Supplementary Information (SI) for Analyst.
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Supporting Information

Impact of Preparation Methods and Storage Conditions for Optimization of the Fecal Metabolome Storage Stability

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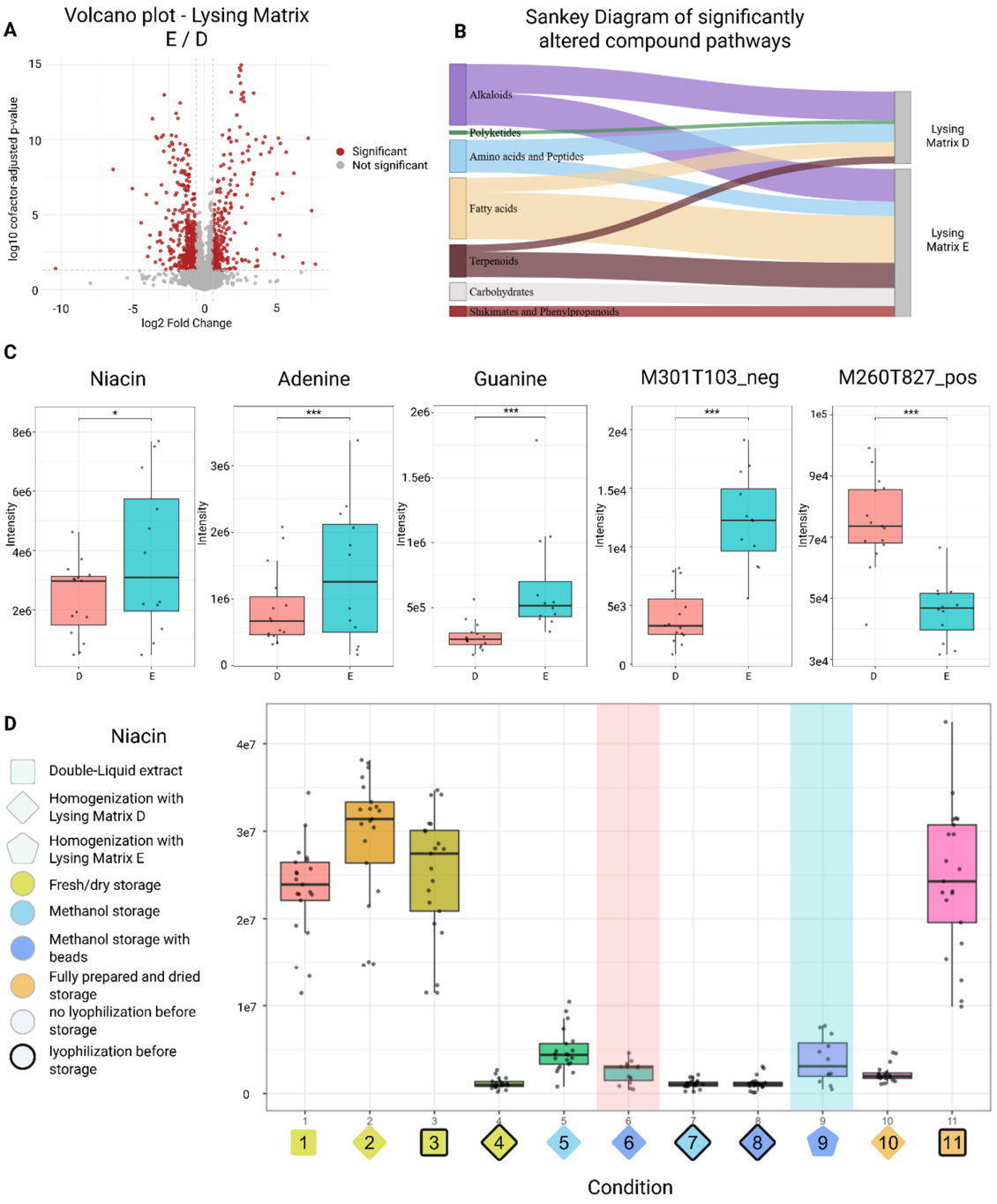

Figure S1. Statistical overview of lysing matrix E vs Lysing matrix D.

A) Volcano plot of the lysing matrix effect of individual metabolomic features (n = 8895, significance = 745, upregulated for lysing matrix E = 312, upregulated for lysing matrix D = 433). Y-axis utilizing -log10 of p-value (< 0.05) obtained with linear model with cofactor adjustment, where collection day, lyophilization, and methanol storage status before storage were adjusted for. The x-axis represents the log2 Fold change (>1.5 or <1/1.5) of estimated marginal means (EMM). Significantly altered features denoted with red color. B) Sankey diagram of NPClassifier-predicted pathways of significantly altered metabolites (n = 61). Line thickness corresponds to the relative number of metabolites per pathway. C) Boxplots of annotated significantly altered metabolites (annotated metabolites confidence level = 1). Statistical significance within a factor is indicated as: *** p < 0.001, ** p < 0.01, * p < 0.05. Group colors: Lysing matrix D – magenta; Lysing matrix E – cyan. D) Extended boxplot of Nicotinic acid with all 11 experimental conditions compared. Each condition denoted with different color-shape-border combination, with legend to the left of the plot area.

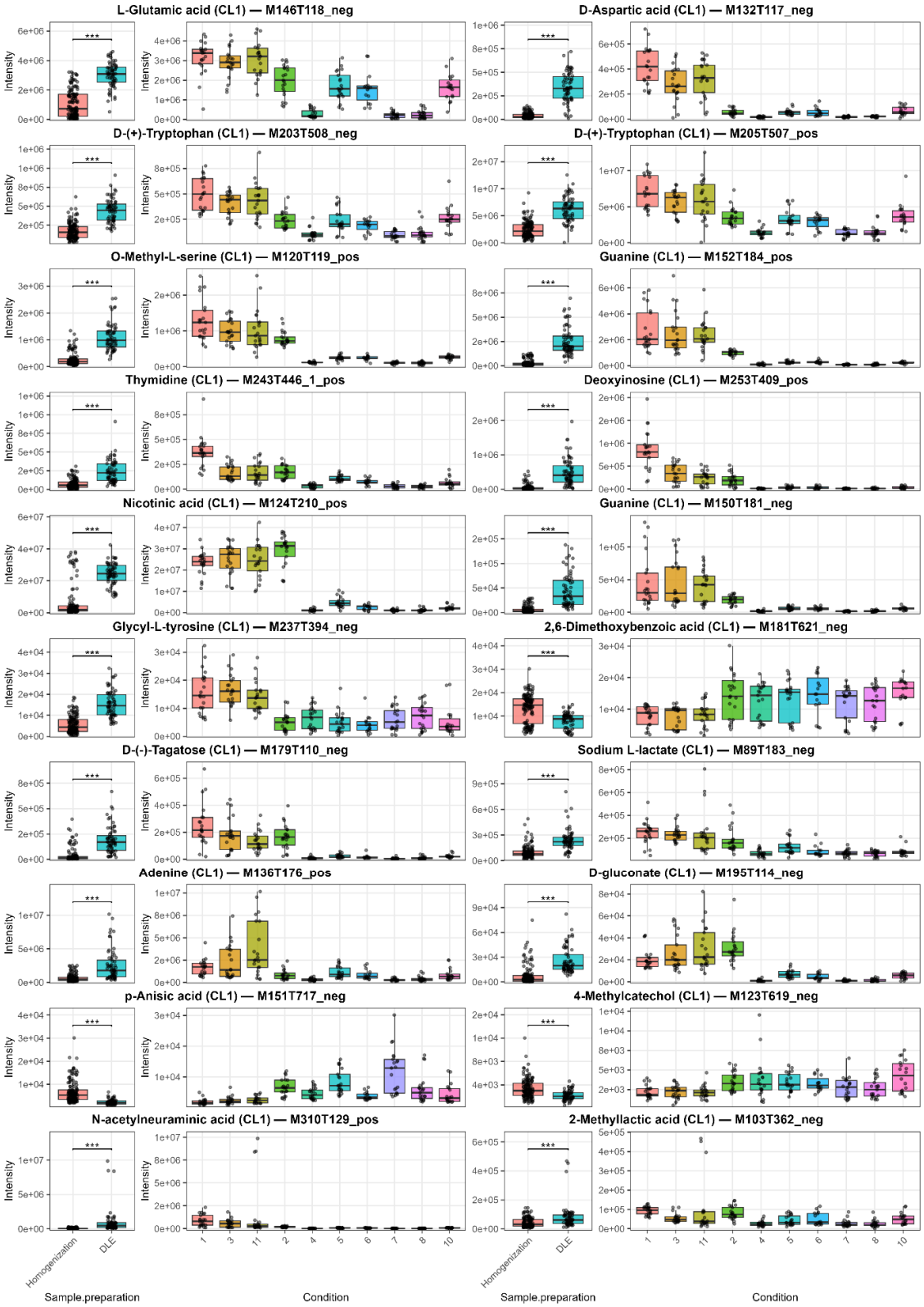

Figure S2. Top 20 significantly altered features for sample preparation method comparison.

For each metabolite 2 plots are presented. Title contains structure annotation at achieved confidence level (CL) and XCMS feature ID with ionization mode indication. 2-group boxplots indicate statistical significance within a factor with asterisks, coded as: *** p < 0.001, ** p < 0.01, * p < 0.05. Group colors: Homogenization – magenta; DLE – cyan. Extended boxplots with all 11 experimental conditions. Each condition denoted with different color.

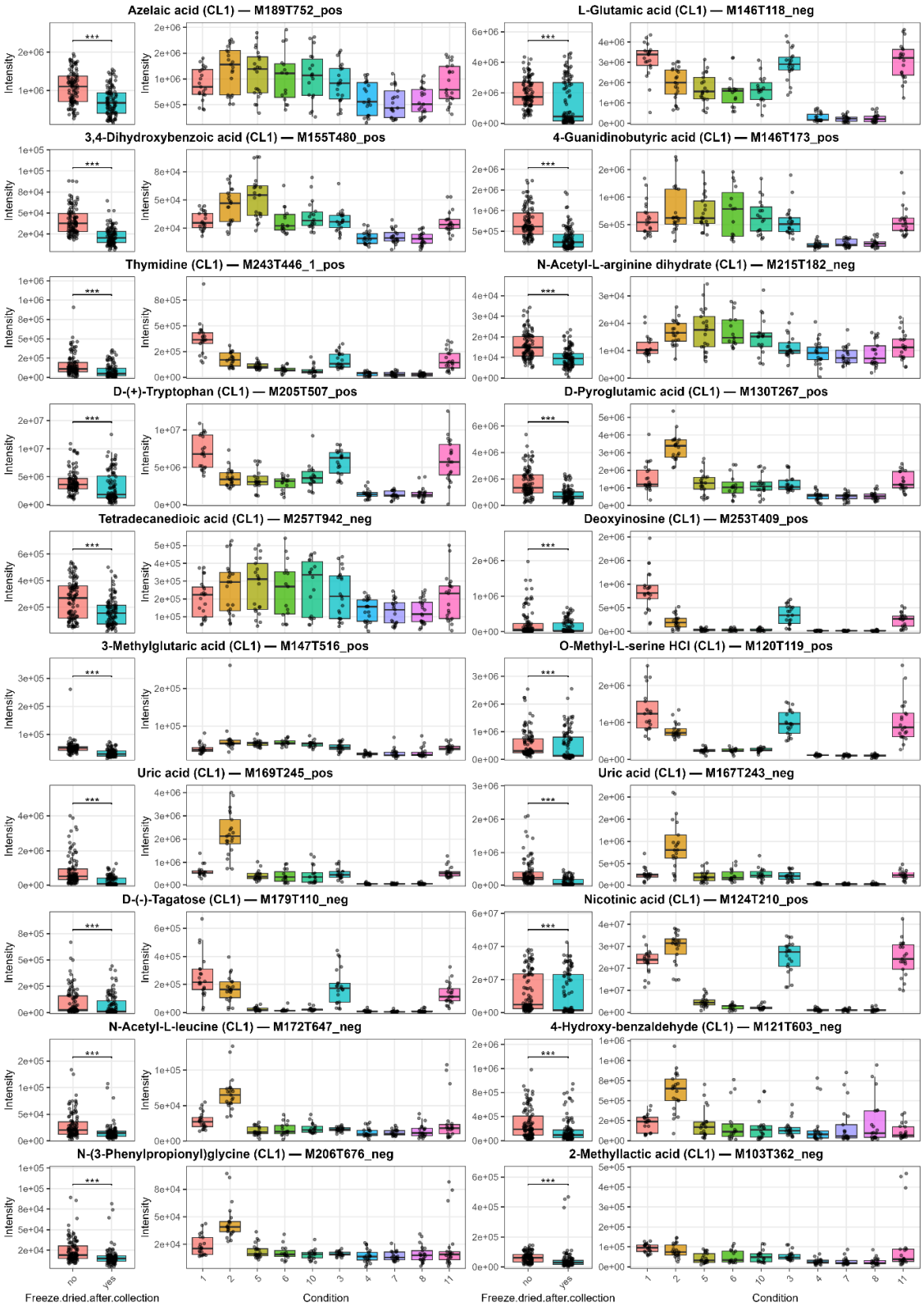

Figure S3. Top 20 significantly altered features for lyophilized storage comparison.

For each metabolite 2 plots are presented. Title contains structure annotation at achieved confidence level (CL) and XCMS feature ID with ionization mode indication. 2-group boxplots indicate statistical significance within a factor with asterisks, coded as: *** $p < 0.001$, ** $p < 0.01$, * $p < 0.05$. Group colors: not lyophilized – magenta; lyophilized – cyan. Extended boxplots with all 11 experimental conditions. Each condition denoted with different color.

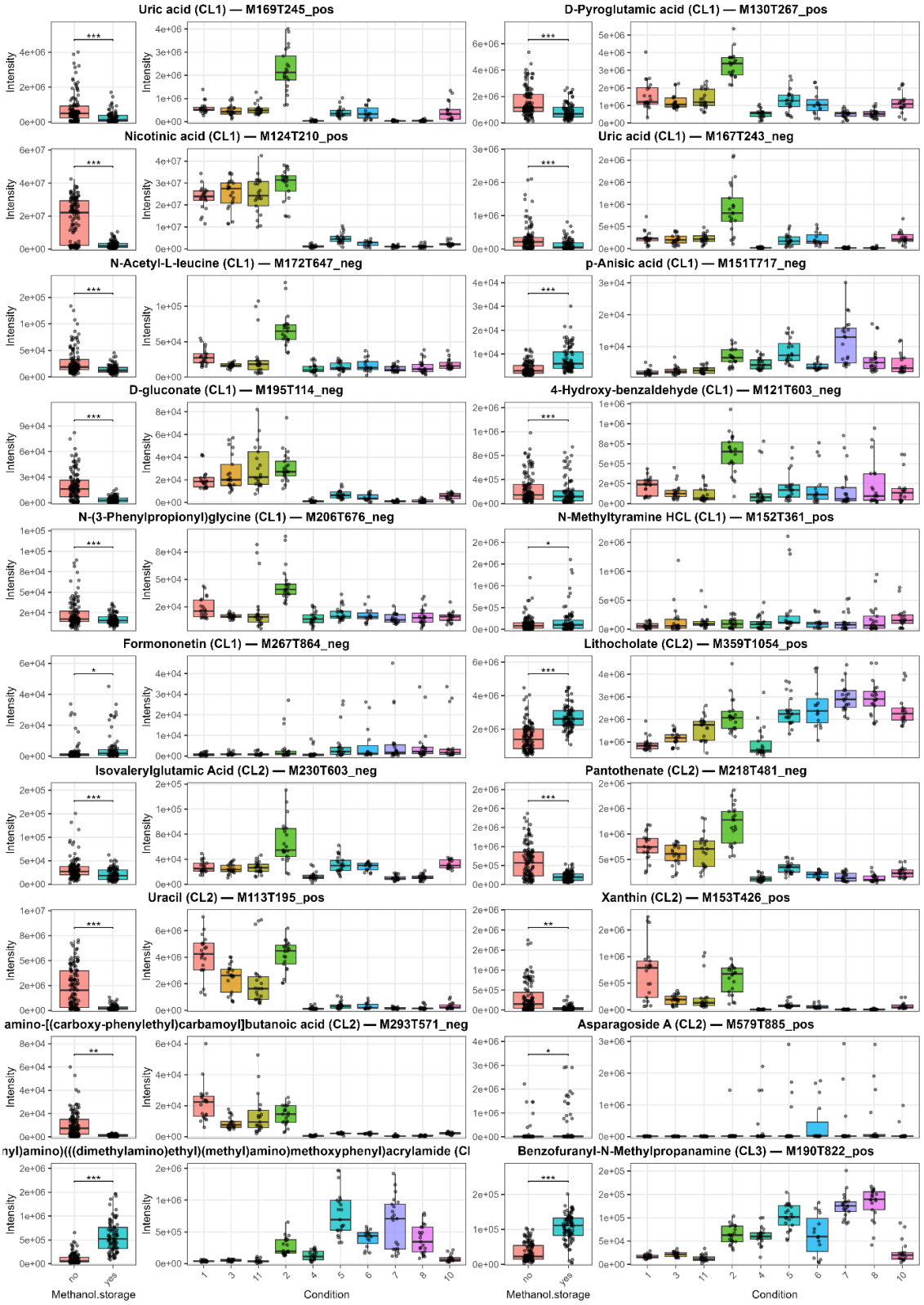

Figure S4. Top 20 significantly altered features for methanol storage comparison.

For each metabolite 2 plots are presented. Title contains structure annotation at achieved confidence level (CL) and XCMS feature ID with ionization mode indication. 2-group boxplots indicate statistical significance within a factor with asterisks, coded as: *** p < 0.001, ** p < 0.01, * p < 0.05. Group colors: fresh/dry – magenta; in methanol – cyan. Extended boxplots with all 11 experimental conditions. Each condition denoted with different color.

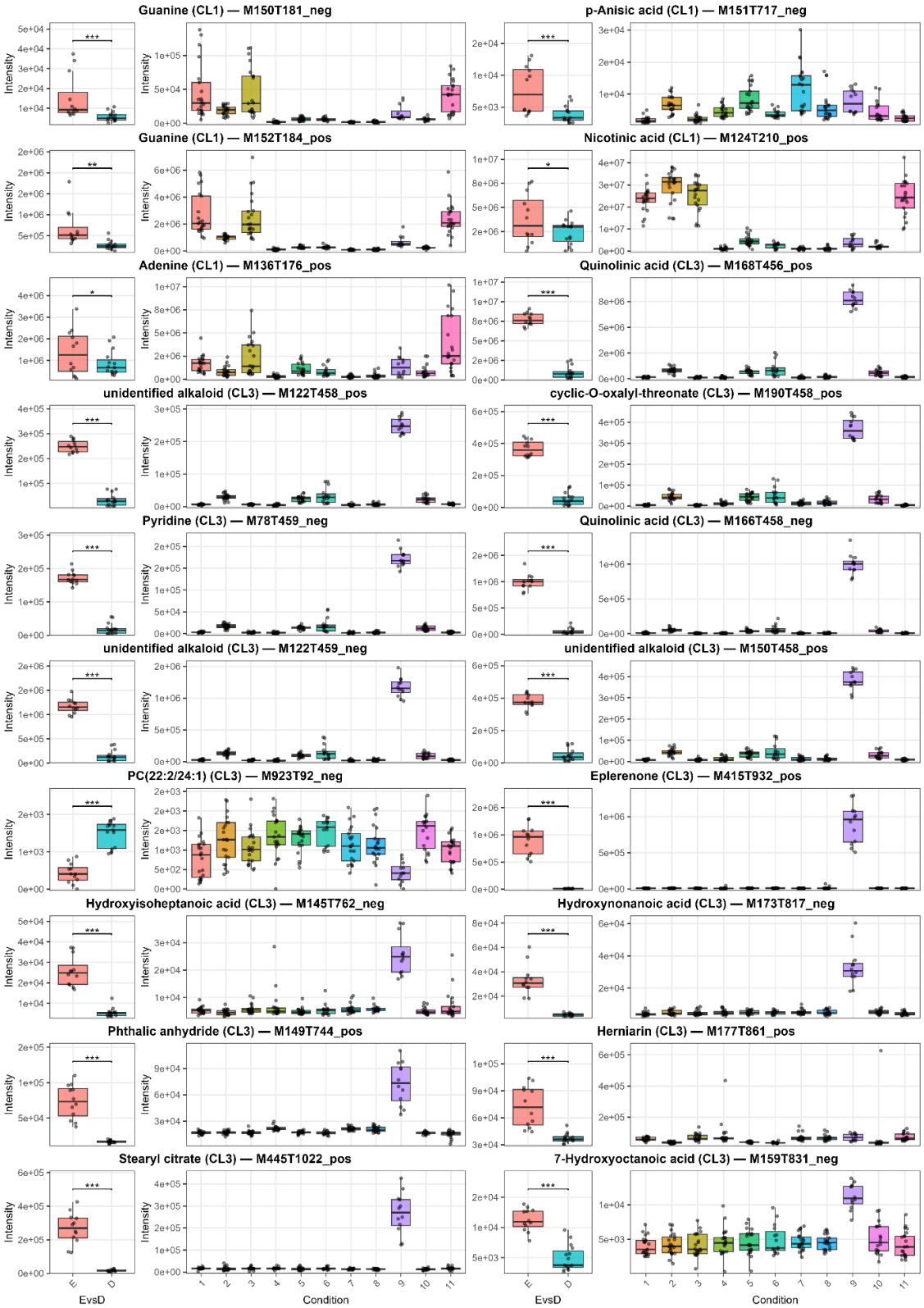

Figure S5. Top 20 significantly altered features for lysing matrix E vs D comparison.

For each metabolite 2 plots are presented. Title contains structure annotation at achieved confidence level (CL) and XCMS feature ID with ionization mode indication. 2-group boxplots indicate statistical significance within a factor with asterisks, coded as: *** p < 0.001, ** p < 0.01, * p < 0.05. Group colors: Lysing matrix D – magenta; Lysing matrix E – cyan. Extended boxplots with all 11 experimental conditions. Each condition denoted with different color.

Table S1. Table of annotated features.

