

Supporting Information:

Metabolomic Analysis of Liver Tissues for Characterization of Hepatocellular Carcinoma

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S1 Fig.

BATCH 1	
Sequence	Sample name
1	wash
2	C18_A_01
3	C18_A_02
4	wash
5	blank
6	wash
7	RI (Alcane+FAME)
8	QC_all_01
9	QC_all_02
10	QC_all_03
11	QC_all_04
12	QC_all_05
13	QC_ADJ/C_01
14	QC_HCC/C_01
15	QC_ADJ/N_01
16	QC_HCC/N_01
17	ADJ-Cirrhosis
18	HCC-Cirrhosis
19	ADJ-Normal
20	HCC-Normal
21	ADJ-Cirrhosis
22	HCC-Cirrhosis
23	ADJ-Normal
24	QC_ADJ/C_02
25	QC_HCC/C_02
26	QC_ADJ/N_02
27	QC_HCC/N_02
28	HCC-Normal
29	ADJ-Cirrhosis
30	HCC-Cirrhosis
31	ADJ-Cirrhosis
32	HCC-Cirrhosis
33	ADJ-Normal
34	HCC-Normal
35	ADJ-Cirrhosis
36	HCC-Cirrhosis
37	QC_ADJ/C_03
38	QC_HCC/C_03
39	QC_ADJ/N_03
40	QC_HCC/N_03
41	wash
42	RI (Alcane+FAME)

BATCH 2	
Sequence	Sample name
1	wash
2	C18_B_01
3	C18_B_02
4	wash
5	blank
6	wash
7	RI (Alcane+FAME)
8	QC_all_01
9	QC_all_02
10	QC_all_03
11	QC_all_04
12	QC_all_05
13	QC_ADJ/C_04
14	QC_HCC/C_04
15	QC_ADJ/N_04
16	QC_HCC/N_04
17	ADJ-Cirrhosis
18	HCC-Cirrhosis
19	ADJ-Normal
20	HCC-Normal
21	ADJ-Cirrhosis
22	HCC-Cirrhosis
23	ADJ-Normal
24	QC_HCC/C_05
25	QC_ADJ/C_05
26	QC_HCC/N_05
27	QC_ADJ/N_05
28	HCC-Normal
29	ADJ-Cirrhosis
30	HCC-Cirrhosis
31	ADJ-Cirrhosis
32	HCC-Cirrhosis
33	ADJ-Normal
34	HCC-Normal
35	ADJ-Cirrhosis
36	HCC-Cirrhosis
37	QC_ADJ/C_06
38	QC_HCC/C_06
39	QC_ADJ/N_06
40	QC_HCC/N_06
41	wash
42	RI (Alcane+FAME)

BATCH 3	
Sequence	Sample name
1	wash
2	C18_C_01
3	C18_C_02
4	wash
5	blank
6	wash
7	RI (Alcane+FAME)
8	QC_all_01
9	QC_all_02
10	QC_all_03
11	QC_all_04
12	QC_all_05
13	QC_ADJ/N_07
14	QC_HCC/N_07
15	ADJ-Normal
16	HCC-Normal
17	ADJ-Normal
18	HCC-Normal
19	ADJ-Normal
20	HCC-Normal
21	ADJ-Normal
22	QC_ADJ/N_08
23	QC_HCC/N_08
24	HCC-Normal
25	ADJ-Normal
26	HCC-Normal
27	ADJ-Normal
28	HCC-Normal
29	ADJ-Normal
30	HCC-Normal
31	ADJ-Normal
32	HCC-Normal
33	QC_ADJ/N_09
34	QC_HCC/N_09
35	wash
36	RI (Alcane+FAME)

BATCH 4	
Sequence	Sample name
1	wash
2	C18_D_01
3	C18_D_02
4	wash
5	blank
6	wash
7	RI (Alcane+FAME)
8	QC_all_01
9	QC_all_02
10	QC_all_03
11	QC_all_04
12	QC_all_05
13	QC_ADJ/N_10
14	QC_HCC/N_10
15	ADJ-Normal
16	HCC-Normal
17	ADJ-Normal
18	HCC-Normal
19	ADJ-Normal
20	HCC-Normal
21	ADJ-Normal
22	HCC-Normal
23	QC_ADJ/N_11
24	QC_HCC/N_11
25	ADJ-Normal
26	HCC-Normal
27	ADJ-Normal
28	HCC-Normal
29	ADJ-Normal
30	HCC-Normal
31	ADJ-Normal
32	HCC-Normal
33	QC_ADJ/N_12
34	QC_HCC/N_12
35	wash
36	RI (Alcane+FAME)

BATCH 5	
Sequence	Sample name
1	wash
2	C18_E_01
3	C18_E_02
4	wash
5	blank
6	wash
7	RI (Alcane+FAME)
8	QC_all_01
9	QC_all_02
10	QC_all_03
11	QC_all_04
12	QC_all_05
13	QC_ADJ/N_13
14	QC_HCC/N_13
15	ADJ-Normal
16	HCC-Normal
17	ADJ-Normal
18	HCC-Normal
19	ADJ-Normal
20	HCC-Normal
21	ADJ-Normal
22	QC_ADJ/N_14
23	QC_HCC/N_14
24	HCC-Normal
25	ADJ-Normal
26	HCC-Normal
27	ADJ-Normal
28	HCC-Normal
29	ADJ-Normal
30	HCC-Normal
31	ADJ-Normal
32	HCC-Normal
33	QC_ADJ/N_15
34	QC_HCC/N_15
35	wash
36	RI (Alcane+FAME)

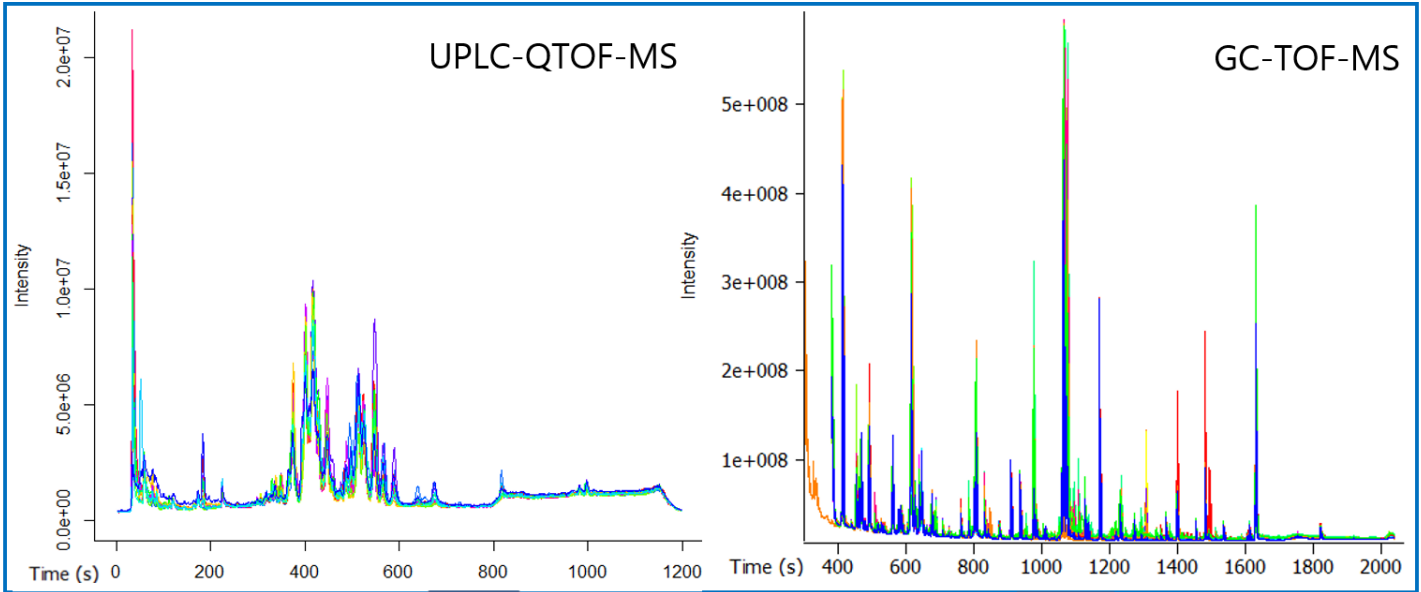
S2 Fig.

Positive		Negative	
Sequence	Sample Name	Sequence	Sample Name
1	ACN	1	ACN
2	Metmix	2	Metmix
3	water	3	water
4	Blank_A	4	Blank_A
5	Blank_B	5	Blank_B
6	Blank_C	6	Blank_C
7	Blank_D	7	Blank_D
8	Blank_E	8	Blank_E
9	QC_all_01	9	QC_all_01
10	QC_all_02	10	QC_all_02
11	QC_all_03	11	QC_all_03
12	QC_all_04	12	QC_all_04
13	QC_all_05	13	QC_all_05
14	QC_all_06	14	QC_all_06
15	QC_all_07	15	QC_all_07
16	QC_ADJ/C_01	16	QC_ADJ/C_01
17	QC_HCC/C_01	17	QC_HCC/C_01
18	QC_ADJ/N_01	18	QC_ADJ/N_01
19	QC_HCC/N_01	19	QC_HCC/N_01
20	ADJ-Cirrhosis	20	ADJ-Cirrhosis
21	HCC-Cirrhosis	21	HCC-Cirrhosis
22	ADJ-Normal	22	ADJ-Normal
23	HCC-Normal	23	HCC-Normal
24	ADJ-Cirrhosis	24	ADJ-Cirrhosis
25	HCC-Cirrhosis	25	HCC-Cirrhosis
26	ADJ-Normal	26	ADJ-Normal
27	HCC-Normal	27	HCC-Normal
28	ADJ-Cirrhosis	28	ADJ-Cirrhosis
29	HCC-Cirrhosis	29	HCC-Cirrhosis
30	ADJ-Cirrhosis	30	ADJ-Cirrhosis
31	HCC-Cirrhosis	31	HCC-Cirrhosis
32	ADJ-Normal	32	ADJ-Normal
33	HCC-Normal	33	HCC-Normal
34	ADJ-Cirrhosis	34	ADJ-Cirrhosis
35	HCC-Cirrhosis	35	HCC-Cirrhosis
36	QC_ADJ/C_02	36	QC_ADJ/C_02
37	QC_HCC/C_02	37	QC_HCC/C_02
38	QC_ADJ/N_02	38	QC_ADJ/N_02
39	QC_HCC/N_02	39	QC_HCC/N_02
40	ADJ-Cirrhosis	40	ADJ-Cirrhosis
41	HCC-Cirrhosis	41	HCC-Cirrhosis
42	ADJ-Normal	42	ADJ-Normal
43	HCC-Normal	43	HCC-Normal
44	ADJ-Cirrhosis	44	ADJ-Cirrhosis
45	HCC-Cirrhosis	45	HCC-Cirrhosis
46	ADJ-Normal	46	ADJ-Normal
47	HCC-Normal	47	HCC-Normal
48	ADJ-Cirrhosis	48	ADJ-Cirrhosis
49	HCC-Cirrhosis	49	HCC-Cirrhosis
50	ADJ-Cirrhosis	50	ADJ-Cirrhosis
51	HCC-Cirrhosis	51	HCC-Cirrhosis
52	ADJ-Normal	52	ADJ-Normal
53	HCC-Normal	53	HCC-Normal
54	ADJ-Cirrhosis	54	ADJ-Cirrhosis
55	HCC-Cirrhosis	55	HCC-Cirrhosis
56	QC_ADJ/C_03	56	QC_ADJ/C_03
57	QC_HCC/C_03	57	QC_HCC/C_03
58	QC_ADJ/N_03	58	QC_ADJ/N_03
59	QC_HCC/N_03	59	QC_HCC/N_03
60	ADJ-Normal	60	ADJ-Normal
61	HCC-Normal	61	HCC-Normal

S2 Fig. (continue)

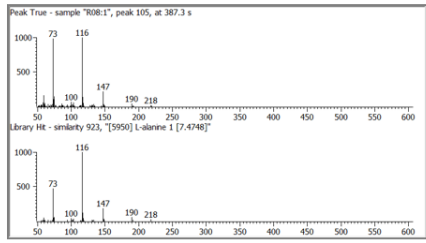
Positive (continue)		Negative (continue)	
Sequence	Sample Name	Sequence	Sample Name
62	ADJ-Normal	62	ADJ-Normal
63	HCC-Normal	63	HCC-Normal
64	ADJ-Normal	64	ADJ-Normal
65	HCC-Normal	65	HCC-Normal
66	ADJ-Normal	66	ADJ-Normal
67	HCC-Normal	67	HCC-Normal
68	ADJ-Normal	68	ADJ-Normal
69	HCC-Normal	69	HCC-Normal
70	ADJ-Normal	70	ADJ-Normal
71	HCC-Normal	71	HCC-Normal
72	ADJ-Normal	72	ADJ-Normal
73	HCC-Normal	73	HCC-Normal
74	ADJ-Normal	74	ADJ-Normal
75	HCC-Normal	75	HCC-Normal
76	QC_ADJ/C_04	76	QC_ADJ/C_04
77	QC_HCC/C_04	77	QC_HCC/C_04
78	QC_ADJ/N_04	78	QC_ADJ/N_04
79	QC_HCC/N_04	79	QC_HCC/N_04
80	ADJ-Normal	80	ADJ-Normal
81	HCC-Normal	81	HCC-Normal
82	ADJ-Normal	82	ADJ-Normal
83	HCC-Normal	83	HCC-Normal
84	ADJ-Normal	84	ADJ-Normal
85	HCC-Normal	85	HCC-Normal
86	ADJ-Normal	86	ADJ-Normal
87	HCC-Normal	87	HCC-Normal
88	ADJ-Normal	88	ADJ-Normal
89	HCC-Normal	89	HCC-Normal
90	ADJ-Normal	90	ADJ-Normal
91	HCC-Normal	91	HCC-Normal
92	ADJ-Normal	92	ADJ-Normal
93	HCC-Normal	93	HCC-Normal
94	ADJ-Normal	94	ADJ-Normal
95	HCC-Normal	95	HCC-Normal
96	QC_ADJ/C_05	96	QC_ADJ/C_05
97	QC_HCC/C_05	97	QC_HCC/C_05
98	QC_ADJ/N_05	98	QC_ADJ/N_05
99	QC_HCC/N_05	99	QC_HCC/N_05
100	ADJ-Normal	100	ADJ-Normal
101	HCC-Normal	101	HCC-Normal
102	ADJ-Normal	102	ADJ-Normal
103	HCC-Normal	103	HCC-Normal
104	ADJ-Normal	104	ADJ-Normal
105	HCC-Normal	105	HCC-Normal
106	ADJ-Normal	106	ADJ-Normal
107	HCC-Normal	107	HCC-Normal
108	ADJ-Normal	108	ADJ-Normal
109	HCC-Normal	109	HCC-Normal
110	ADJ-Normal	110	ADJ-Normal
111	HCC-Normal	111	HCC-Normal
112	ADJ-Normal	112	ADJ-Normal
113	HCC-Normal	113	HCC-Normal
114	ADJ-Normal	114	ADJ-Normal
115	HCC-Normal	115	HCC-Normal
116	QC_ADJ/C_06	116	QC_ADJ/C_06
117	QC_HCC/C_06	117	QC_HCC/C_06
118	QC_ADJ/N_06	118	QC_ADJ/N_06
119	QC_HCC/N_06	119	QC_HCC/N_06
120	ACN	120	ACN
121	Metmix	121	Metmix
122	water	122	water

S3 Fig.



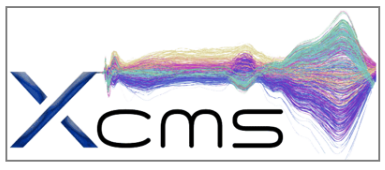
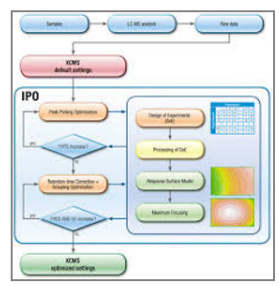
GC-TOF-MS

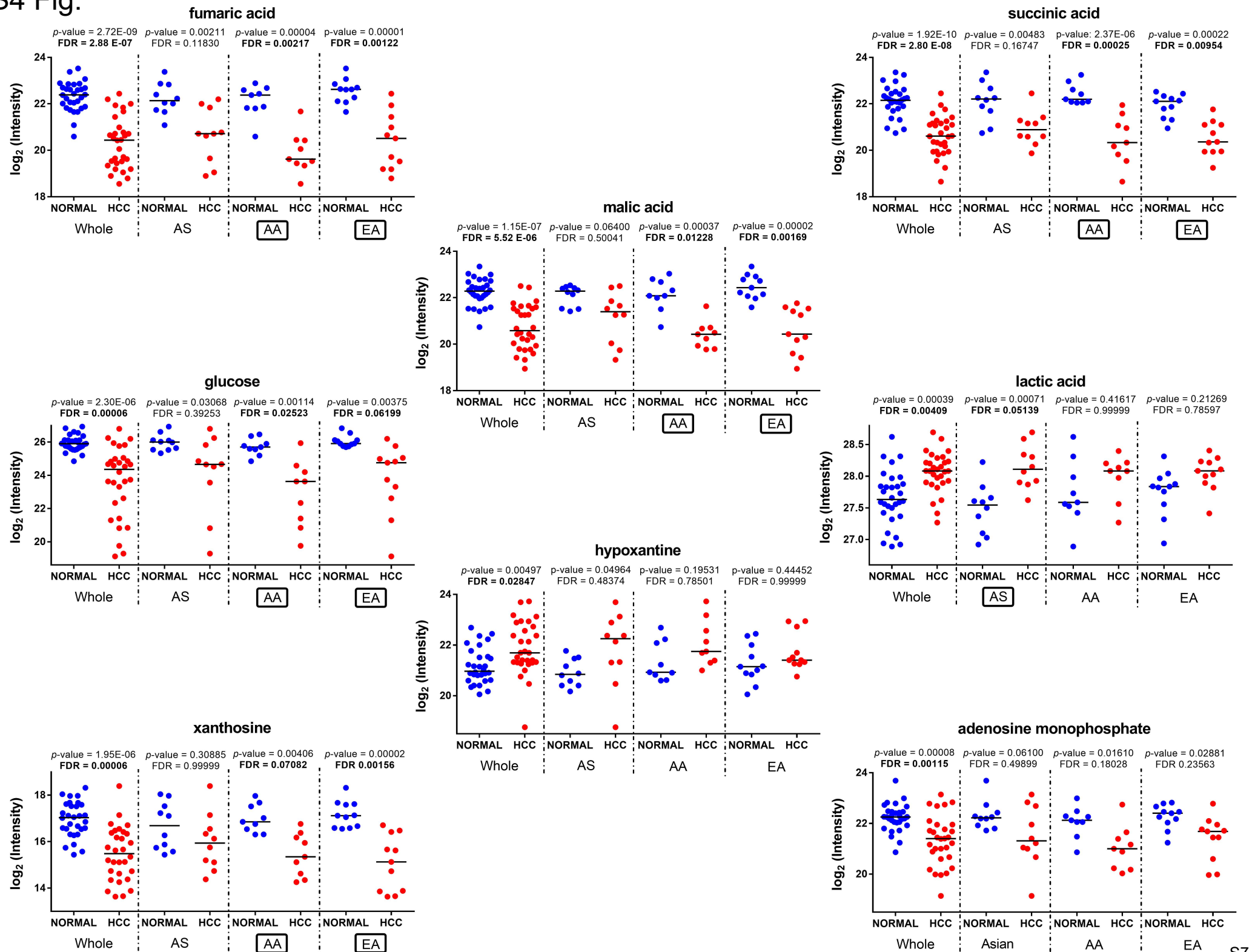
- LECO ChromaTOF:
 - Peak finding
 - True signal deconvolution
 - Library for metabolite identification: Fiehn 2013 & NIST 2011
 - Alignment with Statistical Compare



UPLC-QTOF-MS

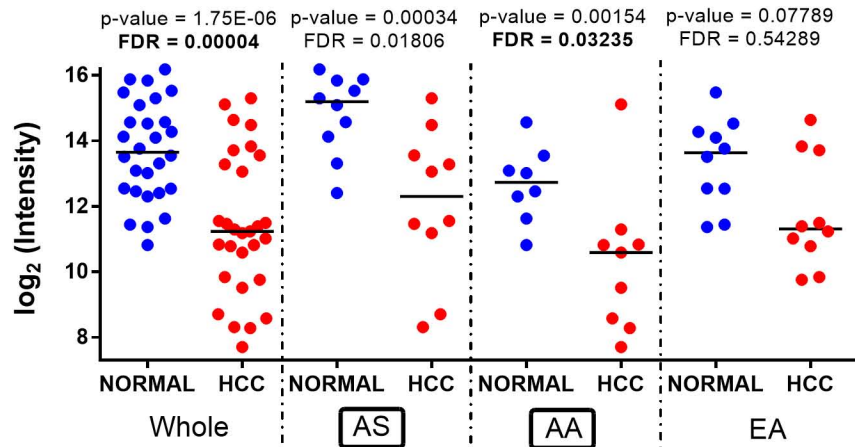
- IPO
 - Optimizing XCMS parameter for peak detection, RT correction and alignment
- XCMS (version 1.44)
 - Filtration and peak finding
 - RT correction & alignment
 - Filling missing peaks
- Annotation with CAMERA
 - Grouping all adducts, cluster ions and charge states entities derived from same analyte



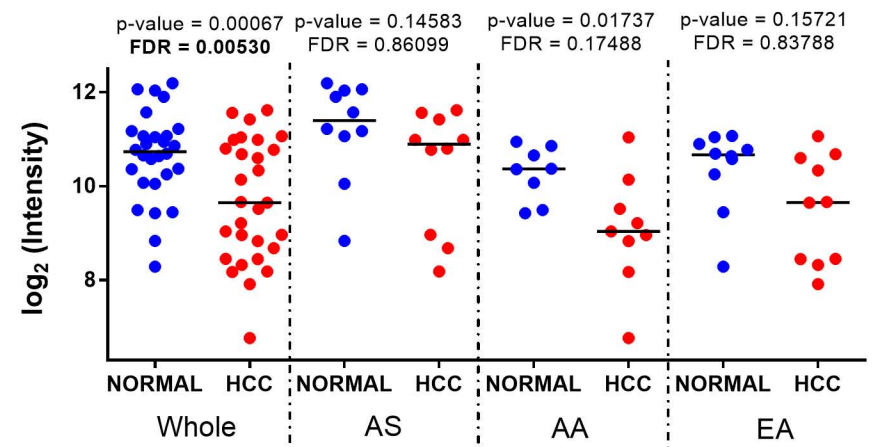


S5 Fig.

