

Supplementary Materials

Figure S1 Water intake and food intake

Figure S2 OPLS-DA score plot

Table S1 Cardiac function, blood pressure and body weight of each group of mice after 6-week modeling.

Table S2 Differentially expressed genes in Limonin-treated mice compared to HFpEF mice based on transcriptomics analysis (fold change >2 or <0.5 and adj. P <0.05)

Table S3 Differential metabolites in Limonin-treated mice compared to HFpEF mice based on metabolomics analysis (VIP>1, fold change >2 or <0.5 and P <0.05)

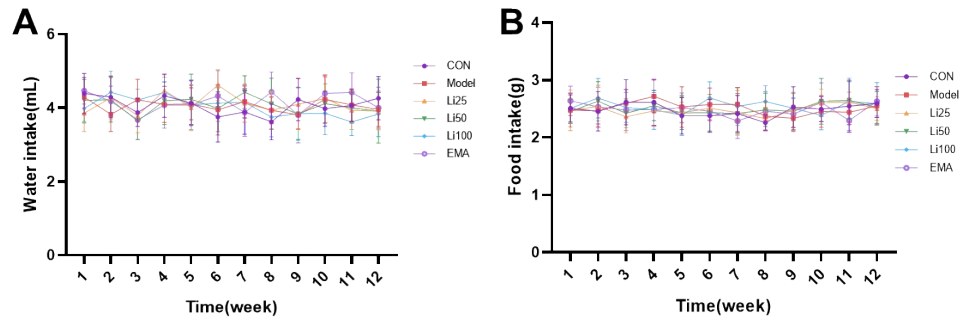


Fig. S1 (A) Water intake during the experiments (n=7). (B) Food intake during the experiments (n=7). All data were expressed as mean $\pm$ SD. * $P < 0.05$; ** $P < 0.01$; *** $P < 0.001$ evaluated using one-way ANOVA.

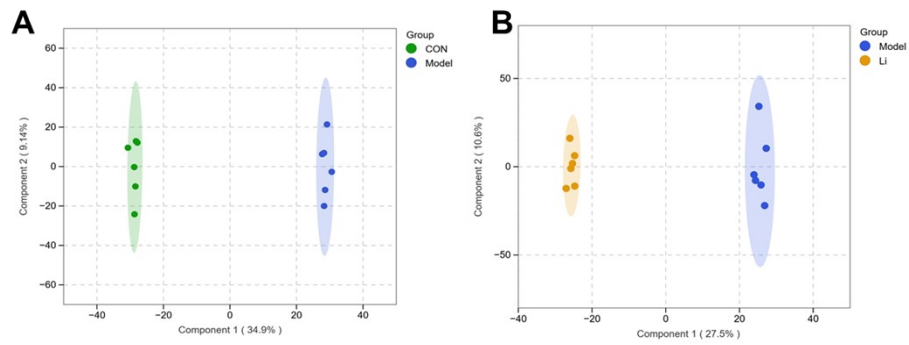


Fig. S2 (A) OPLSDA score plot of the HFpEF group compared to the control group. (n=6). (B) OPLSDA score plot of the Li group compared to the HFpEF group. (n=6).

Table S1 Cardiac function, blood pressure and body weight of each group of mice after 6-week modeling. All data were expressed as mean $\pm$ SD. * $P < 0.05$; ** $P < 0.01$; *** $P < 0.001$ compared with the control group evaluated using one-way ANOVA.

Group	EF%	LVAW;d (mm)	LVAW;s (mm)	LVID;d (mm)	LVID;s (mm)	LVPW;d (mm)	LVPW;s (mm)
CON	74.13 $\pm$ 5.55	0.84 $\pm$ 0.11	1.4 $\pm$ 0.12	3.62 $\pm$ 0.31	2.08 $\pm$ 0.23	0.63 $\pm$ 0.04	1.11 $\pm$ 0.11
Model	71.93 $\pm$ 6.29	0.88 $\pm$ 0.13	1.51 $\pm$ 0.16	3.41 $\pm$ 0.36	2.04 $\pm$ 0.35	0.77 $\pm$ 0.06	1.09 $\pm$ 0.06
Li25	72.71 $\pm$ 5.50	0.88 $\pm$ 0.10	1.44 $\pm$ 0.16	3.42 $\pm$ 0.30	2.02 $\pm$ 0.27	0.74 $\pm$ 0.04	1.08 $\pm$ 0.15
Li50	71.89 $\pm$ 5.57	0.86 $\pm$ 0.19	1.51 $\pm$ 0.10	3.48 $\pm$ 0.14	2.07 $\pm$ 0.15	0.73 $\pm$ 0.06	1.12 $\pm$ 0.10
Li100	71.84 $\pm$ 8.27	0.88 $\pm$ 0.14	1.49 $\pm$ 0.12	3.41 $\pm$ 0.24	2.02 $\pm$ 0.24	0.75 $\pm$ 0.04	1.10 $\pm$ 0.16
EMA	71.65 $\pm$ 7.92	0.87 $\pm$ 0.11	1.50 $\pm$ 0.21	3.61 $\pm$ 0.29	2.15 $\pm$ 0.37	0.75 $\pm$ 0.09	1.15 $\pm$ 0.19

