Table SI. List of differentially expressed metabolites.

Metabolites	Compound ID	Adducts	Formula	Score	Fragmentation score	Mass error, ppm	VIP	P-value
11-deoxy-PGF1α	LMFA03010068	M+H, M+Na	$C_{20}H_{36}O_4$	38.9	5.01	0.936	1.053	<0.001
D-glucuronic acid	HMDB0000127	M-H	$C_6H_{10}O_7$	52.2	69.6	2.939	1.438	<0.001
12-hydroxy-12-octadecanoylcarnitine	HMDB0013154	M+H-H_2O	$C_{25}H_{49}NO_5$	41.5	13.9	0.049	2.676	<0.001
Palmitoyl-L-carnitine	961	M+H, M+Na	$C_{23}H_{45}NO_4$	44.1	22.5	-0.133	2.471	<0.001
Aminocaproic acid	HMDB0001901	M+H, M+K, 2M+K, 2M+Na, 2M+H, M+Na	$C_6H_{13}NO_2$	44.9	30.4	-1.941	2.011	<0.001
MG(0:0/22:4(7Z,10Z,13Z,16Z)/0:0)	HMDB0011554	M+NH_4	$C_{25}H_{42}O_4$	39.5	3.07	-0.332	2.652	<0.001
L-arginine	13	M+H	$C_6H_{14}N_4O_2$	50.8	60.8	-2.596	1.241	<0.001
6-keto-PGF1α	2558	M-H_2O-H, M-H	$C_{20}H_{34}O_6$	43.9	24.4	-2.669	1.798	<0.001
Cervonyl carnitine	HMDB0006510	M+H	$C_{29}H_{45}NO_4$	39.1	3.55	-0.2661	2.588	<0.001
N-[(4E,8Z)-1,3-dihydroxyoctadeca-4,8-dien-2-yl]hexadecanamide 1-glucoside	HMDB0034623	M+H-H_2O, M+Na	$C_{40}H_{75}NO_8$	40	10.3	-0.965	3.135	<0.001
Riboflavin cyclic-4',5'-phosphate	HMDB0059614	M+H-H_2O, M+H	$C_17H_{19}N_4O_8P$	40.9	10.1	-0.674	1.444	<0.001
Stearoylcarnitine	HMDB0000848	M+H, M+Na	$C_{25}H_{49}NO_4$	42.2	12.6	0.036	1.908	<0.001
Felodipine	HMDB0015158	M-H, M+Hac-H	$C_{18}H_{19}C_{12}NO_4$	31.3	0	-0.345	1.120	<0.001
PGF2α methyl ether	LMFA03010073	M+H-H_2O	$C_{21}H_{38}O_4$	41	12.9	0.160	1.350	<0.001
Lyciumin D	HMDB0040695	M+H	$C_{45}H_{57}N_9O_{11}$	32.3	0	-4.009	1.208	<0.001
Hypoxanthine	83	2M+H, 2M+K, M+H, M+H-H_2O	$C_5H_4N_4O$	55.5	79	0.4007	3.566	<0.001
MG(0:0/24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0)	HMDB0011560	M+NH_4	$C_{27}H_{42}O_4$	40.6	5.11	-0.301	3.114	<0.001
SM(d16:1/18:1)	LMSP03010040	M+Na	$C_{39}H_{77}N_2O_6P$	42.5	23.4	-0.467	6.857	<0.001
Ala Phe Arg	19527	M+H-H_2O, M+H	$C_{18}H_{28}N_6O_4$	48.2	43.7	0.587	1.122	<0.001
2-acetyl-4-methylpyridine	HMDB0037071	M+H-H_2O, M+H	C_8H_9NO	43.4	28.2	-0.894	1.087	<0.001
PA(17:2(9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	LMGP10010305	M+H-H_2O	$C_{42}H_{67}O_8P$	39.1	1.72	0.655	1.242	<0.001
Adenosine monophosphate	34478	M+H	$C_{10}H_{14}N_5O_7P$	43.2	20.9	-0.311	1.174	<0.001
PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	LMGP04050016	M-H	$C_{28}H_{45}O_9P$	43.4	21.9	-3.019	3.168	<0.001
3α,7β-dihydroxy-5β-cholest-24-en-26-oic Acid	HMDB0062712	M+NH_4	$C_{27}H_{44}O_4$	40.2	11	-0.245	1.095	<0.001
Delphinidin 3-sambubioside	HMDB0038003	M+NH_4	$C_{26}H_{29}O_{16}$+	38.9	2.38	0.118	1.093	<0.001
Hexaethylene glycol	HMDB0061822	M+Na	$C_{12}H_{26}O_7$	43.5	24.2	0.369440074	1.27462	<0.001
AS 1-5	HMDB0032843	M-H_2O-H	$C_{40}H_{77}NO_9$	38.5	0	-2.577	1.05961	<0.001
9-deoxy-9-methylene-16,16-dimethyl-PGE2	LMFA03010059	M+H-H_2O	$C_{23}H_{38}O_4$	45	25.7	0.095609464	5.74638	<0.001

Table SI. Continued.