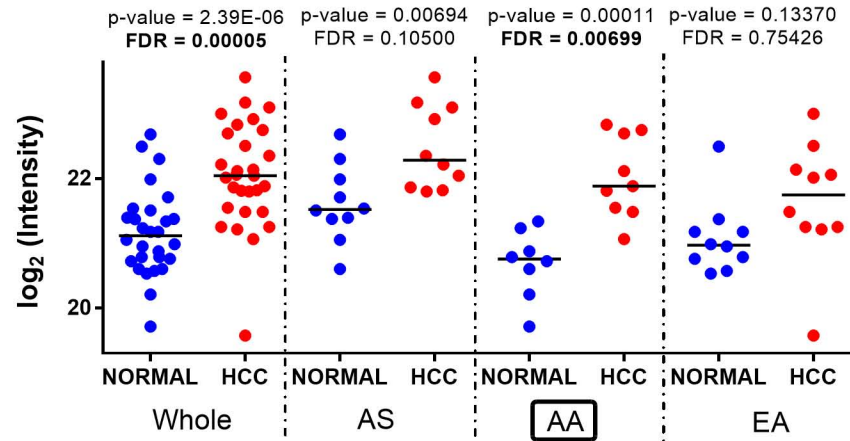
propionylcarnitine



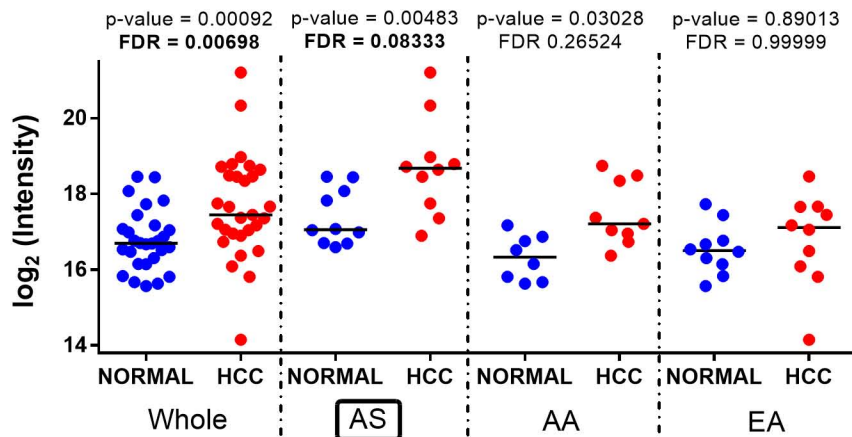
PC(34:2)



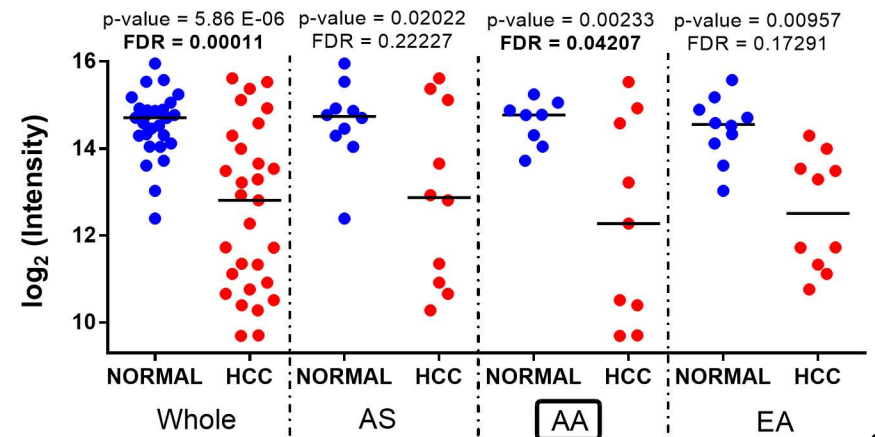
PC(36:1)



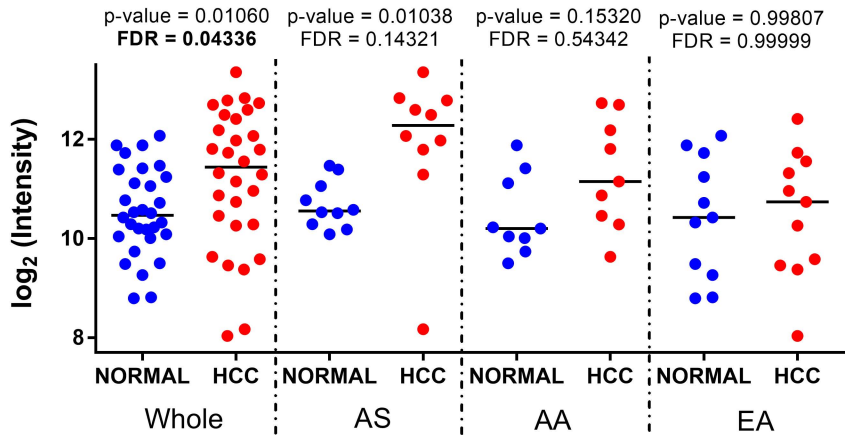
PC(38:2)



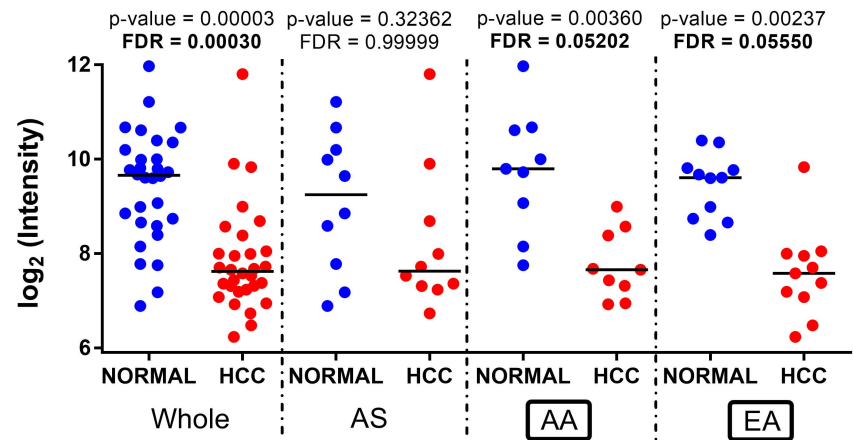
glycerophosphocholine



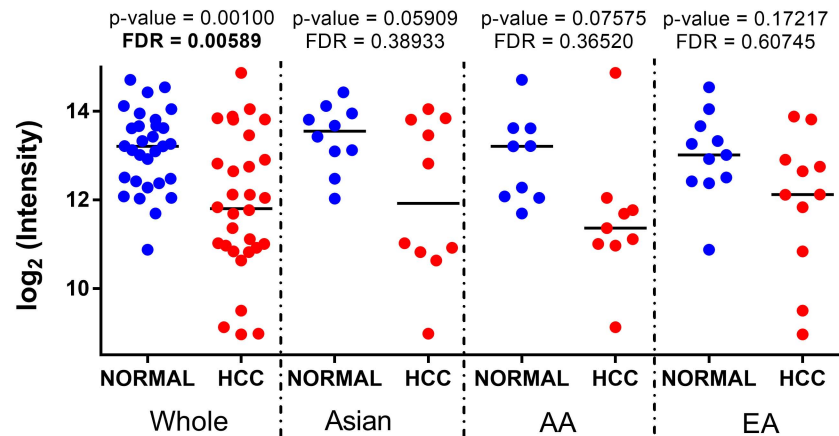
hypoxanthine



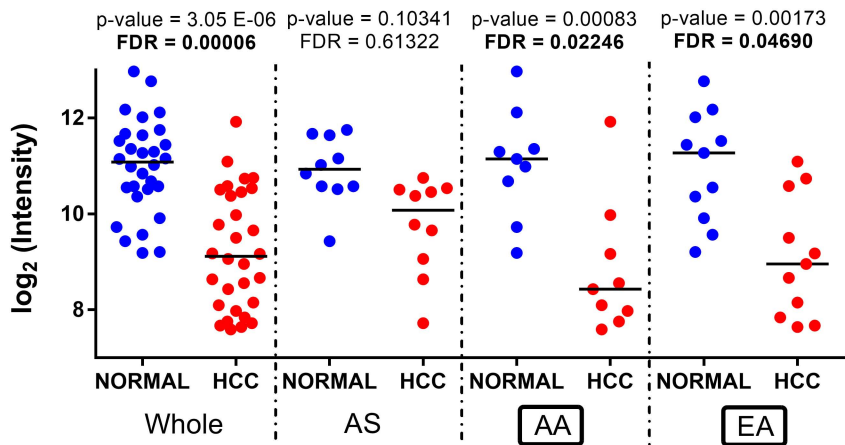
xanthosine



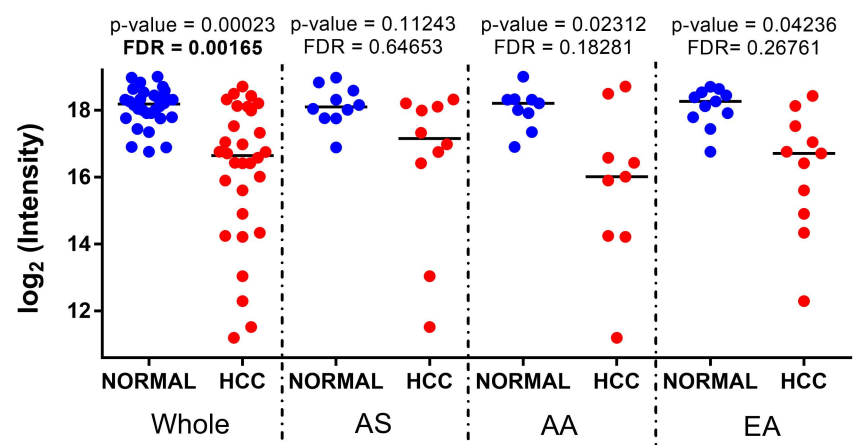
adenosine monophosphate



glycerol 3-phosphate



glycerylphosphorylethanolamine



p-value
adj. p-value (FDR)
Fold change > +1.5
Fold change < -1.5

PLATFORM	extract mass	rt (')	IDENTIFICATION	HCC v adj. C								
				WP			AA			EA		
				p-value	FDR	FC*	p-value	FDR	FC*	p-value	FDR	FC*
GC-MS	315	16.2	[668] dihydroxyacetone phosphate 1 [15.804]	0.00002	0.01736	-4.87	0.00007	0.04937	-9.14	0.04384	1.00000	-3.04
	315	16.3	[668] dihydroxyacetone phosphate 2 [15.929]	0.00060	0.08737	-5.03	0.00303	0.20690	-8.73	0.08079	1.00000	-3.24
	357	20.0	[5459862] D-erythrose-4-phosphate 1 [17.508]	0.00195	0.11825	-2.55	0.00030	0.07851	-3.86	0.76720	1.00000	-1.70
LC-POS-MS	141.0706	11.8	5-Phenyl-1,3-pentadiyne; Norcapillene; 1,4-Methanoazulene; Boron, trifluoro(tetrahydrofuran)	0.00009	0.08938	-37.52	0.02411	1.00000	-22.87	0.00072	0.11467	-40.42
	159.1174	11.8	Butadiene-styrene rubber; 4-Methyl-2-[(propan-2-yl)oxy]-1,3,2-dioxaborinane; 1,3-	0.00013	0.08938	-24.13	0.05975	1.00000	-13.69	0.00046	0.11467	-26.43
	145.1019	11.8	2,2-Dimethyl-2H-indene; 4,4,6-Trimethyl-1,3,2-dioxaborinan-2-ol; Boric acid pinacol ester; 1H-	0.00017	0.08938	-16.25	0.04287	1.00000	-13.51	0.00099	0.11467	-18.20
	218.1392	0.6	Propionylcarnitine;tert-Butyl 2-(hydroxymethyl)morpholine-4-carboxylate; ethyl 3-[(2-ethoxy-2-	0.00020	0.08938	-4.27	0.00362	1.00000	-12.46	0.01220	0.13158	-4.62
	128.0628	11.8	2-Fluoro-5-hydrazinylpyridine	0.00024	0.08940	-21.38	0.06085	1.00000	-14.19	0.00107	0.11467	-26.05
	171.1175	11.8	1,6,7-Trimethylnaphthalene; Aethusin,(3,4-Dimethylcyclopenta-1,3-dien-1-yl)benzene	0.00033	0.08940	-18.83	0.03802	1.00000	-12.57	0.00285	0.11467	-19.07
	269.2269	12.1	anhydroretinol,2-decyl-naphthalene	0.00033	0.08940	-79.69	0.11551	1.00000	-46.53	0.00078	0.11467	-105.65
177.1644	11.8	(6E,8E)-4,6,8-Megastigmatriene; 1-Phenylheptane; 3,5,7-Trimethyl-2E,4E,6E,8E-decatetraene; 1-tert-Butyl-2-(propan-2-yl)benzene; 1,4-Diisopropyl-2-methylbenzene; 1-Hexyl-4-methylbenzene	0.00035	0.08940	-30.46	0.05923	1.00000	-22.37	0.00191	0.11467	-34.69	
LC-NEG-MS	349.0936	0.59	3-Feruloyl-1,5-quinolactone; 6-[2,3-Dihydroxy-1-(hydroxymethyl)propyl]-1,2-dihydro-7-hydroxy-9-methoxy-cyclopenta[c][1]benzopyran-3,4-dione; CAY10648; 4-[(1-benzoyl-3-methyl-5-oxo-4H-pyrazol-4-yl)diazenyl]benzoic acid; 2,3-diphenyl-5-(trifluoromethyl)quinoxaline; N~1~,N~3~-Bis(2-nitrophenyl)benzene-1,3-diamine	0.00031	0.09336	-4.12	0.00741	0.33780	-3.20	0.01633	1.00000	-2.05
	337.0936	0.59	Coumaroyl quinic acid, alpha-Hydrojuglone 4-O-b-D-glucoside, Hydrojuglone glucoside, 1-Caffeoyl-4-deoxyquinic acid; N-(tert-Butoxycarbonyl)-6-chloro-L-tryptophan; Benzhydryl 4-methylbenzenesulfonate; 1,2,4,5-Benzenetetracarboxylic acid, dipropyl ester 4-Methylumbelliferyl-galactopyranoside	0.00060	0.09336	-4.06	0.03935	0.80467	-2.74	0.00708	1.00000	-3.26
	346.0544	0.63	2'-Deoxyguanosine 5'-monophosphate;(1,3-dioxoisindol-2-yl)methyl 4-(difluoromethoxy)benzoate; Pamabrom [USAN:USP],Anthraquinone, 1-amino-4-hydroxy-2-(mercaptophenyl)-; 1H-Pyrazole-4-carboxamide, 4,5-dihydro-3,4-bis(4-chlorophenyl)-N-methyl-	0.00063	0.09336	-4.17	0.00078	0.23035	-11.91	0.23008	1.00000	-3.17
	845.6739	11.32	TG(104:16); TG(52:8)	0.00068	0.09336	-4.87	0.00067	0.23035	-10.10	0.26977	1.00000	-1.26
	402.0692	0.55	1-[(2-bromophenyl)-(2-ethoxyphenyl)methyl]pyrrolidine-2-carboxylic Acid	0.00079	0.09336	-2.88	0.04738	0.83971	-2.45	0.00821	1.00000	-3.47

*Fold change between HCC-C and adj.C

S2 Table (continue)

L
C
-
P
O
S
-
M
S

184.0741	10.4	4-Nitrosobiphenyl; Phosphocholine; 3-Dibenzofuranamine; 4-Hydroxycarbazole; 4-Benzoylpyridine; 2-Aminodiphenylene oxide; 6-Methoxy-2-naphthonitrile; 5-(Furan-3-yl)-1H-indole; 1-Hydroxycarbazole; Methanone, phenyl-2-pyridinyl-; 2-Propenal, 3-(2-quinolinyl)-; 6-(Furan-2-yl)-1H-indole	0.00000	0.00003	2.44	0.00382	0.07345	2.46	0.00017	0.00793	2.87	0.04300	0.39475	2.13
624.3705	0.6	Apicidin	0.01387	0.07104	2.34	0.97689	1.00000	1.87	0.25660	1.00000	1.94	0.01127	0.18676	3.01
524.6421	0.6		0.01845	0.09108	2.24	0.96680	1.00000	1.91	0.08955	0.53312	2.11	0.08696	0.58297	2.46
633.5811	12.9	9-Octadecenoic acid (9Z)-, 2,2-dimethyl-1,3-propanediyl ester	0.00005	0.00063	2.17	0.00947	0.12881	1.94	0.02420	0.21956	2.50	0.06155	0.47697	2.07
800.6152	10.1	PC(37:2); PE(40:2)	0.00134	0.00968	2.08	0.01357	0.16587	5.26	0.11703	0.62671	4.30	0.42523	1.00000	1.62
452.3733	1.3	(11Z,14Z)-eicosadienoylcarnitine; 1-Octadecanaminium, N-ethyl-N,N-dimethyl-, ethyl sulfate	0.00819	0.04524	2.05	0.06894	0.51167	4.89	0.52119	1.00000	1.81	0.17867	0.90305	2.40
706.5384	8.3	PC(30:0); PE(33:0)	0.00000	0.00003	1.95	0.00020	0.01361	2.71	0.00115	0.02647	4.05	0.09244	0.60378	1.65
786.5278	7.8	PS(36:3)	0.00866	0.04711	1.92	0.13855	0.83568	1.87	0.44813	1.00000	2.25	0.13000	0.74441	2.09
229.1550	0.6	L-isoleucyl-L-proline ; AC1NPXVC	0.00097	0.00730	1.90	0.00358	0.06950	2.52	0.08477	0.51539	2.59	0.70753	1.00000	1.32
788.6166	10.4	PC(36:1); PC(72:2); PE(39:1)	0.00000	0.00005	1.90	0.00694	0.10500	1.70	0.00011	0.00699	2.18	0.13370	0.75426	1.75
744.4945	8.3	1-[6-[5]-ladderane-hexanoyl]-2-[8-[3]-ladderane-octanyl]-sn-glycerophosphoethanolamine, Pilocereine	0.00285	0.01838	1.86	0.00726	0.10779	2.47	0.17648	0.83009	2.01	0.70410	1.00000	1.03
786.6008	9.7	PC(72:4), PC(36:2), PE(39:2), Dioloeylphosphatidylcholine, GPCho(18:2(2E,4E)/O-18:0)[U]	0.00011	0.00120	1.82	0.00255	0.05720	2.24	0.04579	0.34973	2.30	0.22806	0.98270	1.46
762.5606	10.0	PS(O-35:1); PS(P-35:0)	0.01868	0.09182	1.73	0.99057	1.00000	1.12	0.14493	0.72828	1.98	0.03410	0.33203	1.62
655.5652	9.4	5-Hydroxy-7-methoxy-2-tritriacontyl-4H-1-benzopyran-4-one	0.02420	0.11430	1.72	0.00132	0.03616	2.73	0.41905	1.00000	1.32	0.98015	1.00000	1.17
814.6320	10.5	PC(38:2); PE(41:2)	0.00092	0.00698	1.69	0.00483	0.08333	3.08	0.03028	0.26524	1.82	0.89013	1.00000	1.53
909.5456	8.6	PI(40:7); 7-Hydroxychlorophyll a; Bacterio-chlorophyll b	0.29443	0.77632	1.68	0.97623	1.00000	1.26	0.00596	0.07874	4.12	0.69662	1.00000	-1.33
102.0921	0.6	5-Aminopentanal; N-butylformamide; pentanamide; 2-Methylpropanal O-methylloxime; 4-Methylaminobutanal; 3-Methylbutyraldehyde oxime;(E)-2-Methylbutanal oxime;Betaine aldehyde; Diethylformamide; tetrahydro-2H-pyran-3-amine; (3R)-N-Methyloxolan-3-amine; N-Propylacetamide; Piperidin-4-ol; 4-Methylmorpholine; Formamide, N-(1-methylpropyl)-; 2,3,4-trimethyl-1,3-oxazetidine; 4,4-Dimethylloxazolidine; 4-Ethylloxazolidine; 2-methylmorpholine; 4-Aminotetrahydropyran; [(1S,2S)-2-(Aminomethyl)cyclopropyl]methanol; 3-Methoxycyclobutan-1-amine; Butanamide, 3-methyl-; Pentanamide; N-Ethylpropionamide	0.00003	0.00040	1.68	0.63312	1.00000	1.37	0.01999	0.19559	2.17	0.00007	0.00658	3.38
605.5499	12.8	9-Octadecenoic acid (9Z)-, 1-methyl-1,2-ethanediy ester	0.00411	0.02494	1.68	0.02234	0.23735	1.73	0.17457	0.82794	1.35	0.58556	1.00000	1.50
748.5844	9.9	PC(33:0); PE(36:0); Distearyl phosphatidyl ethanolamine; phosphatidylethanolamine; PE(34:0)	0.00825	0.04531	1.65	0.04041	0.36953	1.74	0.50458	1.00000	1.51	0.29938	1.00000	1.44
751.5260	10.4	PA(40:5)	0.00364	0.02252	1.64	0.07827	0.56088	1.55	0.08516	0.51640	1.61	0.56397	1.00000	1.55
697.4771	9.5	1,2-Di-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphate; PA(36:4); 1-(Hexadecanoyloxy)-3-(phosphonoxy)propan-2-yl icoso-5,8,11,14-tetraenoate	0.00292	0.01870	1.56	0.02184	0.23490	1.64	0.36388	1.00000	1.40	0.22310	0.98154	1.61
734.5696	9.5	PC(32:0); PE(35:0); 1,2-dipalmitoyl-sn-glycero-3-PC; Colfosceril palmitate; 1,3-Dipalmitoyl-2-phosphatidylcholine;(7S)-7-(Hexadecanoyloxy)-4-hydroxy-N,N,N-trimethyl-10-oxo-3,5,9-trioxa-4-phosphapentacosan-1-aminium 4-oxide	0.00014	0.00143	1.54	0.00470	0.08200	1.53	0.11455	0.62053	1.59	0.07542	0.53438	1.33
762.6007	10.3	PC(34:0); PE(37:0); 1,1-Cyclobutanedicarboxamide, N,N'-bis(2,4,6-tribromophenyl)-	0.01292	0.06711	1.53	0.07931	0.56656	1.38	0.37890	1.00000	1.36	0.42236	1.00000	1.16
259.1697	8.8	Linalyl benzoate; Geranyl benzoate; Falcariolone; Ginsenoyne; Flavidulol B; (all-E)-1,8,10-Heptadecatriene-4,6-diyne-3,12-diol; 5,8,11-heptadecatriynoic acid; 1,9Z,16-heptadecatrien-4,6-diyne-3,8-diol; CICUTOXIN; Enanthotoxin; O-1602; O-1821; Cicutoxin; 5,8,11-Heptadecatriynoic acid; heptadeca-1,9Z,16-trien-4,6-diyne-3,8-diol; Benzyl 2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate	0.00285	0.01838	1.50	0.32143	1.00000	1.34	0.00555	0.07558	2.22	0.63348	1.00000	1.26
188.0838	8.8	Phenylpropanolamine hydrochloride; 4-(Pyridin-4-yl)butan-1-ol--hydrogen chloride (1/1)	0.00037	0.00320	1.46	0.98955	1.00000	1.04	0.00029	0.01101	2.01	0.04547	0.40799	1.18
848.5391	8.7	PS(41:7)	0.01298	0.06730	1.46	0.22982	1.00000	1.76	0.45274	1.00000	1.37	0.12940	0.74326	1.67
786.6537	10.3	SM(40:2)	0.01326	0.06843	1.46	0.07216	0.52502	2.39	0.37520	1.00000	1.66	0.44245	1.00000	1.27
137.0467	0.6	Hypoxanthine; tetrazolo[1,5-a]pyridin-8-ol; 4H-Pyrazolo[3,4-b]pyrazin-4-ol; 3-Nitrobenzyl radical	0.00494	0.02935	1.46	0.00134	0.03616	3.81	0.07677	0.48751	1.80	0.98892	1.00000	1.02
785.6612	12.4	TG(94:8); TG(47:4)	0.01389	0.07104	1.36	0.53273	1.00000	1.43	0.07998	0.49953	1.62	0.34468	1.00000	1.26
365.1575	0.6	Gibberellin A55; (7R*,8R*)-3-Methoxy-3',4,7,9,9'-pentahydroxy-8,4'-oxyneolignan; N-Acetylmuramoyl-Ala; Vernomygdin; Zexbrevin B; 1-methoxy-4-(3-methylsulfinyl-1,1-diphenylpropan-2-yl)benzene; Methyltris(phenylmethoxy)silane	0.01701	0.08472	1.21	0.40947	1.00000	1.26	0.05246	0.38434	1.01	0.65691	1.00000	1.41
779.5575	9.6	PA(42:5); PS(34:1)	0.01962	0.09624	-1.15	0.02211	0.23624	-1.67	0.92629	1.00000	-1.43	0.28318	1.00000	-1.11
775.5542	0.5	PG(36:2); PG(72:4); LBPA(18:1(9Z)/18:1(9Z))	0.64470	1.00000	-1.20	0.94146	1.00000	17.74	0.00484	0.06879	-57.47	0.58823	1.00000	1.46

