	0.00490381 7	1.78015643 7	up
PC(32:2COOH)	pos	PC	5.07165031	0.00023205 6	1.08960307 8	up
PC(33:5)	pos	PC	3.731606505	0.00109680 7	2.38802720 3	up
PC(33:5)	pos	PC	2.458053091	0.01576083 5	1.64056497	up
PC(33:7)	pos	PC	4.115351254	0.00292987 4	1.33028034 7	up
PC(36:2COOH)	pos	PC	1.757646298	0.03923835	1.06723784 2	up
PC(36:6)	pos	PC	3.521630938	0.00228774 5	1.1444193	up
PC(40:4COOH)	pos	PC	3.165420177	0.00156325 7	1.64686182 6	up
PC(40:4COOH)	pos	PC	2.519661089	0.04978807 8	1.05421012 7	up
PC(46:8)	pos	PC	2.038282071	0.04730996 8	1.24724384 1	up

PC(14:1/20:1)	pos	PC	0.566717499	0.04148751 2	1.02773988 1	down
PC(15:0/18:0)	pos	PC	0.400169765	0.01318556 5	1.22734796 2	down
PC(15:0/20:5)	pos	PC	0.283184581	0.00088338 5	2.00074812 6	down
PC(17:0/18:2)	pos	PC	0.400043342	0.04935750 7	1.95960332 5	down
PC(18:1/17:0)	pos	PC	0.392909538	0.03816344 8	1.91633012 6	down
PC(18:3/15:0)	pos	PC	0.236056904	0.00014652 6	1.67398072 5	down
PC(18:3/15:0)	pos	PC	0.427207962	0.00960585 8	1.46006885	down
PC(18:3/16:0)	pos	PC	0.451656241	0.03681194 2	1.51618397 4	down
PC(19:4/18:0)	pos	PC	0.372674842	0.02056265 2	1.93626910 8	down
PC(22:2)	pos	PC	0.18914768	0.04499938 3	1.91976683 9	down
PC(22:5/18:0)	pos	PC	0.405860793	0.01377615 4	1.06311522 4	down
PC(28:3)	pos	PC	0.316808924	0.00532065 1	1.75340345 8	down
PC(28:3)	pos	PC	0.354918673	0.00702632 3	2.05081643 8	down
PC(29:3)	pos	PC	0.530745945	0.04950177	1.22244267 1	down
PC(29:3)	pos	PC	0.212716361	0.00044171 8	2.75949624 8	down
PC(30:3)	pos	PC	0.24836147	0.04891543 1	2.50568607 5	down
PC(30:3)	pos	PC	0.363215115	0.01412020 4	2.00044239 1	down
PC(30:4)	pos	PC	0.375255583	0.01747292 1	1.20191324 1	down
PC(30:4)	pos	PC	0.35271955	0.01532786 6	2.29758527 7	down
PC(31:1)	pos	PC	0.211903035	0.00071116 8	1.54969505 3	down
PC(32:5)	pos	PC	0.379301603	0.02560506 3	1.27212022 9	down
PC(32:5)	pos	PC	0.403116347	0.03559486 4	1.69765239 2	down
PC(33:3)	pos	PC	0.165348934	0.00212866 2	1.23137526 6	down
PC(35:0)	pos	PC	0.31247096	0.03824702 5	1.77012398 2	down
PC(36:2CHO)	pos	PC	0.441185626	0.01626636 7	1.15233031 9	down
PC(36:7COOH)	pos	PC	0.154127258	0.01421006 2	2.56507646 7	down
PC(37:2)	pos	PC	0.490110443	0.03482532 2	1.64522984	down
PC(38:2CHO)	pos	PC	0.287104657	0.00112546 5	2.83399548 9	down
PC(38:3CHO)	pos	PC	0.341801838	0.01310833 6	1.94120181 6	down

PC(38:4CHO)	pos	PC	0.346500341	0.00945897 4	1.83791185 6	down