Metabolites	Compound ID	Adducts	Formula	Score	Fragmentation score	Mass error, ppm	VIP	P-value
6-hydroxy flavin adenine dinucleotide	HMDB0011612	M-H_2O-H	$C_{27}H_{33}N_9Oz_6P_2$	39	5.34	-1.42055575	1.03462	<0.001
Toluene	HMDB0034168	M+H	C_7H_8	49.5	52.6	3.097667019	1.38517	<0.001
12-[5]-ladderane-dodecanoic acid	LMFA01140015	M-H	$C_{24}H_{38}O_2$	39.6	6.97	-2.334969157	1.47043	<0.001
Trandolapril-d5 diketopiperazine	HMDB0061178	M+FA-H	$C_{24}H_{32}N_2O_4$	40	3.21	0.375411892	3.78873	<0.001
MG(0:0/16:0/0:0)	HMDB0011533	M+H, M+Na	$C_{19}H_{38}O_4$	44	30.1	-1.25487032	1.29048	<0.001
PS(20:4(5Z,8Z,11Z,14Z)/0:0)	LMGP03050007	M-H	$C_{26}H_{44}NO_9P$	44.5	30.1	-3.521304611	3.47253	<0.001
11-oxo-androsterone glucuronide	HMDB0010338	M+Hac-H	$C_{25}H_{36}O_9$	39.3	4.29	-2.996648425	2.30143	<0.001
Ganoderal A	HMDB0035983	2M+K	$C_{30}H_{44}O_2$	39.4	13	-4.280978437	6.53651	<0.001
4,4α,5,6-tetrahydro-7-methyl-2(3H)-naphthalenone	HMDB0039803	M+H-H_2O, M+Na, M+H	$C_{11}H_{14}O$	46.8	40.7	-2.467005136	1.0493	<0.001
PI(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	LMGP06050012	M-H	$C_{31}H_{49}O_{12}P$	41	8.63	-2.496628516	5.39964	<0.001
MG(18:0/0:0/0:0)	HMDB0011131	M+H-H_2O, M+NH_4	$C_{21}H_{42}O_4$	40.8	6.27	0.387794015	3.17609	<0.001
Heptaethylene glycol	HMDB0061835	M+Na	$C_{14}H_{30}O_8$	45.3	35.7	0.403545076	1.13066	<0.001
Riboflavin (vitamin B2)	233	M+H, M+Na, M+K, M+H-H_2O	$C_{17}H_{20}N_4O_6$	49	47.3	0.703055462	1.54734	<0.001
Stearic acid	HMDB0000827	M-H	$C_{18}H_{36}O_2$	40.3	2.47	0.754702182	2.72861	<0.001
7-epizucchini factor A	HMDB0036405	M+NH_4	$C_{44}H_{59}NO_5$	39.6	14.2	3.750409481	1.77523	<0.001
5(Z),11(Z),14(Z)-eicosatrienoic acid	35044	M-H_2O-H, M-H	$C_{20}H_{34}O_2$	41.4	9.3	1.155640631	2.69857	<0.001
Acolamone	HMDB0035020	M+H-H_2O	$C_{15}H_{24}O$	43.4	24.8	-2.180931903	1.32868	<0.001
p-cresol	HMDB0001858	M+H-H_2O	C_7H_8O	38.9	0	4.051543613	2.00779	<0.001
LysoPE(0:0/20:4(8Z,11Z,14Z,17Z))	HMDB0011488	M+H, M+Na	$C_{25}H_{44}NO_7P$	43.3	24.5	-0.48028325	2.45924	<0.001
Eicosapentaenoyl ethanolamide	HMDB0013649	M+H, 2M+Na, 2M+H	$C_{22}H_{35}NO_2$	36.9	0.0906	-2.175164142	3.61464	<0.001