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660.6643	12.2	Cer(m18:1(4E)/26:1(17Z))	0.00294	0.01880	-1.22	0.05541	0.45076	-1.99	0.06848	0.45770	-1.75	0.50845	1.00000	1.04
184.0743	8.8	4-Nitrosobiphenyl;Phosphocholine;3-Dibenzofuranamine;4-Hydroxycarbazole;4-Benzoylpyridine;2-Aminodiphenylene oxide;6-Methoxy-2-naphthonitrile;5-(Furan-3-yl)-1H-indole;4-Dibenzofuranamine;Methanone, phenyl-2-pyridinyl;-2-Propenal, 3-(2-quinolinyl)-;6-(Furan-2-yl)-1H-indole	0.00009	0.00099	-1.24	0.13688	0.82781	-1.18	0.00608	0.07977	-2.14	0.02843	0.31248	-1.14
786.6020	9.8	PC(72:4);PC(36:2);PE(39:2);Dioleoylphosphatidylcholine; GPCho(18:2(2E,4E)/O-18:0)[U];1,2-Dioleoyl PC	0.01499	0.07579	-1.26	0.27215	1.00000	-1.27	0.37814	1.00000	-1.29	0.17594	0.89579	-1.20
832.5851	8.5	PC(40:7)	0.00971	0.05172	-1.34	0.31469	1.00000	-1.41	0.43241	1.00000	-1.08	0.06382	0.48472	-1.34
184.0742	9.8	4-Nitrosobiphenyl; Phosphocholine; 3-Dibenzofuranamine; 4-Hydroxycarbazole; 4-Benzoylpyridine; 2-Aminodiphenylene oxide; 6-Methoxy-2-naphthonitrile; 5-(Furan-3-yl)-1H-indole; 4-Dibenzofuranamine;Methanone, phenyl-2-pyridinyl;- 2-Propenal, 3-(2-quinolinyl)-	0.00536	0.03136	-1.37	0.56243	1.00000	-1.30	0.09369	0.54778	-1.55	0.08217	0.56581	-1.49
768.5540	9.9	PC(35:4); PE(38:4); PE(36:4); PE(76:8); PE(P-38:4)	0.02031	0.09920	-1.37	0.75613	1.00000	1.18	0.58121	1.00000	-1.36	0.01920	0.25155	-1.56
125.0006	8.8	Phosphonoacetaldehyde	0.00085	0.00659	-1.40	0.90157	1.00000	1.01	0.00745	0.09301	-2.43	0.01742	0.24129	-1.29
758.5697	8.8	PC(34:2); PC(68:4); PE(37:2); PE(72:4); PE(36:2)	0.00003	0.00037	-1.41	0.08903	0.61083	-1.28	0.00156	0.03239	-2.60	0.02807	0.30996	-1.28
589.5184	12.6	Mayolene-20	0.00227	0.01520	-1.41	0.09007	0.61463	-1.72	0.02656	0.23904	-2.02	0.68066	1.00000	-1.16
561.4878	12.6	Mayolene-18; 2-methylbacteriohopane-32,33,34,35-tetrol	0.00149	0.01051	-1.43	0.05271	0.43500	-1.90	0.05473	0.39335	-3.17	0.35437	1.00000	-1.41
603.5350	10.0	DG(O-34:1)	0.01865	0.09182	-1.43	0.60174	1.00000	-1.31	0.46609	1.00000	-1.61	0.04896	0.43053	-1.25
780.5508	9.0	PC(36:5); PE(39:5)	0.00252	0.01658	-1.44	0.52710	1.00000	-1.22	0.11583	0.62320	-1.43	0.02381	0.28303	-1.59
830.5662	9.1	PC(40:8); PC(80:16)	0.00320	0.02016	-1.44	0.16326	0.91983	-1.19	0.74904	1.00000	-1.77	0.00627	0.13791	-2.55
830.5663	8.9	PC(40:8); PC(80:16)	0.01746	0.08678	-1.45	0.67797	1.00000	-1.36	0.19562	0.88375	-1.23	0.12746	0.73768	-2.17
575.5033	12.5	Montecristin, Mayolene-19, Ethylenebis(dioctylphosphine) dioxide	0.00003	0.00037	-1.47	0.01468	0.17517	-1.98	0.00035	0.01231	-2.87	0.40998	1.00000	-1.19
730.5380	7.3	PC(32:2); PC(64:4); PE(35:2)	0.00369	0.02271	-1.50	0.75045	1.00000	-1.22	0.07962	0.49953	-2.19	0.02747	0.30488	-1.67
269.2269	12.1	anhydroretinol, 1,4-Dimethyl-5-octyl-naphthalene; 2-decyl-naphthalene	0.00000	0.00000	-41.05	0.00001	0.00454	-38.55	0.00000	0.00104	-42.71	0.00000	0.00044	-79.39
716.7480	9.1	Hydrocinnamic acid, 4-(4-hydroxy-3-iodophenoxy)-3,5-diiodo-, sulfate	0.00094	0.00711	-24.42	0.20407	1.00000	-23.91	0.03298	0.28618	-10.83	0.09126	0.59775	-19.55
141.0706	11.8	5-Phenyl-1,3-pentadiene; Norcapillene; 1,4-Methanoazulene; Boron, trifluoro(tetrahydrofuran)-, (T-4)-	0.00000	0.00000	-15.91	0.00001	0.00454	-14.54	0.00005	0.00481	-15.12	0.00000	0.00034	-51.82
873.0201	12.5	Ubistatin A	0.00000	0.00000	-14.81	0.00028	0.01621	-12.45	0.00000	0.00094	-77.72	0.07005	0.51459	-2.44
875.1823	12.6	Quercetin 3-(2''-caffeoylglucoside)-(1->2)-(6''-malonylglucoside); Monodemalonylsalviadelphin	0.00000	0.00000	-14.56	0.00003	0.00461	-13.39	0.00000	0.00011	-66.54	0.00292	0.08145	-4.13
414.3007	0.7	N-Docosahexaenoyl GABA; N-docosahexaenoyl GABA; N-oleoyl methionine	0.00043	0.00360	-13.12	0.42796	1.00000	-2.81	0.00650	0.08400	-19.94	0.05353	0.44274	-18.40
177.1644	11.8	(6E,8E)-4,6,8-Megastigmatriene; 1-Phenylheptane; 1-Methyl-2-n-hexylbenzene; 3,5,7-Trimethyl-2E,4E,6E,8E-decatetraene; 1,2,3-Triethyl-4-methylbenzene; 1-tert-Butyl-2-(propan-2-yl)benzene; 5-tert-Butyl-1,2,3-trimethylbenzene; 1,4-Diisopropyl-2-methylbenzene; 1-Methyl-2,4-diisopropylbenzene; 1-Hexyl-4-methylbenzene	0.00000	0.00000	-12.38	0.00020	0.01361	-8.46	0.00002	0.00291	-9.64	0.00001	0.00195	-31.39
159.1174	11.8	Butadiene-styrene rubber; 1,2-Bis(1-methylethenyl)benzene; 4-Methyl-2-[(propan-2-yl)oxy]-1,3,2-dioxaborinane; 1,3-Diisopropenylbenzene; 1,4-Bis(1-methylethenyl)benzene; 4-Phenyl-1-cyclohexene	0.00000	0.00000	-12.29	0.00001	0.00454	-12.26	0.00007	0.00561	-10.48	0.00000	0.00043	-31.55
762.5069	7.8	PE(38:7)	0.00000	0.00001	-11.86	0.00117	0.03467	-12.55	0.00140	0.02981	-11.43	0.00147	0.05506	-4.98
792.5530	7.5	PC(37:6); PE(40:6); PE(P-40:6)	0.00000	0.00000	-10.89	0.00017	0.01353	-22.62	0.00037	0.01293	-15.94	0.00949	0.17291	-7.08
128.0628	11.8	2-Fluoro-5-hydrazinylpyridine	0.00000	0.00000	-10.75	0.00008	0.00736	-10.46	0.00012	0.00699	-7.65	0.00000	0.00043	-31.68
337.2740	11.2	Pregnanetriol; 5beta-Pregnane-3alpha,17alpha,20alpha-triol; 3-Methyl-5-pentyl-2-furanundecanoic acid; Isolinderanolide; 2alpha-(Hydroxymethyl)-17-methyl-5alpha-androstane-3beta,17beta-diol; 2,2'-(1R,2R)-Cyclohexane-1,2-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)	0.00000	0.00000	-10.19	0.00018	0.01361	-3.75	0.00000	0.00011	-35.11	0.00018	0.01187	-9.78
171.1175	11.8	1,6,7-Trimethylnaphthalene; Aethusin;(3,4-Dimethylcyclopenta-1,3-dien-1-yl)benzene; 2-Isopropyl-naphthalene; 1-Ethyl-8-methylnaphthalene	0.00000	0.00000	-9.93	0.00004	0.00548	-9.44	0.00025	0.01019	-7.31	0.00000	0.00053	-25.62
173.1330	11.8	1,2-Dihydro-1,1,6-trimethylnaphthalene; 2-Ethoxy-4,4,6-trimethyl-1,3,2-dioxaborinane; 2,3,4,4a,9,9a-Hexahydro-1H-fluorene	0.00000	0.00000	-9.85	0.00021	0.01361	-8.99	0.00041	0.01301	-8.72	0.00002	0.00287	-31.43
671.5600	11.1	LDG(40:5)	0.00000	0.00001	-9.51	0.00852	0.11904	-4.41	0.00052	0.01525	-13.19	0.00134	0.05363	-9.99
714.5063	8.2	PE(34:3); PC(31:3)	0.00000	0.00001	-9.22	0.00670	0.10282	-7.05	0.00088	0.02160	-10.26	0.00311	0.08451	-3.92
304.3004	1.2	Cetylpyridinium; 1-hexadecylpyridinium; BENZALKONIUM	0.00083	0.00648	-8.77	0.05690	0.45796	-7.91	0.15084	0.74476	-7.88	0.06503	0.49227	-20.87
808.5121	6.8	PS(38:6)	0.00002	0.00027	-8.58	0.00040	0.01971	-14.55	0.07346	0.47573	-6.38	0.05332	0.44274	-10.21

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337.2741	5.1	Pregnanetriol; 5beta-Pregnane-3alpha,17alpha,20alpha-triol; 3-Methyl-5-pentyl-2-furanundecanoic acid; Isolinderanolide; 2alpha-(Hydroxymethyl)-17-methyl-5alpha-androstane-3beta,17beta-diol; 2,2'-[(1R,2R)-Cyclohexane-1,2-diy]bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)	0.00000	0.00000	-8.56	0.00225	0.05308	-9.07	0.00175	0.03580	-7.45	0.00009	0.00824	-12.86
829.7146	11.7	SM(43:1)	0.00000	0.00000	-8.36	0.00100	0.03260	-10.92	0.00027	0.01057	-9.63	0.00232	0.07129	-6.31
145.1019	11.8	2,2-Dimethyl-2H-indene; 4,4,6-Trimethyl-1,3,2-dioxaborinan-2-ol; Boric acid pinacol ester; 1H-Cyclobut(f)indene, 2,4,5,6-tetrahydro-; Bicyclo(4.4.1)undeca-1,3,5,8-tetralene	0.00000	0.00000	-7.99	0.00002	0.00454	-7.61	0.00011	0.00699	-7.29	0.00000	0.00041	-20.77
341.3053	11.2	Polyoxyethylene (600) monoricinoleate; 2-oxo-heneicosanoic acid; Glycidyl stearate	0.00000	0.00000	-7.79	0.00007	0.00684	-3.32	0.00000	0.00026	-13.32	0.00014	0.01040	-7.59
286.2017	0.6	2-Octenoylcarnitine; (2E)-octenoylcarnitine; 2-octenoyl-L-carnitine; 1-tert-Butyl 4-ethyl 4-ethylpiperidine-1,4-dicarboxylate	0.00003	0.00045	-7.76	0.04497	0.39538	-3.40	0.00735	0.09237	-8.59	0.01970	0.25155	-6.40
778.5380	9.2	PC(36:6); PC(72:12); PE(39:6)	0.00000	0.00007	-7.22	0.00359	0.06950	-7.98	0.00588	0.07874	-9.54	0.01203	0.19466	-2.89
779.5409	9.2	1,28-Octacosanediol diferulate	0.00000	0.00004	-7.08	0.00300	0.06321	-8.62	0.00321	0.05096	-8.86	0.00876	0.16691	-2.78
175.1487	11.8	5,7alpha-Dihydro-1,4,4,7a-tetramethyl-4H-indene; 1,2,3,4-Tetrahydro-1,5,7-trimethylnaphthalene; alpha-Ionene; 1-Methyl-4-(1-methyl-2-propenyl)-benzene; 1,2,3,4-tetrahydro-2,5,8-trimethyl naphthalene; 1,2,3,4-Tetrahydro-1,1,6-trimethylnaphthalene; 2,2,6-Trimethyl-1,2,3,4-tetrahydronaphthalene; Benzene, (1-(1,1-dimethylethyl)cyclopropyl)-	0.00000	0.00000	-6.67	0.00056	0.02343	-7.02	0.00295	0.04820	-5.28	0.00004	0.00440	-16.60
621.4872	7.8	1-(6-[5]-ladderane-hexanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerol; PA(O-31:0)	0.00000	0.00000	-6.60	0.00003	0.00461	-9.56	0.00099	0.02353	-5.64	0.00053	0.02822	-6.33
832.5845	8.6	PC(40:7)	0.00000	0.00000	-6.25	0.00010	0.00881	-5.90	0.00011	0.00699	-3.88	0.00012	0.01016	-5.70
203.1799	11.1	(6alpha,7alpha,10alpha)-1(5),3-Aromadendradiene; beta-Spathulene; (1alpha,6alpha,7alphaH)-2,4(15)-Copadiene; 1,4,9-Cadinatriene; beta-Vatirenene; alpha-Curcumene; (-)-alpha-Curcumene; (E)-Calamene; Cuparene; Patchoula-2,4-diene; 2-Dodecanone, 12-fluoro-	0.00000	0.00000	-5.83	0.00294	0.06278	-3.82	0.00075	0.01985	-5.22	0.00023	0.01338	-6.63
573.4876	8.2	Dieporeticenin	0.00002	0.00026	-5.78	0.04297	0.38067	-4.87	0.01694	0.17232	-3.88	0.01414	0.21260	-3.49
789.6836	11.2	SM(40:0)	0.00003	0.00044	-5.78	0.00501	0.08416	-8.93	0.00358	0.05419	-11.07	0.24997	1.00000	-2.52
761.6519	10.6	SM(38:0)	0.00004	0.00051	-5.71	0.04552	0.39716	-5.91	0.00388	0.05728	-6.91	0.05564	0.45263	-3.39
361.2742	11.1	1alpha,23-dihydroxy-24,25,26,27-tetranorvitamin D3; 1alpha,23-dihydroxy-24,25,26,27-tetranorcholecalciferol; 17beta-Hydroxy-6beta-methyl; 5alpha-androstan-3-one propionate; 3beta-Hydroxy-5alpha-pregnan-20-one acetate; 1f1t,23-dihydroxy-24,25,26,27-tetranorvitamin D3; 1f1t,23-dihydroxy-24,25,26,27-tetranorcholecalciferol; O-Arachidonoyl Glycidol; 12-shogaol; Dromostanolone propionate;(Oxiran-2-yl)methyl icosane-5,8,11,14-tetraenoate	0.00000	0.00001	-5.65	0.00491	0.08375	-2.77	0.00142	0.02999	-7.36	0.00059	0.02976	-8.76
645.5344	11.2	N-palmitoyl-D-sphingosyl-1-(2-aminoethyl)phosphonate	0.00000	0.00000	-5.64	0.00012	0.01058	-2.99	0.00000	0.00044	-7.03	0.00023	0.01338	-3.70
820.5843	8.9	PE(42:6); PC(39:6)	0.00000	0.00007	-5.51	0.00228	0.05330	-6.66	0.00590	0.07874	-6.86	0.01716	0.23914	-2.97
218.1392	0.6	Propionylcarnitine; tert-Butyl 2-(hydroxymethyl)morpholine-4-carboxylate; ethyl 3-[[2-ethoxy-2-oxoethyl)-methylamino]propanoate; 4-(4-Methylpiperazin-1-yl)-7H-pyrrolo[2,3-d]pyrimidine; butyl 2-(ethylcarbamoyloxy)propanoate; Zindotrine; Diethyl 3,3'-Iminodipropionate; Guanidine, 1-butyl-2-cyano-3-(3-pyridyl)-	0.00000	0.00004	-5.38	0.00034	0.01806	-6.53	0.00154	0.03235	-4.50	0.07789	0.54289	-5.03
786.5035	8.6	PE(40:9)	0.00003	0.00043	-5.28	0.01613	0.18723	-3.73	0.06801	0.45730	-6.19	0.00485	0.11555	-6.03
133.1019	11.8	p-Mentha-1,3,5,8-tetraene; Tetralin; Dicyclopentadiene; 3,4-Dimethylstyrene; Benzene, 1-ethenyl-3,5-dimethyl- (9CI); (1-Fluorocyclohexyl)methanol; Dispiro(2.0.2.4)deca-1,5-diene; 1-Methyl-4-(prop-1-en-2-yl)benzene; 1,4-Cyclohexadiene, 1,4-dimethyl-3,6-bis(methylene)-	0.00000	0.00000	-5.25	0.00034	0.01806	-4.80	0.00039	0.01295	-4.78	0.00002	0.00260	-14.10
814.5342	9.7	PE(42:9)	0.00000	0.00003	-5.22	0.00041	0.01971	-10.44	0.02188	0.20753	-5.21	0.00282	0.07970	-3.79
337.2739	6.9	Pregnanetriol; 5beta-Pregnane-3alpha,17alpha,20alpha-triol; 3-Methyl-5-pentyl-2-furanundecanoic acid; Isolinderanolide; 2alpha-(Hydroxymethyl)-17-methyl-5alpha-androstane-3beta,17beta-diol; 2,2'-[(1R,2R)-Cyclohexane-1,2-diy]bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)	0.00000	0.00000	-5.12	0.00707	0.10561	-3.91	0.00371	0.05544	-8.56	0.00004	0.00405	-11.50
769.4774	8.3	PA(42:10); Pittoside A; HMT-toxin	0.00000	0.00007	-5.10	0.01285	0.16115	-5.63	0.00236	0.04207	-5.73	0.00958	0.17291	-1.95

S2 Table (continue)