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M124T210_pos	124.0393	210	1	Nicotinic acid	124.0393	213	C6H5NO2	Nicotinic acid	Alkaloids	HMDB0001488	Nicotinic acid	C6H5NO2	0.2
M314T375_pos	314.0921	375	1	Methylthioadenosine sulfoxide	314.0921	369			Carbohydrates	HMDB0245242	2-Methylthioadenosine	C11H15N5O4S	1.1
M121T603_neg	121.0296	603	1	4-Hydroxy-benzaldehyde	121.0298	603				HMDB0001870	Benzoic acid	C7H6O2	0.5
M151T717_neg	151.0402	717	1	p-Anisic acid	151.0400	721				HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.6
M163T540_pos	163.0393	540	1	6-Hydroxycoumaran	163.0391	528				HMDB0002149	3 Hydroxycoumarin	C9H6O3	1.9
M205T507_pos	205.0972	507	1	D-(+)-Tryptophan	205.0975	504				HMDB0000929	L-Tryptophan	C11H12N2O2	0.1
M120T119_pos	120.0656	119	1	O-Methyl-L-serine HCl	120.0655	118				HMDB0000167	L-Threonine	C4H9NO3	0.6
M130T267_pos	130.0499	267	1	D-Pyroglutamic acid	130.0498	263			Amino acids and Peptides	HMDB0000267	Pyroglutamic acid	C5H7NO3	0.4
M136T176_pos	136.0618	176	1	Adenine	136.0617	175			Alkaloids	HMDB0000034	Adenine	C5H5N5	0.3
M152T184_pos	152.0563	184	1	Guanine	152.0566	186			Amino acids and Peptides	HMDB0249989	Amino-4-methylsulfanyl-butane-1	C5H13NS2	0.6
M169T245_pos	169.0357	245	1	Uric acid	169.0356	244				HMDB0000289	Uric acid	C5H4N4O3	0.5
M243T446_1_pos	243.0977	446	1	Thymidine	243.0974	449				HMDB0000273	Thymidine	C10H14N2O5	0.8
M253T409_pos	253.0932	409	1	Deoxyinosine	253.0931	405				HMDB0000071	Deoxyinosine	C10H12N4O4	0.1
M146T118_neg	146.0459	118	1	L-Glutamic acid	146.0458	115			Amino acids and Peptides	HMDB0000148	L-Glutamic acid	C5H9NO4	0.2
M206T676_neg	206.0823	676	1	N-(3-Phenylpropionyl)glycine	206.0822	675	C11H13NO3	Afalanine	Amino acids and Peptides	HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	0.3
M103T362_neg	103.0401	362	1	2-Methyllactic acid	103.0400	360				HMDB0000008	2-Hydroxybutyric acid	C4H8O3	0.2
M150T181_neg	150.0421	181	1	Guanine	150.0420	186			Alkaloids	HMDB0000132	Guanine	C5H5N5O	0.3
M167T243_neg	167.0211	243	1	Uric acid	167.0210	246			Alkaloids	HMDB0000289	Uric acid	C5H4N4O3	0.3
M172T647_neg	172.0980	647	1	N-Acetyl-L-leucine	172.0978	650				HMDB0000701	Hexanoylglycine	C8H15NO3	0.5
M179T110_neg	179.0561	110	1	D-(-)-Tagatose	179.0560	109				HMDB0000122	D-Glucose	C6H12O6	0.1
M195T114_neg	195.0510	114	1	D-gluconate	195.0483	116				HMDB0000565	Galactonic acid	C6H12O7	0.0
M267T864_neg	267.0665	864	1	Formononetin	267.0663	865			Shikimates and Phenylpropanoids	HMDB0005808	Formononetin	C16H12O4	0.8
M152T361_pos	152.1070	361	1	N-Methyltyramine HCL	152.1070	361				HMDB0001387	N-Methylphenylethanolamine	C9H13NO	0.2
M189T752_pos	189.1122	752	1	Azelaic acid	189.1118	751			Fatty acids	HMDB0000784	Azelaic acid	C9H16O4	0.2
M146T173_pos	146.0924	173	1	4-Guanidinobutyric acid	146.0924	173				HMDB0003464	4-Guanidinobutanoic acid	C5H11N3O2	0.3
M147T516_pos	147.0652	516	1	3-Methylglutaric acid	147.0652	516				HMDB0000422	2-Methylglutaric acid	C6H10O4	0.2
M155T480_pos	155.0335	480	1	3,4-Dihydroxybenzoic acid	155.0339	478				HMDB0000152	Gentisic acid	C7H6O4	2.5
M310T129_pos	310.1135	129	1	N-acetylneuraminic acid	310.1134	129				HMDB0000230	N-Acetylneuraminic acid	C11H19NO9	0.7
M203T508_neg	203.0827	508	1	D-(+)-Tryptophan	203.0825	503	C11H12N2O2	Tryptophan	Amino acids and Peptides	HMDB0000929	L-Tryptophan	C11H12N2O2	0.3
M257T942_neg	257.1758	942	1	Tetradecanedioic acid	257.1762	939			Fatty acids	HMDB0000872	Tetradecanedioic acid	C14H26O4	0.1
M89T183_neg	89.0244	183	1	Sodium L-lactate	89.0243	181				HMDB0244144	1,2,4-Trioxane	C3H6O3	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M124T210_pos	124.0393	210	1	2.63E-27	0.23	TRUE	2.08E-08	1.82	TRUE	5.16E-07	1.58	TRUE	2.37E-02	1.85	TRUE
M314T375_pos	314.0921	375	1	3.47E-03	1.67	TRUE	7.21E-04	0.55	TRUE	9.36E-12	0.30	TRUE	2.78E-03	1.66	TRUE
M121T603_neg	121.0296	603	1	4.53E-04	1.64	TRUE	2.56E-04	1.69	TRUE	3.40E-06	1.79	TRUE	7.14E-01	1.05	FALSE
M151T717_neg	151.0402	717	1	1.79E-09	1.68	TRUE	2.29E-05	0.59	TRUE	9.74E-03	0.83	FALSE	5.67E-04	1.54	TRUE
M163T540_pos	163.0393	540	1	8.95E-03	0.53	TRUE	2.91E-02	1.78	TRUE	5.62E-05	2.44	TRUE	5.07E-01	1.46	FALSE
M205T507_pos	205.0972	507	1	6.89E-44	0.37	TRUE	1.36E-01	1.08	FALSE	7.61E-18	1.52	TRUE	2.89E-02	1.17	FALSE
M120T119_pos	120.0656	119	1	1.76E-42	0.22	TRUE	2.95E-04	1.32	FALSE	1.85E-11	1.58	TRUE	8.39E-01	0.98	FALSE
M130T267_pos	130.0499	267	1	5.29E-02	0.82	FALSE	1.34E-08	1.84	TRUE	1.94E-17	2.38	TRUE	4.19E-01	1.10	FALSE
M136T176_pos	136.0618	176	1	3.88E-17	0.26	TRUE	9.62E-01	1.01	FALSE	7.50E-01	1.04	FALSE	2.49E-02	1.64	TRUE
M152T184_pos	152.0563	184	1	2.45E-42	0.10	TRUE	1.25E-01	1.16	FALSE	3.10E-03	1.27	FALSE	1.61E-03	2.55	TRUE
M169T245_pos	169.0357	245	1	7.51E-01	0.93	FALSE	8.93E-09	5.73	TRUE	2.71E-11	6.29	TRUE	1.24E-01	1.43	FALSE
M243T446_1_pos	243.0977	446	1	8.48E-34	0.26	TRUE	3.92E-01	1.08	FALSE	3.55E-20	2.09	TRUE	2.30E-01	1.20	FALSE
M253T409_pos	253.0932	409	1	5.23E-32	0.08	TRUE	4.58E-01	1.10	FALSE	2.69E-12	2.29	TRUE	5.26E-01	0.88	FALSE
M146T118_neg	146.0459	118	1	4.64E-58	0.32	TRUE	3.59E-02	1.10	FALSE	6.46E-31	1.73	TRUE	7.91E-02	0.80	FALSE
M206T676_neg	206.0823	676	1	7.37E-01	0.96	FALSE	3.15E-04	1.51	TRUE	8.49E-06	1.55	TRUE	6.14E-01	1.07	FALSE
M103T362_neg	103.0401	362	1	3.65E-07	0.48	TRUE	1.23E-01	1.24	FALSE	3.73E-04	1.53	TRUE	6.46E-02	1.20	FALSE
M150T181_neg	150.0421	181	1	4.29E-27	0.12	TRUE	2.49E-01	1.16	FALSE	1.79E-02	1.30	FALSE	4.53E-04	3.56	TRUE
M167T243_neg	167.0211	243	1	9.93E-01	1.00	FALSE	3.51E-07	4.79	TRUE	1.40E-10	6.59	TRUE	4.41E-01	1.22	FALSE
M172T647_neg	172.0980	647	1	8.19E-01	0.96	FALSE	5.54E-07	2.46	TRUE	1.53E-06	2.11	TRUE	5.18E-01	0.83	FALSE
M179T110_neg	179.0561	110	1	2.26E-24	0.16	TRUE	2.05E-03	1.49	FALSE	9.15E-08	1.85	TRUE	2.85E-01	1.51	FALSE
M195T114_neg	195.0510	114	1	2.87E-16	0.26	TRUE	5.98E-05	1.77	TRUE	8.03E-04	1.48	FALSE	8.16E-01	1.03	FALSE
M267T864_neg	267.0665	864	1	8.37E-05	2.68	TRUE	2.01E-02	0.55	TRUE	5.75E-01	1.12	FALSE	8.82E-01	0.97	FALSE
M152T361_pos	152.1070	361	1	3.02E-01	1.18	FALSE	1.21E-02	0.63	TRUE	4.58E-01	1.11	FALSE	7.15E-01	1.08	FALSE
M189T752_pos	189.1122	752	1	2.87E-03	0.90	FALSE	2.84E-03	1.12	FALSE	1.28E-31	1.55	TRUE	2.61E-01	0.93	FALSE
M146T173_pos	146.0924	173	1	4.90E-07	0.67	FALSE	8.55E-01	1.01	FALSE	1.50E-22	2.17	TRUE	7.08E-01	0.94	FALSE
M147T516_pos	147.0652	516	1	4.68E-01	0.95	FALSE	3.25E-01	1.08	FALSE	7.53E-12	1.60	TRUE	7.46E-02	0.92	FALSE
M155T480_pos	155.0335	480	1	4.94E-04	0.83	FALSE	7.46E-01	0.98	FALSE	2.77E-25	1.77	TRUE	1.42E-01	1.13	FALSE
M310T129_pos	310.1135	129	1	8.93E-08	0.06	TRUE	7.40E-01	1.12	FALSE	9.72E-01	1.01	FALSE	2.80E-01	1.14	FALSE
M203T508_neg	203.0827	508	1	2.66E-46	0.37	TRUE	1.09E-01	1.09	FALSE	1.36E-15	1.45	FALSE	1.42E-02	1.21	FALSE
M257T942_neg	257.1758	942	1	7.17E-03	0.87	FALSE	3.64E-01	1.05	FALSE	2.28E-17	1.53	TRUE	7.45E-01	1.03	FALSE
M89T183_neg	89.0244	183	1	1.34E-21	0.38	TRUE	1.90E-01	1.12	FALSE	1.32E-03	1.27	FALSE	7.40E-01	1.09	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M123T619_neg	123.0450	619	1	4-Methylcatechol	123.0452	617				HMDB0000873	4-Methylcatechol	C7H8O2	1.2
M132T117_neg	132.0303	117	1	D-Aspartic acid	132.0302	113	C4H7NO4	Aspartic acid	Amino acids and Peptides	HMDB0000191	L-Aspartic acid	C4H7NO4	0.5
M181T621_neg	181.0507	621	1	2,6-Dimethoxybenzoic acid	181.0506	621				HMDB0000118	Homovanillic acid	C9H10O4	0.3
M215T182_neg	215.1149	182	1	N-Acetyl-L-arginine dihydrate	215.1149	184			Amino acids and Peptides	HMDB0004620	N-a-Acetyl-L-arginine	C8H16N4O3	0.2
M237T394_neg	237.0886	394	1	Glycyl-L-tyrosine	237.0881	395	C11H14N2O4	2-(2-aminoacetamido)-3-(4-hydroxyphenyl)propanoic acid	Amino acids and Peptides	HMDB0015084	Felbamate	C11H14N2O4	2.4
M297T784_neg	297.1131	784	1	Enterolactone	297.1140	777	C18H18O4	Hpmf	Shikimates and Phenylpropanoids	HMDB0004808	7C-aglycone	C18H18O4	0.5
M290T356_pos	290.1349	356	1	Ophtalmic acid	290.1347	346				HMDB0005765	Ophthalmic acid	C11H19N3O6	0.7
M299T784_pos	299.1279	784	1	Enterolactone	299.1280	777				HMDB0004808	7C-aglycone	C18H18O4	0.5
M203T807_pos	203.1279	807	1	Sebacic acid	203.1271	807			Fatty acids	HMDB0000792	Sebacic acid	C10H18O4	0.5
M286T923_pos	286.1440	923	1	Piperine	286.1437	920				HMDB0014440	Morphine	C17H19NO3	0.7
M538T1074_pos	537.5356	1074	1	β-Carotene	537.5330	1074							
M103T82_pos	103.1230	82	1	1,5-Diaminopentane	103.1231	87				HMDB0002322	Cadaverine	C5H14N2	0.7
M153T601_pos	153.0546	601	1	o-Hydroxyphenylacetic acid	153.0547	603				HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.1
M196T475_1_pos	196.0605	475	1	2-[(4-Hydroxyphenyl)formamido]acetic acid	196.0604	471				HMDB0000840	Salicyluric acid	C9H9NO4	0.6
M208T676_pos	208.0968	676	1	N-(3-Phenylpropionyl)glycine	208.0968	674				HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	0.0
M303T858_pos	303.1607	858	1	Nordihydroguaiaretic Acid	303.1595	861							
M151T600_neg	151.0401	600	1	o-Hydroxyphenylacetic acid	151.0400	603				HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.5
M117T436_neg	117.0558	436	1	β-Hydroxyisovaleric acid	117.0556	438				HMDB0000351	(3R)-3-Hydroxy-2-methylbutanoic a	C5H10O3	0.8
M130T126_neg	130.0623	126	1	Creatine	130.0605	125				HMDB0000064	Creatine	C4H9N3O2	0.6
M145T526_neg	145.0507	526	1	2-Methylglutaric acid	145.0506	525				HMDB0000422	2-Methylglutaric acid	C6H10O4	0.6
M121T777_pos	121.0648	777	1	4-Vinylphenol	121.0649	772				HMDB0004072	4-Hydroxystyrene	C8H8O	0.2
M113T195_pos	113.0346	195	2				C4H4N2O2	Uracil		HMDB0000300	Uracil	C4H4N2O2	0.3
M153T426_pos	153.0408	426	2				C5H4N4O2	Xanthin	Alkaloids	HMDB0000292	Xanthine	C5H4N4O2	0.4
M218T481_neg	218.1034	481	2				C9H17NO5	Pantothenate	Fatty acids	HMDB0000210	Pantothenic acid	C9H17NO5	0.1
M293T571_neg	293.1144	571	2				C14H18N2O5	2-amino-4-[(1-carboxy-2-phenylethyl)carbamoyl]butanoic acid	Amino acids and Peptides	HMDB0000594	gamma-Glutamylphenylalanine	C14H18N2O5	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M123T619_neg	123.0450	619	1	3.45E-09	1.57	TRUE	6.46E-04	1.30	FALSE	1.12E-02	1.17	FALSE	5.37E-01	1.05	FALSE
M132T117_neg	132.0303	117	1	6.13E-58	0.10	TRUE	8.30E-01	0.98	FALSE	6.84E-07	1.37	FALSE	1.99E-01	1.22	FALSE
M181T621_neg	181.0507	621	1	3.60E-25	1.64	TRUE	1.74E-01	1.06	FALSE	2.60E-03	1.11	FALSE	2.13E-01	0.90	FALSE
M215T182_neg	215.1149	182	1	5.76E-01	1.03	FALSE	9.38E-01	1.00	FALSE	2.59E-18	1.55	TRUE	6.07E-01	1.05	FALSE
M237T394_neg	237.0886	394	1	9.24E-26	0.37	TRUE	7.29E-01	1.03	FALSE	1.06E-01	0.90	FALSE	3.72E-01	1.70	FALSE
M297T784_neg	297.1131	784	1	3.56E-51	4.89	TRUE	2.18E-05	0.75	FALSE	2.46E-06	0.76	FALSE	4.20E-01	0.91	FALSE
M290T356_pos	290.1349	356	1	6.66E-04	0.87	FALSE	9.61E-01	1.00	FALSE	1.86E-28	1.61	TRUE	8.96E-01	1.01	FALSE
M299T784_pos	299.1279	784	1	1.64E-47	2.84	TRUE	1.41E-03	0.85	FALSE	3.09E-02	1.10	FALSE	9.68E-01	1.00	FALSE
M203T807_pos	203.1279	807	1	4.95E-01	0.98	FALSE	3.63E-02	1.08	FALSE	7.38E-10	1.21	FALSE	1.72E-01	0.89	FALSE
M286T923_pos	286.1440	923	1	6.40E-02	3.51	FALSE	4.06E-01	0.56	FALSE	4.27E-01	1.52	FALSE	1.28E-01	-0.26	FALSE
M538T1074_pos	537.5356	1074	1	7.32E-01	0.98	FALSE	5.19E-01	1.03	FALSE	9.26E-01	1.00	FALSE	3.76E-01	1.13	FALSE
M103T82_pos	103.1230	82	1	1.72E-02	0.80	FALSE	1.41E-01	1.15	FALSE	8.27E-04	1.32	FALSE	1.66E-01	0.62	FALSE
M153T601_pos	153.0546	601	1	2.99E-05	1.22	FALSE	6.68E-01	1.02	FALSE	1.46E-05	1.20	FALSE	2.09E-01	0.96	FALSE
M196T475_1_pos	196.0605	475	1	4.09E-01	0.92	FALSE	8.67E-01	0.98	FALSE	1.61E-01	1.13	FALSE	3.45E-01	1.17	FALSE
M208T676_pos	208.0968	676	1	1.11E-03	1.21	FALSE	7.91E-04	1.23	FALSE	2.68E-11	1.44	FALSE	7.83E-01	0.97	FALSE
M303T858_pos	303.1607	858	1	1.69E-01	0.92	FALSE	1.51E-02	1.16	FALSE	2.22E-04	1.20	FALSE	2.48E-01	1.10	FALSE
M151T600_neg	151.0401	600	1	2.02E-07	1.23	FALSE	7.20E-01	1.01	FALSE	7.64E-09	1.22	FALSE	2.86E-01	1.06	FALSE
M117T436_neg	117.0558	436	1	5.70E-09	1.32	FALSE	2.29E-01	1.06	FALSE	1.59E-01	1.06	FALSE	7.93E-01	1.01	FALSE
M130T126_neg	130.0623	126	1	9.62E-02	1.58	FALSE	5.98E-02	0.61	FALSE	4.09E-01	0.82	FALSE	6.00E-01	0.91	FALSE
M145T526_neg	145.0507	526	1	3.93E-01	0.91	FALSE	4.82E-01	1.09	FALSE	6.37E-04	1.41	FALSE	9.86E-01	0.99	FALSE
M121T777_pos	121.0648	777	1	9.80E-03	1.22	FALSE	1.37E-01	0.89	FALSE	2.31E-01	1.08	FALSE	3.82E-01	0.90	FALSE
M113T195_pos	113.0346	195	2	7.96E-18	0.23	TRUE	1.19E-06	1.98	TRUE	1.15E-11	2.39	TRUE	8.12E-01	1.09	FALSE
M153T426_pos	153.0408	426	2	2.04E-11	0.25	TRUE	1.56E-03	1.77	TRUE	2.74E-14	4.07	TRUE	3.18E-01	1.42	FALSE
M218T481_neg	218.1034	481	2	3.26E-10	0.48	TRUE	2.16E-07	1.84	TRUE	7.05E-11	1.95	TRUE	3.49E-02	1.26	FALSE
M293T571_neg	293.1144	571	2	1.70E-21	0.17	TRUE	3.15E-03	1.52	TRUE	8.17E-10	2.20	TRUE	2.30E-01	1.17	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M116T129_pos	116.0706	129	2				C5H9NO2	Proline	Amino acids and Peptides	HMDB0000162	L-Proline	C5H9NO2	0.1
M359T1054_pos	359.2941	1054	2				C24H40O3	Lithocholate	Terpenoids	HMDB0006322	Tetracosapentaenoic acid (24:5n-6	C24H38O2	1.1
M786T984_pos	785.5906	984	2				C48H80O8	10-Undecenoic acid 7alpha,12alpha-dihydroxy-24-[2-(10-undecenoyloxy)ethoxy]-24-oxo-5beta-cholane-3alpha-yl ester	Terpenoids				
M786T1024_2_pos	785.5925	1024	2				C48H80O8	10-Undecenoic acid 7alpha,12alpha-dihydroxy-24-[2-(10-undecenoyloxy)ethoxy]-24-oxo-5beta-cholane-3alpha-yl ester	Terpenoids				
M217T572_pos	217.1548	572	2				C10H20N2O3	Val-Val	Amino acids and Peptides	HMDB0029140	Valylvaline	C10H20N2O3	0.6
M579T885_pos	579.3899	885	2				C33H54O8	Asparagoside A	Terpenoids	HMDB0030046	Asparagoside A	C33H54O8	1.2
M784T1024_neg	783.5781	1024	2				C48H80O8	10-Undecenoic acid 7alpha,12alpha-dihydroxy-24-[2-(10-undecenoyloxy)ethoxy]-24-oxo-5beta-cholane-3alpha-yl ester	Terpenoids				
M230T603_neg	230.1034	603	2				C10H17NO5	Isovalerylglutamic Acid	Amino acids and Peptides	HMDB0000726	Isovalerylglutamic acid	C10H17NO5	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M116T129_pos	116.0706	129	2	3.00E-18	0.43	TRUE	2.40E-05	1.44	FALSE	2.87E-15	1.90	TRUE	3.97E-01	0.94	FALSE
M359T1054_pos	359.2941	1054	2	3.80E-13	1.66	TRUE	4.32E-13	0.63	TRUE	5.86E-01	0.97	FALSE	3.84E-02	1.16	FALSE
M786T984_pos	785.5906	984	2	1.48E-12	2.40	TRUE	3.03E-07	0.56	TRUE	5.19E-02	1.20	FALSE	2.07E-01	1.28	FALSE
M786T1024_2_pos	785.5925	1024	2	1.47E-23	2.40	TRUE	4.62E-14	0.58	TRUE	7.88E-01	0.98	FALSE	4.11E-01	1.09	FALSE
M217T572_pos	217.1548	572	2	8.54E-33	0.10	TRUE	3.35E-01	1.12	FALSE	1.94E-12	2.15	TRUE	4.54E-01	0.83	FALSE
M579T885_pos	579.3899	885	2	6.46E-03	7.72	TRUE	4.94E-02	0.32	TRUE	4.78E-01	0.70	FALSE	1.61E-01	0.06	FALSE
M784T1024_neg	783.5781	1024	2	2.02E-20	1.97	TRUE	2.35E-10	0.66	TRUE	8.42E-01	0.99	FALSE	3.66E-01	1.09	FALSE
M230T603_neg	230.1034	603	2	9.80E-01	1.00	FALSE	6.82E-08	1.82	TRUE	2.22E-18	2.55	TRUE	3.32E-01	1.08	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M291T458_neg	291.0990	458	2				C14H16N2O5	3-(4-hydroxyphenyl)-2-[(5-oxopyrrolidin-2-yl)formamido]propanoic acid	Amino acids and Peptides	HMDB0041309	(2S,4S)-Monatin	C14H16N2O5	1.4
M518T411_neg	518.1757	411	2				C25H25N7O6	6-O-diphenylcarbamoyl-2-N-methylcarbamoyl deoxyguanosine	Carbohydrates				
M784T974_neg	783.5767	974	2				C48H80O8	10-Undecenoic acid 7alpha,12alpha-dihydroxy-24-[2-(10-undecenoyloxy)ethoxy]-24-oxo-5beta-cholane-3alpha-yl ester	Terpenoids				
M269T395_pos	269.0884	395	2				C10H12N4O5	Inosin	Carbohydrates	HMDB0000195	Inosine	C10H12N4O5	1.3
M284T396_pos	284.0992	396	2				C10H13N5O5	Guanosin	Carbohydrates	HMDB0000133	Guanosine	C10H13N5O5	0.9
M341T1054_pos	341.2835	1054	2				C24H40O3	Lithocholate	Terpenoids				
M398T788_pos	398.3419	788	2				C27H43NO	Solatubine	Alkaloids	HMDB0003236	Solanidine	C27H43NO	0.4
M808T1026_pos	807.5747	1026	2				C48H80O8	10-Undecenoic acid 7alpha,12alpha-dihydroxy-24-[2-(10-undecenoyloxy)ethoxy]-24-oxo-5beta-cholane-3alpha-yl ester	Terpenoids				
M96T364_pos	96.0444	364	2				C5H5NO	pyridin-3-ol	Alkaloids	HMDB0013751	2-Hydroxypyridine	C5H5NO	0.3
M272T889_2_pos	272.2588	889	2				C16H33NO2	Hexadecasphingosine	Fatty acids	HMDB0242181	Hexadecasphingosine	C16H33NO2	1.4
M300T930_pos	300.2899	930	2				C18H37NO2	Sphingoid	Fatty acids	HMDB0000252	Sphingosine	C18H37NO2	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M291T458_neg	291.0990	458	2	1.02E-26	0.10	TRUE	9.60E-01	1.01	FALSE	2.54E-08	1.98	TRUE	2.87E-01	1.16	FALSE
M518T411_neg	518.1757	411	2	2.53E-23	0.01	TRUE	8.35E-01	0.96	FALSE	2.93E-09	2.77	TRUE	1.32E-01	3.33	FALSE
M784T974_neg	783.5767	974	2	3.28E-17	2.44	TRUE	6.50E-10	0.54	TRUE	3.85E-01	1.07	FALSE	8.97E-01	1.02	FALSE
M269T395_pos	269.0884	395	2	2.62E-66	0.11	TRUE	1.01E-01	1.11	FALSE	1.38E-03	1.18	FALSE	1.36E-01	1.67	FALSE
M284T396_pos	284.0992	396	2	1.94E-31	0.20	TRUE	5.07E-01	1.07	FALSE	2.53E-03	1.29	FALSE	4.01E-01	1.22	FALSE
M341T1054_pos	341.2835	1054	2	1.58E-10	1.53	TRUE	5.71E-05	0.77	FALSE	8.25E-02	0.91	FALSE	6.46E-02	1.18	FALSE
M398T788_pos	398.3419	788	2	4.55E-03	5.13	TRUE	6.58E-01	0.83	FALSE	3.97E-01	1.42	FALSE	9.27E-01	1.04	FALSE
M808T1026_pos	807.5747	1026	2	5.89E-26	1.73	TRUE	1.04E-10	0.75	FALSE	1.13E-02	0.91	FALSE	9.48E-02	1.13	FALSE
M96T364_pos	96.0444	364	2	2.75E-02	0.89	FALSE	8.95E-01	1.01	FALSE	3.33E-21	1.67	TRUE	1.62E-01	0.85	FALSE
M272T889_2_pos	272.2588	889	2	4.07E-04	3.51	TRUE	4.49E-01	0.80	FALSE	2.37E-01	1.38	FALSE	6.44E-01	0.89	FALSE
M300T930_pos	300.2899	930	2	9.99E-04	5.45	TRUE	8.77E-02	0.54	FALSE	5.60E-01	1.23	FALSE	7.44E-01	0.92	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M180T324_neg	180.0667	324	2				C9H11NO3	L-Tyr	Amino acids and Peptides	HMDB0000158	L-Tyrosine	C9H11NO3	0.4
M215T404_neg	215.1402	404	2				C10H20N2O3	Val-Val	Amino acids and Peptides	HMDB0029140	Valylvaline	C10H20N2O3	0.4
M327T985_neg	327.1814	985	2				C17H28O6	Spiculisporic Acid	Fatty acids	HMDB0061062	7-hydroxygranisetron	C18H24N4O2	3.8
M328T973_neg	328.2132	973	2				C17H31NO5	N-Lauroyl-L-glutamic acid	Fatty acids	HMDB0013202	6-Keto-decanoylcarnitine	C17H31NO5	0.6
M437T973_neg	437.2908	973	2				C25H42O6	methyl 4-{4,5,7,11-tetrahydroxy-9a,11a-dimethyl-hexadecahydro-1H-cyclopenta[a]phenanthren-1-yl}pentanoate	Terpenoids	HMDB0297051	DG(2:0/20:3(6,8,11)-OH(5)/0:0)	C25H42O6	0.2
M221T495_neg	221.0932	495	2				C11H14N2O3	Gf Zwitterion	Amino acids and Peptides	HMDB0028848	Glycyl-Phenylalanine	C11H14N2O3	0.4
M259T601_neg	259.0726	601	2				C13H12N2O4	1H,2H,3H,4H,9H-pyrido[3,4-b]indole-1,3-dicarboxylic acid	Alkaloids	HMDB0032102	etrahydro-b-carboline-1,3-dicarbo	C13H12N2O4	0.7
M263T531_neg	263.1405	531	2				C14H20N2O3	0	Amino acids and Peptides	HMDB0015568	Vorinostat	C14H20N2O3	1.4
M265T503_neg	265.1195	503	2				C13H18N2O4	0	Amino acids and Peptides	HMDB0029005	Phenylalanylthreonine	C13H18N2O4	0.6
M429T789_neg	429.1780	789	2				C21H26N4O6	0		HMDB0032622	Phenethyl rutinoside	C20H30O10	3.2
M280T1020_pos	280.2636	1020	2				C18H33NO	Linoleamide	Fatty acids	HMDB0062656	Linoleamide	C18H33NO	0.4
M410T1027_pos	410.3266	1027	2				C24H40O4	Cdca	Terpenoids				
M123T722_pos	123.0441	722	2				C7H6O2	Benzoic Acid	Shikimates and Phenylpropanoids	HMDB0001870	Benzoic acid	C7H6O2	0.2
M394T1054_pos	394.3310	1054	2				C24H40O3	Lithocholate	Terpenoids	HMDB0241978	N-Linoleoyl Isoleucine	C24H43NO3	1.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M180T324_neg	180.0667	324	2	2.16E-28	0.28	TRUE	2.37E-01	1.11	FALSE	1.12E-03	1.28	FALSE	4.99E-01	1.12	FALSE
M215T404_neg	215.1402	404	2	1.21E-38	0.15	TRUE	1.88E-01	1.13	FALSE	2.41E-03	1.27	FALSE	2.14E-01	0.67	FALSE
M327T985_neg	327.1814	985	2	1.85E-01	0.85	FALSE	5.05E-02	1.29	FALSE	4.07E-11	2.24	TRUE	2.95E-01	1.24	FALSE
M328T973_neg	328.2132	973	2	6.35E-12	0.64	TRUE	3.69E-03	0.83	FALSE	3.97E-08	1.36	FALSE	7.10E-01	0.90	FALSE
M437T973_neg	437.2908	973	2	6.56E-25	1.55	TRUE	2.08E-15	0.75	FALSE	8.79E-01	1.00	FALSE	9.78E-01	1.00	FALSE
M221T495_neg	221.0932	495	2	1.84E-46	0.13	TRUE	3.86E-01	1.08	FALSE	1.60E-04	1.31	FALSE	1.18E-01	0.71	FALSE
M259T601_neg	259.0726	601	2	1.38E-06	0.41	TRUE	6.51E-01	1.08	FALSE	1.98E-01	1.21	FALSE	7.22E-01	0.96	FALSE
M263T531_neg	263.1405	531	2	1.81E-12	0.26	TRUE	5.85E-01	1.10	FALSE	5.72E-03	1.47	FALSE	8.98E-02	0.56	FALSE
M265T503_neg	265.1195	503	2	8.44E-40	0.23	TRUE	4.21E-01	1.07	FALSE	8.10E-04	1.25	FALSE	3.99E-01	0.83	FALSE
M429T789_neg	429.1780	789	2	1.91E-01	0.89	FALSE	3.18E-04	1.41	FALSE	5.90E-27	2.99	TRUE	5.96E-01	0.93	FALSE
M280T1020_pos	280.2636	1020	2	6.35E-05	0.92	FALSE	2.14E-04	1.08	FALSE	6.86E-03	0.95	FALSE	7.86E-01	0.99	FALSE
M410T1027_pos	410.3266	1027	2	4.29E-14	1.24	FALSE	9.92E-04	0.91	FALSE	1.73E-05	0.90	FALSE	4.07E-01	1.04	FALSE
M123T722_pos	123.0441	722	2	3.42E-06	1.24	FALSE	7.90E-02	0.92	FALSE	5.52E-02	0.93	FALSE	5.12E-01	1.04	FALSE
M394T1054_pos	394.3310	1054	2	5.27E-02	1.10	FALSE	5.41E-09	0.73	FALSE	2.97E-07	0.79	FALSE	5.78E-02	1.18	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M424T925_1_pos	424.3063	925	2				C24H41NO5	(4R)-N-hydroxy-4-[(3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-3,7,12-trihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanamide	Terpenoids	HMDB0241825	thyl-5-propylfuran-2-yl)nonanoylo	C24H41NO5	1.3
M437T1024_neg	437.2909	1024	2				C25H42O6	methyl 4-{4,5,7,11-tetrahydroxy-9a,11a-dimethyl-hexadecahydro-1H-cyclopenta[a]phenanthren-1-yl}pentanoate	Terpenoids	HMDB0297051	DG(2:0/20:3(6,8,11)-OH(5)/0:0)	C25H42O6	0.2
M270T880_neg	270.1711	880	2				C14H25NO4	3-hydroxy-N-(2-oxooxolan-3-yl)decanamide	Fatty acids	HMDB0241681	Hept-3-enoylcarnitine	C14H25NO4	0.1
M462T438_pos	462.2333	438	3							HMDB0015232	Pimozide	C28H29F2N3O	3.9
M532T323_pos	532.2607	323	3							HMDB0254750	Mirodenafil	C26H37N5O5S	3.5
M267T1008_pos	267.2320	1008	3							HMDB0031050	Methyl 2E,4Z-hexadecadienoate	C17H30O2	0.6
M283T839_pos	283.1177	839	3							HMDB0249246	Bis(2-methoxyethyl) phthalate	C14H18O6	0.4
M537T275_pos	537.2046	275	3						Carbohydrates	HMDB0254391	Mecapegfilgrastim	C21H36N4O8S2	0.3
M167T648_neg	167.0352	648	3						Shikimates and Phenylpropanoids	HMDB0000130	Homogentisic acid	C8H8O4	1.3
M508T676_neg	508.2667	676	3							HMDB0253969	Landiolol	C25H39N3O8	0.4
M78T205_neg	78.0349	205	3							HMDB0000926	Pyridine	C5H5N	0.6
M135T529_neg	135.0453	529	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.8
M189T494_neg	189.0405	494	3							HMDB0012710	3-Dehydroquinic acid	C7H10O6	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M424T925_1_pos	424.3063	925	2	2.03E-01	1.14	FALSE	3.05E-01	0.89	FALSE	6.66E-01	0.96	FALSE	9.19E-01	1.01	FALSE
M437T1024_neg	437.2909	1024	2	9.49E-20	1.36	FALSE	2.14E-05	0.88	FALSE	2.41E-01	0.97	FALSE	2.01E-01	1.07	FALSE
M270T880_neg	270.1711	880	2	4.47E-04	1.50	FALSE	4.13E-03	1.39	FALSE	2.31E-01	1.12	FALSE	7.23E-02	1.29	FALSE
M462T438_pos	462.2333	438	3	3.90E-09	0.43	TRUE	2.51E-03	1.51	TRUE	1.69E-04	1.56	TRUE	4.78E-03	2.19	TRUE
M532T323_pos	532.2607	323	3	5.04E-03	0.54	TRUE	1.92E-02	1.66	TRUE	4.36E-04	1.96	TRUE	3.82E-02	1.66	TRUE
M267T1008_pos	267.2320	1008	3	1.99E-04	1.76	TRUE	1.40E-09	2.68	TRUE	2.16E-04	0.61	TRUE	1.48E-02	1.50	TRUE
M283T839_pos	283.1177	839	3	3.76E-07	1.53	TRUE	1.31E-13	0.57	TRUE	6.67E-09	1.53	TRUE	5.68E-04	0.53	TRUE
M537T275_pos	537.2046	275	3	3.15E-12	0.15	TRUE	1.18E-02	1.68	TRUE	4.08E-03	1.67	TRUE	2.77E-03	2.95	TRUE
M167T648_neg	167.0352	648	3	9.36E-14	1.85	TRUE	2.19E-04	0.62	TRUE	2.32E-12	1.64	TRUE	1.00E-05	1.64	TRUE
M508T676_neg	508.2667	676	3	5.26E-03	1.53	TRUE	2.34E-04	1.82	TRUE	2.35E-06	1.92	TRUE	3.54E-03	1.58	TRUE
M78T205_neg	78.0349	205	3	1.17E-13	0.29	TRUE	1.87E-06	2.05	TRUE	2.23E-06	1.82	TRUE	3.16E-02	2.08	TRUE
M135T529_neg	135.0453	529	3	7.48E-10	0.20	TRUE	1.21E-02	1.75	TRUE	1.86E-04	2.05	TRUE	3.44E-02	1.70	TRUE
M189T494_neg	189.0405	494	3	9.12E-04	2.33	TRUE	1.06E-04	3.04	TRUE	1.26E-12	8.32	TRUE	4.01E-03	2.35	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M259T554_neg	259.1294	554	3						Amino acids and Peptides	HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	2.1
M395T707_neg	395.1048	707	3							HMDB0254193	e oxide, diphenyl(2,4,6-trimethoxy	C22H21O5P	1.5
M412T384_neg	412.1364	384	3							HMDB0249302	-chlorophenyl)-2-methyl-1H-pyrro	C23H25Cl2N3	2.8
M460T438_neg	460.2191	438	3							HMDB0015232	Pimozide	C28H29F2N3O	3.3
M643T892_neg	643.3348	892	3							HMDB0030736	Capsianoside IV	C32H52O13	2.1
M860T961_neg	859.6093	961	3							HMDB0266373	PA(24:0/PGF1alpha)	C47H89O11P	2.7
M72T158_pos	72.0806	158	3							HMDB0031641	Pyrrolidine	C4H9N	2.8
M86T323_pos	86.0963	323	3							HMDB0034301	Piperidine	C5H11N	1.8
M120T439_pos	120.0808	439	3							HMDB0253472	Indoline	C8H9N	0.1
M152T747_pos	152.0165	747	3							HMDB0247072	6-Hydroxybenzothiazole	C7H5NOS	0.2
M168T456_pos	168.0292	456	3							HMDB0000232	Quinolinic acid	C7H5NO4	0.3
M190T458_pos	190.0112	458	3							HMDB0304308	cyclic- 3,4-O-oxalyl-L-threonate	C6H5O7	0.8
M190T822_pos	190.1229	822	3							HMDB0243800	nzofuran-5-yl)-N-Methylpropan-2-	C12H15NO	1.6
M220T480_pos	220.1180	480	3							HMDB0000210	Pantothenic acid	C9H17NO5	0.3
M276T386_pos	276.1079	386	3							HMDB0030697	Sarmentosin	C11H17NO7	0.6
M294T387_pos	294.1185	387	3						Carbohydrates	HMDB0029353	Galactosyl 4-hydroxyproline	C11H19NO8	0.6
M301T1039_pos	301.2731	1039	3							HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	C18H36O3	2.1
M328T949_2_pos	328.3212	949	3						Fatty acids	HMDB0013078	Stearoylethanolamide	C20H41NO2	0.7
M330T961_pos	330.3368	961	3						Fatty acids				
M358T686_pos	358.2702	686	3							HMDB0094648	Leu-Leu-Leu	C18H35N3O4	0.5
M369T920_2_pos	369.2423	920	3							HMDB0254439	Menoctone	C24H32O3	0.2
M409T920_pos	409.2351	920	3							HMDB0062190	almitoyl-dihydroxyacetone-phosph	C19H37O7P	0.3
M439T606_pos	439.1016	606	3						Alkaloids	HMDB0059614	Thiomorpholine 3-carboxylate	C17H19N4O8P	0.6
M454T1050_2_pos	454.2928	1050	3							HMDB0011473	LysoPE(0:0/16:0)	C21H44NO7P	0.0
M486T900_pos	486.2602	900	3							HMDB0248754	o)-2-((2-(dimethylamino)ethyl)(m	C27H31N7O2	2.1
M496T1049_pos	496.3401	1049	3							HMDB0240262	LysoPC(0:0/16:0)	C24H50NO7P	0.7
M547T630_pos	547.3380	630	3							HMDB0248383	Anamorelin	C31H42N6O3	2.0
M583T893_pos	583.2558	893	3							HMDB0303975	(3Z)-phytochromobilin	C33H34N4O6	0.6
M602T1039_pos	601.5404	1039	3						Fatty acids				
M610T980_pos	610.3894	980	3						Terpenoids				
M641T913_pos	641.3186	913	3						Amino acids and Peptides				
M69T304_pos	69.0697	304	3							HMDB0249189	Bicyclo[2.1.0]pentane	C5H8	2.8
M84T88_pos	84.0806	88	3							HMDB0033529	+)-2,3-Dihydro-3-methyl-1H-pyrrol	C5H9N	1.7
M113T593_pos	113.0597	593	3						Fatty acids	HMDB0001164	trans-1,2-Dihydrobenzene-1,2-dio	C6H8O2	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M259T554_neg	259.1294	554	3	2.60E-09	0.29	TRUE	5.73E-04	1.93	TRUE	2.23E-06	2.22	TRUE	2.25E-02	1.96	TRUE
M395T707_neg	395.1048	707	3	2.45E-14	2.62	TRUE	4.97E-06	0.39	TRUE	1.49E-10	0.51	TRUE	2.98E-04	1.86	TRUE
M412T384_neg	412.1364	384	3	9.90E-14	0.31	TRUE	8.19E-06	1.87	TRUE	1.33E-13	2.67	TRUE	1.60E-02	1.85	TRUE
M460T438_neg	460.2191	438	3	1.25E-08	0.38	TRUE	1.01E-03	1.69	TRUE	2.92E-04	1.65	TRUE	1.83E-03	2.66	TRUE
M643T892_neg	643.3348	892	3	3.62E-11	0.49	TRUE	5.40E-08	1.76	TRUE	7.95E-07	1.55	TRUE	1.87E-02	1.53	TRUE
M860T961_neg	859.6093	961	3	1.64E-07	2.23	TRUE	4.57E-03	0.61	TRUE	8.00E-05	1.65	TRUE	4.23E-05	2.73	TRUE
M72T158_pos	72.0806	158	3	6.09E-26	0.28	TRUE	1.36E-06	1.60	TRUE	9.85E-12	1.81	TRUE	6.52E-01	1.06	FALSE
M86T323_pos	86.0963	323	3	2.96E-27	0.26	TRUE	4.16E-06	1.57	TRUE	1.82E-11	1.81	TRUE	5.15E-01	1.15	FALSE
M120T439_pos	120.0808	439	3	5.87E-42	0.23	TRUE	3.25E-08	1.51	TRUE	1.57E-15	1.73	TRUE	1.94E-01	1.20	FALSE
M152T747_pos	152.0165	747	3	3.25E-02	0.82	FALSE	9.67E-05	0.67	TRUE	4.58E-23	0.38	TRUE	1.94E-02	1.56	TRUE
M168T456_pos	168.0292	456	3	2.92E-08	2.43	TRUE	6.65E-01	0.94	FALSE	5.70E-21	5.01	TRUE	9.93E-16	6.01	TRUE
M190T458_pos	190.0112	458	3	4.18E-15	3.85	TRUE	2.69E-01	0.86	FALSE	3.73E-17	3.52	TRUE	1.65E-14	5.81	TRUE
M190T822_pos	190.1229	822	3	1.03E-24	2.77	TRUE	1.88E-24	0.39	TRUE	4.64E-09	0.65	TRUE	6.15E-02	1.48	FALSE
M220T480_pos	220.1180	480	3	4.74E-09	0.49	TRUE	2.65E-07	1.89	TRUE	8.16E-11	2.02	TRUE	4.38E-02	1.27	FALSE
M276T386_pos	276.1079	386	3	2.48E-07	0.39	TRUE	1.13E-08	2.91	TRUE	2.16E-10	2.86	TRUE	6.01E-01	1.10	FALSE
M294T387_pos	294.1185	387	3	8.35E-08	0.37	TRUE	3.47E-08	2.82	TRUE	7.29E-10	2.77	TRUE	1.57E-01	1.23	FALSE
M301T1039_pos	301.2731	1039	3	1.49E-08	2.88	TRUE	8.39E-06	0.43	TRUE	4.30E-01	0.89	FALSE	6.17E-05	1.54	TRUE
M328T949_2_pos	328.3212	949	3	3.03E-06	3.22	TRUE	7.03E-04	0.53	TRUE	1.71E-03	0.53	TRUE	5.20E-01	0.90	FALSE
M330T961_pos	330.3368	961	3	4.68E-04	2.34	TRUE	8.62E-05	0.47	TRUE	9.93E-04	0.50	TRUE	5.53E-01	0.91	FALSE
M358T686_pos	358.2702	686	3	1.46E-32	0.32	TRUE	4.37E-01	0.94	FALSE	3.51E-13	1.64	TRUE	2.45E-03	0.54	TRUE
M369T920_2_pos	369.2423	920	3	1.13E-09	1.87	TRUE	1.15E-05	1.55	TRUE	1.11E-15	2.13	TRUE	9.03E-02	0.76	FALSE
M409T920_pos	409.2351	920	3	9.61E-12	1.83	TRUE	2.05E-07	1.56	TRUE	1.69E-08	1.52	TRUE	1.07E-01	0.75	FALSE
M439T606_pos	439.1016	606	3	9.53E-15	1.91	TRUE	1.42E-04	0.68	FALSE	1.70E-24	2.24	TRUE	2.06E-07	1.85	TRUE
M454T1050_2_pos	454.2928	1050	3	3.86E-05	2.57	TRUE	3.63E-02	0.63	TRUE	2.96E-08	3.22	TRUE	1.69E-01	0.82	FALSE
M486T900_pos	486.2602	900	3	3.23E-09	1.69	TRUE	1.72E-25	0.19	TRUE	4.53E-01	1.06	FALSE	2.88E-05	1.51	TRUE
M496T1049_pos	496.3401	1049	3	3.66E-04	2.38	TRUE	3.27E-03	0.43	TRUE	1.68E-02	1.62	TRUE	7.89E-01	0.93	FALSE
M547T630_pos	547.3380	630	3	1.89E-09	4.16	TRUE	1.87E-07	0.36	TRUE	6.35E-03	0.62	TRUE	1.14E-01	0.66	FALSE
M583T893_pos	583.2558	893	3	5.78E-12	2.83	TRUE	3.78E-06	0.61	TRUE	4.55E-01	1.09	FALSE	1.87E-03	1.63	TRUE
M602T1039_pos	601.5404	1039	3	4.39E-04	2.62	TRUE	6.29E-04	0.37	TRUE	7.26E-01	0.93	FALSE	1.29E-03	1.63	TRUE
M610T980_pos	610.3894	980	3	9.44E-03	0.54	TRUE	3.97E-03	0.53	TRUE	1.81E-09	0.23	TRUE	7.77E-01	1.04	FALSE
M641T913_pos	641.3186	913	3	4.29E-03	0.66	TRUE	1.06E-05	2.01	TRUE	7.22E-14	2.98	TRUE	3.89E-01	1.20	FALSE
M69T304_pos	69.0697	304	3	2.58E-28	0.29	TRUE	1.20E-07	1.61	TRUE	1.36E-12	1.78	TRUE	9.51E-01	1.01	FALSE
M84T88_pos	84.0806	88	3	6.59E-35	0.38	TRUE	8.60E-01	1.01	FALSE	4.58E-17	1.62	TRUE	4.60E-03	1.76	TRUE
M113T593_pos	113.0597	593	3	1.65E-08	0.36	TRUE	3.23E-04	1.85	TRUE	2.96E-05	1.84	TRUE	7.49E-01	1.07	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M117T447_pos	117.0546	447	3							HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	0.1
M122T458_pos	122.0239	458	3						Alkaloids				
M123T603_pos	123.0441	603	3							HMDB0001870	Benzoic acid	C7H6O2	0.1
M125T459_pos	125.0709	459	3							HMDB0004181	Methylimidazole acetaldehyde	C6H8N2O	0.5
M144T431_pos	144.0478	431	3							HMDB0246712	-(1-Hydroxyethyl)-4-methylthiazol	C6H9NOS	0.4
M148T596_pos	148.0757	596	3						Alkaloids	HMDB0005785	Indole-3-carbinol	C9H9NO	0.4
M150T458_pos	150.0186	458	3						Alkaloids				
M153T823_pos	153.0910	823	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.3
M162T598_pos	162.0912	598	3						Alkaloids	HMDB0003447	Tryptophol	C10H11NO	0.9
M179T151_pos	179.1105	151	3							HMDB0041608	Methional diethyl acetal	C8H18O2S	2.7
M186T700_pos	186.0913	700	3							HMDB0032597	4-Hydroxydiphenylamine	C12H11NO	0.1
M191T630_pos	191.0851	630	3							HMDB0248124	Aldicar	C7H14N2O2S	1.2
M210T581_pos	210.1349	581	3							HMDB0014494	Minoxidil	C9H15N5O	0.0
M213T491_pos	213.1599	491	3							HMDB0060336	1,2-Dihydronaphthalene-1,2-diol	C11H20N2O2	0.6
M220T982_pos	220.1122	982	3							HMDB0032865	N-Phenyl-2-naphthylamine	C16H13N	0.6
M224T418_pos	224.0555	418	3							HMDB0004083	no-3-hydroxyphenyl)-2,4-dioxobuta	C10H9NO5	0.5
M228T445_pos	228.1595	445	3							HMDB0255213	OCTANOYL-L-HOMOSERINE LACTO	C12H21NO3	0.5
M236T346_pos	236.1130	346	3							HMDB0255309	o-4,5,6-trihydroxy-3-[(2R)-1-oxopr	C9H17NO6	0.6
M248T810_pos	248.1758	810	3							HMDB0246918	methylphenyl)-2-(piperazin-1-yl)a	C14H21N3O	0.2
M250T209_pos	250.1287	209	3							HMDB0243858	1-Deoxy-1-morpholino-D-fructose	C10H19NO6	0.9
M261T552_pos	261.1445	552	3							HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	0.1
M275T518_2_pos	275.1971	518	3							HMDB0248003	Adelmidrol	C13H26N2O4	1.9
M276T439_pos	276.1079	439	3							HMDB0030697	Sarmentosin	C11H17NO7	0.5
M276T497_pos	276.1084	497	3							HMDB0030697	Sarmentosin	C11H17NO7	2.1
M281T523_pos	281.1002	523	3							HMDB0028979	Methionyl-Methionine	C10H20N2O3S2	4.8
M285T426_pos	285.0838	426	3							HMDB0304399	L-arginino-succinate	C10H12N4O6	0.9
M307T1033_2_pos	307.2265	1033	3							HMDB0000523	5-Androstene-3b,16b,17a-triol	C19H30O3	0.8
M316T620_pos	316.2229	620	3						Amino acids and Peptides	HMDB0094676	Val-Val-Val	C15H29N3O4	0.6
M317T988_pos	317.2688	988	3							HMDB0011532	MG(0:0/15:0/0:0)	C18H36O4	0.7
M321T630_pos	321.1479	630	3							HMDB0303294	Sodium decylbenzenesulfonate	C16H25NaO3S	4.9
M335T814_pos	335.1966	814	3							HMDB0256796	Proglumide	C18H26N2O4	0.1
M335T965_pos	335.2584	965	3							HMDB0000879	Tetrahydrodeoxycorticosterone	C21H34O3	0.9
M343T630_pos	343.1301	630	3							HMDB0040442	Dictyoquinazol C	C18H18N2O5	3.7
M349T762_pos	349.1786	762	3							HMDB0253427	Imidocar	C19H20N6O	4.3
M382T877_pos	382.1548	877	3							HMDB0301782	ylthio-N6-(delta2-isopentenyl)ade	C16H23N5O4S	1.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M117T447_pos	117.0546	447	3	1.46E-03	0.53	TRUE	3.19E-02	1.57	TRUE	1.38E-03	1.74	TRUE	6.59E-01	0.94	FALSE
M122T458_pos	122.0239	458	3	4.71E-07	2.04	TRUE	8.74E-01	0.98	FALSE	6.08E-22	4.32	TRUE	2.33E-15	5.84	TRUE
M123T603_pos	123.0441	603	3	3.68E-03	1.67	TRUE	4.09E-03	1.67	TRUE	3.90E-06	2.10	TRUE	9.04E-01	0.98	FALSE
M125T459_pos	125.0709	459	3	1.33E-01	1.27	FALSE	2.07E-05	2.16	TRUE	5.77E-07	2.13	TRUE	4.17E-02	0.60	TRUE
M144T431_pos	144.0478	431	3	2.52E-09	0.54	TRUE	9.21E-06	1.57	TRUE	6.47E-21	2.61	TRUE	2.15E-02	0.73	FALSE
M148T596_pos	148.0757	596	3	1.99E-09	1.90	TRUE	2.14E-05	0.59	TRUE	1.39E-01	0.88	FALSE	4.89E-03	0.59	TRUE
M150T458_pos	150.0186	458	3	1.07E-09	2.73	TRUE	8.71E-01	1.02	FALSE	2.26E-15	3.39	TRUE	2.79E-13	6.87	TRUE
M153T823_pos	153.0910	823	3	2.15E-09	3.05	TRUE	8.04E-02	0.76	FALSE	2.31E-04	0.58	TRUE	3.48E-02	0.19	TRUE
M162T598_pos	162.0912	598	3	1.19E-08	2.00	TRUE	1.68E-05	0.54	TRUE	1.96E-01	0.88	FALSE	4.44E-03	0.55	TRUE
M179T151_pos	179.1105	151	3	1.55E-40	0.31	TRUE	2.85E-02	1.15	FALSE	7.76E-21	1.78	TRUE	6.07E-04	1.52	TRUE
M186T700_pos	186.0913	700	3	1.35E-02	1.66	TRUE	1.96E-02	0.59	TRUE	6.69E-03	0.62	TRUE	3.22E-01	1.19	FALSE
M191T630_pos	191.0851	630	3	2.34E-05	3.56	TRUE	1.63E-02	0.55	TRUE	9.22E-15	38.59	TRUE	2.93E-01	1.25	FALSE
M210T581_pos	210.1349	581	3	5.95E-03	0.45	TRUE	4.79E-01	0.83	FALSE	8.61E-03	1.91	TRUE	1.49E-02	0.09	TRUE
M213T491_pos	213.1599	491	3	9.90E-29	0.40	TRUE	8.89E-05	1.31	FALSE	3.80E-19	1.78	TRUE	7.74E-04	0.54	TRUE
M220T982_pos	220.1122	982	3	1.52E-05	0.40	TRUE	1.13E-02	0.63	TRUE	2.86E-10	0.28	TRUE	2.78E-01	0.72	FALSE
M224T418_pos	224.0555	418	3	1.36E-06	0.64	TRUE	3.28E-01	1.10	FALSE	7.74E-19	2.24	TRUE	1.63E-02	0.51	TRUE
M228T445_pos	228.1595	445	3	6.68E-03	2.64	TRUE	3.51E-03	2.61	TRUE	4.46E-07	6.95	TRUE	7.11E-01	1.08	FALSE
M236T346_pos	236.1130	346	3	3.65E-04	4.04	TRUE	6.39E-07	22.69	TRUE	4.65E-11	-174.36	FALSE	1.43E-03	1.85	TRUE
M248T810_pos	248.1758	810	3	2.41E-35	0.17	TRUE	4.07E-02	1.22	FALSE	7.78E-08	1.59	TRUE	7.67E-03	0.41	TRUE
M250T209_pos	250.1287	209	3	4.73E-15	0.16	TRUE	5.52E-03	1.63	TRUE	6.07E-09	2.62	TRUE	4.11E-01	1.09	FALSE
M261T552_pos	261.1445	552	3	8.05E-13	0.21	TRUE	6.52E-05	2.08	TRUE	1.59E-07	2.34	TRUE	6.37E-01	1.13	FALSE
M275T518_2_pos	275.1971	518	3	1.86E-03	1.51	TRUE	7.70E-04	1.58	TRUE	2.01E-09	2.08	TRUE	4.01E-01	0.88	FALSE
M276T439_pos	276.1079	439	3	3.32E-04	0.42	TRUE	1.24E-06	3.50	TRUE	2.17E-06	2.78	TRUE	4.89E-01	1.08	FALSE
M276T497_pos	276.1084	497	3	2.28E-14	0.39	TRUE	1.15E-04	1.55	TRUE	1.23E-17	2.59	TRUE	7.34E-01	1.09	FALSE
M281T523_pos	281.1002	523	3	1.53E-06	0.43	TRUE	1.90E-04	1.91	TRUE	1.45E-05	1.90	TRUE	1.96E-01	1.25	FALSE
M285T426_pos	285.0838	426	3	7.53E-07	0.49	TRUE	1.15E-05	1.92	TRUE	1.68E-11	2.44	TRUE	3.36E-01	1.40	FALSE
M307T1033_2_pos	307.2265	1033	3	4.37E-09	2.10	TRUE	2.45E-01	0.86	FALSE	3.81E-05	1.54	TRUE	1.45E-02	0.40	TRUE
M316T620_pos	316.2229	620	3	1.13E-28	0.26	TRUE	5.50E-01	1.06	FALSE	2.21E-08	1.59	TRUE	2.05E-02	0.29	TRUE
M317T988_pos	317.2688	988	3	2.06E-06	1.76	TRUE	2.15E-04	0.62	TRUE	7.47E-01	0.97	FALSE	3.73E-02	1.51	TRUE
M321T630_pos	321.1479	630	3	5.55E-04	2.03	TRUE	2.34E-02	0.66	TRUE	1.70E-15	6.54	TRUE	2.01E-01	1.24	FALSE
M335T814_pos	335.1966	814	3	6.79E-06	2.06	TRUE	1.45E-12	0.25	TRUE	7.87E-04	0.64	TRUE	7.93E-01	1.06	FALSE
M335T965_pos	335.2584	965	3	1.26E-09	3.82	TRUE	6.35E-01	1.08	FALSE	1.18E-02	1.51	TRUE	1.41E-02	0.60	TRUE
M343T630_pos	343.1301	630	3	8.82E-06	2.30	TRUE	8.90E-03	0.64	TRUE	2.68E-17	5.69	TRUE	8.45E-02	1.29	FALSE
M349T762_pos	349.1786	762	3	3.05E-04	1.71	TRUE	5.83E-05	0.56	TRUE	2.14E-11	2.60	TRUE	6.49E-02	1.42	FALSE
M382T877_pos	382.1548	877	3	2.42E-03	0.60	TRUE	4.70E-06	2.25	TRUE	2.21E-05	1.88	TRUE	4.00E-01	1.11	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M383T724_pos	383.2182	724	3							HMDB0062321	etradecanoyl-sn-glycero-3-phosph	C17H35O7P	3.0
M387T921_pos	387.2532	921	3							HMDB0000385	12a-Hydroxy-3-oxocholadienic acid	C24H34O4	0.4
M391T1049_pos	391.2247	1049	3							HMDB0251364	Dilept	C21H30N2O5	4.9
M457T836_pos	457.2337	836	3							HMDB0259814	Vindoline	C25H32N2O6	0.8
M478T1039_pos	478.2929	1039	3							HMDB0011477	LysoPE(0:0/18:2(9Z,12Z))	C23H44NO7P	0.3
M480T1056_pos	480.3090	1056	3							HMDB0011475	LysoPE(0:0/18:1(11Z))	C23H46NO7P	1.0
M494T1035_pos	494.3850	1035	3							HMDB0241838	ethyl-5-propylfuran-2-yl)tridecan	C29H51NO5	2.1
M560T175_pos	560.0797	175	3							HMDB0248024	ADP Ribose	C15H23N5O14P2	1.4
M627T743_pos	627.3657	743	3							HMDB0262689	A(10:0/20:4(6E,8Z,11Z,14Z)+=O(5	C33H55O9P	0.1
M645T881_pos	645.3496	881	3						Amino acids and Peptides	HMDB0030736	Capsianoside IV	C32H52O13	2.3
M111T190_neg	111.0200	190	3							HMDB0000300	Uracil	C4H4N2O2	0.2
M122T459_neg	122.0248	459	3							HMDB0001488	Nicotinic acid	C6H5NO2	0.7
M129T598_neg	129.0558	598	3							HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	0.5
M134T385_neg	134.0474	385	3							HMDB0000034	Adenine	C5H5N5	1.2
M151T323_neg	151.0262	323	3						Alkaloids	HMDB0000292	Xanthine	C5H4N4O2	0.5
M166T458_neg	166.0147	458	3						Alkaloids	HMDB0000232	Quinolinic acid	C7H5NO4	0.5
M181T529_neg	181.0507	529	3							HMDB0000118	Homovanillic acid	C9H10O4	0.4
M187T651_neg	187.0071	651	3							HMDB0240655	o-Cresol sulfate	C7H8O4S	0.3
M188T315_neg	188.0565	315	3							HMDB0000590	Glutarylglycine	C7H11NO5	0.2
M199T862_neg	199.1340	862	3							HMDB0032662	(S)-9-Hydroxy-10-undecenoic acid	C11H20O3	0.1
M215T116_neg	215.0327	116	3							HMDB0304061	-C-methyl-D-erythritol-4-phosphat	C5H13O7P	0.5
M256T120_neg	256.0593	120	3						Carbohydrates				
M292T388_neg	292.1038	388	3						Carbohydrates	HMDB0029353	Galactosyl 4-hydroxyproline	C11H19NO8	0.2
M312T385_neg	312.0950	385	3						Carbohydrates				
M385T920_neg	385.2385	920	3						Terpenoids	HMDB0000385	12a-Hydroxy-3-oxocholadienic acid	C24H34O4	0.2
M431T920_neg	431.2441	920	3						Terpenoids	HMDB0029656	Erinacine E	C25H36O6	0.5
M437T610_neg	437.0870	610	3						Carbohydrates	HMDB0059614	Thiomorpholine 3-carboxylate	C17H19N4O8P	0.6
M437T481_neg	437.2144	481	3						Fatty acids				
M451T480_neg	451.1396	480	3						Amino acids and Peptides				
M452T1049_neg	452.2784	1049	3						Fatty acids	HMDB0011473	LysoPE(0:0/16:0)	C21H44NO7P	0.2
M461T1043_neg	461.3638	1043	3							HMDB0034430	6-Deoxohomodolichosterone	C29H50O4	0.3
M491T613_neg	491.2289	613	3							HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.4
M600T1039_neg	599.5256	1039	3						Fatty acids				
M692T1038_neg	691.5513	1038	3						Terpenoids	HMDB0296107	(19:0/20:3(8Z,11Z,14Z)-2OH(5,6)/(	C42H76O7	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M383T724_pos	383.2182	724	3	9.99E-05	3.18	TRUE	1.38E-08	0.23	TRUE	3.47E-04	0.41	TRUE	4.77E-01	0.87	FALSE
M387T921_pos	387.2532	921	3	4.49E-09	1.84	TRUE	3.97E-06	1.60	TRUE	1.33E-16	2.23	TRUE	1.70E-01	0.79	FALSE
M391T1049_pos	391.2247	1049	3	2.30E-01	1.35	FALSE	1.46E-02	0.41	TRUE	9.21E-05	2.48	TRUE	2.28E-03	0.37	TRUE
M457T836_pos	457.2337	836	3	2.20E-02	2.06	TRUE	1.54E-07	12.17	TRUE	1.06E-06	4.89	TRUE	9.94E-01	1.00	FALSE
M478T1039_pos	478.2929	1039	3	7.11E-06	3.15	TRUE	8.80E-05	0.38	TRUE	9.19E-03	1.69	TRUE	7.63E-01	0.84	FALSE
M480T1056_pos	480.3090	1056	3	6.50E-05	2.61	TRUE	1.86E-02	0.57	TRUE	2.87E-06	2.69	TRUE	5.32E-01	0.84	FALSE
M494T1035_pos	494.3850	1035	3	2.74E-18	1.88	TRUE	5.40E-01	0.96	FALSE	2.47E-13	1.55	TRUE	9.41E-03	0.63	TRUE
M560T175_pos	560.0797	175	3	6.14E-05	2.58	TRUE	7.55E-07	0.26	TRUE	1.03E-03	1.91	TRUE	2.89E-01	1.37	FALSE
M627T743_pos	627.3657	743	3	5.19E-12	3.92	TRUE	1.15E-23	0.15	TRUE	3.99E-05	0.54	TRUE	9.60E-01	1.01	FALSE
M645T881_pos	645.3496	881	3	1.09E-14	0.55	TRUE	2.13E-08	1.52	TRUE	8.05E-16	1.74	TRUE	8.58E-01	1.01	FALSE
M111T190_neg	111.0200	190	3	5.75E-26	0.16	TRUE	5.84E-05	1.65	TRUE	1.04E-10	2.07	TRUE	6.18E-01	1.19	FALSE
M122T459_neg	122.0248	459	3	2.39E-07	2.25	TRUE	9.87E-01	1.00	FALSE	2.87E-22	5.49	TRUE	1.98E-13	5.94	TRUE
M129T598_neg	129.0558	598	3	1.65E-07	0.18	TRUE	1.25E-02	2.03	TRUE	7.21E-03	1.87	TRUE	9.60E-01	0.96	FALSE
M134T385_neg	134.0474	385	3	2.07E-06	1.84	TRUE	2.89E-05	0.55	TRUE	3.78E-19	3.20	TRUE	1.13E-01	1.21	FALSE
M151T323_neg	151.0262	323	3	1.04E-17	0.14	TRUE	3.11E-04	1.84	TRUE	4.22E-10	2.65	TRUE	3.45E-01	1.31	FALSE
M166T458_neg	166.0147	458	3	5.77E-07	2.55	TRUE	8.34E-01	1.03	FALSE	6.96E-21	7.99	TRUE	7.51E-14	10.94	TRUE
M181T529_neg	181.0507	529	3	1.61E-09	0.19	TRUE	3.70E-02	1.62	TRUE	8.70E-04	1.93	TRUE	3.34E-02	1.48	FALSE
M187T651_neg	187.0071	651	3	3.19E-04	0.48	TRUE	6.05E-08	3.32	TRUE	1.44E-09	3.26	TRUE	5.68E-02	0.48	FALSE
M188T315_neg	188.0565	315	3	1.35E-08	0.56	TRUE	7.95E-01	0.97	FALSE	1.37E-07	1.59	TRUE	3.97E-02	0.41	TRUE
M199T862_neg	199.1340	862	3	5.68E-22	2.71	TRUE	5.17E-07	0.65	TRUE	3.75E-01	1.07	FALSE	5.27E-06	0.50	TRUE
M215T116_neg	215.0327	116	3	9.03E-17	0.25	TRUE	4.71E-05	1.77	TRUE	1.28E-08	2.02	TRUE	2.97E-01	1.54	FALSE
M256T120_neg	256.0593	120	3	9.79E-08	0.44	TRUE	5.79E-04	1.71	TRUE	3.47E-12	2.65	TRUE	5.43E-01	1.20	FALSE
M292T388_neg	292.1038	388	3	1.64E-05	0.44	TRUE	6.14E-08	2.99	TRUE	2.02E-10	3.16	TRUE	6.19E-03	1.38	FALSE
M312T385_neg	312.0950	385	3	3.16E-06	1.87	TRUE	3.84E-05	0.54	TRUE	3.85E-20	3.63	TRUE	7.56E-02	1.24	FALSE
M385T920_neg	385.2385	920	3	7.95E-10	2.13	TRUE	1.28E-05	1.68	TRUE	2.51E-14	2.34	TRUE	2.53E-01	0.76	FALSE
M431T920_neg	431.2441	920	3	7.58E-10	1.84	TRUE	1.27E-05	1.53	TRUE	3.50E-15	2.03	TRUE	2.40E-01	0.81	FALSE
M437T610_neg	437.0870	610	3	4.98E-12	2.00	TRUE	1.50E-03	0.68	FALSE	4.37E-23	2.61	TRUE	1.25E-06	2.09	TRUE
M437T481_neg	437.2144	481	3	5.51E-04	0.48	TRUE	4.92E-07	3.37	TRUE	1.70E-06	2.53	TRUE	5.17E-02	1.45	FALSE
M451T480_neg	451.1396	480	3	8.92E-07	0.56	TRUE	1.94E-04	1.56	TRUE	2.83E-08	1.79	TRUE	8.31E-01	1.02	FALSE
M452T1049_neg	452.2784	1049	3	1.57E-05	2.50	TRUE	1.09E-02	0.60	TRUE	1.17E-07	2.73	TRUE	1.22E-01	0.74	FALSE
M461T1043_neg	461.3638	1043	3	8.46E-05	2.04	TRUE	4.98E-05	0.52	TRUE	6.52E-03	0.66	TRUE	7.46E-01	1.11	FALSE
M491T613_neg	491.2289	613	3	6.93E-05	1.57	TRUE	2.56E-04	1.52	TRUE	9.21E-04	1.38	FALSE	3.99E-03	1.63	TRUE
M600T1039_neg	599.5256	1039	3	1.51E-06	2.58	TRUE	1.80E-05	0.37	TRUE	2.33E-01	0.83	FALSE	2.83E-02	1.76	TRUE
M692T1038_neg	691.5513	1038	3	2.67E-12	3.10	TRUE	3.98E-10	0.38	TRUE	3.26E-02	0.77	FALSE	2.16E-02	1.58	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M841T881_neg	841.4965	881	3							HMDB0034624	Vinaginsenoside R1	C44H74O15	1.2
M930T734_neg	929.5030	734	3							HMDB0276514	11Z)/20:5(7Z,9Z,11E,13E,17Z)-3OH	C47H79O16P	0.4
M939T719_neg	939.4398	719	3							HMDB0257223	Rifalazil	C51H64N4O13	0.1
M78T459_neg	78.0349	459	3							HMDB0000926	Pyridine	C5H5N	0.4
M88T481_neg	88.0405	481	3							HMDB0000056	beta-Alanine	C3H7NO2	1.1
M89T388_neg	89.0244	388	3							HMDB0244144	1,2,4-Trioxane	C3H6O3	0.0
M116T641_neg	116.0506	641	3							HMDB0000738	Indole	C8H7N	0.4
M116T160_neg	116.0718	160	3							HMDB0000883	L-Valine	C5H11NO2	0.5
M119T110_neg	119.0350	110	3							HMDB0000337	(S)-3,4-Dihydroxybutyric acid	C4H8O4	0.4
M122T205_neg	122.0248	205	3							HMDB0001488	Nicotinic acid	C6H5NO2	0.5
M130T324_neg	130.0875	324	3							HMDB0000172	L-Isoleucine	C6H13NO2	0.8
M137T193_neg	137.0357	193	3							HMDB0000301	Urocanic acid	C6H6N2O2	0.4
M141T112_neg	140.9181	112	3							HMDB0012190	Arsenate	AsH3O4	4.8
M145T505_neg	145.0143	505	3							HMDB0000208	Oxoglutaric acid	C5H6O5	0.7
M146T481_neg	146.0824	481	3							HMDB0029449	-2-Amino-4-hydroxy-3-methylpent	C6H13NO3	0.8
M147T674_neg	147.0453	674	3						Shikimates and Phenylpropanoids	HMDB0000567	Cinnamic acid	C9H8O2	0.7
M147T435_neg	147.0664	435	3							HMDB0000227	Mevalonic acid	C6H12O4	0.6
M148T188_neg	148.0438	188	3							HMDB0252040	thyl 2-amino-3-sulfanylpropanoat	C5H11NO2S	0.4
M151T514_neg	151.0401	514	3						Shikimates and Phenylpropanoids	HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.0
M157T494_neg	157.0143	494	3							HMDB0031210	Zymonic acid	C6H6O5	0.3
M165T674_neg	165.0558	674	3							HMDB0000375	3-(3-Hydroxyphenyl)propanoic acid	C9H10O3	0.6
M182T113_neg	181.9632	113	3							HMDB0304085	2-phospho-D-glycerate	C3H4O7P	3.5
M184T106_neg	184.0018	106	3							HMDB0000272	Phosphoserine	C3H8NO6P	0.8
M185T127_neg	185.0221	127	3						Fatty acids				
M188T641_neg	188.0354	641	3							HMDB0000715	Kynurenic acid	C10H7NO3	0.5
M214T105_neg	214.0207	105	3							HMDB0259067	Tiamenidine	C8H10ClN3S	1.8
M218T99_neg	218.0157	99	3							HMDB0250532	Creatinine nitrite nitrate	C4H5N5O6	4.8
M225T107_neg	225.0616	107	3							HMDB0240292	3,4,5,6,7-Hexahydroxyheptanoic a	C7H14O8	0.2
M228T868_neg	228.1605	868	3							HMDB0013267	N-Decanoylglycine	C12H23NO3	0.1
M237T1033_neg	237.1860	1033	3							HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	0.1
M243T194_neg	243.0622	194	3							HMDB0000296	Uridine	C9H12N2O6	0.2
M247T629_neg	246.9919	629	3							HMDB0125151	hydroxy-3-(sulfooxy)phenyl]acetic	C8H8O7S	0.3
M262T411_neg	262.0725	411	3							HMDB0246176	Bolton-Hunter reagent	C13H13NO5	1.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M841T881_neg	841.4965	881	3	3.41E-06	0.65	TRUE	8.81E-05	1.45	FALSE	6.37E-08	1.56	TRUE	5.38E-03	1.56	TRUE
M930T734_neg	929.5030	734	3	5.85E-06	1.83	TRUE	1.49E-03	0.67	FALSE	2.24E-05	1.62	TRUE	1.02E-03	1.58	TRUE
M939T719_neg	939.4398	719	3	1.26E-08	1.80	TRUE	3.48E-07	0.58	TRUE	2.41E-15	2.13	TRUE	1.44E-01	1.23	FALSE
M78T459_neg	78.0349	459	3	4.43E-07	2.33	TRUE	8.60E-01	0.97	FALSE	6.93E-22	6.30	TRUE	6.64E-14	6.65	TRUE
M88T481_neg	88.0405	481	3	2.16E-11	0.47	TRUE	2.06E-07	1.77	TRUE	5.45E-12	1.96	TRUE	3.20E-02	1.26	FALSE
M89T388_neg	89.0244	388	3	1.58E-06	0.45	TRUE	1.74E-08	2.64	TRUE	1.89E-10	2.66	TRUE	7.49E-02	1.18	FALSE
M116T641_neg	116.0506	641	3	1.09E-21	0.28	TRUE	1.85E-05	1.62	TRUE	3.02E-16	2.38	TRUE	4.99E-01	1.16	FALSE
M116T160_neg	116.0718	160	3	1.28E-09	0.46	TRUE	3.66E-07	1.87	TRUE	5.38E-11	2.08	TRUE	3.54E-01	1.10	FALSE
M119T110_neg	119.0350	110	3	4.67E-19	0.29	TRUE	2.02E-04	1.55	TRUE	5.52E-13	2.19	TRUE	1.21E-01	1.15	FALSE
M122T205_neg	122.0248	205	3	6.30E-13	0.33	TRUE	4.25E-08	2.21	TRUE	4.55E-06	1.74	TRUE	4.66E-02	1.46	FALSE
M130T324_neg	130.0875	324	3	1.12E-10	0.41	TRUE	1.10E-04	1.67	TRUE	1.96E-04	1.51	TRUE	8.47E-01	1.06	FALSE
M137T193_neg	137.0357	193	3	1.15E-27	0.21	TRUE	1.02E-04	1.53	TRUE	3.19E-03	1.30	FALSE	4.62E-02	1.59	TRUE
M141T112_neg	140.9181	112	3	3.07E-38	5.12	TRUE	1.55E-02	0.81	FALSE	6.62E-16	0.52	TRUE	5.77E-05	0.51	TRUE
M145T505_neg	145.0143	505	3	3.77E-07	0.40	TRUE	2.04E-03	1.68	TRUE	1.14E-07	2.26	TRUE	1.07E-01	0.05	FALSE
M146T481_neg	146.0824	481	3	4.24E-09	0.49	TRUE	1.01E-07	1.90	TRUE	1.00E-10	1.97	TRUE	8.00E-03	1.35	FALSE
M147T674_neg	147.0453	674	3	6.53E-09	0.17	TRUE	3.10E-02	1.72	TRUE	9.60E-04	2.05	TRUE	9.12E-01	1.02	FALSE
M147T435_neg	147.0664	435	3	8.36E-04	0.63	TRUE	2.80E-04	1.68	TRUE	5.46E-04	1.51	TRUE	6.14E-01	0.92	FALSE
M148T188_neg	148.0438	188	3	2.00E-34	0.21	TRUE	2.39E-07	1.60	TRUE	1.14E-13	1.86	TRUE	4.61E-01	0.90	FALSE
M151T514_neg	151.0401	514	3	2.61E-08	0.33	TRUE	3.26E-03	1.75	TRUE	3.86E-05	1.95	TRUE	6.44E-01	0.92	FALSE
M157T494_neg	157.0143	494	3	1.03E-01	1.46	FALSE	9.71E-04	2.43	TRUE	6.65E-12	6.37	TRUE	1.17E-02	2.49	TRUE
M165T674_neg	165.0558	674	3	3.11E-08	0.23	TRUE	1.60E-02	1.75	TRUE	8.09E-04	1.94	TRUE	5.29E-01	0.85	FALSE
M182T113_neg	181.9632	113	3	1.78E-01	1.23	FALSE	2.58E-05	2.03	TRUE	2.34E-08	2.27	TRUE	1.78E-03	0.43	TRUE
M184T106_neg	184.0018	106	3	2.60E-29	0.42	TRUE	3.54E-03	1.21	FALSE	3.42E-19	1.73	TRUE	4.92E-04	0.51	TRUE
M185T127_neg	185.0221	127	3	3.47E-02	1.90	TRUE	1.30E-02	2.74	TRUE	6.96E-10	10.69	TRUE	7.57E-01	0.89	FALSE
M188T641_neg	188.0354	641	3	4.13E-22	0.23	TRUE	3.36E-05	1.67	TRUE	1.03E-17	2.78	TRUE	6.95E-01	0.91	FALSE
M214T105_neg	214.0207	105	3	1.04E-29	0.43	TRUE	2.27E-02	1.15	FALSE	2.70E-16	1.60	TRUE	3.16E-03	0.66	TRUE
M218T99_neg	218.0157	99	3	5.53E-49	0.09	TRUE	2.93E-02	1.21	FALSE	4.44E-09	1.57	TRUE	2.25E-04	0.12	TRUE
M225T107_neg	225.0616	107	3	4.31E-23	0.14	TRUE	3.34E-03	1.52	TRUE	4.72E-07	1.87	TRUE	1.74E-01	1.59	FALSE
M228T868_neg	228.1605	868	3	3.54E-02	0.58	TRUE	2.31E-06	4.09	TRUE	2.45E-06	3.23	TRUE	5.36E-02	1.45	FALSE
M237T1033_neg	237.1860	1033	3	3.15E-10	2.42	TRUE	1.28E-04	0.57	TRUE	5.01E-01	1.08	FALSE	9.29E-03	1.61	TRUE
M243T194_neg	243.0622	194	3	3.88E-18	0.20	TRUE	3.20E-03	1.53	TRUE	4.27E-11	2.45	TRUE	8.53E-01	1.03	FALSE
M247T629_neg	246.9919	629	3	1.94E-04	1.49	FALSE	3.77E-04	0.49	TRUE	3.20E-17	2.45	TRUE	6.62E-03	1.80	TRUE
M262T411_neg	262.0725	411	3	1.36E-06	0.38	TRUE	2.72E-03	1.74	TRUE	7.95E-11	3.30	TRUE	3.14E-01	0.78	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M273T721_neg	273.0437	721	3							HMDB0059981	droxy-5-(phenyl)-valeric acid-O-sul	C11H14O6S	0.4
M274T440_neg	274.0933	440	3						Carbohydrates	HMDB0030697	Sarmentosin	C11H17NO7	0.3
M277T700_neg	277.1219	700	3							HMDB0003426	Pantetheine	C11H22N2O4S	3.0
M279T524_neg	279.0854	524	3							HMDB0028979	Methionyl-Methionine	C10H20N2O3S2	4.2
M280T350_neg	280.1044	350	3							HMDB0037843	N-(1-Deoxy-1-fructosyl)threonine	C10H19NO8	2.1
M283T427_neg	283.0685	427	3						Carbohydrates	HMDB0000299	Xanthosine	C10H12N4O6	0.2
M297T541_neg	297.0661	541	3						Carbohydrates	HMDB0242752	6-Methylthioinosine	C11H14N4O4S	0.8