Group	e'/a'	E/A	E/e'	BW (g)	SBP (mmhg)	DBP (mmhg)
CON	1.23 $\pm$ 0.09	1.28 $\pm$ 0.12	21.93 $\pm$ 2.61	27.14 $\pm$ 1.13	99.14 $\pm$ 5.07	74.79 $\pm$ 4.16
Model	0.61 $\pm$ 0.08***	1.31 $\pm$ 0.32	47.92 $\pm$ 5.29***	35.47 $\pm$ 2.77***	127.95 $\pm$ 4.70***	100.45 $\pm$ 6.04***
Li25	0.63 $\pm$ 0.12***	1.34 $\pm$ 0.34	47.33 $\pm$ 4.60***	35.15 $\pm$ 2.64***	124.37 $\pm$ 3.73***	101.89 $\pm$ 6.77***
Li50	0.64 $\pm$ 0.11***	1.26 $\pm$ 0.34	47.19 $\pm$ 6.54***	35.18 $\pm$ 2.85***	127.15 $\pm$ 5.41***	101.94 $\pm$ 6.62***
Li100	0.63 $\pm$ 0.14***	1.32 $\pm$ 0.11	47.40 $\pm$ 6.30***	35.35 $\pm$ 3.39***	124.43 $\pm$ 4.54***	99.63 $\pm$ 8.20***
EMA	0.65 $\pm$ 0.08***	1.30 $\pm$ 0.30	47.89 $\pm$ 5.14***	35.24 $\pm$ 2.97***	124.06 $\pm$ 4.42***	98.52 $\pm$ 6.51***

Table S2 Differentially expressed genes in Limonin-treated mice compared to HFpEF mice based on transcriptomics analysis (fold change >2 or <0.5 and adj. $P < 0.05$)

Gene symbol	Foldchange	adj. P	regulated
1700030J22Rik	7.635188367	0.01911711	up
Glde	6.12384819	0.03675976	up
Marco	5.176190565	0.01197432	up
Slc7a11	4.842615605	0.0169048	up
Gm39772	4.386307345	1.66E-05	up
Mmp8	4.13632962	0.0165301	up
Fth1	4.118596437	2.50E-62	up
Slc19a3	4.101933192	0.02708431	up
Serpina3c	3.883417986	0.0403186	up
Sost	3.085724766	0.03659569	up
CN725425	2.881529155	3.51E-06	up
Gm42326	2.788830953	0.02089071	up
2610035D17Rik	2.788061769	2.83E-06	up
Clec4e	2.78275482	0.02829886	up
Gdf15	2.748857685	6.65E-05	up
E130119H09Rik	2.672459625	6.78E-06	up
Ccl5	2.645265227	0.00157331	up
Bcat1	2.637879906	0.02731634	up
Gpx4	2.632532337	1.29E-21	up
Sv2b	2.628725101	0.03936581	up
Myc	2.563770897	9.94E-05	up

Mmp12	2.498903379	0.01692877	up
Nfe2l2	2.484024724	1.13E-15	up
Scx	2.483530966	2.49E-05	up
Shld1	2.42203226	9.65E-14	up
Ahsg	2.403449557	0.00693586	up
Gm4151	2.365175576	0.00033311	up
Ahrr	2.300105056	2.22E-05	up
D7Ertd443e	2.298191832	0.00042915	up
Ddit4l	2.24210641	0.0100068	up
Ftl1	2.225432698	1.16E-11	up
Pdk4	2.216822953	0.00157779	up
Klhl34	2.205928153	0.02877392	up
Lincrd1	2.094299012	0.01450713	up
Gm32954	2.093797097	1.12E-05	up
Tnfrsf12a	2.064531824	0.04457691	up
Arhgap11a	0.495587492	0.02348345	down
Mest	0.495450987	2.09E-10	down
Kif21b	0.489886647	0.02536297	down
Gm38585	0.48584227	0.02872308	down
Kcnqlot1	0.469263209	0.02294698	down
9430062P05Rik	0.462896695	0.02816088	down
Cd109	0.462087376	0.00606277	down
Gm47814	0.44441647	0.03576085	down
Lama3	0.442778461	0.00847576	down
Mki67	0.442550536	0.00233014	down
Prc1	0.440592869	0.03327468	down
Slfn9	0.438395978	0.00083368	down
Top2a	0.429475962	0.00174687	down
Potefam3e	0.420980993	0.03955316	down
Prkcg	0.414539388	0.00644673	down
Mybl1	0.409858728	0.0147939	down
Adam12	0.40728007	0.04485385	down
Gm42127	0.404583335	0.01907278	down
Plekhh1	0.387600276	0.02296996	down
Lrrc36	0.376148069	0.01816955	down
Nppb	0.37191412	0.00121609	down
Tpsb2	0.359444143	0.0287005	down
Tmprss13	0.342898057	0.02036056	down
Gm33583	0.3394046	0.0003504	down
Gm29040	0.332855445	0.03170942	down
Ptgs2	0.332256717	0.0026872	down
Aspm	0.317812424	0.02717035	down
Gm41949	0.317253445	0.02399523	down
Kif23	0.315025588	0.00078173	down

