

## DATA FILE S2

### CD vs non-IBD

ESI mode	Ion	Log2 FC	Q-value	Validated ID	Overlap with metabotype
Positive	479.2784_3.8324	7.84	0.002		
Positive	752.4485_4.3337	6.15	0.011		
Positive	708.4223_4.2912	5.85	0.027		
Positive	783.479_4.3649	5.80	0.027		
Positive	509.8048_4.0186	5.79	0.013		
Positive	488.7993_3.8092	5.66	0.036		
Positive	173.1647_2.242	5.48	0.045		
Positive	321.1808_4.5154	-4.12	0.027		x
Positive	611.3437_4.3716	-4.51	0.027		x

### UC vs non-IBD

ESI mode	Ion	Log2 FC	Q-value	Validated ID	Overlap with metabotype
Negative	150.0546_3.2145	6.76	0.027		
Negative	108.0437_0.993	6.05	0.014		
Positive	154.0509_0.9254	5.86	1.0E-04	5-aminosalicylic acid	
Positive	196.0604_2.9493	5.75	0.008		
Positive	136.0407_0.9222	5.60	0.007		
Negative	194.0443_3.2148	5.48	0.014		
Negative	152.0343_0.9903	4.56	0.002	5-aminosalicylic acid	
Negative	202.0712_0.9967	2.83	0.014		x
Positive	373.274_6.5337	-3.48	0.027		

### Metabotype 2 vs. 1

ESI mode	Ion	Log2 FC	Q-value	Validated ID
Negative	589.3029_4.8287	9.57	4.7E-16	
Negative	556.3314_5.6626	8.98	8.1E-11	
Negative	611.2826_4.6855	8.67	4.7E-16	
Positive	632.4107_5.9785	8.60	1.2E-07	
Positive	407.2797_5.5815	8.12	1.8E-10	7-Ketodeoxycholic acid
Negative	385.1334_5.3172	8.03	2.9E-07	
Positive	613.2999_4.583	8.00	4.7E-16	
Positive	357.2783_5.8275	7.97	6.0E-06	
Negative	405.2631_5.8089	7.93	0.003	
Positive	371.2584_5.555	7.71	7.8E-07	3-Oxo-4,6-choladienoic acid
Negative	397.2052_5.4302	7.49	2.1E-05	
Negative	498.2867_5.4288	7.47	1.2E-06	Taurochenodeoxycholate
Positive	335.2365_5.5524	7.46	3.4E-04	
Negative	587.2878_5.274	7.44	5.7E-08	

Positive	389.2688_5.5598	7.41	5.7E-08	
Negative	493.2234_5.8191	7.34	1.9E-07	3-Sulfodeoxycholic acid
Negative	443.2574_6.0663	7.33	2.9E-05	
Negative	536.3226_5.3551	7.24	3.1E-05	
Positive	337.2541_5.9828	7.22	9.4E-04	
Negative	405.2632_5.6659	7.21	1.8E-06	7-Ketodeoxycholic acid
Negative	545.3117_4.691	7.19	1.7E-07	
Positive	353.248_5.5509	7.17	2.1E-06	
Positive	247.1287_1.9494	7.08	1.2E-07	
Negative	194.0487_1.2085	7.02	8.3E-07	
Positive	629.2674_4.5797	7.02	3.4E-08	
Positive	424.3058_5.5396	7.00	1.9E-07	
Negative	475.2688_6.2292	6.99	1.1E-04	
Positive	468.2506_6.0942	6.95	5.7E-04	
Positive	799.5687_5.9584	6.85	1.4E-04	
Positive	274.144_4.9738	6.79	2.8E-08	
Positive	632.9135_5.9509	6.71	2.6E-05	
Negative	399.1489_5.4445	6.62	1.1E-06	
Positive	373.2741_4.7803	6.60	5.5E-05	
Negative	375.1827_5.4724	6.55	6.4E-06	
Positive	607.3145_5.3077	6.51	0.013	
Negative	272.1296_5.1129	6.48	6.4E-06	
Positive	429.2621_5.5639	6.45	4.5E-03	
Positive	355.2632_5.9773	6.39	3.5E-08	
Negative	498.2895_5.6354	6.35	7.0E-05	Taurochenodeoxycholate
Negative	591.318_6.2442	6.34	5.5E-07	
Positive	357.2788_6.8897	6.31	1.9E-07	
Negative	476.2727_6.1139	6.29	2.7E-05	
Negative	453.2315_6.2465	6.28	0.003	
Negative	415.1864_3.6039	6.27	0.020	
Positive	431.2786_5.9801	6.15	1.1E-06	Cholic Acid
Negative	143.0712_1.4524	6.08	0.025	
Positive	468.2492_4.2929	6.05	6.0E-07	
Positive	315.1348_4.575	6.04	3.7E-07	
Negative	613.2984_6.2629	6.04	0.002	
Positive	591.3154_6.0937	6.03	0.026	
Positive	785.5953_6.8808	5.97	0.027	
Positive	229.1553_0.9898	5.96	1.2E-06	
Positive	389.2685_5.188	5.95	0.028	
Positive	593.3334_6.0881	5.95	3.7E-07	
Negative	466.1253_0.8949	5.89	9.8E-04	
Positive	426.322_5.4095	5.88	0.030	
Negative	357.0757_1.8091	5.87	0.009	
Positive	615.3156_6.1003	5.82	3.6E-05	
Negative	514.2822_4.9444	5.80	0.002	
Negative	426.1955_5.0671	5.79	0.033	
Negative	442.1897_4.8568	5.79	0.033	