M299T575_neg	299.0990	575	3							HMDB0253183	Histidine glutamate	C11H16N4O6	2.4
M313T839_neg	313.1290	839	3						Polyketides				
M314T633_neg	314.2086	633	3						Amino acids and Peptides	HMDB0094676	Val-Val-Val	C15H29N3O4	0.2
M327T424_neg	327.0947	424	3							HMDB0004256	Hydroxy-6-methyl-8-ribityl lumazi	C12H16N4O7	0.2
M328T374_neg	328.0453	374	3							HMDB0000058	Cyclic AMP	C10H12N5O6P	0.3
M329T449_neg	329.1830	449	3						Amino acids and Peptides				
M334T701_neg	334.1518	701	3							HMDB0242692	N6-Cyclopentyladenosine	C15H21N5O4	0.8
M349T792_neg	349.1769	792	3							HMDB0251479	Disofenin	C18H26N2O5	0.0
M396T973_neg	396.2156	973	3							HMDB0249521	ylamino)carbonyl]oxiran-2-Yl}carb	C19H31N3O6	4.0
M434T1043_neg	434.2677	1043	3						Fatty acids				
M450T1030_neg	450.2628	1030	3						Fatty acids	HMDB0011474	LysoPE(0:0/16:1(9Z))	C21H42NO7P	0.5
M457T743_neg	457.1846	743	3							HMDB0252405	Fluprostenol	C23H29F3O6	0.6
M478T1056_neg	478.2941	1056	3						Fatty acids	HMDB0011475	LysoPE(0:0/18:1(11Z))	C23H46NO7P	0.4
M487T85_neg	487.0395	85	3							HMDB0303488	Iron(III) ammonium citrate	C12H22FeN3O14	3.3
M517T1012_neg	517.3535	1012	3							HMDB0297155	S(8:0/20:4(6E,8Z,11Z,14Z)+=O(5)/0	C31H50O6	0.0
M530T457_neg	530.1297	457	3						Carbohydrates				
M566T1057_neg	566.3465	1057	3						Fatty acids	HMDB0243883	eneicosanoyl-glycero-3-phosphose	C27H54NO9P	0.3
M624T459_neg	624.2148	459	3						Alkaloids				
M652T461_neg	652.2110	461	3						Amino acids and Peptides	HMDB0015331	Bromocriptine	C32H40BrN5O5	4.6
M659T723_neg	659.3299	723	3							HMDB0002318	Capsianoside I	C32H52O14	2.2
M770T452_neg	770.2839	452	3							HMDB0035904	Phyllanthusol B	C35H49NO18	4.9
M829T776_neg	829.4491	776	3						Amino acids and Peptides				
M852T958_neg	851.5682	958	3							HMDB0061395	PC(DiMe(11,3)/MonoMe(11,3))	C47H83NO10P	0.0
M87T463_pos	87.0439	463	3							HMDB0245045	2-Butyne-1,4-diol	C4H6O2	1.7
M87T418_pos	87.0439	418	3							HMDB0245045	2-Butyne-1,4-diol	C4H6O2	1.7
M97T665_pos	97.0648	665	3							HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M273T721_neg	273.0437	721	3	1.82E-05	0.37	TRUE	4.16E-03	1.95	TRUE	9.20E-08	3.07	TRUE	4.15E-01	1.21	FALSE
M274T440_neg	274.0933	440	3	1.92E-02	0.54	TRUE	1.94E-06	4.30	TRUE	6.04E-06	3.09	TRUE	4.34E-01	1.08	FALSE
M277T700_neg	277.1219	700	3	8.66E-03	1.80	TRUE	3.56E-02	0.64	TRUE	4.90E-08	3.29	TRUE	4.78E-01	1.20	FALSE
M279T524_neg	279.0854	524	3	3.35E-03	0.64	TRUE	7.05E-05	1.88	TRUE	3.63E-09	2.33	TRUE	4.27E-01	1.10	FALSE
M280T350_neg	280.1044	350	3	1.05E-04	3.59	TRUE	8.68E-06	5.73	TRUE	1.43E-12	33.51	TRUE	5.71E-02	1.50	FALSE
M283T427_neg	283.0685	427	3	3.25E-08	0.44	TRUE	2.22E-06	2.03	TRUE	2.96E-12	2.56	TRUE	2.29E-01	1.51	FALSE
M297T541_neg	297.0661	541	3	3.64E-20	0.30	TRUE	7.96E-05	1.55	TRUE	9.08E-11	1.92	TRUE	9.02E-01	0.98	FALSE
M299T575_neg	299.0990	575	3	5.62E-06	0.55	TRUE	4.48E-01	1.10	FALSE	6.35E-05	1.56	TRUE	3.72E-02	0.65	TRUE
M313T839_neg	313.1290	839	3	3.87E-07	1.58	TRUE	6.78E-14	0.54	TRUE	1.84E-05	1.39	FALSE	1.71E-03	0.50	TRUE
M314T633_neg	314.2086	633	3	3.14E-25	0.29	TRUE	7.19E-01	1.04	FALSE	1.66E-07	1.55	TRUE	2.10E-02	0.66	TRUE
M327T424_neg	327.0947	424	3	2.15E-13	0.55	TRUE	3.65E-01	1.07	FALSE	4.08E-10	1.54	TRUE	2.26E-03	1.51	TRUE
M328T374_neg	328.0453	374	3	5.00E-04	0.65	TRUE	9.63E-01	0.99	FALSE	4.92E-13	2.38	TRUE	1.32E-02	1.56	TRUE
M329T449_neg	329.1830	449	3	5.38E-07	0.54	TRUE	4.24E-01	0.90	FALSE	2.61E-13	2.28	TRUE	3.17E-05	0.33	TRUE
M334T701_neg	334.1518	701	3	3.23E-04	3.46	TRUE	2.78E-02	0.54	TRUE	4.55E-12	67.51	TRUE	1.17E-01	1.39	FALSE
M349T792_neg	349.1769	792	3	2.52E-03	1.63	TRUE	3.86E-13	0.33	TRUE	5.99E-07	0.48	TRUE	4.47E-01	0.91	FALSE
M396T973_neg	396.2156	973	3	3.59E-03	1.87	TRUE	2.69E-02	0.61	TRUE	1.38E-06	2.62	TRUE	9.98E-01	1.00	FALSE
M434T1043_neg	434.2677	1043	3	1.66E-04	2.29	TRUE	3.48E-02	0.59	TRUE	1.54E-04	2.05	TRUE	8.10E-01	1.04	FALSE
M450T1030_neg	450.2628	1030	3	1.43E-05	2.31	TRUE	1.56E-02	0.64	TRUE	6.21E-04	1.74	TRUE	6.27E-01	0.90	FALSE
M457T743_neg	457.1846	743	3	2.63E-06	0.53	TRUE	8.59E-10	2.36	TRUE	3.90E-12	2.38	TRUE	7.27E-01	1.04	FALSE
M478T1056_neg	478.2941	1056	3	7.10E-06	2.34	TRUE	1.60E-04	0.48	TRUE	6.48E-05	1.90	TRUE	6.40E-01	0.81	FALSE
M487T85_neg	487.0395	85	3	3.31E-46	0.15	TRUE	4.40E-04	1.33	FALSE	3.33E-16	1.86	TRUE	1.57E-02	0.54	TRUE
M517T1012_neg	517.3535	1012	3	2.13E-07	1.65	TRUE	4.78E-10	0.51	TRUE	7.18E-01	0.97	FALSE	3.91E-05	1.68	TRUE
M530T457_neg	530.1297	457	3	2.53E-21	0.00	TRUE	8.55E-01	0.96	FALSE	8.41E-06	2.18	TRUE	1.11E-02	3.03	TRUE
M566T1057_neg	566.3465	1057	3	8.26E-03	13.77	TRUE	6.89E-03	0.14	TRUE	3.02E-02	0.24	TRUE	9.86E-01	0.98	FALSE
M624T459_neg	624.2148	459	3	3.37E-03	3.21	TRUE	2.87E-01	0.71	FALSE	1.23E-05	5.50	TRUE	2.35E-04	38.87	TRUE
M652T461_neg	652.2110	461	3	2.07E-11	0.06	TRUE	8.60E-01	1.05	FALSE	3.51E-02	0.63	TRUE	4.95E-02	0.28	TRUE
M659T723_neg	659.3299	723	3	9.77E-07	1.82	TRUE	1.57E-02	0.75	FALSE	6.68E-08	1.79	TRUE	3.25E-03	1.65	TRUE
M770T452_neg	770.2839	452	3	1.13E-10	0.16	TRUE	5.83E-04	2.25	TRUE	2.15E-07	3.02	TRUE	3.77E-01	2.06	FALSE
M829T776_neg	829.4491	776	3	1.17E-04	5.10	TRUE	7.11E-08	0.08	TRUE	2.69E-03	0.38	TRUE	9.11E-01	1.01	FALSE
M852T958_neg	851.5682	958	3	8.15E-07	1.92	TRUE	6.02E-01	1.07	FALSE	1.53E-18	3.23	TRUE	8.10E-03	0.63	TRUE
M87T463_pos	87.0439	463	3	2.07E-24	0.59	TRUE	1.30E-01	1.07	FALSE	5.64E-31	1.73	TRUE	7.35E-05	0.77	FALSE
M87T418_pos	87.0439	418	3	1.30E-06	0.63	TRUE	9.84E-01	1.00	FALSE	1.36E-14	1.98	TRUE	2.28E-01	0.88	FALSE
M97T665_pos	97.0648	665	3	9.17E-20	0.63	TRUE	8.39E-03	1.13	FALSE	6.37E-29	1.69	TRUE	3.86E-05	0.71	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M113T349_pos	113.0346	349	3							HMDB0000300	Uracil	C4H4N2O2	0.3
M114T547_pos	114.0914	547	3							HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	0.3
M118T161_pos	118.0863	161	3							HMDB0000883	L-Valine	C5H11NO2	0.1
M123T239_pos	123.0553	239	3						Alkaloids	HMDB0001406	Niacinamide	C6H6N2O	0.1
M127T375_pos	127.0501	375	3						Alkaloids	HMDB0000262	Thymine	C5H6N2O2	0.6
M130T517_pos	130.1591	517	3							HMDB0247306	Diisopropylethylamine	C8H19N	0.4
M132T324_pos	132.1019	324	3							HMDB0000172	L-Isoleucine	C6H13NO2	0.2
M133T191_pos	133.0318	191	3							HMDB0059667	3-Methyl sulfolene	C5H8O2S	0.3
M136T384_pos	136.0618	384	3						Alkaloids	HMDB0000034	Adenine	C5H5N5	0.2
M139T201_pos	139.0503	201	3							HMDB0000301	Urocanic acid	C6H6N2O2	0.4
M141T520_pos	141.0910	520	3						Fatty acids	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	0.3
M143T665_pos	143.0703	665	3						Fatty acids	HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.1
M146T687_pos	146.0601	687	3						Alkaloids	HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.2
M146T514_pos	146.1652	514	3						Alkaloids	HMDB0001257	Spermidine	C7H19N3	0.2
M148T120_pos	148.0604	120	3							HMDB0000148	L-Glutamic acid	C5H9NO4	0.0
M150T191_pos	150.0583	191	3							HMDB0000696	L-Methionine	C5H11NO2S	0.1
M152T422_pos	152.0706	422	3							HMDB0001859	Acetaminophen	C8H9NO2	0.2
M156T655_pos	156.0421	655	3							HMDB0060173	-Methylethanolaminium phosphat	C3H10NO4P	0.4
M157T793_pos	157.0496	793	3							HMDB0029610	Ascladiol	C7H8O4	0.4
M157T1039_pos	157.1223	1039	3							HMDB0004362	4-Hydroxynonenal	C9H16O2	0.3
M162T421_pos	162.0550	421	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.4
M167T439_pos	167.0895	439	3							HMDB0038183	3-(4-Methyl-3-pentenyl)thiophene	C10H14S	3.8
M181T1039_pos	181.1587	1039	3							HMDB0031181	Homodihydrojasmone	C12H20O	0.3
M182T487_pos	182.0449	487	3							HMDB0006954	-3-hydroxy-5-formylpyridine-4-ca	C8H7NO4	0.5
M190T485_pos	190.0500	485	3						Alkaloids	HMDB0000715	Kynurenic acid	C10H7NO3	0.6
M191T707_pos	191.0816	707	3							HMDB0031173	6-Hydroxy-1H-indole-3-acetamide	C10H10N2O2	0.7
M193T923_pos	193.1224	923	3							HMDB0031571	Methyl-1-phenyl-2-propanyl aceta	C12H16O2	0.4
M203T429_pos	203.1392	429	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.7
M206T471_pos	206.0449	471	3						Alkaloids	HMDB0000881	Xanthurenic acid	C10H7NO4	0.6
M209T949_pos	209.1173	949	3							HMDB0029867	Isoelemicin	C12H16O3	0.3
M211T923_pos	211.1329	923	3						Fatty acids	HMDB0032797	Jasmonic acid	C12H18O3	0.2
M213T1039_pos	213.1850	1039	3						Fatty acids	HMDB0031017	10-Undecenyl acetate	C13H24O2	0.5
M218T398_pos	218.0483	398	3							HMDB0006409	Tyramine-O-sulfate	C8H11NO4S	0.7
M219T113_pos	219.0298	113	3							HMDB0031823	Diphenyl disulfide	C12H10S2	0.6
M219T438_pos	219.1341	438	3							HMDB0014515	Meprobamate	C9H18N2O4	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M113T349_pos	113.0346	349	3	3.82E-12	0.61	TRUE	7.71E-01	0.98	FALSE	7.57E-21	1.86	TRUE	8.31E-01	0.98	FALSE
M114T547_pos	114.0914	547	3	1.13E-24	2.04	TRUE	9.30E-05	0.77	FALSE	2.04E-07	0.76	FALSE	1.30E-04	1.65	TRUE
M118T161_pos	118.0863	161	3	5.88E-44	0.21	TRUE	3.17E-05	1.37	FALSE	1.14E-10	1.54	TRUE	6.24E-02	1.33	FALSE
M123T239_pos	123.0553	239	3	1.61E-06	1.72	TRUE	6.64E-04	0.64	TRUE	4.59E-01	1.07	FALSE	7.75E-03	1.35	FALSE
M127T375_pos	127.0501	375	3	3.33E-23	0.12	TRUE	4.65E-02	1.33	FALSE	4.13E-10	2.31	TRUE	5.14E-01	1.26	FALSE
M130T517_pos	130.1591	517	3	2.15E-13	1.78	TRUE	7.32E-01	0.98	FALSE	4.31E-04	0.80	FALSE	2.12E-03	0.38	TRUE
M132T324_pos	132.1019	324	3	1.41E-20	0.28	TRUE	5.33E-05	1.60	TRUE	1.12E-04	1.46	FALSE	8.64E-01	1.05	FALSE
M133T191_pos	133.0318	191	3	4.93E-52	0.14	TRUE	1.29E-05	1.39	FALSE	8.09E-12	1.59	TRUE	7.28E-02	1.19	FALSE
M136T384_pos	136.0618	384	3	2.78E-01	1.11	FALSE	6.25E-05	0.66	TRUE	1.25E-26	3.03	TRUE	1.99E-01	1.14	FALSE
M139T201_pos	139.0503	201	3	7.26E-43	0.16	TRUE	1.89E-04	1.37	FALSE	1.93E-04	1.31	FALSE	4.86E-02	1.53	TRUE
M141T520_pos	141.0910	520	3	1.01E-35	1.79	TRUE	6.08E-01	1.02	FALSE	8.81E-28	0.66	TRUE	4.55E-01	1.04	FALSE
M143T665_pos	143.0703	665	3	3.95E-23	0.57	TRUE	1.36E-01	1.08	FALSE	2.44E-29	1.79	TRUE	9.12E-05	0.68	FALSE
M146T687_pos	146.0601	687	3	6.21E-01	0.91	FALSE	4.88E-07	2.80	TRUE	6.21E-11	3.48	TRUE	1.51E-02	0.78	FALSE
M146T514_pos	146.1652	514	3	1.62E-01	1.16	FALSE	1.97E-05	0.62	TRUE	3.48E-06	1.56	TRUE	3.12E-01	1.15	FALSE
M148T120_pos	148.0604	120	3	8.93E-79	0.27	TRUE	2.54E-02	1.09	FALSE	9.73E-33	1.58	TRUE	2.25E-01	0.92	FALSE
M150T191_pos	150.0583	191	3	8.05E-58	0.11	TRUE	2.24E-04	1.31	FALSE	7.97E-11	1.52	TRUE	2.90E-02	1.23	FALSE
M152T422_pos	152.0706	422	3	3.02E-25	0.30	TRUE	7.01E-01	1.04	FALSE	8.90E-10	1.67	TRUE	1.27E-01	1.15	FALSE
M156T655_pos	156.0421	655	3	5.45E-35	5.92	TRUE	1.12E-01	1.17	FALSE	1.81E-16	0.46	TRUE	9.56E-01	0.99	FALSE
M157T793_pos	157.0496	793	3	1.69E-06	0.58	TRUE	4.69E-01	1.09	FALSE	2.83E-22	0.31	TRUE	9.84E-01	1.00	FALSE
M157T1039_pos	157.1223	1039	3	4.42E-09	1.76	TRUE	1.73E-05	0.66	TRUE	7.06E-01	0.97	FALSE	8.39E-05	1.34	FALSE
M162T421_pos	162.0550	421	3	1.11E-02	0.79	FALSE	3.30E-01	1.10	FALSE	1.48E-20	2.49	TRUE	1.09E-02	0.49	TRUE
M167T439_pos	167.0895	439	3	9.85E-41	0.22	TRUE	4.31E-07	1.49	FALSE	2.32E-14	1.73	TRUE	1.51E-01	1.23	FALSE
M181T1039_pos	181.1587	1039	3	1.09E-13	1.79	TRUE	2.17E-08	0.66	TRUE	8.55E-01	1.01	FALSE	8.08E-04	1.25	FALSE
M182T487_pos	182.0449	487	3	5.54E-07	0.48	TRUE	6.21E-01	1.07	FALSE	3.61E-06	1.79	TRUE	4.33E-01	1.11	FALSE
M190T485_pos	190.0500	485	3	6.43E-01	0.96	FALSE	4.99E-01	1.07	FALSE	9.30E-16	2.13	TRUE	1.13E-03	0.45	TRUE
M191T707_pos	191.0816	707	3	7.34E-22	2.08	TRUE	3.47E-01	1.06	FALSE	2.18E-32	2.35	TRUE	2.86E-01	0.91	FALSE
M193T923_pos	193.1224	923	3	8.12E-12	0.38	TRUE	5.95E-01	1.07	FALSE	1.69E-05	1.62	TRUE	4.74E-01	0.90	FALSE
M203T429_pos	203.1392	429	3	9.04E-12	0.36	TRUE	1.36E-01	1.24	FALSE	2.89E-06	1.75	TRUE	1.34E-01	0.63	FALSE
M206T471_pos	206.0449	471	3	3.33E-19	0.44	TRUE	4.89E-01	1.06	FALSE	3.21E-15	1.82	TRUE	3.58E-01	0.89	FALSE
M209T949_pos	209.1173	949	3	4.66E-24	0.61	TRUE	2.29E-03	1.15	FALSE	3.27E-29	1.64	TRUE	7.33E-01	1.02	FALSE
M211T923_pos	211.1329	923	3	5.21E-12	0.36	TRUE	6.75E-01	1.06	FALSE	1.65E-05	1.65	TRUE	4.59E-01	0.88	FALSE
M213T1039_pos	213.1850	1039	3	1.22E-14	2.11	TRUE	3.20E-08	0.60	TRUE	9.41E-01	0.99	FALSE	1.31E-04	1.36	FALSE
M218T398_pos	218.0483	398	3	3.65E-17	0.50	TRUE	9.15E-01	0.99	FALSE	2.91E-16	1.78	TRUE	2.77E-04	0.72	FALSE
M219T113_pos	219.0298	113	3	6.88E-09	0.36	TRUE	9.59E-04	1.76	TRUE	1.41E-02	1.40	FALSE	7.69E-01	1.15	FALSE
M219T438_pos	219.1341	438	3	2.69E-21	0.27	TRUE	6.62E-01	0.95	FALSE	8.52E-06	1.54	TRUE	1.58E-01	0.83	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M229T768_1_pos	229.0497	768	3							HMDB0013695	Urolithin A	C13H8O4	0.9
M229T923_pos	229.1436	923	3							HMDB0000933	Traumatic acid	C12H20O4	0.5
M231T793_pos	231.0864	793	3							HMDB0246021	lactitol, 1,2:5,6-dianhydro-, diacet	C10H14O6	0.4
M231T640_2_pos	231.1704	640	3						Amino acids and Peptides	HMDB0028920	Isoleucyl-Valine	C11H22N2O3	0.3
M233T544_pos	233.1497	544	3							HMDB0013075	Spermic acid 2	C10H20N2O4	0.3
M246T646_pos	246.1702	646	3							HMDB0000378	2-Methylbutyroylcarnitine	C12H23NO4	0.9
M247T549_pos	247.1080	549	3							HMDB0013713	N-Acetyltryptophan	C13H14N2O3	1.0
M247T854_pos	247.1727	854	3							HMDB0038947	(S)-3-Methylthiohexyl hexanoate	C13H26O2S	0.3
M248T488_pos	248.0589	488	3							HMDB0252436	Forchlorfenuron	C12H10ClN3O	1.6
M249T570_pos	249.0872	570	3							HMDB0004185	5-Hydroxyindoleacetylglycine	C12H12N2O4	0.9
M251T949_pos	251.1279	949	3							HMDB0002012	Ubiquinone-1	C14H18O4	0.4
M253T486_pos	253.1188	486	3							HMDB0013940	N-Desmethylpromazine	C12H16N2O4	2.0
M257T675_pos	257.0812	675	3							HMDB0005760	Dihydrodaidzein	C15H12O4	1.3
M259T818_pos	259.0966	818	3							HMDB0004629	O-Desmethylangolensin	C15H14O4	0.4
M259T829_pos	259.1443	829	3							HMDB0246654	hylaminomethyl-gamma-aminobut	C15H18N2O2	0.9
M260T447_pos	260.1606	447	3							HMDB0028800	Glutaminylisoleucine	C11H21N3O4	0.6
M269T412_pos	269.1498	412	3							HMDB0247322	(2-hydroxyethyl)amino-L-phenylala	C13H20N2O4	1.0
M275T649_pos	275.1030	649	3							HMDB0035115	rahydro-1-methyl-beta-carboline-1	C14H14N2O4	1.4
M277T793_pos	277.1284	793	3							HMDB0034263	Triethyl citrate	C12H20O7	0.7
M282T483_pos	282.1339	483	3							HMDB0255476	3-Hydroxy-4-pivaloyloxyphenyl)ala	C14H19NO5	1.1
M282T1074_pos	282.2217	1074	3							HMDB0015554	Alverine	C20H27N	0.1
M283T1039_pos	283.2635	1039	3						Fatty acids	HMDB0000207	Oleic acid	C18H34O2	1.2
M286T946_pos	286.3107	946	3							HMDB0258433	Spisulosine	C18H39NO	0.8
M288T919_pos	288.2899	919	3						Fatty acids				
M289T598_pos	289.1186	598	3							HMDB0034881	-tetrahydro-1H-pyrido[3,4-b]indole	C15H16N2O4	1.1
M289T953_pos	289.2164	953	3						Terpenoids	HMDB0000077	Dehydroepiandrosterone	C19H28O2	0.6
M292T759_pos	292.2272	759	3							HMDB0015447	Penbutolol	C18H29NO2	0.4
M295T956_pos	295.1905	956	3							HMDB0005783	Gingerol	C17H26O4	0.4
M299T793_pos	299.1104	793	3							HMDB0247416	8-Aminoguanosine	C10H14N6O5	1.8
M299T906_pos	299.1655	906	3							HMDB0030729	Gravelliferone	C19H22O3	4.6
M305T1062_pos	305.2475	1062	3							HMDB0001043	Arachidonic acid	C20H32O2	0.0
M307T847_pos	307.2014	847	3							HMDB0255251	N,N-Diallylpentobarbital	C17H26N2O3	0.9
M311T684_pos	311.0918	684	3							HMDB0040357	xy-2,2-dimethylpyrano[3,2-c]xanth	C18H14O5	1.1
M311T524_pos	311.1604	524	3							HMDB0250969	Delgocitini	C16H18N6O	3.3
M317T1055_pos	317.2688	1055	3							HMDB0011532	MG(0:0/15:0/0:0)	C18H36O4	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M229T768_1_pos	229.0497	768	3	1.18E-05	2.37	TRUE	2.06E-02	0.64	TRUE	9.37E-01	0.99	FALSE	4.72E-02	1.41	FALSE
M229T923_pos	229.1436	923	3	3.82E-12	0.35	TRUE	6.28E-01	1.07	FALSE	2.17E-05	1.66	TRUE	5.27E-01	0.90	FALSE
M231T793_pos	231.0864	793	3	8.25E-06	0.62	TRUE	4.82E-01	1.08	FALSE	1.77E-19	0.37	TRUE	3.95E-02	0.94	FALSE
M231T640_2_pos	231.1704	640	3	1.12E-41	0.04	TRUE	5.07E-01	1.08	FALSE	2.41E-08	1.72	TRUE	3.72E-01	0.65	FALSE
M233T544_pos	233.1497	544	3	5.07E-43	0.09	TRUE	4.58E-01	1.08	FALSE	1.18E-10	1.76	TRUE	1.78E-01	0.87	FALSE
M246T646_pos	246.1702	646	3	4.33E-12	1.66	TRUE	8.00E-01	0.98	FALSE	1.25E-02	1.16	FALSE	2.55E-02	0.62	TRUE
M247T549_pos	247.1080	549	3	1.53E-16	0.65	TRUE	3.31E-02	1.11	FALSE	1.39E-35	1.92	TRUE	6.39E-02	0.88	FALSE
M247T854_pos	247.1727	854	3	5.82E-21	2.56	TRUE	1.64E-04	0.74	FALSE	2.06E-02	0.85	FALSE	1.12E-04	0.27	TRUE
M248T488_pos	248.0589	488	3	3.43E-21	0.52	TRUE	6.24E-02	1.12	FALSE	5.66E-23	1.81	TRUE	7.15E-01	1.02	FALSE
M249T570_pos	249.0872	570	3	1.51E-38	0.45	TRUE	1.89E-01	1.07	FALSE	1.36E-30	1.76	TRUE	1.11E-01	0.91	FALSE
M251T949_pos	251.1279	949	3	4.72E-26	0.55	TRUE	9.89E-05	1.22	FALSE	8.81E-30	1.76	TRUE	7.21E-02	1.12	FALSE
M253T486_pos	253.1188	486	3	1.28E-28	0.33	TRUE	8.16E-01	1.02	FALSE	2.56E-09	1.53	TRUE	8.23E-02	0.85	FALSE
M257T675_pos	257.0812	675	3	1.35E-29	0.54	TRUE	4.91E-02	1.10	FALSE	1.36E-36	1.88	TRUE	4.92E-01	1.04	FALSE
M259T818_pos	259.0966	818	3	5.78E-10	2.79	TRUE	1.49E-03	0.61	TRUE	1.70E-01	1.19	FALSE	6.57E-01	1.07	FALSE
M259T829_pos	259.1443	829	3	2.55E-14	1.94	TRUE	4.90E-03	0.82	FALSE	5.55E-06	1.38	FALSE	2.20E-06	0.61	TRUE
M260T447_pos	260.1606	447	3	5.84E-31	0.24	TRUE	4.29E-01	0.93	FALSE	3.46E-07	1.51	TRUE	1.12E-01	0.66	FALSE
M269T412_pos	269.1498	412	3	8.88E-11	0.61	TRUE	1.09E-01	1.13	FALSE	6.63E-23	2.08	TRUE	4.87E-01	0.96	FALSE
M275T649_pos	275.1030	649	3	8.00E-41	0.33	TRUE	1.17E-01	1.10	FALSE	2.74E-17	1.62	TRUE	1.62E-04	0.75	FALSE
M277T793_pos	277.1284	793	3	8.84E-08	0.53	TRUE	4.53E-01	1.09	FALSE	6.33E-21	0.32	TRUE	2.77E-01	0.91	FALSE
M282T483_pos	282.1339	483	3	7.56E-13	0.63	TRUE	3.83E-02	1.14	FALSE	4.89E-27	1.94	TRUE	8.05E-01	0.98	FALSE
M282T1074_pos	282.2217	1074	3	8.63E-02	0.65	FALSE	2.57E-03	0.49	TRUE	2.18E-09	0.20	TRUE	3.75E-01	0.72	FALSE
M283T1039_pos	283.2635	1039	3	3.51E-14	2.34	TRUE	3.96E-08	0.56	TRUE	7.72E-01	0.98	FALSE	1.08E-04	1.39	FALSE
M286T946_pos	286.3107	946	3	1.74E-05	8.65	TRUE	2.55E-02	0.53	TRUE	7.96E-01	0.92	FALSE	9.52E-01	1.01	FALSE
M288T919_pos	288.2899	919	3	6.66E-06	4.45	TRUE	2.38E-02	0.58	TRUE	7.02E-01	1.10	FALSE	6.06E-01	0.90	FALSE
M289T598_pos	289.1186	598	3	1.03E-14	0.57	TRUE	1.23E-01	1.11	FALSE	3.79E-21	1.88	TRUE	3.52E-04	0.80	FALSE
M289T953_pos	289.2164	953	3	1.07E-12	1.78	TRUE	9.16E-01	0.99	FALSE	9.67E-15	1.74	TRUE	5.46E-01	0.95	FALSE
M292T759_pos	292.2272	759	3	1.46E-08	1.90	TRUE	1.36E-08	0.56	TRUE	3.08E-01	0.91	FALSE	5.65E-02	0.65	FALSE
M295T956_pos	295.1905	956	3	4.67E-12	2.31	TRUE	9.20E-12	0.36	TRUE	4.95E-02	0.83	FALSE	7.72E-01	1.07	FALSE
M299T793_pos	299.1104	793	3	2.07E-05	0.61	TRUE	3.49E-01	1.12	FALSE	1.81E-23	0.29	TRUE	4.51E-01	1.23	FALSE
M299T906_pos	299.1655	906	3	2.72E-17	1.90	TRUE	4.89E-11	0.63	TRUE	9.47E-09	0.70	FALSE	3.54E-01	0.91	FALSE
M305T1062_pos	305.2475	1062	3	5.83E-06	3.46	TRUE	3.59E-02	0.64	TRUE	9.91E-01	1.00	FALSE	9.33E-01	0.98	FALSE
M307T847_pos	307.2014	847	3	1.34E-07	0.65	TRUE	3.92E-07	1.51	TRUE	4.76E-03	1.21	FALSE	9.39E-02	1.18	FALSE
M311T684_pos	311.0918	684	3	2.76E-27	0.49	TRUE	1.64E-01	1.08	FALSE	1.53E-23	1.73	TRUE	3.29E-02	0.83	FALSE
M311T524_pos	311.1604	524	3	2.41E-23	0.54	TRUE	4.56E-03	1.17	FALSE	1.71E-34	2.05	TRUE	6.14E-01	1.02	FALSE
M317T1055_pos	317.2688	1055	3	4.65E-04	2.36	TRUE	3.67E-01	0.81	FALSE	3.07E-08	3.68	TRUE	2.96E-01	0.84	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M318T1039_pos	318.3003	1039	3						Fatty acids	HMDB0004610	Phytosphingosine	C18H39NO3	0.1
M318T919_pos	318.3003	919	3						Fatty acids	HMDB0004610	Phytosphingosine	C18H39NO3	0.3
M321T738_pos	321.1446	738	3							HMDB0038970	Formylfusarochromanone	C16H20N2O5	0.4
M321T867_pos	321.2176	867	3							HMDB0253572	Iprovalicar	C18H28N2O3	0.9
M327T955_1_pos	327.2168	955	3							HMDB0031963	2-Epoxy-7(11)-eremophilene-6,8,1	C18H30O5	0.5
M336T690_pos	336.2279	690	3							HMDB0060098	eroxy-5Z,7E,11Z,14Z-eicosatetraen	C20H31O4	4.7
M337T1063_pos	337.2732	1063	3						Fatty acids	HMDB0006070	Pregnanetriol	C21H36O3	1.6
M348T801_pos	348.1444	801	3							HMDB0255456	Naproxcinod	C18H21NO6	0.7
M349T562_pos	349.1766	562	3							HMDB0253427	Imidocar	C19H20N6O	1.6
M349T982_pos	349.2739	982	3							HMDB0029683	-Hydroxy-6-pentadecylbenzoic aci	C22H36O3	0.5
M356T545_pos	356.1859	545	3							HMDB0246890	y)anthracen-9-yl]methylamino]-2-	C21H25NO4	0.8
M375T842_pos	375.2013	842	3							HMDB0029782	6-Epi-7-isocucurbic acid glucoside	C18H30O8	0.1
M375T1047_pos	375.2511	1047	3						Fatty acids				
M377T619_pos	377.1457	619	3							HMDB0000244	Riboflavin	C17H20N4O6	0.3
M379T426_pos	379.2077	426	3							HMDB0003933	Pentosidine	C17H26N6O4	3.1
M389T1056_pos	389.3051	1056	3							HMDB0038523	2-(10-heptadecenyl)-6-hydroxybe	C25H40O3	0.3
M393T1062_pos	393.2401	1062	3							HMDB0007003	CPA(16:0/0:0)	C19H37O6P	0.1
M399T963_pos	399.2893	963	3							HMDB0258854	Benzotest	C26H38O3	0.2
M400T808_pos	400.3575	808	3						Alkaloids	HMDB0032023	3-Epidemissidine	C27H45NO	0.3
M408T931_pos	408.1557	931	3							HMDB0255119	N-Desmethyl Topotecan	C22H21N3O5	0.8
M410T382_pos	410.1672	382	3							HMDB0011596	Queuosine	C17H23N5O7	0.5
M414T794_pos	414.3368	794	3							HMDB0031913	5alpha-Tomatidan-3-one	C27H43NO2	0.3
M414T649_pos	414.3370	649	3							HMDB0031913	5alpha-Tomatidan-3-one	C27H43NO2	0.7
M416T847_pos	416.3524	847	3							HMDB0034731	Tomatidine	C27H45NO2	0.2
M416T759_pos	416.3525	759	3							HMDB0034731	Tomatidine	C27H45NO2	0.5
M419T1059_pos	419.3159	1059	3							HMDB0012515	10-HETE	C26H42O4	0.7
M420T719_pos	420.2494	719	3							HMDB0247141	N-Formyl-Nle-Leu-Phe	C22H33N3O5	0.2
M420T653_pos	420.2494	653	3							HMDB0247141	N-Formyl-Nle-Leu-Phe	C22H33N3O5	0.2
M420T778_pos	420.2494	778	3							HMDB0247141	N-Formyl-Nle-Leu-Phe	C22H33N3O5	0.2
M422T953_pos	422.1714	953	3							HMDB0015164	Topotecan	C23H23N3O5	0.9
M426T1016_pos	426.2621	1016	3							HMDB0011470	LysoPE(0:0/14:0)	C19H40NO7P	1.4
M432T805_pos	432.2751	805	3							HMDB0061045	alpha-hydroxysalmeterol	C25H37NO5	1.5
M440T1034_pos	440.2773	1034	3							HMDB0240697	sphocholine (isomer 1) (LPC(12:0) i	C20H42NO7P	0.2
M445T1043_pos	445.3675	1043	3						Terpenoids	HMDB0011662	eta-methyl-5-alpha-cholest-7-ene-	C29H48O3	0.4
M450T989_pos	450.3222	989	3						Terpenoids	HMDB0000631	Deoxycholic acid glycine conjugate	C26H43NO5	1.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M318T1039_pos	318.3003	1039	3	6.53E-16	1.93	TRUE	7.76E-09	0.63	TRUE	2.25E-01	0.93	FALSE	5.62E-05	1.35	FALSE
M318T919_pos	318.3003	919	3	1.64E-04	3.75	TRUE	7.31E-03	0.48	TRUE	6.44E-02	0.61	FALSE	8.25E-01	0.92	FALSE
M321T738_pos	321.1446	738	3	4.01E-02	1.20	FALSE	1.53E-01	1.13	FALSE	4.01E-09	1.61	TRUE	9.75E-05	0.55	TRUE
M321T867_pos	321.2176	867	3	1.57E-06	0.66	TRUE	6.94E-08	1.61	TRUE	7.78E-02	1.14	FALSE	3.54E-02	1.31	FALSE
M327T955_1_pos	327.2168	955	3	3.40E-10	1.77	TRUE	1.10E-09	0.52	TRUE	2.35E-01	0.92	FALSE	7.37E-01	1.06	FALSE
M336T690_pos	336.2279	690	3	2.82E-04	2.65	TRUE	3.92E-01	0.82	FALSE	2.26E-02	1.65	TRUE	4.35E-01	0.87	FALSE
M337T1063_pos	337.2732	1063	3	2.88E-01	1.26	FALSE	7.45E-03	0.40	TRUE	2.41E-07	3.09	TRUE	5.60E-01	0.76	FALSE
M348T801_pos	348.1444	801	3	2.42E-09	0.62	TRUE	8.11E-01	1.02	FALSE	2.15E-12	1.65	TRUE	7.55E-01	1.05	FALSE
M349T562_pos	349.1766	562	3	1.58E-14	0.60	TRUE	1.18E-01	1.10	FALSE	4.19E-27	1.99	TRUE	2.52E-01	0.94	FALSE
M349T982_pos	349.2739	982	3	2.41E-09	2.48	TRUE	4.93E-05	0.57	TRUE	1.19E-01	1.20	FALSE	1.14E-01	1.58	FALSE
M356T545_pos	356.1859	545	3	3.88E-10	1.51	TRUE	4.66E-01	1.05	FALSE	2.18E-13	1.53	TRUE	8.51E-02	0.90	FALSE
M375T842_pos	375.2013	842	3	1.14E-34	0.50	TRUE	2.10E-01	1.06	FALSE	8.49E-35	1.81	TRUE	3.16E-03	0.78	FALSE
M375T1047_pos	375.2511	1047	3	4.17E-01	1.22	FALSE	5.20E-02	0.50	FALSE	1.44E-04	2.41	TRUE	1.11E-03	0.28	TRUE
M377T619_pos	377.1457	619	3	1.04E-10	0.55	TRUE	2.17E-04	1.42	FALSE	3.59E-23	2.46	TRUE	6.19E-02	1.28	FALSE
M379T426_pos	379.2077	426	3	3.32E-25	0.42	TRUE	3.61E-01	1.07	FALSE	1.26E-17	1.77	TRUE	9.47E-01	1.00	FALSE
M389T1056_pos	389.3051	1056	3	6.92E-11	1.72	TRUE	8.60E-01	1.01	FALSE	3.59E-13	1.70	TRUE	1.66E-02	1.33	FALSE
M393T1062_pos	393.2401	1062	3	1.21E-01	1.25	FALSE	1.90E-02	0.64	TRUE	4.78E-08	2.12	TRUE	5.76E-01	0.84	FALSE
M399T963_pos	399.2893	963	3	9.51E-15	1.63	TRUE	3.70E-01	1.05	FALSE	8.17E-14	1.50	TRUE	4.29E-01	0.95	FALSE
M400T808_pos	400.3575	808	3	5.45E-05	4.02	TRUE	2.82E-02	0.55	TRUE	7.05E-01	1.10	FALSE	9.08E-01	1.04	FALSE
M408T931_pos	408.1557	931	3	1.49E-17	1.91	TRUE	2.66E-01	0.93	FALSE	1.79E-18	1.79	TRUE	7.56E-01	0.98	FALSE
M410T382_pos	410.1672	382	3	2.35E-34	0.40	TRUE	6.33E-02	1.12	FALSE	3.32E-17	1.59	TRUE	4.76E-01	1.08	FALSE
M414T794_pos	414.3368	794	3	2.40E-06	3.88	TRUE	1.74E-02	0.59	TRUE	5.51E-01	1.14	FALSE	4.42E-01	0.86	FALSE
M414T649_pos	414.3370	649	3	4.68E-34	5.10	TRUE	1.03E-03	1.37	FALSE	1.79E-15	2.03	TRUE	3.69E-02	0.82	FALSE
M416T847_pos	416.3524	847	3	5.53E-07	5.19	TRUE	1.13E-03	0.47	TRUE	6.56E-01	0.90	FALSE	6.68E-01	0.92	FALSE
M416T759_pos	416.3525	759	3	4.63E-04	4.64	TRUE	4.38E-02	0.55	TRUE	2.16E-01	1.49	FALSE	7.52E-01	0.81	FALSE
M419T1059_pos	419.3159	1059	3	1.96E-04	0.65	TRUE	8.15E-06	1.71	TRUE	7.98E-02	0.84	FALSE	1.21E-01	0.58	FALSE
M420T719_pos	420.2494	719	3	4.49E-03	0.65	TRUE	1.53E-01	1.23	FALSE	2.16E-05	1.78	TRUE	9.87E-01	1.00	FALSE
M420T653_pos	420.2494	653	3	2.12E-11	4.16	TRUE	3.11E-06	0.53	TRUE	7.63E-02	1.31	FALSE	9.70E-01	0.99	FALSE
M420T778_pos	420.2494	778	3	1.29E-17	0.59	TRUE	8.36E-08	1.36	FALSE	9.27E-21	1.68	TRUE	1.62E-01	1.08	FALSE
M422T953_pos	422.1714	953	3	2.67E-16	2.19	TRUE	1.21E-01	0.87	FALSE	1.55E-11	1.70	TRUE	9.52E-01	1.01	FALSE
M426T1016_pos	426.2621	1016	3	3.28E-03	2.82	TRUE	2.46E-01	0.66	FALSE	3.07E-06	5.09	TRUE	5.46E-01	0.86	FALSE
M432T805_pos	432.2751	805	3	2.17E-03	2.28	TRUE	7.83E-01	0.94	FALSE	2.24E-03	2.02	TRUE	9.46E-01	1.04	FALSE
M440T1034_pos	440.2773	1034	3	4.46E-04	2.95	TRUE	2.34E-01	0.70	FALSE	1.35E-07	4.87	TRUE	1.55E-01	0.79	FALSE
M445T1043_pos	445.3675	1043	3	5.99E-07	1.97	TRUE	1.38E-04	0.64	TRUE	5.98E-01	1.06	FALSE	6.60E-01	0.94	FALSE
M450T989_pos	450.3222	989	3	9.37E-03	2.56	TRUE	8.59E-03	0.31	TRUE	9.68E-02	0.61	FALSE	6.10E-01	1.42	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M452T514_pos	452.3234	514	3						Amino acids and Peptides				
M452T456_pos	452.3235	456	3						Amino acids and Peptides				
M459T1037_pos	459.3465	1037	3							HMDB0032669	E,24R)-3,5,9-Trihydroxy-23-methy	C29H46O4	0.8
M468T1034_pos	468.3687	1034	3							HMDB0241576	Z,11Z)-3-Icosa-8,11-dienoylcarniti	C27H49NO5	0.8
M471T1048_pos	471.3468	1048	3						Terpenoids	HMDB0011628	Glycyrrhetinic acid	C30H46O4	0.3
M474T821_pos	474.2599	821	3							HMDB0011480	LysoPE(0:0/18:4(6Z,9Z,12Z,15Z))	C23H40NO7P	3.5
M474T852_pos	474.3579	852	3							HMDB0006321	osa-4,7,10,13,16-pentaenoyl carni	C29H47NO4	0.2
M476T1050_pos	476.2760	1050	3							HMDB0011478	LysoPE(0:0/18:3(6Z,9Z,12Z))	C23H42NO7P	2.4
M479T1039_pos	479.2970	1039	3							HMDB0250805	Valyl-leucyl-lysine 4-nitroanilide	C23H38N6O5	1.4
M488T822_pos	488.3373	822	3							HMDB0241616	Z)-17-Hydroxydocosa-4,7,10,13,15	C29H45NO5	0.6
M490T857_pos	490.3528	857	3						Alkaloids	HMDB0242406	Chenodeoxycholylproline	C29H47NO5	0.3
M493T1016_pos	493.3526	1016	3							HMDB0033907	Homodolicholide	C29H48O6	0.5
M496T759_pos	496.3090	759	3							HMDB0242393	Chenodeoxycholylcysteine	C27H45NO5S	0.3
M509T998_pos	509.3239	998	3							HMDB0115485	PA(8:0/14:0)	C25H49O8P	0.2
M512T960_pos	512.4790	960	3						Fatty acids				
M520T1038_pos	520.3394	1038	3							HMDB0010386	LysoPC(18:2(9Z,12Z)/0:0)	C26H50NO7P	0.7
M522T1056_pos	522.3556	1056	3							HMDB0061701	LysoPC(0:0/18:1(9Z))	C26H52NO7P	0.4
M524T707_pos	524.2981	707	3							HMDB0240603	LysoPS(18:1(9Z)/0:0)	C24H46NO9P	0.4
M524T1075_pos	524.3698	1075	3						Fatty acids	HMDB0010384	LysoPC(18:0/0:0)	C26H54NO7P	2.5
M551T789_pos	551.3592	789	3							HMDB0297203	20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,	C31H50O8	2.5
M554T1063_pos	554.2846	1063	3							HMDB0033599	Vignatic acid A	C30H39N3O7	2.7
M560T725_pos	560.3949	725	3							HMDB0033678	gamma-Chaconine	C33H53NO6	0.5
M571T1017_pos	571.2807	1017	3							HMDB0036360	Pipercyclobutanamide A	C34H38N2O6	0.8
M573T993_pos	573.3415	993	3							HMDB0250071	Chemistry 2	C34H44N4O4	3.6
M593T1022_pos	593.3333	1022	3							HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.1
M611T696_pos	611.1975	696	3						Shikimates and Phenylpropanoids	HMDB0003265	Hesperidin	C28H34O15	0.7
M613T846_pos	613.3960	846	3							HMDB0010355	lestane-3,7,12,25-tetrol-3-glucuro	C33H56O10	2.3
M619T1038_pos	619.4914	1038	3							HMDB0295183	15:0/20:3(5Z,8Z,11Z)-O(14R,15S)/	C38H66O6	3.0
M631T925_pos	631.2763	925	3							HMDB0040917	apus non-fluorescent chlorophyll c	C34H38N4O8	0.2
M635T846_pos	635.3783	846	3						Amino acids and Peptides	HMDB0251275	Digitoxigenin bisdigitoxide	C35H54O10	1.0
M641T785_pos	641.3547	785	3						Polyketides				
M694T1038_pos	693.5661	1038	3							HMDB0296107	(19:0/20:3(8Z,11Z,14Z)-2OH(5,6)/(	C42H76O7	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M452T514_pos	452.3234	514	3	9.47E-01	0.99	FALSE	4.45E-04	0.64	TRUE	6.59E-07	1.72	TRUE	3.49E-01	1.15	FALSE
M452T456_pos	452.3235	456	3	9.97E-01	1.00	FALSE	3.10E-04	0.65	TRUE	2.04E-06	1.62	TRUE	1.99E-01	1.22	FALSE
M459T1037_pos	459.3465	1037	3	8.61E-13	2.84	TRUE	1.94E-06	0.56	TRUE	2.12E-01	0.87	FALSE	1.04E-01	1.19	FALSE
M468T1034_pos	468.3687	1034	3	1.06E-14	1.90	TRUE	4.96E-10	0.61	TRUE	3.84E-02	0.87	FALSE	2.63E-01	1.10	FALSE
M471T1048_pos	471.3468	1048	3	4.48E-13	2.44	TRUE	1.33E-04	0.65	TRUE	4.89E-01	1.07	FALSE	5.57E-03	1.23	FALSE
M474T821_pos	474.2599	821	3	1.09E-11	0.63	TRUE	3.27E-05	1.31	FALSE	2.71E-14	1.57	TRUE	3.70E-01	1.05	FALSE
M474T852_pos	474.3579	852	3	3.93E-07	3.62	TRUE	2.18E-04	0.50	TRUE	2.35E-01	0.80	FALSE	6.21E-01	0.90	FALSE
M476T1050_pos	476.2760	1050	3	5.23E-07	1.80	TRUE	4.80E-03	0.73	FALSE	6.63E-07	1.66	TRUE	6.49E-01	0.89	FALSE
M479T1039_pos	479.2970	1039	3	5.76E-05	2.15	TRUE	1.47E-04	0.48	TRUE	1.09E-02	1.50	FALSE	8.85E-01	0.93	FALSE
M488T822_pos	488.3373	822	3	3.76E-06	2.58	TRUE	2.27E-01	0.80	FALSE	6.65E-04	1.78	TRUE	7.29E-01	1.04	FALSE
M490T857_pos	490.3528	857	3	3.67E-07	2.86	TRUE	8.05E-03	0.62	TRUE	8.98E-02	1.31	FALSE	3.76E-01	1.13	FALSE
M493T1016_pos	493.3526	1016	3	1.29E-16	2.33	TRUE	1.71E-12	0.54	TRUE	4.88E-01	1.05	FALSE	1.38E-02	0.80	FALSE
M496T759_pos	496.3090	759	3	5.23E-22	2.06	TRUE	2.72E-01	0.93	FALSE	5.57E-16	1.65	TRUE	2.18E-02	0.85	FALSE
M509T998_pos	509.3239	998	3	1.23E-06	1.89	TRUE	6.54E-01	0.94	FALSE	1.29E-01	0.85	FALSE	9.24E-03	2.84	TRUE
M512T960_pos	512.4790	960	3	2.60E-04	2.33	TRUE	3.34E-05	0.45	TRUE	1.98E-01	0.78	FALSE	5.37E-01	1.14	FALSE
M520T1038_pos	520.3394	1038	3	2.18E-03	3.39	TRUE	4.10E-04	0.23	TRUE	3.41E-01	1.34	FALSE	8.55E-01	0.87	FALSE
M522T1056_pos	522.3556	1056	3	7.32E-04	3.23	TRUE	3.07E-04	0.24	TRUE	9.53E-01	1.02	FALSE	9.52E-01	0.95	FALSE
M524T707_pos	524.2981	707	3	2.58E-02	1.43	FALSE	3.57E-04	1.85	TRUE	7.68E-04	1.62	TRUE	2.52E-01	1.34	FALSE
M524T1075_pos	524.3698	1075	3	2.32E-02	1.91	TRUE	2.21E-01	0.67	FALSE	1.01E-02	1.90	TRUE	5.37E-01	0.81	FALSE
M551T789_pos	551.3592	789	3	2.34E-10	1.79	TRUE	2.65E-03	1.30	FALSE	3.41E-11	1.70	TRUE	1.05E-02	1.29	FALSE
M554T1063_pos	554.2846	1063	3	3.46E-04	4.18	TRUE	1.42E-01	0.62	FALSE	7.09E-03	2.33	TRUE	5.31E-01	0.89	FALSE
M560T725_pos	560.3949	725	3	1.01E-04	7.19	TRUE	9.82E-01	0.99	FALSE	7.59E-03	2.62	TRUE	2.24E-01	1.49	FALSE
M571T1017_pos	571.2807	1017	3	2.31E-04	3.65	TRUE	3.73E-02	0.51	TRUE	3.25E-01	1.30	FALSE	2.42E-01	0.40	FALSE
M573T993_pos	573.3415	993	3	7.20E-01	0.95	FALSE	1.14E-03	1.61	TRUE	6.73E-01	0.95	FALSE	3.61E-03	1.87	TRUE
M593T1022_pos	593.3333	1022	3	9.28E-03	0.73	FALSE	5.70E-06	1.76	TRUE	1.73E-07	1.80	TRUE	2.37E-01	0.79	FALSE
M611T696_pos	611.1975	696	3	1.71E-01	1.78	FALSE	9.72E-01	0.98	FALSE	3.15E-02	2.26	TRUE	1.60E-02	4.77	TRUE
M613T846_pos	613.3960	846	3	4.43E-05	0.54	TRUE	1.24E-05	1.95	TRUE	2.42E-02	1.33	FALSE	4.41E-02	1.41	FALSE
M619T1038_pos	619.4914	1038	3	5.65E-06	2.21	TRUE	9.27E-03	0.66	TRUE	3.92E-02	1.34	FALSE	4.33E-01	1.16	FALSE
M631T925_pos	631.2763	925	3	2.49E-18	0.50	TRUE	3.87E-03	1.23	FALSE	1.21E-13	1.63	TRUE	2.80E-02	1.12	FALSE
M635T846_pos	635.3783	846	3	3.49E-07	0.59	TRUE	1.25E-08	1.79	TRUE	3.41E-01	1.08	FALSE	3.47E-02	1.33	FALSE
M641T785_pos	641.3547	785	3	5.66E-07	1.70	TRUE	2.75E-08	0.60	TRUE	2.49E-04	1.39	FALSE	6.92E-01	0.95	FALSE
M694T1038_pos	693.5661	1038	3	8.31E-15	2.76	TRUE	1.25E-05	0.60	TRUE	2.29E-01	0.89	FALSE	2.28E-01	1.22	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M750T973_pos	749.5722	973	3						Terpenoids				
M752T1055_pos	751.5874	1055	3						Terpenoids				
M774T795_pos	774.4443	795	3						Amino acids and Peptides				
M778T960_pos	777.5303	960	3							HMDB0263673	PA(18:0/PGF1alpha)	C41H77O11P	3.4
M797T840_pos	797.4489	840	3						Polyketides				
M833T1029_pos	832.5702	1029	3							HMDB0282101	PS(20:0/18:1(12Z)-O(9S,10R))	C44H82NO11P	0.4
M70T128_pos	70.0649	128	3							HMDB0012497	1-Pyrroline	C4H7N	2.9
M73T305_pos	73.0282	305	3							HMDB0001167	Pyruvaldehyde	C3H4O2	2.5
M77T439_pos	77.0384	439	3							HMDB0248980	Cyclohexa-1,2,4,5-tetraene	C6H4	2.1
M79T439_pos	79.0540	439	3							HMDB0001505	Benzene	C6H6	2.3
M84T120_pos	84.0442	120	3							HMDB0255970	Oxazine	C4H5NO	1.9
M89T408_pos	89.0597	408	3							HMDB0000039	Butyric acid	C4H8O2	0.6
M90T120_pos	90.0550	120	3							HMDB0000056	beta-Alanine	C3H7NO2	0.6
M101T306_pos	101.0234	306	3							HMDB0032523	Succinic anhydride	C4H4O3	0.5
M102T120_pos	102.0550	120	3							HMDB0029387	L-3-Aminodihydro-2(3H)-furanone	C4H7NO2	0.4
M104T191_pos	104.0529	191	3							HMDB0258908	tetrahydrothiazine	C4H9NS	0.4
M107T439_pos	107.0492	439	3							HMDB0006115	Benzaldehyde	C7H6O	0.6
M108T486_pos	108.0445	486	3							HMDB0245308	2-Pyridinecarboxaldehyde	C6H5NO	0.7
M112T231_pos	112.0505	231	3							HMDB0000630	Cytosine	C4H5N3O	0.1
M115T418_pos	115.0390	418	3							HMDB0031859	Norfuraneol	C5H6O3	0.3
M115T665_pos	115.0754	665	3						Fatty acids	HMDB0000453	delta-Hexanolactone	C6H10O2	0.2
M116T84_pos	116.0707	84	3							HMDB0000162	L-Proline	C5H9NO2	0.7
M118T688_pos	118.0652	688	3							HMDB0000738	Indole	C8H7N	0.9
M119T322_pos	119.0492	322	3							HMDB0030968	2,4,6-Octatriyn-1-ol	C8H6O	0.4
M122T117_pos	122.0713	117	3							HMDB0242314	(1E)-1-Phenyltriaz-1-ene	C6H7N3	0.3
M122T446_pos	122.0965	446	3							HMDB0001020	N,N-Dimethylaniline	C8H11N	0.2
M123T327_pos	123.0442	327	3						Shikimates and Phenylpropanoids	HMDB0001870	Benzoic acid	C7H6O2	1.1
M123T162_pos	123.1031	162	3						Alkaloids				
M127T446_pos	127.0502	446	3						Alkaloids	HMDB0000262	Thymine	C5H6N2O2	0.1
M128T448_pos	128.0533	448	3							HMDB0029730	2-Ethyl-4-methylthiazole	C6H9NS	3.7
M130T119_pos	130.0499	119	3							HMDB0000267	Pyroglutamic acid	C5H7NO3	0.1
M130T90_pos	130.0863	90	3						Amino acids and Peptides	HMDB0000070	Pipecolic acid	C6H11NO2	0.7
M131T217_pos	131.0340	217	3							HMDB0000620	Glutaconic acid	C5H6O4	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M750T973_pos	749.5722	973	3	1.05E-15	2.33	TRUE	9.75E-09	0.58	TRUE	3.05E-02	1.19	FALSE	4.30E-01	1.11	FALSE
M752T1055_pos	751.5874	1055	3	1.62E-13	2.88	TRUE	7.43E-03	0.71	FALSE	1.19E-06	1.73	TRUE	6.17E-03	1.35	FALSE
M774T795_pos	774.4443	795	3	7.11E-13	0.58	TRUE	8.75E-01	1.01	FALSE	3.77E-16	1.73	TRUE	7.05E-03	1.20	FALSE
M778T960_pos	777.5303	960	3	6.18E-11	2.25	TRUE	8.01E-04	1.48	FALSE	1.34E-25	3.85	TRUE	1.01E-01	0.73	FALSE
M797T840_pos	797.4489	840	3	8.49E-01	0.96	FALSE	9.72E-03	1.83	TRUE	9.61E-04	1.95	TRUE	8.99E-01	1.08	FALSE
M833T1029_pos	832.5702	1029	3	1.24E-03	3.36	TRUE	1.77E-01	0.62	FALSE	5.31E-06	5.14	TRUE	5.31E-01	0.86	FALSE
M70T128_pos	70.0649	128	3	7.53E-17	0.45	TRUE	2.17E-04	1.38	FALSE	3.16E-12	1.73	TRUE	3.41E-01	0.87	FALSE
M73T305_pos	73.0282	305	3	1.44E-21	0.43	TRUE	2.44E-01	1.10	FALSE	8.75E-12	1.61	TRUE	2.82E-02	1.43	FALSE
M77T439_pos	77.0384	439	3	1.44E-40	0.24	TRUE	4.20E-07	1.47	FALSE	1.42E-14	1.71	TRUE	1.75E-01	1.22	FALSE
M79T439_pos	79.0540	439	3	9.20E-38	0.28	TRUE	4.51E-07	1.45	FALSE	2.13E-14	1.68	TRUE	9.99E-01	1.00	FALSE
M84T120_pos	84.0442	120	3	8.22E-61	0.33	TRUE	1.22E-01	1.07	FALSE	3.64E-31	1.67	TRUE	5.79E-02	0.81	FALSE
M89T408_pos	89.0597	408	3	3.47E-19	1.61	TRUE	8.49E-01	1.01	FALSE	2.29E-03	1.14	FALSE	7.99E-03	0.50	TRUE
M90T120_pos	90.0550	120	3	1.25E-09	0.53	TRUE	6.94E-02	1.20	FALSE	1.13E-06	1.54	TRUE	2.42E-01	0.79	FALSE
M101T306_pos	101.0234	306	3	1.15E-19	0.43	TRUE	3.14E-01	1.09	FALSE	2.45E-13	1.75	TRUE	7.75E-01	0.97	FALSE
M102T120_pos	102.0550	120	3	4.01E-78	0.26	TRUE	2.99E-02	1.09	FALSE	8.82E-31	1.57	TRUE	5.86E-02	0.83	FALSE
M104T191_pos	104.0529	191	3	2.13E-49	0.15	TRUE	1.83E-05	1.39	FALSE	7.49E-11	1.57	TRUE	3.19E-01	1.12	FALSE
M107T439_pos	107.0492	439	3	5.28E-37	0.32	TRUE	2.08E-05	1.34	FALSE	7.91E-12	1.52	TRUE	7.66E-02	1.18	FALSE
M108T486_pos	108.0445	486	3	4.04E-08	0.54	TRUE	4.58E-01	1.08	FALSE	2.43E-09	1.78	TRUE	7.58E-01	1.03	FALSE
M112T231_pos	112.0505	231	3	4.69E-17	0.24	TRUE	4.81E-01	1.11	FALSE	2.97E-04	1.55	TRUE	2.08E-01	1.27	FALSE
M115T418_pos	115.0390	418	3	6.74E-10	0.49	TRUE	8.02E-01	1.03	FALSE	3.86E-06	1.56	TRUE	2.32E-01	0.89	FALSE
M115T665_pos	115.0754	665	3	1.03E-21	0.61	TRUE	1.06E-01	1.08	FALSE	7.95E-30	1.71	TRUE	5.15E-05	0.67	FALSE
M116T84_pos	116.0707	84	3	2.74E-14	0.44	TRUE	7.73E-04	1.39	FALSE	4.85E-07	1.55	TRUE	2.02E-01	0.79	FALSE
M118T688_pos	118.0652	688	3	8.69E-01	1.04	FALSE	2.16E-07	3.58	TRUE	2.13E-03	1.82	TRUE	2.20E-01	1.81	FALSE
M119T322_pos	119.0492	322	3	7.97E-40	0.31	TRUE	2.65E-04	1.27	FALSE	2.06E-13	1.54	TRUE	3.12E-02	1.23	FALSE
M122T117_pos	122.0713	117	3	3.91E-03	0.69	FALSE	2.03E-08	2.19	TRUE	2.50E-09	2.07	TRUE	1.52E-01	0.81	FALSE
M122T446_pos	122.0965	446	3	2.79E-05	2.06	TRUE	1.75E-04	1.94	TRUE	8.44E-01	1.03	FALSE	3.22E-01	0.94	FALSE
M123T327_pos	123.0442	327	3	2.45E-16	0.51	TRUE	1.10E-02	1.21	FALSE	1.19E-11	1.59	TRUE	8.94E-01	1.02	FALSE
M123T162_pos	123.1031	162	3	5.27E-01	0.95	FALSE	8.80E-01	1.01	FALSE	1.29E-08	1.51	TRUE	3.40E-05	0.28	TRUE
M127T446_pos	127.0502	446	3	8.31E-39	0.31	TRUE	2.61E-01	1.08	FALSE	1.02E-35	2.51	TRUE	5.85E-01	1.07	FALSE
M128T448_pos	128.0533	448	3	3.53E-19	0.45	TRUE	8.26E-01	1.02	FALSE	1.65E-14	1.77	TRUE	1.57E-01	1.24	FALSE
M130T119_pos	130.0499	119	3	2.02E-79	0.28	TRUE	5.09E-02	1.07	FALSE	8.64E-34	1.58	TRUE	6.41E-02	0.86	FALSE
M130T90_pos	130.0863	90	3	9.76E-57	0.25	TRUE	1.69E-03	1.19	FALSE	2.31E-22	1.68	TRUE	1.30E-01	0.92	FALSE
M131T217_pos	131.0340	217	3	5.72E-26	0.31	TRUE	9.07E-04	1.34	FALSE	9.43E-08	1.52	TRUE	9.26E-02	0.64	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M131T590_pos	131.0702	590	3							HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	0.2
M131T142_pos	131.1180	142	3							HMDB0002064	N-Acetylputrescine	C6H14N2O	0.7
M133T92_pos	133.0973	92	3							HMDB0000214	Ornithine	C5H12N2O2	1.4
M136T486_pos	136.0394	486	3							HMDB0032931	2-Benzoxazolol	C7H5NO2	0.5
M136T326_pos	136.0757	326	3							HMDB0001250	N-Acetylarylamine	C8H9NO	0.4
M137T528_pos	137.0597	528	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.1
M138T424_pos	138.0914	424	3							HMDB0000306	Tyramine	C8H11NO	0.3
M138T675_2_pos	138.0914	675	3							HMDB0000306	Tyramine	C8H11NO	0.3
M138T360_pos	138.0914	360	3							HMDB0000306	Tyramine	C8H11NO	0.5
M141T329_pos	141.0182	329	3							HMDB0060459	4-Carboxymethylenebut-2-en-4-o	C6H4O4	0.1
M142T410_pos	142.0611	410	3							HMDB0251409	Dimetridazole	C5H7N3O2	0.3
M145T698_pos	145.0495	698	3							HMDB0000393	3-Hexenedioic acid	C6H8O4	0.1
M145T205_pos	145.1336	205	3							HMDB0002284	N-Acetylcadaverine	C7H16N2O	0.4
M146T507_pos	146.0601	507	3							HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.5
M147T119_pos	147.0765	119	3							HMDB0000641	L-Glutamine	C5H10N2O3	0.5
M147T109_pos	147.1130	109	3							HMDB0000182	L-Lysine	C6H14N2O2	1.2
M148T413_pos	148.0604	413	3						Amino acids and Peptides	HMDB0000148	L-Glutamic acid	C5H9NO4	0.2
M148T732_pos	148.0757	732	3						Alkaloids	HMDB0005785	Indole-3-carbinol	C9H9NO	0.1
M148T386_pos	148.0757	386	3							HMDB0005785	Indole-3-carbinol	C9H9NO	0.2
M149T439_pos	149.0598	439	3							HMDB0000567	Cinnamic acid	C9H8O2	0.3
M151T374_pos	151.0615	374	3							HMDB0003162	7-Methylhypoxanthine	C6H6N4O	0.2
M151T413_pos	151.0965	413	3							HMDB0259193	TRIETHYLENE GLYCOL	C6H14O4	0.1
M152T407_pos	152.0567	407	3							HMDB0000132	Guanine	C5H5N5O	0.3
M157T568_pos	157.0972	568	3							HMDB0242468	(2-Ethylcrotonoyl)urea	C7H12N2O2	0.4
M157T429_pos	157.1337	429	3							HMDB0246231	3-(Dimethylamino)propyl)acrylam	C8H16N2O	0.9
M158T273_pos	158.0925	273	3							HMDB0259734	V-Pyrro/NO	C6H11N3O2	0.4
M158T449_2_pos	158.1176	449	3							HMDB0014447	Tranexamic Acid	C8H15NO2	0.4
M158T580_pos	158.1176	580	3							HMDB0014447	Tranexamic Acid	C8H15NO2	0.2
M159T120_pos	159.0765	120	3						Amino acids and Peptides	HMDB0031670	methyl)-5,5-dimethyl-2,4-imidazo	C6H10N2O3	0.3
M163T698_pos	163.0598	698	3						Carbohydrates	HMDB0000321	2-Hydroxyadipic acid	C6H10O5	1.7
M163T722_pos	163.0866	722	3							HMDB0001297	Norcotinine	C9H10N2O	0.0
M164T362_pos	164.0568	362	3							HMDB0000802	Pterin	C6H5N5O	0.9
M165T528_pos	165.0547	528	3							HMDB0000205	Phenylpyruvic acid	C9H8O3	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M131T590_pos	131.0702	590	3	2.15E-05	0.76	FALSE	2.67E-01	1.08	FALSE	5.06E-13	1.53	TRUE	2.52E-02	0.63	TRUE
M131T142_pos	131.1180	142	3	2.76E-01	1.25	FALSE	2.26E-05	2.56	TRUE	5.12E-05	2.13	TRUE	6.09E-02	1.24	FALSE
M133T92_pos	133.0973	92	3	3.17E-17	0.38	TRUE	4.00E-04	1.44	FALSE	1.71E-10	1.80	TRUE	7.34E-01	1.09	FALSE
M136T486_pos	136.0394	486	3	4.09E-04	0.66	TRUE	9.79E-01	1.00	FALSE	1.30E-08	1.86	TRUE	2.57E-01	0.92	FALSE
M136T326_pos	136.0757	326	3	2.28E-08	0.64	TRUE	2.47E-01	1.10	FALSE	1.15E-09	1.54	TRUE	2.29E-01	0.85	FALSE
M137T528_pos	137.0597	528	3	4.79E-05	0.64	TRUE	5.75E-02	1.24	FALSE	1.14E-07	1.68	TRUE	2.72E-01	1.21	FALSE
M138T424_pos	138.0914	424	3	9.18E-07	-41.54	FALSE	1.45E-17	-3.56	FALSE	4.60E-05	7.07	TRUE	1.76E-04	0.45	TRUE
M138T675_2_pos	138.0914	675	3	1.74E-08	1.57	TRUE	6.14E-01	0.96	FALSE	2.62E-11	1.61	TRUE	4.64E-01	1.12	FALSE
M138T360_pos	138.0914	360	3	2.33E-05	1.60	TRUE	6.85E-02	0.82	FALSE	5.93E-02	1.19	FALSE	1.88E-02	0.43	TRUE
M141T329_pos	141.0182	329	3	3.07E-32	0.12	TRUE	9.26E-01	1.01	FALSE	2.22E-01	0.89	FALSE	6.97E-05	0.42	TRUE
M142T410_pos	142.0611	410	3	1.61E-06	2.00	TRUE	4.07E-08	0.48	TRUE	2.40E-03	1.44	FALSE	2.11E-01	0.79	FALSE
M145T698_pos	145.0495	698	3	6.80E-03	2.00	TRUE	2.71E-02	0.58	TRUE	4.81E-01	1.16	FALSE	3.18E-01	0.50	FALSE
M145T205_pos	145.1336	205	3	3.29E-02	1.61	TRUE	8.01E-01	1.06	FALSE	3.94E-03	1.77	TRUE	1.25E-01	0.72	FALSE
M146T507_pos	146.0601	507	3	1.12E-32	0.47	TRUE	1.67E-01	1.08	FALSE	4.36E-20	1.58	TRUE	6.63E-02	0.80	FALSE
M147T119_pos	147.0765	119	3	2.21E-36	0.30	TRUE	5.10E-02	1.16	FALSE	4.55E-12	1.57	TRUE	7.17E-01	1.07	FALSE
M147T109_pos	147.1130	109	3	2.56E-69	0.18	TRUE	6.23E-04	1.20	FALSE	6.86E-23	1.66	TRUE	4.79E-01	1.04	FALSE
M148T413_pos	148.0604	413	3	2.06E-16	0.63	TRUE	3.31E-03	1.17	FALSE	4.35E-34	1.98	TRUE	7.07E-01	1.02	FALSE
M148T732_pos	148.0757	732	3	7.15E-12	1.86	TRUE	9.86E-02	0.84	FALSE	2.10E-10	0.61	TRUE	1.30E-01	0.81	FALSE
M148T386_pos	148.0757	386	3	3.45E-03	0.54	TRUE	5.64E-01	0.88	FALSE	8.31E-03	1.61	TRUE	3.72E-01	0.36	FALSE
M149T439_pos	149.0598	439	3	4.73E-41	0.23	TRUE	3.68E-07	1.48	FALSE	9.55E-15	1.72	TRUE	2.41E-01	1.16	FALSE
M151T374_pos	151.0615	374	3	5.88E-01	1.13	FALSE	6.35E-09	4.74	TRUE	2.71E-08	3.53	TRUE	7.31E-02	1.27	FALSE
M151T413_pos	151.0965	413	3	1.24E-18	1.89	TRUE	1.34E-01	0.90	FALSE	6.87E-22	0.54	TRUE	2.93E-03	1.45	FALSE
M152T407_pos	152.0567	407	3	1.05E-27	0.18	TRUE	1.43E-02	1.32	FALSE	1.18E-11	2.03	TRUE	9.56E-02	1.45	FALSE
M157T568_pos	157.0972	568	3	8.62E-44	0.20	TRUE	4.87E-02	1.17	FALSE	1.55E-03	1.23	FALSE	5.91E-03	0.61	TRUE
M157T429_pos	157.1337	429	3	1.26E-15	0.36	TRUE	1.57E-01	1.19	FALSE	2.22E-07	1.69	TRUE	1.96E-01	0.71	FALSE
M158T273_pos	158.0925	273	3	1.43E-07	0.61	TRUE	3.04E-01	1.10	FALSE	1.82E-08	1.59	TRUE	4.57E-01	0.90	FALSE
M158T449_2_pos	158.1176	449	3	3.18E-11	0.60	TRUE	6.78E-02	0.87	FALSE	8.78E-11	1.53	TRUE	6.50E-01	0.98	FALSE
M158T580_pos	158.1176	580	3	5.51E-03	1.96	TRUE	8.66E-05	2.87	TRUE	5.17E-01	1.14	FALSE	9.22E-01	1.05	FALSE
M159T120_pos	159.0765	120	3	9.07E-65	0.09	TRUE	7.40E-04	1.25	FALSE	1.59E-14	1.61	TRUE	7.57E-01	0.96	FALSE
M163T698_pos	163.0598	698	3	3.96E-02	2.11	TRUE	9.45E-03	0.39	TRUE	9.16E-01	1.03	FALSE	3.74E-01	0.43	FALSE
M163T722_pos	163.0866	722	3	7.33E-01	0.96	FALSE	5.78E-05	1.78	TRUE	5.05E-12	2.36	TRUE	5.11E-01	1.15	FALSE
M164T362_pos	164.0568	362	3	5.41E-24	0.57	TRUE	3.52E-01	1.05	FALSE	4.62E-28	1.73	TRUE	8.52E-01	1.03	FALSE
M165T528_pos	165.0547	528	3	1.37E-06	0.58	TRUE	1.55E-01	1.18	FALSE	5.98E-06	1.56	TRUE	2.81E-01	1.12	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M165T325_pos	165.0547	325	3						Shikimates and Phenylpropanoids	HMDB0000205	Phenylpyruvic acid	C9H8O3	0.4
M165T1038_1_pos	165.0910	1038	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.2
M166T121_pos	166.0533	121	3							HMDB0002005	Methionine sulfoxide	C5H11NO3S	0.4
M166T438_pos	166.0863	438	3						Alkaloids	HMDB0000159	L-Phenylalanine	C9H11NO2	0.3
M168T375_pos	168.0881	375	3							HMDB0255369	no-2,3,6,7-tetrahydro-1H-pteridin-	C6H9N5O	0.5
M171T1039_pos	171.1380	1039	3							HMDB0004980	cis-4-Decenoic acid	C10H18O2	0.4
M173T166_pos	173.0922	166	3						Amino acids and Peptides	HMDB0000721	Glycylproline	C7H12N2O3	0.7
M173T457_pos	173.1649	457	3							HMDB0246342	mino-2,2,6,6-tetramethylpiperidin-	C9H20N2O	0.4
M176T123_pos	176.1026	123	3							HMDB0000904	Citrulline	C6H13N3O3	2.1
M177T335_pos	177.0395	335	3							HMDB0000044	Ascorbic acid	C6H8O6	0.7
M177T670_pos	177.0547	670	3							HMDB0029758	Herniarin	C10H8O3	0.4
M181T920_pos	181.1224	920	3							HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.3
M182T106_pos	181.9619	106	3							HMDB0304153	3-phospho-hydroxypyruvate	C3H2O7P	4.6
M182T355_pos	182.0450	355	3							HMDB0006954	-3-hydroxy-5-formylpyridine-4-ca	C8H7NO4	1.0
M184T351_pos	184.0967	351	3							HMDB0000068	Epinephrine	C9H13NO3	0.9
M185T637_pos	185.1284	637	3							HMDB0061384	(3-acetamidopropyl)pyrrolidin-2-o	C9H16N2O2	0.2
M185T1039_pos	185.1537	1039	3						Terpenoids	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	0.3
M186T113_pos	186.0163	113	3						Amino acids and Peptides	HMDB0000272	Phosphoserine	C3H8NO6P	0.8
M187T564_pos	187.1078	564	3							HMDB0028695	Alanylproline	C8H14N2O3	0.2
M189T270_pos	189.1235	270	3						Amino acids and Peptides	HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.8
M190T700_pos	190.0864	700	3							HMDB0002302	Indole-3-propionic acid	C11H11NO2	0.6
M190T417_pos	190.1075	417	3						Amino acids and Peptides	HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.7
M192T425_pos	192.0659	425	3						Alkaloids	HMDB0000763	5-Hydroxyindoleacetic acid	C10H9NO3	1.8
M192T515_pos	192.1022	515	3							HMDB0001896	5-Methoxytryptophol	C11H13NO2	1.5
M197T546_pos	197.1286	546	3						Alkaloids	HMDB0029741	propyl-3,5-dimethoxy-6-methylpyr	C10H16N2O2	0.5
M198T374_pos	198.0765	374	3							HMDB0000181	L-Dopa	C9H11NO4	2.1
M198T763_pos	198.1490	763	3							HMDB0258508	Estreptoquinasa	C11H19NO2	0.8
M201T370_pos	201.1235	370	3							HMDB0304430	N-alpha-acetyl lysine methyl ester	C9H16N2O3	3.6
M203T377_pos	203.1392	377	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.8
M203T524_pos	203.1391	524	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.5
M204T128_pos	204.0971	128	3							HMDB0028682	Alanylasparagine	C7H13N3O4	3.9
M204T662_pos	204.1241	662	3							HMDB0245646	Methylbut-2-EN-1-YL)-9H-purin-6-	C10H13N5	1.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M165T325_pos	165.0547	325	3	6.31E-24	0.37	TRUE	1.77E-03	1.30	FALSE	4.45E-09	1.54	TRUE	2.44E-01	1.26	FALSE
M165T1038_1_pos	165.0910	1038	3	2.82E-09	3.35	TRUE	6.37E-04	0.57	TRUE	5.27E-01	0.91	FALSE	5.65E-01	1.12	FALSE
M166T121_pos	166.0533	121	3	1.17E-45	0.17	TRUE	4.86E-04	1.31	FALSE	1.93E-14	1.74	TRUE	1.86E-01	1.24	FALSE
M166T438_pos	166.0863	438	3	2.52E-43	0.29	TRUE	7.04E-09	1.45	FALSE	1.24E-17	1.67	TRUE	1.34E-01	1.24	FALSE
M168T375_pos	168.0881	375	3	1.07E-10	1.55	TRUE	6.89E-02	1.13	FALSE	4.83E-17	1.68	TRUE	2.15E-01	0.86	FALSE
M171T1039_pos	171.1380	1039	3	8.32E-12	1.83	TRUE	6.14E-07	0.65	TRUE	9.86E-01	1.00	FALSE	2.00E-04	1.33	FALSE
M173T166_pos	173.0922	166	3	6.79E-43	0.17	TRUE	4.51E-03	1.27	FALSE	2.10E-09	1.56	TRUE	5.54E-01	0.88	FALSE
M173T457_pos	173.1649	457	3	2.71E-01	1.22	FALSE	6.80E-07	2.73	TRUE	2.62E-04	1.83	TRUE	4.53E-01	0.91	FALSE
M176T123_pos	176.1026	123	3	2.11E-56	0.08	TRUE	2.65E-03	1.26	FALSE	4.53E-12	1.63	TRUE	6.11E-01	1.18	FALSE
M177T335_pos	177.0395	335	3	2.59E-27	0.11	TRUE	9.67E-01	0.99	FALSE	5.66E-01	0.94	FALSE	5.10E-04	0.54	TRUE
M177T670_pos	177.0547	670	3	1.42E-02	0.72	FALSE	4.75E-04	1.67	TRUE	3.93E-05	1.65	TRUE	3.33E-01	1.15	FALSE
M181T920_pos	181.1224	920	3	5.45E-13	3.37	TRUE	1.87E-04	0.61	TRUE	5.14E-03	0.71	FALSE	1.09E-01	0.52	FALSE
M182T106_pos	181.9619	106	3	1.20E-18	0.14	TRUE	5.37E-01	1.11	FALSE	2.39E-03	1.52	TRUE	5.98E-01	1.09	FALSE
M182T355_pos	182.0450	355	3	9.95E-15	0.60	TRUE	5.32E-01	0.96	FALSE	8.67E-19	1.68	TRUE	9.38E-01	1.01	FALSE
M184T351_pos	184.0967	351	3	2.88E-08	0.53	TRUE	7.26E-01	0.96	FALSE	1.51E-05	1.52	TRUE	3.90E-01	0.88	FALSE
M185T637_pos	185.1284	637	3	1.89E-22	0.36	TRUE	9.29E-01	0.99	FALSE	4.87E-04	1.30	FALSE	3.51E-02	0.50	TRUE
M185T1039_pos	185.1537	1039	3	3.55E-14	2.04	TRUE	3.27E-08	0.61	TRUE	7.14E-01	1.03	FALSE	4.32E-04	1.32	FALSE
M186T113_pos	186.0163	113	3	1.56E-36	0.39	TRUE	4.53E-01	1.04	FALSE	4.93E-17	1.57	TRUE	6.90E-01	0.95	FALSE
M187T564_pos	187.1078	564	3	3.75E-41	0.25	TRUE	5.07E-01	1.05	FALSE	1.30E-03	1.22	FALSE	2.56E-02	0.51	TRUE
M189T270_pos	189.1235	270	3	2.09E-17	0.26	TRUE	2.59E-01	1.17	FALSE	3.53E-05	1.60	TRUE	8.84E-02	0.65	FALSE
M190T700_pos	190.0864	700	3	7.17E-02	1.22	FALSE	1.04E-07	1.89	TRUE	2.90E-14	2.25	TRUE	1.27E-01	0.77	FALSE
M190T417_pos	190.1075	417	3	4.91E-18	0.35	TRUE	6.61E-01	0.96	FALSE	4.95E-06	1.51	TRUE	4.66E-01	0.97	FALSE
M192T425_pos	192.0659	425	3	4.61E-01	0.93	FALSE	7.67E-02	1.19	FALSE	1.34E-10	1.81	TRUE	2.64E-02	0.65	TRUE
M192T515_pos	192.1022	515	3	1.49E-10	0.34	TRUE	5.19E-01	1.10	FALSE	7.98E-06	1.83	TRUE	2.58E-02	0.86	FALSE
M197T546_pos	197.1286	546	3	3.01E-15	0.48	TRUE	3.31E-01	1.09	FALSE	2.78E-08	1.52	TRUE	6.85E-02	0.90	FALSE
M198T374_pos	198.0765	374	3	2.15E-15	0.45	TRUE	2.80E-01	1.10	FALSE	8.80E-08	1.55	TRUE	2.02E-01	0.76	FALSE