PC(39:5)	pos	PC	0.402106108	0.02242876 3	1.81483697 7	down
PC(40:2CHO)	pos	PC	0.101777327	4.07212E-05 8	4.01215945 8	down
PC(40:2CHO)	pos	PC	0.365006211	0.00309687 9	2.59509882 9	down
PC(40:4CHO)	pos	PC	0.465032466	0.02210324 6	1.76207707 2	down
PC(41:2)	pos	PC	0.371726402	0.00942507 5	1.71572695 3	down
PC(42:3)	pos	PC	0.307280814	0.00655448 3	1.66291519 3	down
PC(42:3)	pos	PC	0.42825759	0.02728955 3	1.84181605 9	down
PC(15:2COOH/18:2)	neg	PC	2.562993016	0.00352334 4	1.51092480 7	up
PC(16:1/17:5CHO)	neg	PC	1.581268104	0.02122162 2	1.78783106 1	up
PC(17:0/16:1)	neg	PC	2.267728593	0.00140486 4	1.29315281 2	up
PC(17:0/16:1)	neg	PC	1.832944722	0.01003248 8	1.32137812 5	up
PC(19:4COOH/18:2)	neg	PC	1.754653085	0.02858129 1	2.01200276 1	up
PC(12:1/18:3)	neg	PC	0.323698959	0.00379374 7	1.40328239 8	down
PC(14:0/15:0)	neg	PC	0.123391818	0.00121379 7	1.86793251 2	down
PC(14:0/15:0)	neg	PC	0.178338471	0.01276237 6	2.14779324 7	down
PC(15:0/15:0)	neg	PC	0.240853792	0.00047849 1	2.63514090 1	down
PC(15:0/15:0)	neg	PC	0.369075111	0.00657874 3	2.35022459 7	down
PC(15:0/18:3)	neg	PC	0.155016485	0.00023195 3	1.82534843 3	down
PC(15:0/18:3)	neg	PC	0.325045889	0.01596899 2	1.22013284 8	down
PC(15:0/20:4)	neg	PC	0.146267803	7.80168E-05 2	3.46548539 2	down
PC(15:0/20:4)	neg	PC	0.334059356	0.00053183 2	2.27505382 2	down
PC(15:0/22:5)	neg	PC	0.421961515	0.01013683 1	2.46762881 4	down
PC(15:0/22:5)	neg	PC	0.426374305	0.01454001 8	1.77459878 6	down
PC(15:1/18:3)	neg	PC	0.248574094	0.00036377 5	1.60433926 4	down
PC(15:1/20:4)	neg	PC	0.500783386	0.01297250 4	1.98729069 5	down
PC(16:0/19:1COOH)	neg	PC	0.302732783	0.00019441 3	1.54654351 3	down
PC(16:0/19:4)	neg	PC	0.778660752	0.04810158 4	1.27505282 2	down
PC(16:0/19:4)	neg	PC	0.356435705	0.00832299 5	1.12223111 2	down

PC(16:0/22:5)	neg	PC	0.447500297	0.02035791 2	1.10608193 3	down
PC(16:1/16:0)	neg	PC	0.406418696	0.01975146 8	1.84231004 2	down
PC(16:1/19:1)	neg	PC	0.440881424	0.00724007 8	1.82805123 8	down
PC(16:1/19:1)	neg	PC	0.480784728	0.00288414 6	1.51387405 8	down
PC(16:1/22:5)	neg	PC	0.468347194	0.00841026 6	1.39562573 2	down
PC(16:2/18:3)	neg	PC	0.405292101	0.00883908 8	1.65754764 8	down
PC(16:2/22:4)	neg	PC	0.566179029	0.03915418 3	1.09068341 8	down
PC(18:0/17:1)	neg	PC	0.187750942	0.00024024 5	2.40748317	down
PC(18:0/17:1)	neg	PC	0.414606357	0.00267039 3	1.41745905 1	down
PC(18:0/20:1)	neg	PC	0.475662051	0.01080322 5	1.61631205 4	down
