

Supplementary Table S2. LC-MS positive mode significant features

QC note: Feature_ID, m/z, and RT were checked and restored from intact feature identifiers; 168 positive-mode features were retained.

Feature_ID	m/z	RT (min)
311	126.0220	0.74
1067	137.0652	2.62
3692	950.6321	7.70
1240	267.1340	3.15
3772	114.0631	7.78
1432	265.1545	3.91
384	219.1337	0.83
548	253.1183	1.19
926	189.1234	2.15
5109	766.5733	9.33
5012	701.5583	9.10
1907	149.0296	5.43
9084	321.9873	15.41
6809	124.0917	12.46
1790	986.2586	4.79
1551	253.0999	4.29
4947	748.5272	8.96
8771	141.9515	14.86
8577	110.0162	14.62
9099	111.0392	15.46
5098	113.0709	9.33
8828	149.0297	14.93
8140	811.6664	13.98
5886	138.1026	10.83
4902	744.5532	8.88
1489	432.2803	4.12
5127	124.0912	9.38
8860	154.9968	14.95
8721	110.0252	14.77
2675	194.1257	6.58
2528	496.3015	6.39
5151	413.2661	9.42
2300	178.1227	6.08
5581	122.0991	10.22
4014	832.5825	8.04
2612	313.2370	6.51
8991	131.9700	15.19
618	107.0492	1.33

Feature_ID	m/z	RT (min)
5092	780.5528	9.30
835	301.4740	1.88
2397	114.0631	6.22
6661	124.0944	12.28
1840	504.2370	5.00
2702	114.0631	6.63
1091	235.1992	2.69
4714	746.5687	8.75
8586	227.9826	14.65
8973	115.9621	15.14
8719	183.9854	14.77
9172	149.0154	15.67
8931	109.5241	15.08
341	310.0865	0.77
6496	784.5834	12.06
6575	784.5838	12.18
7616	804.5514	13.43
6768	810.5992	12.41
6905	149.0822	12.58
1208	189.1274	3.08
1634	305.1315	4.51
4359	730.5373	8.37
8688	109.5156	14.74
2474	115.0697	6.31
7797	780.5509	13.62
5939	153.1134	10.96
738	149.0284	1.65
118	114.0733	0.41
5668	781.5546	10.38
1202	348.1763	3.04
5925	810.5991	10.92
5615	780.5514	10.28
5748	149.0822	10.53
6609	138.1026	12.21
7381	124.0916	13.17
3492	383.2790	7.52
8720	156.9940	14.77
1576	569.3139	4.34
390	322.1066	0.85
4178	756.5518	8.20
5455	784.5831	10.01

Feature_ID	m/z	RT (min)
9067	177.1638	15.36
143	149.0184	0.48
8812	158.9860	14.89
6485	128.1182	12.04
4737	836.6132	8.76
4517	902.5387	8.55
4532	265.2526	8.56
5699	780.5513	10.43
5440	167.0928	9.99
1096	289.9661	2.71
2758	372.2440	6.70
7069	732.5534	12.79
5703	100.0631	10.43
9078	182.9809	15.40
6074	758.5689	11.28
8482	110.0150	14.54
277	738.1732	0.71
6507	758.5689	12.09
1367	243.1828	3.71
1470	402.2333	4.04
1385	192.1182	3.79
6277	808.5843	11.73
9213	227.1640	15.81
1059	289.9661	2.59
342	613.1588	0.80
1164	149.0284	2.91
676	137.0652	1.49
2216	151.1481	5.97
6398	810.5993	11.92
1464	205.0905	4.01
3077	478.3139	7.06
3499	730.5374	7.54
3686	488.3580	7.73
5950	784.5832	10.97
6539	810.5991	12.11
6033	128.1182	11.17
632	341.0032	1.38
533	149.0333	1.16
1737	907.2410	4.75
6439	369.3513	12.00
8449	115.9620	14.51

Feature_ID	m/z	RT (min)
3950	475.7696	7.97
1603	344.2539	4.42
429	129.0489	0.94
5549	111.0917	10.17
1036	508.0030	2.51
8959	115.9641	15.12
915	149.0332	2.13
5776	153.1134	10.59
6608	760.5834	12.20
331	320.0909	0.79
662	235.1992	1.45
8797	122.5472	14.88
2611	177.0547	6.51
1038	149.0154	2.52
1821	741.0114	4.93
8887	129.1274	15.01
5839	179.0928	10.74
7644	790.5345	13.49
1373	314.1809	3.71
1221	149.0314	3.11
3460	497.8177	7.51
1831	1077.3778	4.97
8563	214.0035	14.62
8641	199.9829	14.69
818	128.0426	1.85
7608	151.0978	13.42
7272	151.0978	13.03
1569	1057.5905	4.32
5448	732.5525	10.00
5007	804.5512	9.07
1128	149.0284	2.79
8301	704.5224	14.10
4332	748.5268	8.36
5104	731.6060	9.34
8971	122.5472	15.15
9103	127.1094	15.46
3643	598.3644	7.65
1254	217.1798	3.18
5388	784.5830	9.88
7681	113.0710	13.50
3992	403.2321	8.01

Feature_ID	m/z	RT (min)
4989	828.5501	9.05
4043	828.5501	8.06
704	359.1035	1.57
6933	128.1182	12.62
6385	153.1134	11.90
5660	149.0822	10.35
7037	810.5992	12.75