Arachidyl carnitine	HMDB0006460	M+H	$C_{27}H_{53}NO_4$	39.4	2.8	-0.23054379	1.09282	<0.001
Docosapentaenoic acid (22n-6)	HMDB0001976	M-H	$C_{22}H_{34}O_2$	38.2	0	-2.250128806	1.25945	<0.001
(3-methyl-2-butenyl)-benzene	HMDB0061808	M+H, M+Na, 2M+H	$C_{11}H_{14}$	40.4	7.71	-3.525414412	1.38468	<0.001
MG(0:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	HMDB0011555	M+H-H_2O	$C_{25}H_{40}O_4$	39.7	5.03	-0.517161158	1.66874	<0.001
PA(18:0/18:2(9Z,12Z))	HMDB0007861	M-H_2O-H	$C_{39}H_{73}O_8P$	38.6	0.187	-2.438278767	1.54643	<0.001
PE(15:1(9Z)/20:1(11Z))	LMGP02010494	M+H, M+Na	$C_{40}H_{76}NO_8P$	35	6.52	-3.94834109	3.13399	<0.001
PA(O-18:0/14:0)	LMGP10020021	M-H	$C_{35}H_{71}O_7P$	38.5	0	-2.78804082	1.58585	<0.001
1,2-dihydro-1,1,6-trimethylnaphthalene	HMDB0040284	M+H, M+Na	$C_{13}H_{16}$	42	18.9	-3.129995921	1.04528	<0.001
p-mentha-1,3,5,8-tetraene	HMDB0029641	M+H, M+Na, 2M+H	$C_{10}H_{12}$	44	28.5	-3.177236638	1.0562	<0.001
2-hydroxy-4-oxo-5,12-heneicosadien-1-yl acetate	HMDB0039403	M+H-H_2O	$C_{23}H_{40}O_4$	41.3	11.1	-0.202571598	2.44876	<0.001
Licocoumarin A	HMDB0033611	M-H	$C_{25}H_{26}O_5$	39.9	10.2	4.640976391	1.1576	0.0012
PC(16:0/0:0)[U] / PC(16:0/0:0)[rac]	182	M+H, M+K, 2M+H, M+Na, M+H-H_2O	$C_{24}H_{50}NO_7P$	43.8	27.4	1.155047716	11.4853	0.0012

Table SI. Continued.

Metabolites	Compound ID	Adducts	Formula	Score	Fragmentation score	Mass error, ppm	VIP	P-value
N-docosahexaenoyl phenylalanine	LMFA08020094	M-H	$C_{31}H_{41}NO_3$	39.3	7.14	-3.143293611	1.24534	0.0012
1-(2E,6E-phytadienyl)-2-(2E,6E-phytadienyl)-sn-glycero-3-phosphocholine	LMGP01040096	M+K	$C_{48}H_{92}NO_6P$	37.8	3.12	0.928315763	4.68706	0.0013
MG(0:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:0)	HMDB0011550	M+H-H_2O	$C_{23}H_{36}O_4$	41.6	11.8	0.007579726	1.23764	0.0014
10E,12Z-octadecadienoic acid	34801	M-H	$C_{18}H_{32}O_2$	42.3	15.7	-1.021395532	1.38636	0.0014
1,4-dithiane-2,5-diol	HMDB0033670	M+Hac-H	$C_4H_8O_2S_2$	37.4	0	1.514065385	2.06615	0.0014
2-methyl-1,3-cyclohexadiene	HMDB0032395	M+H, M+Na, 2M+Na, 2M+H	C_7H_{10}	41.1	15.1	3.873560245	1.01297	0.0017
1-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphate	HMDB0062312	M+Na	$C_{23}H_{39}O_7P$	46	38.5	-0.552860399	1.01968	0.0018