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287.2375	11.1	Vitamin A;(x)-p-Menth-1-en-4-yl 5-isopropyl-2-methylphenyl ether; Abietinal; ent-16-Kauren-19-al; ent-kaur-16-en-19-al; Kaur-16-en-18-al;ent-19-Trachylobanal;8,13-Abietadien-18-al; Palustradienal;Helicallenal;levopimaradienal;dehydroabietadienol;(+) Totarol;isopimara-7,15-dienal; 9beta-Pimara-7,15-dien-19-al;(-)-13(16),14-Spongiadiene;(+) -15-Beyeren-3-one;pregna-5-20-dien-3beta-ol;Ferruginol;Neobietal;Retinol;TOTAROL;Sandaracopimarinal;(3beta)-17-Methylideneandrost-5-en-3-ol;6'-(tert-Butyl)-2',3'-dihydro-3',3'-dimethylspiro(cyclohexane-1,1'-(1H)indene)-5'-ol;1,2,3,6,7,8-Hexahydro-1,1,3,3,6,6,8,8-octamethyl-as-indacen-4-ol;Totarol;Kaurenal;levopimaral	0.00000	0.00001	-5.10	0.00429	0.07872	-2.59	0.00086	0.02160	-7.25	0.00033	0.01856	-7.54
129.0697	11.8	Naphthalene; Azulene	0.00000	0.00000	-5.06	0.00048	0.02205	-5.39	0.00051	0.01525	-4.68	0.00001	0.00096	-19.16
803.6986	11.5	SM(41:0)	0.00001	0.00019	-5.01	0.00311	0.06407	-6.41	0.00019	0.00819	-9.80	0.59551	1.00000	-1.90
290.1601	0.6	3-Methylglutaryl carnitine;O-Adipoyl carnitine;4-Amino-6,7-dimethoxy-2-(1-piperazinyl)quinazoline;2,4-Pyrimidinediamine, 5-((4-(aminomethyl)-3,5-dimethoxyphenyl)methyl)-;Etazolate;2-(1-Piperazinyl)-4-amino-6,7-dimethoxyquinazoline	0.00029	0.00262	-4.86	0.01287	0.16115	-4.82	0.14950	0.74287	-4.18	0.05766	0.46248	-8.94
147.1174	11.8	(3-Methyl-2-butenyl)-benzene;3-Methylidenebicyclo[4.2.2]deca-7,9-diene;Octahydro-1H-2,4,1-(ethane[1,1,2]triyil)cyclobuta[cd]pentalene;1-(But-3-en-1-yl)-3-methylbenzene;2-Ethylindan;Triethyl borate;Dispiro(2.0.2.5)undeca-1,5-diene;2-Octanone, 1-fluoro-;1,2-Dimethyl-alpha-methylstyrene;1,2-Dimethyl-4-(1-methylethenyl)-benzene;5-Phenyl-1-pentene;(1-Isopropylvinyl)benzene;Octanoyl fluoride	0.00000	0.00000	-4.86	0.00073	0.02702	-4.54	0.00185	0.03675	-3.32	0.00000	0.00053	-13.87
621.5446	11.2	LDG(36:2);1,2-Dioleoyl-sn-glycerol;1,2-Dioleoyl-rac-glycerol	0.00000	0.00000	-4.86	0.05792	0.46433	-2.41	0.00000	0.00035	-16.15	0.00280	0.07970	-5.50
653.5407	8.5	7226-96-2	0.00004	0.00054	-4.82	0.03628	0.34415	-6.25	0.02278	0.21170	-3.20	0.01284	0.20195	-2.37
689.5903	11.1		0.00000	0.00004	-4.67	0.01902	0.21110	-3.47	0.00027	0.01057	-6.56	0.00936	0.17291	-4.54
770.5653	8.5	PC(35:3);PE(38:3)	0.00048	0.00405	-4.66	0.05860	0.46433	-4.26	0.04050	0.32599	-4.58	0.11005	0.68363	-2.68
118.0870	0.6	Betaine;L-Valine; 2-Amino-3-methylbutanoic acid; D-Valine;Vaporole;N-Methyl-a-aminoisobutyric acid;5-Aminopentanoic acid;Norvaline; 2S-amino-pentanoic acid;Amyl Nitrite;4R-aminopentanoic acid; 4S-aminopentanoic acid; 4-amino-pentanoic acid;2-Amino-2-methylbutanoate;4-Methylaminobutyrate;isoamyl nitrite;Valine;Pentanoic acid, 4-amino-, (R)-; Valeric acid, 4-amino-, (R)-(+); (R)-(+)-4-Aminovaleric acid; (R)-4-Aminopentanoic acid;Pentanoic acid, 4-amino-, (S)-; (S)-4-Aminopentanoic acid; (S)-4-Aminovaleric acid;Pentanoic acid, 4-amino-, (1)-; Valeric acid, 4-amino-, (1)-; (1)-4-Aminopentanoic acid; (RS)-4-Aminopentanoic acid; (RS)-4-Methyl-gamma-aminobutyric acid;L-Norvaline;3-Nitropentane;2-Ethoxypropanamide;Pentyl nitrite;3-Methylbutyl nitrite;N-Ethyl-N-methylglycine;4-Methylmorpholine 4-oxide;N-(3-methoxypropyl)formamide;1,3-Dioxolane-2-methanamine, N-methyl-;1,3-Dioxolane-2-ethylamine;Butane, 2-methyl-2-nitro-;Ethyl 3-aminopropanoate;Formamide, N-(2-hydroxy-1,1-dimethylethyl)-;3-Methyl-1-nitrobutane;1-Nitropentane;Carbamic acid, 2-methylpropyl ester;Carbamic acid, butyl ester;Ethyl ethylcarbamate	0.00004	0.00054	-4.64	0.19077	1.00000	-2.22	0.00534	0.07401	-4.91	0.00753	0.15508	-2.73
339.2895	6.9	Glycidyl oleate; 4-(4,8-Dimethylnonyl)-2,6-dimethyl-1-phenylpyridin-1-ium	0.00000	0.00001	-4.63	0.00447	0.07883	-3.79	0.00765	0.09504	-3.82	0.00002	0.00247	-11.03
837.5467	8.5	PI(34:1)	0.00015	0.00147	-4.56	0.05919	0.46497	-11.87	0.18064	0.84104	-3.24	0.00327	0.08744	-3.19
651.5344	8.5	1-(8-[3]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerol	0.00010	0.00105	-4.56	0.06045	0.46688	-10.10	0.11870	0.63105	-3.30	0.00329	0.08744	-3.32

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429.3728	6.1	Cholesteryl acetate;4alpha-Formyl-4beta-methyl-5alpha-cholesta-8-en-3beta-ol; 4i±-formyl-4i²-methyl-5i±-cholesta-8-en-3i²-ol;4alpha-Hydroxymethyl-4beta-methyl-5alpha-cholesta-8,24-dien-3beta-ol; 4i±-hydroxymethyl-4i²-methyl-5i±-cholesta-8,24-dien-3i²-ol;3-Hydroxystigmast-5-en-7-one; 3beta-hydroxy-stigmast-5-en-7-one;Mangiferdesmethylursanone;(6beta,24R)-6-Hydroxystigmast-4-en-3-one;Stigmastane-3,6-dione;(3alpha,5alpha,7alpha)-14-Methylergosta-9(11),24(28)-dien-3,7-diol;3-beta-Hydroxy-4-beta-methyl-5-alpha-cholest-7-ene-4-alpha-carbaldehyde; 3beta-hydroxy-4beta-methyl-5alpha-cholest-7-ene-4alpha-;carbaldehyde; 3beta-Hydroxy-4beta-methyl-5alpha-cholest-7-ene-4alpha-carbaldehyde;(3beta,24R,24'R)-fucosterol epoxide; (3beta,24S,24'S)-fucosterol epoxide;Saringosterol ;22S-hydroxyisofucosterol;halosterol A;halosterol B;leucisterol;(25R)-5alpha,6alpha-epoxy-24R,26R-dimethyl-26,27-cyclo-cholestan-3beta-ol;1alpha-hydroxy-26,27-dimethylvitamin D3 / 1alpha-hydroxy-26,27-dimethylcholecalciferol;25-hydroxy-26,27-dimethylvitamin D3 / 25-hydroxy-26,27-dimethylcholecalciferol;(6S)-6,19-ethano-25-hydroxy-6,19-dihydrovitamin D3 / (6S)-6,19-ethano-25-hydroxy-6,19-dihydrocholecalciferol; (6R)-6,19-ethano-25-hydroxy-6,19-dihydrovitamin D3 / (6R)-6,19-ethano-25-hydroxy-6,19-dihydrocholecalciferol;25-Hydroxy-6,19-dihydro-6,19-ethanovitamin D3;1-Hydroxyvitamin D5;4a-Hydroxymethyl-4b-methyl-5a-cholesta-8,24-dien-3b-ol;1i±-hydroxy-26,27-dimethylvitamin D3 / 1i±-hydroxy-26,27-dimethylcholecalciferol;4alpha-formyl-4beta-methyl-5alpha-cholesta-8-en-3beta-ol;4alpha-hydroxymethyl-4beta-methyl-5alpha-cholesta-8,24-dien-3beta-ol;3-beta-hydroxy-4-beta-methyl-5-alpha-cholest-7-ene-4-alpha-carbaldehyde	0.00125	0.00917	-4.55	0.23805	1.00000	-4.12	0.01197	0.13281	-4.05	0.27337	1.00000	-3.78
896.5381	8.3	Chlorophyll d	0.00003	0.00044	-4.34	0.01715	0.19506	-5.23	0.03379	0.29042	-3.65	0.01291	0.20195	-2.05
855.7429	12.5	TG(104:8);TG(52:4);Glycerol 1,3-di-(9Z,12Z-octadecadienoate) 2-hexadecanoate;	0.00000	0.00000	-4.32	0.00014	0.01172	-4.14	0.00001	0.00212	-6.38	0.08598	0.57977	-1.75
780.5537	7.7	PC(36:5);PE(39:5)	0.00003	0.00046	-4.21	0.02976	0.29822	-3.18	0.02322	0.21491	-6.09	0.01071	0.18264	-3.75
751.5096	7.9	1,26-Hexacosanediol diferulate; 1,28-Dicaffeoyloctacosanediol	0.00000	0.00004	-4.21	0.00065	0.02469	-7.18	0.00951	0.11035	-5.34	0.00934	0.17291	-3.57
298.0655	0.6	Asn-Gly-OH;Gly-Asn-OH;Benzoic acid, 2-((3-chloro-1-naphthalenyl)amino)-;Glybuzole;1-Amino-1-oxobutan-2-yl 3,5-dinitrobenzoate;1-Amino-2-methyl-1-oxopropan-2-yl 3,5-dinitrobenzoate;1,4-Naphthalenedione, 2-chloro-3-((4-methylphenyl)amino)-;2-Naphthalenecarboxamide, N-(4-chlorophenyl)-3-hydroxy-;2-Chloro-5-(4-methylnaphthalen-1-yl)pyridine-4-carboxylic acid;N-(5-Isopropyl-1,3,4-thiadiazol-2-yl)-p-toluenesulphonamide;2-Naphthalenecarboxamide, N-(2-chlorophenyl)-1-hydroxy-	0.00001	0.00020	-4.20	0.05293	0.43521	-3.55	0.08753	0.52794	-1.47	0.00013	0.01036	-3.99
881.7185	12.3	22:2-Glc-Campesterol	0.00001	0.00018	-4.20	0.35461	1.00000	-1.78	0.00015	0.00712	-8.34	0.01089	0.18446	-6.88
647.5606	11.4	LDG(38:3)	0.00007	0.00080	-4.17	0.04303	0.38067	-2.78	0.02386	0.21821	-4.32	0.01838	0.24819	-4.77
140.0689	0.6	(3S)-3-(Trifluoromethyl)pyrrolidine; SBB013287	0.00005	0.00058	-4.11	0.16002	0.91352	-3.00	0.00270	0.04506	-5.91	0.02345	0.28303	-4.51
806.5697	8.3	Lactosylceramide (d18:1/12:0); LacCer(d18:1/12:0);PC(76:12);PC(38:6);PE(41:6);LacCer(d14:1/16:0);Galabiosylceramide (d18:1/12:0)	0.00000	0.00006	-4.08	0.00529	0.08645	-7.41	0.00351	0.05353	-5.65	0.00886	0.16733	-2.27
341.3057	11.1	Polyoxyethylene (600) monoricinoleate; 2-oxo-heneicosanoic acid; Glycidyl stearate	0.00000	0.00002	-4.05	0.00291	0.06273	-2.32	0.00338	0.05288	-4.84	0.00170	0.05868	-4.74
848.6816	12.3	PS(O-41:0)	0.00006	0.00073	-4.05	0.00026	0.01588	-8.37	0.00856	0.10243	-5.99	0.87353	1.00000	-1.29
899.7096	12.3	TG(56:10); TG(112:20)	0.00012	0.00121	-4.04	0.00092	0.03092	-5.26	0.00837	0.10074	-5.28	0.82324	1.00000	-1.68
653.5106	10.8	LDG(38:7);LDG(40:7);LDG(39:7)	0.00000	0.00003	-4.01	0.00063	0.02445	-4.60	0.00306	0.04919	-4.93	0.02024	0.25683	-4.17
645.5454	11.1	LDG(38:4);LDG(36:4);LDG(40:4);1-(9Z,12Z,15Z-octadecatrienoyl)-2-(11Z-eicosenoyl)-sn-glycerol	0.00000	0.00001	-4.01	0.00207	0.05078	-1.97	0.00217	0.04058	-3.92	0.00102	0.04594	-4.39
125.0005	0.6	Phosphonoacetaldehyde	0.00002	0.00029	-3.94	0.09361	0.62941	-2.33	0.01240	0.13558	-3.16	0.00160	0.05711	-3.99
296.0665	0.6	5-Aminoimidazole ribonucleotide;2,2,2-trifluoro-N-(8-fluoro-9H-fluoren-2-yl)acetamide;5,8-Quinolinedione, 6-amino-2-(2-nitrophenyl)-;N-(5-Bromopentyl)-3-phenylprop-2-enamide	0.00004	0.00054	-3.84	0.15773	0.90598	-2.70	0.03543	0.30001	-2.61	0.00106	0.04663	-4.94
764.5228	8.6	PE(38:6);PC(35:6);PE(P-38:6)	0.00004	0.00047	-3.84	0.00859	0.11904	-5.84	0.08045	0.50112	-5.45	0.00968	0.17291	-2.75
897.5409	8.3	PI(39:6)	0.00000	0.00007	-3.73	0.00183	0.04595	-8.56	0.01912	0.18917	-3.68	0.00577	0.12872	-2.40

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258.1100	0.7	Glycerophosphocholine;5-Methylcytidine;Tolmetin;Pyro-L-glutaminy-L-glutamine;Isimine;Benserazide;sn-glycero-3-Phosphocholine;N4-Methylcytidine;NSC359093;6-Chloro-N ⁴ ~-[2-(morpholin-4-yl)ethyl]pyrimidine-4,5-diamine;4-Methoxy-N-(2-methoxyphenyl)benzamide;2-phenoxyethyl N-phenylcarbamate;2-(4-aminophenyl)-2-(4-methoxyphenyl)acetic acid;2-[[4-(Trifluoromethyl)phenyl]methyl]piperidin-4-one;3'-O-Methylcytidine N-(4'-Hydroxy-3'-methoxy[1,1'-biphenyl]-3-yl)acetamide;4'-Hydroxy-3'-methoxy-N-methyl[1,1'-biphenyl]-3-carboxamide;N1-(Tris(hydroxymethyl)methyl-4-nitro-1,2-phenylenediamine;5-(2,5-Dimethylphenyl)-2-methoxypyridine-3-carboxylic acid;6-(4-Ethoxy-2-methylphenyl)pyridine-3-carboxylic acid;5-Amino-2'-methoxy-5'-methyl[1,1'-biphenyl]-3-carboxylic acid;5-Amino-3'-ethoxy[1,1'-biphenyl]-3-carboxylic acid;Uridine, 2'-deoxy-, 4-(O-methylxime);4-(4-Ethoxy-2-methylphenyl)pyridine-3-carboxylic acid;Dinoseb, ammonium salt;STK047859;Acetamide, N-[2-(2-methoxyphenoxy)phenyl]-;Pyridazine, 3,6-dipropoxy-4-nitro-, 1-oxide;Benzamide, 2-hydroxy-N-(4-methoxyphenyl)-4-methyl-	0.00001	0.00011	-3.73	0.02022	0.22227	-3.65	0.00233	0.04207	-5.66	0.00957	0.17291	-3.59
836.5438	8.5	PS(40:6)	0.00015	0.00149	-3.70	0.06689	0.50297	-8.90	0.22295	0.95878	-2.72	0.00210	0.06860	-2.79
792.5547	9.7	PC(37:6); PE(40:6); PE(P-40:6)	0.00002	0.00031	-3.69	0.00327	0.06606	-7.64	0.10571	0.59230	-2.81	0.00836	0.16580	-2.35
257.1476	0.6	Pulcherrimic acid; 6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)quinazoline; NSC520792; 4,7,10,13-Tetraoxahexadecanedinitrile	0.00036	0.00314	-3.66	0.52528	1.00000	-1.87	0.00165	0.03392	-6.28	0.09524	0.62030	-3.85
568.3397	0.9	LPC(22:6); Penitrem D	0.00039	0.00331	-3.64	0.08808	0.60831	-3.97	0.08183	0.50522	-2.94	0.02990	0.31938	-2.88
781.6119	12.3	3-Demethylubiquinone-9	0.00017	0.00169	-3.63	0.16214	0.91746	-2.67	0.00123	0.02752	-6.67	0.21269	0.96984	-3.17
86.0971	0.6	Piperidine;(R)-2-Methylpyrrolidine;N-Methylpyrrolidine;cyclobutylmethanamine	0.00004	0.00052	-3.57	0.13056	0.80883	-2.50	0.03656	0.30616	-3.19	0.00108	0.04667	-4.77
655.4689	10.5	PA(O-34:4); PA(P-34:3)	0.00001	0.00011	-3.55	0.01278	0.16115	-3.60	0.00124	0.02752	-4.05	0.03048	0.31960	-3.52
197.0815	12.3	Homoveratric acid;Xanthoxylin;2,4,5-Trimethoxybenzaldehyde;(+)3-(3,4-Methylenedioxyphenyl)-1,2-propanediol;Maltlyl isobutyrate;(S)-Batatic acid;1-(2,4,5-Trihydroxyphenyl)-1-butanone;2-Hydroxy-3-(4-methoxyphenyl)propanoic acid;(S)-2-(4-Methoxyphenoxy)propanoic acid;4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one;5-Hydroxyconiferyl alcohol;3-(3-Hydroxyphenyl)-2-methylactic acid;3-(3,4-Dihydroxyphenyl)-2-methylpropionic acid;Hydroferulic acid;2,3-Dihydroxy-p-cumate;Phlorisobutyrophenone;Acetosyringone;2',6'-Dimethoxy-4'-hydroxyacetophenone;Cantharidin;Paeonilactone B;α-Methyl-3,4-dihydroxyphenylpropionic acid;3-(4-Hydroxy-3-methoxyphenyl)propionic acid;ASARYLALDEHYDE;ORSELLINIC ACID, ETHYL ESTER;ACETOSYRINGONE;XANTHOXYLIN;CANTHARIDIN;SAFROLGLYCOL;5-Hydroxy-4-pentenoic acid d-lactone;(7E)-2-acetyl-2,3,4,5-tetrahydrooxonine-6,9-dione;Atracic acid;3-(3-Methoxyphenoxy)propionic acid;2,4-Dimethoxy-5-methylbenzoic acid;[3-(Propylsulfanyl)phenyl]boronic acid;NSC361563;Ethyl 4-(furan-2-yl)-3-oxobutanoate;4-(2-Hydroperoxypropan-2-yl)benzoic acid;4-Ethoxyphenoxyacetic acid;4,5-Diethoxycyclohexa-3,5-diene-1,2-dione;4-Hydroxy-1-oxaspiro[5.5]undec-4-ene-2,3-dione;4-Ethoxy-2-methoxybenzoic acid;2',4',5'-Trihydroxybutyrophenone;2-methoxyethyl 2-hydroxybenzoate;4-[1,3]dioxolan-2-yl-2-methoxyphenol;Dimethyl Octa-2,4,6-trienedioate;3-Methoxy-4-(methoxymethoxy)benzaldehyde;2,3,6-Trimethoxybenzaldehyde;2,4-Dimethoxyphenylacetic acid;Methyl 2,4-dihydroxy-3,6-dimethylbenzoate;(2-Ethoxy-phenoxy)-acetic acid;2-(3-Methoxyphenoxy)propanoic acid;2-[4-(hydroxymethyl)phenoxy]propanoic acid;2-pyrazinylbenzimidazole;Diprop-2-en-1-yl (2Z)-but-2-enedioate;4-methoxy-2-(methoxymethoxy)benzaldehyde;1,2,4-Triazol[4,3-a]pyridine, 3-(2-pyridinyl)-;Maltol isobutyrate;2,5-Cyclohexadiene-1-acetic acid, 1-hydroxy-4-	0.00056	0.00455	-3.48	0.53395	1.00000	-1.82	0.00094	0.02255	-6.58	0.24023	1.00000	-3.65
773.6520	10.7	SM(39:1)	0.00203	0.01385	-3.44	0.19636	1.00000	-1.97	0.07423	0.47802	-3.50	0.12201	0.72447	-1.94
569.3432	0.9	(24E)-3α,15α-Diacetoxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid;(-)-Helvolic acid;Karatavigenin B;6,8a-Seco-6,8a-deoxy-5-oxoavermectin "1a" aglycone	0.00022	0.00208	-3.41	0.02891	0.29118	-3.91	0.03845	0.31503	-3.48	0.08798	0.58638	-1.96
358.2953	0.8	N-palmitoyl threonine	0.00063	0.00510	-3.41	0.00609	0.09667	-3.01	0.10744	0.59327	-2.91	0.34297	1.00000	-1.47
845.5280	8.3	PG(42:9)	0.00002	0.00026	-3.31	0.01377	0.16745	-5.24	0.06302	0.43261	-3.41	0.00230	0.07129	-2.59
797.5087	9.4	PA(44:10)	0.00000	0.00006	-3.31	0.00141	0.03706	-5.32	0.00437	0.06319	-2.72	0.02515	0.28458	-2.53
540.4985	7.6	Hexacosanoyl carnitine	0.00000	0.00003	-3.20	0.69829	1.00000	-1.71	0.00240	0.04255	-3.28	0.00000	0.00049	-5.72