Positive	251.1602_0.7512	5.78	2.8E-05	
Positive	303.1713_4.2478	5.78	5.5E-03	
Positive	253.1566_1.3107	5.78	0.033	
Negative	405.2648_6.2066	5.77	0.034	
Negative	407.2791_4.877	5.71	7.6E-06	
Positive	276.1598_4.9131	5.69	0.001	
Positive	407.2795_4.978	5.68	0.004	7-Ketodeoxycholic acid
Negative	274.1458_5.0667	5.63	0.038	
Positive	373.2737_5.978	5.62	6.1E-07	
Negative	405.2646_6.0966	5.62	0.035	
Negative	459.2716_6.238	5.59	0.038	
Negative	487.2369_5.254	5.54	1.9E-05	7-Sulfocholic acid
Positive	267.1711_2.4522	5.53	0.003	
Positive	159.1483_1.2432	5.52	0.005	
Positive	355.2626_6.1642	5.51	7.5E-04	
Positive	426.3214_5.9814	5.51	1.4E-10	
Positive	575.3707_5.5478	5.51	0.042	
Positive	371.2558_5.1913	5.48	0.043	
Positive	126.0235_0.8442	5.47	9.1E-08	
Positive	355.2629_5.1581	5.47	7.8E-07	7,10,13,16-Docosatetraenoic acid
Negative	407.2788_6.2278	5.47	2.0E-04	
Negative	437.2906_6.2075	5.46	7.1E-04	
Positive	302.2326_5.1092	5.46	0.044	
Negative	412.1797_4.8941	5.44	0.044	
Positive	426.3204_6.2157	5.43	0.005	
Positive	265.1514_5.9857	5.43	0.001	
Positive	355.2632_4.7754	5.43	0.010	
Positive	247.1295_2.2814	5.42	0.002	
Positive	373.2738_5.3622	5.40	7.6E-06	
Positive	339.2674_6.8928	5.37	0.047	
Positive	391.2851_5.9897	5.33	3.0E-06	
Negative	205.036_0.8938	5.32	0.005	
Positive	389.2686_4.9418	5.31	0.049	
Negative	173.0099_0.9894	5.26	0.035	
Negative	367.1585_5.2159	5.26	3.8E-06	
Positive	426.3208_5.1578	5.22	4.3E-05	
Negative	475.2671_6.081	5.16	1.2E-04	
Positive	346.2703_8.6613	5.13	3.6E-04	
Negative	407.2794_5.4892	5.12	7.2E-06	
Positive	143.0726_0.8995	5.12	0.005	
Positive	256.1461_5.9852	5.09	6.6E-04	
Positive	291.1693_5.6892	5.08	0.039	
Positive	355.2615_5.4202	5.04	0.009	
Negative	799.5738_6.183	5.04	0.002	
Negative	269.0444_5.1218	4.95	0.035	
Negative	589.3019_4.6741	4.91	5.7E-08	
Positive	391.2844_5.1658	4.90	5.1E-04	