Gm36556	0.303935521	0.04903806	down
Gm30259	0.285497977	0.0015828	down
C2	0.284856354	0.03662855	down
Slc39a8	0.281671032	0.01614246	down
Muc3a	0.273091289	0.03244944	down
Cdca8	0.266129785	0.0470079	down
Nppa	0.262709906	4.53E-41	down
Fmod	0.260090061	0.02435349	down
Tfrc	0.255702675	3.10E-09	down
Cenpe	0.252600863	0.00075037	down
Gm46565	0.243537412	0.00035843	down
Sorcs1	0.243149798	0.04316906	down
Ptch2	0.230613413	0.00203338	down
Ckap2	0.207103513	0.00774491	down
Scart1	0.207100822	0.04718766	down
Tll2	0.193807096	2.43E-06	down
Gtse1	0.174919854	0.03105451	down
Gm36371	0.129835388	0.01000531	down
Ccnb1	0.124356087	0.00177701	down
Krt8	0.089753186	0.01441321	down
Lrrn4	0.028989155	0.00706817	down
Krt19	0.02586669	0.00565152	down
Upk3b	0.020757764	0.0379223	down
Msln	0.012565335	0.00132615	down

Table S3 Differential metabolites in Limonin-treated mice compared to HFpEF mice based on metabolomics analysis (VIP>1, fold change >2 or <0.5 and P<0.05)

Metabolites	VIP	Fold_Change	P-value	Type	m/z	Retention time (min)	Ion mode	Adducts
(-)-Arctigenin	1.621195	2.086046	0.000357	up	353.1410297	12.43226667	neg	M-H ₂ O-H
(11E,13E)-9-Hydroxyoctadeca-11,13-dienoylcarnitine	1.50406	4.532316	0.001442	up	462.3187117	9.196816667	pos	M+Na
(1S)-1-(3-Methoxyphenyl)-2-[4-[4-[(propan-2-ylideneamino)oxymethyl]phenyl]triazol-1-yl]ethanol	1.576784	2.363364	0.000333	up	379.1776718	13.52261667	neg	M-H
(2xi,6xi)-7-Methyl-3-methylene-1,2,6,7-octanetetrol	1.903401	5073345	0.001666	up	407.2635427	7.925816667	neg	2M-H
(4Z,7Z,10Z,13Z,16Z)-18-(3-Ethylloxiran-2-yl)octadeca-4,7,10,13,16-pentaenoylcarnitine	1.751049	0.141885	0.000989	down	510.3171602	11.35298333	pos	M+Na
(6beta,7alpha,12beta,13beta)-7-Hydroxy-11,16-dioxo-8,14-apianadien-22,6-olide	1.393879	5.916003	0.003747	up	429.1932747	12.499	neg	M+FA-H
(R)-1-O-[b-D-Apiofuranosyl-(1->2)-b-D-glucopyranoside]-1,3-octanediol	1.696457	0.137763	0.006389	down	475.2310208	9.991016667	pos	M+K
1(3)-glyceryl-PGE2	1.837397	64.38952	0.004532	up	425.2564014	14.50213333	neg	M-H
1,1'-Ethylidenebistryptophan	1.71076	0.306436	0.003203	down	434.1931225	4.611133333	pos	M+
1,2,3-Trihydroxyhenicos-12-en-4-one	1.789925	4.185692	3.93E-07	up	357.2988756	11.37606667	pos	M+H
1,2,5,6-Tetrahydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one	1.663789	0.178061	0.006184	down	218.0807902	4.90855	neg	M+FA-H
1,2-Ethanediol monoricinoleate	1.590732	0.457802	0.003821	down	342.280113	10.77791667	pos	M+
1,4,7,10,13,16-Hexaoxacyclooctadecane	1.740506	0.28338	0.002968	down	245.1380546	4.9602	neg	M-H ₂ O-H
1,6-Dihydroxy-3,7-dimethoxy-2-(3-methyl-2-butenyl)-8-(2-oxo-3-methyl-3-butenyl)-xanthone	1.223462	2.179594	0.003365	up	419.1514916	10.91725	neg	M-H ₂ O-H
10-Hydroxyloganin	1.902663	985218.9	0.001664	up	405.1421392	3.91495	neg	M-H