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258.1108	0.6	Glycerophosphocholine;5-Methylcytidine;Tolmetin;Pyro-L-glutaminy-L-glutamine;Isimine;Benserazide;sn-glycero-3-Phosphocholine;N4-Methylcytidine;NSC359093;6-Chloro-N ⁴ ~-[2-(morpholin-4-yl)ethyl]pyrimidine-4,5-diamine;4-Methoxy-N-(2-methoxyphenyl)benzamide;2-phenoxyethyl N-phenylcarbamate;2-(4-aminophenyl)-2-(4-methoxyphenyl)acetic acid;2-[[4-(Trifluoromethyl)phenyl]methyl]piperidin-4-one;3'-O-Methylcytidine;N-(4'-Hydroxy-3'-methoxy[1,1'-biphenyl]-3-yl)acetamide;4'-Hydroxy-3'-methoxy-N-methyl[1,1'-biphenyl]-3-carboxamide;N1-(Tris(hydroxymethyl)methyl-4-nitro-1,2-phenylenediamine;5-(2,3-Dimethylphenyl)-2-methoxypyridine-3-carboxylic acid;5-(4-Ethylphenyl)-2-methoxypyridine-3-carboxylic acid;5-(2,4-Dimethylphenyl)-2-methoxypyridine-3-carboxylic acid;2-(4-Ethoxy-2-methylphenyl)pyridine-4-carboxylic acid;5-Amino-2'-methoxy-5'-methyl[1,1'-biphenyl]-3-carboxylic acid;5-Amino-3'-ethoxy[1,1'-biphenyl]-3-carboxylic acid;Uridine, 2'-deoxy-, 4-(O-methylxime);4-(4-Ethoxy-2-methylphenyl)pyridine-3-carboxylic acid;Dinoseb, ammonium salt;STK047859;Acetamide, N-[2-(2-methoxyphenoxy)phenyl]-;Pyridazine, 3,6-dipropoxy-4-nitro-, 1-oxide;Benzamide, 2-hydroxy-N-(4-methoxyphenyl)-4-methyl-	0.00001	0.00023	-3.20	0.13056	0.80883	-2.14	0.00584	0.07874	-2.43	0.00126	0.05144	-2.79
744.5535	8.1	PC(33:2); 1,2-Dioleoyl phosphatidyl ethanolamine	0.00000	0.00003	-3.20	0.03791	0.35307	-3.94	0.00014	0.00712	-6.89	0.00425	0.10449	-2.48
635.5440	10.4	1-(8-[5]-ladderane-octanyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerol	0.00494	0.02935	-3.19	0.10325	0.68215	-2.79	0.18314	0.84578	-3.99	0.24860	1.00000	-2.37
795.6462	12.3	TG(96:12); TG(48:6)	0.00635	0.03675	-3.17	0.03586	0.34295	-2.06	0.13763	0.70228	-2.74	0.72339	1.00000	-1.94
313.2740	10.6	10-oxo-nonadecanoic acid;Ricinoleic Acid methyl ester;Methyl ricinoleate;Glycidyl Palmitate	0.00000	0.00004	-3.17	0.05069	0.42443	-2.51	0.00011	0.00699	-12.36	0.06291	0.48257	-2.72
169.1017	11.8	2,4,6,8-Tridecatetrayne;4-Methylbiphenyl;(E,E)-1,3,5,11-Tridecatetraene-7,9-diyne;Diphenylmethane;4-Phenyltoluene;4-Fluoro-1-methoxy-2-(propan-2-yl)benzene	0.00000	0.00000	-3.17	0.00078	0.02840	-5.10	0.01615	0.16706	-2.30	0.00016	0.01090	-9.83
575.5035	10.6	LDG(34:2); cis-Uvariamicin IB; Reticulatin 2; cis-Uvariamicin IV; Neoreticulatacin A; LDG(33:2); LDG(35:2)	0.00002	0.00026	-3.13	0.05176	0.42875	-3.09	0.00043	0.01318	-11.17	0.08437	0.57310	-2.41
827.6992	11.2	SM(43:2)	0.00206	0.01400	-3.12	0.06176	0.47378	-4.46	0.07603	0.48701	-2.39	0.34192	1.00000	-2.90
796.5842	9.1	PC(37:4); PE(40:4)	0.00003	0.00046	-3.11	0.18359	1.00000	-1.35	0.00309	0.04941	-4.14	0.01002	0.17478	-3.66
795.6889	11.7	1-N-[(4-tert-butylcyclohexyl)-[(4-tert-butylcyclohexyl)-[(4-(dihydroxyamino)-2,6-di(propan-2-yl)cyclohexyl)amino]methyl]peroxymethyl]-4-N,4-N-dihydroxy-2,6-di(propan-2-yl)cyclohexane-1,4-diamine	0.00083	0.00648	-3.08	0.01034	0.13660	-2.65	0.98780	1.00000	-1.69	0.00226	0.07129	-4.11
755.6031	9.8	SM(38:2);SM(38:3)	0.00148	0.01051	-3.05	0.42183	1.00000	-2.45	0.08199	0.50522	-6.05	0.02578	0.28749	-2.63
339.2897	8.3	Glycidyl oleate, 4-(4,8-Dimethylnonyl)-2,6-dimethyl-1-phenylpyridin-1-ium	0.00089	0.00685	-3.02	0.21332	1.00000	-2.22	0.67540	1.00000	-2.72	0.00057	0.02950	-8.65
337.2740	10.6	Pregnanetriol; 5beta-Pregnane-3alpha,17alpha,20alpha-triol, 3-Methyl-5-pentyl-2-furanundecanoic acid; Isolinderanolide; 2alpha-(Hydroxymethyl)-17-methyl-5alpha-androstane-3beta,17beta-diol; 2,2'-(1R,2R)-Cyclohexane-1,2-diyl]bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)	0.00000	0.00002	-3.02	0.03815	0.35307	-3.11	0.00005	0.00480	-12.97	0.06084	0.47466	-2.81
810.5274	7.8	PS(38:5); PE(0:0)	0.00083	0.00648	-3.02	0.13556	0.82779	-2.31	0.17075	0.81288	-1.67	0.01965	0.25155	-2.47
297.0697	0.6	N-Methoxyspirobrassinol methyl ether; NSC153740; 2-Chloro-4-(4-methylnaphthalen-1-yl)benzoic acid	0.00108	0.00802	-3.01	0.51601	1.00000	-2.30	0.09088	0.53861	-2.66	0.00852	0.16580	-3.20
730.5376	9.6	PC(32:2); PC(64:4); PE(35:2)	0.00040	0.00338	-3.00	0.28214	1.00000	-2.74	0.03518	0.29897	-3.41	0.01698	0.23812	-2.18
184.0742	0.6	4-Nitrosobiphenyl;Phosphocholine;3-Dibenzofuranamine;4-Hydroxycarbazole;4-Benzoylpyridine;2-Aminodiphenylene oxide;6-Methoxy-2-naphthonitrile;5-(Furan-3-yl)-1H-indole;1-Hydroxycarbazole;4-Dibenzofuranamine;Methanone, phenyl-2-pyridinyl;-2-Propenal, 3-(2-quinolinyl)-	0.00001	0.00022	-2.99	0.12150	0.76938	-2.22	0.00611	0.07977	-2.33	0.00145	0.05506	-3.45
778.5352	7.9	PC(36:6); PC(72:12); PE(39:6)	0.00003	0.00045	-2.98	0.30094	1.00000	-2.11	0.00080	0.02070	-10.08	0.01450	0.21668	-2.04
827.7112	12.4	TG(100:8); TG(50:4)	0.00001	0.00023	-2.94	0.00097	0.03226	-5.96	0.00415	0.06040	-4.33	0.26259	1.00000	-1.54
795.6279	12.1	Coenzyme Q9	0.00009	0.00094	-2.92	0.09738	0.65094	-3.23	0.00129	0.02801	-4.57	0.30426	1.00000	-1.92
778.5351	8.1	PC(36:6); PC(72:12); PE(39:6)	0.02046	0.09973	-2.88	0.29308	1.00000	-2.32	0.44210	1.00000	-5.36	0.23595	1.00000	-3.83
104.1077	0.6	Neurine;Choline;2-Amino-3-methyl-1-butanol;[(2-Methylpropyl)amino]methanol;Dimepranol;(S)-(+)-1-Dimethylamino-2-propanol;1-Butanamine, N-hydroxy-3-methyl-;2-methyl-2-(methylamino)propan-1-ol;2-(Isopropylamino)ethanol	0.00001	0.00017	-2.86	0.06805	0.50669	-2.20	0.00873	0.10344	-2.32	0.00115	0.04884	-3.27
817.7140	11.7	SM(42:0)	0.00028	0.00261	-2.85	0.00753	0.11012	-5.19	0.00440	0.06332	-5.21	0.83166	1.00000	-1.22
863.6913	12.4	Coenzyme Q10; Ubisemiquinone; Ubidecarenone	0.00015	0.00153	-2.82	0.53056	1.00000	-1.64	0.00267	0.04506	-4.28	0.01850	0.24819	-2.92
679.4691	10.2	PA(P-36:5)	0.00264	0.01731	-2.79	0.21267	1.00000	-3.25	0.00723	0.09180	-5.37	0.67750	1.00000	-1.92
617.5137	12.1	LDG(36:4)	0.00002	0.00025	-2.76	0.00986	0.13211	-2.50	0.00727	0.09180	-4.52	0.03528	0.33886	-3.04

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835.6816	11.7	TG(51:7);TG(102:14);PG(O-41:0)	0.00287	0.01841	-2.74	0.01157	0.14948	-2.48	0.99999	1.00000	-1.24	0.00725	0.15383	-3.38
811.5302	7.8	PI(32:0); PC(0:0)	0.00142	0.01019	-2.73	0.11172	0.72554	-1.72	0.43906	1.00000	-1.00	0.01155	0.18972	-4.15
733.6212	9.8	SM(36:0)	0.00125	0.00917	-2.72	0.19814	1.00000	-1.91	0.07059	0.46371	-3.08	0.07182	0.51791	-2.13
589.5187	9.6	Mayolene-20	0.00034	0.00301	-2.70	0.40768	1.00000	-2.06	0.02019	0.19559	-2.76	0.01282	0.20195	-2.70
816.7070	12.3	SM(42:1); TG(96:8); TG(48:4)	0.00034	0.00302	-2.67	0.00851	0.11904	-5.75	0.00787	0.09676	-6.99	0.76251	1.00000	-1.38
801.6843	11.3	SM(41:1)	0.00023	0.00218	-2.64	0.02705	0.27859	-2.13	0.01975	0.19462	-3.69	0.18509	0.91530	-1.91
770.5687	8.3	PC(35:3); PE(38:3)	0.00427	0.02567	-2.61	0.67026	1.00000	-2.23	0.07130	0.46705	-2.29	0.05372	0.44274	-1.95
659.5006	11.2	PA(O-34:2); PA(P-34:1)	0.00000	0.00000	-2.58	0.01398	0.16903	-1.74	0.00001	0.00165	-4.81	0.03200	0.32513	-2.92
617.5142	10.4	LDG(36:4)	0.00485	0.02893	-2.55	0.07234	0.52502	-2.70	0.10707	0.59327	-2.60	0.47298	1.00000	-1.97
337.2744	0.9	Pregnanetriol; 5beta-Pregnane-3alpha,17alpha,20alpha-triol;3-Methyl-5-pentyl-2-furanundecanoic acid;isolinderanolide;2alpha-(Hydroxymethyl)-17-methyl-5alpha-androstane-3beta,17beta-diol;2,2'-[1(R,2R)-Cyclohexane-1,2-diy]bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)	0.00030	0.00270	-2.55	0.13141	0.81127	-2.70	0.64365	1.00000	-1.10	0.00022	0.01338	-3.92
156.0430	0.6	N-Methylethanolaminium phosphate; D-1-Aminopropan-2-ol O-phosphate; L-1-Aminopropan-2-ol O-phosphate; N-Methylethanolamine phosphate; (2S,3S)-3-Amino-2-hydroxybutanoic acid--hydrogen chloride (1/1); 1-(Methoxycarbonyl)cyclobut-2-ene-1-carboxylate; 1-Oxo-1H-indene-2-carbonitrile; 3-(hydroxyamino)propylphosphonic acid; Potassium N,N-dimethyl-beta-alaninate	0.00003	0.00041	-2.54	0.51672	1.00000	-1.41	0.00256	0.04359	-3.54	0.00145	0.05506	-4.33
901.7251	12.5	TG(112:18); TG(56:9)	0.00004	0.00053	-2.52	0.00753	0.11012	-3.81	0.00093	0.02255	-3.80	0.55178	1.00000	-1.61
339.2898	8.2	Glycidyl oleate; 4-(4,8-Dimethylnonyl)-2,6-dimethyl-1-phenylpyridin-1-ium	0.00803	0.04466	-2.47	0.50746	1.00000	-1.87	0.98014	1.00000	-1.78	0.00068	0.03285	-10.82
918.7016	12.4	PC(46:6)	0.00004	0.00052	-2.40	0.00056	0.02343	-4.90	0.00202	0.03929	-3.32	0.87251	1.00000	-1.14
756.5537	7.6	PC(34:3); PE(37:3)	0.00036	0.00315	-2.39	0.26540	1.00000	-1.87	0.04182	0.33543	-3.91	0.01299	0.20195	-2.05
794.5689	9.2	PC(37:5); PE(40:5)	0.00004	0.00053	-2.38	0.49936	1.00000	-1.64	0.00398	0.05829	-3.30	0.00206	0.06832	-3.38
226.1205	0.6	Nnal-N-oxide;alpha-[3-[(Hydroxymethyl)nitrosoamino]propyl]-3-pyridinemethanol;2-[2-(4-Pyridinyl)-1-butenyl]phenol;Navenone A;1-(Methylnitrosoamino)-4-(3-pyridinyl)-1,4-butanediol;4-(Methylnitrosamino)-1-(3-pyridyl-N-oxide)-1-butanol;NSC400085;2,3-diphenylpropanamide;3,3-diphenylpropanamide;Propionanilide, o-phenyl;-N-(2,5-Dimethylphenyl)benzamide;Hexazinone (Metab D);Benzamide, 2-methyl-N-(3-methylphenyl)-;Benzamide, 2-ethyl-N-phenyl;-N'-[[3-hydroxy-5-(hydroxymethyl)-2-methylpyridin-4-yl]methyl]acetohydrazide;N-methyl-alpha-phenylbenzeneacetamide;Oletimol;AC1L9QXK;4-[1-(4-Methoxyphenyl)prop-1-en-2-yl]pyridine;4-{2-[4-(Methylamino)phenyl]ethenyl}phenol;1-[3-(Aminomethyl)phenyl]-2-phenylethan-1-one;1-Phenyl-5,6,7,8-tetrahydroquinolin-2(1H)-one;Methanone, [4-(dimethylamino)phenyl]phenyl;-o-Acetotoluidide, 4'-phenyl-	0.00001	0.00010	-2.36	0.02189	0.23490	-1.83	0.00195	0.03834	-2.41	0.00747	0.15508	-1.75
832.5781	8.7	PC(40:7)	0.00002	0.00036	-2.33	0.00262	0.05755	-3.68	0.02753	0.24486	-2.11	0.05124	0.43824	-2.44
782.5697	8.1	PC(36:4);PC(72:8);PE(39:4)	0.00268	0.01748	-2.31	0.36809	1.00000	-1.97	0.10272	0.58555	-2.46	0.05155	0.43824	-2.27
794.5696	10.0	PC(37:5); PE(40:5)	0.00003	0.00042	-2.29	0.04609	0.40065	-1.99	0.05489	0.39335	-2.65	0.00153	0.05556	-1.71
624.6282	11.8	Cer(d18:0/22:0);Cer(d20:0/20:0)	0.00070	0.00559	-2.29	0.09182	0.62249	-3.01	0.01026	0.11847	-2.37	0.37401	1.00000	-1.78
650.6437	12.0	N-Lignoceroylsphingosine; Cer(d18:1/24:0)	0.00002	0.00026	-2.29	0.00129	0.03594	-3.07	0.01679	0.17212	-2.75	0.07967	0.55357	-1.93
781.6186	10.3	SM(40:3)	0.00049	0.00410	-2.27	0.04145	0.37309	-2.35	0.05310	0.38615	-2.17	0.12855	0.74209	-2.68
683.5640	8.7	LDG(40:6); LDG(42:6); LDG(41:6)	0.00826	0.04531	-2.26	0.41364	1.00000	-2.64	0.74682	1.00000	-1.72	0.00729	0.15383	-4.17
667.5922	11.1	Glycerol 1,2-didodecanoate 3-tetradecanoate; TG(12:0/12:0/14:0)[iso3]; TG(76:0); Glyceryl 2-acetate distearate	0.00000	0.00003	-2.26	0.00050	0.02234	-2.42	0.06726	0.45627	-1.68	0.00061	0.03051	-2.96
530.4034	0.6	Rocuronium	0.00143	0.01026	-2.26	0.97265	1.00000	-1.49	0.02801	0.24819	-2.80	0.00531	0.12272	-6.61
593.5130	10.6	LDG(34:2); cis-Uvariamicin IB; Reticulatain 2; cis-Uvariamicin IV; Neoreticulatain A; LDG(33:2); LDG(35:2)	0.00004	0.00051	-2.25	0.05870	0.46433	-2.91	0.00293	0.04819	-4.58	0.05616	0.45368	-2.42
415.1926	1.2	Octadecanoic acid trichloroethyl ester; SU 11652; AGN-PC-OLONAA; Acridine, 9,9'-ethylenediiminobis-	0.01002	0.05328	-2.23	0.00988	0.13211	-3.06	0.36552	1.00000	-2.43	0.83758	1.00000	-1.82
806.5695	7.7	Lactosylceramide (d18:1/12:0);PC(38:6);PE(41:6); LacCer(d14:1/16:0);	0.00304	0.01931	-2.19	0.99414	1.00000	-1.06	0.01119	0.12543	-3.25	0.03121	0.32280	-4.13
531.4062	0.6	alpha-Tocopherol succinate, VITAMIN E SUCCINATE(TOCOPHEROL SUCCINATE); d-alpha-Tocopheryll succinate; NSC375717	0.00363	0.02252	-2.17	0.94415	1.00000	-1.68	0.09129	0.53861	-3.19	0.00778	0.15879	-5.60
496.3398	8.8	LPC(32:0);PC(O-16:0);LPC(16:0);LPE(19:0);Cytosine, 1-beta-D-arabinofuranosyl-N(sup 4)-margaroyl-	0.00067	0.00530	-2.13	0.14583	0.86099	-1.43	0.01737	0.17488	-2.51	0.15721	0.83788	-2.02
603.5350	8.8	1-(14-methyl-pentadecanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerol, 1-Hexadecyl-2-arachidonoyl-glycerol	0.00003	0.00038	-2.09	0.15741	0.90598	-1.86	0.00039	0.01295	-4.33	0.05157	0.43824	-1.49