PC(18:0/22:4)	neg	PC	0.569328065	0.04791306 8	1.31623240 8	down
PC(18:0/22:5)	neg	PC	0.414332476	0.01195344 2	1.32316745 2	down
PC(18:1/19:2)	neg	PC	0.558477853	0.00813754 1	1.00763018 7	down
PC(18:2/18:2)	neg	PC	0.475491242	0.04951139 3	1.39053764 6	down
PC(18:2/19:2)	neg	PC	0.51931336	0.01657116 2	1.44501340 5	down
PC(18:2/22:6)	neg	PC	0.383213297	0.00891429 7	1.52157305	down
PC(18:4/18:1)	neg	PC	0.470350763	0.00216631 2	1.30804896 2	down
PC(18:4COOH/18:1)	neg	PC	0.38776054	0.01102540 3	1.87034038 6	down
PC(18:4COOH/18:1)	neg	PC	0.46192647	0.03511811 6	1.83499498 3	down
PC(19:0/18:1)	neg	PC	0.38515281	0.00094930 2	1.56421424 3	down
PC(19:0/18:2)	neg	PC	0.362098138	0.00130734 6	2.12968363 9	down
PC(19:0/18:2)	neg	PC	0.550192393	0.03786622 1	1.50963182 3	down
PC(19:4COOH/24:0)	neg	PC	0.410810879	0.00962223	1.09101805 9	down
PC(20:0/18:2)	neg	PC	0.551007058	0.02268407 4	1.02772525 6	down
PC(20:3COOH/18:2)	neg	PC	0.405597789	0.00122336 9	1.86564504 7	down
PC(20:3COOH/18:2)	neg	PC	0.573129824	0.03057369 4	1.55812108 6	down
PC(21:4/21:4COOH)	neg	PC	0.236517746	0.01118179 9	1.84815802 3	down
PC(23:0/18:1)	neg	PC	0.603955869	0.01102636 5	2.24059694 1	down
PC(23:0/18:1)	neg	PC	0.267400909	4.15665E-05	2.42960930 3	down

PC(23:0/18:2)	neg	PC	0.211659808	0.00181175 6	2.58456959 2	down
PC(23:0/18:2)	neg	PC	0.34776808	0.00415504 7	2.06473179 2	down
PC(24:0/18:2)	neg	PC	0.55081334	0.02184927 8	2.09298149 7	down
PC(24:0/18:2)	neg	PC	0.330651678	0.00358125 7	2.25232947 3	down
PC(37:4COOH)	neg	PC	0.397780104	0.00792581 6	1.42533545 3	down
Phosphatidyl ethanolamine (83)						
PE(14:0/16:1)	pos	PE	2.809962573	0.03071029 3	1.02710436 2	up
PE(14:0/18:2)	pos	PE	9.15655524	0.00051847 3	2.20149933 7	up
PE(14:0/18:2)	pos	PE	2.556538404	0.01302687 5	1.27887425 5	up
PE(14:1/20:2)	pos	PE	3.900256238	0.00043431 1	1.70913683 9	up
PE(16:0/18:2)	pos	PE	4.234071927	0.00047292 3	2.62966834 7	up
PE(16:0/18:2)	pos	PE	2.267838876	0.02004248 9	1.53829372 7	up
PE(16:0/18:2CHO)	pos	PE	10.2803324	0.00021163 2	1.90779182	up
PE(16:0/18:2CHO)	pos	PE	3.147980857	0.00611406 2	1.33506824 8	up
PE(16:0/20:4)	pos	PE	2.702406485	0.00975386 1	1.67786710 8	up
PE(16:1/18:1)	pos	PE	4.475013628	0.00374548 2	1.54254269 8	up
PE(18:1/16:1)	pos	PE	4.475013628	0.00374548 2	1.58834241	up
PE(18:1/18:2)	pos	PE	2.588443408	0.01527473	1.84832897 6	up
PE(18:3/16:1)	pos	PE	2.996980625	0.00323555 4	1.30217577 7	up