11-Oxo-androsterone glucuronide	1.76144	0.185636	0.003794	down	463.2310299	9.513083333	pos	M+H-H ₂ O
11-oxo-undeca-5,8-dienoic acid	1.731885	0.173057	0.003818	down	195.1011728	7.547333333	neg	M-H
12,13-Dihydroxyoleic acid	1.746561	0.398594	0.002564	down	313.2372063	9.696733333	neg	M-H
15,16-dihydroxy-octadecanoic acid	1.726982	0.176513	0.005616	down	315.2524069	9.892816667	neg	M-H
16,16-dimethyl-6-keto Prostaglandin E1	1.485748	715.6226	0.006367	up	441.251055	14.02606667	neg	M+FA-H
16b-Hydroxystanozolol	1.740396	3.162251	3.72E-06	up	389.2447279	11.9608	neg	M+FA-H
17(20)-Dehydrocryptogenin	1.493604	2.464096	0.006517	up	446.3239936	9.7215	pos	M+NH ₄
18-fluoro-9Z,12Z-octadecadienoic acid	1.669205	0.474256	0.00144	down	316.2647992	10.46566667	pos	M+NH ₄
1-O-(2R-hydroxy-4Z-octadecenyl)-sn-glycerol	1.471401	2.130176	0.004669	up	381.2973056	12.30043333	pos	M+Na
1-O-all-trans-retinoyl-beta-glucuronic acid	1.79125	0.168309	0.002778	down	477.2463427	9.911716667	pos	M+H
2-(5,8-Tetradecadienyl)cyclobutanone	1.707309	3.336972	0.001647	up	263.2352732	12.15255	pos	M+H
2-(Methylthio)pyrazine	1.74807	2.767259	6.03E-06	up	109.0220667	11.1589	pos	M+H-H ₂ O
2-[2-[Bis(carboxymethyl)amino]ethyl-[2-[bis(carboxymethyl)amino]-3-phenylpropyl]amino]acetic acid	1.689765	0.237224	0.001284	down	466.1828934	4.540116667	pos	M+H-H ₂ O
21-Desacetyl Deflazacort	1.710248	0.317221	0.001279	down	422.1931748	4.497066667	pos	M+Na
22:5(4Z,7Z,10Z,13Z,16Z)	1.599683	0.474255	0.006527	down	331.2607605	12.96523333	pos	M+H
2-Decarboxybetanin	1.646171	0.191954	0.005302	down	552.1584787	4.639166667	neg	M+FA-H
2-ethylacryloylcarnitine	1.719222	0.339487	5.84E-06	down	266.1373132	4.20325	pos	M+Na
2-Hydroxy-2,6,6-trimethylcyclohexanone	1.836004	2.158157	2.37E-06	up	139.1110487	6.97935	pos	M+H-H ₂ O
2-Hydroxy-imipramine glucuronide	1.070778	0.07522	0.002604	down	490.2537411	9.87285	pos	M+NH ₄
2-Methoxyestrone 3-glucuronide	1.632863	0.236513	0.007034	down	476.2033708	5.046933333	pos	M+
3-methyl-tridecanedioic acid	1.238746	0.469928	0.00593	down	239.1640528	9.556516667	neg	M-H ₂ O-H
3-O-Demethylfortimicin A	1.601216	140.1173	0.000731	up	409.2771115	7.941316667	pos	M+NH ₄
3Z,6Z,9Z-Heptadecatriene	1.750277	2.919985	0.00218	up	279.2318046	13.8029	neg	M+FA-H
4-Dodecylbenzenesulfonic Acid	1.668771	2.56179	0.006485	up	325.1828916	13.88943333	neg	M-H