Positive	373.2737_5.1357	4.87	2.8E-07	
Negative	166.0176_0.9396	4.86	6.7E-05	
Negative	353.0999_3.9251	4.80	0.001	
Negative	485.2209_4.8745	4.74	0.002	
Negative	515.3057_6.2301	4.74	0.033	
Positive	392.3166_5.673	4.73	2.6E-05	
Positive	235.632_5.9721	4.72	1.3E-04	
Positive	309.1644_0.8126	4.67	0.001	
Positive	589.3026_5.154	4.67	2.7E-05	
Negative	289.1555_5.8038	4.61	2.3E-04	
Negative	133.0499_1.0336	4.60	0.006	
Positive	493.2449_5.9568	4.54	0.005	
Positive	357.2791_5.6808	4.54	6.5E-04	
Positive	244.6374_5.9809	4.48	8.0E-05	
Positive	145.0499_0.8983	4.46	1.2E-04	
Negative	344.1809_3.4212	4.40	0.010	
Negative	407.2793_6.4209	4.36	0.009	
Positive	201.9346_0.8002	4.34	4.6E-06	
Negative	317.1464_0.8437	4.31	0.025	
Positive	243.1349_2.3083	4.28	7.5E-05	
Positive	303.1714_4.0203	4.27	0.003	
Positive	591.3179_4.5766	4.27	1.3E-09	
Positive	241.1552_0.9974	4.23	9.4E-04	
Negative	156.0666_1.0014	4.22	9.4E-04	
Positive	324.29_8.6656	4.22	9.0E-04	
Positive	442.2693_3.4706	4.20	0.026	
Positive	319.1921_6.0283	4.15	3.2E-04	
Negative	124.0067_0.8872	4.14	7.4E-08	Taurine
Negative	124.9904_0.9145	4.09	4.2E-04	
Negative	469.228_5.1926	4.06	0.005	
Positive	319.1603_0.8174	4.04	5.3E-06	
Negative	539.1375_0.8801	4.02	0.016	
Negative	286.0016_2.6719	4.01	0.003	
Negative	243.1231_4.6191	4.01	0.013	
Negative	121.0655_3.9387	3.97	7.9E-05	
Negative	319.191_4.398	3.93	0.021	
Positive	255.0672_4.4672	3.92	0.031	
Negative	327.0515_3.2674	3.86	0.003	
Negative	253.1193_2.328	3.84	0.008	
Negative	379.0978_0.8896	3.83	0.004	
Positive	442.2104_5.701	3.83	0.002	
Positive	114.0874_0.8408	3.82	1.4E-04	
Negative	405.2646_5.0509	3.74	0.032	
Positive	269.1752_3.3247	3.72	0.005	
Positive	171.1495_0.7788	3.70	0.005	
Positive	373.2749_7.0789	3.68	0.010	
Positive	242.0429_0.9223	3.68	1.1E-04	