PE(18:4/16:1)	pos	PE	2.959244516	0.00398022 6	1.26826428 6	up
PE(20:5/16:1)	pos	PE	8.407976083	0.00015465 7	1.71645214 1	up
PE(20:5/16:1)	pos	PE	2.646540858	0.00744725	1.03378323 1	up
PE(34:2CHO)	pos	PE	2.541070913	0.00312377 8	1.09703501 4	up
PE(36:4)	pos	PE	2.674810158	0.02110304 7	1.44016980 1	up
PE(36:5)	pos	PE	4.742646912	0.00036402 5	2.70527375 7	up
PE(36:5)	pos	PE	2.34906439	0.02200295 4	1.49772586 3	up
PE(36:7)	pos	PE	5.181048341	0.01222467 6	1.50628561 8	up
PE(38:6)	pos	PE	3.652644051	0.00305308 6	1.93445321 8	up
PE(18:0/22:2CHO)	pos	PE	0.304115769	0.00182729 1	1.21813308 5	down

PE(18:0/22:2CHO)	pos	PE	0.472476919	0.02623480 1	1.22238759 3	down
PE(18:0/22:4)	pos	PE	0.449596356	0.03365964 9	1.49579243 9	down
PE(18:1/22:2CHO)	pos	PE	0.188822323	0.00141554 4	3.24258937 8	down
PE(18:1/22:2CHO)	pos	PE	0.371634716	0.04199330 6	2.86414505 7	down
PE(22:3CHO/18:1)	pos	PE	0.325039143	0.03427879 7	1.53367003 8	down
PE(40:3CHO)	pos	PE	0.362467231	0.04382912 9	1.92809638 2	down
PE(16:1/18:2)	neg	PE	4.001778621	0.00044323 7	1.67093814 7	up
PE(16:1/18:2)	neg	PE	1.900686952	0.02694391 4	1.22085230 4	up
PE(16:1/19:3COOH)	neg	PE	3.573731416	0.00127800 7	1.97006362 8	up
PE(16:1/20:4)	neg	PE	2.489554429	0.00863808 8	1.54323308 8	up
PE(16:1/20:5)	neg	PE	3.505650783	0.03428119 4	3.14963213 3	up
PE(17:1CHO/18:2)	neg	PE	1.694569474	0.04819182 1	1.01783697 2	up
PE(18:0/18:2)	neg	PE	2.928234989	0.03330491 6	2.06243881 8	up
PE(18:2/18:2)	neg	PE	1.893782821	0.02558321 9	1.77259226 3	up
PE(18:2/19:3COOH)	neg	PE	3.083122473	0.00152017 8	1.80934254 up	up
PE(18:2/21:4COOH)	neg	PE	2.416539493	0.01101483 4	2.63940847 9	up
PE(19:2COOH/20:5)	neg	PE	1.70235245	0.02596387 1	1.34572256 up	up
PE(12:0/17:0)	neg	PE	0.373759656	0.0014931	1.47777717 5	down
PE(14:0/15:0)	neg	PE	0.185863101	0.00762930 6	3.84642444 2	down
PE(14:0/22:2CHO)	neg	PE	0.269320373	0.00440059 5	1.53584290 1	down
PE(14:0/22:2CHO)	neg	PE	0.255345728	0.00354379 8	1.76873685 7	down
PE(14:1/16:0)	neg	PE	0.257458695	0.00910251 9	1.95634425 6	down
PE(14:1/16:0)	neg	PE	0.304754373	0.03477338 8	1.88971148 1	down
PE(15:0/16:0)	neg	PE	0.265510546	0.00271321	1.32193914 1	down
PE(15:0/16:0)	neg	PE	0.417669402	0.03805561 1	1.06203861 6	down
PE(15:0/18:3)	neg	PE	0.273955579	0.00203535	1.68548606 3	down
PE(15:0/18:3)	neg	PE	0.339397246	0.00779138 1	1.82478707 1	down
