

Supplementary Table 1. Features that were found to be differentially regulated in the HCC as defined in figure 4.

No.	M/Z	Rt	Name	Formula	Fold	P value	Trend
1	301.0575	2.1	5-(3,4-Dihydroxy-1,5-cyclohexadien-1-yl)-5-ethylbarbituric acid	C ₁₂ H ₁₄ N ₂ O ₅	1.6	0.00003	↓
2	113.0255	2.11	2-Hydroxy-2,4-pentadienoate	C ₅ H ₆ O ₃	1.5	0.00005	↓
3	203.0032	4.17	NA	NA	1.7	0.00007	↓
4	125.0254	1.56	Methyl 2-furoate	C ₆ H ₆ O ₃	1.8	0.00016	↓
5	204.9813	1.56	4-Chlorophenylacetic acid	C ₈ H ₇ ClO ₂	1.9	0.00026	↓
6	113.025	4.62	Norfuraneol	C ₅ H ₆ O ₃	2	0.00065	↓
7	246.9933	2.73	Vanillic acid 4-sulfate	C ₈ H ₈ O ₇ S	1.6	0.00071	↓
8	192.0668	4.26	(3-Arylcarbonyl)-alanine	C ₁₀ H ₁₁ NO ₃	1.8	0.00078	↓
9	175.0253	4.62	Ascorbic acid	C ₆ H ₈ O ₆	1.9	0.00086	↓
10	258.9946	1.85	NA	NA	1.5	0.00103	↓
11	283.08	4.62	p-Cresol glucuronide	C ₁₃ H ₁₆ O ₇	2.2	0.00106	↓
12	197.047	2.61	3,4-O-Dimethylgallic acid	C ₉ H ₁₀ O ₅	1.6	0.00121	↓
13	407.9502	4.62	NA	NA	1.7	0.00131	↓
14	409.9471	4.62	NA	NA	1.8	0.00247	↓
15	167.0355	2.73	3-Hydroxymandelic acid	C ₈ H ₈ O ₄	1.6	0.00375	↓
16	188.0113	4.51	NA	NA	2.2	0.0039	↓
17	428.0051	4.62	NA	NA	1.5	0.00392	↓
18	187.0051	4.51	NA	NA	2.2	0.00422	↓
19	107.051	4.51	Benzyl alcohol	C ₇ H ₈ O	2.3	0.00435	↓
20	231.0758	4.79	NA	C ₁₂ H ₁₂ N ₂ O ₃	1.7	0.00524	↓
21	112.9866	0.45	Trifluoroacetic acid	C ₂ HF ₃ O ₂	1.5	0.00576	↑
22	152.0122	2.73	L-Aspartic acid b-semialdehyde	C ₄ H ₇ NO ₃	1.5	0.00597	↓
23	174.9575	0.42	Phosphonoacetate	C ₂ H ₅ O ₅ P	1.5	0.00625	↓
24	315.0745	1.83	L-beta-aspartyl-L-phenylalanine	C ₁₃ H ₁₆ N ₂ O ₅	2.2	0.00643	↓
25	212.0035	4	Indoxylsulfuric acid	C ₈ H ₇ NO ₄ S	1.6	0.00715	↓
26	335.0106	5.62	NA	NA	1.7	0.00917	↓