PE(17:0/17:2(9Z,12Z))	LMGP02010545	M+Na	$C_{39}H_{74}NO_8P$	39	9.27	-1.064717548	1.54816	0.0019
LysoPE(0:0/24:6(6Z,9Z,12Z,15Z,18Z,21Z))	HMDB0011499	M-H	$C_{29}H_{48}NO_7P$	40.1	3.96	-2.581547544	5.66736	0.0022
7b-hydroxy-3-oxo-5b-cholanoic acid	HMDB0000541	M+H-H_2O, M+Na	$C_{25}H_{38}O_4$	40.7	5.82	1.405353363	7.5402	0.0022
Deserpidine	HMDB0015221	M+H, M+Na	$C_{32}H_{38}N_2O_8$	36.9	0	-1.599308383	1.21072	0.0023
Tetrahydrofurfuryl butyrate	HMDB0036188	M+H	$C_9H_{16}O_3$	40.7	12.5	-1.426859358	1.60112	0.0023
1,4'-bipiperidine-1'-carboxylic acid	HMDB0060336	2M+Na	$C_{11}H_{20}N_2O_2$	38.3	0	-1.262923705	1.34887	0.0024
PC(22:1(13Z)/24:1(15Z))	HMDB0008585	M+K	$C_{54}H_{104}NO_8P$	38.5	7.38	1.273308171	5.10614	0.0025
N-[(4E,8E)-1,3-dihydroxyoctadeca-4,8-dien-2-yl]hexadecanamide	HMDB0035480	M-H, M+FA-H	$C_{34}H_{65}NO_3$	42.4	16.8	-3.365385075	1.4173	0.0026
PA(O-16:0/16:1(9Z))	LMGP10020008	M-H	$C_{35}H_{69}O_7P$	38.6	0	-2.890732288	1.67385	0.0029
Cardanolmonoene	HMDB0030482	M-H_2O-H	$C_{21}H_{34}O$	39.9	0.528	0.239540982	3.21802	0.0029
PA(12:0/20:5(5Z,8Z,11Z,14Z,17Z))	LMGP10010061	M+Hac-H	$C_{35}H_{59}O_8P$	38.2	0	-1.285039539	1.22159	0.0030
(4Z,7Z,10Z,13Z,16Z,19Z)-4,7,10,13,16,19-docosahexaenoic acid	3457	M-H_2O-H, M-H	$C_{22}H_{32}O_2$	40.9	7.54	-2.441494868	4.22328	0.0032
5,8,11-octadecatrienoic acid	LMFA01030341	M-H	$C_{18}H_{30}O_2$	41.1	11.5	-0.565135898	1.02818	0.0033
Docosahexaenoic acid	HMDB0002183	M-H_2O-H, M-H	$C_{22}H_{32}O_2$	55	75.8	-0.257441246	6.18154	0.0034
DG(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)	HMDB0007121	M+Na	$C_{41}H_{68}O_5$	37.7	1.83	-1.777013958	2.20181	0.0035
PI(18:2(9Z,12Z)/0:0)	LMGP06050010	M-H	$C_{27}H_{49}O_{12}P$	40.1	7.28	-3.225199678	2.48507	0.0035
Decanoylcholine	HMDB0013228	M+Hac-H, M+FA-H	$C_{15}H_{32}N_{O2}^{+}$	48.7	50.1	-1.70550808	3.59039	0.0041
5Z,7E,9E,14Z,17Z-eicosapentaenoic acid	LMFA01030760	M-H_2O-H, M-H	$C_{20}H_{30}O_2$	48.1	45.1	-0.373322352	1.78508	0.0044
LysoPC(P-16:0)	HMDB0010407	M+H, M+Na	$C_{24}H_{50}NO_6P$	40.1	6.21	-0.215707178	1.62161	0.0045
11,14-trans-eicosadienoic acid	24088	M-H	$C_{20}H_{36}O_2$	50.4	55.4	-1.006365351	1.20199	0.0046

Table SI. Continued.