Positive	144.0814_2.9765	3.64	0.005	Phenethylamine
Negative	471.2406_5.8057	3.64	8.6E-04	Chenodeoxycholic acid sulfate
Positive	295.1437_5.688	3.63	2.7E-04	
Positive	543.1309_0.8156	3.63	4.3E-04	
Positive	496.3379_7.9889	3.62	0.015	
Positive	226.1518_0.9523	3.61	0.004	
Positive	325.1119_0.8692	3.61	2.5E-04	
Negative	321.1292_0.8173	3.58	0.020	
Positive	383.0944_0.8064	3.55	7.1E-04	
Negative	285.1703_3.4399	3.50	0.001	
Negative	254.0699_1.0384	3.48	0.032	
Positive	203.054_0.8276	3.47	4.7E-05	
Negative	259.1451_3.7921	3.45	0.002	
Positive	310.1301_1.5025	3.45	0.035	
Negative	469.2261_5.4088	3.42	0.008	
Negative	130.0861_2.1345	3.39	0.031	
Negative	407.2789_6.08	3.37	8.0E-05	Cholic Acid
Negative	181.0362_1.1213	3.36	7.9E-04	
Negative	305.0698_3.4475	3.31	0.021	
Positive	146.1176_1.0253	3.30	0.047	
Positive	300.1559_5.4295	3.25	0.009	
Negative	187.0373_3.9347	3.22	0.007	
Positive	307.1868_0.8774	3.18	0.004	
Negative	163.0601_0.9071	3.16	0.012	
Negative	435.1276_0.9265	3.15	0.016	
Negative	119.0348_0.8648	3.13	0.009	
Positive	466.3176_5.3628	3.13	0.046	
Positive	393.3195_5.6367	3.13	0.041	
Negative	96.9615_0.9836	3.12	2.0E-04	
Negative	124.0078_1.0052	3.05	0.003	Taurine
Negative	487.2364_5.0286	3.04	0.035	
Positive	105.0698_2.322	3.03	0.020	
Positive	101.0606_0.8469	3.01	1.2E-05	
Positive	287.2434_0.7876	3.00	5.3E-04	
Negative	471.2406_5.2037	3.00	0.023	Chenodeoxycholic acid sulfate
Negative	407.279_5.2626	2.99	6.1E-04	
Negative	471.2407_5.4898	2.98	0.016	Chenodeoxycholic acid sulfate
Negative	607.3141_5.1374	2.98	0.050	
Negative	284.0996_0.8839	2.97	0.044	
Negative	240.9688_0.8143	2.96	0.003	
Positive	223.1081_2.6583	2.95	0.019	
Positive	171.0794_0.827	2.94	0.002	
Negative	87.0089_0.9968	2.91	0.043	
Negative	377.085_0.892	2.89	2.0E-04	
Positive	277.1186_2.7869	2.87	0.009	
Negative	343.1957_3.3207	2.86	0.029	
Negative	701.1903_0.891	2.86	0.042	

Negative	159.066_1.0792	2.83	0.047
Positive	189.1614_0.8254	2.82	0.009
Positive	201.123_1.0094	2.81	0.024
Positive	331.1872_5.621	2.77	0.010
Positive	219.0281_0.8177	2.76	2.6E-06
Positive	365.0997_0.8288	2.72	0.009
Positive	317.0235_0.7582	2.71	0.009
Negative	329.2329_5.4488	2.71	0.007
Positive	271.0821_2.3981	2.70	0.027
Negative	202.0712_0.9967	2.69	2.7E-05
Negative	229.155_3.0436	2.69	0.020
Positive	280.1392_0.8706	2.68	6.1E-04
Negative	341.1082_0.8545	2.64	0.013
Positive	221.15_0.7462	2.60	0.035
Negative	317.1502_4.6189	2.57	0.019
Positive	215.1028_0.9795	2.57	0.008
Negative	359.0763_3.0846	2.54	0.049
Positive	131.1172_0.8442	2.52	0.033
Positive	323.1604_3.6842	2.51	0.031
Negative	165.055_3.9364	2.50	0.003
Positive	146.0609_2.6208	2.47	0.030
Negative	119.0498_3.9309	2.47	0.019
Positive	243.1407_0.8621	2.43	0.004
Positive	183.0852_0.8744	2.35	0.035
Positive	85.0282_0.8849	2.33	0.010
Negative	305.0694_3.2644	2.32	0.011
Positive	277.0759_0.8885	2.31	0.005
Positive	381.0802_0.8154	2.30	2.5E-04
Negative	193.0344_0.8947	2.29	0.003
Positive	183.1119_1.0703	2.28	0.046
Positive	166.0777_0.9135	2.27	0.009
Negative	149.0456_0.9022	2.24	0.009
Positive	580.6564_5.1435	2.18	0.050
Positive	204.0902_0.9568	2.17	3.8E-04
Positive	243.1342_1.9576	2.17	0.024
Positive	233.1155_1.0717	2.16	0.043
Positive	532.0042_4.9757	2.15	0.046
Positive	123.0505_0.8741	2.12	0.013
Positive	128.1069_0.8991	2.07	0.015
Positive	230.1854_0.8989	2.07	0.007
Positive	159.1492_1.0029	2.06	0.015
Positive	100.0764_1.5459	2.05	0.007
Positive	244.0808_0.8577	2.02	0.007
Positive	263.1393_3.2193	2.02	0.019
Positive	145.1336_0.8918	2.00	0.009
Positive	332.9965_0.7666	2.00	0.029
Positive	152.028_0.8402	1.99	0.005