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499.1159	0.7	N,N'-Bis(gamma-glutamyl)cystine; Bis-gamma-glutamylcystine; Bis- β -glutamylcystine; Triphenylead acetate; 2-Bromo-6beta-fluoro-11alpha,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-acetate	0.00000	0.00009	-2.09	0.11332	0.73178	-1.25	0.04268	0.33850	-1.64	0.00003	0.00388	-2.35
526.2941	1.0	LPE(22:6)	0.00530	0.03114	-2.09	0.00216	0.05245	-3.05	0.62602	1.00000	-2.13	0.65574	1.00000	-1.40
280.0928	0.6	Thieno(3,2-c)pyridine, 4,5,6,7-tetrahydro-5-(2-phenylethyl)-, monohydrochloride; 1,3,4-Oxadiazole-2-methanol, 5-(3,4-dimethoxyphenyl)-, carbamate (ester)	0.00007	0.00074	-2.07	0.04743	0.40758	-2.50	0.03621	0.30432	-1.47	0.00874	0.16691	-2.14
839.7478	12.6	TG(52:5)	0.00000	0.00000	-2.07	0.00014	0.01172	-2.70	0.00006	0.00481	-2.92	0.07169	0.51791	-1.58
769.4984	7.8	PG(36:5)	0.00018	0.00180	-2.06	0.29567	1.00000	-1.93	0.00806	0.09851	-2.40	0.02368	0.28303	-2.12
645.4859	12.4	PA(O-33:2); PA(P-33:1)	0.00126	0.00923	-2.06	0.51392	1.00000	-1.61	0.00046	0.01413	-3.42	0.74373	1.00000	-1.68
660.5039	11.2	Acidissiminin	0.00000	0.00009	-2.06	0.12951	0.80673	-1.80	0.00053	0.01525	-3.55	0.01820	0.24765	-2.64
535.3781	12.3	Pyrohyferforin; Piloplex; Decanoic acid, 2-(4-(1-oxododecyl)-1-piperazinylolethyl ester, monomethanesulfonate	0.00023	0.00215	-2.05	0.40000	1.00000	-1.77	0.00038	0.01295	-4.61	0.35671	1.00000	-1.92
98.9846	0.6	Phosphoric acid	0.00173	0.01195	-2.04	0.63352	1.00000	-1.62	0.17969	0.83830	-2.22	0.00404	0.10264	-2.51
859.5290	8.5	PI(36:4)	0.00371	0.02280	-2.04	0.44871	1.00000	-1.31	0.09355	0.54778	-3.11	0.07541	0.53438	-1.65
184.0741	11.6	4-Nitrosobiphenyl; Phosphocholine; 3-Dibenzofuranamine; 4-Hydroxycarbazole; 4-Benzoylpyridine; 2-Aminodiphenylene oxide; 6-Methoxy-2-naphthonitrile; 5-(Furan-3-yl)-1H-indole; 1-Hydroxycarbazole; Methanone, phenyl-2-pyridinyl; 2-Propenal, 3-(2-quinolinyl)-	0.00245	0.01618	-2.04	0.00851	0.11904	-2.06	0.17104	0.81288	-2.41	0.62536	1.00000	-1.73
885.5456	8.7	PI(38:5)	0.00153	0.01077	-2.04	0.13976	0.83811	-2.22	0.01231	0.13535	-3.92	0.47115	1.00000	-1.42
834.6005	9.5	PC(40:6); PE(43:6); LacCer(d18:1/14:0)	0.00008	0.00085	-2.03	0.00619	0.09690	-3.90	0.12439	0.65070	-1.83	0.02366	0.28303	-1.61
761.6425	10.3	PA(O-41:0)	0.01069	0.05669	-2.03	0.27340	1.00000	-1.55	0.23000	0.97729	-2.46	0.20723	0.96171	-2.99
889.7275	12.5	TG(55:8); TG(110:16); Sodium L-throxine pentahydrate	0.00002	0.00029	-2.03	0.00053	0.02265	-3.89	0.11775	0.62745	-2.10	0.03047	0.31960	-1.49
182.0592	12.3	L-2-Amino-4-(hydroxymethylphosphinyl)butanoate; Glufosinate;Phosphinothricin;(Morpholin-4-yl)acetic acid--hydrogen chloride (1/1);2-chloro-N,N-bis(2-hydroxyethyl)acetamide;9H-Indeno(2,1-b)pyridin-9-one;Methyl aminolevulinate hydrochloride;Methyl (3R)-3-hydroxy-L-prolinate--hydrogen chloride (1/1);4-Hydroxypiperidine-4-carboxylic acid--hydrogen chloride (1/1)	0.00050	0.00416	-2.03	0.13981	0.83811	-1.88	0.00055	0.01526	-2.83	0.77712	1.00000	-1.62
561.4875	12.5	TG(102:8); TG(51:4)	0.00001	0.00012	-2.02	0.00007	0.00684	-2.73	0.01753	0.17579	-2.10	0.22477	0.98154	-1.48
782.5694	7.9	PC(36:4); PC(72:8); PE(39:4)	0.00000	0.00004	-2.02	0.03006	0.29876	-1.73	0.00008	0.00590	-2.96	0.01941	0.25155	-1.25
857.7583	12.6	TG(104:6); TG(52:3); 1-Palmitoyl-2-oleoyl-3-linoleoyl-rac-glycerol	0.00000	0.00002	-2.00	0.00120	0.03529	-2.63	0.00013	0.00712	-3.83	0.12099	0.72447	-1.51
616.6017	11.5	Bromopentakis(bromomethyl)benzene; Cer(m18:1(4E)/24:1(15Z))	0.00053	0.00431	-2.00	0.57458	1.00000	-1.45	0.00480	0.06858	-6.93	0.09661	0.62745	-1.71
879.7415	12.4	TG(108:12); TG(54:6); Trilinolein C18:2	0.00049	0.00408	-1.93	0.04115	0.37180	-3.50	0.00550	0.07527	-7.54	0.59062	1.00000	-1.37
716.5228	9.1	PE(34:2); PC(31:2); 1-Palmitoyl-2-linoleoyl PE	0.00760	0.04309	-1.93	0.42745	1.00000	-2.13	0.24799	1.00000	-2.21	0.06329	0.48368	-1.87
772.5851	9.2	PC(35:2); PE(38:2)	0.00618	0.03587	-1.92	0.95105	1.00000	-1.23	0.05812	0.40508	-3.51	0.02961	0.31938	-2.03
631.5818	11.5	Solanisol	0.00032	0.00289	-1.92	0.18612	1.00000	-1.70	0.02004	0.19559	-2.18	0.03390	0.33203	-1.47
339.2895	10.6	Glycidyl oleate, 4-(4,8-Dimethylnonyl)-2,6-dimethyl-1-phenylpyridin-1-ium	0.00372	0.02281	-1.91	0.37551	1.00000	-1.85	0.05656	0.40033	-3.68	0.15606	0.83546	-2.41
575.5036	9.1	Montecristin; Mayolene-19; Ethylenebis(diocetylphosphine) dioxide	0.00534	0.03129	-1.91	0.42639	1.00000	-2.25	0.24612	1.00000	-2.33	0.05812	0.46454	-1.86
306.2796	10.0	Clavepictine B	0.01516	0.07648	-1.91	0.54212	1.00000	-1.30	0.40705	1.00000	-1.58	0.05367	0.44274	-2.00
865.7251	12.6	TG(106:12); TG(53:6)	0.00008	0.00085	-1.90	0.01323	0.16407	-2.41	0.01073	0.12271	-2.95	0.15745	0.83788	-1.40
573.4879	12.5	Dieporeticenin	0.00015	0.00147	-1.89	0.00780	0.11210	-2.69	0.01385	0.14937	-2.81	0.34254	1.00000	-1.38
772.5853	9.4	PC(35:2);PE(38:2);PE(72:4);PE(36:2)	0.00002	0.00025	-1.88	0.06950	0.51287	-2.45	0.00107	0.02532	-3.66	0.03161	0.32513	-1.70
818.5692	9.2	PE(42:7); PC(39:7)	0.00009	0.00102	-1.88	0.18598	1.00000	-1.10	0.00776	0.09588	-2.39	0.01659	0.23696	-2.29
264.2688	12.0	(2S,5R)-5-(hex-5-en-1-yl)-2-propyldecahydroquinoline;1-methyl-4-(oct-7-en-1-yl)octahydro-2H-quinolizine;7-ethyl-3,5-dipropyldecahydropropyrolo[2,1,5-cd]indolizine;9-Octadecenenitrile, (9Z)-	0.00005	0.00056	-1.87	0.00431	0.07872	-2.32	0.06913	0.45805	-2.09	0.03032	0.31960	-1.89
844.7386	12.4	SM(44:1)	0.00034	0.00301	-1.83	0.01670	0.19091	-3.22	0.01091	0.12348	-2.29	0.51072	1.00000	-1.56
759.6374	10.3	SM(38:1)	0.00678	0.03892	-1.83	0.18632	1.00000	-1.41	0.21307	0.93154	-1.90	0.19232	0.92362	-2.02
587.5033	12.6	Erythrasinate A	0.00023	0.00218	-1.81	0.00331	0.06641	-3.29	0.05002	0.37009	-2.69	0.36500	1.00000	-1.28
123.0560	0.6	2-Acetylpyrazine;Picolinamide;Isonicotineamide;Isonicotinamide;(Ethylphosphanediyl)dimethanol;Benzenediazonium hydroxide;6-Aminopyridine-3-carbaldehyde;1-(Pyridazin-3-yl)ethanone;Acetylpyrazine;Propanedinitrile, (ethoxymethylene)-;1-Chloro-3-ethoxypropane	0.00803	0.04466	-1.78	0.95332	1.00000	-1.07	0.36987	1.00000	-1.09	0.00015	0.01054	-2.71
788.5202	9.4	PE(40:8); N-Acetyl-leu-leu-leu-leu-tyr-amide	0.00780	0.04400	-1.75	0.43489	1.00000	-2.03	0.61715	1.00000	-1.54	0.01098	0.18461	-4.45
756.5537	7.8	PC(36:3); PC(72:6); PE(39:3)	0.00005	0.00056	-1.69	0.32556	1.00000	-1.53	0.00228	0.04204	-2.91	0.00853	0.16580	-1.55
836.6161	9.7	PC(40:5); LacCer(d18:0/14:0)	0.00001	0.00017	-1.69	0.00113	0.03440	-2.28	0.04636	0.35206	-1.46	0.01474	0.21793	-2.23
815.7002	11.6	SM(42:1)	0.00012	0.00122	-1.67	0.00059	0.02350	-2.17	0.07667	0.48751	-1.91	0.32415	1.00000	-1.41

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838.5568	8.9	PS(40:5)	0.00224	0.01504	-1.66	0.24405	1.00000	-1.86	0.11299	0.61793	-2.41	0.06805	0.50340	1.20
575.5033	7.8	Montecristin; Mayolene-19; Ethylenebis(dioctylphosphine) dioxide	0.00825	0.04531	-1.66	0.42915	1.00000	-1.82	0.08434	0.51539	-3.77	0.23892	1.00000	-1.55
782.5703	8.6	PC(36:4); PC(72:8); PE(39:4)	0.00125	0.00917	-1.66	0.11114	0.72380	-1.12	0.08799	0.52933	-1.70	0.10054	0.64743	-1.23
787.6686	11.0	SM(40:1)	0.00312	0.01971	-1.64	0.06955	0.51287	-1.71	0.17963	0.83830	-1.83	0.22601	0.98225	-1.61
760.4874	9.1	PE(38:8)	0.00408	0.02478	-1.63	0.22369	1.00000	-1.49	0.12088	0.63882	-1.87	0.22778	0.98270	-1.82
219.1422	0.6	(S)-3-Mercaptohexyl pentanoate;(S)-3-Methylthiohexyl butyrate; Ethyl (heptylthio)acetate	0.05873	0.23472	-1.63	0.00314	0.06407	-4.65	0.99438	1.00000	-1.08	0.92710	1.00000	-1.13
810.5212	9.4	PS(38:5);PE(0:0)	0.00714	0.04088	-1.59	0.79917	1.00000	-1.10	0.17929	0.83830	-2.19	0.02217	0.27397	-1.57
829.7268	12.5	TG(100:6); TG(50:3); 15-Oleoylsolamin	0.00400	0.02445	-1.59	0.04817	0.41238	-2.32	0.07982	0.49953	-2.22	0.63524	1.00000	-1.37
1004.6282	9.7	MIPC(t18:0/18:0(2OH))	0.00962	0.05148	-1.57	0.04105	0.37180	1.08	0.64647	1.00000	-1.50	0.22491	0.98154	-1.69
186.0443	0.6	Dextrosil	0.00000	0.00001	4.41	0.00046	0.03377	5.04	0.00554	0.06587	3.18	0.00010	0.00770	5.83
830.5910	9.7	PS(39:1)	0.00004	0.00036	3.91	0.00285	0.07405	5.26	0.04084	0.25688	4.57	0.07016	0.32716	2.62
187.0411	0.6	Isoplumbagin;1-Hydroxy-2-naphthoate;Ramentaceone;F-Honauin A;4-(Furan-2-yl)-2-hydroxybenzaldehyde;1,4-Naphthalenedione, 2-(hydroxymethyl)-;Phenyl 2-furoate;2-acetyl-3-hydroxy-1H-inden-1-one;(1-Oxo-1,3-dihydro-2H-inden-2-ylidene)acetic acid;(Oxan-4-yl)hydrazine--hydrogen chloride (1/1);Pyridinium, 4-(methoxycarbonyl)-1-methyl-;2-Butylisouronium chloride	0.00000	0.00000	3.51	0.00016	0.01562	4.24	0.00557	0.06587	2.65	0.00010	0.00770	4.44
772.5853	10.4	PC(35:1);PE(38:1)	0.00000	0.00007	3.37	0.01165	0.15700	2.76	0.00043	0.01907	3.87	0.07038	0.32716	3.47
770.5696	9.7	PC(35:2);PE(38:2);PE(72:4);PE(36:2)	0.00020	0.00145	3.33	0.00582	0.10150	4.14	0.10404	0.43448	5.01	0.11650	0.47053	2.50
511.2136	0.8	gibberellin A2 O-beta-D-glucoside;Raucaffricine;4-[(2H-1,3-Benzodioxol-5-yl)methyl]piperazin-1-yl}[1-(2,4-dimethylphenyl)-3-(4-fluorophenyl)-1H-pyrazol-5-yl]methanone	0.00000	0.00000	3.21	0.00001	0.00302	4.35	0.00015	0.01441	3.81	0.00308	0.06280	1.79
236.0162	0.6	9-Oxo-9H-thioxanthene-3-carbonitrile;[2-(Methylsulfonyl)-5-(trifluoromethyl)pyridin-3-yl]boronic acid;Butanoic acid, 4,4,4-trinitro-, methyl ester (9CI)	0.02207	0.08077	2.92	0.15067	0.72969	2.44	0.09182	0.41977	4.05	0.95766	1.00000	-1.29
832.6069	10.4	PS(39:0); Sulfobromophthalein	0.00001	0.00009	2.76	0.01411	0.16401	2.37	0.00066	0.02246	3.80	0.05732	0.29445	2.95
390.9777	0.5	4,4'-Sulfonylbis(tetrafluoroaniline);(4-Iodoacetanilido)iminodiacetic acid	0.00012	0.00089	2.70	0.02348	0.22297	2.47	0.04351	0.25688	3.23	0.04431	0.26761	3.81
751.5312	8.3	PA(40:4)	0.00000	0.00004	2.69	0.00004	0.01042	5.94	0.01869	0.15874	3.22	0.06290	0.31344	1.85
281.2476	2.8	Oleic acid; Elaidic acid; Octadec-9-enoic Acid;Vaccenic acid; trans-vaccenic acid;Ethyl 9-hexadecenoate; ethyl 9Z-hexadecenoate;2-methyl-16-heptadecenoic acid;17:1(12)(7Me);3-octadecylenic acid; ;18:1(14E); ;17:1(4)(15Me);11-Cycloheptylundecanoic acid;11E-Hexadecenyl acetate; ;Methyl 14-methyl-8E-hexadecenoate; Methyl 14-methyl-8Z-hexadecenoate;18-Octadecanolide;Petroselinic acid;Palmitoleic Acid ethyl ester;formyl 14-methyl-8E-hexadecenoate;(13R)-13-Hexyl-1-oxacyclotridecan-2-one;2-Propenoic acid, 2-methyl-, tetradecyl ester;(Z)-11-Hexadecenyl acetate;Cyclohexyl laurate;Hexadecanoic acid, ethenyl ester	0.00466	0.02234	2.37	0.16188	0.76796	1.90	0.18362	0.60416	2.22	0.17188	0.60745	2.36
483.1946	0.8	ethyl 4-[[4-(4-methylanilino)-6-[2-(pyridine-4-carbonyl)hydrazinyl]-1,3,5-triazin-2-yl]amino]benzoate;RMI 61,220	0.00000	0.00000	2.26	0.00028	0.02357	2.54	0.00371	0.05235	2.22	0.00001	0.00427	2.18
394.9840	0.5	F0817-0263	0.00043	0.00289	2.25	0.03029	0.24500	2.59	0.11646	0.46042	3.38	0.06873	0.32716	4.00
718.5382	9.5	PC(31:0); PE(34:0); PE(32:0)	0.00077	0.00480	2.20	0.00719	0.11225	2.82	0.24371	0.72624	1.70	0.29491	0.84092	1.75
203.0127	0.6	CCCP; aluminum acetate; Honauin A; 3,5-Diamino-4-hydroxybenzene-1-sulfonic acid; [hydroxy-(4-hydroxyphenyl)methyl]phosphonic acid;Buta-1,3-diene-1,1,2,3,4,4-hexacarbonitrile;Carbonyl cyanide chlorophenylhydrazone;NSC690029;Allyl pentafluoropropionate;2,2,3,3,3-Pentafluoropropyl acrylate;1,1,3,3,3-Pentafluoropropyl prop-2-enoate	0.00011	0.00084	2.16	0.00015	0.01562	5.85	0.32336	0.89162	2.22	0.19588	0.64755	1.35
115.0194	0.6	Diammonium sulfite	0.00135	0.00781	2.12	0.51135	1.00000	1.55	0.14106	0.50998	1.76	0.00610	0.08413	3.53
714.5069	9.0	PE(34:2);PC(31:2);1-Palmitoyl-2-linoleoyl PE	0.02664	0.09461	2.06	0.12792	0.66543	1.51	0.30847	0.86694	4.15	0.75706	1.00000	1.77

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245.0423	0.6	PE(34:2);PC(31:2);1-Palmitoyl-2-linoleoyl PE;Glycerophosphoglycerol;Phosphatidyl glycerol;2-Deoxyglucose-1-phosphate;Phosphorothioic acid, O,O-diethyl O-phenyl ester;Butanedioic acid, tetrafluoro-, diethyl ester;Ethanedione, bis(4-fluorophenyl)-;Dibenzo[a,h]pyrene;Bicozamycin;3"-Deamino-3"-oxonicotianamine;Dibenzo[a,h]pyrene;Dibenzo[a,e]fluoranthene;Naphtho[1,2-b]fluoranthene;Naphtho[2,3-e]pyrene;Diphenylphosphine Acid;Thiopyrophosphoramidate, octamethyl-;NSC404668;Bicyclomycin;N-Allyl-7,8-dimethoxy-4,5-dihydronaphtho(1,2-d)[1,3]thiazol-2-amine;5-Amino-4-(ethylcarbonyl)-3'-fluoro[1,1'-biphenyl]-3-carboxylic acid;Dibenzo(a,e)pyrene	0.01030	0.04243	2.03	0.01267	0.15988	4.75	0.17117	0.58063	2.15	0.98622	1.00000	1.39
135.0299	0.6	Hypoxanthine, Erythronic acid; Threonic acid; L-threonic Acid, 1-Pentanesulfenothioic acid, Ethyl propyl disulfide, Threonate, D-threonic acid, DL-erythronic acid, tetrazolo[1,5-a]pyridin-8-ol, [1,2,4]Triazolo[4,3-c]pyrimidin-5(1H)-one, 4H-Pyrazolo[3,4-b]pyrazin-4-ol	0.01060	0.04336	1.97	0.01038	0.14321	3.34	0.15320	0.54342	1.93	0.99807	1.00000	1.25
399.2551	1.4	11'-Carboxy-gamma-tocotrienol;Colupulone;Ophiobolin A;16alpha,17-Isopropylidenedioxy-6alpha-methylprogesterone	0.00033	0.00228	1.94	0.29391	1.00000	2.05	0.16506	0.56578	-1.18	0.00133	0.04566	2.45
775.5479	9.7	PG(36:1);1-Stearoyl-2-Oleoyl-sn-Glycero-3-[Phospho-rac-(1-glycerol)]; CHAULMOSULFONE	0.00485	0.02280	1.84	0.02008	0.21263	4.31	0.04972	0.28907	1.88	0.97948	1.00000	1.34
173.0073	0.6	Phenylmethanesulfonyl fluoride, Perchloric acid--carbonohydrazonic diamide (1/1), Benzenemethanesulfonyl fluoride, Benzenesulfonyl fluoride, 4-methyl-	0.00467	0.02234	1.74	0.04217	0.30873	2.05	0.11026	0.45094	1.86	0.66502	1.00000	1.03
279.0306	0.6	Furo[2,3-b]quinoxaline, 3-chloro-2-phenyl-	0.00097	0.00580	1.60	0.00205	0.06075	1.73	0.66635	1.00000	1.76	0.12647	0.49999	1.41
331.0834	0.6	Sanguinarine;2',3,5-Trihydroxy-5',7-dimethoxyflavanone;3'-Deoxydryopteracid;Parvisoflavanone;Dihydrotricetin;7,3'-dimethyl ether;Dioclein;5,7,4'-Trihydroxy-8,3'-dimethoxyflavanone;Sulochrin;3-(Tris(acetoxy)silyl)propyl methacrylate;Evernic acid;5-Chloro-2-hydroxy-N-[4-(morpholin-4-yl)phenyl]benzamide;Sodium 1,4-diisobutyl sulfosuccinate	0.00036	0.00242	1.59	0.53911	1.00000	1.23	0.04081	0.25688	1.78	0.00687	0.08665	1.72
913.5800	9.4	PI(40:4); PI(40:3)	0.03642	0.12273	1.56	0.00150	0.04939	4.20	0.37326	0.98374	-1.04	0.81288	1.00000	-1.28
157.0301	0.6	1,4-Naphthoquinone;2-Methylidene-1H-indene-1,3(2H)-dione;Piperazine dihydrochloride;4-Chloro-2-hydrazinyl-6-methylpyrimidine;Guanidinoproclavaminc acid;1-Benzyl-3-(trifluoromethyl)piperazine	0.00897	0.03771	1.47	0.14773	0.72398	1.71	0.36701	0.97159	1.34	0.24044	0.73496	1.47
427.2861	1.9	Schidigeragenin B;Spirostane-3,6-dione;25-Hydroxyvitamin D3-26,23-lactone;(23S,25R)-25-hydroxycholecalciferol 26,23-lactone;15,20-dihydroxycholest-4,14-dien-3,16-dione;17(20)-Dehydrocryptogenin ;delta5-Convallamarogenin;1,25-Dihydroxy-24-oxo-16-ene-vitamin D3;12-epi-Scalaradial;(22E)-(24S,25S)-25,26-epoxy-11z,24-dihydroxy-22,23-didehydrovitamin D3 / (22E)-(24S,25S)-25,26-epoxy-11z,24-dihydroxy-22,23-didehydrocholecalciferol;Homostypolhydroperoxide;cholest-4,14-dien-15,20-diol-3,16-dione	0.00014	0.00104	1.46	0.01304	0.16108	1.69	0.02825	0.21477	1.79	0.14292	0.53983	1.19
769.6210	10.4	SM(39:2)	0.01715	0.06478	1.46	0.32871	1.00000	1.70	0.01874	0.15874	3.55	0.96141	1.00000	1.26
455.3172	2.8	Norselic acid B;(25R)-12alpha-hydroxy-24R,26R-dimethyl-26,27-cyclo-cholest-4-en-3,6-dione;(22S)-1alpha,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydrovitamin D3 / (22S)-1alpha,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydrocholecalciferol; (22R)-1alpha,22,25-trihydroxy-23,24-tetradehydro-24a,24b-dihomo-20-epivitamin D3 / (22R)-1alpha,22,25-trihydroxy-23,24-tetradehydro-24a,24b-dihomo-20-epicholecalciferol;1alpha-hydroxy-18-(5-hydroxy-5-methyl-2-hexynyl)-23,24,25,26,27-pentanolvitamin D3 / 1alpha-hydroxy-18-(5-hydroxy-5-methyl-2-hexynyl)-23,24,25,26,27-pentanolcholecalciferol;Callystatin A;(22S)-11z,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydrovitamin D3 / (22S)-11z,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetradehydrocholecalciferol;Dequalinium	0.00324	0.01643	1.28	0.00301	0.07442	1.86	0.59528	1.00000	1.24	0.44887	1.00000	1.14
485.3073	7.5	Trihexyl 2-(acetyloxy)propane-1,2,3-tricarboxylate	0.01903	0.07143	-1.00	0.97534	1.00000	1.01	0.05673	0.31147	-1.06	0.01609	0.15385	-1.21
802.6368	8.8	PC(37:0); PE(40:0)	0.00439	0.02135	-1.03	0.88410	1.00000	-1.20	0.00721	0.07912	91.15	0.18611	0.62809	1.02
355.1756	0.6	Xanthoplanine;Pibutidine;1alpha,5alpha-Dimercaptoandrostane-3alpha,17beta-diol;5H-Pyridazino(3,4-b)(1,4)benzoxazine, 7-acetyl-2-(2-(diethylamino)ethoxy)-	0.00544	0.02539	-1.09	0.00084	0.04128	-1.92	0.48795	1.00000	-1.10	0.96186	1.00000	-1.17