M198T763_pos	198.1490	763	3	7.76E-01	0.98	FALSE	1.20E-02	1.15	FALSE	6.52E-17	1.54	TRUE	9.40E-03	0.66	TRUE
M201T370_pos	201.1235	370	3	7.44E-13	0.58	TRUE	6.13E-01	1.04	FALSE	2.16E-11	1.55	TRUE	5.65E-01	0.90	FALSE
M203T377_pos	203.1392	377	3	6.42E-13	0.36	TRUE	4.93E-01	1.10	FALSE	2.27E-04	1.50	TRUE	1.93E-01	0.70	FALSE
M203T524_pos	203.1391	524	3	1.35E-23	0.08	TRUE	9.39E-01	1.01	FALSE	1.23E-03	1.54	TRUE	3.12E-01	0.78	FALSE
M204T128_pos	204.0971	128	3	2.26E-06	0.44	TRUE	5.70E-01	1.10	FALSE	4.95E-05	1.81	TRUE	5.25E-01	0.85	FALSE
M204T662_pos	204.1241	662	3	5.61E-15	0.48	TRUE	4.86E-06	1.50	FALSE	3.30E-10	1.64	TRUE	6.24E-01	0.95	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M204T453_pos	204.1231	453	3							HMDB0062176	N-Lactoylleucine	C9H17NO4	0.4
M205T368_pos	205.1196	368	3							HMDB0259195	Triethylenemelamine	C9H12N6	0.1
M206T418_pos	206.0450	418	3							HMDB0000881	Xanthurenic acid	C10H7NO4	0.9
M207T421_pos	207.0482	421	3							HMDB0033995	)-5-(5-methyl-2-thienyl)-2-penten	C11H10O2S	3.8
M207T864_pos	207.0960	864	3							HMDB0247786	thiophen-2-ylethenyl)-5,6-dihydro	C11H14N2S	4.5
M210T664_pos	210.1115	664	3							HMDB0248234	alpha-Methyltyrosine methyl este	C11H15NO3	4.7
M212T436_pos	212.0555	436	3							HMDB0011639	Topaquinone	C9H9NO5	0.9
M212T200_pos	212.0555	200	3							HMDB0011639	Topaquinone	C9H9NO5	0.8
M212T525_pos	212.0556	525	3							HMDB0011639	Topaquinone	C9H9NO5	1.4
M212T980_pos	212.2011	980	3							HMDB0037834	Ethyl menthane carboxamide	C13H25NO	0.8
M215T415_pos	215.1392	415	3							HMDB0003581	Dethiobiotin	C10H18N2O3	0.6
M216T111_pos	216.0354	111	3						Amino acids and Peptides	HMDB0259067	Tiamenidine	C8H10ClN3S	1.1
M216T753_pos	216.1022	753	3							HMDB0032888	Acetyl vitamin K5	C13H13NO2	1.3
M216T822_pos	216.1596	822	3							HMDB0013279	N-Nonanoylglycine	C11H21NO3	0.8
M218T546_pos	218.0482	546	3							HMDB0006409	Tyramine-O-sulfate	C8H11NO4S	0.3
M218T572_pos	218.1578	572	3							HMDB0249477	Butylate	C11H23NOS	2.3
M220T508_pos	220.0607	508	3							HMDB0039387	yl 2,6-dihydroxy-4-quinolinecarbox	C11H9NO4	1.2
M224T330_pos	224.0920	330	3							HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	1.2
M226T248_pos	226.0712	248	3						Alkaloids	HMDB0037264	4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	1.0
M229T533_pos	229.1255	533	3							HMDB0037386	(S)-Menthone 8-thioacetate	C12H20O2S	0.6
M229T477_pos	229.1548	477	3							HMDB0011174	Isoleucylproline	C11H20N2O3	0.7
M230T725_pos	230.1390	725	3							HMDB0013126	Butenylcarnitine	C11H19NO4	1.3
M232T269_pos	232.1289	269	3							HMDB0028744	Asparaginyl-Valine	C9H17N3O4	1.2
M234T344_pos	234.1338	344	3							HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	0.8
M239T502_pos	239.1077	502	3							HMDB0029700	Cinnamyl benzoate	C16H14O2	4.5
M240T447_pos	240.0870	447	3							HMDB0250058	(3s)-3-(Benzyloxy)-L-Aspartic Acid	C11H13NO5	1.4
M242T947_pos	242.2844	947	3							HMDB0243891	Hexadecylamine	C16H35N	0.8
M243T564_pos	243.0768	564	3							HMDB0240720	mino-7-methoxy-3H-phenoxazin-3	C13H10N2O3	1.6
M243T591_pos	243.1335	591	3							HMDB0246097	Pueraria glycoside	C11H18N2O4	1.7
M245T348_pos	245.0771	348	3							HMDB0000296	Uridine	C9H12N2O6	1.2
M245T201_pos	245.0771	201	3							HMDB0000296	Uridine	C9H12N2O6	1.3
M245T699_pos	245.1857	699	3							HMDB0028910	Isoleucyl-Isoleucine	C12H24N2O3	1.1
M246T694_pos	246.1341	694	3							HMDB0241651	3-Oxobutanoylcarnitine	C11H19NO5	2.2
M246T299_pos	246.1445	299	3							HMDB0028734	Asparaginylisoleucine	C10H19N3O4	1.2
M246T116_pos	246.1814	116	3							HMDB0028964	Lysylvaline	C11H23N3O3	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M204T453_pos	204.1231	453	3	2.48E-27	0.23	TRUE	5.35E-01	0.94	FALSE	2.23E-12	1.94	TRUE	6.99E-01	0.97	FALSE
M205T368_pos	205.1196	368	3	2.48E-36	0.13	TRUE	6.19E-01	1.05	FALSE	4.60E-10	1.77	TRUE	9.16E-01	0.98	FALSE
M206T418_pos	206.0450	418	3	5.41E-03	0.78	FALSE	3.05E-01	1.10	FALSE	1.14E-21	2.48	TRUE	1.96E-02	0.55	TRUE
M207T421_pos	207.0482	421	3	1.98E-03	0.76	FALSE	4.36E-01	1.08	FALSE	4.17E-20	2.31	TRUE	1.81E-02	0.54	TRUE
M207T864_pos	207.0960	864	3	3.62E-05	0.57	TRUE	3.16E-02	0.75	FALSE	2.36E-04	0.65	TRUE	7.93E-01	1.09	FALSE
M210T664_pos	210.1115	664	3	6.44E-06	6.02	TRUE	2.44E-01	0.73	FALSE	2.21E-02	0.53	TRUE	6.57E-01	0.83	FALSE
M212T436_pos	212.0555	436	3	8.63E-15	0.45	TRUE	8.57E-01	0.98	FALSE	1.27E-08	1.61	TRUE	6.58E-02	0.61	FALSE
M212T200_pos	212.0555	200	3	2.32E-05	0.53	TRUE	9.10E-01	0.98	FALSE	7.15E-04	1.54	TRUE	4.71E-01	0.80	FALSE
M212T525_pos	212.0556	525	3	4.42E-05	0.64	TRUE	3.66E-01	1.10	FALSE	1.04E-05	1.52	TRUE	2.04E-01	0.69	FALSE
M212T980_pos	212.2011	980	3	2.91E-07	1.37	FALSE	5.46E-19	0.53	TRUE	9.28E-02	0.92	FALSE	7.50E-04	1.81	TRUE
M215T415_pos	215.1392	415	3	6.90E-33	0.22	TRUE	1.60E-02	1.25	FALSE	4.31E-09	1.61	TRUE	6.95E-01	0.91	FALSE
M216T111_pos	216.0354	111	3	9.53E-35	0.43	TRUE	1.68E-01	1.08	FALSE	2.97E-22	1.67	TRUE	1.75E-02	0.76	FALSE
M216T753_pos	216.1022	753	3	9.94E-14	0.11	TRUE	8.15E-01	0.95	FALSE	3.25E-03	1.70	TRUE	8.14E-01	0.96	FALSE
M216T822_pos	216.1596	822	3	6.23E-02	0.74	FALSE	9.28E-07	2.32	TRUE	3.75E-06	1.97	TRUE	7.17E-01	1.04	FALSE
M218T546_pos	218.0482	546	3	2.46E-27	0.43	TRUE	8.84E-01	1.01	FALSE	5.41E-15	1.60	TRUE	5.68E-03	0.72	FALSE
M218T572_pos	218.1578	572	3	1.69E-27	0.12	TRUE	6.42E-01	1.06	FALSE	8.95E-09	1.95	TRUE	1.54E-01	0.72	FALSE
M220T508_pos	220.0607	508	3	4.45E-11	0.63	TRUE	5.17E-01	1.04	FALSE	3.30E-23	1.95	TRUE	3.84E-01	0.92	FALSE
M224T330_pos	224.0920	330	3	2.45E-07	0.66	TRUE	7.63E-01	1.02	FALSE	6.23E-19	1.99	TRUE	4.78E-01	0.87	FALSE
M226T248_pos	226.0712	248	3	2.05E-14	0.48	TRUE	6.32E-01	1.04	FALSE	6.23E-16	1.98	TRUE	2.67E-01	0.91	FALSE
M229T533_pos	229.1255	533	3	4.96E-05	0.55	TRUE	8.34E-01	1.03	FALSE	7.67E-09	2.18	TRUE	6.70E-01	1.04	FALSE
M229T477_pos	229.1548	477	3	1.98E-22	0.21	TRUE	5.94E-03	1.42	FALSE	1.73E-08	1.88	TRUE	3.34E-01	0.79	FALSE
M230T725_pos	230.1390	725	3	6.34E-04	0.81	FALSE	4.47E-13	1.61	TRUE	2.52E-14	1.56	TRUE	1.67E-01	1.10	FALSE
M232T269_pos	232.1289	269	3	1.53E-45	0.07	TRUE	1.90E-01	1.14	FALSE	2.78E-02	1.20	FALSE	2.86E-03	0.22	TRUE
M234T344_pos	234.1338	344	3	8.52E-09	0.59	TRUE	5.35E-01	0.95	FALSE	4.95E-15	1.94	TRUE	1.24E-01	0.82	FALSE
M239T502_pos	239.1077	502	3	1.13E-15	0.57	TRUE	3.70E-01	1.06	FALSE	9.32E-22	1.84	TRUE	3.09E-01	0.91	FALSE
M240T447_pos	240.0870	447	3	8.24E-12	0.64	TRUE	9.15E-01	1.01	FALSE	3.33E-16	1.60	TRUE	7.86E-01	0.98	FALSE
M242T947_pos	242.2844	947	3	1.82E-05	3.96	TRUE	2.74E-02	0.59	TRUE	5.64E-01	1.15	FALSE	5.80E-01	0.92	FALSE
M243T564_pos	243.0768	564	3	5.50E-14	1.51	TRUE	5.27E-01	0.97	FALSE	6.49E-23	1.65	TRUE	3.63E-01	1.06	FALSE
M243T591_pos	243.1335	591	3	1.64E-21	0.28	TRUE	7.10E-01	0.96	FALSE	6.16E-07	1.61	TRUE	6.89E-01	0.96	FALSE
M245T348_pos	245.0771	348	3	7.40E-17	0.52	TRUE	7.27E-01	0.97	FALSE	3.07E-18	1.82	TRUE	9.15E-01	1.01	FALSE
M245T201_pos	245.0771	201	3	1.03E-23	0.35	TRUE	4.42E-03	1.28	FALSE	5.83E-13	1.77	TRUE	7.63E-01	0.97	FALSE
M245T699_pos	245.1857	699	3	1.35E-25	0.06	TRUE	3.66E-01	1.15	FALSE	6.46E-03	1.42	FALSE	2.73E-02	0.26	TRUE
M246T694_pos	246.1341	694	3	5.66E-01	0.96	FALSE	2.10E-08	1.57	TRUE	6.31E-19	1.97	TRUE	6.68E-01	1.03	FALSE
M246T299_pos	246.1445	299	3	5.78E-43	0.08	TRUE	4.21E-01	1.09	FALSE	3.02E-01	1.09	FALSE	3.06E-03	2.10	TRUE
M246T116_pos	246.1814	116	3	1.35E-06	0.62	TRUE	9.70E-01	1.00	FALSE	5.46E-07	1.54	TRUE	5.23E-02	1.26	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M247T428_pos	247.1081	428	3							HMDB0013713	N-Acetyltryptophan	C13H14N2O3	1.4
M248T367_1_pos	248.1142	367	3							HMDB0242235	(+-)-Carbovir	C11H13N5O2	0.1
M248T484_pos	248.1130	484	3							HMDB0002095	Malonylcarnitine	C10H17NO6	0.7
M253T412_pos	253.0830	412	3							HMDB0244958	2-(Trifluoromethyl)benzhydrol	C14H11F3O	2.0
M255T360_pos	255.0984	360	3							HMDB0245609	acid, [(diethoxyphosphinyl)oxy]me	C9H19O6P	3.1
M255T569_pos	255.0982	569	3							HMDB0029445	L-Agaridoxin	C11H14N2O5	2.6
M255T157_pos	255.0979	157	3							HMDB0029445	L-Agaridoxin	C11H14N2O5	1.5
M259T434_pos	259.0928	434	3							HMDB0000884	Ribothymidine	C10H14N2O6	1.1
M260T117_pos	260.0534	117	3							HMDB0250754	D-Glucosamine-6-phosphate	C6H14NO8P	1.7
M260T545_pos	260.0666	545	3							HMDB0243786	Carboxypropylcarbamoyl)-5-fluoro	C9H10FN3O5	4.5
M260T827_pos	260.1284	827	3							HMDB0248485	Ilepcimide	C15H17NO3	1.3
M261T494_pos	261.0876	494	3							HMDB0245532	2-Acetylacteoside	C10H13FN2O5	2.0
M261T446_pos	261.0979	446	3							HMDB0248997	Benznidazole	C12H12N4O3	1.3
M263T388_pos	263.1064	388	3							HMDB0060337	1,6-Dimethoxypyrene	C18H14O2	1.1
M265T531_pos	265.1549	531	3							HMDB0015568	Vorinostat	C14H20N2O3	0.7
M265T1038_pos	265.2527	1038	3						Fatty acids	HMDB0247717	Octadeca-9,12-dienal	C18H32O	0.4
M266T378_pos	266.1137	378	3							HMDB0040694	Agaritinal	C12H15N3O4	0.5
M266T457_pos	266.1248	457	3							HMDB0244841	rin-9-yl)-5-(hydroxymethyl)cyclope	C11H15N5O3	0.0
M266T376_pos	266.1395	376	3							HMDB0243530	diol, 2-(p-methoxybenzyl)-, 3-aceta	C14H19NO4	3.1
M266T936_pos	266.2844	936	3						Fatty acids				
M267T869_pos	267.1229	869	3							HMDB0040891	bis(4-hydroxyphenyl)-1,4,6-heptat	C14H18O5	0.7
M267T405_pos	267.1345	405	3							HMDB0029005	Phenylalanylthreonine	C13H18N2O4	2.0
M268T231_pos	268.1042	231	3							HMDB0000050	Adenosine	C10H13N5O4	0.8
M268T389_pos	268.1042	389	3							HMDB0000050	Adenosine	C10H13N5O4	0.8
M268T952_2_pos	268.3001	952	3							HMDB0244390	9-Octadecen-1-amine	C18H37N	0.8
M269T540_pos	269.0771	540	3							HMDB0304685	Glycine-betaxanthin	C11H12N2O6	1.0
M269T865_pos	269.0809	865	3						Shikimates and Phenylpropanoids	HMDB0005808	Formononetin	C16H12O4	0.4
M269T950_pos	269.1385	950	3							HMDB0038935	Kamahine C	C14H20O5	0.4
M270T368_pos	270.0978	368	3							HMDB0247197	phenyl)-7H-[1,2,3]triazolo[4,5-d]py	C13H11N5O2	2.7
M272T825_pos	272.1285	825	3							HMDB0014004	Norhydromorphone	C16H17NO3	1.3
M273T264_pos	273.0848	264	3							HMDB0061177	Pyridine N-oxide glucuronide	C11H14NO7	1.7
M275T605_pos	275.0703	605	3							HMDB0041120	yl-1H,3H-naphtho[1,8-cd]pyran-1,	C18H10O3	0.1
M276T355_pos	276.1552	355	3							HMDB0003869	epsilon-(gamma-Glutamyl)lysine	C11H21N3O5	0.6
M277T597_pos	277.1186	597	3							HMDB0062178	N-lactoyl-Tryptophan	C14H16N2O4	1.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M247T428_pos	247.1081	428	3	6.42E-05	0.60	TRUE	9.31E-01	1.01	FALSE	2.13E-08	1.89	TRUE	6.23E-02	0.85	FALSE
M248T367_1_pos	248.1142	367	3	1.81E-10	0.58	TRUE	3.33E-01	1.08	FALSE	3.95E-09	1.54	TRUE	7.65E-01	0.96	FALSE
M248T484_pos	248.1130	484	3	3.11E-25	0.52	TRUE	7.82E-02	1.10	FALSE	1.20E-27	1.83	TRUE	3.53E-02	0.88	FALSE
M253T412_pos	253.0830	412	3	2.21E-35	0.07	TRUE	4.90E-01	1.08	FALSE	4.89E-10	1.94	TRUE	7.16E-01	0.96	FALSE
M255T360_pos	255.0984	360	3	1.43E-18	0.48	TRUE	9.33E-01	0.99	FALSE	7.37E-22	2.03	TRUE	9.89E-01	1.00	FALSE
M255T569_pos	255.0982	569	3	6.09E-08	0.46	TRUE	7.08E-01	1.05	FALSE	3.95E-04	1.52	TRUE	6.61E-01	0.94	FALSE
M255T157_pos	255.0979	157	3	2.01E-04	2.31	TRUE	1.06E-01	0.72	FALSE	2.26E-15	8.28	TRUE	9.03E-02	1.29	FALSE
M259T434_pos	259.0928	434	3	4.31E-41	0.38	TRUE	3.55E-01	1.05	FALSE	2.01E-26	1.77	TRUE	4.67E-01	1.03	FALSE
M260T117_pos	260.0534	117	3	6.09E-12	0.44	TRUE	8.96E-03	1.34	FALSE	9.56E-12	2.00	TRUE	7.51E-01	1.04	FALSE
M260T545_pos	260.0666	545	3	1.02E-15	0.62	TRUE	2.64E-02	1.13	FALSE	4.85E-30	1.94	TRUE	8.99E-02	1.08	FALSE
M260T827_pos	260.1284	827	3	8.55E-20	2.17	TRUE	3.29E-04	0.79	FALSE	6.00E-05	1.30	FALSE	1.00E-06	0.55	TRUE
M261T494_pos	261.0876	494	3	4.32E-15	0.64	TRUE	1.24E-01	1.09	FALSE	2.61E-26	1.76	TRUE	9.57E-01	1.00	FALSE
M261T446_pos	261.0979	446	3	4.88E-05	0.12	TRUE	8.60E-01	0.93	FALSE	1.09E-02	2.45	TRUE	3.81E-01	0.81	FALSE
M263T388_pos	263.1064	388	3	6.71E-18	0.56	TRUE	2.55E-01	1.07	FALSE	4.90E-23	1.84	TRUE	2.17E-02	0.83	FALSE
M265T531_pos	265.1549	531	3	2.81E-12	0.26	TRUE	5.89E-01	1.10	FALSE	3.69E-03	1.51	TRUE	1.05E-01	0.65	FALSE
M265T1038_pos	265.2527	1038	3	9.62E-14	1.90	TRUE	4.03E-08	0.63	TRUE	7.28E-01	0.98	FALSE	2.10E-04	1.31	FALSE
M266T378_pos	266.1137	378	3	1.17E-10	0.55	TRUE	9.52E-01	0.99	FALSE	2.51E-09	1.60	TRUE	3.38E-01	0.88	FALSE
M266T457_pos	266.1248	457	3	1.14E-19	0.18	TRUE	2.74E-01	1.17	FALSE	3.12E-13	2.74	TRUE	3.72E-01	1.24	FALSE
M266T376_pos	266.1395	376	3	7.20E-12	0.62	TRUE	4.62E-01	0.95	FALSE	1.91E-16	1.69	TRUE	5.77E-02	0.87	FALSE
M266T936_pos	266.2844	936	3	1.77E-06	4.38	TRUE	3.47E-02	0.60	TRUE	3.49E-01	1.23	FALSE	7.90E-01	0.96	FALSE
M267T869_pos	267.1229	869	3	3.57E-21	0.67	TRUE	3.71E-02	1.09	FALSE	2.47E-31	1.60	TRUE	3.29E-05	0.81	FALSE
M267T405_pos	267.1345	405	3	2.35E-14	0.27	TRUE	6.10E-01	1.08	FALSE	8.46E-04	1.52	TRUE	5.06E-01	0.86	FALSE
M268T231_pos	268.1042	231	3	6.72E-28	0.37	TRUE	1.21E-02	1.21	FALSE	6.65E-16	1.75	TRUE	1.50E-02	0.70	FALSE
M268T389_pos	268.1042	389	3	6.43E-08	1.79	TRUE	8.56E-04	0.68	FALSE	1.42E-24	3.17	TRUE	7.05E-01	1.03	FALSE
M268T952_2_pos	268.3001	952	3	8.50E-05	3.98	TRUE	2.26E-02	0.53	TRUE	7.20E-01	1.10	FALSE	8.48E-01	0.93	FALSE
M269T540_pos	269.0771	540	3	6.95E-10	0.53	TRUE	2.02E-01	1.14	FALSE	2.92E-12	1.89	TRUE	9.24E-01	0.99	FALSE
M269T865_pos	269.0809	865	3	6.40E-05	2.28	TRUE	1.40E-02	0.59	TRUE	1.41E-01	1.28	FALSE	9.21E-01	0.98	FALSE
M269T950_pos	269.1385	950	3	1.45E-18	0.62	TRUE	8.44E-04	1.19	FALSE	1.21E-23	1.63	TRUE	5.19E-01	1.04	FALSE
M270T368_pos	270.0978	368	3	9.63E-08	0.57	TRUE	9.75E-01	1.00	FALSE	7.10E-08	1.65	TRUE	2.66E-01	1.21	FALSE
M272T825_pos	272.1285	825	3	7.22E-01	0.94	FALSE	1.40E-02	1.56	TRUE	1.40E-03	1.63	TRUE	8.70E-01	1.01	FALSE
M273T264_pos	273.0848	264	3	4.01E-16	0.43	TRUE	7.97E-01	1.02	FALSE	7.64E-08	1.56	TRUE	7.89E-02	0.90	FALSE
M275T605_pos	275.0703	605	3	1.34E-05	0.64	TRUE	9.57E-01	1.01	FALSE	5.17E-12	1.91	TRUE	2.16E-01	0.81	FALSE
M276T355_pos	276.1552	355	3	3.13E-50	0.18	TRUE	1.17E-01	1.12	FALSE	3.28E-11	1.52	TRUE	3.29E-01	0.80	FALSE
M277T597_pos	277.1186	597	3	6.25E-20	0.24	TRUE	9.19E-01	0.99	FALSE	4.29E-06	1.65	TRUE	7.87E-01	1.06	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M277T1015_pos	277.2162	1015	3						Fatty acids	HMDB0002697	19-Norandrosterone	C18H28O2	0.1
M278T476_pos	278.1235	476	3							HMDB0038493	N-(1-Deoxy-1-fructosyl)proline	C11H19NO7	0.3
M280T450_pos	280.1545	450	3							HMDB0031802	(\xc2\xb1)-Metalaxyl	C15H21NO4	0.7
M280T512_pos	280.1546	512	3							HMDB0031802	(\xc2\xb1)-Metalaxyl	C15H21NO4	1.1
M282T575_pos	282.0975	575	3							HMDB0006061	-Hydroxyphenylacetylglutamic aci	C13H15NO6	1.0
M282T449_pos	282.1200	449	3							HMDB0003331	1-Methyladenosine	C11H15N5O4	1.1
M283T585_pos	283.0930	585	3							HMDB0032560	Dinoseb acetate	C12H14N2O6	1.8
M283T350_pos	283.1283	350	3							HMDB0029073	Threonyltyrosine	C13H18N2O5	1.8
M284T935_pos	284.2948	935	3							HMDB0034146	Octadecanamide	C18H37NO	0.1
M286T260_pos	286.1290	260	3							HMDB0241034	dimethylidenebutanedioylcarnitine	C13H19NO6	1.7
M286T511_pos	286.1436	511	3							HMDB0014440	Morphine	C17H19NO3	0.7
M288T575_pos	288.0870	575	3							HMDB0030373	Citrusinine II	C15H13NO5	1.4
M289T534_pos	289.1188	534	3							HMDB0034881	-tetrahydro-1H-pyrido[3,4-b]indole	C15H16N2O4	1.7
M290T411_pos	290.1345	411	3							HMDB0005765	Ophthalmic acid	C11H19N3O6	0.5
M291T369_pos	291.1020	369	3							HMDB0034688	o-2,3-dihydroxy-9-phenyl-1H-phen	C19H14O3	1.4
M291T414_pos	291.1704	414	3							HMDB0015453	Procaterol	C16H22N2O3	0.4
M291T956_pos	291.2684	956	3							HMDB0035083	,6E,10E)-1,6,10,14-Phytatetraen-3	C20H34O	0.5
M293T684_pos	293.0811	684	3							HMDB0039404	ydroxyphenyl)-1H,3H-naphtho[1,8	C18H12O4	1.1
M293T934_pos	293.1857	934	3							HMDB0014662	Carteolol	C16H24N2O3	1.0
M293T1040_pos	293.2467	1040	3							HMDB0000369	3b,17b-Dihydroxyetiocholane	C19H32O2	2.8
M294T697_pos	294.1127	697	3							HMDB0015126	Oxaprozin	C18H15NO3	0.9
M295T598_pos	295.1654	598	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.6
M295T1015_pos	295.2264	1015	3							HMDB0004668	13-OxoODE	C18H30O3	1.4
M296T492_pos	296.1683	492	3							HMDB0042026	Tertatolol	C16H25NO2S	1.6
M296T543_pos	296.1686	543	3							HMDB0042026	Tertatolol	C16H25NO2S	2.3
M296T598_pos	296.1680	598	3							HMDB0042026	Tertatolol	C16H25NO2S	0.4
M297T467_pos	297.0908	467	3							HMDB0256121	Paracetamol mercapturate	C13H16N2O4S	1.4
M297T563_pos	297.1270	563	3							HMDB0029001	Phenylalanylmethionine	C14H20N2O3S	0.9
M298T489_pos	298.1113	489	3							HMDB0259284	Tritiozine	C14H19NO4S	1.9
M299T151_pos	299.1604	151	3							HMDB0035233	Olomoucine	C15H18N6O	3.5
M303T107_1_pos	303.0225	107	3							HMDB0257704	nylidene-3H-purin-9-yl)-3H-purine	C10H6N8S2	1.4
M304T431_pos	304.0967	431	3						Amino acids and Peptides	HMDB0257167	Resorufin benzyl ether	C19H13NO3	0.5
M304T627_2_pos	304.1658	627	3							HMDB0029096	Tryptophyl-Valine	C16H21N3O3	0.8
M304T622_pos	304.1944	622	3							HMDB0242030	N-Lauroyl Cysteine	C15H29NO3S	0.9
M305T786_pos	305.1860	786	3							HMDB0259093	Tilisolol	C17H24N2O3	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M277T1015_pos	277.2162	1015	3	1.39E-02	1.43	FALSE	1.17E-03	0.57	TRUE	1.10E-06	1.90	TRUE	9.18E-01	0.97	FALSE
M278T476_pos	278.1235	476	3	5.04E-40	0.36	TRUE	3.28E-01	1.06	FALSE	6.64E-19	1.63	TRUE	8.91E-01	0.99	FALSE
M280T450_pos	280.1545	450	3	9.18E-14	0.58	TRUE	5.80E-01	1.04	FALSE	3.62E-22	1.92	TRUE	9.83E-01	1.00	FALSE
M280T512_pos	280.1546	512	3	2.76E-08	1.70	TRUE	1.62E-01	1.14	FALSE	2.80E-09	1.64	TRUE	2.43E-01	0.89	FALSE
M282T575_pos	282.0975	575	3	1.01E-11	0.55	TRUE	1.68E-01	1.12	FALSE	2.16E-08	1.51	TRUE	5.07E-01	0.96	FALSE
M282T449_pos	282.1200	449	3	2.12E-32	0.35	TRUE	4.90E-01	0.95	FALSE	1.50E-12	1.56	TRUE	5.83E-01	1.11	FALSE
M283T585_pos	283.0930	585	3	5.36E-14	0.61	TRUE	1.05E-01	1.11	FALSE	1.01E-22	1.83	TRUE	8.18E-01	1.02	FALSE
M283T350_pos	283.1283	350	3	2.96E-10	0.57	TRUE	2.68E-01	1.10	FALSE	8.40E-14	1.83	TRUE	3.44E-01	0.88	FALSE
M284T935_pos	284.2948	935	3	1.97E-04	2.33	TRUE	9.09E-03	0.61	TRUE	1.21E-01	0.75	FALSE	7.44E-01	0.82	FALSE
M286T260_pos	286.1290	260	3	1.03E-16	0.58	TRUE	5.38E-02	1.13	FALSE	1.34E-30	2.10	TRUE	7.32E-01	0.95	FALSE
M286T511_pos	286.1436	511	3	8.45E-12	2.00	TRUE	6.44E-02	1.19	FALSE	8.97E-26	2.90	TRUE	4.44E-03	0.81	FALSE
M288T575_pos	288.0870	575	3	1.46E-15	0.59	TRUE	2.78E-01	1.07	FALSE	2.24E-25	1.90	TRUE	1.72E-01	0.88	FALSE
M289T534_pos	289.1188	534	3	2.75E-07	0.55	TRUE	7.72E-01	1.03	FALSE	1.23E-06	1.63	TRUE	4.71E-01	1.03	FALSE
M290T411_pos	290.1345	411	3	2.18E-14	0.55	TRUE	1.95E-01	1.10	FALSE	1.18E-16	1.76	TRUE	7.38E-01	0.94	FALSE
M291T369_pos	291.1020	369	3	1.69E-10	0.65	TRUE	5.35E-01	1.04	FALSE	1.70E-20	1.82	TRUE	2.13E-02	0.79	FALSE
M291T414_pos	291.1704	414	3	5.80E-22	0.37	TRUE	9.62E-02	1.16	FALSE	9.83E-09	1.56	TRUE	9.86E-01	1.00	FALSE
M291T956_pos	291.2684	956	3	3.64E-07	2.97	TRUE	1.90E-03	0.61	TRUE	4.96E-01	0.89	FALSE	6.26E-01	1.10	FALSE
M293T684_pos	293.0811	684	3	1.26E-25	0.52	TRUE	2.54E-01	1.07	FALSE	1.97E-20	1.62	TRUE	1.04E-01	0.87	FALSE
M293T934_pos	293.1857	934	3	6.04E-09	0.54	TRUE	7.46E-03	1.32	FALSE	1.29E-06	1.55	TRUE	7.61E-01	1.08	FALSE
M293T1040_pos	293.2467	1040	3	5.26E-01	1.47	FALSE	9.94E-01	1.01	FALSE	1.47E-02	4.62	TRUE	2.66E-02	0.52	TRUE
M294T697_pos	294.1127	697	3	2.59E-03	1.50	TRUE	9.47E-02	1.26	FALSE	1.89E-05	1.67	TRUE	7.02E-01	0.95	FALSE
M295T598_pos	295.1654	598	3	2.74E-38	0.08	TRUE	7.41E-01	1.04	FALSE	1.28E-07	1.66	TRUE	9.64E-01	0.99	FALSE
M295T1015_pos	295.2264	1015	3	5.62E-05	1.57	TRUE	4.69E-03	0.71	FALSE	1.31E-07	1.70	TRUE	3.31E-01	1.20	FALSE
M296T492_pos	296.1683	492	3	2.07E-12	0.65	TRUE	3.19E-01	1.06	FALSE	4.80E-28	1.95	TRUE	1.47E-01	0.92	FALSE
M296T543_pos	296.1686	543	3	3.52E-32	0.36	TRUE	7.29E-01	1.03	FALSE	2.38E-19	1.82	TRUE	8.72E-02	0.75	FALSE
M296T598_pos	296.1680	598	3	6.97E-29	0.23	TRUE	5.41E-01	0.94	FALSE	2.28E-09	1.70	TRUE	7.43E-01	1.12	FALSE
M297T467_pos	297.0908	467	3	1.97E-19	0.54	TRUE	4.53E-01	1.05	FALSE	4.01E-22	1.79	TRUE	7.14E-01	1.03	FALSE
M297T563_pos	297.1270	563	3	3.12E-06	0.60	TRUE	6.67E-01	1.05	FALSE	4.66E-13	2.07	TRUE	3.77E-02	0.70	FALSE
M298T489_pos	298.1113	489	3	1.20E-04	0.64	TRUE	2.56E-01	1.14	FALSE	2.78E-11	2.04	TRUE	9.49E-02	1.08	FALSE
M299T151_pos	299.1604	151	3	1.70E-08	0.46	TRUE	8.29E-01	1.03	FALSE	8.42E-07	1.78	TRUE	3.64E-01	0.84	FALSE
M303T107_1_pos	303.0225	107	3	6.31E-19	0.48	TRUE	1.34E-01	1.12	FALSE	5.40E-12	1.60	TRUE	1.08E-02	0.70	FALSE
M304T431_pos	304.0967	431	3	2.60E-06	0.66	TRUE	6.10E-03	1.28	FALSE	6.74E-15	1.91	TRUE	4.83E-02	1.21	FALSE
M304T627_2_pos	304.1658	627	3	1.21E-47	0.12	TRUE	1.67E-01	1.12	FALSE	7.94E-11	1.63	TRUE	8.39E-01	0.98	FALSE
M304T622_pos	304.1944	622	3	3.52E-15	0.25	TRUE	5.30E-01	1.10	FALSE	1.10E-03	1.51	TRUE	1.53E-01	0.84	FALSE
M305T786_pos	305.1860	786	3	8.60E-06	0.68	FALSE	2.73E-06	1.51	TRUE	4.24E-13	1.78	TRUE	9.09E-01	1.03	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M307T913_pos	307.2269	913	3						Terpenoids	HMDB0000523	5-Androstene-3b,16b,17a-triol	C19H30O3	0.4
M308T395_pos	308.1341	395	3							HMDB0059780	1,N2-propanodeoxyguanosine	C13H17N5O4	4.0
M309T453_pos	309.1086	453	3							HMDB0029386	Indicaxanthin	C14H16N2O6	1.4
M309T712_pos	309.1809	712	3							HMDB0060990	8-Hydroxycarteolol	C16H24N2O4	0.2
M309T1078_pos	309.2786	1078	3							HMDB0005060	Eicosadienoic acid	C20H36O2	0.7
M309T956_pos	309.2788	956	3							HMDB0005060	Eicosadienoic acid	C20H36O2	0.2
M311T563_pos	311.1241	563	3							HMDB0011741	gamma-Glutamyltyrosine	C14H18N2O6	1.1
M311T460_pos	311.1256	460	3							HMDB0250310	Cl-amidine	C14H19ClN4O2	4.3
M311T697_pos	311.1397	697	3							HMDB0258528	2-dihydroindol-3-ylidenemethyl)-1	C18H18N2O3	2.2
M311T383_pos	311.1606	383	3							HMDB0250969	Delgocitini	C16H18N6O	3.0
M311T152_pos	311.1613	152	3							HMDB0250969	Delgocitini	C16H18N6O	0.7
M312T473_pos	312.1445	473	3							HMDB0033939	Domoic acid	C15H21NO6	1.1
M312T647_pos	312.1737	647	3							HMDB0249451	BUTACHLOR	C17H26ClNO2	3.8
M313T474_pos	313.1224	474	3							HMDB0256230	Penicillin F	C14H20N2O4S	2.2
M313T1052_pos	313.2739	1052	3						Fatty acids				
M314T365_pos	314.1239	365	3							HMDB0010328	Tyramine glucuronide	C14H19NO7	1.4
M314T826_pos	314.2693	826	3							HMDB0013034	Palmitoylglycine	C18H35NO3	1.0
M316T405_pos	316.1408	405	3							HMDB0245634	9-benzyl-2-(2-methoxyethoxy)-9H-	C15H17N5O3	1.1
M316T949_pos	316.3212	949	3						Fatty acids				
M317T117_pos	317.0831	117	3						Amino acids and Peptides				
M318T661_pos	318.1815	661	3							HMDB0028918	Isoleucyl-Tryptophan	C17H23N3O3	0.8
M319T773_pos	319.1653	773	3							HMDB0255714	Noopept	C17H22N2O4	0.4
M319T499_pos	319.1654	499	3							HMDB0255714	Noopept	C17H22N2O4	0.6
M321T522_pos	321.1553	522	3							HMDB0000901	Valproic acid glucuronide	C14H24O8	2.8
M324T1053_pos	324.2895	1053	3						Fatty acids	HMDB0012252	Linoleoyl ethanolamide	C20H37NO2	0.6
M325T537_pos	325.1761	537	3							HMDB0255924	p-Hydroxyubenimex	C16H24N2O5	0.9
M327T562_pos	327.1017	562	3							HMDB0249367	Brasofensine	C16H20Cl2N2O	2.7
M329T571_pos	329.1502	571	3							HMDB0029007	Phenylalanyltyrosine	C18H20N2O4	1.9
M330T915_1_pos	330.2458	915	3						Fatty acids				
M331T1072_pos	331.2850	1072	3							HMDB0011533	MG(0:0/16:0/0:0)	C19H38O4	2.2
M332T682_pos	332.1650	682	3							HMDB0249389	)-3-(4-hydroxy-3-methoxyphenoxy	C19H22FNO3	2.1
M333T516_pos	333.1086	516	3							HMDB0251046	Desidustat	C16H16N2O6	1.4
M333T529_pos	333.1559	529	3							HMDB0028808	Glutaminyltryptophan	C16H20N4O4	0.4
M333T533_pos	333.1812	533	3							HMDB0253709	Isoxaben	C18H24N2O4	0.9
M335T525_pos	335.1606	525	3							HMDB0037499	1-Ethenylhexyl butanoate	C17H22N2O5	1.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M307T913_pos	307.2269	913	3	5.37E-15	3.33	TRUE	1.65E-01	1.18	FALSE	1.92E-02	1.30	FALSE	8.99E-03	0.60	TRUE
M308T395_pos	308.1341	395	3	2.14E-24	0.05	TRUE	9.82E-01	1.00	FALSE	8.61E-06	1.90	TRUE	8.16E-01	1.02	FALSE
M309T453_pos	309.1086	453	3	1.74E-10	0.45	TRUE	5.71E-01	1.07	FALSE	2.62E-09	1.87	TRUE	2.87E-01	1.10	FALSE
M309T712_pos	309.1809	712	3	1.48E-05	1.64	TRUE	1.02E-08	0.59	TRUE	7.95E-03	0.77	FALSE	5.01E-01	0.94	FALSE
M309T1078_pos	309.2786	1078	3	2.05E-05	1.94	TRUE	1.03E-03	0.62	TRUE	4.74E-01	0.91	FALSE	9.06E-01	0.97	FALSE
M309T956_pos	309.2788	956	3	1.02E-06	2.36	TRUE	1.85E-03	0.63	TRUE	9.50E-01	0.99	FALSE	2.30E-01	0.89	FALSE
M311T563_pos	311.1241	563	3	8.80E-09	0.56	TRUE	7.94E-01	1.03	FALSE	1.95E-13	1.96	TRUE	2.45E-01	0.83	FALSE
M311T460_pos	311.1256	460	3	1.42E-13	0.14	TRUE	1.45E-01	1.34	FALSE	2.52E-03	1.67	TRUE	9.83E-01	1.01	FALSE
M311T697_pos	311.1397	697	3	1.07E-03	1.66	TRUE	6.71E-02	1.33	FALSE	2.39E-05	1.79	TRUE	7.71E-01	0.96	FALSE
M311T383_pos	311.1606	383	3	4.60E-12	0.56	TRUE	3.46E-01	1.08	FALSE	2.63E-10	1.56	TRUE	8.27E-01	1.04	FALSE
M311T152_pos	311.1613	152	3	2.31E-10	0.42	TRUE	9.00E-01	1.02	FALSE	2.00E-05	1.61	TRUE	2.90E-01	0.60	FALSE
M312T473_pos	312.1445	473	3	2.77E-28	0.51	TRUE	2.63E-01	1.06	FALSE	1.00E-20	1.58	TRUE	9.21E-01	0.99	FALSE
M312T647_pos	312.1737	647	3	3.82E-13	0.47	TRUE	9.00E-04	1.38	FALSE	2.28E-09	1.68	TRUE	5.75E-03	1.33	FALSE
M313T474_pos	313.1224	474	3	2.97E-12	0.51	TRUE	2.15E-01	1.13	FALSE	4.63E-08	1.55	TRUE	9.57E-02	1.27	FALSE
M313T1052_pos	313.2739	1052	3	1.03E-02	1.51	TRUE	3.98E-01	1.16	FALSE	1.58E-05	1.87	TRUE	5.04E-01	1.13	FALSE
M314T365_pos	314.1239	365	3	2.65E-19	0.10	TRUE	5.98E-01	1.09	FALSE	1.44E-04	1.76	TRUE	4.80E-01	1.09	FALSE
M314T826_pos	314.2693	826	3	4.11E-09	4.09	TRUE	6.03E-02	0.72	FALSE	1.95E-02	1.51	TRUE	2.81E-01	0.67	FALSE
M316T405_pos	316.1408	405	3	6.47E-12	0.44	TRUE	5.61E-01	1.07	FALSE	1.21E-09	1.85	TRUE	5.98E-01	0.92	FALSE
M316T949_pos	316.3212	949	3	7.22E-05	3.76	TRUE	7.33E-04	0.46	TRUE	8.76E-02	0.65	FALSE	7.24E-01	0.94	FALSE
M317T117_pos	317.0831	117	3	5.74E-35	0.31	TRUE	3.99E-01	1.06	FALSE	2.71E-12	1.58	TRUE	3.24E-01	1.13	FALSE
M318T661_pos	318.1815	661	3	9.63E-42	0.21	TRUE	7.88E-01	0.98	FALSE	2.27E-16	1.81	TRUE	4.91E-01	0.78	FALSE
M319T773_pos	319.1653	773	3	9.69E-09	1.64	TRUE	1.10E-12	0.58	TRUE	3.96E-01	1.06	FALSE	3.60E-02	0.73	FALSE
M319T499_pos	319.1654	499	3	2.13E-18	0.56	TRUE	2.47E-01	1.07	FALSE	2.39E-27	1.95	TRUE	1.36E-01	0.92	FALSE
M321T522_pos	321.1553	522	3	1.12E-16	0.57	TRUE	3.20E-02	1.15	FALSE	3.83E-27	2.02	TRUE	5.99E-01	0.96	FALSE
M324T1053_pos	324.2895	1053	3	3.97E-05	3.10	TRUE	3.97E-02	0.60	TRUE	7.55E-01	1.07	FALSE	5.92E-01	0.87	FALSE
M325T537_pos	325.1761	537	3	8.14E-10	0.65	TRUE	1.33E-01	1.11	FALSE	6.64E-22	1.89	TRUE	6.77E-01	0.93	FALSE
M327T562_pos	327.1017	562	3	1.51E-03	1.53	TRUE	7.21E-01	0.96	FALSE	6.22E-05	1.60	TRUE	4.77E-01	0.89	FALSE
M329T571_pos	329.1502	571	3	2.55E-07	0.65	TRUE	6.82E-01	0.96	FALSE	2.40E-17	1.96	TRUE	9.60E-02	0.76	FALSE
M330T915_1_pos	330.2458	915	3	3.42E-05	2.88	TRUE	4.51E-01	0.85	FALSE	4.54E-03	1.80	TRUE	4.15E-01	0.88	FALSE
M331T1072_pos	331.2850	1072	3	3.76E-04	1.93	TRUE	9.58E-04	0.52	TRUE	4.48E-02	1.37	FALSE	9.35E-01	0.98	FALSE
M332T682_pos	332.1650	682	3	1.62E-08	1.74	TRUE	3.90E-01	0.92	FALSE	2.79E-09	1.66	TRUE	1.66E-01	0.81	FALSE
M333T516_pos	333.1086	516	3	4.70E-08	0.47	TRUE	6.52E-01	1.06	FALSE	1.26E-05	1.67	TRUE	9.99E-02	1.12	FALSE
M333T529_pos	333.1559	529	3	2.72E-07	0.61	TRUE	8.00E-01	0.98	FALSE	9.52E-08	1.57	TRUE	8.56E-02	0.92	FALSE
M333T533_pos	333.1812	533	3	1.19E-20	0.54	TRUE	4.38E-01	1.05	FALSE	4.99E-21	1.72	TRUE	5.73E-01	0.94	FALSE
M335T525_pos	335.1606	525	3	3.74E-23	0.53	TRUE	1.01E-01	1.10	FALSE	3.21E-30	1.94	TRUE	9.01E-02	0.94	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M335T1067_pos	335.2576	1067	3							HMDB0000879	Tetrahydrodeoxycorticosterone	C21H34O3	1.4
M335T909_pos	335.2583	909	3							HMDB0000879	Tetrahydrodeoxycorticosterone	C21H34O3	0.7
M340T440_pos	340.1400	440	3							HMDB0013200	5-Hydroxytryptophol glucuronide	C16H21NO7	2.7
M341T439_pos	341.1711	439	3							HMDB0257669	olidin-1-yl)-6-oxohexanoyl]pyrrolid	C16H24N2O6	1.2
M341T516_pos	341.1710	516	3							HMDB0257669	olidin-1-yl)-6-oxohexanoyl]pyrrolid	C16H24N2O6	0.9
M342T451_pos	342.1186	451	3							HMDB0244642	Nep-IN-2	C16H23NO3S2	1.8
M343T421_pos	343.1140	421	3							HMDB0246183	ethylaminoethoxy)phenyl]-4-(trifl	C14H18N2O8	1.2
M344T468_pos	344.1861	468	3							HMDB0030211	(R)-Laudanidine	C20H25NO4	1.5
M344T956_pos	344.2429	956	3							HMDB0241165	2-Hydroxyundec-3-enoylcarnitine	C18H33NO5	0.7
M344T1060_pos	344.3161	1060	3							HMDB0249513	N-Acetylsphinganine	C20H41NO3	0.6
M345T427_pos	345.1406	427	3							HMDB0002928	Maltitol	C12H24O11	4.3
M347T400_pos	347.1564	400	3							HMDB0253972	Laninamivir	C13H22N4O7	0.7
M349T506_pos	349.1762	506	3							HMDB0041886	Enalaprilat	C18H24N2O5	1.3
M349T1074_pos	349.2738	1074	3							HMDB0029683	-Hydroxy-6-pentadecylbenzoic aci	C22H36O3	0.1
M350T658_pos	350.2075	658	3							HMDB0029225	Coutaric acid	C18H27N3O4	0.3
M351T792_pos	351.1915	792	3							HMDB0251479	Disofenin	C18H26N2O5	0.2
M351T994_pos	351.2527	994	3							HMDB0000268	Tetrahydrocorticosterone	C21H34O4	0.7
M352T363_pos	352.1404	363	3							HMDB0244481	thoxybenzoyl)-4,4-diethyl-3,5-isox	C17H21NO7	3.8
M353T1007_2_pos	353.2687	1007	3						Fatty acids	HMDB0011539	MG(0:0/18:3(6Z,9Z,12Z)/0:0)	C21H36O4	0.0
M355T677_pos	355.1865	677	3							HMDB0251077	-4-yn-2-yl]amino]-4-methyl-1-oxop	C17H26N2O6	0.4
M358T353_pos	358.1138	353	3							HMDB0029833	Cyclodopa glucoside	C15H19NO9	1.4
M358T956_pos	358.2593	956	3							HMDB0240760	9Z)-3-Hydroxydodecenoylcarnitine	C19H35NO5	1.5
M361T382_pos	361.1183	382	3							HMDB0015173	Fenofibrate	C20H21ClO4	5.0
M362T307_pos	362.0173	307	3							HMDB0247566	nyl)thio)-N-(4-(pyridin-2-yl)thiazol	C16H12ClN3OS2	2.9
M363T812_pos	363.1931	812	3							HMDB0257145	Remifentanil Acid	C19H26N2O5	4.6
M365T122_pos	365.1051	122	3							HMDB0254257	Lykurim	C10H24N2O8S2	1.1
M371T318_pos	371.1455	318	3							HMDB0252214	Fenozan 50F	C22H20F2O3	0.5
M371T416_pos	371.1886	416	3							HMDB0002759	Androsterone sulfate	C19H30O5S	0.2
M371T858_pos	371.2064	858	3							HMDB0032841	egastigmen-7-yne-3,9-diol 9-gluco	C19H30O7	0.0
M372T687_pos	372.1115	687	3							HMDB0304919	Hydroxydesmethylpiperine sulfate	C16H21NO7S	0.9
M372T1062_pos	372.3108	1062	3						Fatty acids	HMDB0240823	4-Methyltridecanoylcarnitine	C21H41NO4	0.2
M377T1062_pos	377.2660	1062	3							HMDB0245653	24-Hexaoxa-1,10-diazabicyclo[8.8.	C18H36N2O6	3.8
M378T808_pos	378.1452	808	3							HMDB0247816	ic acid, 9-fluoro-2,3-dihydro-3-me	C18H20FN3O5	2.2
M384T550_pos	384.2131	550	3							HMDB0249520	lamino)carbonyl)oxiranyl)carbony	C18H29N3O6	0.4
M385T447_pos	385.1974	447	3							HMDB0258164	Schiff base	C19H24N6O3	2.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M335T1067_pos	335.2576	1067	3	2.15E-05	2.32	TRUE	8.73E-01	1.03	FALSE	8.99E-08	2.58	TRUE	5.94E-01	0.92	FALSE
M335T909_pos	335.2583	909	3	4.22E-06	1.53	TRUE	4.35E-08	0.59	TRUE	2.74E-01	0.92	FALSE	4.81E-02	0.76	FALSE
M340T440_pos	340.1400	440	3	5.06E-32	0.31	TRUE	2.97E-06	1.45	FALSE	5.34E-17	1.85	TRUE	2.41E-02	1.39	FALSE
M341T439_pos	341.1711	439	3	1.99E-26	0.50	TRUE	6.15E-01	1.03	FALSE	3.03E-20	1.63	TRUE	7.38E-01	0.99	FALSE
M341T516_pos	341.1710	516	3	3.59E-26	0.49	TRUE	3.66E-03	1.19	FALSE	4.19E-29	1.96	TRUE	5.26E-03	1.17	FALSE
M342T451_pos	342.1186	451	3	2.41E-25	0.07	TRUE	9.11E-01	0.98	FALSE	7.82E-05	1.68	TRUE	4.78E-01	0.89	FALSE
M343T421_pos	343.1140	421	3	1.06E-13	0.42	TRUE	5.80E-01	1.06	FALSE	3.58E-10	1.82	TRUE	5.34E-01	0.91	FALSE
M344T468_pos	344.1861	468	3	3.01E-23	0.31	TRUE	1.91E-01	1.13	FALSE	6.95E-13	1.90	TRUE	1.52E-01	0.82	FALSE
M344T956_pos	344.2429	956	3	4.20E-04	2.17	TRUE	4.56E-01	0.84	FALSE	1.53E-02	0.64	TRUE	8.57E-01	1.04	FALSE
M344T1060_pos	344.3161	1060	3	1.70E-02	1.65	TRUE	8.99E-01	0.97	FALSE	1.20E-02	1.58	TRUE	7.90E-01	1.03	FALSE
M345T427_pos	345.1406	427	3	4.39E-11	0.47	TRUE	4.73E-01	1.08	FALSE	3.70E-07	1.61	TRUE	3.90E-01	1.14	FALSE
M347T400_pos	347.1564	400	3	5.92E-12	0.56	TRUE	6.33E-01	1.04	FALSE	3.67E-19	1.99	TRUE	5.82E-01	0.95	FALSE
M349T506_pos	349.1762	506	3	3.77E-14	0.55	TRUE	4.80E-01	1.05	FALSE	1.60E-12	1.61	TRUE	6.26E-02	0.80	FALSE
M349T1074_pos	349.2738	1074	3	9.45E-13	3.51	TRUE	2.78E-03	0.65	TRUE	8.99E-02	1.24	FALSE	8.58E-01	1.07	FALSE
M350T658_pos	350.2075	658	3	8.40E-20	0.40	TRUE	4.47E-01	1.07	FALSE	4.99E-08	1.52	TRUE	1.80E-01	0.87	FALSE
M351T792_pos	351.1915	792	3	1.95E-01	1.19	FALSE	9.50E-11	0.45	TRUE	4.05E-07	0.54	TRUE	2.43E-01	0.75	FALSE
M351T994_pos	351.2527	994	3	2.14E-01	1.26	FALSE	8.53E-03	0.50	TRUE	3.24E-05	2.02	TRUE	3.28E-01	0.86	FALSE
M352T363_pos	352.1404	363	3	2.16E-05	2.03	TRUE	5.52E-02	1.35	FALSE	4.98E-01	0.91	FALSE	2.15E-02	1.52	TRUE
M353T1007_2_pos	353.2687	1007	3	7.04E-02	1.60	FALSE	3.40E-02	0.49	TRUE	1.85E-03	2.08	TRUE	8.24E-01	0.95	FALSE
M355T677_pos	355.1865	677	3	1.45E-09	1.85	TRUE	8.47E-10	0.54	TRUE	3.47E-02	0.84	FALSE	1.94E-02	0.78	FALSE
M358T353_pos	358.1138	353	3	1.09E-27	0.08	TRUE	8.30E-01	0.97	FALSE	1.90E-05	1.68	TRUE	2.38E-01	1.13	FALSE
M358T956_pos	358.2593	956	3	2.29E-10	2.46	TRUE	1.05E-04	0.56	TRUE	1.29E-01	0.85	FALSE	7.94E-01	1.04	FALSE
M361T382_pos	361.1183	382	3	4.38E-07	0.65	TRUE	8.71E-01	0.99	FALSE	2.72E-12	1.72	TRUE	8.02E-02	0.72	FALSE
M362T307_pos	362.0173	307	3	7.82E-06	0.66	TRUE	9.62E-01	1.00	FALSE	5.93E-12	1.80	TRUE	3.00E-01	1.23	FALSE
M363T812_pos	363.1931	812	3	5.83E-01	0.94	FALSE	2.96E-02	0.78	FALSE	2.60E-17	2.49	TRUE	2.10E-02	1.56	TRUE
M365T122_pos	365.1051	122	3	1.14E-05	0.50	TRUE	5.77E-01	0.91	FALSE	5.07E-02	1.29	FALSE	4.22E-03	30.19	TRUE
M371T318_pos	371.1455	318	3	3.24E-46	0.36	TRUE	1.35E-03	1.18	FALSE	5.53E-23	1.64	TRUE	4.40E-02	1.21	FALSE
M371T416_pos	371.1886	416	3	2.90E-08	0.59	TRUE	4.64E-01	1.07	FALSE	4.77E-17	2.10	TRUE	5.98E-01	1.05	FALSE
M371T858_pos	371.2064	858	3	3.71E-34	0.55	TRUE	7.13E-02	1.08	FALSE	7.60E-30	1.60	TRUE	3.16E-01	0.94	FALSE
M372T687_pos	372.1115	687	3	6.29E-06	0.50	TRUE	8.87E-01	1.02	FALSE	9.78E-06	1.79	TRUE	3.28E-01	0.78	FALSE
M372T1062_pos	372.3108	1062	3	9.38E-02	1.40	FALSE	1.49E-03	0.36	TRUE	1.57E-08	3.12	TRUE	5.51E-01	0.75	FALSE
M377T1062_pos	377.2660	1062	3	8.74E-01	0.98	FALSE	4.81E-03	0.55	TRUE	2.68E-09	2.41	TRUE	3.30E-01	0.69	FALSE
M378T808_pos	378.1452	808	3	1.70E-01	0.82	FALSE	5.32E-01	1.10	FALSE	2.10E-08	2.19	TRUE	1.35E-02	0.55	TRUE
M384T550_pos	384.2131	550	3	2.82E-06	0.65	TRUE	5.40E-01	1.06	FALSE	2.32E-15	1.98	TRUE	2.84E-02	0.74	FALSE
M385T447_pos	385.1974	447	3	1.41E-12	0.64	TRUE	5.36E-01	1.04	FALSE	2.06E-27	1.94	TRUE	3.16E-01	1.08	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M385T1034_pos	385.2741	1034	3							HMDB0034952	Persicaxanthin	C25H36O3	0.9
M387T1019_pos	387.3260	1019	3							HMDB0032925	1-Phenyl-1,3-eicosanedione	C26H42O2	0.8
M389T181_pos	389.1922	181	3							HMDB0245138	2-Guanidinobutanoic acid	C18H24N6O4	2.5
M389T402_pos	389.1932	402	3							HMDB0245138	2-Guanidinobutanoic acid	C18H24N6O4	0.0
M389T858_pos	389.2163	858	3							HMDB0031676	xy-7E-megastigmene-3a,9e-diol 3	C19H32O8	1.8
M390T858_pos	390.2190	858	3							HMDB0243857	1-Demethylmethergoline	C24H27N3O2	3.5
M398T726_pos	398.3419	726	3						Alkaloids	HMDB0003236	Solanidine	C27H43NO	0.4
M399T1009_pos	399.2889	1009	3							HMDB0258854	Benzotest	C26H38O3	1.2
M400T569_pos	400.1728	569	3							HMDB0242721	AB-MECA	C18H21N7O4	0.1
M403T598_pos	403.1450	598	3							HMDB0258261	Setipiprant	C24H19FN2O3	0.6
M403T1074_pos	403.2823	1074	3							HMDB0000541	b-Hydroxy-3-oxo-5b-cholanoic aci	C25H38O4	4.9
M409T693_pos	409.2585	693	3							HMDB0260479	MG(PGJ2/0:0/0:0)	C23H36O6	0.0
M412T616_pos	412.2441	616	3							HMDB0003752	LysoPC(10:0/0:0)	C18H38NO7P	4.4
M414T849_pos	414.3364	849	3							HMDB0031913	5alpha-Tomatidan-3-one	C27H43NO2	0.6
M417T527_pos	417.1806	527	3							HMDB0250142	Agelin	C24H29ClO4	5.0
M417T821_pos	417.2025	821	3							HMDB0254818	Mmp inhibitor V	C22H28N2O6	1.1
M419T1034_pos	419.3517	1034	3							HMDB0006280	7-a,25-Dihydroxycholesterol	C27H46O3	0.6
M428T904_pos	428.2548	904	3							HMDB0014388	Ranolazine	C24H33N3O4	0.9
M428T974_pos	428.3732	974	3							HMDB0240867	5-Methylheptadecanoylcarnitine	C25H49NO4	0.6
M430T863_pos	430.3316	863	3							HMDB0062336	N-Oleoyl phenylalanine	C27H43NO3	0.1
M433T698_pos	433.3508	698	3							HMDB0303271	Polyglycerol esters of fatty acids	C24H48O6	3.7
M434T960_pos	434.3277	960	3							HMDB0000698	Lithocholic acid glycine conjugate	C26H43NO4	2.8
M437T1043_pos	437.2861	1043	3							HMDB0029949	Pangamic acid	C20H40N2O8	0.7
M443T693_pos	443.3228	693	3						Amino acids and Peptides				
M445T1037_pos	445.2951	1037	3							HMDB0000969	5-Dihydroxyvitamin D3-26,23-lact	C27H40O5	0.6
M446T965_pos	446.3269	965	3							HMDB0062337	N-Oleoyl tyrosine	C27H43NO4	0.9
M446T780_pos	446.3266	780	3							HMDB0062337	N-Oleoyl tyrosine	C27H43NO4	0.2
M447T946_pos	447.3108	946	3						Terpenoids	HMDB0030913	Cepagenin	C27H42O5	0.6
M452T1030_pos	452.2775	1030	3							HMDB0011474	LysoPE(0:0/16:1(9Z))	C21H42NO7P	0.7
M455T963_pos	455.3518	963	3							HMDB0034963	beta-Elemonic acid	C30H46O3	0.4
M456T994_pos	456.4050	994	3							HMDB0006460	Arachidyl carnitine	C27H53NO4	0.6
M460T155_pos	460.2029	155	3						Amino acids and Peptides				
M463T1033_pos	463.3426	1033	3							HMDB0034336	Dolichosterone	C28H46O5	1.6
M468T698_pos	468.2687	698	3							HMDB0014822	Tobramycin	C18H37N5O9	4.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M385T1034_pos	385.2741	1034	3	2.59E-09	1.65	TRUE	2.01E-02	1.21	FALSE	8.89E-19	2.01	TRUE	1.01E-01	0.74	FALSE
M387T1019_pos	387.3260	1019	3	4.55E-08	1.84	TRUE	4.07E-06	0.61	TRUE	1.85E-01	1.13	FALSE	5.68E-01	0.92	FALSE
M389T181_pos	389.1922	181	3	6.23E-06	0.65	TRUE	6.86E-01	1.04	FALSE	1.85E-19	2.37	TRUE	6.08E-03	0.75	FALSE
M389T402_pos	389.1932	402	3	5.96E-06	0.63	TRUE	1.32E-01	1.16	FALSE	1.47E-09	1.72	TRUE	5.08E-01	0.95	FALSE
M389T858_pos	389.2163	858	3	5.08E-31	0.55	TRUE	1.18E-01	1.07	FALSE	5.65E-33	1.73	TRUE	7.70E-03	0.83	FALSE
M390T858_pos	390.2190	858	3	8.39E-17	0.66	TRUE	3.25E-01	1.05	FALSE	1.57E-20	1.51	TRUE	5.33E-02	0.82	FALSE
M398T726_pos	398.3419	726	3	2.03E-04	5.02	TRUE	9.32E-01	1.03	FALSE	2.56E-03	2.77	TRUE	2.50E-01	1.44	FALSE
M399T1009_pos	399.2889	1009	3	8.61E-11	2.42	TRUE	1.66E-06	0.58	TRUE	7.28E-01	0.96	FALSE	8.23E-01	1.04	FALSE
M400T569_pos	400.1728	569	3	1.79E-07	0.65	TRUE	8.33E-01	1.02	FALSE	3.09E-09	1.54	TRUE	3.50E-01	0.87	FALSE
M403T598_pos	403.1450	598	3	4.75E-15	0.65	TRUE	1.38E-03	1.19	FALSE	9.00E-29	1.81	TRUE	6.95E-01	1.04	FALSE
M403T1074_pos	403.2823	1074	3	5.13E-10	2.70	TRUE	1.11E-01	0.79	FALSE	1.05E-04	1.64	TRUE	8.58E-01	0.94	FALSE
M409T693_pos	409.2585	693	3	5.51E-16	0.34	TRUE	6.92E-01	0.96	FALSE	3.74E-05	1.51	TRUE	9.20E-01	0.99	FALSE
M412T616_pos	412.2441	616	3	2.88E-02	0.69	FALSE	8.73E-01	1.03	FALSE	4.54E-06	2.02	TRUE	1.16E-02	0.45	TRUE
M414T849_pos	414.3364	849	3	1.65E-03	2.16	TRUE	4.17E-02	0.61	TRUE	8.64E-02	1.42	FALSE	8.44E-01	1.03	FALSE
M417T527_pos	417.1806	527	3	2.92E-08	0.52	TRUE	7.46E-01	1.04	FALSE	2.48E-06	1.60	TRUE	2.98E-01	0.82	FALSE
M417T821_pos	417.2025	821	3	3.84E-12	0.38	TRUE	1.78E-01	1.18	FALSE	1.25E-04	1.52	TRUE	3.33E-01	0.88	FALSE
M419T1034_pos	419.3517	1034	3	7.98E-09	2.34	TRUE	9.13E-05	0.61	TRUE	3.97E-01	0.91	FALSE	4.89E-01	0.93	FALSE
M428T904_pos	428.2548	904	3	4.08E-07	0.70	FALSE	2.82E-08	1.50	FALSE	1.18E-10	1.51	TRUE	1.08E-05	1.59	TRUE
M428T974_pos	428.3732	974	3	2.81E-05	3.57	TRUE	4.05E-02	0.59	TRUE	3.44E-01	1.24	FALSE	4.44E-01	0.88	FALSE
M430T863_pos	430.3316	863	3	1.45E-04	2.03	TRUE	1.35E-02	0.66	TRUE	7.15E-01	1.06	FALSE	9.98E-01	1.00	FALSE
M433T698_pos	433.3508	698	3	1.94E-02	6.41	TRUE	7.23E-03	0.16	TRUE	9.27E-01	0.95	FALSE	3.98E-01	0.31	FALSE
M434T960_pos	434.3277	960	3	2.32E-09	1.53	TRUE	9.01E-01	0.99	FALSE	9.21E-11	1.50	TRUE	1.39E-01	0.83	FALSE
M437T1043_pos	437.2861	1043	3	1.25E-02	1.64	TRUE	2.31E-01	0.75	FALSE	6.14E-04	1.82	TRUE	9.28E-02	1.33	FALSE
M443T693_pos	443.3228	693	3	1.56E-16	0.40	TRUE	2.58E-01	1.12	FALSE	1.27E-04	1.39	FALSE	5.39E-03	0.50	TRUE
M445T1037_pos	445.2951	1037	3	1.07E-07	1.75	TRUE	5.39E-01	1.06	FALSE	1.60E-09	1.75	TRUE	5.32E-02	0.77	FALSE
M446T965_pos	446.3269	965	3	2.14E-05	2.42	TRUE	7.56E-04	0.56	TRUE	1.18E-01	0.77	FALSE	5.81E-01	0.93	FALSE
M446T780_pos	446.3266	780	3	2.10E-04	1.96	TRUE	4.50E-01	0.88	FALSE	7.04E-03	1.51	TRUE	1.16E-01	1.20	FALSE
M447T946_pos	447.3108	946	3	1.75E-07	1.53	TRUE	2.44E-01	1.10	FALSE	9.12E-12	1.65	TRUE	4.80E-01	0.89	FALSE
M452T1030_pos	452.2775	1030	3	1.01E-03	2.66	TRUE	8.33E-02	0.59	FALSE	8.67E-06	3.36	TRUE	3.53E-01	0.85	FALSE
M455T963_pos	455.3518	963	3	7.12E-06	1.46	FALSE	7.35E-12	0.54	TRUE	6.10E-03	0.82	FALSE	5.73E-05	2.07	TRUE
M456T994_pos	456.4050	994	3	5.54E-05	2.78	TRUE	2.56E-02	0.61	TRUE	2.01E-01	1.29	FALSE	6.52E-01	0.92	FALSE
M460T155_pos	460.2029	155	3	6.68E-13	0.34	TRUE	3.45E-02	1.33	FALSE	8.13E-10	2.12	TRUE	8.23E-01	1.17	FALSE
M463T1033_pos	463.3426	1033	3	7.18E-06	1.87	TRUE	1.19E-01	0.81	FALSE	4.39E-05	1.63	TRUE	2.87E-01	1.18	FALSE
M468T698_pos	468.2687	698	3	1.49E-02	4.22	TRUE	1.75E-02	0.28	TRUE	5.23E-01	0.75	FALSE	5.12E-01	0.53	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M471T788_pos	471.2164	788	3							HMDB0253951	Lactose-lysine	C18H34N2O12	4.4
M472T955_pos	472.3425	955	3							HMDB0006510	Cervonyl carnitine	C29H45NO4	0.7
M473T951_pos	473.3265	951	3							HMDB0035112	23-Epoxy-3,29-dihydroxy-27-norla	C29H44O5	0.7
M473T1011_pos	473.3617	1011	3							HMDB0002392	Maslinic acid	C30H48O4	1.7
M475T786_pos	475.2552	786	3							HMDB0254939	mTOR-IN-1	C25H30N8O2	2.6
M475T961_pos	475.3421	961	3						Terpenoids	HMDB0035144	-17,23-Epoxy-3,24,29-trihydroxy-2	C29H46O5	0.6
M482T1073_pos	482.3228	1073	3							HMDB0256087	Palmitoyl Ara-C	C25H43N3O6	0.8
M484T689_pos	484.2445	689	3							HMDB0033470	Caffeoylferuloylspermidine	C26H33N3O6	0.6
M490T130_pos	490.1770	130	3							HMDB0258340	mino]propanoylamino]-2-[(4-ethy	C22H27N5O6S	3.1
M490T794_pos	490.3528	794	3						Alkaloids	HMDB0242406	Chenodeoxycholylproline	C29H47NO5	0.3
M493T704_pos	493.2430	704	3							HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.3
M500T866_pos	500.2758	866	3							HMDB0248778	Osimertini	C28H33N7O2	2.1
M505T410_pos	505.1794	410	3						Carbohydrates	HMDB0256657	ro-4-hydroxy-2-oxo-2H-cycloocta(b	C28H28N2O5S	0.5
M506T960_pos	506.3488	960	3							HMDB0241611	9,20-Dihydroxydocosa-4,7,10,13,1	C29H47NO6	2.4
M512T714_pos	512.2794	714	3							HMDB0013863	AFN911	C29H33N7O2	5.0
M512T690_pos	512.3030	690	3							HMDB0242372	Cholylcysteine	C27H45NO6S	2.1
M518T1022_pos	518.3240	1022	3							HMDB0010387	LysoPC(18:3(6Z,9Z,12Z)/0:0)	C26H48NO7P	0.2
M520T821_pos	520.3634	821	3						Alkaloids				
M545T816_pos	545.3118	816	3							HMDB0254457	Meproscillarin	C31H44O8	1.6
M551T984_pos	551.3594	984	3							HMDB0297203	20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,	C31H50O8	2.7
M556T483_pos	556.1559	483	3						Carbohydrates				
M587T870_pos	587.2868	870	3							HMDB0014900	Irinotecan	C33H38N4O6	0.6
M594T698_pos	594.4003	698	3						Alkaloids				
M624T786_pos	624.3749	786	3							HMDB0248512	apicidin	C34H49N5O6	1.0
M643T868_pos	643.3337	868	3							HMDB0036707	Steviobioside	C32H50O13	2.0
M646T868_pos	646.3355	868	3							HMDB0013055	droxy-9-deoxy-delta12-PGD2)-glu	C30H51N3O10S	2.0
M651T894_pos	651.3756	894	3							HMDB0034635	Esculentoside E	C35H54O11	2.6
M683T908_pos	683.3657	908	3							HMDB0032821	Corchorusoside B	C35H54O13	2.9
M692T1023_pos	691.5511	1023	3							HMDB0296095	0/20:4(6Z,8E,10E,14Z)-2OH(5S,12	C42H74O7	0.5
M757T1065_pos	756.6136	1065	3						Alkaloids				
M841T978_pos	840.6002	978	3						Terpenoids				
M87T419_neg	87.0452	419	3							HMDB0000039	Butyric acid	C4H8O2	0.1
M115T803_neg	115.0765	803	3							HMDB0000535	Caproic acid	C6H12O2	0.7
M115T664_neg	115.0765	664	3							HMDB0000535	Caproic acid	C6H12O2	0.7
M125T376_neg	125.0357	376	3							HMDB0000262	Thymine	C5H6N2O2	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M471T788_pos	471.2164	788	3	1.37E-05	0.66	TRUE	1.56E-01	1.15	FALSE	1.08E-07	1.58	TRUE	7.29E-01	1.08	FALSE
M472T955_pos	472.3425	955	3	2.86E-07	3.01	TRUE	1.81E-03	0.58	TRUE	7.70E-01	0.95	FALSE	5.75E-01	1.13	FALSE
M473T951_pos	473.3265	951	3	5.65E-12	2.39	TRUE	3.06E-06	0.59	TRUE	8.51E-02	1.18	FALSE	1.59E-01	0.73	FALSE
M473T1011_pos	473.3617	1011	3	1.04E-05	1.59	TRUE	7.93E-04	0.67	FALSE	3.22E-01	1.09	FALSE	3.62E-02	1.76	TRUE
M475T786_pos	475.2552	786	3	5.78E-18	0.60	TRUE	2.40E-03	1.18	FALSE	1.45E-19	1.60	TRUE	7.80E-01	0.98	FALSE
M475T961_pos	475.3421	961	3	1.27E-11	1.56	TRUE	1.08E-02	0.85	FALSE	5.22E-02	1.11	FALSE	1.56E-03	1.57	TRUE
M482T1073_pos	482.3228	1073	3	2.27E-02	1.61	TRUE	3.27E-01	0.81	FALSE	9.12E-04	1.85	TRUE	9.78E-01	1.01	FALSE
M484T689_pos	484.2445	689	3	4.37E-20	0.48	TRUE	6.42E-01	0.97	FALSE	9.09E-12	1.55	TRUE	1.11E-01	1.26	FALSE
M490T130_pos	490.1770	130	3	9.86E-35	0.14	TRUE	4.75E-01	1.08	FALSE	3.23E-06	1.53	TRUE	2.92E-01	1.80	FALSE
M490T794_pos	490.3528	794	3	4.18E-03	2.19	TRUE	4.15E-01	0.79	FALSE	6.57E-03	1.89	TRUE	8.44E-01	0.91	FALSE
M493T704_pos	493.2430	704	3	7.66E-06	3.93	TRUE	7.63E-03	0.62	TRUE	1.72E-01	0.73	FALSE	7.57E-01	0.93	FALSE
M500T866_pos	500.2758	866	3	2.12E-08	0.59	TRUE	2.39E-02	1.23	FALSE	1.46E-07	1.52	TRUE	5.11E-01	1.06	FALSE
M505T410_pos	505.1794	410	3	6.02E-22	0.03	TRUE	8.69E-01	0.97	FALSE	2.37E-09	2.75	TRUE	6.10E-01	0.93	FALSE
M506T960_pos	506.3488	960	3	7.84E-03	1.19	FALSE	1.43E-02	1.18	FALSE	1.78E-12	1.54	TRUE	3.89E-03	0.51	TRUE
M512T714_pos	512.2794	714	3	5.39E-04	0.78	FALSE	6.56E-09	1.53	TRUE	5.14E-10	1.50	TRUE	1.30E-01	1.16	FALSE
M512T690_pos	512.3030	690	3	2.95E-14	1.51	TRUE	5.65E-01	0.97	FALSE	4.48E-20	1.57	TRUE	9.79E-02	0.89	FALSE
M518T1022_pos	518.3240	1022	3	1.53E-02	2.59	TRUE	6.94E-04	0.23	TRUE	4.78E-01	0.80	FALSE	8.13E-01	1.30	FALSE
M520T821_pos	520.3634	821	3	2.85E-07	2.22	TRUE	4.90E-01	0.91	FALSE	8.42E-06	1.80	TRUE	4.07E-01	1.07	FALSE
M545T816_pos	545.3118	816	3	2.10E-08	1.73	TRUE	5.83E-02	0.85	FALSE	3.12E-08	1.59	TRUE	5.77E-01	1.06	FALSE
M551T984_pos	551.3594	984	3	6.05E-01	0.93	FALSE	3.82E-05	1.83	TRUE	7.19E-03	1.39	FALSE	1.10E-02	1.70	TRUE
M556T483_pos	556.1559	483	3	1.26E-18	0.03	TRUE	8.26E-01	0.96	FALSE	3.49E-04	1.88	TRUE	1.85E-02	1.38	FALSE
M587T870_pos	587.2868	870	3	1.62E-06	1.87	TRUE	6.83E-01	0.96	FALSE	7.23E-09	1.96	TRUE	4.29E-01	0.91	FALSE
M594T698_pos	594.4003	698	3	2.29E-02	6.78	TRUE	6.80E-03	0.15	TRUE	9.70E-01	1.02	FALSE	4.63E-01	0.37	FALSE
M624T786_pos	624.3749	786	3	6.78E-03	1.87	TRUE	3.49E-06	0.32	TRUE	4.96E-01	0.88	FALSE	8.03E-01	0.95	FALSE
M643T868_pos	643.3337	868	3	3.66E-01	0.92	FALSE	9.36E-01	1.01	FALSE	4.59E-07	1.52	TRUE	1.54E-02	1.60	TRUE
M646T868_pos	646.3355	868	3	1.93E-12	0.41	TRUE	1.14E-01	1.20	FALSE	1.45E-05	1.56	TRUE	2.68E-01	1.12	FALSE
M651T894_pos	651.3756	894	3	1.03E-01	1.46	FALSE	5.50E-01	0.89	FALSE	8.04E-06	2.68	TRUE	4.46E-02	0.20	TRUE
M683T908_pos	683.3657	908	3	1.22E-16	0.31	TRUE	2.20E-03	1.47	FALSE	2.07E-10	2.03	TRUE	8.53E-01	1.04	FALSE
M692T1023_pos	691.5511	1023	3	8.07E-10	2.17	TRUE	1.63E-08	0.48	TRUE	8.18E-05	1.50	FALSE	3.71E-01	0.80	FALSE
M757T1065_pos	756.6136	1065	3	3.63E-04	3.40	TRUE	1.61E-03	0.43	TRUE	1.03E-01	0.65	FALSE	8.81E-01	1.04	FALSE
M841T978_pos	840.6002	978	3	9.09E-03	2.43	TRUE	2.52E-02	0.43	TRUE	2.08E-01	0.70	FALSE	6.59E-01	1.28	FALSE
M87T419_neg	87.0452	419	3	6.62E-08	0.56	TRUE	7.86E-01	1.03	FALSE	3.19E-11	1.90	TRUE	2.46E-01	0.89	FALSE
M115T803_neg	115.0765	803	3	4.37E-15	2.33	TRUE	4.28E-01	1.08	FALSE	6.52E-07	0.65	TRUE	4.48E-01	0.85	FALSE
M115T664_neg	115.0765	664	3	4.57E-28	0.55	TRUE	9.03E-02	1.08	FALSE	3.86E-29	1.71	TRUE	2.81E-04	0.72	FALSE
M125T376_neg	125.0357	376	3	5.14E-25	0.11	TRUE	4.74E-02	1.32	FALSE	2.14E-10	2.29	TRUE	3.23E-01	1.42	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M129T441_neg	129.0558	441	3							HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	0.7
M131T418_neg	131.0351	418	3						Fatty acids	HMDB0000576	Monoethyl malonic acid	C5H8O4	0.7
M131T464_neg	131.0351	464	3						Fatty acids	HMDB0000576	Monoethyl malonic acid	C5H8O4	0.7
M131T656_neg	131.0715	656	3						Fatty acids	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.7
M135T657_neg	135.0452	657	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.7
M136T724_neg	136.0769	724	3							HMDB0000306	Tyramine	C8H11NO	0.7
M145T574_neg	145.0507	574	3						Fatty acids	HMDB0000422	2-Methylglutaric acid	C6H10O4	0.5
M146T487_neg	146.0248	487	3							HMDB0006779	Indole-5,6-quinone	C8H5NO2	0.6
M147T368_neg	147.0300	368	3							HMDB0000426	Citramalic acid	C5H8O5	0.6
M147T438_neg	147.0453	438	3							HMDB0000567	Cinnamic acid	C9H8O2	0.8
M155T441_neg	155.0351	441	3							HMDB0029610	Ascladiol	C7H8O4	0.6
M157T332_neg	157.0144	332	3							HMDB0031210	Zymonic acid	C6H6O5	0.7
M159T664_neg	159.0663	664	3						Fatty acids	HMDB0000555	3-Methyladipic acid	C7H12O4	0.4
M164T439_neg	164.0718	439	3						Amino acids and Peptides	HMDB0000159	L-Phenylalanine	C9H11NO2	0.5
M165T551_neg	165.0559	551	3							HMDB0000375	3-(3-Hydroxyphenyl)propanoic acid	C9H10O3	0.8
M175T589_neg	175.0613	589	3						Fatty acids	HMDB0000402	2-Isopropylmalic acid	C7H12O5	0.3
M177T381_neg	177.0406	381	3							HMDB0000150	Gluconolactone	C6H10O6	0.5
M183T923_neg	183.1391	923	3							HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	0.2
M184T741_neg	184.0981	741	3							HMDB0006348	Pseudoecgonine	C9H15NO3	0.8
M185T923_neg	185.1184	923	3							HMDB0010724	3-Oxodecanoic acid	C10H18O3	0.3
M187T925_neg	187.1340	925	3							HMDB0002203	3-Hydroxycapric acid	C10H20O3	0.3
M189T685_neg	189.0769	685	3						Fatty acids	HMDB0000325	3-Hydroxysuberic acid	C8H14O5	0.2
M189T563_neg	189.0769	563	3							HMDB0000325	3-Hydroxysuberic acid	C8H14O5	0.4
M196T795_neg	196.0616	795	3						Alkaloids	HMDB0000181	L-Dopa	C9H11NO4	0.2
M199T1033_neg	199.1704	1033	3						Fatty acids	HMDB0000638	Dodecanoic acid	C12H24O2	0.1
M201T481_neg	200.9864	481	3							HMDB0240374	Benzoic acid sulfate	C7H6O5S	0.3
M201T868_neg	201.1497	868	3							HMDB0032443	3-Hydroxynonyl acetate	C11H22O3	0.3
M206T487_neg	206.0459	487	3						Alkaloids	HMDB0000978	4-Aminophenyl)-2,4-dioxobutanoic	C10H9NO4	0.1
M211T489_neg	211.0252	489	3						Shikimates and Phenylpropanoids				
M214T756_neg	214.1449	756	3							HMDB0013279	N-Nonanoylglycine	C11H21NO3	0.3
M217T715_neg	217.1082	715	3						Fatty acids	HMDB0000350	3-Hydroxysebacic acid	C10H18O5	0.2
M224T569_neg	224.0565	569	3							HMDB0037264	4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	0.2
M226T741_neg	226.1085	741	3						Fatty acids				