4-ethylamino-6-isopropylamino-1,3,5-triazin-2-ol	1.47965	231.008	0.005948	up	393.2480109	9.71395	neg	2M-H
4-formyl Indole	1.534999	0.491071	0.004648	down	146.0592346	5.311633333	pos	M+H
4-Hepteneoylglycine	1.647934	0.375825	0.004048	down	186.1116273	4.760316667	pos	M+H
4-Hydroxynonenal glutathione	1.705492	0.243179	0.004334	down	462.1898295	4.587383333	neg	M-H
4-Oxododecanedioic acid	1.754771	0.390338	0.000636	down	243.122423	5.2036	neg	M-H
5-Hydroxydec-3-enoylcarnitine	1.616246	0.37972	0.00246	down	330.2255856	5.37535	pos	M+H
5Z,8Z,11Z-Eicosatrienedioic acid	1.547816	3.255772	0.003922	up	317.210838	10.50825	neg	M-H ₂ O-H
6-beta-hydroxydexamethasone	1.004998	6.253824	0.000217	up	453.1930875	11.9608	neg	M+FA-H
6-hydroxyphenylpropionylglycine	1.644902	0.375784	0.007247	down	222.0791284	4.297966667	neg	M-H
6-isobutyl-4-hydroxy-2-pyrone	1.778299	86.39481	0.003791	up	333.1340962	11.52545	neg	2M-H
7',8'-Dihydro-8'-hydroxyreticulataxanthin	1.901705	12441070	0.005328	up	473.3421937	14.214	pos	M+H-H ₂ O
7beta-Hydroxycholest-4-en-3-one	1.666176	0.304665	0.00221	down	401.3388145	14.84566667	pos	M+H
7-hydroxygranisetron	1.817584	45.93838	0.005696	up	309.1728565	13.32938333	neg	M-H ₂ O-H
8-Aminohexylamino cAMP	1.646938	0.263721	0.003647	down	442.1609626	4.50105	neg	M-H
8-iso Prostaglandin E2-d4	1.518113	0.493632	0.002386	down	379.238617	10.90236667	pos	M+Na
8-Propanoylneosolaniol	1.700807	0.203295	0.007014	down	456.2226893	10.3205	pos	M+NH ₄
9-(2-Phosphonomethoxypropyl)adenine	1.902381	621702.7	0.0019	up	286.0716066	3.926783333	neg	M-H
9,10,13-TriHOME(11)	1.648122	0.297509	0.001262	down	329.2317935	8.08455	neg	M-H
9,12,13-TriHOME	1.636398	0.302143	0.000262	down	313.2351322	8.255116667	pos	M+H-H ₂ O
Abeado	1.418282	2.332038	0.004255	up	697.3627888	4.50915	neg	2M-H
Acridine, 3,6-bis(2-(1-piperidinyl)ethoxy)-	1.758242	0.188922	0.004279	down	472.2363413	9.501216667	pos	M+K
Aliskiren	1.650242	2.577058	0.000249	up	552.3987697	13.534	pos	M+H
all-trans-heptaprenyl diphosphate	1.713284	0.188661	0.004939	down	672.4164316	12.71466667	pos	M+NH ₄
alpha-15,16-DiHODE	1.700753	0.486674	0.000701	down	311.2216076	9.218666667	neg	M-H
Amodiaquine	1.601225	2.186755	0.000593	up	378.1370081	6.111466667	pos	M+Na
Aprindine	1.579119	2.054987	0.000668	up	303.2226608	11.94938333	neg	M-H ₂ O-H

Arborinine	1.726896	0.414021	0.004076	down	308.0888041	9.742816667	pos	M+Na
Asparagine-betaxanthin	1.688039	0.424991	0.005487	down	308.0892292	4.582933333	pos	M+H-H ₂ O
Aspartyl-Asparagine	1.7969	0.198395	0.000107	down	248.0889426	0.59285	pos	M+H
Bis(perfluorobutyl)ethene	1.193225	0.042185	0.004071	down	464.9944261	4.273516667	pos	M+H
Carbuterol	1.015705	6.321353	0.000376	up	290.1485495	11.60778333	pos	M+Na
CE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))	1.481474	3.094727	9.94E-05	up	751.5403906	12.90346667	pos	M+K
Ceanothine C	1.698434	1955.573	0.005109	up	469.2823528	14.61663333	neg	M-H
chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5a	1.609457	0.458235	0.000694	down	196.0730713	0.71895	neg	M+FA-H
Ciclopirox	1.660511	3.354075	0.00048	up	413.2445873	12.02398333	neg	2M-H
Cinnzeylanine	1.725782	0.159724	0.005735	down	449.2152873	9.932983333	pos	M+Na
Cyclohexanemethylamine	1.841681	10.43303	0.000493	up	114.1273906	4.309233333	pos	M+H
Cyclopropanecarboxamide, 1,2,2,3,3-pentamethyl-	1.811029	8.170146	0.004766	up	200.1279249	6.220216667	neg	M+FA-H
Daucic acid	1.903497	2055816	0.000989	up	185.0110587	0.76955	neg	M-H ₂ O-H
Derenofylline	1.586868	2.450397	0.000207	up	353.1623622	13.33865	neg	M+FA-H
DG(18:1(12Z)-2OH(9,10)/i-18:0/0:0)	1.291771	14.6879	5.06E-05	up	635.5232424	12.73033333	neg	M-H ₂ O-H
DG(LTE4/i-18:0/0:0)	1.44578	2.181564	0.006392	up	780.5467787	13.35265	pos	M+H
Diflucortolone valerate	1.52463	0.297142	0.002092	down	478.2544314	10.50698333	pos	M+
Dihydroxyfomitremorgin C	1.640263	0.308987	0.001282	down	456.1766358	4.858316667	neg	M+FA-H
DL-7-hydroxy stearic acid	1.621198	0.343337	0.005217	down	299.2577921	12.8132	neg	M-H
Enniatin B	1.698281	0.240889	0.005924	down	622.4038304	11.43865	pos	M+H-H ₂ O
Ergothioneine	1.806317	2.540639	0.000588	up	230.0944435	0.758966667	pos	M+H
Erinacine G	1.520589	0.233875	0.006347	down	464.2398256	5.77905	pos	M+
fleroxacin	1.553473	0.355843	0.002149	down	414.129771	3.691566667	neg	M+FA-H
Glu Pro Tyr	1.579159	0.327219	0.000656	down	408.1775139	4.112116667	pos	M+H
Glucose lactate ketone	1.899933	5279620	0.00581	up	365.0715085	11.5101	neg	M-H ₂ O-H
Glutamylalanine	1.448205	0.376834	0.00677	down	217.0814547	0.787383333	neg	M-H ₂ O-H,