N-Acetylcadaverine

Positive	226.0718_0.9278	1.98	0.022	
Positive	673.423_4.9985	1.97	0.028	
Positive	578.8675_5.0025	1.97	0.001	
Positive	276.1462_1.0338	1.89	0.034	
Negative	191.0555_0.9233	1.89	0.014	
Positive	574.2215_5.0989	1.88	0.031	
Positive	262.1303_0.9037	1.87	0.009	
Positive	249.0457_0.8026	1.86	0.011	
Positive	294.1537_1.0299	1.84	0.008	
Negative	89.0243_0.8666	1.83	0.007	
Positive	564.5236_5.0891	1.82	0.041	
Positive	272.1658_0.8523	1.80	0.035	
Positive	250.1286_0.8839	1.77	0.027	
Positive	215.1388_1.1735	1.76	0.024	
Positive	289.0986_0.8846	1.76	0.033	
Negative	215.0323_0.8906	1.74	0.002	
Positive	244.1999_0.9862	1.73	0.038	
Positive	374.2355_0.9052	1.71	0.034	
Negative	161.0455_0.8894	1.70	0.003	
Positive	339.269_7.0521	1.70	0.028	
Negative	117.0188_1.1458	1.69	0.036	
Negative	113.024_0.8863	1.67	0.005	
Positive	156.0769_0.824	1.65	0.020	
Positive	188.1756_0.7768	1.64	0.006	
Positive	600.8812_5.0254	1.62	0.009	
Positive	134.0457_0.8351	1.62	0.024	
Positive	217.1186_0.9427	1.57	0.008	
Positive	630.3982_5.0523	1.56	0.033	
Positive	189.0232_0.8231	1.53	0.018	
Positive	265.0207_0.7657	1.53	0.037	
Negative	174.0404_0.9909	1.48	0.035	
Positive	202.9714_0.7389	1.47	0.033	
Positive	385.9044_0.7337	1.47	0.048	
Positive	146.1179_0.8336	1.46	0.035	
Positive	205.0976_2.5971	1.43	0.037	Tryptophan
Positive	586.3721_5.013	1.42	0.038	
Positive	246.1793_0.8212	1.41	0.034	
Positive	258.1088_0.8635	1.39	0.032	
Negative	131.0415_0.889	1.39	0.038	
Positive	301.1435_8.2587	1.36	0.038	
Positive	188.0711_2.6005	1.33	0.025	Serinyl tryptophan
Positive	335.124_8.1063	1.32	0.026	
Negative	179.0556_0.8637	1.31	0.002	
Positive	260.193_0.9965	1.29	0.044	
Positive	375.2242_0.9817	1.28	0.045	
Positive	410.3264_7.0503	1.28	0.048	
Positive	73.5172_0.7451	1.27	0.024	