Metabolites	Compound ID	Adducts	Formula	Score	Fragmentation score	Mass error, ppm	VIP	P-value
LysoPC(20:4(8Z,11Z,14Z,17Z))	HMDB0010396	M+H, M+Na, M+K, M+H-H_2O	$C_{28}H_{50}NO_7P$	43.2	17.6	0.166113037	4.35766	0.0046
PA(12:0/20:2(11Z,14Z))	LMGP10010058	M-H_2O-H	$C_{35}H_{65}O_8P$	38.5	0.0123	-2.655856225	1.86318	0.0047
Desogestrel	HMDB0014449	M+H-H_2O, M+H	$C_{22}H_{30}O$	41.1	16.7	-0.373116057	1.19534	0.0051
5-hydroxypropafenone	HMDB0060988	M+NH_4	$C_{21}H_{27}NO_4$	37.9	0.311	-2.306194984	1.08599	0.0053
LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	HMDB0011496	M-H	$C_{27}H_{44}NO_7P$	49.9	52.7	-2.467035754	3.27665	0.0054
1-eicosanoyl-glycero-3-phosphate	HMDB0062315	M+FA-H	$C_{23}H_{47}O_7P$	39.8	8.77	-3.784824343	1.21842	0.0056
LysoPC(15:0)	HMDB0010381	M-H, M+FA-H	$C_{23}H_{48}NO_7P$	42.4	15.1	-2.139337108	3.55749	0.0063
PA(22:4(7Z,10Z,13Z,16Z)/14:0)	LMGP10010788	M-H_2O-H	$C_{39}H_{69}O_8P$	38.8	0.848	-2.205621799	5.70366	0.0066
Persicachrome	HMDB0036425	M+Na	$C_{25}H_{36}O_3$	52.5	71.5	-0.342145334	1.4043	0.0068
Acetone	HMDB0001659	2M+H	C_3H_6O	39.6	0	0.631104102	1.28924	0.0084
(all-E)-3,5,7-tridecatriene-9,11-diyn-1-ol	HMDB0038526	M+H, 2M+H	$C_{13}H_{14}O$	39	5.3	-2.591762785	3.2025	0.0090
PC(15:0/22:4(7Z,10Z,13Z,16Z))	HMDB0007955	M+H-H_2O, M+NH_4	$C_{45}H_{82}NO_8P$	34.6	0	-2.654374634	1.23175	0.0093
(5Z,8Z)-1,5,8-heptadecatriene	HMDB0041082	M+FA-H	$C_{17}H_{30}$	39.8	2.41	-1.38808181	1.40487	0.0097
Acevaltrate	HMDB0034494	M+Na, M+K	$C_{24}H_{32}O_{10}$	37.7	2.21	-4.185762305	1.12576	0.0100
PE(16:0/0:0)	40776	M+H, 2M+Na, 2M+H, M+Na, M+K, M+H-H_2O	$C_{21}H_{44}NO_7P$	56	81.5	-0.172297785	2.4601	0.0120
Cohibin D	HMDB0035398	M+H	$C_{37}H_{68}O_4$	37.1	3.76	-1.178476063	1.0774	0.0123
2,3-dinor-11β-PGF2α	LMFA03010011	2M+NH_4	$C_{18}H_{30}O_5$	39.9	9.72	3.977922796	1.06813	0.0125
Glu Pro Pro Tyr	132539	M+H-H_2O, M+H	$C_{24}H_{32}N_4O_8$	38.6	0.0279	2.395748469	1.34395	0.0130
PC(18:1(9E)/0:0)[U]	46689	M+H, M+Na, M+K	$C_{26}H_{52}NO_7P$	49.4	49	0.743283153	4.35025	0.0151
Pantothenic acid	241	M+Na, M+K, 2M+Na, 2M+K, M+H, M+H-H_2O	$C_9H_{17}NO_5$	55.6	79.8	-0.37069974	1.00615	0.0154
SM(d18:2/16:0)	LMSP03010090	M+H-H_2O, M+H	$C_{39}H_{77}N_2O_6P$	38.8	6.01	-1.912798284	3.14081	0.0158
LysoPC(16:0)	HMDB0010382	M+FA-H	$C_{24}H_{50}NO_7P$	46.4	38.6	-3.952825278	1.73512	0.0160
Isopalmitic acid	4289	M-H	$C_{16}H_{32}O_2$	53.4	70.4	1.485621702	2.05686	0.0165
1-pentadecanoyl-glycero-3-phosphate	HMDB0062324	M-H_2O-H, M-H	$C_{18}H_{37}O7P$	38.8	1.5	-3.83135046	2.05014	0.0171
Butyl dodecanoate	HMDB0032065	M-H	$C_{16}H_{32}O_2$	40.5	4.5	1.098583359	2.32147	0.0176
5-(4-chloro-3-hydroxy-1-butynyl)-2,2'-bithiophene	HMDB0033269	M-H_2O-H	$C_{12}H_9C_lOS_2$	34	7.66	1.067393772	1.1039	0.0186
N-undecylbenzenesulfonic acid	HMDB0032549	M-H	$C_{17}H_{28}O_3S$	41.2	16.4	-1.838887238	1.16964	0.0193
Arachidonic acid (peroxide free)	193	M+H, 2M+H, M+K, M+Na, M+H-H_2O	$C_{20}H_{32}O_2$	50	60.1	-0.250922556	1.0129	0.0197
PS(18:2(9Z,12Z)/0:0)	LMGP03050011	M-H, M+FA-H	$C_{24}H_{44}NO_9P$	41.7	22.7	-3.357918022	1.59867	0.0204

Table SI. Continued.