								M-H
Gluten exorphin C	1.727141	0.2287	0.003976	down	666.3963089	12.12575	neg	M-H
Hexyl glucoside	1.449461	0.424659	0.006537	down	245.1379968	5.0653	neg	M-H ₂ O-H
Hildgardtene	1.703821	4.054303	0.006024	up	365.1388828	11.69593333	neg	M+FA-H
indole-3-acetyl-valine	1.609315	3.052754	0.003823	up	545.2411016	4.355916667	neg	2M-H
Isolariciresinol 9'-O- α -L-arabinofuranoside	1.697053	0.190059	0.006001	down	492.1982562	4.103916667	pos	M+
LacCer(d18:1/14:0)	1.440294	2.270582	0.00391	up	816.5791616	13.35265	pos	M+H-H ₂ O
L-argininium(1+)	1.756765	2.264082	0.000522	up	176.1271539	0.781116667	pos	M+H
Lefradafibanum	1.69283	0.23051	0.003419	down	484.1713448	4.587383333	neg	M+FA-H
Leu Val	1.520745	0.290281	0.000412	down	229.1544076	3.651233333	neg	M-H
Levan	1.772356	0.212251	0.00212	down	549.1671408	4.650883333	neg	M+FA-H
Liquiritigenin 4'-O-apiosyl(1->2)-glucoside	1.727242	0.277722	0.000973	down	551.1811606	4.65935	pos	M+H, M+Na
Lisuride	1.805164	22.46737	0.005207	up	337.2041744	14.32031667	neg	M-H
LY-411575	1.630596	0.233946	0.00437	down	524.163486	4.858316667	neg	M+FA-H
Malvalic acid	1.793301	2.310883	7.11E-07	up	279.2317944	13.58258333	neg	M-H
Maysin 3'-methyl ether	1.808863	0.157063	0.003028	down	571.1487087	4.650883333	neg	M-H ₂ O-H
Melanthugenin	1.511663	2.515416	0.000794	up	455.2081967	12.70988333	neg	M-H
Melledonal A	1.654938	0.16866	0.004585	down	432.1773424	4.760316667	pos	M+
Melleolide	1.571531	2.336308	0.000393	up	381.1721402	13.52261667	neg	M-H ₂ O-H
Methacycline	1.605511	0.381649	0.007171	down	460.1721563	4.760316667	pos	M+NH ₄
Methionyl-Asparagine	1.634068	16.50584	0.000513	up	246.0890589	0.758966667	pos	M+H-H ₂ O
Methyl jasmonate	1.609658	2.716254	0.000612	up	247.1307205	11.9627	pos	M+Na
MG(0:0/18:1(9Z)/0:0)	1.626528	2.721804	9.31E-05	up	339.2871222	12.71466667	pos	M+H-H ₂ O
MG(16:0/0:0/0:0)	1.717699	2.56115	0.000242	up	313.2715699	12.48783333	pos	M+H-H ₂ O
MG(18:1(11Z)/0:0/0:0)	1.613076	2.844759	3.31E-05	up	401.2890037	12.73033333	neg	M+FA-H
MG(18:1(9Z)/0:0/0:0)	1.769915	4.794544	0.000133	up	401.2893269	12.9318	neg	M+FA-H