Positive	130.0533_0.8546	1.27	0.004	
Positive	104.1061_0.8037	1.25	0.034	
Positive	571.5299_5.0028	1.22	0.048	
Positive	176.1187_3.3908	1.18	0.024	
Positive	260.0539_0.8273	1.15	0.015	
Positive	255.1371_0.8587	1.14	0.041	
Negative	101.0246_0.8738	1.10	0.024	
Negative	132.0296_0.9036	0.90	0.043	
Negative	188.0559_1.0259	-0.76	0.044	Acetyl-glutamic acid
Negative	251.0776_1.021	-1.12	0.016	
Positive	520.333_3.5639	-1.19	0.043	
Negative	283.1182_4.5585	-1.32	0.047	
Positive	652.4109_3.7945	-1.38	0.037	
Negative	187.0971_4.3188	-1.42	0.010	Azaleic acid
Negative	125.0967_4.2984	-1.46	0.043	
Positive	414.7607_4.0011	-1.47	0.013	
Negative	184.0015_0.8462	-1.49	0.011	
Positive	445.2873_4.0565	-1.59	0.049	
Positive	226.1048_0.9746	-1.64	0.035	
Negative	349.0712_0.9498	-1.71	0.044	
Positive	337.6653_4.5708	-1.74	0.038	
Positive	362.221_3.9171	-1.78	0.035	
Positive	696.4379_3.8367	-1.82	0.043	
Positive	560.3285_3.5157	-1.82	0.029	
Negative	227.0225_0.8685	-1.83	0.018	
Negative	591.3178_4.6332	-1.85	0.043	Mesobilirubinogen
Negative	172.0615_1.0129	-1.86	0.009	
Positive	180.1023_0.9652	-1.96	0.045	
Positive	209.1175_3.5483	-1.97	0.034	
Positive	686.9183_4.1458	-1.97	0.049	
Negative	212.925_0.8376	-1.97	0.016	
Negative	267.0733_1.0368	-2.04	3.9E-04	
Positive	164.0702_3.9596	-2.05	0.046	
Negative	410.8636_0.8271	-2.07	0.011	
Positive	290.8487_0.7967	-2.10	0.005	
Positive	295.1654_2.8735	-2.14	0.043	Estradiol
Negative	257.9333_0.8656	-2.20	5.7E-04	
Negative	267.9633_0.832	-2.25	0.011	
Negative	201.1128_4.7648	-2.27	2.2E-05	
Positive	182.0816_3.977	-2.27	0.002	
Positive	196.0971_0.9926	-2.28	0.005	
Negative	440.8814_0.8072	-2.30	0.021	
Negative	115.076_3.7638	-2.33	0.005	
Negative	139.1124_4.7645	-2.34	4.2E-04	
Negative	159.0659_3.7654	-2.35	0.012	
Positive	443.2693_3.9619	-2.39	0.016	
Negative	211.0276_0.8806	-2.40	0.018	



Positive	303.1694_4.492	-2.41	0.048
Positive	549.3463_5.0632	-2.42	0.012
Negative	227.0673_1.0436	-2.45	0.037
Positive	344.2515_3.7491	-2.45	0.044
Negative	184.0618_1.16	-2.46	0.033
Positive	218.1381_0.9957	-2.47	0.029
Negative	229.1439_5.5632	-2.48	2.3E-04
Negative	297.113_5.4414	-2.50	0.021
Positive	768.4697_4.3531	-2.52	0.012
Positive	740.4628_3.9154	-2.57	0.017
Negative	138.0556_1.0851	-2.58	0.004
Positive	421.256_3.9007	-2.65	0.007
Negative	367.0807_0.8921	-2.67	0.014
Negative	206.0453_1.8664	-2.67	0.035
Negative	380.8445_0.8199	-2.76	0.020
Negative	326.9018_0.8129	-2.77	0.005
Negative	145.05_2.475	-2.79	0.049
Negative	197.0671_0.9601	-2.84	0.048
Positive	174.1221_0.9965	-2.85	0.014
Positive	665.7434_4.2095	-2.86	0.049
Negative	227.1285_5.3716	-2.89	0.007
Positive	659.7361_4.4323	-2.91	0.020
Positive	399.2402_3.8135	-2.91	0.045
Negative	167.1438_5.5621	-2.95	6.3E-04
Positive	210.113_0.9352	-2.95	0.036
Positive	133.0863_3.9597	-2.95	0.020
Positive	225.1151_3.6524	-3.02	0.013
Positive	539.833_4.0684	-3.05	0.029
Negative	297.1126_5.2941	-3.08	1.9E-04
Positive	377.2273_3.7823	-3.10	0.040
Negative	241.1076_3.7694	-3.12	0.006
Positive	783.479_4.3649	-3.12	0.019
Positive	377.7291_3.8236	-3.13	0.035
Positive	451.7792_3.8998	-3.13	0.022
Positive	181.1226_3.5359	-3.16	0.041
Positive	231.1135_3.4172	-3.18	0.005
Negative	131.0344_1.4294	-3.19	0.016
Positive	227.129_3.5401	-3.21	4.0E-04
Positive	741.465_3.8812	-3.22	0.006
Positive	466.7836_3.7877	-3.30	0.034
Positive	545.8179_3.8941	-3.31	0.029
Negative	229.0975_3.3707	-3.32	0.019
Positive	615.5551_5.2136	-3.37	0.035
Negative	245.1386_4.2957	-3.39	0.006
Negative	163.1148_3.6399	-3.41	0.010
Negative	331.1907_8.1156	-3.42	0.010
Negative	229.1456_3.6622	-3.47	2.1E-04