PE(15:1/16:0)	neg	PE	0.366421976	0.00519132 1	2.07428759 8	down
PE(15:1/16:0)	neg	PE	0.330159325	0.00496935 8	1.83779226 8	down

PE(15:1/18:2)	neg	PE	0.594152244	0.02694362 2	1.07570905 3	down
PE(15:1/18:3)	neg	PE	0.307965854	0.00078611 2	1.78867847 1	down
PE(15:1/18:3)	neg	PE	0.441657733	0.00751776 8	1.35230022 4	down
PE(15:1/20:4)	neg	PE	0.478754212	0.01087276 7	1.15770112 4	down
PE(16:1/15:0)	neg	PE	0.297335601	0.02043804 9	1.79405597 3	down
PE(16:1/15:0)	neg	PE	0.17422387	0.02380870 1	2.82989060 1	down
PE(16:1/17:0)	neg	PE	0.340100105	0.00483783 2	1.90170089 6	down
PE(16:1/17:0)	neg	PE	0.339000323	0.00267659 3	1.65242978 9	down
PE(17:0/18:0)	neg	PE	0.285956065	0.00170014 8	2.43112142 1	down
PE(17:0/18:0)	neg	PE	0.246384055	0.00106032 3	2.88587890 7	down
PE(17:0/18:1)	neg	PE	0.368576921	0.00283963 2	1.56148923 5	down
PE(17:0/22:2CHO)	neg	PE	0.104184892	2.33717E-05	2.67165539 7	down
PE(17:0/22:2CHO)	neg	PE	0.232559351	0.00025038	1.90347654	down
PE(17:1/22:3)	neg	PE	0.423821521	0.02476052 8	1.82698219 1	down
PE(17:1/22:5)	neg	PE	0.219294588	3.34359E-05	2.47355462 4	down
PE(17:1/22:5)	neg	PE	0.512099116	0.01805222 5	1.38674577 2	down
PE(18:0/18:0)	neg	PE	0.306625607	0.04938730 1	1.84435753 4	down
PE(18:0/20:3)	neg	PE	0.465091407	0.01957033	1.20612582 2	down
PE(18:0/22:1)	neg	PE	0.671753082	0.03744296 5	1.69238818 8	down
PE(18:0/22:2COOH)	neg	PE	0.291560081	0.01328147 7	1.05603150 1	down
PE(18:0/22:2COOH)	neg	PE	0.297297053	0.00702426 9	1.17693549 9	down
PE(18:0/22:3)	neg	PE	0.496084316	0.03057902	1.0449858	down
PE(18:1/17:0)	neg	PE	0.316038708	0.00235485	2.60820673 6	down
PE(18:1/18:1)	neg	PE	0.520426616	0.02793230 6	1.46710753 6	down
PE(20:0/18:3)	neg	PE	0.446240738	0.03402688 1	2.00666118 9	down
PE(20:2COOH/18:1)	neg	PE	0.384903742	0.01559031 3	1.32620624 7	down
PE(22:0/18:1)	neg	PE	0.676325986	0.03587103 3	1.61785704 2	down
PE(23:0/21:3COOH)	neg	PE	0.528281577	0.02924984	1.33648437 1	down
PE(23:0/21:3COOH)	neg	PE	0.480433599	0.01904177 8	1.45103666 1	down
PE(24:0/18:1)	neg	PE	0.382056657	0.01932276 4	1.92014498	down

PE(9:0CHO/18:0)	neg	PE	0.383966572	0.00019251 2	2.40016012 9	down
Phosphatidylethanolamine ethyl ester (2)						
PEt(18:4/21:2)	pos	PEt	4.063027387	0.00131568 4	1.62569474	up
PEt(20:0)	pos	PEt	3.130726416	0.02280702 5	1.04031163	up
Perfluoroalkyl acid (1)						
PFAA(15:0)	pos	PFAA	2.155224487	0.03980086 9	1.38647560 4	up
Phosphatidylinositol (11)						