MG(18:1(9Z)/0:0/0:0)[rac]	1.630642	2.670053	0.000117	up	357.2977539	12.73443333	pos	M+H
MG(18:2(9Z,12Z)/0:0/0:0)	1.705012	3.036224	1.16E-05	up	337.2714243	11.9627	pos	M+H-H ₂ O, M+H
MG(18:2(9Z,12Z)/0:0/0:0)[rac]	1.648527	2.557737	0.001491	up	355.281758	12.15255	pos	M+H
MG(5-iso PGF ₂ VI/0:0/0:0)	1.822951	33.38785	0.006123	up	381.2302041	14.48291667	neg	M-H ₂ O-H
MITOGUAZONE	1.769716	4.303827	0.003515	up	367.2298297	14.47506667	neg	2M-H
N-(2-Hydroxyethyl)ethylenediaminetriacetic acid	1.807983	2.028649	2.55E-06	up	296.1445004	10.6132	pos	M+NH ₄
N-(gamma-Glutamyl)ethanolamine	1.416708	0.468615	0.00413	down	189.0866272	0.729966667	neg	M-H
N-(hexadecanoyl)-deoxysphing-4-enine-1-sulfonate	1.561646	2.02311	0.002002	up	584.4691892	13.09098333	pos	M+H-H ₂ O
N-(tetradecanoyl)-deoxysphing-4-enine-1-sulfonate	1.42508	115.3278	0.005016	up	556.4387299	14.23423333	pos	M+H-H ₂ O
Naltrindole	1.742013	3.386894	0.000335	up	459.1944122	2.831816667	neg	M+FA-H
Neuromedin B (1-3)	1.689071	0.284449	0.002335	down	320.1915659	9.84935	pos	M+NH ₄
Neuromedin N (1-4)	1.901362	49757286	0.006366	up	485.2770932	14.09375	neg	M-H ₂ O-H
Nicotine imine	1.549475	2.546391	0.006216	up	321.2093649	14.50213333	neg	2M-H
Nitrazine	1.196827	8.695125	8.26E-05	up	234.1305925	12.46706667	pos	M+H
N-Linoleoyl Glutamine	1.464677	2.415931	0.003878	up	407.2897961	10.80345	neg	M-H
N-T-Boc-leu-gly-arg P-nitroanilide	1.71668	0.214597	0.00649	down	582.3365274	11.54663333	pos	M+NH ₄
Octadec-11-en-9-ynoic acid	1.746183	2.024333	2.44E-05	up	277.2159448	12.07468333	neg	M-H
PA(16:0/20:4(8Z,11Z,14Z,17Z))	1.670414	0.440191	7.64E-05	down	677.4522863	12.36233333	neg	M-H ₂ O-H
PA(18:1(9Z)-O(12,13)/12:0)	1.657532	0.249485	0.00453	down	650.4345214	12.30043333	pos	M+NH ₄
PA(22:1(11Z)/0:0)	1.731166	0.376065	0.001061	down	531.2836018	10.90236667	pos	M+K
PA(8:0/i-19:0)	1.605185	2.502193	0.003347	up	561.3939554	11.85861667	pos	M+H-H ₂ O
Palmitoyl Serotonin	1.697398	0.170773	0.002222	down	415.3323647	14.11098333	pos	M+H
PC(0:0/20:4(5Z,8Z,11Z,14Z))	1.786873	0.411421	6.77E-07	down	582.2913502	10.1986	pos	M+K
PC(13:0/22:1(11Z))	1.771187	2.335066	2.22E-06	up	796.5827872	12.34228333	pos	M+Na
PC(15:1(9Z)/19:0)	1.542163	3.024343	0.001385	up	782.5640984	12.71466667	pos	M+H, M+Na

PC(16:0/3:0)	1.634721	0.136655	0.006212	down	552.3617395	11.46158333	pos	M+H
PC(16:0/3:1(2E))	1.61155	0.16963	0.001365	down	594.3391805	11.58748333	neg	M+FA-H
PC(16:0/4:0)	1.620774	0.178773	0.002032	down	566.3763967	11.83721667	pos	M+H
PC(16:0/PGF1alpha)	1.594674	3.503058	0.00026	up	816.5777939	11.18	pos	M+H-H2O
PC(18:1(11Z)/18:1(12Z)-2OH(9,10))	1.751347	4.065712	4.84E-06	up	818.5955688	12.34228333	pos	M+H
PC(P-16:0/PGF1alpha)	1.7162	5.958668	5.32E-09	up	818.5930939	13.534	pos	M+H
PC(P-18:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))	1.593378	0.480942	0.005104	down	878.5885039	11.14158333	neg	M+FA-H
PC(P-18:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	1.75229	0.417316	0.001667	down	878.5883892	12.46871667	neg	M+FA-H
Pcera-1	1.636957	0.307823	0.001286	down	432.1790854	5.043483333	neg	M+FA-H
PE(0:0/20:4;O2)	1.527243	0.384305	0.005247	down	551.3088527	10.36043333	pos	M+NH4
PE(0:0/20:5(5Z,8Z,11Z,14Z,17Z))	1.767879	0.313717	0.004412	down	498.2606878	9.71395	neg	M-H
PE(0:0/22:4(7Z,10Z,13Z,16Z))	1.796792	0.499779	3.40E-06	down	528.3072048	10.74098333	neg	M-H
PE(0:0/24:6(6Z,9Z,12Z,15Z,18Z,21Z))	1.678519	0.314157	0.00297	down	571.3532682	4.640716667	pos	M+NH4
PE(15:0/18:0)	1.371969	5.175501	0.000516	up	706.5343966	12.55136667	pos	M+H
PE(18:3(9Z,12Z,15Z)/20:0)	1.824343	21.73885	2.25E-05	up	792.5487382	10.05593333	pos	M+Na
PE(22:2(13Z,16Z)/0:0)	1.778179	0.232076	0.002239	down	578.343987	12.00658333	neg	M+FA-H
PE(22:2(13Z,16Z)/17:1(9Z))	1.841056	2.62928	5.24E-05	up	766.5683236	12.71466667	pos	M+H-H2O
PE(22:5(7Z,10Z,13Z,16Z,19Z)/20:2(11Z,14Z))	1.435321	2.8666	0.003606	up	817.5649385	11.79555	pos	M+
PE(P-18:1(11Z)/20:4(6E,8Z,11Z,13E)-2OH(5S,15S))	1.751198	0.49295	9.98E-05	down	764.5174492	10.79823333	pos	M+H-H2O
Pelargonic acid	1.772561	0.311098	0.001683	down	315.2524731	10.23358333	neg	2M-H
PE-NMe(16:0/18:2(9Z,12Z))	1.806224	0.447333	0.000201	down	752.5174662	12.13153333	pos	M+Na
PE-NMe(18:1(9Z)/20:2(11Z,14Z))	1.876512	0.340232	2.76E-06	down	766.5692424	11.52583333	pos	M+H-H2O
PE-NMe(20:1(11Z)/16:1(9Z))	1.694218	2.775444	0.000241	up	758.5645811	12.71466667	pos	M+H, M+Na
Perindoprilat	1.457474	10.87655	0.002759	up	385.1982213	10.50825	neg	M+FA-H
Phenylalanyl-leucyl-leucyl-arginyl-asparagine	1.748586	0.139984	0.003656	down	644.385093	11.43865	pos	M+H-H2O
Phosphonoacetate	1.845281	0.234309	6.43E-05	down	139.9871321	0.620716667	pos	M+, M+H