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834.5257	9.9	PS(40:6)	0.00697	0.03039	-1.20	0.21171	0.91640	-1.30	0.64169	1.00000	-1.11	0.02659	0.20478	-1.23
187.1078	0.6	N6-Acetyl-L-lysine;N-Alpha-acetyllysine; ;Glycyl-L-leucine;Alanyl-Valine;Isoleucyl-Glycine;Leucyl-Glycine;Valyl-Alanine;6-Acetamido-3-aminohexanoate;N μ -Acetyl-L-lysine;Nitrosoamylurethane;N-Butyl-N-(2-carboxyethyl)nitrosamine;Pentanamide, N-((hydroxyamino)carbonyl)-2,2-dimethyl-;5-Oxo-L-proline, compound with trimethylamine (1:1);4-(2-Nitrobutyl)morpholine;Carbamic acid, N-(4-morpholinomethyl)-, ethyl ester;Hydrazinecarboxylic acid, (1-ethoxypropylidene)-, ethyl ester;Butanoic acid, 4-((1,1-dimethylethyl)nitrosoamino)-	0.50687	0.91083	-1.23	0.52432	1.00000	1.34	0.99056	1.00000	-1.06	0.00433	0.06692	-2.84
277.0729	0.6	Isophthalic diglycidyl ester; 4-(3,4-Dimethoxybenzoyl)-3-methoxyfuran-2(5H)-one	0.02414	0.08676	-1.32	0.24747	0.96512	-1.26	0.12808	0.48338	-1.83	0.75611	1.00000	-1.22
397.2254	0.9	tert-Butyl (2S,4S)-2-{4-[2-(azetidin-1-yl)-2-oxoethyl]piperazine-1-carbonyl}-4-fluoropyrrolidine-1-carboxylate; Lapyrium chloride; Carbanilic acid, m-butoxy-N-propyl-, 2-piperidinoethyl ester, hydrochloride	0.02709	0.09563	-1.36	0.19173	0.85007	-1.72	0.84600	1.00000	-1.18	0.12930	0.50736	-1.50
885.5501	8.6	PI(38:4);Glc-GP(18:0/20:4(5Z,8Z,11Z,14Z))	0.01555	0.05948	-1.41	0.92527	1.00000	-1.26	0.58440	1.00000	-1.21	0.00354	0.06280	-1.72
742.5392	10.0	PC(33:2); 1,2-Dioleoyl phosphatidyl ethanolamine	0.02838	0.09841	-1.46	0.73613	1.00000	-1.10	0.44402	1.00000	-1.61	0.06043	0.30521	-1.33
766.5394	9.9	PC(35:4);PE(38:4);PE(36:4);PE(76:8);PE(P-38:4)	0.02770	0.09720	-1.46	0.87379	1.00000	1.07	0.45001	1.00000	-1.57	0.02924	0.21404	-1.74
464.3009	0.7	Glycocholic acid; 3a,7b,12a-Trihydroxyoxocholanyl-Glycine; Sodium glycocholate; Glycocholic Acid; N-[4-(Morpholin-4-yl)-2-[2-(morpholin-4-yl)ethyl]-2-(naphthalen-1-yl)butyl]-4,5-dihydro-1H-imidazol-2-amine	0.00001	0.00018	-21.45	0.03772	0.28678	-23.48	0.00045	0.01907	-115.29	0.10245	0.43086	-6.11
514.2835	0.6	Taurocholic acid; Tauroursocolic acid; Taurallocholic acid; Taurocholate; Tauro-b-muricholic acid; Taurohydrocholate; Taurohydrocholic acid;Candoxatril;Atracurium (Quaternary alcohol);2,4-D, dimethylethylamine salt	0.00187	0.01019	-11.45	0.23853	0.95802	-4.70	0.00780	0.08415	-40.29	0.50386	1.00000	-7.61
448.3059	0.7	Chenodeoxycholic acid glycine conjugate; Glycoursodeoxycholic acid; Chenodeoxyglycocholic acid; Chenodeoxyglycocholate;Glycochenodeoxycholic acid;Glycodeoxycholate;N-(3 β ,12 β -dihydroxy-5 β -cholan-24-oyl)-glycine	0.00008	0.00066	-9.59	0.30006	1.00000	-2.74	0.00189	0.03289	-57.34	0.02839	0.21314	-18.32
769.5014	5.1	PG(36:4)	0.00000	0.00000	-9.46	0.00148	0.04939	-6.21	0.00003	0.00850	-10.82	0.00001	0.00427	-10.06
215.0310	0.6	2-C-Methyl-D-erythritol 4-phosphate; 2,4-Difluoro-9H-fluoren-9-one; 4,4,4-Trifluoro-1-phenyl-1,3-butanedione;	0.00094	0.00577	-8.80	0.05430	0.37035	-6.59	0.39566	1.00000	-2.63	0.01831	0.16965	-15.95
561.3787	2.8	Cholesterol glucuronide; Rhodoxanthin	0.00347	0.01745	-8.00	0.18430	0.84071	-7.73	0.04327	0.25688	-6.40	0.38760	0.98467	-6.04
771.5172	6.9	PG(36:3)	0.00000	0.00000	-7.65	0.00148	0.04939	-3.92	0.00035	0.01907	-7.38	0.00006	0.00741	-8.55
850.5600	8.3	PE(0:0); PS(41:5)	0.00000	0.00005	-7.39	0.00394	0.08338	-9.94	0.00337	0.05029	-10.45	0.00792	0.09768	-3.25
806.4967	6.8	PS(38:6)	0.00000	0.00006	-7.31	0.00065	0.04128	-9.36	0.03475	0.23684	-6.23	0.00542	0.07680	-12.31
712.4910	8.2	PE(34:3); PC(31:3)	0.00000	0.00004	-7.29	0.02999	0.24500	-5.86	0.00152	0.02818	-7.29	0.00164	0.04690	-5.65
366.1080	0.6	ethyl 6'-amino-5'-cyano-2,2'-dimethyl-1,3-dioxospiro[isoquinoline-4,4'-pyran]-3'-carboxylate;Chromone-2-carboxylic acid, 7-hydroxy-8-(1-piperidinomethyl)-, ethyl ester, hydrochloride;2-cyano-3-(2,3-dimethoxyphenyl)-N-(4-methyl-2-nitrophenyl)prop-2-enamide;2,4-dinitro-6-[2-(1,3,3-trimethylindol-2-ylidene)ethylidene]cyclohexa-2,4-dien-1-one;2,4,6-Trinitrophenol--3-methyl-1,5,6,7,8,8a-hexahydroimidazo[1,5-a]pyridine (1/1)	0.00000	0.00001	-6.54	0.00513	0.09563	-3.79	0.00133	0.02623	-7.43	0.00091	0.03644	-15.24
367.1048	0.6	3-O-Feruloylquinic acid;3-O-Caffeoyl-4-O-methylquinic acid; ;3-(4-Aminophenyl)-7-(isoquinolin-4-yl)thieno[3,2-c]pyridin-4-amine ;tert-Butyl 4-(((4-bromophenyl)methyl)amino)piperidine-1-carboxylate;Dihydrorhodamine 123;ethyl 6-amino-5-cyano-2,4-diphenyl-4H-pyran-3-carboxylate;Hexananilide, 4'-sulfanyl-;9-(9H-Fluoren-9-yl)-9H-xanthen;spiro[9H-anthracene-10,9'-xanthen];phenyl-(9-phenylfluoren-9-yl)methanone;2-(3-(4-Fluorophenyl)propoxy)-4-phenanthrenol	0.00000	0.00007	-5.68	0.01452	0.16564	-3.70	0.00386	0.05323	-6.20	0.00663	0.08665	-10.68
824.5436	7.7	PS(39:4)	0.00001	0.00010	-5.24	0.00924	0.13371	-6.73	0.02092	0.17227	-6.37	0.00294	0.06231	-5.13
834.5285	8.5	PS(40:6)	0.00001	0.00018	-5.21	0.02999	0.24500	-7.34	0.05576	0.31147	-4.54	0.00068	0.03644	-6.38
140.0107	0.6	O-Phosphoethanolamine; 5-Hydroxymethyl-2-furanoate; (2E,4E)-5-carboxypenta-2,4-dienoate; 1-Hydroxy-2-aminoethylphosphonate; O-Phosphorylethanolamine; 3-nitro-1-oxidopyridazin-1-ium; 2-Hydroxy-5-nitropyrimidine	0.00002	0.00022	-5.14	0.07402	0.46694	-2.41	0.00819	0.08673	-8.78	0.00407	0.06692	-5.44
507.2714	0.9	LPG(18:2); 26,26,26,27,27-hexafluoro-1alpha-hydroxyvitamin D3 / 26,26,26,27,27-hexafluoro-1alpha-hydroxycholecalciferol;2-[[2-[bis(2-hydroxyethyl)amino]-4,8-dimorpholin-4-yl]pyrimido[5,4-d]pyrimidin-6-yl]-[2-hydroxyethyl]amino]ethanol	0.00000	0.00007	-5.12	0.05674	0.37808	-3.83	0.04189	0.25688	-2.85	0.00004	0.00741	-7.94

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468.1281	0.6	BUCLADESINE;2-[4-(6-Amino-5-cyano-3-methyl-2,4-dihydropyranol[2,3-c]pyrazol-4-yl)phenoxy]-N-[2-(trifluoromethyl)phenyl]acetamide	0.00050	0.00326	-5.02	0.24718	0.96512	-1.42	0.01662	0.14708	-3.09	0.06381	0.31534	-3.42
524.2771	1.0	LPE(22:6); Desmosine	0.00000	0.00001	-4.91	0.00091	0.04137	-8.54	0.00548	0.06587	-4.22	0.00086	0.03644	-3.88
762.5079	8.6	PE(38:6);PC(35:6);PE(P-38:6)	0.00007	0.00057	-4.72	0.02279	0.22297	-5.43	0.05638	0.31147	-6.61	0.01520	0.14781	-2.80
861.5495	8.8	PI(36:2)	0.00000	0.00007	-4.67	0.19165	0.85007	-2.33	0.00008	0.01115	-20.46	0.01383	0.14144	-2.43
817.5011	4.4	PG(40:8);Quinquenoside F1;LBPA(20:4(SZ,8Z,11Z,14Z)/20:4(SZ,8Z,11Z,14Z))	0.00005	0.00040	-4.57	0.18367	0.84071	-2.51	0.01189	0.11557	-10.37	0.00355	0.06280	-4.70
788.5433	8.1	PS(36:1)	0.00000	0.00004	-4.57	0.01748	0.18849	-4.97	0.00056	0.02086	-4.69	0.00873	0.09768	-2.78
288.1188	0.6	Ophthalmic acid;Chlophedianol;Tabtoxin;;(S)-3,4,5,6-Tetrahydro-5-methyl-1-phenyl-1H-2,5-benzoxazocine hydrochloride;Propiophenone, 3-(benzylmethylamino)-, hydrochloride;4-allyl-5-[1-(3,4-dimethylphenoxy)ethyl]-4H-1,2,4-triazole-3-thiol;Nefopam hydrochloride;Butamisolol	0.00026	0.00183	-4.56	0.33712	1.00000	-1.85	0.12346	0.47233	-3.45	0.00104	0.03860	-6.50
283.0672	0.6	Xanthosine;Mazindol;2(1H)-Quinolinone, 3-amino-6-chloro-1-methyl-4-phenyl-;N-[[Furan-2-yl)methyl]-N'-quinazolin-6-ylthiourea;Ethanol, 2,2'-((7-nitro-4-benzofurazanyl)imino)bis-, oxide;Nolatrexed;2-Chloro-5-nitro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine;Dibenz(b,f)imidazo(1,2-d)(1,4)oxazepine, 3-methyl-, hydrochloride;4-Chloro-2-(4-methoxyphenyl)-5-methylquinazoline;Dihydrosterigmatocystin;Atroviridin;O-Demethylforbexanthone;Demethoxykanugin;Cuneatin methyl ether;Fujikinetin methyl ether;3',4'-Dimethoxy-6,7-methylenedioxyisoflavone;Maximaisoflavone D;Derrustone;Tlatlancauyin;Irisolone methyl ether;Boeravinone A;5,7-Dimethoxy-3',4'-methylenedioxy-4-phenylcoumarin;Millettocalyxin A;Milletenin C;7,8-Dimethoxy-3',4'-methylenedioxyflavone;Jacareubin;Ophiopogonone A;NSC345136;Ethyl 3'-hydroxy-5'-(trifluoromethoxy)[1,1'-biphenyl]-4-carboxylate;2',4'-Dimethoxy-5-(trifluoromethyl)[1,1'-biphenyl]-3-carboxylic acid;7,9-Dimethoxy-6-phenyl-[1,3]dioxolo[4,5-g]chromen-8-one;2(1H)-Pyrimidinethione, 3,4-dihydro-1-(4-methyl-2-sulfonyl)-4,4,6-trimethyl-	0.00003	0.00030	-4.11	0.32362	1.00000	-3.18	0.00360	0.05202	-4.41	0.00237	0.05550	-4.07
273.0372	0.6	1-Deoxy-D-alto-heptulose 7-phosphate; O,O-diethyl S-[2-(ethylsulfanyl)-ethyl]phosphorothioate	0.00000	0.00001	-4.03	0.00698	0.11191	-2.56	0.00074	0.02246	-7.69	0.00008	0.00770	-6.90
515.2865	0.6	L-Olivosyl-oleandolide	0.00867	0.03697	-4.01	0.31552	1.00000	-2.72	0.00992	0.09968	-10.47	0.90885	1.00000	-3.42
764.5228	9.2	PC(35:5);PE(38:5);PE(P-38:5)	0.00001	0.00018	-3.99	0.12757	0.66543	-2.80	0.00212	0.03487	-5.30	0.00544	0.07680	-3.19
171.0051	0.6	Glycerol 3-phosphate; sn-Glycerol 1-phosphate; DL-Glycerol 1-phosphate;Beta-Glycerophosphoric acid;((2-Chloroethyl)thio)benzene;Butane-1,4-diyl bis(thiocyanate);1-Chloro-4-((methylthio)methyl)benzene;4-Chloro-2,5-dimethylbenzenethiol;sn-Glycerol 3-phosphate;Phosphoric acid, diethyl p-(methylsulfonyl)phenyl ester	0.00000	0.00006	-3.91	0.10341	0.61322	-1.77	0.00083	0.02246	-6.55	0.00173	0.04690	-4.97
776.5234	9.2	PC(36:6);PC(72:12);PE(39:6)	0.00001	0.00013	-3.90	0.00328	0.07791	-4.61	0.00843	0.08770	-5.01	0.03763	0.25652	-1.93
858.5255	9.7	PS(42:8)	0.00000	0.00006	-3.83	0.00376	0.08250	-7.76	0.01304	0.12271	-3.63	0.00355	0.06280	-2.28
816.5746	9.4	PS(38:1)	0.00000	0.00002	-3.52	0.03888	0.29187	-2.18	0.00004	0.00850	-5.30	0.00814	0.09768	-2.45
833.5176	7.3	PI(34:2); PG(42:7)	0.00207	0.01106	-3.48	0.12368	0.66543	-3.76	0.01261	0.12060	-6.26	0.75493	1.00000	-2.09
747.4954	8.5	Azythromycin; PA(40:6); Bis(dodecylthio)diocystannane	0.00003	0.00031	-3.47	0.01730	0.18849	-6.34	0.05262	0.30003	-4.23	0.00674	0.08665	-2.93
788.5249	8.9	PE(40:7); PC(37:7)	0.00000	0.00004	-3.42	0.01249	0.15988	-3.59	0.00104	0.02528	-4.25	0.00440	0.06692	-3.00
830.4942	8.7	PS(40:8)	0.00000	0.00006	-3.30	0.00689	0.11191	-4.21	0.00339	0.05029	-6.14	0.00841	0.09768	-3.06
498.2886	0.6	Tauroursodeoxycholic acid; ;Taurodeoxycholic acid;;5Î²-CHOLANIC ACID-3Î±, 12Î±-DIOL N-(2-SULPHOETHYL)-AMIDE;Taurochenodeoxycholic acid;N-bis[[1-hydroxy-2,2,6,6-tetramethylpiperidin-4-yl)oxy]phosphorylbutan-2-amine	0.02017	0.07475	-3.23	0.69486	1.00000	-2.01	0.04251	0.25688	-11.32	0.50785	1.00000	-1.65
878.5906	9.5	PE(0:0)	0.00011	0.00084	-3.19	0.00887	0.13155	-7.90	0.09554	0.42599	-3.72	0.03881	0.26149	-2.21
773.5327	8.3	PG(36:2);PG(72:4);LBPA(18:1(9Z)/18:1(9Z));PA(O-40:4);PA(P-40:3)	0.00029	0.00199	-3.16	0.22575	0.94275	-1.73	0.18062	0.60386	-4.64	0.00139	0.04566	-8.88
845.6739	11.3	TG(104:16);TG(52:8)	0.00001	0.00018	-3.15	0.04458	0.31849	-1.62	0.00078	0.02246	-5.26	0.05577	0.29445	-2.42
800.5435	7.6	PS(37:2)	0.00098	0.00580	-3.00	0.12479	0.66543	-3.89	0.05583	0.31147	-3.17	0.10923	0.44981	-3.13
859.5277	9.7	PI(36:3)	0.00000	0.00006	-3.00	0.00549	0.09859	-3.90	0.01143	0.11300	-2.66	0.00224	0.05541	-2.60
856.6867	11.7	PE(44:1);PC(41:1)	0.00159	0.00897	-2.94	0.06004	0.39127	-2.08	0.75478	1.00000	-2.84	0.00684	0.08665	-3.06

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214.0477	0.6	Glycerylphosphorylethanolamine;sn-glycero-3-Phosphoethanolamine; ;2-Phenylthiomorpholine-hydrogen chloride (1/1);3,4'-Difluoro[1,1'-biphenyl]-4-carbonitrile;2-Propanethiol, 1-(p-chloroanilino)-2-methyl-;Galactosamine hydrochloride;Glucosamine hydrochloride;NSC632482;D-Glucose, 3-amino-3-deoxy-, hydrochloride;(Carboxylatomethyl)trimethylammonium phosphate;cycloguanil;1H-Pyrrolo(2,3-d)pyrimidine-5-acetic acid, 2,3,4,7-tetrahydro-2,4-dioxo-1,3,6-trimethyl-;Methyl 4-(dimethoxyphosphoryl)piperidine-1-carboxylate;MLS003171529;NSC403094;2-Methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-amine;Methyl 1-(5-nitropyridin-2-yl)-L-prolinate	0.00023	0.00165	-2.91	0.11243	0.64653	-1.91	0.02312	0.18281	-4.59	0.04236	0.26761	-2.94
817.6423	10.7	3-Decaprenyl-4-hydroxybenzoic acid;TG(100:16);TG(50:8);2-decaprenyl-6-methoxy-1,4-benzoquinone	0.00952	0.03977	-2.90	0.41084	1.00000	-1.37	0.09412	0.42284	-3.78	0.27317	0.80882	-1.90
785.6533	11.3	SM(40:1)	0.00001	0.00017	-2.75	0.04291	0.31034	-1.63	0.00030	0.01907	-8.15	0.09717	0.41453	-2.28
790.5396	9.7	PC(37:6);PE(40:6);PE(P-40:6)	0.00003	0.00031	-2.73	0.02369	0.22297	-4.80	0.06328	0.33599	-2.83	0.00342	0.06280	-1.68
346.0544	0.6	2'-Deoxyguanosine 5'-monophosphate;3'-AMP;2-hydroxy-dAMP;7-alpha-D-Ribosyladenine 5'-phosphate;deoxyguanosine 5'-monophosphate (dGMP);2-Hydroxy-dAMP;PUBCHEM_17796798;(1,3-dioxoisindol-2-yl)methyl 4-(difluoromethoxy)benzoate;Pamabrom [USAN:USP];Anthraquinone, 1-amino-4-hydroxy-2-(mercaptophenyl)-;1H-Pyrazole-4-carboxamide, 4,5-dihydro-3,4-bis(4-chlorophenyl)-N-methyl-	0.00100	0.00589	-2.65	0.05909	0.38933	-2.59	0.07575	0.36520	-3.59	0.17217	0.60745	-1.85
509.2874	1.0	LPG(18:1)	0.07299	0.20909	-2.64	0.88367	1.00000	-1.61	0.99858	1.00000	-1.27	0.00432	0.06692	-4.97
818.5692	9.5	PE(42:6);PC(39:6)	0.00003	0.00029	-2.54	0.00417	0.08523	-5.64	0.03094	0.22375	-3.53	0.04117	0.26761	-1.93
805.5037	11.1	N-di-Demethyl roxithromycin; PG(39:7)	0.00000	0.00000	-2.52	0.00009	0.01325	-2.60	0.00044	0.01907	-3.12	0.00006	0.00741	-2.12
229.0097	0.6	D-Ribulose 5-phosphate; Xylulose 5-phosphate; L-Ribulose 5-phosphate; L-Xylulose 5-phosphate; Endothal-disodium; Disodium endothal; 7-Hydroxy-4-trifluoromethylcoumarin; 5,5'-Dithiobis(1-methyltetrazole)	0.00010	0.00079	-2.44	0.00131	0.04939	-2.94	0.11306	0.45300	-1.84	0.13875	0.53084	-2.40
792.5545	10.0	PC(37:5); PE(40:5)	0.00001	0.00008	-2.41	0.02141	0.22274	-2.14	0.01792	0.15632	-2.96	0.00092	0.03644	-1.86
619.2873	0.8	1-Arachidonoylglycerophosphoinositol; PI(20:4(5Z,8Z,11Z,14Z)/0:0);1-Benzyl-2-octadecyl-1H-benzimidazole-6-sulfonic acid	0.00052	0.00337	-2.41	0.50093	1.00000	-1.74	0.06688	0.33900	-1.73	0.00371	0.06280	-3.04
337.0936	0.6	3-O-p-Coumaroylquinic acid; ;alpha-Hydrojuglone 4-O-b-D-glucoside;Hydrojuglone glucoside;1-Caffeoyl-4-deoxyquinic acid;N-(tert-Butoxycarbonyl)-5-chloro-L-tryptophan;Benzhydryl 4-methylbenzenesulfonate;BIS(ETHOXYCARBONYLMETHYL) BENZENE-1,4-DICARBOXYLATE;1,2,4,5-Benzenetetracarboxylic acid, dipropyl ester;4-Methylumbelliferyl-galactopyranoside	0.00000	0.00005	-2.40	0.02614	0.23395	-2.31	0.00150	0.02818	-2.47	0.00254	0.05575	-2.00
880.6061	9.7	PS(43:4)	0.00019	0.00141	-2.39	0.00809	0.12301	-3.04	0.10177	0.43420	-1.76	0.08744	0.38408	-1.82
349.0936	0.6	3-Feruloyl-1,5-quinolactone;6-[2,3-Dihydroxy-1-(hydroxymethyl)propyl]-1,2-dihydro-7-hydroxy-9-methoxy-cyclopenta[c][1]benzopyran-3,4-dione;CAY10648;4-[(1-benzoyl-3-methyl-5-oxo-4H-pyrazol-4-yl)diazenyl]benzoic acid;2,3-diphenyl-5-(trifluoromethyl)quinoxaline;N~1~,N~3~-Bis(2-nitrophenyl)benzene-1,3-diamine	0.00000	0.00001	-2.36	0.00100	0.04237	-2.27	0.00128	0.02623	-1.83	0.00184	0.04734	-3.34
831.4976	8.7	PI(34:3)	0.00000	0.00006	-2.36	0.01246	0.15988	-2.44	0.00611	0.06840	-2.79	0.01927	0.17295	-1.53
911.5642	8.7	PI(40:5)	0.00097	0.00580	-2.36	0.47846	1.00000	-1.49	0.03969	0.25688	-5.50	0.02233	0.17893	-3.30
788.5232	8.8	PE(40:7); PC(37:7)	0.00623	0.02776	-2.36	0.27484	1.00000	-3.43	0.12961	0.48338	-3.66	0.19948	0.64995	-1.16
773.5329	8.2	PG(36:2); PG(72:4); LBPA(18:1(9Z)/18:1(9Z))	0.02999	0.10278	-2.36	0.74202	1.00000	-1.11	0.87972	1.00000	-3.22	0.00861	0.09768	-6.74