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M129T441_neg	129.0558	441	3	2.92E-18	0.64	TRUE	3.11E-02	1.11	FALSE	1.45E-32	1.81	TRUE	5.53E-01	1.02	FALSE
M131T418_neg	131.0351	418	3	1.03E-08	0.55	TRUE	9.62E-01	1.00	FALSE	2.09E-11	1.86	TRUE	2.59E-01	0.88	FALSE
M131T464_neg	131.0351	464	3	1.28E-31	0.50	TRUE	4.58E-02	1.10	FALSE	1.67E-29	1.76	TRUE	2.43E-04	0.79	FALSE
M131T656_neg	131.0715	656	3	7.17E-01	0.85	FALSE	7.87E-05	30.66	TRUE	3.89E-03	3.63	TRUE	6.66E-02	1.45	FALSE
M135T657_neg	135.0452	657	3	4.93E-19	0.63	TRUE	9.06E-02	1.09	FALSE	2.09E-30	1.76	TRUE	1.71E-01	1.15	FALSE
M136T724_neg	136.0769	724	3	1.72E-03	1.52	TRUE	5.91E-05	1.72	TRUE	2.07E-03	1.43	FALSE	1.14E-01	1.42	FALSE
M145T574_neg	145.0507	574	3	6.98E-20	0.55	TRUE	1.93E-01	1.08	FALSE	2.24E-17	1.61	TRUE	8.25E-01	0.96	FALSE
M146T487_neg	146.0248	487	3	1.69E-01	0.84	FALSE	4.06E-01	1.12	FALSE	9.05E-11	2.19	TRUE	9.60E-03	0.38	TRUE
M147T368_neg	147.0300	368	3	1.83E-09	0.63	TRUE	1.55E-02	1.20	FALSE	6.82E-22	2.04	TRUE	1.13E-01	1.08	FALSE
M147T438_neg	147.0453	438	3	1.44E-42	0.20	TRUE	2.11E-06	1.45	FALSE	1.29E-14	1.74	TRUE	6.81E-02	1.28	FALSE
M155T441_neg	155.0351	441	3	2.25E-17	0.63	TRUE	4.10E-02	1.11	FALSE	1.07E-34	1.92	TRUE	7.93E-01	0.98	FALSE
M157T332_neg	157.0144	332	3	1.31E-54	0.09	TRUE	7.23E-01	1.03	FALSE	3.35E-02	1.15	FALSE	1.31E-02	0.62	TRUE
M159T664_neg	159.0663	664	3	3.97E-29	0.54	TRUE	6.75E-02	1.09	FALSE	1.84E-29	1.71	TRUE	5.24E-04	0.73	FALSE
M164T439_neg	164.0718	439	3	4.13E-40	0.20	TRUE	2.06E-06	1.49	FALSE	3.74E-14	1.78	TRUE	8.33E-02	1.30	FALSE
M165T551_neg	165.0559	551	3	4.92E-25	0.37	TRUE	2.59E-01	1.10	FALSE	1.89E-10	1.58	TRUE	1.30E-01	0.91	FALSE
M175T589_neg	175.0613	589	3	3.33E-14	0.52	TRUE	3.69E-02	1.19	FALSE	7.77E-15	1.80	TRUE	1.18E-01	0.85	FALSE
M177T381_neg	177.0406	381	3	1.02E-56	0.28	TRUE	1.71E-01	1.07	FALSE	4.58E-22	1.62	TRUE	4.44E-01	0.94	FALSE
M183T923_neg	183.1391	923	3	3.35E-10	0.42	TRUE	2.77E-01	1.15	FALSE	1.41E-07	1.82	TRUE	6.01E-01	0.94	FALSE
M184T741_neg	184.0981	741	3	1.67E-04	0.55	TRUE	5.33E-01	1.11	FALSE	7.11E-02	1.27	FALSE	1.96E-03	1.79	TRUE
M185T923_neg	185.1184	923	3	2.68E-25	0.26	TRUE	7.82E-01	1.03	FALSE	6.91E-12	0.52	TRUE	8.80E-01	0.93	FALSE
M187T925_neg	187.1340	925	3	2.48E-16	1.58	TRUE	4.67E-05	0.81	FALSE	1.73E-17	1.51	TRUE	3.51E-01	1.06	FALSE
M189T685_neg	189.0769	685	3	6.93E-30	0.28	TRUE	4.56E-02	1.19	FALSE	1.46E-13	1.81	TRUE	4.75E-02	0.67	FALSE
M189T563_neg	189.0769	563	3	3.34E-10	0.58	TRUE	2.15E-01	1.11	FALSE	2.37E-08	1.51	TRUE	8.89E-01	0.99	FALSE
M196T795_neg	196.0616	795	3	1.05E-31	0.50	TRUE	8.04E-02	1.09	FALSE	2.18E-29	1.75	TRUE	3.25E-03	0.81	FALSE
M199T1033_neg	199.1704	1033	3	9.32E-04	1.69	TRUE	8.16E-05	0.49	TRUE	4.81E-01	0.91	FALSE	8.19E-01	1.15	FALSE
M201T481_neg	200.9864	481	3	1.65E-40	0.40	TRUE	4.97E-01	1.04	FALSE	1.57E-20	1.60	TRUE	5.60E-01	0.95	FALSE
M201T868_neg	201.1497	868	3	1.26E-12	2.16	TRUE	6.89E-08	0.51	TRUE	6.11E-01	0.96	FALSE	1.95E-01	0.72	FALSE
M206T487_neg	206.0459	487	3	2.69E-01	0.92	FALSE	9.18E-01	1.01	FALSE	8.01E-20	2.09	TRUE	1.44E-03	0.56	TRUE
M211T489_neg	211.0252	489	3	7.29E-16	0.50	TRUE	6.95E-02	1.16	FALSE	2.17E-14	1.75	TRUE	9.20E-01	1.01	FALSE
M214T756_neg	214.1449	756	3	5.77E-03	3.42	TRUE	6.97E-01	1.15	FALSE	4.42E-02	0.49	TRUE	4.92E-01	1.03	FALSE
M217T715_neg	217.1082	715	3	6.33E-13	0.63	TRUE	8.64E-01	1.01	FALSE	8.82E-21	1.76	TRUE	9.27E-01	1.01	FALSE
M224T569_neg	224.0565	569	3	1.46E-19	0.52	TRUE	7.31E-01	1.02	FALSE	1.59E-25	1.99	TRUE	9.86E-01	1.00	FALSE
M226T741_neg	226.1085	741	3	7.31E-06	0.49	TRUE	5.21E-01	1.11	FALSE	4.44E-02	1.30	FALSE	2.11E-03	1.91	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M227T768_neg	227.0351	768	3						Shikimates and Phenylpropanoids	HMDB0013695	Urolithin A	C13H8O4	0.3
M227T383_neg	227.0674	383	3						Carbohydrates	HMDB0000012	Deoxyuridine	C9H12N2O5	0.1
M227T923_neg	227.1289	923	3						Fatty acids	HMDB0000933	Traumatic acid	C12H20O4	0.1
M239T878_neg	239.0925	878	3						Fatty acids	HMDB0030254	,4,5-Trimethoxyphenyl)propanoic	C12H16O5	0.1
M240T473_neg	240.0514	473	3							HMDB0037548	y-6,7-dimethoxy-2H-1,4-benzoxaz	C10H11NO6	0.2
M241T449_neg	241.0830	449	3							HMDB0000273	Thymidine	C10H14N2O5	0.1
M243T349_neg	243.0623	349	3						Carbohydrates	HMDB0000296	Uridine	C9H12N2O6	0.1
M246T490_neg	246.0442	490	3						Fatty acids	HMDB0252436	Forchlorfenuron	C12H10ClN3O	0.9
M251T412_neg	251.0785	412	3						Carbohydrates	HMDB0000071	Deoxyinosine	C10H12N4O4	0.2
M254T510_neg	254.0671	510	3							HMDB0304540	beta-D-ribosylnicotinate	C11H13NO6	0.2
M257T818_neg	257.0820	818	3						Shikimates and Phenylpropanoids	HMDB0004629	O-Desmethylangolensin	C15H14O4	0.1
M266T387_neg	266.0895	387	3						Carbohydrates	HMDB0000050	Adenosine	C10H13N5O4	0.2
M267T949_neg	267.1238	949	3							HMDB0038935	Kamahine C	C14H20O5	0.1
M273T867_neg	273.1611	867	3						Alkaloids				
M275T738_neg	275.1402	738	3						Alkaloids				
M276T479_neg	276.1089	479	3							HMDB0038493	N-(1-Deoxy-1-fructosyl)proline	C11H19NO7	0.0
M277T1068_neg	277.2173	1068	3							HMDB0001388	alpha-Linolenic acid	C18H30O2	0.1
M283T869_neg	283.1187	869	3							HMDB0029819	Phenylethyl beta-D-glucopyranosi	C14H20O6	0.2
M287T448_neg	287.0883	448	3						Carbohydrates	HMDB0031768	Iprobenfos	C13H21O3PS	2.4
M289T349_neg	289.0678	349	3						Carbohydrates	HMDB0252808	Glutamic acid glutamate	C10H14N2O8	0.2
M299T487_neg	299.0344	487	3						Amino acids and Peptides				
M299T1039_neg	299.2591	1039	3						Fatty acids	HMDB0010737	(R)-3-Hydroxy-Octadecanoic acid	C18H36O3	0.3
M301T674_neg	301.0718	674	3						Shikimates and Phenylpropanoids	HMDB0005782	Hesperetin	C16H14O6	0.1
M301T1066_neg	301.2173	1066	3							HMDB0001999	Eicosapentaenoic acid	C20H30O2	0.1
M307T983_neg	307.1915	983	3						Fatty acids	HMDB0029852	Methylgingerol	C18H28O4	0.1
M308T539_neg	308.0777	539	3							HMDB0010319	Indoxyl glucuronide	C14H15NO7	0.4
M309T524_neg	309.1457	524	3							HMDB0250969	Delgocitini	C16H18N6O	4.1
M311T1017_2_neg	311.2228	1017	3						Fatty acids	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	0.0
M313T845_neg	313.1656	845	3							HMDB0029848	(-)-trans-Carveol glucoside	C16H26O6	0.1
M313T1034_neg	313.2384	1034	3						Fatty acids	HMDB0000782	Octadecanedioic acid	C18H34O4	0.0
M323T913_neg	323.2227	913	3						Fatty acids	HMDB0031007	etoxy-2-hydroxy-16-heptadecyn-4	C19H32O4	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M227T768_neg	227.0351	768	3	1.09E-05	2.21	TRUE	2.95E-03	0.57	TRUE	9.69E-01	0.99	FALSE	1.21E-01	1.45	FALSE
M227T383_neg	227.0674	383	3	1.28E-33	0.14	TRUE	2.45E-03	1.38	FALSE	3.75E-18	2.48	TRUE	4.85E-01	1.09	FALSE
M227T923_neg	227.1289	923	3	8.07E-11	0.43	TRUE	3.80E-01	1.11	FALSE	6.02E-08	1.80	TRUE	3.75E-01	0.87	FALSE
M239T878_neg	239.0925	878	3	2.58E-17	0.56	TRUE	5.69E-05	1.30	FALSE	1.59E-15	1.59	TRUE	6.49E-03	1.29	FALSE
M240T473_neg	240.0514	473	3	4.42E-19	0.36	TRUE	4.98E-01	1.07	FALSE	7.65E-09	1.67	TRUE	3.88E-01	0.89	FALSE
M241T449_neg	241.0830	449	3	7.08E-41	0.26	TRUE	3.42E-01	1.07	FALSE	6.42E-32	2.47	TRUE	6.46E-01	1.06	FALSE
M243T349_neg	243.0623	349	3	5.44E-11	0.59	TRUE	7.57E-01	1.03	FALSE	3.12E-18	1.93	TRUE	7.67E-01	1.04	FALSE
M246T490_neg	246.0442	490	3	1.05E-19	0.52	TRUE	2.46E-02	1.16	FALSE	2.24E-23	1.89	TRUE	1.10E-01	1.12	FALSE
M251T412_neg	251.0785	412	3	4.07E-36	0.04	TRUE	4.14E-01	1.10	FALSE	1.89E-12	2.25	TRUE	1.00E+00	1.00	FALSE
M254T510_neg	254.0671	510	3	6.75E-15	0.50	TRUE	2.68E-01	1.10	FALSE	8.31E-18	1.97	TRUE	6.62E-01	0.95	FALSE
M257T818_neg	257.0820	818	3	3.06E-08	3.10	TRUE	2.55E-03	0.56	TRUE	3.89E-01	1.14	FALSE	9.40E-01	1.01	FALSE
M266T387_neg	266.0895	387	3	1.44E-18	0.38	TRUE	2.10E-02	0.79	FALSE	3.13E-23	2.65	TRUE	1.24E-01	1.22	FALSE
M267T949_neg	267.1238	949	3	3.71E-25	0.57	TRUE	2.38E-06	1.26	FALSE	4.85E-28	1.71	TRUE	1.90E-03	1.24	FALSE
M273T867_neg	273.1611	867	3	7.61E-18	2.54	TRUE	2.01E-07	0.65	TRUE	1.18E-02	1.23	FALSE	5.05E-02	1.21	FALSE
M275T738_neg	275.1402	738	3	7.95E-05	0.76	FALSE	9.65E-04	1.26	FALSE	1.02E-14	1.66	TRUE	6.23E-05	0.64	TRUE
M276T479_neg	276.1089	479	3	1.22E-26	0.39	TRUE	7.36E-01	1.03	FALSE	1.26E-16	1.78	TRUE	9.31E-01	0.98	FALSE
M277T1068_neg	277.2173	1068	3	4.24E-01	1.22	FALSE	7.80E-04	0.31	TRUE	1.24E-02	1.76	TRUE	3.88E-01	0.57	FALSE
M283T869_neg	283.1187	869	3	1.07E-29	0.53	TRUE	1.07E-03	1.17	FALSE	1.60E-35	1.87	TRUE	2.67E-01	0.94	FALSE
M287T448_neg	287.0883	448	3	1.40E-39	0.25	TRUE	3.66E-01	1.07	FALSE	1.42E-30	2.51	TRUE	8.44E-01	1.03	FALSE
M289T349_neg	289.0678	349	3	2.95E-11	0.60	TRUE	7.52E-01	1.03	FALSE	5.01E-19	1.89	TRUE	6.10E-01	1.06	FALSE
M299T487_neg	299.0344	487	3	1.10E-12	0.52	TRUE	5.02E-01	1.06	FALSE	6.38E-16	1.93	TRUE	2.41E-01	0.86	FALSE
M299T1039_neg	299.2591	1039	3	1.89E-12	1.99	TRUE	1.88E-08	0.57	TRUE	5.61E-01	0.96	FALSE	6.05E-02	1.30	FALSE
M301T674_neg	301.0718	674	3	4.46E-29	0.48	TRUE	6.01E-02	1.11	FALSE	1.15E-28	1.86	TRUE	1.09E-01	1.14	FALSE
M301T1066_neg	301.2173	1066	3	2.59E-03	1.66	TRUE	8.89E-03	0.64	TRUE	9.63E-01	1.01	FALSE	4.47E-01	1.43	FALSE
M307T983_neg	307.1915	983	3	1.96E-07	1.70	TRUE	7.83E-01	0.97	FALSE	8.95E-07	1.54	TRUE	6.71E-01	1.06	FALSE
M308T539_neg	308.0777	539	3	2.60E-01	0.93	FALSE	2.05E-11	1.58	TRUE	3.06E-13	1.57	TRUE	1.08E-01	1.13	FALSE
M309T524_neg	309.1457	524	3	2.68E-18	0.61	TRUE	7.95E-04	1.19	FALSE	2.05E-35	2.03	TRUE	2.39E-01	1.06	FALSE
M311T1017_2_neg	311.2228	1017	3	3.36E-09	1.59	TRUE	7.99E-01	1.02	FALSE	1.56E-11	1.60	TRUE	5.49E-01	0.96	FALSE
M313T845_neg	313.1656	845	3	1.06E-13	0.62	TRUE	3.48E-02	1.14	FALSE	1.46E-23	1.83	TRUE	3.21E-01	0.93	FALSE
M313T1034_neg	313.2384	1034	3	4.41E-09	2.07	TRUE	2.59E-01	0.87	FALSE	9.64E-12	2.11	TRUE	1.18E-02	1.42	FALSE
M323T913_neg	323.2227	913	3	2.86E-12	7.61	TRUE	3.04E-02	1.48	FALSE	1.82E-01	1.27	FALSE	3.03E-02	0.51	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M327T923_neg	327.0541	923	3							HMDB0033622	Cabbage identification factor 2	C15H12N4O3S	4.9
M327T684_neg	327.0875	684	3							HMDB0029677	Zapotinin	C18H16O6	0.2
M327T1078_neg	327.2330	1078	3						Fatty acids	HMDB0002183	Docosahexaenoic acid	C22H32O2	0.0
M339T1021_neg	339.2176	1021	3							HMDB0302961	2-alpha-Ethoxydihydrophytuberin	C19H32O5	0.3
M343T942_neg	343.1552	942	3							HMDB0031753	yphenoxy)-1-(4-hydroxy-3-methox	C20H24O5	0.3
M345T1044_neg	345.2071	1044	3						Terpenoids	HMDB0000015	Cortexolone	C21H30O4	0.2
M349T986_neg	349.1658	986	3							HMDB0034915	Calonectrin	C19H26O6	0.3
M354T1058_neg	354.2651	1058	3						Fatty acids	HMDB0241309	Tridec-3-enoylcarnitine	C20H37NO4	0.3
M359T823_neg	359.1712	823	3						Polyketides				
M363T772_neg	363.1562	772	3						Alkaloids				
M373T841_neg	373.1866	841	3						Fatty acids	HMDB0029782	6-Epi-7-isocucurbic acid glucoside	C18H30O8	0.4
M375T620_neg	375.1311	620	3							HMDB0000244	Riboflavin	C17H20N4O6	0.3
M387T858_neg	387.2024	858	3						Fatty acids	HMDB0031676	xy-7E-megastigmene-3a,9e-diol 3	C19H32O8	0.1
M399T1039_neg	399.1844	1039	3						Fatty acids				
M407T982_neg	407.1169	982	3							HMDB0245109	nethylsulfonyloxyphenyl)ethoxy]p	C20H24O7S	0.4
M433T1015_neg	433.3324	1015	3							HMDB0000359	pha,7alpha-Dihydroxycoprostanic a	C27H46O4	0.1
M448T989_neg	448.3077	989	3						Terpenoids	HMDB0000631	Deoxycholic acid glycine conjugate	C26H43NO5	2.0
M471T643_neg	471.2252	643	3							HMDB0254095	Linagliptin	C25H28N8O2	2.2
M475T1037_neg	475.3431	1037	3						Polyketides	HMDB0034079	Homodolichosterone	C29H48O5	0.5
M491T1016_neg	491.3378	1016	3							HMDB0033907	Homodolicholide	C29H48O6	0.1
M540T1049_neg	540.3310	1049	3						Fatty acids				
M550T398_neg	550.1655	398	3						Carbohydrates	HMDB0060904	Haloperidol glucuronide	C27H31ClFNO8	1.0
M583T797_neg	583.1823	797	3						Polyketides	HMDB0249055	Benzoylpaeoniflorin	C30H32O12	0.3
M589T834_neg	589.3034	834	3						Alkaloids	HMDB0004158	Urobilinogen	C33H42N4O6	0.4
M615T982_neg	615.3902	982	3							HMDB0244453	-O-Tetradecanoylphorbol 12-aceta	C36H56O8	0.1
M622T1039_neg	621.5078	1039	3						Terpenoids	HMDB0295719	DG(17:0/18:1(12Z)-O(9S,10R)/0:0)	C38H70O6	3.5
M676T1040_neg	675.5567	1040	3							HMDB0296219	DG(19:0/20:3(6,8,11)-OH(5)/0:0)	C42H76O6	0.3
M750T1055_neg	749.5725	1055	3						Terpenoids				
M776T960_neg	775.5155	960	3							HMDB0263673	PA(18:0/PGF1alpha)	C41H77O11P	3.2
M778T958_neg	777.5285	958	3						Terpenoids	HMDB0038065	1,28-Octacosanediol diferulate	C48H74O8	3.3
M785T778_neg	785.4233	778	3						Amino acids and Peptides				
M808T960_neg	807.5419	960	3						Terpenoids	HMDB0268817	PG(18:0/18:1(12Z)-2OH(9,10))	C42H81O12P	3.2
M822T962_neg	821.5573	962	3						Terpenoids	HMDB0271830	PG(i-19:0/18:1(12Z)-2OH(9,10))	C43H83O12P	2.9
M1029T856_neg	1028.5410	856	3							HMDB0115980	DP-DG(20:2(11Z,14Z)/18:2(9Z,12Z	C50H85N3O15P2	2.6
M1049T854_neg	1048.5674	854	3							HMDB0294146	DP-DG(i-20:0/18:1(12Z)-O(9S,10R	C50H89N3O16P2	2.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M327T923_neg	327.0541	923	3	1.34E-12	0.40	TRUE	9.77E-01	1.00	FALSE	2.18E-07	1.71	TRUE	4.15E-01	0.83	FALSE
M327T684_neg	327.0875	684	3	4.94E-26	0.45	TRUE	2.64E-01	1.08	FALSE	2.98E-20	1.77	TRUE	1.11E-01	0.83	FALSE
M327T1078_neg	327.2330	1078	3	1.41E-02	1.60	TRUE	8.84E-03	0.62	TRUE	8.82E-01	0.98	FALSE	6.50E-01	1.26	FALSE
M339T1021_neg	339.2176	1021	3	2.11E-07	1.64	TRUE	4.97E-03	0.76	FALSE	1.55E-07	1.54	TRUE	1.03E-03	1.45	FALSE
M343T942_neg	343.1552	942	3	2.23E-06	1.86	TRUE	9.61E-01	1.01	FALSE	6.40E-11	2.19	TRUE	1.33E-02	1.44	FALSE
M345T1044_neg	345.2071	1044	3	9.08E-06	2.05	TRUE	2.86E-02	0.69	FALSE	8.47E-01	1.03	FALSE	1.96E-02	2.11	TRUE
M349T986_neg	349.1658	986	3	2.89E-01	0.90	FALSE	4.67E-01	1.08	FALSE	7.80E-07	1.58	TRUE	7.95E-03	0.46	TRUE
M354T1058_neg	354.2651	1058	3	2.70E-07	0.65	TRUE	9.98E-07	1.54	TRUE	1.02E-03	0.79	FALSE	6.00E-01	1.09	FALSE
M359T823_neg	359.1712	823	3	1.18E-34	0.49	TRUE	2.08E-02	1.12	FALSE	6.33E-29	1.71	TRUE	5.09E-02	0.85	FALSE
M363T772_neg	363.1562	772	3	2.90E-42	0.45	TRUE	2.73E-02	1.11	FALSE	9.61E-24	1.56	TRUE	1.45E-01	1.11	FALSE
M373T841_neg	373.1866	841	3	6.13E-34	0.49	TRUE	3.54E-02	1.11	FALSE	8.69E-35	1.87	TRUE	1.49E-01	0.90	FALSE
M375T620_neg	375.1311	620	3	9.62E-09	0.59	TRUE	3.48E-04	1.41	FALSE	8.13E-24	2.54	TRUE	5.73E-02	1.27	FALSE
M387T858_neg	387.2024	858	3	1.31E-23	0.55	TRUE	2.45E-02	1.13	FALSE	2.29E-28	1.82	TRUE	2.95E-01	0.89	FALSE
M399T1039_neg	399.1844	1039	3	6.53E-12	1.94	TRUE	1.16E-06	0.61	TRUE	6.24E-01	1.04	FALSE	2.20E-03	1.36	FALSE
M407T982_neg	407.1169	982	3	3.95E-08	1.58	TRUE	4.28E-01	1.07	FALSE	9.16E-10	1.56	TRUE	4.13E-01	1.10	FALSE
M433T1015_neg	433.3324	1015	3	3.82E-21	2.14	TRUE	1.36E-10	0.63	TRUE	8.34E-01	0.99	FALSE	1.98E-04	1.33	FALSE
M448T989_neg	448.3077	989	3	1.21E-02	3.12	TRUE	2.38E-02	0.32	TRUE	8.58E-02	0.53	FALSE	3.72E-01	1.75	FALSE
M471T643_neg	471.2252	643	3	1.50E-06	1.93	TRUE	1.81E-03	1.52	TRUE	1.29E-02	1.33	FALSE	2.60E-02	1.39	FALSE
M475T1037_neg	475.3431	1037	3	6.54E-11	2.80	TRUE	6.45E-06	0.54	TRUE	3.49E-01	0.89	FALSE	4.17E-01	1.24	FALSE
M491T1016_neg	491.3378	1016	3	2.06E-15	2.10	TRUE	2.67E-10	0.58	TRUE	9.40E-01	1.01	FALSE	3.67E-01	1.10	FALSE
M540T1049_neg	540.3310	1049	3	1.58E-02	2.31	TRUE	4.77E-02	0.45	TRUE	9.59E-02	0.62	FALSE	7.06E-01	1.19	FALSE
M550T398_neg	550.1655	398	3	2.05E-30	0.06	TRUE	4.88E-01	1.10	FALSE	9.09E-01	1.01	FALSE	4.08E-02	3.44	TRUE
M583T797_neg	583.1823	797	3	5.08E-32	0.23	TRUE	3.35E-01	1.09	FALSE	6.36E-09	1.60	TRUE	2.72E-02	1.34	FALSE
M589T834_neg	589.3034	834	3	1.76E-07	1.80	TRUE	3.82E-03	1.35	FALSE	1.93E-04	1.42	FALSE	1.53E-02	0.61	TRUE
M615T982_neg	615.3902	982	3	3.59E-05	2.97	TRUE	4.15E-01	1.24	FALSE	6.32E-07	3.23	TRUE	7.55E-02	1.61	FALSE
M622T1039_neg	621.5078	1039	3	3.07E-08	3.00	TRUE	3.70E-04	0.50	TRUE	2.04E-02	0.70	FALSE	5.72E-01	1.36	FALSE
M676T1040_neg	675.5567	1040	3	1.09E-11	3.42	TRUE	3.49E-08	0.39	TRUE	6.64E-01	0.94	FALSE	1.45E-01	1.42	FALSE
M750T1055_neg	749.5725	1055	3	4.10E-10	1.92	TRUE	1.05E-02	0.77	FALSE	2.74E-08	1.64	TRUE	6.48E-03	1.44	FALSE
M776T960_neg	775.5155	960	3	1.44E-12	1.85	TRUE	1.91E-03	1.29	FALSE	1.42E-25	2.43	TRUE	5.13E-02	0.70	FALSE
M778T958_neg	777.5285	958	3	4.21E-14	1.68	TRUE	1.53E-01	1.10	FALSE	5.96E-21	1.80	TRUE	3.65E-02	0.76	FALSE
M785T778_neg	785.4233	778	3	4.72E-03	1.70	TRUE	8.89E-01	0.98	FALSE	1.59E-04	1.87	TRUE	1.69E-01	1.16	FALSE
M808T960_neg	807.5419	960	3	7.58E-12	1.88	TRUE	5.25E-03	1.28	FALSE	1.33E-24	2.53	TRUE	7.72E-02	0.71	FALSE
M822T962_neg	821.5573	962	3	4.99E-08	2.06	TRUE	2.84E-02	1.32	FALSE	5.68E-14	2.52	TRUE	6.16E-01	0.93	FALSE
M1029T856_neg	1028.5410	856	3	2.96E-14	3.13	TRUE	5.31E-01	1.09	FALSE	2.91E-07	1.82	TRUE	3.06E-01	1.17	FALSE
M1049T854_neg	1048.5674	854	3	2.63E-12	2.59	TRUE	8.63E-01	0.98	FALSE	6.37E-08	1.82	TRUE	4.97E-01	1.09	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M71T526_neg	71.0502	526	3							HMDB0000246	Tetrahydrofuran	C4H8O	0.3
M73T309_neg	73.0295	309	3							HMDB0244090	1,2-Dioxolane	C3H6O2	0.3
M85T441_neg	85.0659	441	3							HMDB0006478	Isovaleraldehyde	C5H10O	0.0
M85T656_neg	85.0659	656	3							HMDB0006478	Isovaleraldehyde	C5H10O	0.1
M87T464_neg	87.0452	464	3							HMDB0000039	Butyric acid	C4H8O2	0.0
M91T466_neg	90.9859	466	3							HMDB0254464	mercaptoacetic acid	C2H4O2S	0.2
M92T489_neg	92.0506	489	3							HMDB0003012	Aniline	C6H7N	0.1
M92T437_neg	92.0506	437	3							HMDB0003012	Aniline	C6H7N	0.1
M93T191_neg	93.0458	191	3							HMDB0033112	Methylpyrazine	C5H6N2	0.1
M97T453_neg	97.0659	453	3							HMDB0003315	Cyclohexanone	C6H10O	0.4
M101T592_neg	101.0608	592	3							HMDB0000718	Isovaleric acid	C5H10O2	0.3
M102T117_neg	102.0560	117	3							HMDB0000092	Dimethylglycine	C4H9NO2	0.2
M110T403_neg	110.0248	403	3							HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	0.3
M111T441_neg	111.0452	441	3							HMDB0001164	trans-1,2-Dihydrobenzene-1,2-dio	C6H8O2	0.3
M113T463_neg	113.0245	463	3							HMDB0031859	Norfuraneol	C5H6O3	0.6
M115T517_neg	115.0037	517	3							HMDB0000134	Fumaric acid	C4H4O4	0.5
M115T473_neg	115.0038	473	3							HMDB0000134	Fumaric acid	C4H4O4	0.8
M117T315_neg	117.0194	315	3							HMDB0000202	Methylmalonic acid	C4H6O4	0.6
M117T499_neg	117.0558	499	3						Fatty acids	HMDB0000351	3R)-3-Hydroxy-2-methylbutanoic a	C5H10O3	0.7
M119T674_neg	119.0503	674	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.7
M121T551_neg	121.0661	551	3							HMDB0029306	4-Ethylphenol	C8H10O	1.3
M122T436_neg	122.0612	436	3							HMDB0029300	p-Anisidine	C7H9NO	0.4
M124T471_neg	124.0405	471	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.9
M126T582_neg	126.0020	582	3							HMDB0256222	Penem	C5H5NOS	0.7
M128T118_neg	128.0354	118	3							HMDB0000267	Pyroglutamic acid	C5H7NO3	0.5
M129T212_neg	129.0194	212	3							HMDB0000620	Glutaconic acid	C5H6O4	0.5
M129T868_neg	129.0922	868	3							HMDB0000666	Heptanoic acid	C7H14O2	0.7
M131T117_neg	131.0827	117	3							HMDB0000214	Ornithine	C5H12N2O2	0.4
M133T153_neg	133.0143	153	3						Fatty acids	HMDB0000156	Malic acid	C4H6O5	0.4
M134T176_neg	134.0473	176	3							HMDB0000034	Adenine	C5H5N5	0.6
M134T487_neg	134.0612	487	3							HMDB0001250	N-Acetylarylamine	C8H9NO	0.7
M135T598_neg	135.0565	598	3						Alkaloids	HMDB0003152	N-Methylnicotinamide	C7H8N2O	0.6
M136T490_neg	136.0405	490	3							HMDB0000875	Trigonelline	C7H7NO2	0.5
M137T441_neg	137.0245	441	3							HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.7
M137T490_neg	137.0437	490	3							HMDB0031314	Benzyl methyl sulfide	C8H10S	4.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M71T526_neg	71.0502	526	3	1.08E-01	1.29	FALSE	1.76E-05	2.08	TRUE	1.78E-05	1.87	TRUE	6.61E-01	1.04	FALSE
M73T309_neg	73.0295	309	3	2.31E-18	0.40	TRUE	5.36E-02	1.20	FALSE	8.68E-08	1.55	TRUE	6.83E-01	1.10	FALSE
M85T441_neg	85.0659	441	3	2.00E-16	0.57	TRUE	7.83E-02	1.12	FALSE	7.12E-31	2.14	TRUE	3.75E-01	1.06	FALSE
M85T656_neg	85.0659	656	3	5.01E-01	0.74	FALSE	1.08E-04	28.17	TRUE	3.50E-03	3.77	TRUE	5.20E-01	1.22	FALSE
M87T464_neg	87.0452	464	3	1.07E-32	0.48	TRUE	6.73E-02	1.10	FALSE	5.90E-28	1.76	TRUE	3.82E-05	0.74	FALSE
M91T466_neg	90.9859	466	3	7.16E-29	0.45	TRUE	9.62E-04	1.22	FALSE	7.68E-33	2.12	TRUE	3.89E-01	0.94	FALSE
M92T489_neg	92.0506	489	3	2.28E-07	0.43	TRUE	6.47E-01	1.07	FALSE	1.17E-05	1.81	TRUE	6.70E-01	0.97	FALSE
M92T437_neg	92.0506	437	3	4.46E-09	0.37	TRUE	6.98E-01	1.06	FALSE	9.39E-06	1.84	TRUE	9.73E-01	1.01	FALSE
M93T191_neg	93.0458	191	3	1.04E-27	0.13	TRUE	3.66E-04	1.57	TRUE	1.11E-02	1.31	FALSE	5.37E-01	1.31	FALSE
M97T453_neg	97.0659	453	3	5.17E-15	2.16	TRUE	3.46E-15	2.08	TRUE	5.78E-03	0.81	FALSE	8.42E-01	1.03	FALSE
M101T592_neg	101.0608	592	3	1.17E-12	0.62	TRUE	2.45E-02	1.16	FALSE	8.28E-22	1.83	TRUE	2.03E-02	0.79	FALSE
M102T117_neg	102.0560	117	3	2.03E-31	0.38	TRUE	2.63E-02	1.16	FALSE	1.60E-17	1.71	TRUE	1.92E-01	0.82	FALSE
M110T403_neg	110.0248	403	3	9.50E-29	0.21	TRUE	3.19E-01	1.11	FALSE	3.64E-07	1.58	TRUE	7.89E-01	0.95	FALSE
M111T441_neg	111.0452	441	3	1.54E-17	0.62	TRUE	6.91E-02	1.10	FALSE	1.15E-33	1.94	TRUE	6.41E-01	0.98	FALSE
M113T463_neg	113.0245	463	3	1.94E-15	2.23	TRUE	2.19E-01	0.89	FALSE	8.31E-32	0.29	TRUE	6.12E-04	0.79	FALSE
M115T517_neg	115.0037	517	3	6.20E-23	0.50	TRUE	3.16E-01	1.06	FALSE	5.98E-20	1.71	TRUE	3.79E-02	0.84	FALSE
M115T473_neg	115.0038	473	3	2.65E-20	0.43	TRUE	2.79E-01	1.09	FALSE	9.67E-09	1.50	TRUE	5.11E-01	0.92	FALSE
M117T315_neg	117.0194	315	3	7.58E-18	0.36	TRUE	4.35E-02	1.24	FALSE	4.57E-07	1.59	TRUE	2.57E-01	1.71	FALSE
M117T499_neg	117.0558	499	3	8.99E-03	0.64	TRUE	6.85E-01	1.08	FALSE	5.12E-01	1.10	FALSE	8.31E-03	1.59	TRUE
M119T674_neg	119.0503	674	3	3.25E-06	0.41	TRUE	1.99E-01	1.27	FALSE	1.04E-03	1.67	TRUE	8.19E-01	1.08	FALSE
M121T551_neg	121.0661	551	3	1.05E-23	0.38	TRUE	2.32E-01	1.10	FALSE	1.29E-11	1.65	TRUE	3.64E-02	0.81	FALSE
M122T436_neg	122.0612	436	3	6.37E-09	0.41	TRUE	6.34E-01	1.07	FALSE	5.31E-06	1.78	TRUE	5.39E-01	1.08	FALSE
M124T471_neg	124.0405	471	3	1.44E-17	0.51	TRUE	3.46E-01	1.07	FALSE	1.43E-18	1.83	TRUE	5.89E-01	0.93	FALSE
M126T582_neg	126.0020	582	3	2.75E-15	0.47	TRUE	6.28E-03	1.29	FALSE	3.63E-19	2.16	TRUE	7.75E-01	1.06	FALSE
M128T118_neg	128.0354	118	3	6.15E-30	0.39	TRUE	1.28E-01	1.11	FALSE	3.32E-14	1.59	TRUE	1.58E-01	0.81	FALSE
M129T212_neg	129.0194	212	3	6.90E-20	0.34	TRUE	3.24E-04	1.44	FALSE	2.06E-09	1.71	TRUE	1.57E-01	0.87	FALSE
M129T868_neg	129.0922	868	3	3.79E-14	1.86	TRUE	6.50E-01	1.03	FALSE	8.38E-13	0.61	TRUE	4.07E-01	0.85	FALSE
M131T117_neg	131.0827	117	3	2.36E-44	0.13	TRUE	9.57E-04	1.33	FALSE	8.54E-11	1.66	TRUE	3.81E-01	1.07	FALSE
M133T153_neg	133.0143	153	3	4.12E-23	0.03	TRUE	8.46E-01	1.03	FALSE	2.03E-03	1.58	TRUE	5.93E-01	1.15	FALSE
M134T176_neg	134.0473	176	3	2.49E-11	0.42	TRUE	8.65E-01	0.98	FALSE	5.19E-01	0.94	FALSE	1.42E-02	1.56	TRUE
M134T487_neg	134.0612	487	3	1.84E-01	0.85	FALSE	4.06E-01	1.11	FALSE	2.03E-11	2.22	TRUE	8.23E-03	0.39	TRUE
M135T598_neg	135.0565	598	3	1.50E-04	0.63	TRUE	8.87E-01	0.98	FALSE	5.15E-07	1.73	TRUE	9.31E-01	0.98	FALSE
M136T490_neg	136.0405	490	3	9.41E-08	0.43	TRUE	6.70E-01	1.07	FALSE	6.24E-06	1.81	TRUE	1.64E-01	1.14	FALSE
M137T441_neg	137.0245	441	3	4.08E-15	0.65	TRUE	7.97E-02	1.10	FALSE	6.46E-34	1.97	TRUE	2.80E-01	1.06	FALSE
M137T490_neg	137.0437	490	3	7.55E-08	0.44	TRUE	7.01E-01	1.06	FALSE	2.77E-06	1.82	TRUE	6.27E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M141T664_neg	141.0558	664	3							HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.6
M143T707_neg	143.0350	707	3							HMDB0000393	3-Hexenedioic acid	C6H8O4	0.4
M144T687_neg	144.0455	687	3						Alkaloids	HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.4
M144T487_neg	144.0456	487	3							HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.7
M145T717_neg	145.0506	717	3							HMDB0000422	2-Methylglutaric acid	C6H10O4	0.1
M146T578_neg	146.0824	578	3							HMDB0029449	-2-Amino-4-hydroxy-3-methylpent	C6H13NO3	0.9
M147T213_neg	147.0300	213	3						Fatty acids	HMDB0000426	Citramalic acid	C5H8O5	0.4
M149T515_neg	149.0278	515	3							HMDB0037115	1)-2-Hydroxy-4-(methylthio)butar	C5H10O3S	0.2
M149T112_neg	149.0456	112	3							HMDB0000098	D-Xylose	C5H10O5	0.4
M150T747_neg	150.0020	747	3							HMDB0247072	6-Hydroxybenzothiazole	C7H5NOS	0.6
M151T818_neg	151.0401	818	3							HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.4
M152T581_neg	152.0356	581	3							HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	1.7
M154T548_neg	154.0148	548	3							HMDB0002916	4-Nitrocatechol	C6H5NO4	1.6
M154T404_neg	154.0147	404	3							HMDB0002916	4-Nitrocatechol	C6H5NO4	0.7
M157T481_neg	156.9966	481	3							HMDB0248986	Benzenesulfonic acid	C6H6O3S	0.6
M157T954_neg	157.1235	954	3							HMDB0000798	Oenanthic ether	C9H18O2	0.5
M161T670_neg	161.0245	670	3							HMDB0002149	3 Hydroxycoumarin	C9H6O3	0.6
M161T383_neg	161.0456	383	3						Fatty acids	HMDB0000321	2-Hydroxyadipic acid	C6H10O5	0.6
M162T363_neg	162.0425	363	3							HMDB0000802	Pterin	C6H5N5O	2.0
M163T466_neg	163.0071	466	3							HMDB0245081	2-Chloroquinoxaline	C8H5ClN2	1.7
M163T517_neg	163.0071	517	3							HMDB0245081	2-Chloroquinoxaline	C8H5ClN2	1.7
M165T506_neg	165.0306	506	3						Alkaloids	HMDB0245946	3-Nitrobenzaldoxime	C7H6N2O3	0.3
M166T436_neg	166.0511	436	3							HMDB0001545	Pyridoxal	C8H9NO3	0.6
M167T413_neg	167.0827	413	3							HMDB0001431	Pyridoxamine	C8H12N2O2	0.6
M168T553_neg	168.0303	553	3							HMDB0000439	2-Furoylglycine	C7H7NO4	0.7
M170T308_neg	170.0460	308	3							HMDB0012289	Tetrahydrodipicolinate	C7H9NO4	0.5
M171T554_neg	171.0122	554	3							HMDB0059933	p-Toluenesulfonic acid	C7H8O3S	0.5
M174T118_neg	174.0884	118	3						Amino acids and Peptides	HMDB0000904	Citrulline	C6H13N3O3	0.1
M175T201_neg	175.0725	201	3							HMDB0028696	Alanylserine	C6H12N2O4	0.4
M179T595_neg	179.0353	595	3							HMDB0000707	4-Hydroxyphenylpyruvic acid	C9H8O4	1.9
M180T489_neg	180.0304	489	3							HMDB0006954	-3-hydroxy-5-formylpyridine-4-car	C8H7NO4	1.1
M180T357_neg	180.0303	357	3							HMDB0006954	-3-hydroxy-5-formylpyridine-4-car	C8H7NO4	0.5
M180T352_neg	180.0528	352	3							HMDB0006037	8-Hydroxy-7-methylguanine	C6H7N5O2	0.6
M181T666_neg	181.0143	666	3							HMDB0245171	2-Hydroxyterephthalic acid	C8H6O5	0.4
M181T549_neg	181.0143	549	3							HMDB0245171	2-Hydroxyterephthalic acid	C8H6O5	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M141T664_neg	141.0558	664	3	2.27E-26	0.57	TRUE	9.49E-02	1.08	FALSE	1.17E-27	1.66	TRUE	2.52E-03	0.77	FALSE
M143T707_neg	143.0350	707	3	1.80E-04	0.73	FALSE	4.92E-07	1.56	TRUE	3.13E-09	1.58	TRUE	3.74E-03	1.34	FALSE
M144T687_neg	144.0455	687	3	6.95E-01	0.94	FALSE	1.50E-07	2.60	TRUE	6.73E-12	3.26	TRUE	4.92E-01	0.92	FALSE
M144T487_neg	144.0456	487	3	1.75E-01	0.85	FALSE	3.92E-01	1.12	FALSE	3.15E-11	2.16	TRUE	7.86E-03	0.42	TRUE
M145T717_neg	145.0506	717	3	8.04E-02	1.20	FALSE	6.79E-10	2.00	TRUE	5.19E-08	1.70	TRUE	1.88E-01	0.85	FALSE
M146T578_neg	146.0824	578	3	4.36E-01	1.26	FALSE	9.91E-03	2.59	TRUE	1.49E-06	4.41	TRUE	1.58E-01	1.29	FALSE
M147T213_neg	147.0300	213	3	1.57E-29	0.25	TRUE	2.73E-04	1.40	FALSE	8.83E-09	1.60	TRUE	1.87E-01	0.88	FALSE
M149T515_neg	149.0278	515	3	3.50E-01	0.77	FALSE	2.18E-05	4.38	TRUE	8.55E-04	2.41	TRUE	5.87E-01	0.94	FALSE
M149T112_neg	149.0456	112	3	1.99E-01	0.78	FALSE	1.01E-06	2.84	TRUE	1.45E-03	1.73	TRUE	1.39E-01	2.08	FALSE
M150T747_neg	150.0020	747	3	1.20E-01	0.84	FALSE	1.05E-04	0.61	TRUE	2.15E-23	0.29	TRUE	8.75E-02	1.77	FALSE
M151T818_neg	151.0401	818	3	8.20E-10	3.06	TRUE	2.44E-03	0.60	TRUE	9.21E-01	1.01	FALSE	6.92E-01	1.07	FALSE
M152T581_neg	152.0356	581	3	5.56E-29	0.09	TRUE	8.97E-01	0.98	FALSE	9.67E-05	1.56	TRUE	2.94E-01	1.24	FALSE
M154T548_neg	154.0148	548	3	1.61E-32	0.43	TRUE	1.82E-02	1.15	FALSE	9.37E-25	1.80	TRUE	7.32E-01	1.03	FALSE
M154T404_neg	154.0147	404	3	4.81E-40	0.17	TRUE	3.82E-01	1.08	FALSE	2.41E-08	1.54	TRUE	5.52E-01	0.93	FALSE
M157T481_neg	156.9966	481	3	3.07E-44	0.40	TRUE	4.66E-01	1.04	FALSE	2.42E-24	1.62	TRUE	3.09E-01	0.93	FALSE
M157T954_neg	157.1235	954	3	4.53E-01	1.16	FALSE	1.91E-01	1.32	FALSE	3.60E-06	0.42	TRUE	3.91E-03	2.03	TRUE
M161T670_neg	161.0245	670	3	3.43E-02	4.38	TRUE	6.27E-02	3.15	FALSE	3.96E-02	3.28	TRUE	4.69E-01	0.60	FALSE
M161T383_neg	161.0456	383	3	1.25E-11	0.65	TRUE	6.47E-05	1.28	FALSE	1.40E-13	1.51	TRUE	9.11E-01	1.01	FALSE
M162T363_neg	162.0425	363	3	2.37E-16	0.55	TRUE	6.39E-01	1.03	FALSE	6.94E-21	1.85	TRUE	8.42E-01	0.97	FALSE
M163T466_neg	163.0071	466	3	2.00E-22	0.51	TRUE	7.89E-04	1.23	FALSE	5.65E-32	2.15	TRUE	9.29E-03	1.21	FALSE
M163T517_neg	163.0071	517	3	6.19E-27	0.44	TRUE	5.67E-03	1.20	FALSE	8.97E-28	2.07	TRUE	3.54E-04	0.74	FALSE
M165T506_neg	165.0306	506	3	1.62E-03	0.63	TRUE	3.83E-01	0.87	FALSE	9.51E-07	1.91	TRUE	7.31E-01	1.04	FALSE
M166T436_neg	166.0511	436	3	1.79E-09	0.40	TRUE	5.36E-01	1.09	FALSE	5.61E-05	1.64	TRUE	4.76E-01	1.19	FALSE
M167T413_neg	167.0827	413	3	4.13E-08	0.64	TRUE	7.55E-02	1.16	FALSE	6.06E-19	2.00	TRUE	9.75E-01	1.00	FALSE
M168T553_neg	168.0303	553	3	6.70E-20	0.40	TRUE	1.60E-01	1.13	FALSE	9.93E-12	1.72	TRUE	5.60E-01	0.96	FALSE
M170T308_neg	170.0460	308	3	1.91E-08	0.66	TRUE	3.29E-02	1.17	FALSE	8.88E-23	2.04	TRUE	7.65E-01	1.05	FALSE
M171T554_neg	171.0122	554	3	1.37E-01	1.29	FALSE	1.70E-03	0.62	TRUE	3.56E-03	1.55	TRUE	9.31E-02	0.32	FALSE
M174T118_neg	174.0884	118	3	6.54E-48	0.12	TRUE	1.78E-04	1.37	FALSE	6.07E-11	1.64	TRUE	6.81E-01	0.93	FALSE
M175T201_neg	175.0725	201	3	1.29E-09	0.58	TRUE	4.47E-02	1.19	FALSE	8.15E-15	1.89	TRUE	1.15E-01	1.32	FALSE
M179T595_neg	179.0353	595	3	1.35E-02	0.48	TRUE	6.72E-01	1.14	FALSE	1.34E-02	1.90	TRUE	1.27E-01	2.64	FALSE
M180T489_neg	180.0304	489	3	6.75E-07	0.39	TRUE	7.04E-01	1.07	FALSE	1.84E-04	1.79	TRUE	7.80E-01	0.92	FALSE
M180T357_neg	180.0303	357	3	4.57E-11	0.61	TRUE	8.83E-01	1.01	FALSE	1.41E-14	1.67	TRUE	4.22E-01	0.90	FALSE
M180T352_neg	180.0528	352	3	2.94E-18	0.57	TRUE	4.64E-06	1.31	FALSE	4.19E-25	1.84	TRUE	1.46E-01	1.16	FALSE
M181T666_neg	181.0143	666	3	3.99E-08	0.66	TRUE	5.41E-02	1.16	FALSE	2.07E-24	2.14	TRUE	5.75E-01	1.04	FALSE
M181T549_neg	181.0143	549	3	3.16E-36	0.39	TRUE	2.23E-01	1.08	FALSE	6.38E-25	1.83	TRUE	1.91E-01	0.83	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M181T490_neg	181.0336	490	3							HMDB0257850	ercapto)methylidene]-1-cyclohexa	C9H10O2S	4.1
M181T109_neg	181.0718	109	3							HMDB0000107	Galactitol	C6H14O6	0.2
M182T741_neg	182.1187	741	3							HMDB0015239	Methyprylon	C10H17NO2	0.4
M186T714_neg	186.1137	714	3							HMDB0013010	N-Heptanoylglycine	C9H17NO3	0.5
M188T430_neg	188.0022	430	3							HMDB0004823	Lanthionine ketimine	C6H7NO4S	0.5
M188T101_neg	188.0022	101	3							HMDB0004823	Lanthionine ketimine	C6H7NO4S	0.5
M188T161_neg	188.0023	161	3							HMDB0004823	Lanthionine ketimine	C6H7NO4S	0.2
M188T211_neg	188.0929	211	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.2
M189T410_neg	188.9864	410	3							HMDB0240263	Hydroquinone sulfate	C6H6O5S	0.3
M189T707_neg	189.0670	707	3							HMDB0031173	6-Hydroxy-1H-indole-3-acetamide	C10H10N2O2	0.4
M190T537_neg	190.0541	537	3							HMDB0011745	N-Acetyl-L-methionine	C7H13NO3S	1.5
M193T670_neg	193.0507	670	3						Shikimates and Phenylpropanoids	HMDB0000954	Ferulic acid	C10H10O4	0.5
M194T356_neg	194.0460	356	3							HMDB0000840	Salicyluric acid	C9H9NO4	0.6
M195T878_neg	195.1027	878	3							HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	0.1
M196T581_neg	196.0252	581	3							HMDB0006955	roxy-2-methylpyridine-4,5-dicarbo	C8H7NO5	0.3
M196T373_neg	196.0252	373	3							HMDB0006955	roxy-2-methylpyridine-4,5-dicarbo	C8H7NO5	0.4
M197T532_neg	197.0092	532	3						Shikimates and Phenylpropanoids				
M198T504_neg	198.0409	504	3							HMDB0014904	Clavulanate	C8H9NO5	0.5
M199T552_neg	199.1087	552	3							HMDB0304430	N-alpha-acetyl lysine methyl ester	C9H16N2O3	2.0
M200T769_2_neg	200.1293	769	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.2
M201T430_neg	201.1245	430	3						Amino acids and Peptides	HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.4
M202T628_neg	202.0722	628	3							HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	0.5
M202T459_neg	202.0723	459	3							HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	1.1
M202T380_neg	202.1086	380	3							HMDB0062176	N-Lactoylleucine	C9H17NO4	0.3
M203T447_neg	203.0020	447	3							HMDB0240459	4-Methylcatechol 1-sulfate	C7H8O5S	0.2
M203T609_neg	203.0354	609	3							HMDB0244212	1,4-Dihydroxy-2-naphthoic acid	C11H8O4	2.2
M204T616_neg	204.0699	616	3							HMDB0094704	N-Propionylmethionine	C8H15NO3S	0.7
M204T671_neg	204.0667	671	3						Alkaloids	HMDB0000671	Indolelactic acid	C11H11NO3	0.5
M205T414_neg	204.9815	414	3							HMDB0301770	Saccharin sodium	C7H5NNaO3S	0.3
M205T373_neg	205.0354	373	3							HMDB0000379	2-Methylcitric acid	C7H10O7	0.0
M207T508_neg	207.0332	508	3							HMDB0245985	3-Sulfopropyl methacrylate	C7H12O5S	0.4
M209T551_neg	209.0457	551	3							HMDB0011714	Vanilpyruvic acid	C10H10O5	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M181T490_neg	181.0336	490	3	7.13E-07	0.39	TRUE	6.65E-01	1.08	FALSE	2.38E-04	1.78	TRUE	8.80E-01	0.94	FALSE
M181T109_neg	181.0718	109	3	3.54E-03	0.57	TRUE	4.27E-01	1.18	FALSE	7.84E-05	1.98	TRUE	6.70E-01	1.30	FALSE
M182T741_neg	182.1187	741	3	5.73E-06	0.52	TRUE	5.39E-01	1.09	FALSE	2.35E-02	1.31	FALSE	1.52E-03	1.85	TRUE
M186T714_neg	186.1137	714	3	7.38E-01	1.10	FALSE	1.77E-06	5.76	TRUE	7.61E-05	3.10	TRUE	3.43E-01	1.20	FALSE
M188T430_neg	188.0022	430	3	3.42E-01	0.89	FALSE	3.03E-01	1.14	FALSE	2.54E-06	1.68	TRUE	3.92E-02	1.98	TRUE
M188T101_neg	188.0022	101	3	4.53E-17	0.15	TRUE	2.66E-01	1.21	FALSE	2.05E-05	1.88	TRUE	1.71E-01	0.75	FALSE
M188T161_neg	188.0023	161	3	2.79E-02	1.32	FALSE	1.16E-03	1.52	TRUE	5.92E-04	1.47	FALSE	1.36E-02	1.64	TRUE
M188T211_neg	188.0929	211	3	3.86E-11	0.42	TRUE	5.61E-01	1.07	FALSE	2.09E-08	1.84	TRUE	8.99E-01	0.98	FALSE
M189T410_neg	188.9864	410	3	3.13E-12	0.45	TRUE	2.15E-01	1.14	FALSE	2.10E-08	1.70	TRUE	8.61E-01	0.98	FALSE
M189T707_neg	189.0670	707	3	5.92E-18	2.04	TRUE	4.09E-01	1.06	FALSE	4.90E-28	2.36	TRUE	9.19E-01	1.01	FALSE
M190T537_neg	190.0541	537	3	5.76E-02	0.79	FALSE	2.05E-07	2.06	TRUE	1.02E-06	1.75	TRUE	9.97E-01	1.00	FALSE
M193T670_neg	193.0507	670	3	7.10E-03	0.69	FALSE	1.08E-04	1.77	TRUE	2.16E-05	1.68	TRUE	2.61E-01	1.39	FALSE
M194T356_neg	194.0460	356	3	4.32E-07	0.53	TRUE	5.15E-01	1.08	FALSE	2.37E-05	1.57	TRUE	2.16E-01	1.26	FALSE
M195T878_neg	195.1027	878	3	3.22E-18	0.52	TRUE	1.30E-04	1.31	FALSE	1.16E-15	1.66	TRUE	1.03E-01	1.21	FALSE
M196T581_neg	196.0252	581	3	2.37E-21	0.03	TRUE	8.60E-01	0.97	FALSE	1.41E-03	1.66	TRUE	3.22E-01	1.26	FALSE
M196T373_neg	196.0252	373	3	3.69E-23	0.44	TRUE	2.18E-01	1.09	FALSE	7.76E-26	2.14	TRUE	7.49E-01	0.96	FALSE
M197T532_neg	197.0092	532	3	4.40E-22	0.24	TRUE	5.16E-01	1.08	FALSE	8.36E-06	1.57	TRUE	3.18E-01	0.86	FALSE
M198T504_neg	198.0409	504	3	3.31E-09	0.66	TRUE	4.48E-02	1.15	FALSE	9.70E-26	2.06	TRUE	6.45E-01	0.97	FALSE
M199T552_neg	199.1087	552	3	2.65E-02	1.55	TRUE	7.32E-01	0.94	FALSE	1.31E-01	0.77	FALSE	1.73E-02	1.80	TRUE
M200T769_2_neg	200.1293	769	3	5.77E-01	0.90	FALSE	3.45E-06	2.76	TRUE	3.88E-05	2.10	TRUE	6.03E-01	1.06	FALSE
M201T430_neg	201.1245	430	3	4.12E-11	0.41	TRUE	1.98E-01	1.19	FALSE	1.26E-05	1.62	TRUE	1.41E-01	0.64	FALSE
M202T628_neg	202.0722	628	3	9.50E-28	0.43	TRUE	4.10E-01	1.06	FALSE	3.37E-16	1.64	TRUE	3.71E-01	1.13	FALSE
M202T459_neg	202.0723	459	3	2.34E-24	0.50	TRUE	5.40E-05	1.27	FALSE	1.95E-28	1.96	TRUE	9.56E-01	1.00	FALSE
M202T380_neg	202.1086	380	3	1.31E-11	0.05	TRUE	8.69E-01	1.04	FALSE	2.01E-01	1.33	FALSE	2.84E-02	1.79	TRUE
M203T447_neg	203.0020	447	3	1.70E-61	0.33	TRUE	4.65E-02	1.09	FALSE	1.17E-32	1.70	TRUE	2.65E-01	0.92	FALSE
M203T609_neg	203.0354	609	3	2.43E-14	0.63	TRUE	1.26E-01	1.09	FALSE	2.50E-28	1.93	TRUE	7.01E-01	0.95	FALSE
M204T616_neg	204.0699	616	3	4.62E-01	1.08	FALSE	1.55E-04	1.52	TRUE	7.36E-06	1.53	TRUE	1.39E-01	0.83	FALSE
M204T671_neg	204.0667	671	3	2.86E-13	0.15	TRUE	3.49E-01	1.21	FALSE	1.47E-02	1.51	TRUE	1.14E-01	1.21	FALSE
M205T414_neg	204.9815	414	3	3.19E-13	0.49	TRUE	2.85E-02	1.23	FALSE	3.27E-18	2.18	TRUE	8.05E-04	1.43	FALSE
M205T373_neg	205.0354	373	3	5.96E-59	0.23	TRUE	1.50E-01	1.08	FALSE	8.24E-17	1.53	TRUE	8.58E-01	1.03	FALSE
M207T508_neg	207.0332	508	3	5.58E-40	0.38	TRUE	2.76E-03	1.18	FALSE	5.63E-26	1.79	TRUE	7.72E-01	0.98	FALSE
M209T551_neg	209.0457	551	3	3.12E-22	0.41	TRUE	1.19E-01	1.13	FALSE	2.57E-13	1.70	TRUE	1.96E-01	0.93	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M209T633_neg	209.0456	633	3							HMDB0011714	Vanilpyruvic acid	C10H10O5	0.1
M209T114_neg	209.0667	114	3						Carbohydrates	HMDB0003219	Sedoheptulose	C7H14O7	0.0
M210T529_neg	210.0410	529	3							HMDB0011639	Topaquinone	C9H9NO5	0.8
M211T409_neg	211.0725	409	3						Amino acids and Peptides	HMDB0245547	hydroxy-5-(hydroxymethyl)oxolan-	C9H12N2O4	0.1
M212T685_neg	212.0929	685	3							HMDB0253757	kainic acid	C10H15NO4	0.3
M212T677_neg	212.1292	677	3							HMDB0094807	2-nonenoylglycine	C11H19NO3	0.1
M215T571_neg	215.1402	571	3							HMDB0029140	Valylvaline	C10H20N2O3	0.4
M216T558_neg	215.9973	558	3							HMDB0304922	2-Aminophenol N-formate sulfate	C7H7NO5S	0.3
M216T547_neg	216.0336	547	3							HMDB0006409	Tyramine-O-sulfate	C8H11NO4S	0.0
M216T399_neg	216.0336	399	3						Amino acids and Peptides	HMDB0006409	Tyramine-O-sulfate	C8H11NO4S	0.2
M216T493_neg	216.0878	493	3							HMDB0241791	acetyl)oxy]-4-(trimethylazaniumyl)	C9H15NO5	0.3
M216T539_neg	216.1242	539	3							HMDB0240784	O-Propanoyl-D-carnitine	C10H19NO4	0.5
M217T436_neg	217.1194	436	3						Amino acids and Peptides	HMDB0014515	Meprobamate	C9H18N2O4	0.1
M220T111_neg	220.0827	111	3						Amino acids and Peptides	HMDB0000212	N-Acetylgalactosamine	C8H15NO6	0.1
M220T727_neg	220.0979	727	3						Amino acids and Peptides	HMDB0014798	Metaxalone	C12H15NO3	0.1
M221T851_neg	221.0820	851	3							HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	0.2
M221T456_neg	221.0934	456	3							HMDB0028848	Glycyl-Phenylalanine	C11H14N2O3	0.9
M222T675_neg	222.0231	675	3							HMDB0255449	Naphthionic acid	C10H9NO3S	0.3
M222T356_neg	222.0409	356	3							HMDB0004083	no-3-hydroxyphenyl)-2,4-dioxobuta	C10H9NO5	0.7
M223T363_neg	223.0725	363	3							HMDB0000732	Hydroxykynurenine	C10H12N2O4	0.4
M223T949_neg	223.1340	949	3							HMDB0029670	Epoxyeremopetasinorol	C13H20O3	0.2
M224T468_neg	224.0929	468	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.5
M226T521_neg	226.0358	521	3							HMDB0006794	Epimelibiose	C9H9NO6	0.3
M227T454_neg	227.1402	454	3							HMDB0011174	Isoleucylproline	C11H20N2O3	0.2
M229T565_neg	229.1080	565	3							HMDB0041448	Dicyclohexyl disulfide	C12H22S2	4.4
M229T638_neg	229.1557	638	3						Amino acids and Peptides	HMDB0028920	Isoleucyl-Valine	C11H22N2O3	0.1
M230T478_neg	230.0129	478	3							HMDB0240381	HPAA sulfate	C8H9NO5S	0.0
M230T377_neg	230.0671	377	3							HMDB0001180	uccinyl-L-glutamic acid 5-semialde	C9H13NO6	0.4
M231T542_neg	231.1350	542	3							HMDB0013075	Spermic acid 2	C10H20N2O4	0.3
M232T440_1_neg	232.0828	440	3							HMDB0035923	Hirsutin	C10H19NOS2	3.2
M232T578_neg	232.1192	578	3						Fatty acids	HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	0.5
M233T658_neg	233.0125	658	3							HMDB0240530	Homovanillyl alcohol sulfate	C8H10O6S	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M209T633_neg	209.0456	633	3	1.32E-14	0.64	TRUE	6.07E-01	1.03	FALSE	9.80E-31	1.93	TRUE	2.77E-01	0.95	FALSE
M209T114_neg	209.0667	114	3	1.22E-14	0.27	TRUE	7.99E-03	1.47	FALSE	3.06E-05	1.68	TRUE	8.34E-01	0.98	FALSE
M210T529_neg	210.0410	529	3	7.30E-09	0.66	TRUE	2.87E-01	1.08	FALSE	6.49E-14	1.64	TRUE	9.93E-01	1.00	FALSE
M211T409_neg	211.0725	409	3	6.69E-07	0.48	TRUE	3.69E-02	1.35	FALSE	4.50E-07	1.89	TRUE	2.29E-01	1.15	FALSE
M212T685_neg	212.0929	685	3	3.81E-09	0.12	TRUE	4.59E-01	1.22	FALSE	4.63E-02	1.57	TRUE	5.27E-01	1.11	FALSE
M212T677_neg	212.1292	677	3	2.78E-01	0.87	FALSE	1.38E-03	1.60	TRUE	2.11E-06	1.79	TRUE	2.50E-01	0.79	FALSE
M215T571_neg	215.1402	571	3	2.41E-03	2.32	TRUE	2.35E-01	0.73	FALSE	3.03E-02	1.65	TRUE	4.62E-01	1.36	FALSE
M216T558_neg	215.9973	558	3	1.11E-11	0.58	TRUE	6.35E-01	1.04	FALSE	2.53E-22	2.07	TRUE	6.11E-02	1.30	FALSE
M216T547_neg	216.0336	547	3	1.70E-26	0.40	TRUE	5.00E-01	1.05	FALSE	4.70E-16	1.72	TRUE	4.69E-02	0.80	FALSE
M216T399_neg	216.0336	399	3	7.87E-27	0.40	TRUE	7.20E-01	1.03	FALSE	4.85E-17	1.77	TRUE	9.67E-02	0.81	FALSE
M216T493_neg	216.0878	493	3	2.04E-01	0.89	FALSE	5.62E-04	1.42	FALSE	9.25E-14	2.01	TRUE	1.14E-04	2.02	TRUE
M216T539_neg	216.1242	539	3	7.51E-02	0.86	FALSE	7.59E-02	1.17	FALSE	1.66E-12	1.80	TRUE	6.07E-03	0.66	TRUE
M217T436_neg	217.1194	436	3	5.13E-21	0.27	TRUE	9.89E-01	1.00	FALSE	2.91E-05	1.51	TRUE	1.78E-01	0.80	FALSE
M220T111_neg	220.0827	111	3	2.55E-13	0.40	TRUE	2.73E-02	1.29	FALSE	9.08E-18	2.66	TRUE	3.61E-02	1.31	FALSE
M220T727_neg	220.0979	727	3	7.03E-02	0.70	FALSE	2.54E-05	2.46	TRUE	2.23E-05	2.15	TRUE	1.51E-01	1.23	FALSE
M221T851_neg	221.0820	851	3	3.01E-11	0.21	TRUE	9.39E-01	0.99	FALSE	1.95E-01	0.81	FALSE	5.38E-06	183.84	TRUE
M221T456_neg	221.0934	456	3	2.72E-19	0.24	TRUE	7.84E-01	1.04	FALSE	3.40E-02	1.25	FALSE	4.71E-04	0.29	TRUE
M222T675_neg	222.0231	675	3	1.12E-20	0.51	TRUE	7.82E-01	0.98	FALSE	1.36E-14	1.58	TRUE	2.84E-01	1.17	FALSE
M222T356_neg	222.0409	356	3	1.62E-05	0.47	TRUE	1.24E-01	1.32	FALSE	6.93E-04	1.66	TRUE	3.65E-02	0.73	FALSE
M223T363_neg	223.0725	363	3	1.88E-16	0.57	TRUE	6.44E-02	1.13	FALSE	7.16E-26	1.95	TRUE	6.15E-01	1.07	FALSE
M223T949_neg	223.1340	949	3	6.29E-25	0.62	TRUE	8.04E-07	1.23	FALSE	6.60E-27	1.56	TRUE	5.06E-03	1.21	FALSE
M224T468_neg	224.0929	468	3	7.54E-25	0.54	TRUE	8.13E-01	1.01	FALSE	4.91E-26	1.72	TRUE	1.31E-02	0.82	FALSE
M226T521_neg	226.0358	521	3	1.01E-19	0.53	TRUE	8.98E-02	1.11	FALSE	3.84E-29	2.10	TRUE	2.82E-01	0.88	FALSE