Positive	680.421_4.2548	-3.47	0.029	
Positive	465.7782_3.795	-3.52	0.009	
Positive	179.107_3.6549	-3.55	0.003	
Positive	207.1035_3.6551	-3.56	0.037	
Negative	301.2015_5.4483	-3.56	5.5E-05	
Positive	307.2029_5.2062	-3.63	0.026	
Positive	595.3488_4.583	-3.63	3.9E-06	
Positive	479.2784_3.8324	-3.65	0.015	
Negative	319.166_4.5962	-3.65	5.0E-10	Androsta-1,4-diene-3,17-dione
Negative	263.0896_3.7683	-3.68	4.9E-02	
Negative	359.1897_5.7837	-3.69	0.001	
Negative	265.1055_3.6138	-3.69	0.044	
Negative	181.0869_3.7611	-3.71	4.5E-04	
Negative	321.2072_5.9243	-3.74	0.021	
Positive	619.3484_6.1341	-3.76	0.011	
Negative	443.0079_3.5033	-3.78	0.030	
Positive	519.3238_3.8593	-3.80	0.026	
Negative	87.0446_1.4442	-3.81	0.015	
Negative	277.0502_0.9365	-3.82	1.9E-04	
Positive	210.1132_1.3534	-3.82	0.029	
Positive	584.3554_4.2064	-3.83	0.024	
Positive	211.1329_3.6523	-3.85	0.008	
Positive	488.7993_3.8092	-3.85	0.002	
Positive	271.1652_2.8472	-3.85	0.004	
Positive	135.1169_3.5732	-3.88	0.002	
Negative	209.0796_4.304	-3.90	0.013	
Negative	131.0713_2.5122	-3.91	0.002	
Positive	455.2477_3.3201	-3.93	0.009	
Positive	211.134_5.033	-3.93	0.011	
Positive	611.3472_4.111	-3.95	2.4E-04	
Negative	315.1227_4.174	-3.97	1.1E-04	
Positive	121.1027_3.5352	-3.97	3.8E-04	
Positive	191.106_3.5461	-3.98	3.1E-04	
Positive	343.1625_4.4913	-4.04	0.003	
Positive	309.1775_3.0874	-4.04	0.006	Androstenedione
Negative	379.2119_5.1469	-4.10	0.003	
Positive	509.8048_4.0186	-4.14	3.3E-04	
Positive	267.121_3.5344	-4.15	0.002	
Negative	373.2739_8.5093	-4.15	0.009	
Positive	636.3947_4.2305	-4.16	0.024	
Positive	156.103_2.8948	-4.23	2.1E-05	
Negative	231.0984_0.8264	-4.24	1.2E-04	
Negative	305.1863_5.2337	-4.24	0.007	
Positive	321.1808_4.5154	-4.25	3.6E-09	
Positive	313.1082_4.169	-4.29	0.003	
Positive	221.1444_3.9338	-4.29	0.007	
Negative	201.0118_0.997	-4.30	0.046	