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289.0724	0.6	Epicatechin; Catechin; ;3-Hydroxyphloretin;gamma-Pyrufuluran;alpha-Cotonefuran;cis-3 and trans-2-Hexenyl propionate;Marshrin;Fonsecin;Cartorimine;6-Hydroxy-alpha-pyrufuluran;Luteoforol;Robinetinidol; ;Mesquitol;(2R-cis)-2-(2,5-Dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol;(2R,3R)-3,5,7,3',5'-Pentahydroxyflavan;Fisetinidol-4beta-ol; Fisetinidol-4alpha-ol; Epifisetinidol-4alpha-ol; ent-Fisetinidol-4beta-ol; ent-Epifisetinidol-4beta-ol;Oritin-4beta-ol; Epioritin-4alpha-ol; Epioritin-4beta-ol;Nubigenol;3,4,2',4',alpha-Pentahydroxydihydrochalcone;2,8-Dihydroxy-3,4,7-trimethoxydibenzofuran;Ptaeroglycol;Mikanolide;Isolepimericin; Plumericin;Chloroxuron;cis-3,4-Leucopelargonidin;Cianidanol;dimethyl 5,9-dioxo-7,8-dihydro-6H-benzo[7]annulene-6,8-dicarboxylate;[1,2,5]Oxadiazolo[3,4-d]pyridazine, diphenyl-, 1-oxide;(-)-Epicatechin;Gerfelin;Naphthoquinone, 2-chloro-3-(4-methylpiperazin-1-yl);-1,3-Disiloxanediol, 1,3-dimethyl-1,3-diphenyl-	0.00002	0.00025	-2.35	0.05518	0.37183	-1.91	0.02897	0.21748	-2.46	0.00174	0.04690	-3.48
179.0544	0.6	D-Glucose; D-Galactose; D-Mannose; Beta-D-Glucose; Allose; Alpha-D-Glucose; Beta-D-Galactose; L-Gulose; L-Galactose; Alpha-D-Glucopyranoside; D-Glucopyranoside; 3(S)-hydroxy-all-cis-8,11,14,17-eicosatetraenoyl-CoA; D-Aldose; alpha-D-Mannose; D-Allose; beta-D-Mannose; D-Altrose; D-Gulose; D-Idose; D-Talose; L-Altrose; L-Idose;Myoinositol; Scyllitol; Levoinositol; 1L-chiro-Inositol; muco-Inositol; scyllo-Inositol;3-Deoxyarabinohehexonic acid;Dihydroxyacetone (dimer);Glycoprotein-phospho-D-mannose; Galactose;D-Fuconate; L-Fuconate; L-Rhamnonate;D-Hamamelose; beta-D-Hamamelopyranose;2-Deoxy-D-gluconate;1,3-Dihydroxyacetone;tetrahydrobenzothiepine-1-oxide;2,3,4,5-tetrahydro-1-benzothiepin-5-ol;1,3-Dihydroxyacetone dimer;NSC625042;alpha-L-Sorbopyranose	0.00000	0.00006	-2.32	0.00077	0.04128	-2.15	0.01489	0.13583	-2.32	0.01749	0.16466	-1.55
326.0626	0.6	Fluazifop;O-Desmethyloxotolrestat;Asn-Ser-OH;2-Methoxy-5-[2-methoxy-5-(trifluoromethyl)phenyl]pyridine-3-carboxylic acid;Glysobuzole;2-(4-Fluorophenyl)-5-[(2-methyl-5-nitrophenyl)methyl]thiophene	0.00621	0.02776	-2.27	0.94017	1.00000	-1.04	0.03180	0.22458	-3.32	0.05663	0.29445	-3.16
792.5541	10.2	PC(37:5); PE(40:5)	0.02833	0.09841	-2.25	0.39647	1.00000	-1.70	0.49990	1.00000	-2.04	0.16537	0.60289	-2.02
714.5077	9.1	PE(34:2); PC(31:2); 1-Palmitoyl-2-linoleoyl PE	0.00478	0.02269	-2.24	0.40753	1.00000	-2.07	0.20275	0.64295	-2.80	0.06864	0.32716	-2.47
353.1594	0.7	Valganciclovir;1H-Indole-2-carboxamide, N-(2-ethoxyphenyl)-3-(2-hydrazinoethoxy)-;1,3-Propanediamine, N'-(2-methoxy-1-nitro-9-acridinyl)-N,N-dimethyl-;Morphinan-3,14-diol, 6-azido-4,5-epoxy-17-(2-propenyl)-(5-alpha,6-beta)-	0.00000	0.00001	-2.17	0.00516	0.09563	-2.27	0.00017	0.01441	-5.18	0.00488	0.07230	-1.69
467.1551	0.6	PRIM-O-GLUCOSYLICMIFUGIN;AC1NPXPU;N-[(4-tert-butylphenyl)methylideneamino]-4-(4-pyrrolidin-1-ylsulfonylphenyl)-1,3-thiazol-2-amine;Strychnine phosphate dihydrate	0.01602	0.06089	-2.15	0.03057	0.24500	-2.51	0.47887	1.00000	-1.99	0.67667	1.00000	-1.70
540.0524	0.6	Cyclic ADP-ribose;GW 4064	0.00276	0.01410	-2.15	0.29142	1.00000	-1.98	0.06403	0.33599	-3.15	0.13473	0.51879	-2.69
756.5531	9.4	PC(34:2);PC(68:4);PE(37:2)	0.00002	0.00023	-2.07	0.06777	0.43215	-1.76	0.00556	0.06587	-2.39	0.00834	0.09768	-2.32
764.5229	9.4	PC(35:5), PE(38:5); PE(P-38:5)	0.01995	0.07442	-2.03	0.36847	1.00000	-2.15	0.56832	1.00000	-2.69	0.08549	0.37830	-1.61
279.2317	8.8	Linoleic acid; Linoelaidic acid; 9Z,12E-octadecadienoic acid; 9E,12Z-octadecadienoic acid;Bovinic acid; 9E,11E-Octadecadienoic acid; 10E,12Z-Octadecadienoic acid; Ricinenic acid;Mangiferic acid;Linalyl caprylate;Ethyl 2E,4Z-hexadecadienoate;5-Octadecynoic acid;Octadecadienoate;16-methyl-6Z,9Z-heptadecadienoic acid;16:2[2E,4E](4Me,6Me[S]);Sebaleic acid;Tariric acid;8-octadecynoic acid;Stearolic acid;Malvalic acid;Chaulmoogric acid;10E,12E-Hexadecadienyl acetate; 10E,12Z-Hexadecadienyl acetate; 10Z,12E-Hexadecadienyl acetate;11-Hexadecynyl acetate;Ethyl (Z,Z)-11,13-hexadecadienoate;(E)-3,7-Dimethyl-2,6-octadienyl octanoate; (Z)-3,7-Dimethyl-2,6-octadienyl octanoate;9-octadecen-4-olide; 9Z-octadecadien-4R-olide;9(Z),11(E)-Conjugated Linoleic Acid;5E,12Z-otadecadienoic acid;6-octadecynoic acid;C18:2n-12;6-Octadecynoic acid; Tariric acid; 6,7-Stearolic acid; 6-Stearolic acid;4-Dodecyl-5-ethyl-2(5H)-furanone;Hexadeca-7,11-dien-1-yl acetate (Z,E)-;trans-10,cis-12-Conjugated linoleic acid	0.00003	0.00031	-2.02	0.02878	0.24500	-1.47	0.00326	0.05029	-3.97	0.07603	0.34681	-1.56
648.6290	12.0	N-Lignoceroylsphingosine; Ceramide (d18:1/24:0);Cer(d18:0/24:1(15Z))	0.00022	0.00159	-1.98	0.01392	0.16401	-2.35	0.04007	0.25688	-2.30	0.17046	0.60745	-1.56

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807.4976	8.9	PI(32:1);Hebevoside I	0.00378	0.01882	-1.98	0.19133	0.85007	-1.61	0.18096	0.60386	-2.44	0.16546	0.60289	-1.96
783.4973	9.1	Ginsenoside C; Gypenoside LXXV	0.01406	0.05412	-1.97	0.90706	1.00000	-1.61	0.12902	0.48338	-2.33	0.06638	0.32265	-1.85
723.4957	8.8	PA(38:4)	0.00627	0.02776	-1.96	0.83660	1.00000	-1.37	0.89052	1.00000	-1.98	0.00019	0.01227	-5.59
620.5980	11.7	Ceramide (d18:1/22:0)	0.00079	0.00486	-1.92	0.40920	1.00000	-1.48	0.04078	0.25688	-2.27	0.02115	0.17416	-1.64
840.5739	9.2	PS(40:3)	0.00272	0.01400	-1.90	0.24901	0.96512	-1.64	0.04185	0.25688	-2.73	0.23291	0.71935	-1.71
247.0624	0.6	Coriandrone E; Propanoic acid, 2-hydroxy-3-[[4-hydroxy-1-naphthalenyl]oxy]-; EX-527; 1-Benzyl-4-carbamoylpyridin-1-ium chloride; 3-[[[(Thiophen-2-yl)methoxymethyl]phenyl]boronic acid; 9-Aminoacridine, monohydrochloride, monohydrate; N-(2-Phenylpyridin-3-yl)acetamide--hydrogen chloride (1/1); 2H-Pyran-2-one, 6-(2,4-dihydroxy-6-methylphenyl)-4-methoxy-; 4H-1-Benzopyran-2-carboxylic acid, 5-methoxy-4-oxo-, ethyl ester; Ethanone, 1-(4-amino-5-(p-chlorophenyl)-2-methyl-1H-pyrrol-3-yl)-; Propylsilanetriyl triacetate; Harmine hydrochloride; Methyl 4-(acetyloxy)-2-methyl-1-benzofuran-6-carboxylate; Ungeremine; (4R)-4-[[4-Cyanophenyl]methyl]-L-proline--hydrogen chloride (1/1); 3-Acetyl-6-methoxy-1,2-phenylene diacetate; 2(3H)-Benzoxazolone, 6-chloro-3-(1-piperidinylmethyl)-; Toluene-2,4,5-triol, triacetate; (4,6,7-trimethoxy-1-benzofuran-3-yl) acetate; Pyrido(2,3,4,5-lmn)phenanthridine-5,10-dione, 2,7-diamino-4,9-dihydro-; 5,6,7,8-Tetramethoxycoumarin; Metomidate hydrochloride; Pyrrole-3-carboxylic acid, 4-amino-5-phenyl-, ethyl ester, monohydrochloride	0.00670	0.02943	-1.90	0.11817	0.65765	-1.78	0.12103	0.47103	-2.17	0.47853	1.00000	-1.83
831.6588	11.0	TG(102:16); TG(51:8); 2-Decaprenyl-6-methoxy-3-methyl-1,4-benzoquinone	0.00180	0.00989	-1.90	0.25690	0.98284	-1.38	0.09823	0.42856	-2.07	0.05595	0.29445	-2.14
830.6642	9.8	PC(39:0); PE(42:0)	0.00240	0.01273	-1.89	0.86093	1.00000	-1.47	0.00861	0.08806	-3.23	0.08153	0.36350	-1.52
771.6377	11.0	SM(39:1)	0.00140	0.00799	-1.88	0.24875	0.96512	-1.35	0.06970	0.34734	-2.36	0.06073	0.30521	-2.07
859.6901	11.6	TG(106:16); TG(53:8)	0.00005	0.00045	-1.81	0.00171	0.05347	-2.37	0.03181	0.22458	-2.63	0.18547	0.62809	-1.58
799.6690	11.6	SM(41:1)	0.00008	0.00062	-1.79	0.00275	0.07405	-2.33	0.03031	0.22375	-2.57	0.20870	0.67261	-1.48
850.4827	9.1	PS(0:0), Chivosazole B	0.00179	0.00989	-1.78	0.18211	0.84071	-2.48	0.25691	0.75795	-2.19	0.04166	0.26761	-1.42
805.5682	8.8	PA(44:5)	0.00001	0.00017	-1.77	0.10289	0.61322	-1.33	0.00028	0.01907	-5.75	0.04429	0.26761	-1.78
292.0428	0.6	1-(3-Bromophenyl)-3-tert-butyl-1H-pyrazol-5-amine	0.00003	0.00028	-1.74	0.00071	0.04128	-1.96	0.02029	0.16949	-1.49	0.22120	0.70049	-1.31
803.6275	10.3	TG(49:8)	0.00577	0.02629	-1.69	0.44079	1.00000	-1.34	0.11109	0.45122	-2.17	0.11154	0.45617	-2.49
915.5988	8.8	Glycerol 2-(9Z,12Z-octadecadienoate) 1-hexadecanoate 3-O-[alpha-D-galactopyranosyl-(1->6)-beta-D-galactopyranoside]; OH-Chlorobactene glucoside laurate	0.00005	0.00042	-1.68	0.27141	1.00000	-1.20	0.00210	0.03487	-2.16	0.01382	0.14144	-1.48
742.6075	10.1	TG(44:1)	0.02434	0.08693	-1.66	0.91119	1.00000	1.10	0.22351	0.67279	-1.94	0.07272	0.33430	-1.64
724.4819	12.2	Spirolide E	0.00189	0.01021	-1.65	0.94135	1.00000	1.04	0.07882	0.37695	-1.91	0.00243	0.05550	-1.68
766.6175	9.9	1-(10-methylhexadecanyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine; GlcCer(d18:2/21:0); GalCer(d18:2/21:0)	0.02874	0.09909	-1.64	0.84913	1.00000	-1.02	0.48110	1.00000	-1.92	0.03122	0.22576	-1.80
241.0103	0.6	Inositol cyclic phosphate; 6-Deoxy-5-ketofructose 1-phosphate; 5-Dimethyldithiocarbamylpicolinic acid; 2-(Ethylsulphonyl)benzothiazol-6-amine; 2,4-Dinitrophenyl methyl carbonate; NSC522047; Aureothricin; Germane, trimethyl(4-(methylthio)phenyl)-; Ethyl 3-amino-4-cyano-5-(methylsulfanyl)thiophene-2-carboxylate; Ethyl heptafluorobutyrate; 5-[[2-Bromophenyl]methyl]tetrazolidine	0.01114	0.04495	-1.64	0.92262	1.00000	-1.05	0.15790	0.55079	-1.39	0.02443	0.19061	-2.09
826.5603	8.6	PS(39:3)	0.00394	0.01945	-1.61	0.26343	0.99837	-1.19	0.09310	0.42143	-2.37	0.16572	0.60289	-1.48
742.5390	8.8	PC(33:2); PE(36:2); PE(72:4); 1,2-Dioleoyl phosphatidyl ethanolamine	0.00004	0.00035	-1.57	0.13831	0.70704	-1.28	0.00113	0.02585	-4.04	0.04530	0.26863	-1.38
878.5132	10.1	PS(0:0)	0.01092	0.04437	-1.56	0.95895	1.00000	-1.15	0.17135	0.58063	-1.85	0.01491	0.14734	-1.92
743.6062	10.3	SM(37:1); PE(40:1)	0.00251	0.01318	-1.55	0.26435	0.99837	-1.38	0.09202	0.41977	-2.07	0.09279	0.40162	-2.55
217.0512	0.6	Liqcoumarin; 8-Hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone; 4-Methylumbelliferyl acetate; Piperic acid; 2-Hydroxy-6-oxo-6-phenylhexa-2,4-dienoate; 2,2',3'-Trihydroxydiphenylether; Aristolindiquinone; 2,7-Dihydroxy-5-methyl-1-naphthoate; (2-Methyl-4-oxo-4H-1-benzopyran-8-yl)acetic acid; (7R)-7-Methyl-7H-furo[3,2-h][2]benzopyran-3,9(2H,6H)-dione; 3,3'-(1,4-Phenylene)bis-2-propenoic acid; 2-oxo-2-(1-oxo-3,4-dihydro-2H-naphthalen-2-yl)acetic acid; 3-benzoyl-4-methoxy-2H-furan-5-one; 2,3-Dimethoxy-1,4-naphthoquinone; 4-(Furan-2-yl)-3-methoxybenzoic acid; Acifran; 2-[[3,4-Dihydroxyphenyl]methylidene]-5-methylfuran-3(2H)-one; [5-(4-Methylphenyl)thiophen-2-yl]boronic acid; Quinhydrone; Silane, trimethoxy(3,3,3-trifluoropropyl)-; [1,1'-Biphenyl]-3,3',5,5'-tetrol	0.01308	0.05154	-1.53	0.42439	1.00000	-1.44	0.13433	0.49785	-2.22	0.27491	0.80882	-1.17
802.5605	8.8	PT(18:0/18:1(9Z)); PS(37:1)	0.00002	0.00027	-1.52	0.11383	0.64653	-1.27	0.00080	0.02246	-3.42	0.04034	0.26576	-1.34
770.5702	9.8	PC(72:4); PC(36:2); PE(39:2); Dioleoylphosphatidylcholine; GPCCho(18:2(2E,4E)/O-18:0)[U]; 1,2-Dioleoyl PC	0.00581	0.02629	-1.52	0.32707	1.00000	-1.49	0.09767	0.42856	-1.68	0.19621	0.64755	-1.33
803.5638	8.8	PA(44:6)	0.00003	0.00032	-1.52	0.12738	0.66543	-1.28	0.00107	0.02528	-3.67	0.04468	0.26761	-1.36

*Fold change between HCC-N and adj.N

Metabolite	Mode	rt (min)	Monoisotopic mass (Da)	Identification*
fumaric acid	EI	11.2	116.01	UM=245, RI=1030.4, SS= 942, LP=245, 75, 246, 143
malic acid	EI	13.1	134.02	UM=233, RI=1180.2, SS=934, LP=233, 133, 75, 245
succinic acid	EI	10.7	118.02	UM=247, RI=996.5, SS=951, LP=75, 148, 247, 55
glucose	EI	18.1	180.06	UM=205, RI=1631.0, SS=859, LP=205, 319, 103, 160
lactic acid	EI	6.6	90.03	UM=117, RI=752.3, SS=953, LP= 117, 191, 148, 190
hypoxanthine†	EI	16.7	136.03	UM=265, RI=1492.2, SS=935, LP=265, 280, 266, 84
	ESI-	0.6		m/z= 135.0299, ppm=9, fragment ions = 138.019; 108.0212; 92.0254; 134.8931; 134.8636; 136.8914; 134.9011; 135.0289; 80.9644; 135.8908
xanthosine†	EI	24.4	284.07	UM=325, RI=2391.1, SS=895, LP=325, 245, 230, 217
	ESI-	0.6		m/z= 283.0671, ppm=4, fragment ions = 151.026; 283.0682; 124.0075; 108.02; 150.0428; 214.0496; 171.0051; 117.0222; 133.0135; 89.0233
adenosine monophosphate†	EI	27.1	347.06	UM= 169, RI=2781.9, SS=934, LP=315, 169, 230, 192
	ESI-	0.6		m/z= 346.0544, ppm=3, fragment ions = 89.0245; 242.0795; 346.1278; 168.0444; 78.9585; 90.0278; 214.0479; 211.002; 152.997; 345.0321
propionyl carnitine	ESI+	0.6	217.13	m/z= 218.1391, ppm=2, fragment ions = 218.1395; 221.0196; 85.0288; 159.0658; 219.1429; 144.1036; 86.0324; 160.0711; 202.0661; 220.1457
linoleic acid†	ESI-	8.8	280.23	m/z=279.2317, ppm=4, fragment ions = 279.2319; 278.9878; 280.986; 280.2384; 282.9937; 282.9735; 216.988; 240.9896; 260.9781; 261.0001
PC(34:2)	ESI+	8.8	757.56	m/z=758.57, ppm=0, fragments ions = 758.57; 476.98; 283.27; 265.00; 237.02
PC(38:3)	ESI+	10.3	811.60	m/z=812.6162, ppm=0, fragment ions = 184.0746; 812.6171; 813.6202; 814.6226; 185.0771; 627.5352; 184.1160; 628.5384; 812.5215; 184.2872
PC(36:1)	ESI+	10.4	787.60	m/z=788.6164, ppm=0, fragment ions = 184.0737; 787.6017; 788.6042; 185.0765; 651.5328; 789.6071; 184.1149; 186.0779; 792.5530; 790.6093
PC(38:2)	ESI+	10.5	813.62	m/z=814.632, ppm=0, fragment ions = 184.0745; 813.6199; 814.6221; 185.0782; 628.5385; 629.5414; 816.5525; 813.5264; 814.5308; 815.6257
glycerol 3-phosphate	ESI-	0.6	172.01	m/z=171.0051, ppm=7, fragment ions = 78.9589; 171.0056; 146.9597; 96.9695; 118.966; 152.9915; 139.8937; 172.0104; 172.8294; 104.9954
glycerylphosphoryl ethanolamine	ESI-	0.6	215.05	m/z=214.0477, ppm=3, fragment ions = 140.0116; 78.9589; 214.0478; 152.9953; 215.0508; 140.0483; 141.0137; 214.0943; 171.0058; 96.9696
glycerophospho choline	ESI+	0.7	257.10	m/z=258.11, ppm=0, fragment ions = 104.10799; 125.0008; 184.0741; 86.0972; 140.0691; 258.1107; 98.9850; 261.1321; 166.0630; 105.1106
coenzyme Q10†	ESI+	12.4	862.68	m/z=885.6731, ppm=0, fragments ions = 885.6714; 886.6742; 887.6779; 885.7438; 888.6804

*UM = unique mass selected by the deconvolution software, RI = Retention Index, SS = Similarity Score, top 4 Largest Peaks (LP) for GC-MS; precursor ion (m/z), ppm for LC-MS; fragment ions for LC-MS/MS

† Verified by comparison with authentic compounds