M227T454_neg	227.1402	454	3	1.13E-39	0.30	TRUE	8.97E-01	0.99	FALSE	6.95E-15	1.62	TRUE	2.85E-01	0.88	FALSE
M229T565_neg	229.1080	565	3	3.09E-15	1.74	TRUE	1.14E-05	0.66	TRUE	4.52E-01	0.96	FALSE	1.17E-02	1.23	FALSE
M229T638_neg	229.1557	638	3	1.14E-40	0.03	TRUE	5.13E-01	1.08	FALSE	3.10E-08	1.75	TRUE	3.36E-01	0.52	FALSE
M230T478_neg	230.0129	478	3	2.13E-16	0.49	TRUE	2.83E-02	1.19	FALSE	3.30E-24	2.27	TRUE	1.53E-01	0.86	FALSE
M230T377_neg	230.0671	377	3	2.10E-31	0.48	TRUE	2.81E-01	1.06	FALSE	7.47E-24	1.68	TRUE	9.98E-01	1.00	FALSE
M231T542_neg	231.1350	542	3	3.16E-15	0.52	TRUE	2.78E-01	0.92	FALSE	3.06E-20	2.01	TRUE	1.93E-01	0.89	FALSE
M232T440_1_neg	232.0828	440	3	1.72E-17	0.43	TRUE	2.23E-01	1.11	FALSE	4.47E-12	1.74	TRUE	1.32E-01	0.79	FALSE
M232T578_neg	232.1192	578	3	9.41E-03	3.84	TRUE	1.30E-02	6.06	TRUE	4.61E-07	-106.92	FALSE	4.76E-01	1.14	FALSE
M233T658_neg	233.0125	658	3	2.05E-06	0.39	TRUE	8.87E-01	0.97	FALSE	2.10E-03	1.64	TRUE	3.80E-01	0.78	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M234T779_neg	234.1136	779	3							HMDB0033610	Pandamarilactam 3x	C13H17NO3	0.1
M235T452_neg	235.1094	452	3							HMDB0015444	Hexobarbital	C12H16N2O3	2.7
M236T369_neg	236.0928	369	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.1
M239T532_neg	239.0673	532	3							HMDB0032559	b1)-2-(1-Methylpropyl)-4,6-dinitro	C10H12N2O5	0.4
M241T627_neg	241.1192	627	3						Amino acids and Peptides	HMDB0246097	Pueraria glycoside	C11H18N2O4	0.8
M243T715_neg	243.0299	715	3							HMDB0029218	Urolithin C	C13H8O5	0.1
M243T569_neg	243.0510	569	3							HMDB0039177	1-O-Galloylglycerol	C10H12O7	0.0
M243T1031_neg	243.1966	1031	3						Fatty acids	HMDB0002261	2-Hydroxymyristic acid	C14H28O3	0.0
M244T398_neg	244.0777	398	3							HMDB0245815	3-Aminobenzanthrone	C17H11NO	3.7
M244T694_2_neg	244.1199	694	3							HMDB0243753	-Aminopurin-9-yl)cyclohex-3-en-1	C12H15N5O	2.0
M245T117_neg	245.0433	117	3							HMDB0240316	Glycerophosphoglycerol	C6H15O8P	0.5
M245T189_neg	245.0778	189	3							HMDB0000497	5,6-Dihydrouridine	C9H14N2O6	0.5
M245T316_neg	245.1143	316	3						Amino acids and Peptides	HMDB0011166	L-beta-aspartyl-L-leucine	C10H18N2O5	0.1
M245T384_neg	245.1144	384	3						Amino acids and Peptides	HMDB0011166	L-beta-aspartyl-L-leucine	C10H18N2O5	0.6
M245T1033_neg	245.1758	1033	3							HMDB0072866	MG(10:0/0:0/0:0)	C13H26O4	0.1
M245T984_neg	245.1912	984	3							HMDB0030926	Avocadienofuran	C17H26O	0.4
M246T370_neg	246.0620	370	3						Amino acids and Peptides				
M247T569_neg	247.0726	569	3							HMDB0004185	5-Hydroxyindoleacetylglycine	C12H12N2O4	0.6
M252T420_neg	252.0515	420	3							HMDB0039506	N-Salicyloylaspartic acid	C11H11NO6	0.6
M252T802_neg	252.0879	802	3							HMDB0011716	N-Acetylvanilalanine	C12H15NO5	0.4
M253T571_neg	253.0830	571	3							HMDB0029445	L-Agaridoxin	C11H14N2O5	0.0
M253T184_neg	253.0928	184	3						Carbohydrates	HMDB0006790	Galactosylglycerol	C9H18O8	0.2
M256T938_neg	256.1917	938	3							HMDB0013272	N-Lauroylglycine	C14H27NO3	0.4
M257T419_neg	257.0778	419	3						Carbohydrates	HMDB0000884	Ribothymidine	C10H14N2O6	0.4
M257T827_neg	257.1302	827	3							HMDB0246654	hylaminomethyl-gamma-aminobut	C15H18N2O2	2.3
M258T705_1_neg	258.0983	705	3							HMDB0013134	Fumarycarnitine	C11H17NO6	0.1
M258T446_neg	258.1460	446	3						Amino acids and Peptides	HMDB0028800	Glutaminylisoleucine	C11H21N3O4	0.3
M258T705_2_neg	258.1700	705	3							HMDB0241032	4-Methylpentanoylcarnitine	C13H25NO4	4.2
M259T90_neg	259.0787	90	3							HMDB0060917	Etodolac acyl glucuronide	C15H13FO3	4.1
M260T287_neg	260.1140	287	3							HMDB0033865	Lotaustralin	C11H19NO6	0.1
M261T444_neg	261.0074	444	3							HMDB0011719	Homovanillic acid sulfate	C9H10O7S	0.0
M261T396_neg	261.0918	396	3							HMDB0028974	Methionylhydroxyproline	C10H18N2O4S	1.2
M261T715_neg	261.1343	715	3							HMDB0031897	Phaseolic acid	C12H22O6	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M234T779_neg	234.1136	779	3	2.91E-01	0.79	FALSE	1.44E-05	3.01	TRUE	5.61E-05	2.33	TRUE	1.40E-01	1.25	FALSE
M235T452_neg	235.1094	452	3	3.57E-05	0.58	TRUE	1.79E-01	1.20	FALSE	1.69E-07	1.84	TRUE	3.84E-01	0.86	FALSE
M236T369_neg	236.0928	369	3	9.07E-09	0.49	TRUE	7.41E-01	1.04	FALSE	7.06E-06	1.59	TRUE	5.79E-01	0.92	FALSE
M239T532_neg	239.0673	532	3	3.59E-06	0.63	TRUE	3.27E-01	1.10	FALSE	5.64E-07	1.54	TRUE	6.97E-01	0.96	FALSE
M241T627_neg	241.1192	627	3	5.82E-07	0.29	TRUE	9.94E-01	1.00	FALSE	6.36E-03	1.69	TRUE	2.81E-01	1.18	FALSE
M243T715_neg	243.0299	715	3	5.57E-03	1.98	TRUE	7.23E-01	0.92	FALSE	7.12E-10	4.98	TRUE	3.42E-01	0.80	FALSE
M243T569_neg	243.0510	569	3	9.87E-01	1.00	FALSE	1.46E-11	0.48	TRUE	4.53E-03	1.20	FALSE	6.30E-04	1.64	TRUE
M243T1031_neg	243.1966	1031	3	2.36E-02	1.65	TRUE	5.00E-03	0.54	TRUE	6.32E-01	0.91	FALSE	9.29E-01	0.93	FALSE
M244T398_neg	244.0777	398	3	4.37E-05	0.58	TRUE	1.19E-01	1.24	FALSE	3.40E-09	2.07	TRUE	5.53E-01	0.86	FALSE
M244T694_2_neg	244.1199	694	3	9.56E-01	1.01	FALSE	2.48E-06	1.98	TRUE	6.05E-13	2.57	TRUE	5.74E-01	0.96	FALSE
M245T117_neg	245.0433	117	3	1.35E-15	0.34	TRUE	8.75E-03	1.38	FALSE	4.81E-09	1.88	TRUE	4.91E-01	1.16	FALSE
M245T189_neg	245.0778	189	3	2.58E-25	0.35	TRUE	1.44E-04	1.37	FALSE	1.04E-12	1.72	TRUE	2.39E-01	1.16	FALSE
M245T316_neg	245.1143	316	3	3.69E-55	0.07	TRUE	2.71E-01	1.09	FALSE	3.50E-09	1.53	TRUE	6.76E-01	0.91	FALSE
M245T384_neg	245.1144	384	3	2.75E-41	0.20	TRUE	2.16E-01	1.11	FALSE	1.17E-14	1.79	TRUE	2.68E-01	1.05	FALSE
M245T1033_neg	245.1758	1033	3	1.20E-04	1.81	TRUE	4.30E-05	0.49	TRUE	8.74E-01	0.98	FALSE	7.61E-01	1.15	FALSE
M245T984_neg	245.1912	984	3	6.61E-09	2.16	TRUE	7.86E-01	1.04	FALSE	2.48E-08	1.88	TRUE	5.16E-02	1.33	FALSE
M246T370_neg	246.0620	370	3	7.66E-31	0.35	TRUE	6.52E-02	1.14	FALSE	8.23E-11	1.52	TRUE	8.49E-01	1.01	FALSE
M247T569_neg	247.0726	569	3	7.95E-31	0.47	TRUE	4.82E-01	1.04	FALSE	9.34E-25	1.73	TRUE	6.64E-01	1.04	FALSE
M252T420_neg	252.0515	420	3	1.12E-10	0.56	TRUE	8.59E-01	1.02	FALSE	3.73E-10	1.62	TRUE	6.69E-02	0.82	FALSE
M252T802_neg	252.0879	802	3	4.78E-13	0.16	TRUE	7.84E-01	0.95	FALSE	1.45E-02	1.50	TRUE	2.54E-01	1.52	FALSE
M253T571_neg	253.0830	571	3	2.73E-10	0.50	TRUE	7.83E-01	1.03	FALSE	3.27E-08	1.67	TRUE	3.62E-01	0.86	FALSE
M253T184_neg	253.0928	184	3	2.08E-06	0.50	TRUE	4.20E-01	1.12	FALSE	8.70E-04	1.51	TRUE	2.17E-01	0.68	FALSE
M256T938_neg	256.1917	938	3	2.04E-01	1.74	FALSE	8.01E-03	3.33	TRUE	2.22E-02	2.48	TRUE	5.07E-01	1.15	FALSE
M257T419_neg	257.0778	419	3	3.65E-37	0.27	TRUE	1.10E-03	1.27	FALSE	4.59E-20	1.94	TRUE	1.67E-01	1.17	FALSE
M257T827_neg	257.1302	827	3	1.08E-14	2.10	TRUE	3.71E-02	0.85	FALSE	8.72E-03	1.22	FALSE	9.12E-07	0.58	TRUE
M258T705_1_neg	258.0983	705	3	1.34E-47	0.21	TRUE	4.01E-01	1.06	FALSE	3.51E-12	1.55	TRUE	8.34E-01	0.98	FALSE
M258T446_neg	258.1460	446	3	2.02E-23	0.31	TRUE	3.15E-01	0.90	FALSE	2.43E-07	1.55	TRUE	2.70E-02	0.68	FALSE
M258T705_2_neg	258.1700	705	3	2.12E-08	1.57	TRUE	4.11E-01	1.07	FALSE	3.81E-03	1.22	FALSE	1.15E-02	0.65	TRUE
M259T90_neg	259.0787	90	3	3.84E-53	0.26	TRUE	6.42E-05	1.26	FALSE	8.11E-21	1.67	TRUE	4.70E-02	0.76	FALSE
M260T287_neg	260.1140	287	3	1.10E-05	0.60	TRUE	7.87E-01	1.03	FALSE	9.93E-14	2.25	TRUE	1.02E-01	0.81	FALSE
M261T444_neg	261.0074	444	3	1.57E-20	0.32	TRUE	5.68E-01	0.94	FALSE	1.63E-07	1.61	TRUE	1.37E-01	1.21	FALSE
M261T396_neg	261.0918	396	3	2.18E-13	0.58	TRUE	5.11E-01	1.05	FALSE	4.75E-23	1.98	TRUE	8.65E-02	0.85	FALSE
M261T715_neg	261.1343	715	3	3.55E-25	0.59	TRUE	4.14E-01	1.04	FALSE	4.19E-24	1.57	TRUE	7.57E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M262T418_neg	262.0515	418	3							HMDB0254471	Mertiatide	C8H13N3O5S	4.7
M266T111_neg	266.0881	111	3							HMDB0000830	Neuraminic acid	C9H17NO8	0.1
M267T541_neg	267.0622	541	3							HMDB0304685	Glycine-betaxanthin	C11H12N2O6	0.4
M267T574_neg	267.0985	574	3							HMDB0029051	Seryltyrosine	C12H16N2O5	0.6
M268T810_neg	268.0829	810	3							HMDB0247197	henyl)-7H-[1,2,3]triazolo[4,5-d]py	C13H11N5O2	4.2
M273T606_neg	273.0553	606	3							HMDB0240717	Serotonin sulfate	C10H14N2O5S	0.9
M275T411_neg	275.0233	411	3							HMDB0131144	ethoxy-3-(sulfooxy)phenyl]propan	C10H12O7S	0.9
M275T464_neg	275.0678	464	3							HMDB0257564	dihydroxy-5-(1-hydroxyethyl)oxola	C10H13FN2O6	2.7
M275T886_neg	275.0925	886	3							HMDB0030145	Ascochitine	C15H16O5	0.0
M275T597_neg	275.1038	597	3						Amino acids and Peptides	HMDB0062178	N-lactoyl-Tryptophan	C14H16N2O4	0.4
M275T440_neg	275.0967	440	3							HMDB0304054	boxy-4-methylthiazol-5-yl)ethyl ph	C12H20O5S	1.1
M276T575_neg	276.0547	575	3						Amino acids and Peptides	HMDB0240719	Metanephrine sulfate	C10H15NO6S	0.1
M276T807_neg	276.1605	807	3							HMDB0036325	Dinorcapsaicin	C16H23NO3	0.1
M277T630_neg	277.1228	630	3						Fatty acids	HMDB0003426	Pantetheine	C11H22N2O4S	0.2
M279T450_neg	279.1352	450	3						Amino acids and Peptides	HMDB0029118	Tyrosyl-Valine	C14H20N2O4	0.5
M279T505_neg	279.1351	505	3							HMDB0029118	Tyrosyl-Valine	C14H20N2O4	0.1
M281T584_neg	281.0775	584	3							HMDB0032560	Dinoseb acetate	C12H14N2O6	1.4
M283T488_neg	283.0402	488	3						Amino acids and Peptides				
M284T712_neg	284.0598	712	3							HMDB0041892	Faropenem	C12H15NO5S	0.0
M285T606_neg	285.0442	606	3							HMDB0014980	Oxazepam	C15H11ClN2O2	1.9
M286T529_neg	286.0504	529	3							HMDB0255486	xo-1,4-thiazinan-4-yl)-1-(5-nitro-2-	C10H13N3O5S	0.3
M286T577_neg	286.0723	577	3							HMDB0030373	Citrusinine II	C15H13NO5	0.7
M286T785_neg	286.0722	785	3							HMDB0030373	Citrusinine II	C15H13NO5	0.3
M287T103_neg	286.8535	103	3							HMDB0014575	Lindane	C6H6Cl6	2.3
M287T440_neg	287.0348	440	3							HMDB0257244	Ritipenem	C10H12N2O6S	1.8
M287T597_neg	287.1039	597	3							HMDB0034881	-tetrahydro-1H-pyrido[3,4-b]indole	C15H16N2O4	0.6
M287T789_neg	287.1498	789	3						Fatty acids				
M287T1032_neg	287.2227	1032	3							HMDB0037798	)-10,16-Dihydroxyhexadecanoic ac	C16H32O4	0.2
M289T447_neg	289.0928	447	3							HMDB0031304	Osmundalin	C12H18O8	0.2
M289T377_neg	289.1406	377	3						Amino acids and Peptides				
M290T497_neg	290.1244	497	3							HMDB0241030	ydroxy-3-methylbutanedioylcarnit	C12H21NO7	0.4
M291T475_neg	291.0627	475	3							HMDB0258079	1-Galactopyranosyl-5-fluorouracil	C10H13FN2O7	2.6
M292T382_neg	292.1402	382	3							HMDB0037840	N-(1-Deoxy-1-fructosyl)leucine	C12H23NO7	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M262T418_neg	262.0515	418	3	9.03E-08	0.56	TRUE	4.86E-01	1.08	FALSE	4.29E-13	2.05	TRUE	3.55E-01	1.12	FALSE
M266T111_neg	266.0881	111	3	8.43E-14	0.38	TRUE	5.91E-02	1.26	FALSE	7.96E-13	2.20	TRUE	1.81E-02	1.25	FALSE
M267T541_neg	267.0622	541	3	2.86E-11	0.51	TRUE	1.88E-01	1.14	FALSE	7.10E-13	1.88	TRUE	9.51E-01	1.01	FALSE
M267T574_neg	267.0985	574	3	3.68E-28	0.07	TRUE	6.61E-01	0.94	FALSE	6.05E-05	1.63	TRUE	1.53E-01	0.78	FALSE
M268T810_neg	268.0829	810	3	8.97E-11	0.58	TRUE	1.68E-01	1.12	FALSE	4.06E-11	1.63	TRUE	5.34E-01	0.89	FALSE
M273T606_neg	273.0553	606	3	1.11E-06	0.57	TRUE	7.88E-01	1.03	FALSE	1.90E-09	1.86	TRUE	2.30E-01	0.80	FALSE
M275T411_neg	275.0233	411	3	1.23E-10	0.57	TRUE	1.81E-01	1.12	FALSE	1.28E-22	2.32	TRUE	3.30E-02	1.25	FALSE
M275T464_neg	275.0678	464	3	1.56E-03	0.64	TRUE	1.42E-01	1.23	FALSE	9.11E-07	1.89	TRUE	1.12E-01	0.35	FALSE
M275T886_neg	275.0925	886	3	1.56E-13	0.61	TRUE	1.57E-01	1.10	FALSE	2.10E-22	1.85	TRUE	2.61E-01	1.13	FALSE
M275T597_neg	275.1038	597	3	1.37E-21	0.04	TRUE	8.78E-01	1.03	FALSE	4.68E-06	2.08	TRUE	4.43E-01	1.16	FALSE
M275T440_neg	275.0967	440	3	1.21E-01	0.80	FALSE	3.61E-05	1.90	TRUE	1.40E-09	2.35	TRUE	3.68E-01	1.13	FALSE
M276T575_neg	276.0547	575	3	3.58E-01	1.12	FALSE	4.56E-03	0.61	TRUE	4.45E-05	1.58	TRUE	5.04E-01	1.05	FALSE
M276T807_neg	276.1605	807	3	2.75E-13	-3.90	FALSE	4.64E-02	2.08	TRUE	1.39E-05	0.09	TRUE	1.31E-01	0.54	FALSE
M277T630_neg	277.1228	630	3	8.38E-03	1.71	TRUE	3.44E-02	0.68	FALSE	3.59E-13	5.04	TRUE	7.11E-01	1.08	FALSE
M279T450_neg	279.1352	450	3	4.20E-13	0.39	TRUE	4.23E-01	1.10	FALSE	6.39E-07	1.68	TRUE	3.19E-01	0.81	FALSE
M279T505_neg	279.1351	505	3	5.20E-46	0.13	TRUE	4.32E-01	1.07	FALSE	2.96E-09	1.57	TRUE	2.70E-01	1.31	FALSE
M281T584_neg	281.0775	584	3	1.65E-08	0.59	TRUE	4.27E-01	1.08	FALSE	1.88E-12	1.80	TRUE	3.40E-01	1.16	FALSE
M283T488_neg	283.0402	488	3	3.05E-05	0.62	TRUE	2.57E-01	1.14	FALSE	4.53E-11	2.03	TRUE	6.84E-01	1.06	FALSE
M284T712_neg	284.0598	712	3	6.27E-18	0.42	TRUE	6.64E-01	1.04	FALSE	4.45E-09	1.59	TRUE	5.20E-01	0.91	FALSE
M285T606_neg	285.0442	606	3	2.02E-03	0.61	TRUE	9.81E-01	1.00	FALSE	2.28E-08	2.32	TRUE	4.52E-01	0.91	FALSE
M286T529_neg	286.0504	529	3	1.56E-08	0.56	TRUE	2.16E-01	1.13	FALSE	6.02E-12	1.89	TRUE	1.41E-02	1.34	FALSE
M286T577_neg	286.0723	577	3	1.79E-16	0.53	TRUE	4.05E-01	1.06	FALSE	2.05E-18	1.81	TRUE	8.19E-01	0.97	FALSE
M286T785_neg	286.0722	785	3	5.76E-14	0.13	TRUE	7.84E-01	0.95	FALSE	7.67E-04	1.79	TRUE	8.43E-01	1.03	FALSE
M287T103_neg	286.8535	103	3	6.54E-08	1.51	TRUE	9.99E-01	1.00	FALSE	5.53E-05	1.30	FALSE	1.31E-04	0.56	TRUE
M287T440_neg	287.0348	440	3	6.30E-08	0.62	TRUE	9.81E-02	1.16	FALSE	8.53E-20	2.20	TRUE	5.99E-01	1.05	FALSE
M287T597_neg	287.1039	597	3	1.90E-09	0.66	TRUE	2.81E-01	1.08	FALSE	2.32E-15	1.63	TRUE	5.11E-01	0.96	FALSE
M287T789_neg	287.1498	789	3	1.88E-11	0.53	TRUE	1.17E-01	1.15	FALSE	1.18E-08	1.58	TRUE	5.05E-01	0.88	FALSE
M287T1032_neg	287.2227	1032	3	1.97E-02	2.07	TRUE	2.78E-02	0.54	TRUE	4.85E-01	1.20	FALSE	6.28E-01	0.68	FALSE
M289T447_neg	289.0928	447	3	3.43E-17	0.66	TRUE	2.13E-02	1.11	FALSE	4.91E-30	1.70	TRUE	1.47E-01	1.18	FALSE
M289T377_neg	289.1406	377	3	2.45E-04	0.58	TRUE	1.86E-01	1.22	FALSE	2.06E-04	1.62	TRUE	8.44E-01	1.06	FALSE
M290T497_neg	290.1244	497	3	3.76E-10	0.59	TRUE	8.83E-01	0.99	FALSE	2.17E-19	2.04	TRUE	6.94E-02	0.75	FALSE
M291T475_neg	291.0627	475	3	1.91E-11	0.42	TRUE	6.61E-02	0.78	FALSE	5.08E-10	1.97	TRUE	1.07E-01	0.57	FALSE
M292T382_neg	292.1402	382	3	1.68E-06	0.05	TRUE	8.96E-01	1.05	FALSE	8.40E-01	1.07	FALSE	1.49E-02	1.62	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M293T543_neg	293.1507	543	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.2
M293T597_neg	293.1507	597	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.0
M296T688_neg	296.0887	688	3							HMDB0254957	Musk xylene	C12H15N3O6	0.3
M296T391_neg	296.1001	391	3							HMDB0001563	1-Methylguanosine	C11H15N5O5	0.1
M296T466_neg	296.1139	466	3							HMDB0010323	Phenethylamine glucuronide	C14H19NO6	0.2
M299T556_neg	299.0711	556	3						Amino acids and Peptides	HMDB0041849	Carboxytolbutamide	C12H16N2O5S	1.4
M299T1033_neg	299.0956	1033	3							HMDB0252098	Etifoxine	C17H17ClN2O	0.3
M300T1033_neg	300.0983	1033	3							HMDB0259954	methyl-6-nitro-2H-1,4-benzoxazin-	C15H15N3O4	2.4
M300T626_neg	300.1929	626	3						Amino acids and Peptides				
M301T727_neg	301.0718	727	3							HMDB0005782	Hesperetin	C16H14O6	0.2
M302T425_neg	302.0518	425	3						Carbohydrates				
M302T423_neg	302.1357	423	3						Amino acids and Peptides	HMDB0039423	cetyl-N2-gamma-L-glutamyl-L-orni	C12H21N3O6	0.1
M302T625_neg	302.1510	625	3							HMDB0029096	Tryptophyl-Valine	C16H21N3O3	0.0
M303T418_neg	303.0829	418	3						Carbohydrates	HMDB0256818	Propaphos	C13H21O4PS	1.1
M309T462_neg	309.1122	462	3							HMDB0250310	Cl-amidine	C14H19ClN4O2	0.7
M312T365_neg	312.1090	365	3							HMDB0010328	Tyramine glucuronide	C14H19NO7	0.3
M312T551_neg	312.1090	551	3							HMDB0010328	Tyramine glucuronide	C14H19NO7	0.3
M313T603_neg	313.0501	603	3							HMDB0060627	Malaoxon	C10H19O7PS	5.0
M313T1050_neg	313.2747	1050	3							HMDB0061651	3-hydroxypristanic acid	C19H38O3	0.3
M315T392_neg	315.0986	392	3						Alkaloids				
M315T865_neg	315.1812	865	3							HMDB0029346	Neryl glucoside	C16H28O6	0.3
M315T1076_neg	315.2331	1076	3							HMDB0000253	Pregnenolone	C21H32O2	0.4
M315T991_neg	315.2540	991	3						Fatty acids	HMDB0011532	MG(0:0/15:0/0:0)	C18H36O4	0.1
M319T696_neg	319.0856	696	3							HMDB0244280	N(4)-Acetylsulfamethazine	C14H16N4O3S	4.4
M322T526_neg	322.1042	526	3							HMDB0258233	Senicapoc	C20H15F2NO	2.2
M323T947_neg	323.1287	947	3							HMDB0032671	)-4-penten-2-ynylidene]-1,6-dioxa	C20H20O4	0.7
M323T1032_neg	323.2591	1032	3							HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	0.2
M325T563_neg	325.0872	563	3						Amino acids and Peptides	HMDB0249367	Brasofensine	C16H20Cl2N2O	2.4
M327T384_neg	327.0836	384	3							HMDB0247403	in-2-yl)disulfanyl]propanamido}he	C14H20N2O3S2	2.1
M329T943_neg	329.1396	943	3							HMDB0031076	Gibberellin A105	C19H22O5	0.4
M331T113_neg	331.0549	113	3						Amino acids and Peptides				
M331T1034_neg	331.2491	1034	3							HMDB0030935	9,10,13-Trihydroxystearic acid	C18H36O5	0.2
M333T526_neg	333.1457	526	3							HMDB0037499	1-Ethenylhexyl butanoate	C17H22N2O5	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M293T543_neg	293.1507	543	3	6.99E-30	0.26	TRUE	8.53E-01	1.02	FALSE	7.85E-17	2.06	TRUE	5.57E-02	0.66	FALSE
M293T597_neg	293.1507	597	3	2.00E-03	0.52	TRUE	5.30E-01	1.15	FALSE	1.22E-03	1.82	TRUE	9.55E-02	2.36	FALSE
M296T688_neg	296.0887	688	3	7.62E-21	0.38	TRUE	2.02E-01	1.12	FALSE	5.66E-13	1.81	TRUE	2.83E-01	0.84	FALSE
M296T391_neg	296.1001	391	3	4.89E-17	0.34	TRUE	9.90E-01	1.00	FALSE	1.17E-13	2.17	TRUE	7.15E-02	1.37	FALSE
M296T466_neg	296.1139	466	3	1.61E-14	0.21	TRUE	8.36E-01	1.03	FALSE	9.65E-05	1.74	TRUE	3.58E-01	1.09	FALSE
M299T556_neg	299.0711	556	3	1.50E-04	1.64	TRUE	3.62E-01	0.89	FALSE	1.31E-04	1.54	TRUE	1.95E-01	0.82	FALSE
M299T1033_neg	299.0956	1033	3	1.13E-05	1.65	TRUE	5.57E-05	0.60	TRUE	6.56E-01	0.96	FALSE	4.04E-01	1.21	FALSE
M300T1033_neg	300.0983	1033	3	8.58E-06	1.67	TRUE	1.37E-04	0.61	TRUE	6.81E-01	0.96	FALSE	1.03E-01	1.37	FALSE
M300T626_neg	300.1929	626	3	5.92E-40	0.23	TRUE	4.25E-02	1.18	FALSE	4.87E-13	1.66	TRUE	4.52E-01	0.75	FALSE
M301T727_neg	301.0718	727	3	9.48E-11	0.63	TRUE	1.03E-01	1.12	FALSE	3.56E-08	1.39	FALSE	1.26E-03	1.82	TRUE
M302T425_neg	302.0518	425	3	6.40E-22	0.30	TRUE	8.92E-01	0.99	FALSE	9.86E-08	1.63	TRUE	1.18E-01	1.80	FALSE
M302T423_neg	302.1357	423	3	2.55E-26	0.26	TRUE	7.09E-01	0.96	FALSE	5.93E-08	1.60	TRUE	7.54E-01	1.18	FALSE
M302T625_neg	302.1510	625	3	2.26E-41	0.17	TRUE	6.49E-01	1.04	FALSE	2.34E-14	1.82	TRUE	3.56E-01	1.11	FALSE
M303T418_neg	303.0829	418	3	5.06E-32	0.33	TRUE	1.08E-01	1.13	FALSE	4.54E-14	1.67	TRUE	1.98E-01	1.17	FALSE
M309T462_neg	309.1122	462	3	5.95E-24	0.25	TRUE	2.65E-03	1.39	FALSE	3.80E-12	2.02	TRUE	2.96E-01	1.27	FALSE
M312T365_neg	312.1090	365	3	6.14E-16	0.07	TRUE	6.58E-01	1.09	FALSE	1.78E-04	1.97	TRUE	9.92E-01	1.00	FALSE
M312T551_neg	312.1090	551	3	2.51E-20	0.55	TRUE	2.52E-01	1.07	FALSE	4.24E-25	1.83	TRUE	2.83E-01	0.91	FALSE
M313T603_neg	313.0501	603	3	4.87E-02	1.19	FALSE	1.62E-08	1.69	TRUE	1.51E-10	1.68	TRUE	8.49E-03	1.34	FALSE
M313T1050_neg	313.2747	1050	3	1.64E-05	1.86	TRUE	4.34E-05	0.55	TRUE	1.76E-01	0.85	FALSE	1.89E-01	1.36	FALSE
M315T392_neg	315.0986	392	3	1.34E-04	0.57	TRUE	8.51E-01	0.97	FALSE	2.61E-04	1.59	TRUE	2.62E-01	0.73	FALSE
M315T865_neg	315.1812	865	3	5.51E-14	0.50	TRUE	1.53E-01	1.13	FALSE	1.51E-11	1.69	TRUE	4.32E-01	0.85	FALSE
M315T1076_neg	315.2331	1076	3	2.86E-03	2.02	TRUE	2.06E-03	0.49	TRUE	8.59E-02	0.71	FALSE	4.83E-01	1.52	FALSE
M315T991_neg	315.2540	991	3	6.68E-09	1.77	TRUE	1.21E-05	0.63	TRUE	9.60E-01	1.00	FALSE	1.42E-01	1.19	FALSE
M319T696_neg	319.0856	696	3	5.86E-01	1.05	FALSE	1.43E-01	0.86	FALSE	5.54E-09	1.55	TRUE	1.44E-02	1.81	TRUE
M322T526_neg	322.1042	526	3	5.64E-11	0.66	TRUE	4.23E-01	1.05	FALSE	1.38E-26	1.97	TRUE	1.61E-01	1.11	FALSE
M323T947_neg	323.1287	947	3	3.28E-05	7.84	TRUE	1.05E-02	0.40	TRUE	4.32E-01	1.29	FALSE	5.21E-01	0.81	FALSE
M323T1032_neg	323.2591	1032	3	1.50E-04	2.34	TRUE	3.65E-02	0.64	TRUE	9.17E-01	0.98	FALSE	2.48E-01	1.30	FALSE
M325T563_neg	325.0872	563	3	3.29E-02	1.60	TRUE	5.72E-01	0.88	FALSE	1.56E-05	2.42	TRUE	9.87E-01	1.00	FALSE
M327T384_neg	327.0836	384	3	2.95E-24	0.26	TRUE	5.42E-01	1.07	FALSE	2.51E-07	1.60	TRUE	9.95E-01	1.00	FALSE
M329T943_neg	329.1396	943	3	4.51E-10	4.25	TRUE	1.08E-07	0.36	TRUE	2.95E-01	0.84	FALSE	5.77E-01	1.16	FALSE
M331T113_neg	331.0549	113	3	1.30E-38	0.24	TRUE	7.78E-02	1.15	FALSE	3.68E-11	1.60	TRUE	5.28E-02	0.46	FALSE
M331T1034_neg	331.2491	1034	3	1.93E-04	3.25	TRUE	1.54E-02	0.47	TRUE	3.93E-01	0.81	FALSE	5.88E-01	0.86	FALSE
M333T526_neg	333.1457	526	3	2.67E-18	0.59	TRUE	1.19E-01	1.09	FALSE	2.75E-33	2.05	TRUE	8.29E-02	0.91	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M336T890_neg	336.1820	890	3							HMDB0029325	3,6-Ditigloyloxytropan-7-ol	C18H27NO5	1.1
M338T1069_neg	338.2702	1069	3							HMDB0013631	Oleoyl glycine	C20H37NO3	0.5
M341T423_neg	341.0992	423	3							HMDB0246183	ethylaminoethoxy)phenyl]-4-(trifl	C14H18N2O8	0.4
M341T1012_neg	341.2697	1012	3							HMDB0242141	Eicosanedioic acid	C20H38O4	0.0
M345T449_neg	345.0979	449	3							HMDB0037250	Muscomin	C18H18O7	0.2
M345T660_neg	345.0991	660	3						Polyketides	HMDB0037250	Muscomin	C18H18O7	3.1
M347T458_neg	347.1460	458	3							HMDB0248799	Azetirelin	C15H20N6O4	3.9
M347T559_neg	347.1618	559	3							HMDB0041886	Enalaprilat	C18H24N2O5	1.6
M347T1033_neg	347.2591	1033	3							HMDB0029683	-Hydroxy-6-pentadecylbenzoic aci	C22H36O3	0.1
M349T817_neg	349.1296	817	3							HMDB0249307	-ylmethyl)-6-(3-methoxyphenyl)p	C19H18N4O3	2.8
M351T991_neg	351.2540	991	3							HMDB0011539	MG(0:0/18:3(6Z,9Z,12Z)/0:0)	C21H36O4	0.1
M353T489_neg	353.1731	489	3							HMDB0062319	1-dodecanoyl-glycero-3-phosphate	C15H31O7P	1.1
M357T103_neg	356.8384	103	3							HMDB0245362	2,2,6,6-Tetramethylpiperidine	C12H4Cl6	3.6
M359T464_neg	359.0774	464	3							HMDB0003572	Rosmarinic acid	C18H16O8	0.5
M361T349_neg	361.0891	349	3							HMDB0258354	Pentazirinocyclodiphosphathiazene	C10H20N8OP2S	2.2
M361T1074_neg	361.2961	1074	3							HMDB0246913	raethylene glycol monododecyl et	C20H42O5	0.4
M367T949_neg	367.0491	949	3							HMDB0029177	3-Sn-phosphatidylethanolamine	C16H16O8S	0.5
M370T687_neg	370.0967	687	3							HMDB0304919	Hydroxydesmethylpiperine sulfate	C16H21NO7S	0.3
M370T671_neg	370.1513	671	3							HMDB0244645	ylamino)propyl)phenyl beta-D-gluc	C17H25NO8	1.4
M371T103_neg	370.8148	103	3							HMDB0244129	,2,3,4,7,8-Hexachlorodibenzofura	C12H2Cl6O	4.2
M371T687_neg	371.1000	687	3							HMDB0031756	Veranisatin C	C16H20O10	4.3
M371T1033_neg	371.2592	1033	3							HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.1
M373T480_neg	373.1729	480	3						Amino acids and Peptides				
M375T1033_neg	375.2543	1033	3							HMDB0011550	MG(0:0/20:5(5Z,8Z,11Z,14Z,17Z)/0:	C23H36O4	0.4
M377T796_neg	377.1243	796	3							HMDB0029304	3,4-DHPEA-EA	C19H22O8	0.4
M377T427_neg	377.1931	427	3							HMDB0003933	Pentosidine	C17H26N6O4	3.2
M379T804_neg	379.1399	804	3							HMDB0036893	Gibberellin A75	C19H24O8	0.2
M383T694_neg	383.0774	694	3							HMDB0030592	5,6-Dimethoxysterigmatocystin	C20H16O8	0.5
M386T810_neg	386.1472	810	3							HMDB0302642	enzyladenine 3-O-beta-D-glucosid	C18H21N5O5	0.5
M387T723_neg	387.1089	723	3						Shikimates and Phenylpropanoids	HMDB0029227	Coutaric acid	C20H20O8	0.9
M387T576_neg	387.1414	576	3							HMDB0248819	Azoxystrobin	C17H20N6O5	2.1
M388T650_neg	388.1074	650	3							HMDB0258681	Taisho	C17H19N5O4S	2.7
M389T996_neg	389.1972	996	3							HMDB0030844	6,7-Dimethoxy-7-epirosmanol	C22H30O6	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M336T890_neg	336.1820	890	3	4.78E-07	0.63	TRUE	7.22E-01	0.97	FALSE	1.76E-11	1.76	TRUE	1.97E-02	1.25	FALSE
M338T1069_neg	338.2702	1069	3	2.57E-04	3.16	TRUE	9.50E-03	0.46	TRUE	7.99E-01	0.94	FALSE	8.67E-01	1.08	FALSE
M341T423_neg	341.0992	423	3	7.09E-09	0.50	TRUE	6.56E-01	1.05	FALSE	2.38E-05	1.53	TRUE	7.34E-01	0.95	FALSE
M341T1012_neg	341.2697	1012	3	8.30E-15	2.20	TRUE	1.41E-05	0.67	TRUE	2.23E-01	1.10	FALSE	1.89E-01	1.22	FALSE
M345T449_neg	345.0979	449	3	1.85E-01	0.90	FALSE	1.06E-02	1.23	FALSE	6.57E-16	1.84	TRUE	8.87E-03	1.56	TRUE
M345T660_neg	345.0991	660	3	2.24E-11	0.52	TRUE	7.62E-01	1.03	FALSE	6.54E-12	1.80	TRUE	7.31E-01	1.06	FALSE
M347T458_neg	347.1460	458	3	1.54E-10	0.39	TRUE	6.90E-01	1.06	FALSE	3.37E-07	1.87	TRUE	3.90E-01	0.88	FALSE
M347T559_neg	347.1618	559	3	6.55E-08	0.65	TRUE	5.31E-02	1.17	FALSE	3.01E-26	2.34	TRUE	4.35E-01	1.06	FALSE
M347T1033_neg	347.2591	1033	3	4.89E-08	2.17	TRUE	1.44E-07	0.50	TRUE	7.01E-02	0.81	FALSE	1.98E-01	1.31	FALSE
M349T817_neg	349.1296	817	3	5.47E-06	0.64	TRUE	1.96E-01	1.14	FALSE	1.54E-13	1.97	TRUE	3.24E-01	0.90	FALSE
M351T991_neg	351.2540	991	3	1.09E-04	1.94	TRUE	1.03E-02	0.64	TRUE	5.71E-01	1.08	FALSE	1.08E-01	0.69	FALSE
M353T489_neg	353.1731	489	3	1.28E-16	0.50	TRUE	5.97E-01	0.96	FALSE	3.81E-13	1.67	TRUE	5.83E-01	0.93	FALSE
M357T103_neg	356.8384	103	3	5.12E-13	3.07	TRUE	1.56E-03	0.64	TRUE	2.83E-01	0.88	FALSE	3.38E-01	1.20	FALSE
M359T464_neg	359.0774	464	3	3.40E-13	0.42	TRUE	3.19E-01	1.12	FALSE	5.36E-06	1.55	TRUE	1.77E-02	1.46	FALSE
M361T349_neg	361.0891	349	3	1.47E-11	0.56	TRUE	3.25E-01	1.08	FALSE	1.86E-13	1.73	TRUE	4.34E-02	1.42	FALSE
M361T1074_neg	361.2961	1074	3	7.06E-04	2.26	TRUE	1.26E-03	0.50	TRUE	5.69E-01	0.89	FALSE	7.25E-01	0.88	FALSE
M367T949_neg	367.0491	949	3	6.61E-29	0.44	TRUE	8.43E-06	1.32	FALSE	2.70E-20	1.71	TRUE	6.81E-02	1.24	FALSE
M370T687_neg	370.0967	687	3	2.19E-04	0.52	TRUE	8.22E-01	1.04	FALSE	5.45E-05	1.86	TRUE	2.86E-01	0.74	FALSE
M370T671_neg	370.1513	671	3	3.20E-04	1.63	TRUE	1.32E-09	2.42	TRUE	3.43E-02	1.28	FALSE	3.62E-02	0.70	FALSE
M371T103_neg	370.8148	103	3	1.20E-06	1.61	TRUE	9.92E-01	1.00	FALSE	4.41E-04	1.34	FALSE	4.69E-05	0.45	TRUE
M371T687_neg	371.1000	687	3	1.89E-06	0.49	TRUE	7.84E-01	1.04	FALSE	1.50E-07	2.00	TRUE	4.41E-01	0.83	FALSE
M371T1033_neg	371.2592	1033	3	2.67E-04	1.68	TRUE	5.34E-02	1.33	FALSE	5.65E-11	2.41	TRUE	5.20E-02	1.34	FALSE
M373T480_neg	373.1729	480	3	2.19E-39	0.20	TRUE	5.97E-01	1.05	FALSE	6.28E-09	1.53	TRUE	7.15E-01	0.94	FALSE
M375T1033_neg	375.2543	1033	3	3.87E-10	2.90	TRUE	6.93E-02	0.74	FALSE	1.45E-05	1.80	TRUE	8.85E-01	0.98	FALSE
M377T796_neg	377.1243	796	3	2.63E-12	0.46	TRUE	3.48E-01	1.10	FALSE	1.13E-14	2.15	TRUE	6.42E-01	0.94	FALSE
M377T427_neg	377.1931	427	3	2.26E-15	0.51	TRUE	1.72E-01	1.11	FALSE	1.26E-19	1.99	TRUE	6.25E-01	0.97	FALSE
M379T804_neg	379.1399	804	3	8.55E-11	0.52	TRUE	4.80E-01	1.07	FALSE	6.33E-15	2.02	TRUE	1.78E-01	0.84	FALSE
M383T694_neg	383.0774	694	3	2.74E-09	0.67	TRUE	2.15E-01	1.09	FALSE	2.19E-19	1.79	TRUE	1.21E-02	0.80	FALSE
M386T810_neg	386.1472	810	3	8.70E-22	0.47	TRUE	1.75E-01	1.10	FALSE	4.46E-16	1.68	TRUE	2.64E-01	1.10	FALSE
M387T723_neg	387.1089	723	3	9.54E-12	0.49	TRUE	6.08E-01	1.05	FALSE	1.56E-10	1.76	TRUE	2.96E-01	0.80	FALSE
M387T576_neg	387.1414	576	3	2.42E-31	0.30	TRUE	6.34E-02	1.16	FALSE	5.00E-12	1.65	TRUE	4.56E-01	1.27	FALSE
M388T650_neg	388.1074	650	3	9.82E-06	0.42	TRUE	8.86E-01	1.03	FALSE	1.24E-04	1.88	TRUE	3.48E-01	0.76	FALSE
M389T996_neg	389.1972	996	3	5.62E-03	2.17	TRUE	8.96E-01	1.04	FALSE	5.15E-07	3.98	TRUE	4.71E-01	0.84	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M396T899_neg	396.2142	899	3							HMDB0249521	ylamino)carbonyl]oxiran-2-Yl}carb	C19H31N3O6	0.4
M399T1033_neg	399.3481	1033	3							HMDB0072855	MG(a-21:0/0:0/0:0)[rac]	C24H48O4	0.2
M403T627_neg	403.0915	627	3							HMDB0060913	Zopiclone N-oxide	C17H17ClN6O4	3.0
M403T1056_neg	403.2855	1056	3						Polyketides	HMDB0011555	IG(0:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:	C25H40O4	0.2
M407T508_neg	407.1723	508	3						Amino acids and Peptides	HMDB0039084	3-O-Methylniveusin A	C21H28O8	2.8
M409T603_neg	409.1650	603	3							HMDB0029981	1-Isomangostin	C24H26O6	1.6
M410T994_neg	410.2316	994	3						Fatty acids	HMDB0003752	LysoPC(10:0/0:0)	C18H38NO7P	0.7
M413T667_neg	413.1156	667	3							HMDB0014745	Nafcillin	C21H22N2O5S	4.9
M414T818_neg	414.2420	818	3							HMDB0255109	N-Demethyl Mifepristone	C28H33NO2	4.6
M415T527_neg	415.1664	527	3							HMDB0250142	Agelin	C24H29ClO4	4.2
M415T1027_neg	415.2813	1027	3						Amino acids and Peptides				
M415T1069_neg	415.3220	1069	3							HMDB0000430	24,25-Dihydroxyvitamin D	C27H44O3	0.6
M417T1067_neg	417.3012	1067	3							HMDB0012515	10-HETE	C26H42O4	0.4
M418T778_neg	418.2348	778	3							HMDB0247141	N-Formyl-Nle-Leu-Phe	C22H33N3O5	0.0
M424T1017_neg	424.2472	1017	3						Fatty acids	HMDB0011470	LysoPE(0:0/14:0)	C19H40NO7P	0.5
M436T1061_neg	436.2834	1061	3						Fatty acids	HMDB0011152	LysoPE(P-16:0/0:0)	C21H44NO6P	0.1
M438T1034_neg	438.2628	1034	3						Fatty acids	HMDB0240697	sphocholine (isomer 1) (LPC(12:0) i	C20H42NO7P	0.5
M443T611_neg	443.1133	611	3							HMDB0037913	Artomunoxanthentrione	C26H20O7	0.7
M447T598_neg	447.1810	598	3							HMDB0258726	Tarazepide	C28H24N4O2	3.7
M462T1067_neg	462.2992	1067	3							HMDB0240599	LysoPE(P-18:1(9Z)/0:0)	C23H46NO6P	0.5
M465T421_neg	465.1187	421	3							HMDB0030106	Neosilyhermin A	C25H22O9	0.8
M468T712_neg	468.2506	712	3						Alkaloids	HMDB0253814	xaldehyde, 3-(1,3-benzodioxol-5-y	C26H35N3O5	0.4
M471T502_neg	471.1720	502	3							HMDB0039741	anosyl-(1->3)-alpha-D-galactopyran	C18H32O14	0.1
M473T705_neg	473.2405	705	3							HMDB0254939	mTOR-IN-1	C25H30N8O2	3.0
M476T1039_neg	476.2785	1039	3						Fatty acids	HMDB0011477	LysoPE(0:0/18:2(9Z,12Z))	C23H44NO7P	0.4
M477T1040_neg	477.2819	1040	3							HMDB0250805	Valyl-leucyl-lysine 4-nitroanilide	C23H38N6O5	2.6
M480T419_neg	480.1628	419	3							HMDB0243604	hanesulfonamido)-6-(propan-2-yl)	C22H28FN3O6S	3.8
M480T1076_neg	480.3099	1076	3						Fatty acids	HMDB0010381	LysoPC(15:0/0:0)	C23H48NO7P	0.7
M481T1030_neg	481.3534	1030	3						Terpenoids				
M491T658_neg	491.2289	658	3						Terpenoids	HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.5
M503T412_neg	503.1648	412	3						Carbohydrates	HMDB0256657	ro-4-hydroxy-2-oxo-2H-cycloocta(b	C28H28N2O5S	0.3
M507T1043_neg	507.3693	1043	3							HMDB0035853	Fasciculol C	C30H52O6	0.3
M510T691_neg	510.2893	691	3							HMDB0242372	Cholylcysteine	C27H45NO6S	0.3
M510T816_neg	510.2894	816	3							HMDB0242372	Cholylcysteine	C27H45NO6S	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M396T899_neg	396.2142	899	3	6.96E-02	1.59	FALSE	2.82E-01	0.71	FALSE	8.97E-03	1.81	TRUE	7.29E-03	3.14	TRUE
M399T1033_neg	399.3481	1033	3	1.45E-03	1.85	TRUE	1.04E-04	0.42	TRUE	5.22E-01	0.90	FALSE	8.62E-01	1.14	FALSE
M403T627_neg	403.0915	627	3	1.99E-25	3.80	TRUE	1.00E+00	1.00	FALSE	3.35E-09	0.59	TRUE	4.03E-02	1.28	FALSE
M403T1056_neg	403.2855	1056	3	2.43E-07	2.05	TRUE	1.55E-04	0.61	TRUE	3.05E-01	0.89	FALSE	1.66E-01	1.25	FALSE
M407T508_neg	407.1723	508	3	2.80E-36	0.18	TRUE	3.96E-01	1.08	FALSE	2.22E-09	1.65	TRUE	4.86E-02	1.40	FALSE
M409T603_neg	409.1650	603	3	3.03E-02	1.44	FALSE	2.84E-03	1.65	TRUE	2.50E-13	3.58	TRUE	7.12E-01	1.05	FALSE
M410T994_neg	410.2316	994	3	1.06E-02	2.52	TRUE	1.63E-01	0.57	FALSE	8.16E-05	3.85	TRUE	6.49E-01	0.90	FALSE
M413T667_neg	413.1156	667	3	1.05E-07	9.02	TRUE	7.72E-01	1.08	FALSE	2.75E-06	4.13	TRUE	6.58E-01	1.08	FALSE
M414T818_neg	414.2420	818	3	2.67E-10	1.65	TRUE	1.83E-01	0.90	FALSE	3.68E-13	1.67	TRUE	3.36E-01	0.90	FALSE
M415T527_neg	415.1664	527	3	1.82E-11	0.55	TRUE	5.35E-01	1.05	FALSE	8.58E-13	1.73	TRUE	3.09E-01	0.80	FALSE
M415T1027_neg	415.2813	1027	3	1.28E-02	0.57	TRUE	4.81E-01	1.17	FALSE	2.67E-02	1.54	TRUE	8.37E-01	0.91	FALSE
M415T1069_neg	415.3220	1069	3	5.68E-08	3.20	TRUE	4.32E-06	0.40	TRUE	9.36E-01	0.99	FALSE	4.50E-01	1.40	FALSE
M417T1067_neg	417.3012	1067	3	2.16E-07	3.19	TRUE	2.34E-04	0.48	TRUE	2.86E-01	1.20	FALSE	6.54E-01	1.17	FALSE
M418T778_neg	418.2348	778	3	4.11E-15	0.57	TRUE	3.92E-08	1.45	FALSE	1.07E-14	1.62	TRUE	6.58E-02	1.20	FALSE
M424T1017_neg	424.2472	1017	3	8.22E-04	2.95	TRUE	5.39E-02	0.54	FALSE	3.02E-05	3.36	TRUE	4.85E-01	0.84	FALSE
M436T1061_neg	436.2834	1061	3	2.24E-02	1.41	FALSE	9.04E-03	0.61	TRUE	1.35E-07	2.09	TRUE	1.84E-01	0.78	FALSE
M438T1034_neg	438.2628	1034	3	4.92E-05	2.82	TRUE	1.01E-01	0.67	FALSE	4.28E-06	2.80	TRUE	2.50E-01	0.80	FALSE
M443T611_neg	443.1133	611	3	9.03E-24	0.29	TRUE	4.17E-01	1.09	FALSE	3.42E-10	1.76	TRUE	7.80E-01	1.05	FALSE
M447T598_neg	447.1810	598	3	2.98E-01	1.20	FALSE	9.95E-01	1.00	FALSE	3.21E-03	1.59	TRUE	3.95E-02	0.59	TRUE
M462T1067_neg	462.2992	1067	3	4.12E-03	2.02	TRUE	9.73E-02	0.59	FALSE	1.40E-02	1.67	TRUE	9.21E-01	0.98	FALSE
M465T421_neg	465.1187	421	3	3.00E-10	0.39	TRUE	8.36E-01	1.03	FALSE	6.97E-07	1.84	TRUE	1.36E-01	1.18	FALSE
M468T712_neg	468.2506	712	3	3.45E-07	1.72	TRUE	1.16E-08	1.87	TRUE	2.56E-01	1.10	FALSE	3.88E-03	1.43	FALSE
M471T502_neg	471.1720	502	3	2.58E-05	0.66	TRUE	3.49E-01	1.10	FALSE	2.85E-19	2.41	TRUE	6.51E-04	0.74	FALSE
M473T705_neg	473.2405	705	3	7.04E-09	0.53	TRUE	6.53E-05	1.54	TRUE	7.24E-05	1.44	FALSE	2.48E-02	1.39	FALSE
M476T1039_neg	476.2785	1039	3	2.32E-06	2.68	TRUE	1.80E-07	0.33	TRUE	7.16E-02	1.35	FALSE	9.56E-01	0.95	FALSE
M477T1040_neg	477.2819	1040	3	1.85E-08	1.89	TRUE	1.64E-05	0.61	TRUE	1.21E-04	1.44	FALSE	8.37E-01	1.16	FALSE
M480T419_neg	480.1628	419	3	1.07E-13	0.08	TRUE	8.96E-01	1.03	FALSE	2.38E-01	1.24	FALSE	3.30E-02	1.78	TRUE
M480T1076_neg	480.3099	1076	3	1.45E-02	2.16	TRUE	1.47E-01	0.61	FALSE	9.41E-04	2.54	TRUE	2.96E-01	0.83	FALSE
M481T1030_neg	481.3534	1030	3	1.60E-13	2.62	TRUE	4.12E-05	0.63	TRUE	4.79E-02	1.22	FALSE	4.67E-01	1.12	FALSE
M491T658_neg	491.2289	658	3	2.12E-07	1.66	TRUE	1.09E-02	1.27	FALSE	4.41E-03	1.26	FALSE	1.23E-02	1.55	TRUE
M503T412_neg	503.1648	412	3	6.57E-14	0.00	TRUE	5.81E-01	0.87	FALSE	4.70E-08	4.09	TRUE	6.79E-01	0.68	FALSE
M507T1043_neg	507.3693	1043	3	4.88E-09	2.79	TRUE	9.23E-05	0.54	TRUE	8.93E-01	0.98	FALSE	7.95E-02	1.53	FALSE
M510T691_neg	510.2893	691	3	6.64E-24	3.00	TRUE	3.54E-01	0.92	FALSE	6.85E-10	1.65	TRUE	4.89E-01	0.94	FALSE
M510T816_neg	510.2894	816	3	4.78E-14	2.64	TRUE	4.01E-07	0.56	TRUE	9.43E-01	1.01	FALSE	4.91E-01	1.11	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M528T273_neg	528.1938	273	3							HMDB0002060	2)-O-b-D-galactopyranosyl-(1->3)-2	C20H35NO15	0.8
M531T990_neg	531.3329	990	3						Terpenoids				
M537T441_neg	537.1939	441	3							HMDB0030133	Asticolorin A	C33H30O7	3.8
M545T538_neg	545.1294	538	3						Carbohydrates	HMDB0030641	hanin A 7-(6-methylmalonylglucos	C26H26O13	1.3
M545T996_neg	545.3230	996	3							HMDB0248383	Anamorelin	C31H42N6O3	2.9
M554T486_neg	554.1409	486	3						Carbohydrates				
M555T1001_neg	555.4267	1001	3						Terpenoids				
M558T176_neg	558.0646	176	3						Carbohydrates	HMDB0248024	ADP Ribose	C15H23N5O14P2	0.3
M558T797_neg	558.2459	797	3						Amino acids and Peptides				
M559T384_neg	559.2367	384	3							HMDB0250087	Chloramphenicol palmitate	C27H42Cl2N2O6	3.5
M564T1038_neg	564.3309	1038	3						Fatty acids				
M565T1038_neg	565.3339	1038	3							HMDB0303709	clo(glycylleucylvalylleucylprolylser	C27H46N6O7	2.8
M568T803_neg	568.2954	803	3						Alkaloids				
M568T1075_neg	568.3621	1075	3						Fatty acids	HMDB0250380	Tenofovir exalidex	C28H52N5O5P	2.1
M570T491_neg	570.1358	491	3						Carbohydrates				
M574T767_neg	574.3022	767	3							HMDB0029338	Mauritine A	C32H41N5O5	2.3
M577T713_neg	577.1354	713	3							HMDB0013690	Procyanidin	C30H26O12	0.4
M579T723_neg	579.2865	723	3							HMDB0248664	peridinyl]phenyl]-N4-[2-[(1-methy	C29H40N8O3S	1.1
M585T998_neg	585.2527	998	3							HMDB0250832	Dalamid	C28H38N6O6S	4.4
M589T463_neg	589.2353	463	3							HMDB0252583	Galactosylpyridinoline	C24H38N4O13	1.6
M591T1020_neg	591.3188	1020	3							HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.0
M629T925_neg	629.2617	925	3							HMDB0040917	apus non-fluorescent chlorophyll c	C34H38N4O8	0.0
M644T833_neg	644.3192	833	3						Alkaloids	HMDB0013055	droxy-9-deoxy-delta12-PGD2)-glu	C30H51N3O10S	4.8
M645T981_neg	645.4948	981	3							HMDB0012096	SM(d18:1/12:0)	C35H71N2O6P	4.5
M662T1007_neg	661.5047	1007	3							HMDB0295679	0/20:4(6Z,8E,10E,14Z)-2OH(5S,12	C40H70O7	0.2
M688T1015_neg	687.5173	1015	3							HMDB0296087	DG(19:0/PGJ2/0:0)	C42H72O7	4.6
M690T1022_neg	689.5362	1022	3						Terpenoids	HMDB0296095	0/20:4(6Z,8E,10E,14Z)-2OH(5S,12	C42H74O7	0.0
M690T882_neg	690.4336	882	3							HMDB0112275	PS(14:1(9Z)/15:0)	C35H66NO10P	2.2
M706T973_neg	705.5312	973	3							HMDB0296071	DG(19:0/PGE2/0:0)	C42H74O8	0.2
M763T908_neg	763.4172	908	3							HMDB0264167	9Z,12Z)/20:5(7Z,9Z,11E,13E,17Z)-3	C41H65O11P	2.5
M777T782_neg	777.3855	782	3							HMDB0014505	Vinorelbine	C45H54N4O8	1.8
M831T1029_neg	830.5556	1029	3						Amino acids and Peptides	HMDB0282101	PS(20:0/18:1(12Z)-O(9S,10R))	C44H82NO11P	0.4
M894T984_neg	893.6143	984	3							HMDB0061391	PC(DiMe(11,3)/DiMe(11,5))	C50H89NO10P	0.9
M74T342_pos	74.0598	342	3							HMDB0001106	3-Aminopropionaldehyde	C3H7NO	2.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M528T273_neg	528.1938	273	3	4.25E-01	1.29	FALSE	4.55E-02	1.96	TRUE	2.12E-04	3.13	TRUE	5.53E-01	0.80	FALSE
M531T990_neg	531.3329	990	3	5.08E-04	3.11	TRUE	1.36E-01	0.64	FALSE	1.88E-01	0.71	FALSE	1.10E-02	7.38	TRUE
M537T441_neg	537.1939	441	3	4.23E-22	0.07	TRUE	3.76E-02	1.42	FALSE	7.28E-07	2.09	TRUE	2.61E-01	2.20	FALSE
M545T538_neg	545.1294	538	3	7.31E-17	0.01	TRUE	6.95E-01	0.91	FALSE	2.18E-05	2.39	TRUE	1.07E-01	1.72	FALSE
M545T996_neg	545.3230	996	3	2.70E-17	2.57	TRUE	6.69E-04	0.73	FALSE	1.82E-06	1.51	TRUE	4.14E-01	0.91	FALSE
M554T486_neg	554.1409	486	3	2.18E-14	0.01	TRUE	8.57E-01	0.96	FALSE	1.85E-03	1.98	TRUE	1.03E-01	1.85	FALSE
M555T1001_neg	555.4267	1001	3	1.46E-12	4.22	TRUE	4.26E-01	0.87	FALSE	1.53E-01	1.23	FALSE	4.77E-04	1.99	TRUE
M558T176_neg	558.0646	176	3	6.01E-04	2.69	TRUE	7.56E-05	0.25	TRUE	5.75E-02	1.56	FALSE	5.06E-01	0.66	FALSE
M558T797_neg	558.2459	797	3	6.58E-01	0.94	FALSE	2.33E-05	1.92	TRUE	9.75E-06	1.78	TRUE	3.82E-01	0.85	FALSE
M559T384_neg	559.2367	384	3	5.32E-01	0.87	FALSE	1.29E-02	1.81	TRUE	2.67E-11	5.00	TRUE	3.13E-01	1.55	FALSE
M564T1038_neg	564.3309	1038	3	2.78E-03	5.34	TRUE	7.65E-05	0.11	TRUE	1.85E-01	0.58	FALSE	9.40E-01	0.92	FALSE
M565T1038_neg	565.3339	1038	3	1.75E-02	2.39	TRUE	5.30E-04	0.27	TRUE	2.87E-01	0.73	FALSE	9.93E-01	0.99	FALSE
M568T803_neg	568.2954	803	3	3.60E-06	2.64	TRUE	2.68E-02	0.58	TRUE	9.93E-01	1.00	FALSE	2.90E-01	0.83	FALSE
M568T1075_neg	568.3621	1075	3	1.88E-02	1.89	TRUE	4.72E-02	0.52	TRUE	6.02E-01	0.89	FALSE	7.11E-01	0.86	FALSE
M570T491_neg	570.1358	491	3	1.29E-18	0.00	TRUE	9.65E-01	1.01	FALSE	8.10E-03	1.62	TRUE	6.59E-01	0.59	FALSE
M574T767_neg	574.3022	767	3	2.14E-03	2.15	TRUE	2.07E-02	0.55	TRUE	3.10E-01	0.81	FALSE	5.61E-02	0.53	FALSE
M577T713_neg	577.1354	713	3	1.18E-31	0.23	TRUE	6.71E-01	1.04	FALSE	3.81E-09	1.63	TRUE	6.87E-01	1.07	FALSE
M579T723_neg	579.2865	723	3	9.67E-05	0.60	TRUE	5.56E-02	1.29	FALSE	5.58E-07	1.80	TRUE	7.44E-01	0.94	FALSE
M585T998_neg	585.2527	998	3	2.90E-12	2.86	TRUE	2.92E-02	0.75	FALSE	1.65E-04	1.55	TRUE	5.81E-01	1.09	FALSE
M589T463_neg	589.2353	463	3	5.85E-01	0.92	FALSE	6.22E-01	1.09	FALSE	1.53E-07	2.20	TRUE	2.59E-02	0.32	TRUE
M591T1020_neg	591.3188	1020	3	7.88E-15	0.20	TRUE	1.63E-02	1.48	FALSE	7.09E-02	1.28	FALSE	3.40E-02	0.30	TRUE
M629T925_neg	629.2617	925	3	1.22E-18	0.50	TRUE	3.17E-04	1.29	FALSE	2.50E-20	1.87	TRUE	1.53E-01	1.10	FALSE
M644T833_neg	644.3192	833	3	9.09E-12	0.33	TRUE	8.66E-03	1.47	FALSE	2.66E-03	1.45	FALSE	4.35E-02	1.86	TRUE
M645T981_neg	645.4948	981	3	1.83E-17	2.82	TRUE	1.63E-04	0.65	TRUE	1.33E-04	1.42	FALSE	2.81E-01	1.20	FALSE
M662T1007_neg	661.5047	1007	3	3.46E-03	1.46	FALSE	4.42E-05	0.51	TRUE	8.68E-02	0.83	FALSE	1.87E-05	2.49	TRUE
M688T1015_neg	687.5173	1015	3	1.77E-02	2.70	TRUE	6.74E-01	0.83	FALSE	6.28E-04	3.78	TRUE	4.08E-01	1.50	FALSE
M690T1022_neg	689.5362	1022	3	6.44E-07	1.93	TRUE	4.71E-09	0.43	TRUE	2.53E-03	1.39	FALSE	2.85E-01	0.66	FALSE
M690T882_neg	690.4336	882	3	6.37E-01	0.93	FALSE	9.49E-03	1.57	TRUE	2.82E-04	1.72	TRUE	5.94E-01	1.22	FALSE
M706T973_neg	705.5312	973	3	1.00E-04	2.06	TRUE	1.01E-03	0.48	TRUE	7.79E-01	0.96	FALSE	9.00E-01	0.97	FALSE
M763T908_neg	763.4172	908	3	1.52E-04	3.43	TRUE	4.75E-09	12.01	TRUE	7.35E-02	1.57	FALSE	7.85E-02	1.46	FALSE
M777T782_neg	777.3855	782	3	8.68E-10	2.74	TRUE	8.69E-01	1.03	FALSE	4.54E-05	1.71	TRUE	1.55E-01	1.29	FALSE
M831T1029_neg	830.5556	1029	3	3.82E-03	3.51	TRUE	2.41E-01	0.61	FALSE	5.60E-05	5.32	TRUE	3.37E-01	0.72	FALSE
M894T984_neg	893.6143	984	3	1.67E-04	2.45	TRUE	3.49E-01	0.81	FALSE	7.71E-03	1.69	TRUE	8.94E-02	1.57	FALSE
M74T342_pos	74.0598	342	3	5.69E-01	0.83	FALSE	2.52E-02	2.14	TRUE	9.67E-01	1.01	FALSE	5.69E-01	0.90	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M75T407_pos	75.0439	407	3							HMDB0244090	1,2-Dioxolane	C3H6O2	2.6
M79T171_1_pos	79.0211	171	3						Fatty acids	HMDB0002151	Dimethyl sulfoxide	C2H6OS	1.6
M85T488_pos	85.0646	488	3							HMDB0001184	Methyl propenyl ketone	C5H8O	1.7
M86T174_pos	86.0963	174	3						Alkaloids	HMDB0034301	Piperidine	C5H11N	1.9
M89T581_pos	89.0596	581	3							HMDB0000039	Butyric acid	C4H8O2	1.0
M97T525_pos	97.0648	525	3						Fatty acids	HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.3
M97T604_pos	97.0648	604	3							HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.3
M97T753_pos	97.1012	753	3							HMDB0254637	Methylenecyclohexane	C7H12	0.3
M100T684_pos	100.0757	684	3							HMDB0011749	2-Piperidinone	C5H9NO	0.4
M100T600_pos	100.0757	600	3							HMDB0011749	2-Piperidinone	C5H9NO	0.3
M123T562_pos	123.0805	562	3							HMDB0029306	4-Ethylphenol	C8H10O	0.7
M125T604_pos	125.0597	604	3							HMDB0000873	4-Methylcatechol	C7H8O2	0.0
M125T753_pos	125.0961	753	3						Fatty acids	HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.0
M129T809_pos	129.0910	809	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.2
M130T411_pos	130.0499	411	3						Amino acids and Peptides	HMDB0000267	Pyroglutamic acid	C5H7NO3	0.5
M132T124_pos	132.0661	124	3							HMDB0000725	4-Hydroxyproline	C5H9NO3	4.4
M134T655_pos	134.0600	655	3						Alkaloids	HMDB0244886	1H-Indol-2-ol	C8H7NO	0.2
M135T564_pos	135.0806	564	3							HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	1.2
M135T684_pos	135.1169	684	3						Terpenoids	HMDB0005805	p-Cymene	C10H14	0.2
M137T263_pos	137.0458	263	3						Alkaloids	HMDB0000157	Hypoxanthine	C5H4N4O	0.2