Pipotiazine	1.654693	0.212861	0.003765	down	474.1892827	5.077116667	neg	M-H
Pomonic acid	1.511	0.494074	0.00154	down	509.3004273	10.73686667	pos	M+K
PS(13:0/0:0)	1.71125	0.298673	0.005536	down	478.2191801	4.989533333	pos	M+Na
PS(14:0/14:0)	1.0134	0.118857	0.003123	down	680.4447955	12.19545	pos	M+H
PS(21:0/17:1(9Z))	1.7435	3.429802	6.23E-06	up	817.5843981	12.71466667	pos	M+, M+Na
Pseudoecgonine	1.554937	2.213019	0.00092	up	369.2031163	11.94938333	neg	2M-H
quinoneimine	1.618561	0.296503	0.001217	down	454.1609217	5.043483333	neg	M-H ₂ O-H
Risperidone	1.645769	30.97562	0.00209	up	455.2089187	12.9318	neg	M+FA-H
Rumenic acid	1.734842	2.084174	0.001681	up	279.2317123	15.43138333	neg	M-H
S-Butylcysteine sulfoxide	1.542426	2.149567	0.002282	up	176.0731141	3.493016667	pos	M+H-H ₂ O
Ser Tyr Phe	1.610031	0.210026	0.005181	down	460.1739946	4.3641	neg	M+FA-H
Serdexmethylphenidate	1.537659	0.345036	0.001598	down	498.1868542	4.986416667	neg	M-H
Simendan	1.584434	2.044702	0.002082	up	325.1060995	1.524933333	neg	M+FA-H
SM(d18:0/18:1(9Z))	1.850738	8.435563	3.25E-08	up	731.6014525	11.48216667	pos	M+H
Sonchifolin	1.623042	2.173102	7.85E-05	up	355.1566458	13.33865	neg	M-H ₂ O-H
Squalamine	1.672131	0.195185	0.004251	down	666.4296365	11.31085	pos	M+K
Stearoyl-EA	1.743792	0.47299	0.003658	down	328.3187399	13.15526667	pos	M+H
Sudan black B	1.412397	3.172672	0.003218	up	437.190387	11.94938333	neg	M-H ₂ O-H
Taraxinic acid glucosyl ester	1.765393	0.182016	0.006075	down	442.2075708	9.536516667	pos	M+NH ₄
TBS-Corey Lactone Aldehyde	1.770433	13.75159	0.003473	up	283.1362245	10.35895	neg	M-H
Tetradecan-7,9-diynoic acid	1.8089	17.81947	0.003878	up	265.1466075	11.51961667	neg	M+FA-H
TRIMETHYLCOLCHICINIC ACID	1.5866	0.387009	0.006119	down	366.1306138	1.323833333	pos	M+Na
Tryptophyl-Arginine	1.620367	3.123385	0.000544	up	360.1895314	4.423	pos	M+
Tyrosyl-Glutamate	1.269635	46.19409	0.004512	up	311.1242915	11.73278333	pos	M+H
Valylleucine	1.507593	0.438715	0.002605	down	231.1689412	3.851616667	pos	M+H
Vofopitant	1.736854	0.17505	0.006673	down	450.222817	10.52983333	pos	M+NH ₄

Xestoaminol B	1.724452	1493.1	0.00532	up	270.2064026	10.03348333	neg	M+FA-H
zaprinast	1.781755	3.273395	2.06E-06	up	289.1404713	10.83918333	pos	M+NH4
Zileuton	1.702123	0.140379	0.002742	down	281.0605347	5.4819	neg	M+FA-H