Negative	280.029_1.1019	-4.31	0.002	
Negative	159.0659_3.2534	-4.33	0.004	
Positive	182.117_5.0401	-4.34	1.0E-04	
Positive	348.1459_4.1753	-4.36	0.003	
Positive	457.2624_3.8029	-4.37	0.002	
Positive	553.3347_4.1701	-4.43	0.009	
Positive	399.2283_5.1237	-4.56	0.003	
Negative	418.2135_4.6056	-4.57	0.020	
Negative	285.1132_5.0484	-4.58	5.1E-06	
Positive	472.2435_4.5582	-4.61	6.4E-04	
Positive	265.1057_3.6562	-4.61	5.6E-04	
Positive	722.4452_5.9167	-4.62	0.014	
Negative	595.3497_6.2462	-4.64	6.1E-04	
Positive	633.2972_4.5636	-4.65	1.3E-04	
Positive	434.2642_4.4206	-4.67	0.009	
Positive	307.1646_4.3363	-4.69	0.032	
Positive	311.1603_2.4386	-4.74	0.022	
Negative	243.1234_3.6176	-4.81	5.7E-08	
Positive	325.174_3.8063	-4.85	1.2E-04	
Positive	329.184_5.0261	-4.85	1.5E-06	
Positive	564.3587_3.8192	-4.86	0.003	
Negative	209.0673_2.6988	-4.88	3.0E-04	
Negative	295.062_0.8812	-4.89	0.003	
Negative	305.1864_5.0961	-4.90	1.1E-04	
Positive	281.1174_4.0698	-4.90	0.005	
Negative	609.3293_4.4399	-4.92	1.6E-07	
Negative	720.4337_5.9728	-4.95	0.038	
Negative	323.1577_3.9981	-4.99	1.1E-04	
Positive	311.1609_3.0473	-4.99	7.9E-04	
Positive	174.1138_2.9138	-5.04	1.2E-05	
Positive	487.2935_3.9841	-5.04	0.001	
Positive	309.1812_4.1209	-5.08	7.2E-07	
Positive	295.0971_4.2243	-5.09	0.001	
Negative	351.0859_4.2565	-5.15	0.027	
Positive	283.1654_2.3657	-5.19	2.7E-04	
Negative	593.3325_4.6412	-5.19	2.8E-13	Stercobilin
Negative	365.1967_4.8918	-5.22	1.1E-03	
Positive	307.2017_5.0302	-5.22	5.7E-08	
Negative	385.1686_4.3367	-5.28	0.050	
Positive	420.2279_4.5397	-5.30	8.3E-07	
Positive	182.0816_4.2585	-5.34	7.6E-06	
Positive	370.2227_4.4035	-5.37	0.009	
Positive	595.3505_4.8372	-5.37	3.8E-06	
Negative	486.2245_4.4763	-5.40	0.046	
Positive	317.1512_4.5777	-5.42	1.1E-07	
Positive	309.1807_3.958	-5.52	2.3E-05	
Positive	617.3315_4.5958	-5.61	2.8E-13	

Positive	226.1076_1.7987	-5.69	4.2E-04
Negative	549.3429_4.6457	-5.75	4.8E-09
Positive	611.3437_4.3716	-5.79	6.9E-13
Positive	597.3657_6.1306	-5.80	2.1E-07
Negative	615.3157_4.642	-5.81	3.0E-10
Negative	285.1131_4.4155	-5.96	0.001
Negative	472.2444_4.6966	-5.98	0.027
Negative	470.2283_4.6311	-6.03	2.2E-07
Positive	607.3137_4.8497	-6.08	0.002
Negative	307.1662_4.1964	-6.15	1.2E-07
Positive	265.1539_1.9924	-6.18	0.002
Positive	635.3769_5.0283	-6.26	2.8E-05
Positive	641.3519_4.4885	-6.33	4.5E-06
Positive	325.1758_2.7968	-6.33	1.9E-06
Negative	635.3083_4.2934	-6.44	2.8E-08
Positive	470.2656_4.3837	-6.76	2.5E-07
Positive	305.1866_4.2135	-6.87	4.2E-06
Positive	613.3624_5.1518	-6.98	2.4E-08
Positive	638.3293_4.2388	-7.00	4.4E-08
Negative	285.1127_4.2733	-7.16	5.2E-10
Negative	261.1605_4.07	-7.26	4.8E-07
Negative	313.1085_4.5438	-7.49	2.3E-08
Positive	625.3591_4.6659	-7.67	2.1E-10
Negative	593.334_4.8291	-7.70	8.4E-14
Negative	623.3431_4.5972	-7.84	3.3E-11
Negative	611.3452_5.2339	-7.93	2.2E-07
Negative	327.0882_4.1465	-8.01	4.2E-09
Negative	341.1492_4.5729	-8.30	2.1E-07
Negative	261.1602_4.3845	-8.36	1.5E-08
Negative	261.1598_3.8294	-8.62	2.4E-08
Positive	637.322_4.2281	-8.62	4.7E-16
Positive	625.3596_4.495	-8.71	4.7E-16