M141T562_pos	141.0910	562	3						Fatty acids	HMDB0032311	2,4-Hexadienyl acetate	C8H12O2	0.1
M142T464_pos	142.0863	464	3							HMDB0014731	Ethosuximide	C7H11NO2	0.2
M142T326_pos	142.0975	326	3							HMDB0003431	L-Histidinol	C6H11N3O	0.1
M143T604_pos	143.0703	604	3						Fatty acids	HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.2
M145T498_pos	145.1336	498	3							HMDB0002284	N-Acetylcadaverine	C7H16N2O	0.3
M146T473_pos	146.0271	473	3						Amino acids and Peptides				
M151T669_pos	151.1118	669	3						Terpenoids	HMDB0001878	Thymol	C10H14O	0.4
M153T1039_pos	153.1274	1039	3							HMDB0003450	(-)-trans-Carveol	C10H16O	0.2
M156T365_pos	156.1131	365	3						Amino acids and Peptides				
M157T170_pos	157.0352	170	3							HMDB0247204	Allantoxanamide	C4H4N4O3	2.7
M157T440_pos	157.0496	440	3							HMDB0029610	Ascladiol	C7H8O4	0.1
M157T686_pos	157.0859	686	3						Fatty acids	HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	0.1
M158T575_pos	158.0965	575	3							HMDB0302385	2,4-Dimethylquinoline	C11H11N	0.4
M158T623_pos	158.1176	623	3							HMDB0014447	Tranexamic Acid	C8H15NO2	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M75T407_pos	75.0439	407	3	8.03E-21	1.52	TRUE	2.59E-01	1.05	FALSE	2.91E-09	1.24	FALSE	4.03E-01	1.04	FALSE
M79T171_1_pos	79.0211	171	3	2.25E-17	0.34	TRUE	5.47E-01	0.94	FALSE	6.57E-01	0.96	FALSE	2.65E-01	0.64	FALSE
M85T488_pos	85.0646	488	3	1.30E-44	1.86	TRUE	5.35E-02	1.07	FALSE	4.55E-02	1.06	FALSE	5.02E-01	0.97	FALSE
M86T174_pos	86.0963	174	3	1.75E-02	1.21	FALSE	2.89E-01	0.91	FALSE	1.76E-16	1.89	TRUE	3.40E-01	1.08	FALSE
M89T581_pos	89.0596	581	3	3.23E-23	1.56	TRUE	1.09E-01	0.94	FALSE	4.96E-01	1.02	FALSE	7.62E-01	1.02	FALSE
M97T525_pos	97.0648	525	3	5.77E-48	1.68	TRUE	5.38E-01	1.02	FALSE	1.06E-01	1.04	FALSE	8.60E-01	0.99	FALSE
M97T604_pos	97.0648	604	3	7.81E-01	0.99	FALSE	4.26E-03	1.13	FALSE	1.71E-34	1.73	TRUE	8.40E-01	0.99	FALSE
M97T753_pos	97.1012	753	3	1.40E-02	0.92	FALSE	6.19E-03	1.10	FALSE	4.29E-33	1.56	TRUE	3.90E-01	0.95	FALSE
M100T684_pos	100.0757	684	3	8.25E-25	1.58	TRUE	6.56E-01	1.02	FALSE	5.93E-01	1.02	FALSE	9.10E-04	0.79	FALSE
M100T600_pos	100.0757	600	3	5.28E-30	1.70	TRUE	7.87E-01	1.01	FALSE	1.82E-01	1.05	FALSE	3.03E-03	0.88	FALSE
M123T562_pos	123.0805	562	3	2.47E-38	1.61	TRUE	6.08E-01	1.02	FALSE	1.68E-03	1.08	FALSE	1.70E-02	0.94	FALSE
M125T604_pos	125.0597	604	3	4.69E-02	0.91	FALSE	1.91E-02	1.12	FALSE	2.30E-35	1.87	TRUE	8.08E-01	0.98	FALSE
M125T753_pos	125.0961	753	3	3.72E-03	0.90	FALSE	5.41E-03	1.11	FALSE	3.34E-34	1.58	TRUE	1.88E-01	0.93	FALSE
M129T809_pos	129.0910	809	3	8.49E-01	0.97	FALSE	3.53E-02	0.66	TRUE	9.99E-01	1.00	FALSE	8.66E-01	1.05	FALSE
M130T411_pos	130.0499	411	3	2.62E-02	0.88	FALSE	7.24E-04	1.23	FALSE	4.10E-26	1.91	TRUE	7.07E-01	1.02	FALSE
M132T124_pos	132.0661	124	3	8.93E-05	1.68	TRUE	3.05E-01	0.88	FALSE	6.31E-01	1.05	FALSE	9.29E-01	1.00	FALSE
M134T655_pos	134.0600	655	3	1.01E-34	2.24	TRUE	8.60E-03	1.15	FALSE	4.83E-02	0.92	FALSE	5.38E-01	0.94	FALSE
M135T564_pos	135.0806	564	3	7.40E-01	1.03	FALSE	4.26E-01	1.08	FALSE	5.50E-12	1.89	TRUE	5.59E-02	0.75	FALSE
M135T684_pos	135.1169	684	3	1.63E-42	1.62	TRUE	2.79E-01	0.97	FALSE	7.68E-02	0.96	FALSE	1.50E-02	0.89	FALSE
M137T263_pos	137.0458	263	3	1.42E-50	0.05	TRUE	8.51E-03	1.27	FALSE	4.01E-05	1.38	FALSE	1.02E-01	1.66	FALSE
M141T562_pos	141.0910	562	3	4.21E-37	1.68	TRUE	5.23E-01	0.98	FALSE	3.19E-02	1.06	FALSE	2.05E-02	0.92	FALSE
M142T464_pos	142.0863	464	3	2.42E-38	1.66	TRUE	2.59E-01	0.96	FALSE	2.14E-02	1.06	FALSE	3.25E-02	0.90	FALSE
M142T326_pos	142.0975	326	3	2.05E-07	1.51	TRUE	1.79E-01	0.90	FALSE	3.33E-03	1.22	FALSE	1.42E-03	0.78	FALSE
M143T604_pos	143.0703	604	3	1.44E-01	0.94	FALSE	1.86E-02	1.11	FALSE	4.76E-35	1.78	TRUE	8.08E-01	0.98	FALSE
M145T498_pos	145.1336	498	3	1.14E-13	1.60	TRUE	1.83E-01	0.92	FALSE	1.06E-01	0.92	FALSE	4.27E-02	0.82	FALSE
M146T473_pos	146.0271	473	3	9.59E-02	0.90	FALSE	5.42E-01	1.04	FALSE	1.19E-17	1.68	TRUE	3.18E-01	0.88	FALSE
M151T669_pos	151.1118	669	3	1.73E-30	1.68	TRUE	5.38E-01	1.02	FALSE	4.80E-01	1.02	FALSE	4.42E-02	0.86	FALSE
M153T1039_pos	153.1274	1039	3	5.92E-15	1.84	TRUE	9.87E-08	0.67	FALSE	8.05E-01	0.99	FALSE	2.08E-04	1.30	FALSE
M156T365_pos	156.1131	365	3	6.57E-31	1.72	TRUE	3.78E-01	1.04	FALSE	9.99E-11	1.26	FALSE	1.10E-02	0.87	FALSE
M157T170_pos	157.0352	170	3	1.59E-90	0.06	TRUE	7.89E-01	1.01	FALSE	7.49E-03	0.89	FALSE	3.20E-01	0.87	FALSE
M157T440_pos	157.0496	440	3	1.33E-03	0.82	FALSE	6.34E-01	0.97	FALSE	3.58E-27	1.97	TRUE	3.78E-02	0.91	FALSE
M157T686_pos	157.0859	686	3	3.14E-01	0.97	FALSE	1.56E-02	1.08	FALSE	1.29E-39	1.60	TRUE	7.48E-02	0.92	FALSE
M158T575_pos	158.0965	575	3	1.75E-04	1.34	FALSE	1.27E-03	1.29	FALSE	2.31E-10	1.57	TRUE	2.03E-02	1.23	FALSE
M158T623_pos	158.1176	623	3	6.72E-04	1.35	FALSE	2.15E-02	1.24	FALSE	1.05E-09	1.64	TRUE	8.26E-02	0.77	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M159T332_pos	159.0289	332	3							HMDB0031210	Zymonic acid	C6H6O5	0.5
M159T609_pos	159.0441	609	3						Polyketides	HMDB0244101	1,2-Naphthoquinone	C10H6O2	0.4
M159T346_pos	159.1493	346	3						Fatty acids	HMDB0254871	Monopropionylcadaverine	C8H18N2O	0.6
M160T162_pos	160.1332	162	3						Fatty acids	HMDB0000991	DL-2-Aminooctanoic acid	C8H17NO2	0.1
M161T659_pos	161.0961	659	3							HMDB0031567	3-Methyl-4-phenyl-3-buten-2-one	C11H12O	0.0
M163T745_pos	163.1329	745	3						Fatty acids	HMDB0033625	(3R,7R)-1,3,7-Octanetriol	C8H18O3	0.3
M167T1039_pos	167.1431	1039	3							HMDB0030002	(-)-Nopol	C11H18O	0.3
M168T153_pos	168.0656	153	3						Alkaloids	HMDB0001545	Pyridoxal	C8H9NO3	0.5
M169T455_pos	169.0971	455	3						Alkaloids	HMDB0001431	Pyridoxamine	C8H12N2O2	0.1
M171T753_pos	171.1016	753	3							HMDB0030471	1,4-Ipomeadiol	C9H14O3	0.0
M172T309_pos	172.0606	309	3						Amino acids and Peptides	HMDB0012289	Tetrahydrodipicolinate	C7H9NO4	0.7
M174T581_pos	174.0550	581	3							HMDB0000842	Quinaldic acid	C10H7NO2	0.3
M177T861_pos	177.0547	861	3							HMDB0029758	Herniarin	C10H8O3	0.3
M177T684_pos	177.1275	684	3							HMDB0031569	4-Methyl-1-phenyl-2-pentanone	C12H16O	0.4
M179T659_pos	179.1067	659	3							HMDB0002043	5-Phenylvaleric acid	C11H14O2	0.3
M180T544_pos	180.1020	544	3							HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	0.3
M181T946_pos	181.1588	946	3							HMDB0031181	Homodihydrojasmone	C12H20O	0.5
M182T416_pos	182.0922	416	3						Amino acids and Peptides				
M182T846_pos	182.1175	846	3							HMDB0033868	beta-O-Methylynephrine	C10H15NO2	0.2
M186T486_pos	186.0763	486	3							HMDB0244794	bicyclo[3.1.0]hexane-2,6-dicarbox	C8H11NO4	1.4
M186T181_pos	186.0874	181	3							HMDB0034912	hydro-1-methyl-4-oxo-1H-imidazo	C7H11N3O3	0.2
M186T676_pos	186.1125	676	3							HMDB0006348	Pseudoecgonine	C9H15NO3	0.4
M187T498_pos	187.1442	498	3							HMDB0033553	(Methylbutyl)nitrosoamino]-2-buta	C9H18N2O2	0.4
M187T987_pos	187.1693	987	3						Fatty acids	HMDB0000947	Undecanoic acid	C11H22O2	0.4
M188T507_pos	188.0706	507	3						Alkaloids	HMDB0000734	Indoleacrylic acid	C11H9NO2	0.1
M189T659_pos	189.0911	659	3							HMDB0029495	Trigoforin	C12H12O2	0.6
M190T750_pos	190.0499	750	3							HMDB0000715	Kynurenic acid	C10H7NO3	0.4
M191T363_pos	191.0453	363	3							HMDB0015491	Nitroxoline	C9H6N2O3	1.0
M191T396_pos	191.1169	396	3							HMDB0004095	5-Methoxytryptamine	C11H14N2O	5.0
M192T474_pos	192.0326	474	3						Amino acids and Peptides	HMDB0244750	Thiazolidinedicarboxylic acid, 2-me	C6H9NO4S	0.4
M195T684_pos	195.1380	684	3							HMDB0014018	4-Hydroxypropofol	C12H18O2	0.3
M195T1039_pos	195.1744	1039	3							HMDB0031846	Geranylacetone	C13H22O	0.5
M196T364_2_pos	196.0969	364	3							HMDB0014903	Metyrosine	C10H13NO3	0.2
M197T441_pos	197.0423	441	3							HMDB0247453	8-Nitroguanine	C5H4N6O3	2.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M159T332_pos	159.0289	332	3	4.90E-37	0.09	TRUE	9.02E-01	1.01	FALSE	8.59E-01	1.02	FALSE	2.17E-01	0.79	FALSE
M159T609_pos	159.0441	609	3	1.12E-08	0.78	FALSE	7.86E-02	1.08	FALSE	1.40E-36	1.82	TRUE	5.15E-01	0.97	FALSE
M159T346_pos	159.1493	346	3	4.26E-03	1.80	TRUE	6.09E-01	0.89	FALSE	7.21E-01	0.94	FALSE	1.16E-01	0.73	FALSE
M160T162_pos	160.1332	162	3	1.16E-01	1.08	FALSE	9.80E-01	1.00	FALSE	1.82E-20	1.57	TRUE	7.99E-02	0.90	FALSE
M161T659_pos	161.0961	659	3	1.03E-01	1.06	FALSE	5.26E-02	1.07	FALSE	3.49E-32	1.56	TRUE	7.98E-04	0.86	FALSE
M163T745_pos	163.1329	745	3	3.30E-05	1.46	FALSE	8.76E-02	1.17	FALSE	6.58E-06	0.70	FALSE	3.65E-07	44.69	TRUE
M167T1039_pos	167.1431	1039	3	5.91E-12	1.73	TRUE	7.60E-07	0.68	FALSE	8.77E-01	0.99	FALSE	8.49E-05	1.33	FALSE
M168T153_pos	168.0656	153	3	6.08E-02	0.79	FALSE	5.70E-01	0.93	FALSE	1.04E-06	1.76	TRUE	2.40E-01	0.74	FALSE
M169T455_pos	169.0971	455	3	1.86E-08	1.72	TRUE	2.12E-01	0.89	FALSE	7.78E-02	0.87	FALSE	1.85E-01	0.81	FALSE
M171T753_pos	171.1016	753	3	3.74E-02	0.93	FALSE	5.93E-03	1.11	FALSE	5.35E-34	1.61	TRUE	4.54E-01	0.95	FALSE
M172T309_pos	172.0606	309	3	6.12E-05	0.77	FALSE	8.71E-01	0.99	FALSE	3.23E-23	1.92	TRUE	5.50E-01	1.04	FALSE
M174T581_pos	174.0550	581	3	6.40E-01	1.02	FALSE	2.52E-01	1.04	FALSE	8.31E-33	1.59	TRUE	1.80E-01	0.94	FALSE
M177T861_pos	177.0547	861	3	9.36E-01	0.99	FALSE	9.85E-02	1.28	FALSE	1.45E-03	0.67	FALSE	5.75E-09	2.22	TRUE
M177T684_pos	177.1275	684	3	2.64E-37	1.56	TRUE	2.78E-01	0.97	FALSE	1.43E-01	0.97	FALSE	1.66E-02	0.91	FALSE
M179T659_pos	179.1067	659	3	3.81E-01	1.03	FALSE	5.23E-02	1.08	FALSE	2.55E-33	1.64	TRUE	1.06E-03	0.85	FALSE
M180T544_pos	180.1020	544	3	2.67E-03	0.83	FALSE	2.97E-02	1.15	FALSE	1.65E-24	1.92	TRUE	1.91E-02	0.84	FALSE
M181T946_pos	181.1588	946	3	1.47E-15	1.55	TRUE	1.16E-07	0.76	FALSE	3.09E-04	1.17	FALSE	5.42E-01	0.93	FALSE
M182T416_pos	182.0922	416	3	2.08E-14	0.61	TRUE	3.36E-01	0.94	FALSE	7.15E-08	1.33	FALSE	4.54E-01	1.09	FALSE
M182T846_pos	182.1175	846	3	1.29E-05	0.69	FALSE	7.26E-08	1.60	TRUE	2.08E-02	1.18	FALSE	1.08E-01	1.19	FALSE
M186T486_pos	186.0763	486	3	5.42E-01	0.96	FALSE	2.56E-01	1.09	FALSE	3.99E-19	1.85	TRUE	6.63E-01	0.98	FALSE
M186T181_pos	186.0874	181	3	2.93E-01	1.08	FALSE	9.64E-03	0.83	FALSE	1.16E-09	1.52	TRUE	5.72E-03	0.72	FALSE
M186T676_pos	186.1125	676	3	9.09E-01	1.01	FALSE	6.48E-03	1.16	FALSE	1.47E-19	1.54	TRUE	4.32E-01	0.92	FALSE
M187T498_pos	187.1442	498	3	2.33E-12	1.54	TRUE	1.77E-01	0.92	FALSE	2.68E-01	0.95	FALSE	3.27E-02	0.81	FALSE
M187T987_pos	187.1693	987	3	4.33E-06	1.78	TRUE	6.34E-02	0.79	FALSE	1.51E-01	1.16	FALSE	1.78E-01	0.76	FALSE
M188T507_pos	188.0706	507	3	3.34E-47	0.35	TRUE	1.28E-01	1.08	FALSE	2.86E-17	1.50	FALSE	5.40E-02	1.14	FALSE
M189T659_pos	189.0911	659	3	5.46E-02	1.07	FALSE	5.65E-02	1.07	FALSE	1.63E-32	1.57	TRUE	4.90E-03	0.88	FALSE
M190T750_pos	190.0499	750	3	7.83E-07	0.80	FALSE	1.61E-02	1.12	FALSE	1.06E-36	1.86	TRUE	5.16E-03	0.80	FALSE
M191T363_pos	191.0453	363	3	1.54E-05	0.84	FALSE	1.40E-01	1.06	FALSE	6.01E-41	1.88	TRUE	5.41E-01	1.03	FALSE
M191T396_pos	191.1169	396	3	5.93E-08	1.86	TRUE	6.06E-01	1.06	FALSE	7.84E-01	1.03	FALSE	8.87E-02	1.29	FALSE
M192T474_pos	192.0326	474	3	4.18E-02	0.87	FALSE	4.51E-01	1.05	FALSE	8.25E-18	1.75	TRUE	5.16E-01	0.92	FALSE
M195T684_pos	195.1380	684	3	2.66E-28	1.56	TRUE	4.81E-01	0.98	FALSE	4.61E-01	0.98	FALSE	2.49E-02	0.92	FALSE
M195T1039_pos	195.1744	1039	3	8.54E-12	1.66	TRUE	2.04E-07	0.69	FALSE	4.72E-01	0.96	FALSE	1.15E-03	1.25	FALSE
M196T364_2_pos	196.0969	364	3	1.57E-02	0.88	FALSE	9.61E-01	1.00	FALSE	1.56E-21	1.65	TRUE	1.15E-01	0.82	FALSE
M197T441_pos	197.0423	441	3	3.33E-06	1.33	FALSE	5.00E-02	0.89	FALSE	1.51E-21	1.76	TRUE	7.00E-03	1.12	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M197T580_pos	197.0955	580	3							HMDB0059631	Cis-stilbene oxide	C14H12O	3.1
M199T652_pos	199.0966	652	3							HMDB0004998	Guaifenesin	C10H14O4	0.5
M199T595_pos	199.1077	595	3							HMDB0014606	Metharbital	C9H14N2O3	0.2
M199T946_pos	199.1694	946	3						Fatty acids	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	0.6
M200T741_pos	200.1282	741	3							HMDB0006406	Ecgonine methyl ester	C10H17NO3	0.6
M201T1033_pos	201.1850	1033	3						Fatty acids	HMDB0000638	Dodecanoic acid	C12H24O2	0.4
M203T407_pos	203.0002	407	3							HMDB0240374	Benzoic acid sulfate	C7H6O5S	3.2
M203T792_pos	203.0915	792	3							HMDB0032306	Diethyl oxalpropionate	C9H14O5	0.4
M206T517_pos	206.0449	517	3							HMDB0000881	Xanthurenic acid	C10H7NO4	0.8
M207T544_pos	207.0765	544	3							HMDB0248299	Amidinophenylpyruvic acid	C10H10N2O3	0.6
M208T483_pos	208.0605	483	3						Alkaloids	HMDB0000978	-Aminophenyl)-2,4-dioxobutanoic	C10H9NO4	0.3
M209T594_2_pos	209.0381	594	3							HMDB0253686	Isoquinolinesulfonamide	C9H8N2O2S	0.8
M210T484_pos	210.1126	484	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.8
M210T330_pos	210.1127	330	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	1.3
M211T669_pos	211.1329	669	3							HMDB0032797	Jasmonic acid	C12H18O3	0.2
M212T401_pos	212.0924	401	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	3.2
M213T468_pos	213.1236	468	3							HMDB0011180	Prolylproline	C10H16N2O3	0.9
M213T684_pos	213.1487	684	3							HMDB0029388	Cucurbic acid	C12H20O3	0.7
M214T627_pos	214.0477	627	3							HMDB0032357	N-Lactoyl ethanolamine phosphate	C5H12NO6P	1.1
M214T575_pos	214.0864	575	3							HMDB0246312	4-(Phenylamino)benzoic acid	C13H11NO2	0.5
M215T1033_pos	215.2006	1033	3						Fatty acids	HMDB0000910	Tridecanoic acid	C13H26O2	0.4
M216T756_pos	216.1596	756	3							HMDB0013279	N-Nonanoylglycine	C11H21NO3	0.7
M217T531_pos	217.1549	531	3						Amino acids and Peptides	HMDB0029140	Valylvaline	C10H20N2O3	1.2
M218T539_pos	218.1386	539	3							HMDB0240784	O-Propanoyl-D-carnitine	C10H19NO4	0.3
M218T382_pos	218.1388	382	3							HMDB0240784	O-Propanoyl-D-carnitine	C10H19NO4	0.6
M218T362_pos	218.1578	362	3							HMDB0249477	Butylate	C11H23NOS	2.0
M219T308_pos	219.1341	308	3							HMDB0014515	Meprobamate	C9H18N2O4	0.9
M219T880_1_pos	219.1593	880	3						Fatty acids	HMDB0254850	2,3-Dihydroxypropyl octanoate	C11H22O4	0.8
M221T407_pos	221.0108	407	3							HMDB0240694	Methylpyrogallol sulfate 3	C7H8O6S	3.0
M222T752_pos	222.0763	752	3							HMDB0038990	Methyl 5-hydroxyoxindole-3-acetat	C11H11NO4	0.9
M222T666_pos	222.0763	666	3							HMDB0038990	Methyl 5-hydroxyoxindole-3-acetat	C11H11NO4	1.1
M223T410_pos	223.0716	410	3							HMDB0251436	Dioxidine	C10H10N2O4	1.0
M223T552_pos	223.1079	552	3							HMDB0028848	Glycyl-Phenylalanine	C11H14N2O3	0.9
M223T494_2_pos	223.1082	494	3							HMDB0028848	Glycyl-Phenylalanine	C11H14N2O3	2.2
M224T471_1_pos	224.0556	471	3							HMDB0004083	o-3-hydroxyphenyl)-2,4-dioxobut	C10H9NO5	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M197T580_pos	197.0955	580	3	2.24E-13	1.91	TRUE	4.18E-01	0.94	FALSE	1.39E-01	0.90	FALSE	3.52E-01	0.89	FALSE
M199T652_pos	199.0966	652	3	1.17E-14	1.64	TRUE	6.37E-01	1.03	FALSE	1.34E-01	1.08	FALSE	7.34E-02	0.78	FALSE
M199T595_pos	199.1077	595	3	2.96E-01	1.06	FALSE	6.41E-03	1.18	FALSE	1.38E-14	1.52	TRUE	8.15E-02	0.88	FALSE
M199T946_pos	199.1694	946	3	2.47E-14	1.51	TRUE	5.72E-06	0.79	FALSE	9.46E-05	1.19	FALSE	2.11E-01	0.86	FALSE
M200T741_pos	200.1282	741	3	1.51E-11	1.64	TRUE	2.78E-03	0.72	FALSE	1.66E-03	0.83	FALSE	3.91E-01	0.85	FALSE
M201T1033_pos	201.1850	1033	3	2.28E-07	1.55	TRUE	5.49E-05	0.70	FALSE	4.47E-01	1.06	FALSE	2.60E-01	1.15	FALSE
M203T407_pos	203.0002	407	3	1.04E-20	1.73	TRUE	3.73E-01	1.05	FALSE	8.53E-09	1.31	FALSE	6.87E-01	0.98	FALSE
M203T792_pos	203.0915	792	3	4.17E-04	0.68	FALSE	1.52E-01	1.18	FALSE	8.06E-13	0.47	TRUE	8.63E-01	1.06	FALSE
M206T517_pos	206.0449	517	3	5.59E-01	0.98	FALSE	8.88E-02	1.08	FALSE	1.06E-38	1.83	TRUE	4.72E-01	0.98	FALSE
M207T544_pos	207.0765	544	3	1.22E-02	1.11	FALSE	1.77E-01	1.06	FALSE	8.56E-38	1.78	TRUE	8.53E-01	1.01	FALSE
M208T483_pos	208.0605	483	3	4.83E-01	0.95	FALSE	2.95E-01	0.93	FALSE	2.34E-17	1.82	TRUE	2.54E-02	0.69	FALSE
M209T594_2_pos	209.0381	594	3	5.44E-02	1.15	FALSE	3.83E-01	1.07	FALSE	1.22E-12	1.61	TRUE	7.44E-01	1.02	FALSE
M210T484_pos	210.1126	484	3	1.29E-01	0.87	FALSE	3.71E-02	1.22	FALSE	6.49E-14	1.98	TRUE	5.67E-01	0.90	FALSE
M210T330_pos	210.1127	330	3	6.84E-02	0.89	FALSE	3.64E-01	0.94	FALSE	1.99E-21	1.79	TRUE	2.45E-01	0.95	FALSE
M211T669_pos	211.1329	669	3	5.72E-33	1.64	TRUE	3.19E-01	1.04	FALSE	1.40E-02	1.07	FALSE	2.80E-02	0.86	FALSE
M212T401_pos	212.0924	401	3	1.30E-02	0.86	FALSE	1.80E-01	1.09	FALSE	3.03E-17	1.64	TRUE	4.43E-01	0.94	FALSE
M213T468_pos	213.1236	468	3	2.38E-23	1.54	TRUE	1.06E-01	0.94	FALSE	8.64E-02	0.95	FALSE	1.39E-01	0.89	FALSE
M213T684_pos	213.1487	684	3	2.26E-39	1.64	TRUE	4.27E-01	0.98	FALSE	4.05E-01	0.98	FALSE	3.00E-03	0.88	FALSE
M214T627_pos	214.0477	627	3	2.25E-35	1.91	TRUE	8.27E-01	1.01	FALSE	9.87E-04	0.89	FALSE	5.99E-03	1.17	FALSE
M214T575_pos	214.0864	575	3	1.33E-03	1.28	FALSE	1.86E-03	1.28	FALSE	3.28E-11	1.60	TRUE	8.25E-03	1.25	FALSE
M215T1033_pos	215.2006	1033	3	2.55E-07	1.55	TRUE	2.84E-05	0.69	FALSE	4.62E-01	1.05	FALSE	3.64E-01	1.12	FALSE
M216T756_pos	216.1596	756	3	5.56E-11	1.53	TRUE	8.22E-03	1.18	FALSE	6.49E-01	0.98	FALSE	1.72E-02	0.88	FALSE
M217T531_pos	217.1549	531	3	2.46E-03	0.86	FALSE	3.69E-01	1.05	FALSE	7.37E-19	1.55	TRUE	3.58E-02	0.83	FALSE
M218T539_pos	218.1386	539	3	1.73E-02	0.78	FALSE	7.61E-01	1.03	FALSE	6.63E-12	2.01	TRUE	1.04E-01	0.83	FALSE
M218T382_pos	218.1388	382	3	5.94E-10	0.68	FALSE	1.07E-01	1.10	FALSE	1.59E-27	1.98	TRUE	4.19E-02	0.91	FALSE
M218T362_pos	218.1578	362	3	3.37E-12	1.41	FALSE	8.46E-04	1.18	FALSE	7.24E-20	1.52	TRUE	3.14E-01	1.06	FALSE
M219T308_pos	219.1341	308	3	2.36E-48	0.13	TRUE	6.31E-01	1.04	FALSE	6.91E-03	1.21	FALSE	2.73E-01	0.70	FALSE
M219T880_1_pos	219.1593	880	3	4.44E-01	1.33	FALSE	1.48E-01	0.45	FALSE	6.78E-02	1.84	FALSE	1.52E-02	0.29	TRUE
M221T407_pos	221.0108	407	3	5.31E-22	1.74	TRUE	7.34E-01	1.02	FALSE	1.03E-03	1.15	FALSE	5.11E-01	1.05	FALSE
M222T752_pos	222.0763	752	3	8.29E-01	0.99	FALSE	1.02E-01	1.11	FALSE	3.36E-20	1.78	TRUE	1.61E-01	0.90	FALSE
M222T666_pos	222.0763	666	3	5.16E-01	0.97	FALSE	4.39E-01	1.04	FALSE	1.69E-24	1.78	TRUE	7.98E-01	0.99	FALSE
M223T410_pos	223.0716	410	3	1.42E-01	0.92	FALSE	5.56E-01	1.04	FALSE	8.64E-25	1.86	TRUE	6.70E-01	0.98	FALSE
M223T552_pos	223.1079	552	3	3.67E-03	1.13	FALSE	3.72E-01	1.04	FALSE	2.57E-24	1.52	TRUE	9.59E-03	0.88	FALSE
M223T494_2_pos	223.1082	494	3	7.34E-43	0.14	TRUE	4.17E-01	1.08	FALSE	8.06E-05	1.35	FALSE	4.13E-02	0.71	FALSE
M224T471_1_pos	224.0556	471	3	4.28E-12	0.49	TRUE	8.22E-01	0.98	FALSE	2.08E-04	1.36	FALSE	2.49E-01	0.87	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M224T417_pos	224.1283	417	3							HMDB0015168	Cerulenin	C12H17NO3	0.6
M225T659_pos	225.1122	659	3							HMDB0030680	Diplosporin	C12H16O4	0.2
M226T368_pos	226.1076	368	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.9
M226T451_pos	226.1076	451	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.8
M228T634_pos	228.1596	634	3							HMDB0255213	OCTANOYL-L-HOMOSERINE LACTO	C12H21NO3	0.8
M230T570_pos	230.0428	570	3							HMDB0062576	phospho-beta-D-ribosylaminium(1	C5H12NO7P	1.6
M230T380_pos	230.1137	380	3							HMDB0028739	Asparaginyl-Proline	C9H15N3O4	0.5
M231T685_pos	231.1593	685	3							HMDB0000623	Dodecanedioic acid	C12H22O4	0.9
M231T491_pos	231.1705	491	3							HMDB0028920	Isoleucyl-Valine	C11H22N2O3	0.6
M233T458_pos	233.1497	458	3							HMDB0013075	Spermic acid 2	C10H20N2O4	0.4
M233T356_pos	233.1498	356	3							HMDB0013075	Spermic acid 2	C10H20N2O4	0.9
M234T473_pos	234.0432	473	3						Amino acids and Peptides	HMDB0258566	Sulbactam	C8H11NO5S	0.7
M234T380_pos	234.0878	380	3							HMDB0246289	idin-2-yl-[1,2,4]oxadiazol-5-yl)-but	C11H11N3O3	2.1
M237T448_pos	237.1599	448	3							HMDB0014859	Procaine	C13H20N2O2	0.4
M238T388_pos	238.0824	388	3							HMDB0246373	o-7-phenylpyrazolo[1,5-a][1,3,5]tr	C11H7N7	4.8
M239T574_1_pos	239.1028	574	3							HMDB0015084	Felbamate	C11H14N2O4	0.9
M240T701_pos	240.1595	701	3							HMDB0001937	Salbutamol	C13H21NO3	0.5
M243T659_pos	243.1228	659	3							HMDB0251246	Diethylene glycol dimethacrylate	C12H18O5	0.5
M243T1012_pos	243.1957	1012	3							HMDB0010730	3-Oxotetradecanoic acid	C14H26O3	1.0
M244T868_pos	244.1910	868	3						Fatty acids	HMDB0013286	N-Undecanoylglycine	C13H25NO3	0.9
M246T428_pos	246.1450	428	3							HMDB0028734	Asparaginylisoleucine	C10H19N3O4	0.7
M247T764_pos	247.1541	764	3							HMDB0000413	3-Hydroxydodecanedioic acid	C12H22O5	0.5
M249T793_pos	249.1123	793	3							HMDB0029575	-hydroxy-4-methoxy-6-(2-phenyle	C14H16O4	0.7
M252T485_pos	252.1709	485	3							HMDB0256787	Procainamide 4-hydroxylamine	C13H21N3O2	1.0
M254T495_pos	254.1026	495	3							HMDB0011716	N-Acetylvanilalanine	C12H15NO5	1.3
M254T385_pos	254.1134	385	3							HMDB0256959	Pyricarbate	C11H15N3O4	0.5
M254T889_pos	254.2480	889	3							HMDB0256086	Palmitoleamide	C16H31NO	0.7
M256T451_pos	256.0818	451	3							HMDB0304540	beta-D-ribosylnicotinate	C11H13NO6	1.1
M256T769_pos	256.0970	769	3							HMDB0014608	Ketorolac	C15H13NO3	0.9
M257T507_pos	257.0595	507	3							HMDB0258257	Serotonin O-sulfate	C10H12N2O4S	1.6
M258T923_pos	258.2793	923	3						Fatty acids				
M260T524_pos	260.1034	524	3							HMDB0014623	Lenalidomide	C13H13N3O3	1.6
M261T376_pos	261.1812	376	3							HMDB0014539	Carisoprodol	C12H24N2O4	1.3
M263T129_pos	263.1968	129	3							HMDB0244223	,13-Tetraoxa-7,16-diazacyclooctac	C12H26N2O4	1.0
M264T341_pos	264.0982	341	3							HMDB0255930	Olaquindox	C12H13N3O4	1.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M224T417_pos	224.1283	417	3	1.56E-12	1.57	TRUE	5.58E-01	1.04	FALSE	3.06E-01	1.05	FALSE	6.75E-01	1.05	FALSE
M225T659_pos	225.1122	659	3	9.81E-01	1.00	FALSE	8.48E-02	1.08	FALSE	5.70E-33	1.71	TRUE	6.96E-03	0.86	FALSE
M226T368_pos	226.1076	368	3	1.26E-05	0.82	FALSE	3.90E-02	1.10	FALSE	9.29E-35	1.81	TRUE	4.27E-01	0.98	FALSE
M226T451_pos	226.1076	451	3	3.99E-01	1.06	FALSE	1.50E-01	1.11	FALSE	5.25E-11	1.54	TRUE	2.02E-01	0.91	FALSE
M228T634_pos	228.1596	634	3	1.02E-19	1.73	TRUE	5.87E-01	1.03	FALSE	2.19E-02	1.11	FALSE	3.08E-02	0.75	FALSE
M230T570_pos	230.0428	570	3	3.54E-16	1.53	TRUE	5.08E-01	0.97	FALSE	1.76E-02	0.91	FALSE	1.37E-02	1.25	FALSE
M230T380_pos	230.1137	380	3	1.96E-05	0.80	FALSE	4.50E-01	1.04	FALSE	5.29E-25	1.73	TRUE	2.26E-01	0.96	FALSE
M231T685_pos	231.1593	685	3	2.15E-48	1.75	TRUE	9.65E-02	0.95	FALSE	3.25E-07	0.88	FALSE	3.97E-03	0.88	FALSE
M231T491_pos	231.1705	491	3	1.81E-30	0.17	TRUE	2.04E-01	1.15	FALSE	4.71E-03	1.29	FALSE	9.96E-02	0.57	FALSE
M233T458_pos	233.1497	458	3	3.99E-34	0.18	TRUE	5.14E-01	1.07	FALSE	1.34E-03	1.30	FALSE	2.51E-01	0.81	FALSE
M233T356_pos	233.1498	356	3	3.35E-25	0.14	TRUE	4.64E-01	1.10	FALSE	3.61E-02	1.26	FALSE	2.29E-01	0.63	FALSE
M234T473_pos	234.0432	473	3	1.55E-03	0.80	FALSE	4.17E-01	1.06	FALSE	1.60E-15	1.70	TRUE	6.46E-01	0.95	FALSE
M234T380_pos	234.0878	380	3	1.10E-01	0.87	FALSE	3.26E-01	1.09	FALSE	1.55E-15	1.94	TRUE	2.37E-02	0.89	FALSE
M237T448_pos	237.1599	448	3	3.47E-01	1.06	FALSE	4.99E-01	1.05	FALSE	5.80E-15	1.60	TRUE	4.24E-02	0.87	FALSE
M238T388_pos	238.0824	388	3	1.56E-02	0.82	FALSE	9.02E-01	1.01	FALSE	1.43E-13	1.81	TRUE	9.18E-02	0.81	FALSE
M239T574_1_pos	239.1028	574	3	4.07E-01	0.94	FALSE	8.63E-01	1.01	FALSE	1.69E-11	1.58	TRUE	2.92E-01	0.95	FALSE
M240T701_pos	240.1595	701	3	4.08E-19	1.55	TRUE	9.95E-01	1.00	FALSE	1.03E-01	1.06	FALSE	9.34E-04	0.79	FALSE
M243T659_pos	243.1228	659	3	3.45E-01	1.03	FALSE	5.93E-02	1.07	FALSE	3.43E-31	1.56	TRUE	5.42E-03	0.87	FALSE
M243T1012_pos	243.1957	1012	3	5.20E-04	1.75	TRUE	7.58E-01	0.95	FALSE	6.28E-03	1.46	FALSE	5.96E-01	1.03	FALSE
M244T868_pos	244.1910	868	3	6.15E-01	1.06	FALSE	9.30E-01	0.99	FALSE	2.07E-01	0.88	FALSE	5.50E-03	2.29	TRUE
M246T428_pos	246.1450	428	3	2.42E-32	0.20	TRUE	3.70E-01	1.09	FALSE	4.78E-05	1.40	FALSE	2.58E-01	0.86	FALSE
M247T764_pos	247.1541	764	3	1.02E-06	0.84	FALSE	2.44E-04	1.14	FALSE	1.06E-32	1.55	TRUE	6.33E-01	0.98	FALSE
M249T793_pos	249.1123	793	3	8.23E-09	0.78	FALSE	1.43E-09	1.30	FALSE	2.61E-25	1.56	TRUE	2.05E-01	0.94	FALSE
M252T485_pos	252.1709	485	3	5.71E-03	1.23	FALSE	3.31E-01	1.08	FALSE	8.16E-11	1.57	TRUE	9.16E-02	0.81	FALSE
M254T495_pos	254.1026	495	3	4.25E-01	1.04	FALSE	8.29E-01	1.01	FALSE	1.47E-23	1.72	TRUE	2.89E-02	0.84	FALSE
M254T385_pos	254.1134	385	3	1.71E-11	0.67	FALSE	4.68E-01	1.04	FALSE	2.86E-29	1.96	TRUE	3.91E-01	0.96	FALSE
M254T889_pos	254.2480	889	3	8.67E-05	2.37	TRUE	8.83E-01	1.03	FALSE	2.15E-01	1.25	FALSE	7.40E-01	0.94	FALSE
M256T451_pos	256.0818	451	3	6.59E-01	1.02	FALSE	4.06E-01	0.95	FALSE	1.80E-15	1.52	TRUE	2.32E-02	0.79	FALSE
M256T769_pos	256.0970	769	3	8.13E-01	0.99	FALSE	7.62E-02	1.08	FALSE	9.30E-23	1.52	TRUE	3.66E-01	0.93	FALSE
M257T507_pos	257.0595	507	3	1.66E-02	1.22	FALSE	2.16E-01	0.90	FALSE	1.77E-08	1.53	TRUE	2.39E-01	0.80	FALSE
M258T923_pos	258.2793	923	3	1.95E-03	1.68	TRUE	4.05E-01	0.87	FALSE	2.96E-01	1.16	FALSE	7.45E-01	0.91	FALSE
M260T524_pos	260.1034	524	3	3.33E-07	0.73	FALSE	3.03E-01	1.07	FALSE	3.47E-28	2.01	TRUE	3.03E-01	1.06	FALSE
M261T376_pos	261.1812	376	3	4.77E-19	1.61	TRUE	3.90E-01	1.04	FALSE	3.97E-15	1.43	FALSE	1.36E-01	1.12	FALSE
M263T129_pos	263.1968	129	3	3.71E-05	0.74	FALSE	1.76E-03	1.27	FALSE	1.53E-11	1.58	TRUE	5.70E-01	1.03	FALSE
M264T341_pos	264.0982	341	3	1.19E-01	0.90	FALSE	9.67E-01	1.00	FALSE	1.32E-20	1.83	TRUE	9.31E-01	1.00	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M264T554_pos	264.1093	554	3							HMDB0255538	Neplanocin A	C11H13N5O3	0.5
M265T432_pos	265.1548	432	3							HMDB0015568	Vorinostat	C14H20N2O3	0.4
M269T803_pos	269.1174	803	3							HMDB0032056	Eugenyl benzoate	C17H16O3	0.6
M269T348_pos	269.1499	348	3							HMDB0247322	(2-hydroxyethyl)amino-L-phenylal	C13H20N2O4	1.1
M273T972_pos	273.2215	972	3						Terpenoids	HMDB0006046	5a-Androst-3-en-17-one	C19H28O	0.7
M275T1033_2_pos	275.2733	1033	3							HMDB0035152	Digeranyl	C20H34	0.1
M277T894_pos	277.1903	894	3							HMDB0015555	Molindone	C16H24N2O2	2.6
M278T524_pos	278.1138	524	3							HMDB0254231	phosphonomethyl)-3-isoquinoline	C11H20NO5P	5.0
M279T620_pos	279.1705	620	3							HMDB0013243	Leucylphenylalanine	C15H22N2O3	0.8
M281T783_pos	281.1171	783	3							HMDB0015081	Phenprocoumon	C18H16O3	0.3
M283T406_pos	283.1299	406	3							HMDB0029073	Threonyltyrosine	C13H18N2O5	3.7
M287T1061_pos	287.2370	1061	3							HMDB0000305	Vitamin A	C20H30O	0.1
M288T522_pos	288.1802	522	3							HMDB0241685	3-Hydroxyhept-4-enoylcarnitine	C14H25NO5	1.4
M290T397_pos	290.0808	397	3						Amino acids and Peptides				
M294T381_pos	294.1546	381	3							HMDB0037840	N-(1-Deoxy-1-fructosyl)leucine	C12H23NO7	0.4
M297T544_pos	297.1811	544	3							HMDB0248879	Batelapine	C16H20N6	3.9
M298T856_pos	298.2743	856	3						Fatty acids	HMDB0013648	Palmitoleoylethanolamde	C18H35NO2	0.7
M303T946_pos	303.2319	946	3						Fatty acids	HMDB0001999	Eicosapentaenoic acid	C20H30O2	0.2
M303T983_pos	303.2319	983	3						Terpenoids	HMDB0001999	Eicosapentaenoic acid	C20H30O2	0.2
M304T595_pos	304.2120	595	3							HMDB0061634	3-hydroxyoctanoyl carnitine	C15H29NO5	0.5
M305T695_pos	305.1861	695	3							HMDB0259093	Tilisolol	C17H24N2O3	0.4
M305T1044_pos	305.2114	1044	3							HMDB0000309	lpha,16beta-Dihydroxyandrosteno	C19H28O3	0.8
M306T480_pos	306.1340	480	3							HMDB0031929	Zanthodioline	C16H19NO5	1.3
M307T690_pos	307.1084	690	3							HMDB0245142	oxy-1-naphthaldehyde salicyloylhy	C18H14N2O3	2.2
M309T824_pos	309.0872	824	3							HMDB0033459	Flazine	C17H12N2O4	0.6
M311T454_pos	311.1605	454	3							HMDB0250969	Delgocitini	C16H18N6O	3.0
M311T965_pos	311.2947	965	3							HMDB0002231	11Z-Eicosenoic acid	C20H38O2	0.7
M312T808_pos	312.1232	808	3							HMDB0030217	Launobine	C18H17NO4	0.6
M312T774_pos	312.1346	774	3							HMDB0249842	-7,8-dimethoxy-3,5-dihydro-2,3-be	C17H17N3O3	1.2
M313T716_pos	313.1072	716	3							HMDB0030679	Cabreuvin	C18H16O5	0.5
M315T701_pos	315.1230	701	3							HMDB0030567	(-)-3,4,9-Trimethoxypterocarpan	C18H18O5	0.9
M319T1014_pos	319.2266	1014	3						Terpenoids	HMDB0001337	Leukotriene A4	C20H30O3	0.6
M325T676_pos	325.1759	676	3							HMDB0255924	p-Hydroxyubenimex	C16H24N2O5	0.2
M326T541_pos	326.0378	541	3							HMDB0002377	Urothion	C11H11N5O3S2	0.7
M329T452_pos	329.1372	452	3							HMDB0250407	Columbianadin	C19H20O5	3.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M264T554_pos	264.1093	554	3	2.87E-02	0.88	FALSE	1.24E-07	1.37	FALSE	2.35E-27	1.93	TRUE	2.42E-01	1.07	FALSE
M265T432_pos	265.1548	432	3	5.19E-01	1.04	FALSE	2.42E-01	1.08	FALSE	7.83E-19	1.74	TRUE	1.24E-01	0.87	FALSE
M269T803_pos	269.1174	803	3	1.11E-29	1.64	TRUE	9.16E-01	1.00	FALSE	5.61E-07	1.18	FALSE	6.94E-02	1.10	FALSE
M269T348_pos	269.1499	348	3	3.94E-02	0.83	FALSE	3.88E-01	1.08	FALSE	9.08E-12	1.77	TRUE	8.37E-01	0.99	FALSE
M273T972_pos	273.2215	972	3	9.65E-09	1.55	TRUE	2.87E-03	0.81	FALSE	8.81E-04	1.24	FALSE	2.62E-02	1.19	FALSE
M275T1033_2_pos	275.2733	1033	3	8.98E-04	2.72	TRUE	1.03E-01	0.66	FALSE	7.13E-01	0.92	FALSE	7.58E-01	1.12	FALSE
M277T894_pos	277.1903	894	3	2.62E-11	1.90	TRUE	6.04E-04	0.75	FALSE	1.49E-02	1.21	FALSE	7.65E-01	1.04	FALSE
M278T524_pos	278.1138	524	3	3.41E-08	0.73	FALSE	3.74E-01	1.05	FALSE	2.67E-28	1.92	TRUE	7.37E-01	0.98	FALSE
M279T620_pos	279.1705	620	3	2.87E-03	0.68	FALSE	8.75E-01	0.98	FALSE	3.63E-14	2.64	TRUE	1.83E-02	0.69	FALSE
M281T783_pos	281.1171	783	3	1.51E-44	4.74	TRUE	4.64E-05	0.75	FALSE	8.44E-02	0.90	FALSE	7.97E-01	1.03	FALSE
M283T406_pos	283.1299	406	3	1.05E-30	0.28	TRUE	7.48E-01	1.03	FALSE	1.95E-03	1.25	FALSE	3.19E-01	1.21	FALSE
M287T1061_pos	287.2370	1061	3	1.46E-04	2.53	TRUE	6.00E-02	0.68	FALSE	5.01E-01	1.14	FALSE	8.34E-01	1.07	FALSE
M288T522_pos	288.1802	522	3	3.71E-01	1.12	FALSE	8.17E-02	1.24	FALSE	2.28E-16	2.86	TRUE	8.57E-01	0.99	FALSE
M290T397_pos	290.0808	397	3	1.46E-05	0.69	FALSE	3.62E-02	1.20	FALSE	3.48E-17	2.01	TRUE	2.49E-01	0.87	FALSE
M294T381_pos	294.1546	381	3	1.96E-10	0.01	TRUE	9.70E-01	1.01	FALSE	2.43E-01	1.35	FALSE	2.94E-01	0.81	FALSE
M297T544_pos	297.1811	544	3	9.24E-05	0.79	FALSE	9.86E-02	1.11	FALSE	4.06E-26	1.92	TRUE	2.80E-02	0.87	FALSE
M298T856_pos	298.2743	856	3	2.11E-10	2.79	TRUE	4.67E-03	0.68	FALSE	1.98E-01	1.17	FALSE	4.89E-01	1.17	FALSE
M303T946_pos	303.2319	946	3	1.93E-09	2.08	TRUE	1.29E-01	0.84	FALSE	2.61E-01	1.12	FALSE	7.59E-01	0.95	FALSE
M303T983_pos	303.2319	983	3	1.48E-07	2.78	TRUE	1.29E-01	0.77	FALSE	1.84E-02	1.44	FALSE	5.42E-01	1.09	FALSE
M304T595_pos	304.2120	595	3	2.01E-04	0.83	FALSE	1.53E-01	1.07	FALSE	2.10E-30	1.80	TRUE	5.16E-01	0.98	FALSE
M305T695_pos	305.1861	695	3	4.91E-02	1.18	FALSE	1.36E-03	0.77	FALSE	1.28E-09	1.62	TRUE	6.15E-01	0.92	FALSE
M305T1044_pos	305.2114	1044	3	1.36E-11	1.53	TRUE	1.36E-05	0.76	FALSE	2.95E-05	1.24	FALSE	5.47E-06	1.41	FALSE
M306T480_pos	306.1340	480	3	1.38E-01	0.92	FALSE	4.60E-03	1.17	FALSE	3.77E-26	1.79	TRUE	3.53E-01	1.04	FALSE
M307T690_pos	307.1084	690	3	1.26E-03	1.30	FALSE	2.56E-01	1.10	FALSE	2.43E-11	1.66	TRUE	4.73E-01	1.11	FALSE
M309T824_pos	309.0872	824	3	9.32E-02	1.19	FALSE	3.15E-01	1.11	FALSE	6.77E-20	2.72	TRUE	2.04E-01	0.92	FALSE
M311T454_pos	311.1605	454	3	1.14E-09	0.68	FALSE	1.59E-01	1.09	FALSE	2.06E-27	1.98	TRUE	1.85E-01	0.93	FALSE
M311T965_pos	311.2947	965	3	5.33E-05	1.75	TRUE	3.75E-02	0.77	FALSE	5.25E-01	1.08	FALSE	5.06E-02	1.29	FALSE
M312T808_pos	312.1232	808	3	3.26E-01	0.94	FALSE	6.06E-01	0.97	FALSE	3.62E-14	1.58	TRUE	5.62E-01	1.10	FALSE
M312T774_pos	312.1346	774	3	1.45E-03	0.84	FALSE	1.48E-02	1.15	FALSE	4.57E-20	1.63	TRUE	3.59E-01	0.93	FALSE
M313T716_pos	313.1072	716	3	3.01E-12	0.71	FALSE	1.44E-01	1.07	FALSE	1.56E-29	1.71	TRUE	1.56E-01	1.08	FALSE
M315T701_pos	315.1230	701	3	3.49E-51	2.76	TRUE	5.14E-03	0.88	FALSE	5.84E-02	1.08	FALSE	4.65E-01	0.93	FALSE
M319T1014_pos	319.2266	1014	3	5.09E-05	1.42	FALSE	1.94E-06	0.65	TRUE	2.44E-01	1.09	FALSE	8.42E-01	0.98	FALSE
M325T676_pos	325.1759	676	3	8.96E-14	1.69	TRUE	5.74E-09	0.68	FALSE	5.28E-01	0.97	FALSE	3.53E-01	0.90	FALSE
M326T541_pos	326.0378	541	3	9.02E-02	1.12	FALSE	1.74E-01	1.10	FALSE	2.30E-21	1.93	TRUE	3.36E-01	0.91	FALSE
M329T452_pos	329.1372	452	3	2.66E-10	0.15	TRUE	6.40E-01	1.12	FALSE	7.80E-01	1.06	FALSE	9.28E-01	0.99	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M330T687_pos	330.2279	687	3							HMDB0013202	6-Keto-decanoylcarnitine	C17H31NO5	1.1
M333T1057_pos	333.2404	1057	3							HMDB0259700	1-piperidinyl)(1,2,4)triazolo(1,5-a)p	C17H28N6O	2.1
M335T1068_pos	335.1518	1068	3							HMDB0041826	Amifloxacin	C16H19FN4O3	1.3
M341T497_pos	341.2074	497	3							HMDB0060574	Perindoprilat	C17H28N2O5	1.0
M341T942_pos	341.3529	942	3						Fatty acids				
M344T354_pos	344.1350	354	3							HMDB0037845	N-(1-Deoxy-1-fructosyl)tyrosine	C15H21NO8	3.0
M345T953_pos	345.3015	953	3							HMDB0031923	10,20-Dihydroxyeicosanoic acid	C20H40O4	4.5
M347T970_pos	347.2208	970	3							HMDB0000015	Cortexolone	C21H30O4	2.6
M351T988_pos	351.1806	988	3							HMDB0034915	Calonectrin	C19H26O6	1.0
M353T960_pos	353.2474	960	3							HMDB0242660	2,3,4-tetrahydronaphthalene-6-yl	C24H32O2	0.3
M354T595_1_pos	354.1451	595	3							HMDB0248684	nyl)-1,2,4-oxadiazol-3-yl)phenoxy)	C19H19N3O4	0.7
M354T595_2_pos	354.1916	595	3							HMDB0241202	7E)-Undeca-2,5,7-trienedioylcarni	C18H27NO6	1.4
M357T985_pos	357.2787	985	3						Terpenoids	HMDB0002007	Tetracosahexaenoic acid	C24H36O2	0.3
M361T671_pos	361.1397	671	3							HMDB0006045	Dityrosine	C18H20N2O6	0.8
M369T967_pos	369.3841	967	3						Fatty acids				
M371T960_2_pos	371.2581	960	3						Terpenoids	HMDB0000476	3-Oxo-4,6-choladienoic acid	C24H34O3	0.0
M375T1025_pos	375.2893	1025	3						Terpenoids	HMDB0000308	3b-Hydroxy-5-cholenoic acid	C24H38O3	0.2
M376T580_pos	376.1572	580	3							HMDB0254099	Linifani	C21H18FN5O	1.1
M381T121_pos	381.0797	121	3						Carbohydrates				
M381T581_pos	381.1127	581	3							HMDB0015541	Meticillin	C17H20N2O6S	3.3
M383T1010_pos	383.2944	1010	3							HMDB0036368	(4,8,12-trimethyl-3,7,11-tridecatri	C26H38O2	0.2
M385T960_pos	385.2737	960	3						Terpenoids	HMDB0034952	Persicaxanthin	C25H36O3	0.1
M395T908_pos	395.1966	908	3							HMDB0249406	Brucine	C23H26N2O4	0.1
M396T714_pos	396.2317	714	3							HMDB0257030	Quinagolida	C20H33N3O3S	0.4
M397T1034_pos	397.3069	1034	3							HMDB0241955	N-Oleoyl Asparagine	C22H40N2O4	2.1
M401T1011_pos	401.3049	1011	3							HMDB0005814	Testosterone enanthate	C26H40O3	0.2
M403T960_pos	403.2844	960	3						Terpenoids	HMDB0000541	b-Hydroxy-3-oxo-5b-cholanoic aci	C25H38O4	0.4
M411T805_pos	411.1919	805	3							HMDB0042005	Quinaprilat	C23H26N2O5	1.2
M412T818_2_pos	412.3063	818	3							HMDB0013335	-Hydroxyhexadecadienoylcarnitin	C23H41NO5	1.2
M416T819_pos	416.2564	819	3							HMDB0255109	N-Demethyl Mifepristone	C28H33NO2	4.9
M416T904_pos	416.3525	904	3							HMDB0034731	Tomatidine	C27H45NO2	0.5
M417T732_pos	417.1811	732	3							HMDB0250142	Agelin	C24H29ClO4	3.9
M419T925_pos	419.3158	925	3						Terpenoids	HMDB0012515	10-HETE	C26H42O4	0.4
M427T776_pos	427.2478	776	3							HMDB0240225	Oxatomide	C27H30N4O	3.4
M430T773_pos	430.3314	773	3							HMDB0062336	N-Oleoyl phenylalanine	C27H43NO3	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M330T687_pos	330.2279	687	3	1.42E-02	1.39	FALSE	3.11E-02	1.33	FALSE	7.21E-18	3.40	TRUE	6.08E-01	0.94	FALSE
M333T1057_pos	333.2404	1057	3	4.32E-01	1.48	FALSE	8.49E-01	0.87	FALSE	4.35E-03	4.21	TRUE	5.90E-01	0.77	FALSE
M335T1068_pos	335.1518	1068	3	2.06E-01	1.27	FALSE	3.29E-02	0.63	TRUE	6.80E-02	1.35	FALSE	4.51E-01	1.35	FALSE
M341T497_pos	341.2074	497	3	6.29E-03	0.82	FALSE	1.91E-02	1.19	FALSE	3.84E-16	1.76	TRUE	6.95E-01	1.04	FALSE
M341T942_pos	341.3529	942	3	4.65E-04	5.23	TRUE	2.83E-01	0.66	FALSE	1.12E-01	1.72	FALSE	7.94E-01	0.92	FALSE
M344T354_pos	344.1350	354	3	1.42E-06	0.06	TRUE	9.00E-01	1.05	FALSE	8.13E-01	1.08	FALSE	1.13E-01	1.16	FALSE
M345T953_pos	345.3015	953	3	2.75E-05	1.85	TRUE	3.96E-02	0.75	FALSE	5.33E-02	1.27	FALSE	9.58E-01	1.01	FALSE
M347T970_pos	347.2208	970	3	3.60E-27	1.96	TRUE	2.66E-05	0.80	FALSE	9.14E-04	1.16	FALSE	5.08E-04	0.70	FALSE
M351T988_pos	351.1806	988	3	1.96E-01	0.90	FALSE	3.02E-01	1.09	FALSE	9.76E-08	1.48	FALSE	1.10E-02	0.63	TRUE
M353T960_pos	353.2474	960	3	1.02E-14	1.40	FALSE	6.54E-03	1.12	FALSE	9.19E-31	1.63	TRUE	5.05E-02	0.84	FALSE
M354T595_1_pos	354.1451	595	3	2.60E-01	0.95	FALSE	1.57E-01	1.08	FALSE	2.58E-29	1.79	TRUE	4.60E-01	1.05	FALSE
M354T595_2_pos	354.1916	595	3	4.70E-15	1.58	TRUE	3.62E-01	0.95	FALSE	2.70E-03	0.87	FALSE	5.39E-01	1.09	FALSE
M357T985_pos	357.2787	985	3	6.96E-19	1.60	TRUE	5.68E-10	0.74	FALSE	5.94E-01	0.98	FALSE	4.74E-01	1.08	FALSE
M361T671_pos	361.1397	671	3	1.48E-03	0.85	FALSE	4.12E-01	1.04	FALSE	5.23E-27	1.75	TRUE	1.16E-01	0.89	FALSE
M369T967_pos	369.3841	967	3	5.22E-04	4.71	TRUE	6.63E-01	0.85	FALSE	4.29E-01	1.29	FALSE	7.83E-01	0.92	FALSE
M371T960_2_pos	371.2581	960	3	7.19E-15	1.38	FALSE	2.05E-03	1.13	FALSE	4.24E-32	1.62	TRUE	4.28E-02	0.84	FALSE
M375T1025_pos	375.2893	1025	3	2.04E-25	1.59	TRUE	8.24E-12	0.77	FALSE	9.78E-01	1.00	FALSE	1.87E-01	1.08	FALSE
M376T580_pos	376.1572	580	3	7.98E-15	1.96	TRUE	1.71E-01	0.90	FALSE	1.39E-02	0.85	FALSE	2.55E-01	0.81	FALSE
M381T121_pos	381.0797	121	3	2.01E-19	0.24	TRUE	7.11E-02	1.26	FALSE	5.57E-02	1.23	FALSE	3.42E-01	1.30	FALSE
M381T581_pos	381.1127	581	3	6.18E-10	1.50	TRUE	1.21E-01	0.90	FALSE	4.46E-01	0.96	FALSE	4.86E-01	1.09	FALSE
M383T1010_pos	383.2944	1010	3	4.82E-20	1.70	TRUE	2.61E-08	0.76	FALSE	7.64E-02	1.08	FALSE	6.73E-01	0.97	FALSE
M385T960_pos	385.2737	960	3	1.16E-15	1.49	FALSE	1.88E-02	1.12	FALSE	1.43E-25	1.63	TRUE	4.03E-02	0.81	FALSE
M395T908_pos	395.1966	908	3	1.31E-02	1.46	FALSE	7.35E-02	0.76	FALSE	5.34E-04	1.60	TRUE	1.97E-01	1.05	FALSE
M396T714_pos	396.2317	714	3	1.67E-01	0.79	FALSE	2.77E-03	1.69	TRUE	2.68E-02	1.40	FALSE	4.30E-01	0.86	FALSE
M397T1034_pos	397.3069	1034	3	8.17E-12	1.58	TRUE	1.81E-05	0.77	FALSE	1.21E-01	0.92	FALSE	8.23E-01	1.02	FALSE
M401T1011_pos	401.3049	1011	3	1.65E-18	1.77	TRUE	6.61E-07	0.75	FALSE	3.26E-03	1.16	FALSE	1.35E-02	0.86	FALSE
M403T960_pos	403.2844	960	3	7.70E-13	1.38	FALSE	8.36E-04	1.16	FALSE	1.54E-29	1.65	TRUE	6.89E-02	0.83	FALSE
M411T805_pos	411.1919	805	3	5.39E-04	1.78	TRUE	9.84E-02	0.77	FALSE	1.56E-01	1.22	FALSE	8.36E-01	0.98	FALSE
M412T818_2_pos	412.3063	818	3	1.41E-04	1.34	FALSE	6.35E-04	1.30	FALSE	4.13E-22	2.12	TRUE	1.02E-02	1.16	FALSE
M416T819_pos	416.2564	819	3	1.74E-11	1.47	FALSE	3.92E-01	0.95	FALSE	8.63E-22	1.68	TRUE	9.57E-01	1.00	FALSE
M416T904_pos	416.3525	904	3	1.60E-01	1.90	FALSE	2.45E-02	0.28	TRUE	6.19E-01	1.21	FALSE	9.96E-01	1.00	FALSE
M417T732_pos	417.1811	732	3	3.14E-04	1.41	FALSE	7.18E-01	1.04	FALSE	1.98E-08	1.63	TRUE	3.51E-01	1.12	FALSE
M419T925_pos	419.3158	925	3	1.20E-14	1.51	TRUE	3.08E-04	0.84	FALSE	1.06E-01	0.93	FALSE	5.54E-01	1.05	FALSE
M427T776_pos	427.2478	776	3	9.15E-02	0.91	FALSE	1.20E-02	1.15	FALSE	4.55E-15	1.50	TRUE	5.72E-01	1.06	FALSE
M430T773_pos	430.3314	773	3	1.29E-02	1.46	FALSE	1.75E-03	0.64	TRUE	4.44E-01	0.91	FALSE	3.14E-01	0.87	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M431T789_1_pos	431.1926	789	3							HMDB0032622	Phenethyl rutinoside	C20H30O10	3.4
M433T794_pos	433.3508	794	3							HMDB0303271	Polyglycerol esters of fatty acids	C24H48O6	3.7
M438T1062_pos	438.2978	1062	3							HMDB0011152	LysoPE(P-16:0/0:0)	C21H44NO6P	0.1
M445T776_pos	445.2584	776	3							HMDB0033034	Antibiotic GR 95647X	C26H36O6	0.3
M445T1022_pos	445.3147	1022	3							HMDB0032521	Stearyl citrate	C24H44O7	2.9
M448T960_pos	448.3429	960	3							HMDB0062343	N-Stearoyl tyrosine	C27H45NO4	1.7
M457T1033_2_pos	457.3312	1033	3						Terpenoids				
M463T776_pos	463.2690	776	3							HMDB0010340	Retinyl beta-glucuronide	C26H38O7	0.1
M464T658_pos	464.3373	658	3							HMDB0240765	3-Hydroxyarachidonoylcarnitine	C27H45NO5	0.5
M466T945_pos	466.3167	945	3							HMDB0000138	Glycocholic acid	C26H43NO6	0.8
M468T895_pos	468.2132	895	3							HMDB0244824	rbonyl-Val-Ala-Asp(OMe)-fluorom	C22H30FN3O7	1.9
M472T792_pos	472.3425	792	3							HMDB0006510	Cervonyl carnitine	C29H45NO4	0.8
M472T854_pos	472.3427	854	3							HMDB0006510	Cervonyl carnitine	C29H45NO4	1.2
M473T646_pos	473.2399	646	3							HMDB0254095	Linagliptin	C25H28N8O2	2.0
M481T777_pos	481.2797	777	3							HMDB0255516	Neoandrographolide	C26H40O8	0.3
M482T997_pos	482.4191	997	3							HMDB0241601	(13Z)-Docos-13-enoylcarnitine	C29H55NO4	2.7
M486T852_pos	486.2599	852	3							HMDB0248754	o)-2-((2-(dimethylamino)ethyl)(m	C27H31N7O2	2.6
M489T669_pos	489.2696	669	3							HMDB0038732	a-Ionol O-[arabinosyl-(1->6)-gluco	C24H40O10	0.5
M489T985_pos	489.3574	985	3							HMDB0034036	Pitheduloside I	C30H48O5	0.1
M495T726_pos	495.2589	726	3							HMDB0033655	7-(3-methylpentanoate) 11-(3-hyd	C26H38O9	0.1
M511T1048_pos	511.3399	1048	3							HMDB0037893	Ganodermic acid TQ	C32H46O5	3.7
M529T1002_pos	529.3520	1002	3							HMDB0033079	Ganoderic acid V	C32H48O6	0.6
M538T580_pos	538.1925	580	3							HMDB0034773	,4S)-1,8-Epoxy-p-menthan-3-ol glu	C25H31NO12	1.1
M543T123_pos	543.1327	123	3						Carbohydrates				
M543T912_pos	543.2807	912	3							HMDB0010320	Cortolone-3-glucuronide	C27H42O11	1.2
M553T1000_pos	553.3754	1000	3							HMDB0036298	Cyclopassifloic acid E	C31H52O8	3.4
M575T1053_pos	575.3773	1053	3							HMDB0254924	iperidin-1-yl]methyl]-4-(3-fluoroph	C35H47FN4O2	3.0
M591T742_pos	591.3180	742	3							HMDB0004158	Urobilinogen	C33H42N4O6	0.4
M597T893_pos	597.3640	893	3							HMDB0004157	Stercobilinogen	C33H48N4O6	1.1
M605T674_pos	605.3436	674	3							HMDB0258791	Telinavir	C33H44N6O5	1.7
M605T609_pos	605.3437	609	3							HMDB0258791	Telinavir	C33H44N6O5	1.5
M617T734_pos	617.3312	734	3							HMDB0258543	Succinobucol	C35H52O5S2	2.8
M617T939_pos	617.3314	939	3							HMDB0258543	Succinobucol	C35H52O5S2	2.4
M621T780_pos	621.3652	780	3							HMDB0030011	ha,3beta,20S,22R,24S,25S)-Pubes	C34H52O10	3.0
M628T856_pos	628.3165	856	3						Amino acids and Peptides				