Metabolites	Compound ID	Adducts	Formula	Score	Fragmentation score	Mass error, ppm	VIP	P-value
PC(14:0/20:3(5Z,8Z,11Z))	HMDB0007881	M+Na	$C_{42}H_{78}NO_8P$	37.1	0	1.061249909	1.86996	0.0214
PG(18:2(9Z,12Z)/0:0)	LMGP04050014	M-H	$C_{24}H_{45}O_9P$	42.9	18.4	-3.040151599	1.01928	0.0227
Mangiferic acid	HMDB0029800	M+H-H_2O, 2M+H, M+K, M+Na	$C_{18}H_{32}O_2$	42.8	22.9	-0.3490648	1.02684	0.0271
3-(2-heptenyloxy)-2-hydroxypropyl undecanoate	HMDB0034031	M+H-H_2O	$C_{21}H_{40}O_4$	39.4	3.22	-0.383885823	1.44861	0.027
3E,9Z,12Z-octadecatrienoic acid	LMFA01030140	M-H	$C_{18}H_{30}O_2$	40.7	8.31	-0.675724029	1.36013	0.0286
PC(16:0/6:0)	LMGP01010674	M-H, M+Hac-H	$C_{30}H_{60}NO_8P$	43.3	29	1.730435679	1.44876	0.0303
Mangostanol	HMDB0029868	M-H, M+Hac-H	$C_{24}H_{26}O_7$	38.9	4.64	3.922504085	2.08404	0.0303
2E,5Z,8Z,11Z,14Z-eicosapentaenoic acid	LMFA01030396	M-H, M+Hac-H	$C_{20}H_{30}O_2$	47	37.7	-1.897343	4.19893	0.0314
LysoPE(0:0/22:4(7Z,10Z,13Z,16Z))	HMDB0011493	M-H	$C_{27}H_{48}NO_7P$	40.3	5.41	-2.868466583	1.83462	0.0355
PE(18:0/0:0)	40775	M+H, 2M+Na, 2M+H, M+K, M+Na, M+H-H_2O	$C_{23}H_{48}NO_7P$	49.6	54	0.068579509	3.22429	0.0376
PI(13:0/0:0)	LMGP06050001	M+K	$C_{22}H_{43}O_{12}P$	31.1	3.63	-3.671928033	1.35497	0.0381
Xylene	HMDB0031461	M+H	$C_{24}H_{30}$	38.6	0	-1.020918773	1.09412	0.0387
1-O-(cis-9-Octadecenyl)-2-O-acetyl-sn-glycero-3-phosphocholine	43412	M+H, M+Na, M+H-H_2O	$C_{28}H_{56}NO_7P$	40.5	6.3	-0.650154992	1.29248	0.0393
Tolnaftate	HMDB0005005	2M-H	$C_{19}H_{17}NOS$	30.5	0	1.061108155	1.7151	0.0410
PC(17:1(10Z)/0:0)	LMGP01050002	M-H	$C_{25}H_{50}NO_7P$	41.5	15.6	-3.596125703	2.52115	0.0417
(±)-3-hydroxynonanoic acid	HMDB0031513	2M+H	$C_9H_{18}O_3$	40.3	4.17	0.196924099	1.45134	0.0424
Arg Thr Thr Thr	222215	M+H-H_2O, M+H	$C_{18}H_{35}N_7O_8$	38.3	0.0285	0.057700205	2.77341	0.0438
Adrenic acid	HMDB0002226	M-H_2O-H, M-H	$C_{22}H_{36}O_2$	41.7	10.9	-0.818252737	1.45506	0.0442
Sulfolithocholylglycine	HMDB0002639	M+H-H_2O, M+K, M+NH_4, M+Na, M+H	$C_{26}H_{43}NO_7S$	40.1	4.02	-0.523377376	2.87261	0.0450
Muricoreacin	HMDB0032086	M+Hac-H	$C_{35}H_{64}O_9$	39.4	4.04	-2.630257077	3.52974	0.0461

VIP, variable influence on projection.