PI(12:0/18:0)	neg	PI	2.469748843	0.00374044 3	2.13031534 3	up
PI(12:0/18:0)	neg	PI	1.753268	0.03088866 3	2.00145015 3	up
PI(16:0/18:1)	pos	PI	2.253198231	0.0158434	1.40925781 3	up
PI(16:0/20:3)	pos	PI	3.318718654	0.00525211	1.57898552	up
PI(16:0/20:3)	pos	PI	2.316761709	0.02203846 4	1.13306227 8	up
PI(18:0/16:1)	pos	PI	2.322130827	0.01144723 5	1.59094011 7	up
PI(18:0/22:5)	neg	PI	0.496455374	0.03593549 7	1.10982921 1	down
PI(18:1/22:5)	neg	PI	0.22787565	0.03204178	1.84319730 1	down
PI(19:0/20:4)	neg	PI	0.286412637	0.00085057 2	2.80841786 8	down
PI(22:7/16:0)	pos	PI	2.861599772	0.00066495	1.76669106 4	up
PI(22:7/16:0)	pos	PI	2.063221547	0.01714788 4	1.22360605 6	up
Phosphatidylserine (27)						
PS(18:3/18:0)	pos	PS	6.497425338	0.00039507 8	1.78459442	up
PS(18:3/18:0)	pos	PS	2.518510764	0.01436937 1	1.37036130 1	up
PS(19:0/18:2)	neg	PS	2.26051757	0.01753490 2	2.07909801 2	up
PS(19:0/18:2)	neg	PS	2.316580191	0.01686567 5	2.90044406 4	up
PS(22:1/18:2)	neg	PS	1.883771308	0.00607373 2	1.21445172 7	up
PS(22:1/18:2)	neg	PS	1.557307872	0.04570577 6	1.16553448 5	up
PS(22:1/20:4)	neg	PS	2.170696109	0.00039679 7	1.31286087 4	up
PS(22:1/20:4)	neg	PS	2.220759003	0.00297280 1	1.73367465 6	up
PS(15:0/20:1)	neg	PS	0.531786082	0.00348081 5	1.28444853 2	down
PS(17:0/18:1)	neg	PS	0.432372202	0.00171963	1.10341339 5	down

PS(18:0/19:2)	neg	PS	0.04793149	0.00734886 7	2.59297238 8	down
PS(18:0/19:2)	neg	PS	0.044848272	0.00593474 4	3.19759426 7	down
PS(18:0/20:2)	neg	PS	0.59285544	0.04099433 5	1.22029900 8	down
PS(18:1/23:1)	neg	PS	0.436332329	0.00098582 4	1.08974857 3	down
PS(18:1/25:1)	neg	PS	0.436789973	0.01087739 3	1.06523262	down
PS(19:0/22:4)	neg	PS	0.35466424	0.00021315	2.44540489 8	down
PS(20:0/22:4)	neg	PS	0.594511361	0.01037631 9	1.40674753 8	down
PS(21:0/20:3)	neg	PS	0.522080214	0.00782480 3	1.30823487 7	down
PS(22:0/22:5)	neg	PS	0.437147783	0.00146594 4	1.43381564 6	down
PS(23:0/18:1)	neg	PS	0.351963245	0.00030874 6	1.27608380 8	down
PS(23:0/18:2)	neg	PS	0.479901557	0.02197291 2	1.21336775 2	down
PS(23:0/18:3)	neg	PS	0.232944263	5.11618E-05	1.78554965 8	down
PS(23:0/18:3)	neg	PS	0.51486534	0.02428725 6	1.02901220 1	down
PS(23:0/20:4)	neg	PS	0.34921585	0.00118501 8	1.98236906 5	down
PS(23:0/20:5)	neg	PS	0.413010723	0.02106178 7	1.20056424 6	down
PS(25:0/18:1)	neg	PS	0.370662669	0.00273269 4	1.56461414 4	down
PS(25:0/18:2)	neg	PS	0.523964403	0.01578835 4	1.36187429 3	down
Sphingomyelin (16)						
SM(d18:2/20:1)	pos	SM	3.434533038	0.00721794 6	1.57903836 6	up
SM(d18:2/20:1)	pos	SM	1.808038327	0.04887736 8	1.22710967 1	up
SM(d28:1)	pos	SM	3.954373022	0.00016752	1.27062443	up
SM(d28:2)	pos	SM	3.898133919	0.00014329 5	1.46610254 8	up
SM(d32:3)	pos	SM	3.359990449	0.03722160 3	1.28609749 3	up
SM(d34:0)	pos	SM	2.840513561	0.02726379 8	1.59122228	up
SM(d34:1)	pos	SM	2.50000968	0.0119731	1.67094898 3	up
SM(d36:0)	pos	SM	3.203627045	0.00644069 3	1.0983343	up
SM(d36:1)	pos	SM	3.199225848	0.02104460 4	1.64970008 8	up
SM(d38:1)	pos	SM	4.68524095	0.01027685 1	1.89853661 7	up
SM(d38:5)	pos	SM	2.622540298	0.02782266 3	1.36704965 4	up
SM(d39:6)	pos	SM	2.122407366	0.03840126	1.53807684 1	up

SM(t32:0)	pos	SM	2.561315152	0.02391472 2	1.29181893 9	up
SM(t34:0)	pos	SM	2.746310935	0.00935331 9	1.91193750 3	up
SM(t36:1)	pos	SM	2.807143472	0.01841444 1	1.10665008 9	up
SM(d33:4)	pos	SM	0.425758248	0.02364502	1.92430865 1	down
Sphingosine (3)						
SPH(d16:1)	pos	SPH	3.245571304	0.00619424 7	1.99535082 4	up
SPH(d18:1)	pos	SPH	4.021276555	0.00012504 8	2.84413692 4	up
SPH(d18:1)	pos	SPH	2.59447201	0.00227997 7	2.10679749 4	up
Sphingosine-1-phosphate (2)						
SPHP(d18:1)	neg	SPHP	4.551653665	0.00411672	2.86782136 6	up
SPHP(d18:1)	neg	SPHP	2.33620408	0.01484832 6	2.84265955 3	up
Triacylglycerol (10)						
TG(14:0/14:0/18:0CHO)	pos	TG	5.890527721	0.04526779 5	1.51873548 4	up
TG(14:0/15:0/18:1)	pos	TG	2.134816999	0.02157878 4	1.39952664 3	up
TG(14:0/18:0/18:1CHO)	pos	TG	2.323113736	0.03184986 9	1.29171624 1	up
TG(14:1/16:1/18:1)	pos	TG	2.148652137	0.01477249 9	1.18334235 3	up
TG(15:0/19:0CHO/18:1)	pos	TG	5.277282888	0.04603569 9	1.58546583 2	up
TG(19:0CHO/13:0/16:1)	pos	TG	3.842199818	0.02318697 6	1.19863403 3	up
TG(2:0/4:0/18:1)	pos	TG	22.92684255	0.03170886 8	1.17241458 7	up
TG(32:0/19:2COOH)	pos	TG	5.233725165	0.03870194 9	1.18898389 2	up
TG(34:0CHO/16:1)	pos	TG	5.277050521	0.04510394 1	1.29680741 7	up
TG(4:1CHO/18:1/18:1)	pos	TG	8.807411978	0.04639770 8	1.49600047 7	up
Wax ester (6)						
WE(18:1)	pos	WE	2.262149263	0.00742617	1.46798089 3	up
WE(24:0/18:3)	pos	WE	3.040089785	0.01344201 6	1.87259626 8	up
WE(34:3)	pos	WE	2.127240152	0.04878332 1	1.35914556 2	up
WE(42:5)	pos	WE	3.808787163	0.00238638 3	1.49643955	up
WE(42:5)	pos	WE	2.484112897	0.00796984 7	1.22421384 7	up
WE(43:4)	pos	WE	2.018958973	0.02558141 5	1.07827477 6	up