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M431T789_1_pos	431.1926	789	3	7.72E-01	0.97	FALSE	3.61E-04	1.40	FALSE	5.35E-30	3.28	TRUE	4.20E-01	0.89	FALSE
M433T794_pos	433.3508	794	3	7.51E-06	4.55	TRUE	9.89E-02	0.67	FALSE	3.59E-01	1.25	FALSE	5.08E-01	0.87	FALSE
M438T1062_pos	438.2978	1062	3	5.87E-02	1.78	FALSE	4.25E-01	0.75	FALSE	1.14E-05	3.74	TRUE	7.20E-01	0.91	FALSE
M445T776_pos	445.2584	776	3	2.82E-01	0.93	FALSE	5.33E-03	1.21	FALSE	7.51E-13	1.57	TRUE	4.17E-01	1.09	FALSE
M445T1022_pos	445.3147	1022	3	3.80E-02	0.89	FALSE	2.37E-01	1.07	FALSE	7.38E-01	1.02	FALSE	1.97E-08	10.93	TRUE
M448T960_pos	448.3429	960	3	9.91E-10	1.44	FALSE	5.03E-04	1.22	FALSE	8.77E-27	1.88	TRUE	4.51E-02	0.76	FALSE
M457T1033_2_pos	457.3312	1033	3	3.88E-05	1.61	TRUE	3.33E-01	0.89	FALSE	2.72E-03	1.34	FALSE	7.02E-01	0.90	FALSE
M463T776_pos	463.2690	776	3	2.10E-01	0.92	FALSE	4.46E-03	1.22	FALSE	4.13E-13	1.58	TRUE	4.26E-01	1.09	FALSE
M464T658_pos	464.3373	658	3	4.27E-11	1.53	TRUE	1.75E-02	0.86	FALSE	2.97E-03	1.17	FALSE	3.66E-01	0.87	FALSE
M466T945_pos	466.3167	945	3	1.02E-01	2.39	FALSE	3.58E-02	0.18	TRUE	1.11E-01	0.48	FALSE	6.94E-01	1.42	FALSE
M468T895_pos	468.2132	895	3	3.16E-01	1.06	FALSE	5.66E-01	0.97	FALSE	3.34E-16	1.61	TRUE	1.53E-03	0.70	FALSE
M472T792_pos	472.3425	792	3	3.14E-04	2.72	TRUE	3.49E-01	0.82	FALSE	6.33E-01	1.11	FALSE	7.74E-01	0.92	FALSE
M472T854_pos	472.3427	854	3	3.74E-14	2.71	TRUE	2.77E-01	0.89	FALSE	7.70E-01	0.97	FALSE	4.22E-01	0.92	FALSE
M473T646_pos	473.2399	646	3	2.03E-02	1.31	FALSE	1.23E-03	1.48	FALSE	1.04E-05	1.60	TRUE	7.03E-03	1.40	FALSE
M481T777_pos	481.2797	777	3	2.54E-01	0.93	FALSE	7.15E-03	1.20	FALSE	1.27E-12	1.54	TRUE	4.94E-01	1.07	FALSE
M482T997_pos	482.4191	997	3	1.01E-04	2.07	TRUE	8.51E-02	0.74	FALSE	8.58E-02	1.31	FALSE	6.73E-01	0.93	FALSE
M486T852_pos	486.2599	852	3	2.77E-08	0.72	FALSE	2.65E-06	1.31	FALSE	3.77E-18	1.60	TRUE	6.57E-01	1.03	FALSE
M489T669_pos	489.2696	669	3	1.76E-02	0.87	FALSE	6.08E-01	1.03	FALSE	1.58E-20	1.70	TRUE	2.63E-01	0.93	FALSE
M489T985_pos	489.3574	985	3	1.87E-04	1.75	TRUE	7.21E-01	1.05	FALSE	7.20E-01	1.05	FALSE	2.89E-01	1.51	FALSE
M495T726_pos	495.2589	726	3	1.41E-04	0.80	FALSE	2.91E-02	1.14	FALSE	2.84E-16	1.56	TRUE	8.55E-01	1.02	FALSE
M511T1048_pos	511.3399	1048	3	5.70E-07	1.61	TRUE	1.62E-02	0.80	FALSE	3.16E-01	0.92	FALSE	6.51E-03	1.24	FALSE
M529T1002_pos	529.3520	1002	3	4.65E-19	1.90	TRUE	5.32E-06	0.74	FALSE	4.03E-05	1.26	FALSE	7.77E-02	1.13	FALSE
M538T580_pos	538.1925	580	3	2.14E-08	1.70	TRUE	6.96E-01	1.04	FALSE	3.83E-04	1.32	FALSE	8.55E-01	0.97	FALSE
M543T123_pos	543.1327	123	3	3.57E-01	1.34	FALSE	1.85E-01	0.57	FALSE	9.69E-03	2.11	TRUE	7.23E-01	0.79	FALSE
M543T912_pos	543.2807	912	3	9.75E-05	0.81	FALSE	1.05E-01	1.09	FALSE	6.69E-22	1.66	TRUE	5.63E-03	1.12	FALSE
M553T1000_pos	553.3754	1000	3	4.06E-03	0.71	FALSE	6.86E-03	1.39	FALSE	4.53E-01	1.08	FALSE	4.69E-03	1.87	TRUE
M575T1053_pos	575.3773	1053	3	1.13E-08	1.73	TRUE	5.81E-04	0.74	FALSE	1.84E-01	0.90	FALSE	8.04E-03	1.27	FALSE
M591T742_pos	591.3180	742	3	8.64E-13	1.71	TRUE	1.92E-03	0.82	FALSE	5.43E-08	1.41	FALSE	3.88E-02	0.84	FALSE
M597T893_pos	597.3640	893	3	1.14E-05	0.70	FALSE	1.10E-03	1.31	FALSE	4.04E-09	1.54	TRUE	3.13E-01	1.25	FALSE
M605T674_pos	605.3436	674	3	5.53E-01	0.95	FALSE	1.65E-02	0.81	FALSE	1.16E-06	1.47	FALSE	3.91E-02	0.48	TRUE
M605T609_pos	605.3437	609	3	2.01E-02	1.28	FALSE	2.58E-02	0.80	FALSE	4.29E-05	1.48	FALSE	1.49E-02	0.37	TRUE
M617T734_pos	617.3312	734	3	2.61E-18	1.59	TRUE	2.05E-04	1.21	FALSE	5.57E-11	0.75	FALSE	3.66E-01	0.86	FALSE
M617T939_pos	617.3314	939	3	7.97E-23	0.43	TRUE	3.66E-04	1.30	FALSE	1.36E-01	1.10	FALSE	1.98E-01	1.21	FALSE
M621T780_pos	621.3652	780	3	2.93E-02	0.89	FALSE	3.85E-01	1.05	FALSE	1.77E-16	1.56	TRUE	6.35E-02	0.86	FALSE
M628T856_pos	628.3165	856	3	2.89E-02	1.15	FALSE	4.96E-01	1.05	FALSE	2.18E-18	1.73	TRUE	6.06E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M639T883_pos	639.3390	883	3						Amino acids and Peptides				
M652T760_pos	652.4062	760	3						Alkaloids				
M655T1056_pos	654.5461	1056	3							HMDB0290135	20:1/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-	C42H71NO4	0.8
M661T883_pos	661.3220	883	3							HMDB0001261	Coproporphyrinogen III	C36H44N4O8	1.7
M735T785_pos	735.3972	785	3						Polyketides				
M741T884_pos	741.4427	884	3						Terpenoids	HMDB0029623	Torvoside C	C39H64O13	0.9
M748T934_pos	748.4291	934	3						Amino acids and Peptides				
M760T842_pos	760.4286	842	3						Amino acids and Peptides				
M773T1031_pos	772.6089	1031	3						Alkaloids				
M776T944_pos	776.4599	944	3						Polyketides				
M795T960_pos	794.5569	960	3							HMDB0296091	DG(19:0/LTE4/0:0)	C45H79NO8S	3.8
M805T898_pos	805.4864	898	3						Amino acids and Peptides	HMDB0270658	PG(a-15:0/PGE2)	C41H73O13P	0.3
M886T810_pos	885.5120	810	3							HMDB0269934	20:4(5Z,8Z,11Z,14Z)/6 keto-PGF1al	C46H77O14P	0.4
M921T857_pos	921.4996	857	3							HMDB0276264	PI(16:2(9Z,12Z)/6 keto-PGF1alpha)	C45H77O17P	2.7
M61T170_pos	61.0104	170	3							HMDB0258994	Thiirane	C2H4S	3.9
M69T604_pos	69.0697	604	3							HMDB0249189	Bicyclo[2.1.0]pentane	C5H8	3.0
M69T665_pos	69.0697	665	3							HMDB0249189	Bicyclo[2.1.0]pentane	C5H8	2.9
M69T525_pos	69.0697	525	3							HMDB0249189	Bicyclo[2.1.0]pentane	C5H8	3.0
M72T492_pos	72.0806	492	3							HMDB0031641	Pyrrolidine	C4H9N	2.6
M72T403_pos	72.0806	403	3							HMDB0031641	Pyrrolidine	C4H9N	2.7
M73T525_pos	73.0646	525	3							HMDB0000246	Tetrahydrofuran	C4H8O	2.6
M81T561_pos	81.0697	561	3							HMDB0251502	1,3,5-Hexatriene	C6H8	2.1
M83T440_pos	83.0490	440	3							HMDB0013749	2-Methylfuran	C5H6O	1.9
M83T516_pos	83.0490	516	3							HMDB0013749	2-Methylfuran	C5H6O	1.8
M83T1024_pos	83.0602	1024	3							HMDB0015344	Fomepizole	C4H6N2	2.1
M83T687_pos	83.0854	687	3							HMDB0031544	3-Methylcyclopentene	C6H10	1.8
M85T616_pos	85.0283	616	3							HMDB0032330	ydroxy-2-butenoic acid gamma-lac	C4H4O2	1.7
M85T464_pos	85.0282	464	3							HMDB0032330	ydroxy-2-butenoic acid gamma-lac	C4H4O2	1.8
M86T397_pos	86.0963	397	3							HMDB0034301	Piperidine	C5H11N	1.7
M86T471_pos	86.0963	471	3							HMDB0034301	Piperidine	C5H11N	1.6
M86T567_pos	86.0963	567	3							HMDB0034301	Piperidine	C5H11N	1.5
M88T393_pos	88.0756	393	3							HMDB0001080	4-Aminobutyraldehyde	C4H9NO	1.3
M95T562_pos	95.0856	562	3							HMDB0031532	1-Methyl-1,3-cyclohexadiene	C7H10	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M639T883_pos	639.3390	883	3	1.71E-05	0.59	TRUE	1.97E-03	1.44	FALSE	7.27E-03	1.32	FALSE	1.56E-01	1.17	FALSE
M652T760_pos	652.4062	760	3	1.10E-05	1.60	TRUE	1.31E-01	0.85	FALSE	1.12E-02	1.26	FALSE	8.78E-02	0.90	FALSE
M655T1056_pos	654.5461	1056	3	6.65E-02	1.15	FALSE	9.48E-01	1.01	FALSE	2.72E-10	1.55	TRUE	9.94E-03	1.47	FALSE
M661T883_pos	661.3220	883	3	4.45E-08	0.65	TRUE	1.85E-05	1.39	FALSE	5.50E-01	1.04	FALSE	3.96E-02	1.29	FALSE
M735T785_pos	735.3972	785	3	5.38E-02	0.77	FALSE	8.06E-02	1.29	FALSE	6.25E-04	1.50	TRUE	3.55E-01	1.26	FALSE
M741T884_pos	741.4427	884	3	1.80E-02	3.33	TRUE	1.18E-01	0.49	FALSE	9.63E-01	1.02	FALSE	1.30E-01	0.07	FALSE
M748T934_pos	748.4291	934	3	6.84E-08	0.36	TRUE	3.09E-02	1.48	FALSE	5.68E-02	1.33	FALSE	9.73E-01	1.01	FALSE
M760T842_pos	760.4286	842	3	6.71E-02	1.31	FALSE	1.43E-01	1.23	FALSE	2.35E-05	1.75	TRUE	1.11E-01	1.29	FALSE
M773T1031_pos	772.6089	1031	3	1.42E-04	4.07	TRUE	6.33E-02	0.59	FALSE	4.58E-01	1.23	FALSE	8.62E-01	1.04	FALSE
M776T944_pos	776.4599	944	3	2.86E-13	0.50	TRUE	4.77E-04	1.36	FALSE	3.06E-06	1.43	FALSE	1.27E-02	1.20	FALSE
M795T960_pos	794.5569	960	3	1.98E-09	1.30	FALSE	1.59E-04	1.18	FALSE	8.54E-24	1.53	TRUE	6.24E-02	0.87	FALSE
M805T898_pos	805.4864	898	3	1.79E-19	0.26	TRUE	5.03E-03	1.41	FALSE	8.32E-04	1.41	FALSE	1.66E-02	1.38	FALSE
M886T810_pos	885.5120	810	3	9.95E-01	1.00	FALSE	1.81E-01	0.91	FALSE	1.16E-18	1.89	TRUE	8.22E-01	0.97	FALSE
M921T857_pos	921.4996	857	3	1.30E-01	1.16	FALSE	1.80E-03	1.41	FALSE	1.01E-09	1.77	TRUE	7.29E-03	1.31	FALSE
M61T170_pos	61.0104	170	3	1.25E-98	0.10	TRUE	5.85E-01	1.02	FALSE	2.27E-02	0.93	FALSE	5.12E-01	0.83	FALSE
M69T604_pos	69.0697	604	3	1.79E-01	0.95	FALSE	2.69E-02	1.09	FALSE	1.41E-35	1.68	TRUE	2.93E-01	0.95	FALSE
M69T665_pos	69.0697	665	3	8.48E-06	0.84	FALSE	2.10E-03	1.14	FALSE	7.37E-26	1.53	TRUE	2.26E-02	0.85	FALSE
M69T525_pos	69.0697	525	3	2.47E-42	1.61	TRUE	5.31E-01	1.02	FALSE	3.16E-03	1.07	FALSE	4.18E-01	0.97	FALSE
M72T492_pos	72.0806	492	3	6.94E-25	0.41	TRUE	1.92E-01	1.10	FALSE	6.78E-04	1.23	FALSE	4.25E-01	0.85	FALSE
M72T403_pos	72.0806	403	3	7.19E-38	0.32	TRUE	2.06E-01	1.09	FALSE	1.39E-03	1.20	FALSE	1.99E-01	0.84	FALSE
M73T525_pos	73.0646	525	3	2.19E-41	1.59	TRUE	4.21E-02	1.06	FALSE	4.36E-02	1.05	FALSE	7.47E-01	0.99	FALSE
M81T561_pos	81.0697	561	3	3.86E-34	1.58	TRUE	5.08E-01	0.98	FALSE	3.40E-02	1.06	FALSE	1.74E-02	0.92	FALSE
M83T440_pos	83.0490	440	3	3.24E-01	1.06	FALSE	9.56E-01	1.00	FALSE	3.16E-19	1.69	TRUE	2.18E-01	0.85	FALSE
M83T516_pos	83.0490	516	3	5.27E-04	0.88	FALSE	7.27E-02	1.07	FALSE	1.58E-43	1.82	TRUE	6.71E-03	0.92	FALSE
M83T1024_pos	83.0602	1024	3	9.98E-01	1.00	FALSE	4.58E-01	1.05	FALSE	1.02E-02	1.17	FALSE	2.58E-02	0.55	TRUE
M83T687_pos	83.0854	687	3	5.39E-01	0.98	FALSE	3.88E-02	1.07	FALSE	1.20E-36	1.52	TRUE	1.28E-01	0.93	FALSE
M85T616_pos	85.0283	616	3	8.13E-15	1.66	TRUE	3.46E-01	0.94	FALSE	1.41E-02	0.88	FALSE	1.32E-01	0.93	FALSE
M85T464_pos	85.0282	464	3	1.71E-18	1.99	TRUE	1.03E-01	0.89	FALSE	1.29E-02	0.86	FALSE	4.12E-01	0.85	FALSE
M86T397_pos	86.0963	397	3	9.99E-11	0.32	TRUE	6.87E-01	1.06	FALSE	2.43E-01	1.17	FALSE	1.25E-01	1.48	FALSE
M86T471_pos	86.0963	471	3	6.55E-21	0.59	TRUE	7.47E-01	1.02	FALSE	3.46E-05	1.20	FALSE	3.00E-01	0.87	FALSE
M86T567_pos	86.0963	567	3	2.21E-24	0.59	TRUE	1.02E-01	1.08	FALSE	5.29E-03	1.12	FALSE	5.14E-01	0.94	FALSE
M88T393_pos	88.0756	393	3	4.07E-29	1.98	TRUE	1.41E-02	1.13	FALSE	8.01E-05	0.84	FALSE	2.15E-01	0.88	FALSE
M95T562_pos	95.0856	562	3	6.45E-38	1.75	TRUE	7.73E-01	1.01	FALSE	1.33E-01	0.96	FALSE	1.01E-01	0.94	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M97T334_pos	97.0285	334	3							HMDB0032914	2-Furancarboxaldehyde	C5H4O2	0.5
M97T698_pos	97.1012	698	3							HMDB0254637	Methylenecyclohexane	C7H12	0.4
M99T1039_pos	99.1168	1039	3							HMDB0061783	(E)-Hept-2-ene	C7H14	0.2
M100T525_pos	100.0757	525	3							HMDB0011749	2-Piperidinone	C5H9NO	0.4
M100T581_pos	100.1121	581	3							HMDB0031404	Cyclohexylamine	C6H13N	0.6
M101T139_pos	101.0598	139	3							HMDB0000509	Senecioic acid	C5H8O2	0.5
M101T517_pos	101.0598	517	3							HMDB0000509	Senecioic acid	C5H8O2	0.5
M101T424_pos	101.0597	424	3							HMDB0000509	Senecioic acid	C5H8O2	0.4
M102T119_pos	102.0914	119	3							HMDB0012815	5-Aminopentanal	C5H11NO	0.7
M103T722_pos	103.0576	722	3							HMDB0031529	3-Methyl-2-butene-1-thiol	C5H10S	0.3
M106T161_pos	106.0499	161	3							HMDB0000187	L-Serine	C3H7NO3	0.4
M107T636_pos	107.0492	636	3							HMDB0006115	Benzaldehyde	C7H6O	0.7
M107T818_pos	107.0492	818	3							HMDB0006115	Benzaldehyde	C7H6O	0.4
M107T745_pos	107.0704	745	3							HMDB0034778	(2R*,3R*)-1,2,3-Butanetriol	C4H10O3	0.9
M109T603_pos	109.0648	603	3							HMDB0001858	p-Cresol	C7H8O	0.0
M110T631_pos	110.0965	631	3							HMDB0029722	1,2,5-Trimethyl-1H-pyrrole	C7H11N	0.6
M111T721_pos	111.0206	721	3							HMDB0252085	Ethylphosphonic acid	C2H7O3P	0.2
M111T441_pos	111.0441	441	3							HMDB0000957	Pyrocatechol	C6H6O2	0.1
M111T514_pos	111.0441	514	3							HMDB0000957	Pyrocatechol	C6H6O2	0.3
M111T742_pos	111.0441	742	3							HMDB0000957	Pyrocatechol	C6H6O2	0.4
M112T180_pos	112.0506	180	3							HMDB0000630	Cytosine	C4H5N3O	0.3
M112T471_pos	112.0757	471	3							HMDB0031163	N-Acetyl-2,3-dihydro-1H-pyrrole	C6H9NO	0.3
M113T105_pos	112.8957	105	3							HMDB0015106	Selenium Sulfide	SSe	1.2
M113T333_pos	113.0234	333	3							HMDB0000444	3-Furoic acid	C5H4O3	0.5
M113T475_pos	113.0597	475	3							HMDB0001164	trans-1,2-Dihydrobenzene-1,2-dio	C6H8O2	0.2
M115T472_pos	115.0390	472	3							HMDB0031859	Norfuraneol	C5H6O3	0.2
M115T526_pos	115.0754	526	3						Fatty acids	HMDB0000453	delta-Hexanolactone	C6H10O2	0.1
M115T474_pos	115.0753	474	3							HMDB0000453	delta-Hexanolactone	C6H10O2	0.1
M115T604_pos	115.0754	604	3						Fatty acids	HMDB0000453	delta-Hexanolactone	C6H10O2	0.1
M116T119_pos	116.0343	119	3							HMDB0246560	4-Oxo-2-azetidinecarboxylic acid	C4H5NO3	0.6
M116T418_pos	116.0707	418	3							HMDB0000162	L-Proline	C5H9NO2	0.4
M116T601_pos	116.0707	601	3							HMDB0000162	L-Proline	C5H9NO2	1.0
M116T674_1_pos	116.0707	674	3							HMDB0000162	L-Proline	C5H9NO2	0.8
M116T367_pos	116.0707	367	3							HMDB0000162	L-Proline	C5H9NO2	0.5
M116T305_pos	116.0707	305	3							HMDB0000162	L-Proline	C5H9NO2	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M97T334_pos	97.0285	334	3	9.87E-10	1.88	TRUE	1.24E-01	0.86	FALSE	5.76E-01	0.95	FALSE	3.51E-01	0.76	FALSE
M97T698_pos	97.1012	698	3	1.19E-13	1.51	TRUE	1.71E-01	1.07	FALSE	3.72E-01	1.04	FALSE	3.19E-01	0.87	FALSE
M99T1039_pos	99.1168	1039	3	9.70E-14	1.53	TRUE	3.18E-07	0.75	FALSE	7.12E-01	1.02	FALSE	3.23E-04	1.24	FALSE
M100T525_pos	100.0757	525	3	5.99E-31	1.56	TRUE	7.08E-01	0.99	FALSE	1.80E-01	1.04	FALSE	4.16E-03	0.88	FALSE
M100T581_pos	100.1121	581	3	1.32E-17	1.52	TRUE	6.01E-01	0.98	FALSE	3.69E-03	0.89	FALSE	8.88E-01	0.98	FALSE
M101T139_pos	101.0598	139	3	7.88E-01	1.02	FALSE	1.01E-02	1.18	FALSE	3.46E-18	1.71	TRUE	9.85E-01	1.00	FALSE
M101T517_pos	101.0598	517	3	1.17E-03	0.89	FALSE	1.89E-02	1.09	FALSE	3.08E-42	1.79	TRUE	4.50E-02	0.94	FALSE
M101T424_pos	101.0597	424	3	3.78E-29	1.56	TRUE	4.30E-01	1.03	FALSE	1.65E-05	1.13	FALSE	9.46E-01	1.00	FALSE
M102T119_pos	102.0914	119	3	1.37E-12	0.40	TRUE	2.21E-01	0.86	FALSE	2.24E-01	1.13	FALSE	5.28E-01	1.12	FALSE
M103T722_pos	103.0576	722	3	3.62E-02	1.87	TRUE	9.25E-01	0.98	FALSE	3.48E-01	1.27	FALSE	8.69E-01	1.07	FALSE
M106T161_pos	106.0499	161	3	1.81E-02	0.86	FALSE	9.88E-01	1.00	FALSE	1.37E-21	1.82	TRUE	1.88E-01	0.85	FALSE
M107T636_pos	107.0492	636	3	1.27E-03	1.66	TRUE	3.56E-02	0.72	FALSE	2.50E-01	0.86	FALSE	7.10E-01	0.91	FALSE
M107T818_pos	107.0492	818	3	4.64E-07	1.84	TRUE	3.96E-03	0.69	FALSE	3.99E-01	0.92	FALSE	9.29E-01	1.01	FALSE
M107T745_pos	107.0704	745	3	2.17E-01	1.16	FALSE	7.44E-01	1.05	FALSE	4.16E-01	1.09	FALSE	8.75E-07	28.14	TRUE
M109T603_pos	109.0648	603	3	1.51E-33	1.60	TRUE	5.33E-10	1.22	FALSE	7.45E-11	0.83	FALSE	1.42E-01	0.97	FALSE
M110T631_pos	110.0965	631	3	3.93E-12	1.71	TRUE	9.25E-01	1.01	FALSE	9.88E-06	1.33	FALSE	7.93E-01	1.05	FALSE
M111T721_pos	111.0206	721	3	6.42E-11	1.50	TRUE	2.63E-01	1.07	FALSE	2.75E-07	0.76	FALSE	7.28E-01	0.96	FALSE
M111T441_pos	111.0441	441	3	1.19E-02	0.87	FALSE	7.71E-01	0.98	FALSE	5.25E-29	1.98	TRUE	4.62E-02	0.92	FALSE
M111T514_pos	111.0441	514	3	3.21E-02	0.92	FALSE	5.05E-03	1.13	FALSE	1.23E-33	1.72	TRUE	7.63E-03	0.91	FALSE
M111T742_pos	111.0441	742	3	1.70E-03	1.50	FALSE	9.09E-01	0.98	FALSE	3.68E-08	0.52	TRUE	1.10E-01	1.52	FALSE
M112T180_pos	112.0506	180	3	8.86E-10	0.39	TRUE	2.42E-01	0.84	FALSE	7.58E-03	1.38	FALSE	3.09E-01	0.85	FALSE
M112T471_pos	112.0757	471	3	1.41E-13	1.66	TRUE	4.24E-01	1.05	FALSE	5.93E-02	1.11	FALSE	5.96E-01	0.97	FALSE
M113T105_pos	112.8957	105	3	8.49E-11	1.52	TRUE	2.66E-02	0.87	FALSE	1.75E-04	1.22	FALSE	4.16E-01	0.91	FALSE
M113T333_pos	113.0234	333	3	1.74E-35	0.11	TRUE	6.54E-01	1.05	FALSE	7.55E-01	0.97	FALSE	2.48E-01	1.55	FALSE
M113T475_pos	113.0597	475	3	4.33E-13	1.53	TRUE	8.20E-02	1.10	FALSE	4.94E-01	1.03	FALSE	2.88E-01	1.25	FALSE
M115T472_pos	115.0390	472	3	2.77E-49	0.30	TRUE	3.73E-02	0.88	FALSE	6.14E-07	1.27	FALSE	1.19E-05	1.44	FALSE
M115T526_pos	115.0754	526	3	1.83E-45	1.79	TRUE	2.24E-01	1.04	FALSE	6.53E-02	1.05	FALSE	3.71E-01	0.97	FALSE
M115T474_pos	115.0753	474	3	1.14E-21	1.76	TRUE	7.84E-01	0.98	FALSE	2.88E-07	0.79	FALSE	8.11E-01	1.04	FALSE
M115T604_pos	115.0754	604	3	3.04E-01	0.96	FALSE	1.14E-02	1.12	FALSE	1.04E-34	1.75	TRUE	3.80E-01	0.95	FALSE
M116T119_pos	116.0343	119	3	5.01E-06	1.46	FALSE	6.98E-01	0.97	FALSE	7.19E-01	0.98	FALSE	2.56E-02	0.65	TRUE
M116T418_pos	116.0707	418	3	1.60E-16	0.56	TRUE	3.15E-01	1.07	FALSE	3.53E-06	1.30	FALSE	8.74E-01	1.02	FALSE
M116T601_pos	116.0707	601	3	2.76E-16	0.38	TRUE	3.33E-01	1.11	FALSE	3.33E-01	1.09	FALSE	1.66E-01	1.28	FALSE
M116T674_1_pos	116.0707	674	3	5.60E-01	1.05	FALSE	6.37E-01	1.05	FALSE	9.47E-01	0.99	FALSE	2.69E-02	1.63	TRUE
M116T367_pos	116.0707	367	3	4.44E-11	0.50	TRUE	5.41E-01	1.06	FALSE	1.33E-04	1.38	FALSE	6.20E-02	0.54	FALSE
M116T305_pos	116.0707	305	3	4.72E-09	1.95	TRUE	2.68E-01	1.13	FALSE	1.04E-01	0.86	FALSE	7.01E-01	1.04	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M117T268_pos	117.0183	268	3							HMDB0000134	Fumaric acid	C4H4O4	0.7
M117T401_pos	117.0547	401	3							HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	0.4
M117T635_pos	117.0910	635	3							HMDB0000535	Caproic acid	C6H12O2	0.3
M118T507_pos	118.0652	507	3							HMDB0000738	Indole	C8H7N	0.6
M119T219_pos	119.0162	219	3							HMDB0251500	Divinyl sulfone	C4H6O2S	0.7
M119T659_pos	119.0857	659	3							HMDB0059837	Indane	C9H10	1.6
M120T530_pos	120.0808	530	3							HMDB0253472	Indoline	C8H9N	0.4
M121T200_pos	121.0397	200	3							HMDB0249016	Benzofurazan	C6H4N2O	0.3
M121T662_pos	121.0648	662	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.3
M121T328_pos	121.0648	328	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.4
M121T555_pos	121.0649	555	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.5
M121T497_pos	121.0648	497	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.3
M122T555_pos	122.0602	555	3							HMDB0004461	Benzamide	C7H7NO	1.0
M123T769_pos	123.0805	769	3							HMDB0029306	4-Ethylphenol	C8H10O	0.7
M123T812_pos	123.0806	812	3							HMDB0029306	4-Ethylphenol	C8H10O	1.0
M123T521_pos	123.0806	521	3							HMDB0029306	4-Ethylphenol	C8H10O	1.6
M123T666_pos	123.1169	666	3							HMDB0038140	Santene	C9H14	0.2
M124T778_pos	124.0758	778	3							HMDB0029300	p-Anisidine	C7H9NO	1.2
M126T469_pos	126.0550	469	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.1
M126T416_pos	126.0550	416	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.4
M127T461_pos	127.0754	461	3							HMDB0029582	Methyl sorbate	C7H10O2	0.0
M127T96_pos	127.1230	96	3							HMDB0242520	(2R,5R)-Hept-6-yne-2,5-diamine	C7H14N2	0.5
M128T648_pos	128.1070	648	3							HMDB0031667	Nor-psi-tropine	C7H13NO	0.3
M129T517_pos	129.0546	517	3							HMDB0031303	Osmundalactone	C6H8O3	0.2
M129T440_pos	129.0546	440	3							HMDB0031303	Osmundalactone	C6H8O3	0.1
M129T633_pos	129.0911	633	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.5
M129T1039_pos	129.0910	1039	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.3
M129T487_pos	129.1023	487	3							HMDB0256575	piperidine-1-carboxamide	C6H12N2O	0.5
M130T308_pos	130.0499	308	3						Amino acids and Peptides	HMDB0000267	Pyroglutamic acid	C5H7NO3	0.4
M131T96_pos	131.1292	96	3							HMDB0001432	Agmatine	C5H14N4	0.4
M132T507_pos	132.0808	507	3							HMDB0000466	3-Methylindole	C9H9N	0.1
M133T462_pos	133.0496	462	3							HMDB0000576	Monoethyl malonic acid	C5H8O4	0.5
M133T525_pos	133.0859	525	3							HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.1
M133T669_pos	133.1015	669	3							HMDB0029641	p-Mentha-1,3,5,8-tetraene	C10H12	2.1
M133T923_pos	133.1015	923	3							HMDB0029641	p-Mentha-1,3,5,8-tetraene	C10H12	2.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M117T268_pos	117.0183	268	3	1.49E-45	0.10	TRUE	9.61E-01	1.00	FALSE	2.61E-02	1.19	FALSE	2.88E-02	0.70	FALSE
M117T401_pos	117.0547	401	3	1.22E-15	0.59	TRUE	9.61E-02	1.11	FALSE	5.36E-11	1.43	FALSE	9.19E-01	0.99	FALSE
M117T635_pos	117.0910	635	3	3.04E-14	1.68	TRUE	3.78E-01	0.94	FALSE	7.04E-06	0.78	FALSE	6.07E-01	0.88	FALSE
M118T507_pos	118.0652	507	3	1.28E-03	0.61	TRUE	5.29E-02	0.72	FALSE	6.76E-01	0.95	FALSE	1.36E-01	1.11	FALSE
M119T219_pos	119.0162	219	3	2.85E-11	1.89	TRUE	2.75E-04	0.74	FALSE	1.24E-02	1.21	FALSE	1.11E-01	0.71	FALSE
M119T659_pos	119.0857	659	3	8.69E-03	1.10	FALSE	1.14E-01	1.06	FALSE	1.20E-28	1.52	TRUE	2.65E-03	0.85	FALSE
M120T530_pos	120.0808	530	3	1.62E-28	0.28	TRUE	2.03E-01	1.13	FALSE	6.32E-07	1.47	FALSE	3.51E-01	0.84	FALSE
M121T200_pos	121.0397	200	3	9.57E-27	0.31	TRUE	1.21E-02	1.24	FALSE	6.20E-03	1.22	FALSE	9.34E-01	0.99	FALSE
M121T662_pos	121.0648	662	3	1.28E-02	0.67	FALSE	6.38E-01	0.92	FALSE	1.58E-03	1.57	TRUE	5.28E-01	0.88	FALSE
M121T328_pos	121.0648	328	3	1.25E-12	1.91	TRUE	2.66E-01	0.91	FALSE	8.18E-03	1.21	FALSE	1.40E-01	0.91	FALSE
M121T555_pos	121.0649	555	3	1.52E-12	1.69	TRUE	7.04E-01	1.03	FALSE	4.06E-02	1.13	FALSE	3.14E-01	0.83	FALSE
M121T497_pos	121.0648	497	3	2.02E-01	0.91	FALSE	2.68E-01	1.09	FALSE	4.76E-18	1.84	TRUE	6.23E-02	0.84	FALSE
M122T555_pos	122.0602	555	3	2.72E-15	1.71	TRUE	5.72E-09	0.68	FALSE	2.84E-08	0.73	FALSE	6.46E-01	1.06	FALSE
M123T769_pos	123.0805	769	3	9.76E-07	1.32	FALSE	1.24E-14	1.55	TRUE	6.14E-04	0.85	FALSE	3.83E-01	0.97	FALSE
M123T812_pos	123.0806	812	3	5.84E-01	1.03	FALSE	2.90E-12	1.53	TRUE	5.99E-02	1.10	FALSE	9.93E-01	1.00	FALSE
M123T521_pos	123.0806	521	3	8.99E-24	1.77	TRUE	2.93E-01	1.05	FALSE	8.62E-10	0.76	FALSE	1.78E-01	1.21	FALSE
M123T666_pos	123.1169	666	3	3.67E-26	1.53	TRUE	5.09E-02	1.07	FALSE	6.06E-01	0.98	FALSE	5.32E-01	1.03	FALSE
M124T778_pos	124.0758	778	3	5.65E-16	1.87	TRUE	5.78E-01	1.04	FALSE	7.02E-02	1.12	FALSE	8.45E-01	1.02	FALSE
M126T469_pos	126.0550	469	3	2.60E-02	0.85	FALSE	7.91E-01	1.02	FALSE	5.33E-10	1.51	TRUE	1.23E-02	0.79	FALSE
M126T416_pos	126.0550	416	3	1.98E-07	0.64	TRUE	5.27E-01	1.06	FALSE	2.01E-03	1.25	FALSE	2.83E-01	1.04	FALSE
M127T461_pos	127.0754	461	3	2.67E-01	1.18	FALSE	1.26E-02	0.63	TRUE	1.36E-02	1.40	FALSE	2.81E-01	0.90	FALSE
M127T96_pos	127.1230	96	3	5.34E-03	1.46	FALSE	7.38E-02	0.72	FALSE	1.36E-07	1.93	TRUE	8.55E-02	2.22	FALSE
M128T648_pos	128.1070	648	3	3.08E-05	1.84	TRUE	3.41E-01	1.13	FALSE	2.92E-02	1.31	FALSE	7.46E-02	0.79	FALSE
M129T517_pos	129.0546	517	3	2.25E-05	0.73	FALSE	2.27E-01	1.10	FALSE	4.25E-13	1.66	TRUE	1.15E-02	0.93	FALSE
M129T440_pos	129.0546	440	3	9.24E-04	0.82	FALSE	8.93E-01	0.99	FALSE	2.22E-29	2.01	TRUE	8.80E-02	0.93	FALSE
M129T633_pos	129.0911	633	3	1.07E-57	1.90	TRUE	8.21E-02	1.05	FALSE	2.15E-06	0.89	FALSE	2.03E-01	1.07	FALSE
M129T1039_pos	129.0910	1039	3	3.05E-07	1.56	TRUE	8.27E-04	0.74	FALSE	2.03E-01	0.91	FALSE	4.06E-04	1.26	FALSE
M129T487_pos	129.1023	487	3	3.63E-35	0.50	TRUE	1.96E-01	1.06	FALSE	4.16E-04	1.15	FALSE	7.98E-01	1.03	FALSE
M130T308_pos	130.0499	308	3	6.66E-04	0.80	FALSE	2.56E-01	0.93	FALSE	3.53E-19	1.75	TRUE	7.96E-01	1.02	FALSE
M131T96_pos	131.1292	96	3	2.18E-03	0.78	FALSE	1.20E-02	0.81	FALSE	1.24E-13	1.76	TRUE	5.56E-01	0.88	FALSE
M132T507_pos	132.0808	507	3	1.84E-36	0.40	TRUE	4.01E-01	1.05	FALSE	7.31E-13	1.44	FALSE	6.88E-02	1.14	FALSE
M133T462_pos	133.0496	462	3	2.46E-04	1.47	FALSE	4.46E-01	1.08	FALSE	8.02E-09	0.58	TRUE	1.09E-01	0.81	FALSE
M133T525_pos	133.0859	525	3	4.83E-41	2.03	TRUE	3.61E-01	1.04	FALSE	9.41E-02	1.06	FALSE	1.44E-01	0.92	FALSE
M133T669_pos	133.1015	669	3	9.37E-28	1.79	TRUE	6.10E-03	1.13	FALSE	1.42E-01	1.06	FALSE	4.08E-01	0.91	FALSE
M133T923_pos	133.1015	923	3	6.62E-10	0.59	TRUE	8.51E-01	1.02	FALSE	7.74E-05	1.32	FALSE	2.25E-01	0.90	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M134T198_pos	134.0448	198	3							HMDB0000191	L-Aspartic acid	C4H7NO4	0.0
M134T119_pos	134.0448	119	3							HMDB0000191	L-Aspartic acid	C4H7NO4	0.3
M134T399_pos	134.0965	399	3							HMDB0012489	1,2,3,4-Tetrahydroisoquinoline	C9H11N	0.5
M135T658_pos	135.0442	658	3							HMDB0032469	Phthalide	C8H6O2	1.3
M135T652_pos	135.0805	652	3							HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	0.4
M136T435_pos	136.0618	435	3							HMDB0000034	Adenine	C5H5N5	0.2
M137T222_pos	137.0268	222	3							HMDB0244530	etrahydrothiophene-3-ol 1,1-dioxid	C4H8O3S	0.5
M137T399_pos	137.0458	399	3						Alkaloids	HMDB0000157	Hypoxanthine	C5H4N4O	0.1
M137T201_pos	137.0708	201	3							HMDB0003152	N-Methylnicotinamide	C7H8N2O	1.2
M137T400_pos	137.1075	400	3							HMDB0014918	Phenelzine	C8H12N2	1.0
M139T454_pos	139.0754	454	3							HMDB0004284	Tyrosol	C8H10O2	0.2
M139T585_pos	139.0866	585	3							HMDB0031850	2-Ethoxy-3-methylpyrazine	C7H10N2O	0.3
M139T591_pos	139.1118	591	3							HMDB0013824	2-Pentylfuran	C9H14O	0.2
M140T394_pos	140.0343	394	3						Alkaloids	HMDB0001232	4-Nitrophenol	C6H5NO3	0.4
M140T473_pos	140.0707	473	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.8
M140T264_pos	140.0819	264	3							HMDB0012234	Histidinal	C6H9N3O	0.3
M142T408_pos	142.1227	408	3							HMDB0030324	(R)-Pelletierine	C8H15NO	0.4
M143T464_1_pos	143.0703	464	3							HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.3
M143T335_pos	143.0704	335	3							HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.6
M144T405_pos	144.0656	405	3							HMDB0000894	Vinylacetylglycine	C6H9NO3	0.6
M144T556_pos	144.0807	556	3							HMDB0033115	6-Methylquinoline	C10H9N	0.6
M144T463_pos	144.1019	463	3						Fatty acids	HMDB0004827	Proline betaine	C7H13NO2	0.3
M144T145_pos	144.1019	145	3						Amino acids and Peptides	HMDB0004827	Proline betaine	C7H13NO2	0.2
M144T244_pos	144.1020	244	3							HMDB0004827	Proline betaine	C7H13NO2	0.6
M145T405_pos	145.0496	405	3							HMDB0000393	3-Hexenedioic acid	C6H8O4	0.7
M145T537_pos	145.0858	537	3							HMDB0245905	3-Hydroxypropyl methacrylate	C7H12O3	0.7
M146T487_pos	146.1176	487	3						Amino acids and Peptides	HMDB0001161	4-Trimethylammoniobutanoic acid	C7H15NO2	0.1
M146T379_pos	146.1176	379	3							HMDB0001161	4-Trimethylammoniobutanoic acid	C7H15NO2	0.4
M146T455_pos	146.1652	455	3						Alkaloids	HMDB0001257	Spermidine	C7H19N3	0.3
M147T330_pos	147.0444	330	3							HMDB0001218	Coumarin	C9H6O2	2.1
M147T431_pos	147.0474	431	3							HMDB0251128	Diallyl sulfone	C6H10O2S	0.1
M147T384_pos	147.0653	384	3							HMDB0000422	2-Methylglutaric acid	C6H10O4	0.9
M147T923_pos	147.1170	923	3							HMDB0246677	acyclo(5.4.0.02,6.03,10.05,9)unde	C11H14	1.3
M148T438_pos	148.0757	438	3							HMDB0005785	Indole-3-carbinol	C9H9NO	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M134T198_pos	134.0448	198	3	4.95E-02	0.82	FALSE	2.13E-02	0.78	FALSE	1.54E-12	1.99	TRUE	5.21E-01	0.96	FALSE
M134T119_pos	134.0448	119	3	7.80E-69	0.17	TRUE	9.73E-01	1.00	FALSE	4.64E-05	1.20	FALSE	3.68E-01	0.89	FALSE
M134T399_pos	134.0965	399	3	8.96E-12	0.28	TRUE	3.97E-01	0.87	FALSE	9.87E-03	1.42	FALSE	1.63E-01	0.78	FALSE
M135T658_pos	135.0442	658	3	1.16E-08	1.59	TRUE	9.46E-01	1.01	FALSE	1.21E-08	0.67	FALSE	2.56E-01	0.85	FALSE
M135T652_pos	135.0805	652	3	4.64E-24	1.81	TRUE	2.68E-01	1.06	FALSE	2.11E-01	1.06	FALSE	1.03E-01	0.82	FALSE
M136T435_pos	136.0618	435	3	3.58E-21	0.36	TRUE	4.98E-01	0.94	FALSE	6.32E-06	1.43	FALSE	1.13E-01	1.13	FALSE
M137T222_pos	137.0268	222	3	9.50E-08	1.97	TRUE	3.81E-02	0.78	FALSE	3.57E-03	1.36	FALSE	5.30E-01	0.80	FALSE
M137T399_pos	137.0458	399	3	3.77E-55	0.13	TRUE	6.06E-02	1.14	FALSE	1.68E-01	1.09	FALSE	1.34E-01	1.68	FALSE
M137T201_pos	137.0708	201	3	8.36E-01	0.99	FALSE	1.72E-02	1.16	FALSE	5.65E-18	1.64	TRUE	1.40E-01	0.93	FALSE
M137T400_pos	137.1075	400	3	3.06E-16	0.39	TRUE	7.99E-01	1.03	FALSE	1.87E-02	1.22	FALSE	5.40E-01	0.89	FALSE
M139T454_pos	139.0754	454	3	5.66E-31	1.61	TRUE	9.97E-01	1.00	FALSE	7.23E-07	1.16	FALSE	1.90E-01	0.89	FALSE
M139T585_pos	139.0866	585	3	2.27E-03	1.27	FALSE	1.23E-04	0.61	TRUE	1.75E-02	1.17	FALSE	3.35E-02	1.34	FALSE
M139T591_pos	139.1118	591	3	9.94E-19	1.61	TRUE	3.22E-01	0.95	FALSE	4.57E-04	1.16	FALSE	3.98E-02	0.85	FALSE
M140T394_pos	140.0343	394	3	9.05E-02	1.13	FALSE	7.10E-04	1.29	FALSE	1.03E-17	1.85	TRUE	3.14E-01	1.11	FALSE
M140T473_pos	140.0707	473	3	1.16E-05	0.56	TRUE	8.90E-01	1.02	FALSE	5.67E-02	1.24	FALSE	2.22E-01	0.91	FALSE
M140T264_pos	140.0819	264	3	2.57E-03	0.51	TRUE	7.15E-01	1.09	FALSE	9.92E-01	1.00	FALSE	2.15E-01	0.82	FALSE
M142T408_pos	142.1227	408	3	8.29E-04	0.48	TRUE	3.88E-01	0.82	FALSE	8.60E-01	1.03	FALSE	2.18E-01	0.50	FALSE
M143T464_1_pos	143.0703	464	3	8.89E-16	1.76	TRUE	5.90E-01	1.04	FALSE	3.80E-01	0.95	FALSE	6.68E-01	1.05	FALSE
M143T335_pos	143.0704	335	3	5.08E-10	1.73	TRUE	1.32E-01	0.88	FALSE	9.42E-01	0.99	FALSE	6.80E-01	0.92	FALSE
M144T405_pos	144.0656	405	3	1.00E-05	0.76	FALSE	8.00E-02	1.12	FALSE	6.47E-13	1.51	TRUE	7.56E-02	1.10	FALSE
M144T556_pos	144.0807	556	3	2.35E-02	0.86	FALSE	1.21E-01	1.11	FALSE	2.92E-27	2.12	TRUE	6.13E-03	0.88	FALSE
M144T463_pos	144.1019	463	3	6.98E-35	1.52	TRUE	2.53E-01	1.03	FALSE	7.78E-03	1.07	FALSE	6.81E-01	0.98	FALSE
M144T145_pos	144.1019	145	3	2.82E-04	1.66	TRUE	8.63E-01	0.98	FALSE	7.10E-01	1.04	FALSE	3.46E-01	1.53	FALSE
M144T244_pos	144.1020	244	3	7.96E-02	0.87	FALSE	9.64E-01	1.00	FALSE	2.35E-14	1.76	TRUE	5.95E-03	0.73	FALSE
M145T405_pos	145.0496	405	3	8.43E-03	0.38	TRUE	8.52E-01	1.07	FALSE	5.66E-01	0.84	FALSE	6.84E-01	1.12	FALSE
M145T537_pos	145.0858	537	3	2.27E-25	1.57	TRUE	2.60E-01	0.96	FALSE	2.59E-01	1.04	FALSE	8.46E-01	0.99	FALSE
M146T487_pos	146.1176	487	3	1.70E-05	0.44	TRUE	3.53E-01	0.84	FALSE	1.26E-01	1.27	FALSE	8.64E-01	0.86	FALSE
M146T379_pos	146.1176	379	3	5.03E-01	0.81	FALSE	7.88E-01	1.09	FALSE	5.37E-01	0.84	FALSE	1.04E-02	1.69	TRUE
M146T455_pos	146.1652	455	3	7.40E-02	1.20	FALSE	1.06E-05	0.61	TRUE	1.63E-05	1.50	FALSE	9.77E-01	1.00	FALSE
M147T330_pos	147.0444	330	3	1.03E-14	0.56	TRUE	8.57E-01	1.01	FALSE	6.59E-08	1.40	FALSE	3.87E-01	1.21	FALSE
M147T431_pos	147.0474	431	3	1.60E-31	2.15	TRUE	4.12E-02	0.90	FALSE	7.10E-01	0.98	FALSE	3.98E-02	0.80	FALSE
M147T384_pos	147.0653	384	3	1.24E-05	0.70	FALSE	3.02E-02	1.19	FALSE	1.89E-10	1.59	TRUE	3.43E-01	0.86	FALSE
M147T923_pos	147.1170	923	3	2.00E-11	0.49	TRUE	9.92E-01	1.00	FALSE	1.01E-04	1.40	FALSE	2.13E-02	0.78	FALSE
M148T438_pos	148.0757	438	3	1.84E-26	0.52	TRUE	2.32E-04	1.22	FALSE	2.50E-13	1.42	FALSE	2.96E-01	1.15	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M148T474_pos	148.0975	474	3						Amino acids and Peptides	HMDB0029449	-2-Amino-4-hydroxy-3-methylpent	C6H13NO3	4.6
M148T563_pos	148.1122	563	3							HMDB0029709	6,7,8-Tetrahydro-4-methylquinoli	C10H13N	0.6
M148T485_pos	148.1122	485	3							HMDB0029709	6,7,8-Tetrahydro-4-methylquinoli	C10H13N	0.8
M149T861_pos	149.0234	861	3							HMDB0256501	Phthalic anhydride	C8H4O3	0.3
M149T744_pos	149.0234	744	3							HMDB0256501	Phthalic anhydride	C8H4O3	0.4
M149T759_pos	149.0449	759	3							HMDB0000426	Citramalic acid	C5H8O5	2.9
M149T664_pos	149.0598	664	3							HMDB0000567	Cinnamic acid	C9H8O2	0.8
M149T1039_pos	149.1325	1039	3							HMDB0059834	Pentylbenzene	C11H16	0.2
M149T684_pos	149.1325	684	3							HMDB0059834	Pentylbenzene	C11H16	0.2
M150T343_pos	150.0774	343	3							HMDB0002099	6-Methyladenine	C6H7N5	0.2
M151T359_pos	151.0423	359	3							HMDB0037115	)1)-2-Hydroxy-4-(methylthio)butar	C5H10O3S	0.5
M152T524_pos	152.0343	524	3							HMDB0245945	3-Nitrobenzaldehyde	C7H5NO3	0.6
M152T283_pos	152.0568	283	3						Alkaloids	HMDB0000132	Guanine	C5H5N5O	0.5
M152T479_pos	152.0707	479	3						Alkaloids	HMDB0001859	Acetaminophen	C8H9NO2	0.6
M153T170_pos	153.0100	170	3							HMDB0249013	Benzodioxaphosphorin	C7H5O2P	0.2
M153T396_pos	153.0652	396	3						Alkaloids	HMDB0004193	1-Methyl-2-pyridone-5-carboxami	C7H8N2O2	4.3
M153T749_pos	153.0910	749	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.2
M153T652_pos	153.0910	652	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.2
M153T565_pos	153.0911	565	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.3
M155T524_pos	155.0699	524	3							HMDB0005784	Hydroxytyrosol	C8H10O3	2.4
M155T668_pos	155.0702	668	3							HMDB0005784	Hydroxytyrosol	C8H10O3	0.2
M155T410_pos	155.0815	410	3							HMDB0242137	xahydropyrrolo[1,2-a]pyrazine-1,4	C7H10N2O2	0.2
M155T204_pos	155.0815	204	3							HMDB0242137	xahydropyrrolo[1,2-a]pyrazine-1,4	C7H10N2O2	0.3
M155T763_pos	155.1067	763	3							HMDB0031302	Methyl 2-octynoate	C9H14O2	0.2
M155T576_pos	155.1067	576	3							HMDB0031302	Methyl 2-octynoate	C9H14O2	0.3
M155T986_pos	155.1431	986	3							HMDB0004043	alpha-Terpineol	C10H18O	0.3
M155T1039_pos	155.1795	1039	3							HMDB0029551	1-Undecene	C11H22	0.3
M156T110_pos	156.0768	110	3							HMDB0000177	L-Histidine	C6H9N3O2	0.5
M156T632_pos	156.1020	632	3							HMDB0030353	Arecoline	C8H13NO2	0.4
M156T675_pos	156.1020	675	3							HMDB0030353	Arecoline	C8H13NO2	0.4
M156T565_pos	156.1020	565	3							HMDB0030353	Arecoline	C8H13NO2	0.5
M156T412_pos	156.1383	412	3							HMDB0030326	Methylisopelletierine	C9H17NO	0.1
M156T105_pos	156.1496	105	3						Alkaloids	HMDB0244825	-3-(3-dimethylaminopropyl)carbo	C8H17N3	0.5
M157T356_pos	157.0972	356	3							HMDB0242468	(2-Ethylcrotonoyl)urea	C7H12N2O2	0.3
M157T486_pos	157.0973	486	3							HMDB0242468	(2-Ethylcrotonoyl)urea	C7H12N2O2	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M148T474_pos	148.0975	474	3	3.21E-04	0.66	TRUE	9.30E-01	1.01	FALSE	7.61E-02	1.19	FALSE	5.34E-02	0.87	FALSE
M148T563_pos	148.1122	563	3	1.22E-07	0.06	TRUE	9.29E-01	0.97	FALSE	2.48E-01	1.39	FALSE	2.44E-01	0.86	FALSE
M148T485_pos	148.1122	485	3	4.69E-09	0.23	TRUE	9.93E-01	1.00	FALSE	3.90E-02	1.45	FALSE	9.81E-02	0.85	FALSE
M149T861_pos	149.0234	861	3	5.63E-03	0.68	FALSE	1.64E-01	1.22	FALSE	8.03E-03	0.73	FALSE	2.19E-04	1.79	TRUE
M149T744_pos	149.0234	744	3	1.77E-12	1.20	FALSE	9.39E-01	1.00	FALSE	1.28E-12	0.85	FALSE	2.97E-09	6.42	TRUE
M149T759_pos	149.0449	759	3	4.58E-06	1.19	FALSE	4.58E-01	0.97	FALSE	7.16E-06	0.86	FALSE	2.99E-07	1.83	TRUE
M149T664_pos	149.0598	664	3	5.72E-12	1.58	TRUE	9.63E-01	1.00	FALSE	1.29E-04	1.23	FALSE	9.38E-01	1.01	FALSE
M149T1039_pos	149.1325	1039	3	2.27E-09	1.54	TRUE	1.09E-06	0.71	FALSE	2.56E-01	1.07	FALSE	2.06E-02	1.18	FALSE
M149T684_pos	149.1325	684	3	5.11E-25	1.51	TRUE	7.69E-01	0.99	FALSE	4.96E-02	0.94	FALSE	6.47E-01	0.98	FALSE
M150T343_pos	150.0774	343	3	4.03E-16	0.48	TRUE	8.66E-01	1.01	FALSE	1.89E-04	1.30	FALSE	4.71E-01	1.14	FALSE
M151T359_pos	151.0423	359	3	1.74E-13	1.61	TRUE	2.43E-07	0.74	FALSE	4.20E-01	0.96	FALSE	2.36E-02	0.85	FALSE
M152T524_pos	152.0343	524	3	1.55E-02	0.90	FALSE	4.26E-02	1.10	FALSE	3.58E-31	1.73	TRUE	3.20E-01	0.94	FALSE
M152T283_pos	152.0568	283	3	2.41E-02	1.19	FALSE	7.25E-06	1.44	FALSE	3.86E-21	2.08	TRUE	6.87E-01	0.94	FALSE
M152T479_pos	152.0707	479	3	9.50E-03	0.60	TRUE	8.60E-01	1.04	FALSE	8.93E-01	1.02	FALSE	3.62E-02	0.85	FALSE
M153T170_pos	153.0100	170	3	1.81E-52	0.15	TRUE	8.37E-01	1.01	FALSE	4.64E-01	0.96	FALSE	9.08E-01	0.99	FALSE
M153T396_pos	153.0652	396	3	3.33E-04	0.65	TRUE	8.24E-02	0.81	FALSE	5.21E-01	0.94	FALSE	9.10E-01	0.97	FALSE
M153T749_pos	153.0910	749	3	6.23E-02	0.88	FALSE	1.60E-02	1.20	FALSE	5.03E-12	1.57	TRUE	8.37E-01	0.95	FALSE
M153T652_pos	153.0910	652	3	3.48E-08	1.84	TRUE	6.20E-01	1.05	FALSE	7.48E-03	0.78	FALSE	6.88E-01	0.93	FALSE
M153T565_pos	153.0911	565	3	1.93E-01	1.10	FALSE	2.66E-01	1.09	FALSE	5.43E-11	1.58	TRUE	4.17E-02	0.75	FALSE
M155T524_pos	155.0699	524	3	1.15E-45	2.91	TRUE	3.98E-01	0.96	FALSE	1.77E-12	0.71	FALSE	8.90E-01	0.99	FALSE
M155T668_pos	155.0702	668	3	1.25E-19	2.17	TRUE	2.37E-01	1.10	FALSE	4.68E-01	0.95	FALSE	2.11E-01	0.81	FALSE
M155T410_pos	155.0815	410	3	2.34E-15	1.84	TRUE	3.67E-01	0.94	FALSE	6.46E-02	0.89	FALSE	4.84E-01	0.91	FALSE
M155T204_pos	155.0815	204	3	1.32E-01	0.92	FALSE	2.94E-01	1.06	FALSE	5.41E-20	1.68	TRUE	1.20E-01	0.91	FALSE
M155T763_pos	155.1067	763	3	3.98E-15	1.56	TRUE	4.60E-01	0.96	FALSE	3.88E-01	0.96	FALSE	4.40E-01	0.92	FALSE
M155T576_pos	155.1067	576	3	1.87E-13	1.52	TRUE	2.91E-01	1.06	FALSE	4.81E-01	0.97	FALSE	7.21E-01	1.05	FALSE
M155T986_pos	155.1431	986	3	3.91E-03	1.61	TRUE	2.32E-01	0.82	FALSE	7.15E-02	1.29	FALSE	1.52E-01	0.70	FALSE
M155T1039_pos	155.1795	1039	3	9.30E-13	1.51	TRUE	1.27E-08	0.73	FALSE	5.82E-01	0.97	FALSE	1.07E-02	1.18	FALSE
M156T110_pos	156.0768	110	3	3.06E-13	0.60	TRUE	3.73E-02	0.87	FALSE	1.42E-09	1.43	FALSE	8.69E-01	0.98	FALSE
M156T632_pos	156.1020	632	3	2.02E-16	1.59	TRUE	3.95E-02	1.12	FALSE	4.93E-05	1.20	FALSE	9.57E-01	1.00	FALSE
M156T675_pos	156.1020	675	3	2.17E-10	1.74	TRUE	3.44E-01	0.92	FALSE	1.24E-02	1.20	FALSE	6.08E-01	1.11	FALSE
M156T565_pos	156.1020	565	3	4.01E-02	4.11	TRUE	1.76E-01	2.35	FALSE	1.91E-01	0.50	FALSE	9.85E-01	1.00	FALSE
M156T412_pos	156.1383	412	3	1.13E-06	1.63	TRUE	9.79E-01	1.00	FALSE	1.35E-01	1.13	FALSE	3.40E-02	0.72	FALSE
M156T105_pos	156.1496	105	3	2.20E-11	0.54	TRUE	9.07E-01	1.01	FALSE	2.18E-02	1.19	FALSE	1.42E-02	1.45	FALSE
M157T356_pos	157.0972	356	3	2.49E-65	0.19	TRUE	2.48E-02	1.13	FALSE	3.53E-14	1.46	FALSE	1.57E-01	0.82	FALSE
M157T486_pos	157.0973	486	3	8.69E-54	0.15	TRUE	3.03E-03	1.24	FALSE	5.40E-05	1.28	FALSE	4.47E-01	1.33	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M157T524_pos	157.1336	524	3							HMDB0246231	3-(Dimethylamino)propyl)acrylam	C8H16N2O	0.4
M157T187_pos	157.1336	187	3						Alkaloids	HMDB0246231	3-(Dimethylamino)propyl)acrylam	C8H16N2O	0.5
M158T468_pos	158.0813	468	3							HMDB0000459	3-Methylcrotonylglycine	C7H11NO3	0.6
M158T511_pos	158.0814	511	3							HMDB0000459	3-Methylcrotonylglycine	C7H11NO3	1.2
M159T507_pos	159.0917	507	3							HMDB0243836	1-Benzylimidazole	C10H10N2	0.0
M160T388_1_pos	160.0759	388	3							HMDB0001190	Indoleacetaldehyde	C10H9NO	1.0
M160T388_2_pos	160.0969	388	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.4
M160T464_pos	160.0968	464	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.2
M160T481_pos	160.1332	481	3							HMDB0000991	DL-2-Aminooctanoic acid	C8H17NO2	0.2
M161T665_pos	161.0809	665	3							HMDB0000555	3-Methyladipic acid	C7H12O4	0.1
M161T467_pos	161.0808	467	3							HMDB0000555	3-Methyladipic acid	C7H12O4	0.5
M161T604_pos	161.0809	604	3						Fatty acids	HMDB0000555	3-Methyladipic acid	C7H12O4	0.2
M161T403_pos	161.0925	403	3							HMDB0003459	D-Alanyl-D-alanine	C6H12N2O3	2.7
M161T463_pos	161.1001	463	3							HMDB0031572	2-Methyl-4-propyl-1,3-oxathiane	C8H16OS	3.7
M161T139_pos	161.1286	139	3							HMDB0002038	N(6)-Methyllysine	C7H16N2O2	0.8
M162T699_pos	162.0551	699	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.7
M162T248_pos	162.0584	248	3							HMDB0248164	Allyl cysteine	C6H11NO2S	0.4
M163T658_pos	163.0390	658	3						Shikimates and Phenylpropanoids	HMDB0002149	3 Hydroxycoumarin	C9H6O3	0.4
M163T759_pos	163.0605	759	3							HMDB0034426	-1-Methylpropyl 1-propenyl disulfi	C7H14S2	2.6
M163T143_pos	163.0602	143	3							HMDB0000321	2-Hydroxyadipic acid	C6H10O5	0.5
M163T884_pos	163.0601	884	3						Carbohydrates	HMDB0000321	2-Hydroxyadipic acid	C6H10O5	0.2
M163T246_pos	163.0614	246	3							HMDB0243493	1,2,4-Benzotriazin-3-amine 1-oxide	C7H6N4O	0.1
M163T382_pos	163.1157	382	3							HMDB0032380	(S1)-Methoxy-3-heptanethiol	C8H18OS	3.3
M163T946_pos	163.1482	946	3							HMDB0013806	1,3-Diisopropylbenzene	C12H18	0.2
M164T517_pos	164.0707	517	3							HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.4
M164T365_pos	164.0735	365	3							HMDB0002169	S-(2-carboxypropyl)-Cysteamine	C6H13NO2S	2.6
M164T768_pos	164.0705	768	3							HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.9
M165T417_pos	165.0547	417	3							HMDB0000205	Phenylpyruvic acid	C9H8O3	0.6
M165T270_pos	165.0548	270	3							HMDB0000205	Phenylpyruvic acid	C9H8O3	0.8
M165T384_pos	165.0757	384	3							HMDB0000174	L-Fucose	C6H12O5	0.0
M165T994_pos	165.0910	994	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.1
M165T659_pos	165.0911	659	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.3
M165T764_pos	165.1275	764	3							HMDB0029653	ethoxy-1-methylethyl)-4-methylbe	C11H16O	0.4
M165T923_pos	165.1274	923	3							HMDB0029653	ethoxy-1-methylethyl)-4-methylbe	C11H16O	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M157T524_pos	157.1336	524	3	1.51E-06	0.62	TRUE	7.64E-01	1.03	FALSE	3.76E-03	1.28	FALSE	1.11E-03	1.43	FALSE
M157T187_pos	157.1336	187	3	1.41E-19	1.92	TRUE	1.28E-01	0.91	FALSE	1.59E-01	1.08	FALSE	5.07E-01	0.97	FALSE
M158T468_pos	158.0813	468	3	3.09E-16	1.59	TRUE	2.68E-01	1.06	FALSE	5.56E-02	1.09	FALSE	8.73E-01	0.99	FALSE
M158T511_pos	158.0814	511	3	1.11E-27	1.53	TRUE	2.95E-01	1.04	FALSE	1.85E-04	1.11	FALSE	9.08E-02	0.93	FALSE
M159T507_pos	159.0917	507	3	8.75E-47	0.38	TRUE	7.90E-02	1.09	FALSE	1.35E-18	1.50	FALSE	6.95E-02	1.15	FALSE
M160T388_1_pos	160.0759	388	3	4.19E-07	2.21	TRUE	2.43E-01	0.83	FALSE	2.66E-01	1.15	FALSE	2.17E-01	1.39	FALSE
M160T388_2_pos	160.0969	388	3	7.04E-20	1.82	TRUE	3.41E-01	1.06	FALSE	4.51E-02	0.90	FALSE	5.23E-01	1.06	FALSE
M160T464_pos	160.0968	464	3	5.40E-39	1.66	TRUE	7.45E-01	0.99	FALSE	2.08E-01	1.03	FALSE	5.03E-02	0.92	FALSE
M160T481_pos	160.1332	481	3	2.10E-14	1.69	TRUE	7.19E-01	1.02	FALSE	2.17E-03	1.18	FALSE	1.64E-01	0.84	FALSE
M161T665_pos	161.0809	665	3	3.31E-08	0.72	FALSE	9.59E-02	1.10	FALSE	8.19E-15	1.52	TRUE	1.73E-03	0.68	FALSE
M161T467_pos	161.0808	467	3	1.22E-13	1.95	TRUE	3.11E-01	1.09	FALSE	1.85E-01	0.91	FALSE	9.00E-01	0.98	FALSE
M161T604_pos	161.0809	604	3	2.22E-02	1.08	FALSE	1.90E-02	1.09	FALSE	4.71E-35	1.62	TRUE	9.37E-02	0.92	FALSE
M161T403_pos	161.0925	403	3	1.88E-03	1.18	FALSE	2.54E-01	1.07	FALSE	3.02E-16	1.52	TRUE	5.12E-01	0.93	FALSE
M161T463_pos	161.1001	463	3	1.10E-35	1.61	TRUE	5.56E-01	0.98	FALSE	4.27E-01	1.02	FALSE	4.07E-02	0.90	FALSE
M161T139_pos	161.1286	139	3	4.05E-03	1.55	TRUE	9.13E-01	0.98	FALSE	1.03E-02	1.40	FALSE	8.44E-01	1.05	FALSE
M162T699_pos	162.0551	699	3	6.52E-01	1.06	FALSE	7.81E-01	0.96	FALSE	1.01E-07	1.87	TRUE	3.05E-01	0.78	FALSE
M162T248_pos	162.0584	248	3	1.72E-02	0.59	TRUE	8.46E-01	1.05	FALSE	6.70E-02	1.41	FALSE	3.96E-01	0.87	FALSE
M163T658_pos	163.0390	658	3	1.97E-08	0.73	FALSE	2.61E-01	1.06	FALSE	6.71E-28	1.83	TRUE	2.35E-01	1.12	FALSE
M163T759_pos	163.0605	759	3	3.81E-06	1.27	FALSE	2.07E-01	0.94	FALSE	1.81E-03	0.87	FALSE	6.13E-03	1.72	TRUE
M163T143_pos	163.0602	143	3	1.40E-16	0.37	TRUE	4.22E-01	0.92	FALSE	1.52E-03	1.33	FALSE	8.53E-01	0.92	FALSE
M163T884_pos	163.0601	884	3	6.45E-03	3.37	TRUE	9.86E-02	0.55	FALSE	2.03E-01	0.64	FALSE	3.81E-01	0.50	FALSE
M163T246_pos	163.0614	246	3	8.25E-03	0.86	FALSE	9.54E-01	1.00	FALSE	2.21E-21	1.72	TRUE	3.28E-01	0.88	FALSE
M163T382_pos	163.1157	382	3	1.05E-39	0.18	TRUE	7.24E-01	1.03	FALSE	8.09E-02	1.13	FALSE	4.89E-01	1.10	FALSE
M163T946_pos	163.1482	946	3	2.53E-18	1.59	TRUE	1.38E-06	0.79	FALSE	8.85E-06	1.21	FALSE	2.49E-01	0.89	FALSE
M164T517_pos	164.0707	517	3	1.20E-01	1.11	FALSE	5.56E-07	0.72	FALSE	2.83E-17	1.74	TRUE	4.37E-01	0.93	FALSE
M164T365_pos	164.0735	365	3	1.70E-01	1.17	FALSE	4.40E-01	0.91	FALSE	2.73E-09	1.88	TRUE	2.58E-01	0.79	FALSE
M164T768_pos	164.0705	768	3	1.59E-08	1.42	FALSE	2.39E-17	0.46	TRUE	3.52E-07	1.32	FALSE	7.66E-01	0.97	FALSE
M165T417_pos	165.0547	417	3	3.34E-11	1.67	TRUE	5.56E-01	1.05	FALSE	2.63E-01	1.07	FALSE	7.57E-01	1.05	FALSE
M165T270_pos	165.0548	270	3	3.25E-01	0.94	FALSE	6.19E-01	0.97	FALSE	8.44E-14	1.59	TRUE	9.37E-01	0.98	FALSE
M165T384_pos	165.0757	384	3	9.88E-06	0.65	TRUE	1.82E-01	1.14	FALSE	2.80E-04	1.36	FALSE	6.10E-01	1.07	FALSE
M165T994_pos	165.0910	994	3	3.39E-13	1.52	TRUE	5.26E-03	0.86	FALSE	2.53E-01	1.05	FALSE	3.65E-02	1.13	FALSE
M165T659_pos	165.0911	659	3	3.01E-02	1.08	FALSE	1.18E-01	1.06	FALSE	2.20E-29	1.52	TRUE	3.67E-03	0.86	FALSE
M165T764_pos	165.1275	764	3	4.88E-06	1.38	FALSE	4.95E-01	1.05	FALSE	5.11E-02	0.89	FALSE	1.77E-02	1.73	TRUE
M165T923_pos	165.1274	923	3	3.28E-10	0.55	TRUE	9.51E-01	1.01	FALSE	2.71E-05	1.40	FALSE	5.24E-01	0.93	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M165T459_pos	165.1387	459	3							HMDB0039979	2,5-Diethyl-3,6-dimethylpyrazine	C10H16N2	0.3
M166T648_pos	166.0501	648	3							HMDB0003454	4-Pyridoxolactone	C8H7NO3	1.2
M166T477_pos	166.0501	477	3							HMDB0003454	4-Pyridoxolactone	C8H7NO3	1.1
M166T331_pos	166.0725	331	3							HMDB0000897	7-Methylguanine	C6H7N5O	0.7
M166T520_pos	166.0863	520	3							HMDB0000159	L-Phenylalanine	C9H11NO2	0.6
M166T599_pos	166.0863	599	3							HMDB0000159	L-Phenylalanine	C9H11NO2	0.3
M167T503_pos	167.0453	503	3							HMDB0245946	3-Nitrobenzaldoxime	C7H6N2O3	1.1
M167T759_pos	167.0555	759	3							HMDB0034394	S-Propyl 1-propanesulfinothioate	C6H14OS2	2.2
M167T571_pos	167.0816	571	3							HMDB0247540	3,4-Dihydroxyphenylacetamidine	C8H10N2O2	0.8
M167T714_pos	167.1067	714	3						Terpenoids	HMDB0004586	Perillic acid	C10H14O2	0.1
M167T591_pos	167.1067	591	3							HMDB0004586	Perillic acid	C10H14O2	0.2
M168T296_pos	168.0518	296	3							HMDB0000401	2,8-Dihydroxyadenine	C5H5N5O2	0.9
M168T240_pos	168.0656	240	3						Alkaloids	HMDB0001545	Pyridoxal	C8H9NO3	0.7
M169T602_pos	169.0860	602	3							HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	0.2
M169T666_pos	169.1224	666	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.4
M169T1034_pos	169.1587	1034	3							HMDB0031128	10-Undecenal	C11H20O	0.3
M170T397_pos	170.0813	397	3							HMDB0000216	Norepinephrine	C8H11NO3	0.9
M170T569_pos	170.0813	569	3							HMDB0000216	Norepinephrine	C8H11NO3	0.9
M170T655_pos	170.1176	655	3							HMDB0038321	Homoarecoline	C9H15NO2	0.3
M171T441_pos	171.1129	441	3							HMDB0015333	Levetiracetam	C8H14N2O2	0.3
M171T568_2_pos	171.1129	568	3							HMDB0015333	Levetiracetam	C8H14N2O2	0.5
M171T675_pos	171.1207	675	3							HMDB0032251	(+/-)-2,8-Epithio-cis-p-menthane	C10H18S	3.2
M171T361_pos	171.1129	361	3							HMDB0015333	Levetiracetam	C8H14N2O2	0.7
M173T411_pos	173.1649	411	3							HMDB0246342	mino-2,2,6,6-tetramethylpiperidin-	C9H20N2O	0.4
M174T438_pos	174.1126	438	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.6
M174T166_pos	174.1127	166	3							HMDB0000701	Hexanoylglycine	C8H15NO3	1.3
M174T583_pos	174.1125	583	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.4
M174T526_pos	174.1126	526	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.5
M174T660_pos	174.1126	660	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.6
M174T549_pos	174.1489	549	3							HMDB0243489	eridinol, 1-hydroxy-2,2,6,6-tetram	C9H19NO2	0.5
M175T441_pos	175.0601	441	3							HMDB0003070	Shikimic acid	C7H10O5	0.0
M175T123_2_pos	175.1187	123	3							HMDB0000517	L-Arginine	C6H14N4O2	1.6
M175T294_pos	175.1079	294	3							HMDB0003357	N2-Acetylornithine	C7H14N2O3	0.9
M175T189_pos	175.1442	189	3							HMDB0013287	Ne,Ne dimethyllysine	C8H18N2O2	0.7
M176T201_pos	176.0555	201	3						Fatty acids	HMDB0000812	N-Acetyl-L-aspartic acid	C6H9NO5	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M165T459_pos	165.1387	459	3	7.16E-05	0.63	TRUE	8.72E-01	0.98	FALSE	8.08E-04	1.40	FALSE	1.51E-01	1.21	FALSE
M166T648_pos	166.0501	648	3	1.85E-23	0.40	TRUE	1.05E-01	1.14	FALSE	1.23E-03	1.24	FALSE	2.88E-01	0.84	FALSE
M166T477_pos	166.0501	477	3	1.60E-01	0.90	FALSE	5.42E-01	1.05	FALSE	1.43E-15	1.85	TRUE	9.25E-01	1.00	FALSE
M166T331_pos	166.0725	331	3	3.33E-25	0.31	TRUE	4.46E-02	1.20	FALSE	3.64E-03	1.26	FALSE	3.27E-01	1.10	FALSE
M166T520_pos	166.0863	520	3	1.92E-09	0.34	TRUE	1.01E-01	1.32	FALSE	2.47E-02	1.37	FALSE	5.36E-01	0.91	FALSE
M166T599_pos	166.0863	599	3	3.12E-26	0.46	TRUE	1.29E-02	1.17	FALSE	1.31E-07	1.34	FALSE	2.78E-01	0.93	FALSE
M167T503_pos	167.0453	503	3	3.25E-02	0.73	FALSE	2.74E-01	0.83	FALSE	4.84E-06	1.86	TRUE	8.14E-01	0.97	FALSE
M167T759_pos	167.0555	759	3	4.25E-20	1.95	TRUE	1.60E-01	1.10	FALSE	3.66E-05	0.79	FALSE	9.45E-01	1.01	FALSE
M167T571_pos	167.0816	571	3	9.75E-05	0.68	FALSE	1.12E-02	1.29	FALSE	1.60E-08	1.65	TRUE	2.56E-02	0.73	FALSE
M167T714_pos	167.1067	714	3	1.67E-04	1.58	TRUE	2.82E-01	0.87	FALSE	2.18E-02	0.79	FALSE	1.23E-01	0.78	FALSE
M167T591_pos	167.1067	591	3	4.63E-32	1.54	TRUE	4.60E-01	1.02	FALSE	1.48E-01	1.04	FALSE	3.76E-01	0.94	FALSE
M168T296_pos	168.0518	296	3	6.39E-01	0.96	FALSE	9.16E-02	1.15	FALSE	3.55E-16	1.85	TRUE	6.39E-01	0.90	FALSE
M168T240_pos	168.0656	240	3	5.76E-03	0.82	FALSE	5.97E-01	1.04	FALSE	6.74E-13	1.63	TRUE	6.71E-01	0.97	FALSE
M169T602_pos	169.0860	602	3	1.77E-44	1.94	TRUE	5.08E-04	1.13	FALSE	6.18E-07	0.86	FALSE	3.38E-01	0.93	FALSE
M169T666_pos	169.1224	666	3	4.74E-19	1.81	TRUE	9.94E-01	1.00	FALSE	3.44E-01	0.95	FALSE	8.97E-01	1.01	FALSE
M169T1034_pos	169.1587	1034	3	2.57E-07	1.79	TRUE	1.22E-03	0.70	FALSE	6.51E-01	0.96	FALSE	1.50E-01	1.26	FALSE
M170T397_pos	170.0813	397	3	1.19E-17	1.53	TRUE	4.27E-01	0.96	FALSE	3.62E-01	1.04	FALSE	9.28E-01	0.99	FALSE
M170T569_pos	170.0813	569	3	5.08E-04	1.16	FALSE	1.35E-02	1.11	FALSE	6.24E-24	1.53	TRUE	9.26E-01	0.99	FALSE
M170T655_pos	170.1176	655	3	7.41E-07	2.21	TRUE	1.32E-01	1.27	FALSE	2.24E-01	1.17	FALSE	6.00E-01	1.07	FALSE
M171T441_pos	171.1129	441	3	1.74E-61	0.16	TRUE	8.17E-02	1.12	FALSE	8.98E-11	1.43	FALSE	5.66E-01	0.90	FALSE
M171T568_2_pos	171.1129	568	3	8.73E-39	0.24	TRUE	9.39E-02	1.14	FALSE	5.14E-05	1.31	FALSE	3.51E-01	0.79	FALSE
M171T675_pos	171.1207	675	3	7.29E-10	3.15	TRUE	1.16E-01	1.30	FALSE	6.42E-01	1.07	FALSE	9.22E-01	0.99	FALSE
M171T361_pos	171.1129	361	3	2.59E-29	0.45	TRUE	5.44E-01	1.04	FALSE	2.08E-06	1.27	FALSE	8.64E-02	1.27	FALSE
M173T411_pos	173.1649	411	3	2.12E-07	1.91	TRUE	1.61E-01	0.84	FALSE	7.90E-01	0.97	FALSE	2.14E-01	0.79	FALSE
M174T438_pos	174.1126	438	3	2.25E-28	0.62	TRUE	6.04E-01	0.98	FALSE	3.86E-23	1.44	FALSE	3.16E-01	0.90	FALSE
M174T166_pos	174.1127	166	3	8.33E-01	1.02	FALSE	4.10E-02	1.23	FALSE	4.43E-07	1.57	TRUE	6.79E-02	1.33	FALSE
M174T583_pos	174.1125	583	3	2.49E-04	1.73	TRUE	1.85E-01	1.23	FALSE	9.01E-01	1.02	FALSE	9.64E-02	1.24	FALSE
M174T526_pos	174.1126	526	3	7.45E-34	1.63	TRUE	9.53E-01	1.00	FALSE	5.08E-02	1.06	FALSE	1.68E-02	0.88	FALSE
M174T660_pos	174.1126	660	3	5.44E-21	2.01	TRUE	5.58E-01	1.04	FALSE	5.65E-06	1.30	FALSE	4.33E-01	1.10	FALSE
M174T549_pos	174.1489	549	3	3.66E-10	1.36	FALSE	1.61E-01	1.07	FALSE	8.74E-21	1.54	TRUE	5.16E-02	0.88	FALSE
M175T441_pos	175.0601	441	3	1.13E-03	0.82	FALSE	2.67E-01	0.93	FALSE	4.64E-15	1.58	TRUE	1.91E-02	0.90	FALSE
M175T123_2_pos	175.1187	123	3	1.96E-04	0.44	TRUE	9.44E-01	0.98	FALSE	5.54E-01	1.11	FALSE	2.62E-01	1.69	FALSE
M175T294_pos	175.1079	294	3	2.68E-59	0.11	TRUE	3.92E-02	1.16	FALSE	9.41E-08	1.39	FALSE	3.62E-01	0.78	FALSE
M175T189_pos	175.1442	189	3	2.64E-17	1.81	TRUE	7.06E-02	0.89	FALSE	1.51E-02	1.14	FALSE	7.41E-02	0.93	FALSE
M176T201_pos	176.0555	201	3	4.52E-03	0.74	FALSE	1.77E-02	0.77	FALSE	1.26E-09	1.79	TRUE	6.93E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M176T174_pos	176.0920	174	3							HMDB0002201	N-Carboxyethyl-g-aminobutyric aci	C7H13NO4	1.4
M178T652_pos	178.0500	652	3							HMDB0040612	4-Acetyl-2(3H)-benzoxazolone	C9H7NO3	0.9
M178T434_pos	178.0724	434	3							HMDB0247091	1H)-Pteridinone, 2-amino-6-methy	C7H7N5O	0.4
M178T403_pos	178.0865	403	3							HMDB0001855	5-Hydroxytryptophol	C10H11NO2	1.2
M179T462_pos	179.0914	462	3							HMDB0033789	2-O-Methyl-L-fucose	C7H14O5	0.2
M179T953_pos	179.1431	953	3							HMDB0014956	Propofol	C12H18O	0.5
M180T433_pos	180.0657	433	3							HMDB0000714	Hippuric acid	C9H9NO3	1.1
M180T362_pos	180.1366	362	3						Alkaloids				
M181T616_pos	180.9819	616	3							HMDB0304009	1,4-dichlorobenzene dihydrodiol	C6H6Cl2O2	0.7
M181T658_pos	181.0496	658	3							HMDB0000707	4-Hydroxyphenylpyruvic acid	C9H8O4	0.4
M181T597_pos	181.0607	597	3						Amino acids and Peptides	HMDB0003269	Nicotinuric acid	C8H8N2O3	0.4
M181T397_pos	181.0975	397	3							HMDB0004076	5-Hydroxykynurenamine	C9H12N2O2	1.9
M181T523_pos	181.1336	523	3							HMDB0257232	Rilmenidine	C10H16N2O	0.3
M181T822_pos	181.1223	822	3						Terpenoids	HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.2
M182T135_pos	182.0578	135	3							HMDB0252799	Glufosinate	C5H12NO4P	0.4
M182T267_pos	182.0813	267	3							HMDB0000158	L-Tyrosine	C9H11NO3	0.6
M182T761_pos	182.0812	761	3							HMDB0000158	L-Tyrosine	C9H11NO3	0.2
M182T536_pos	182.0812	536	3							HMDB0000158	L-Tyrosine	C9H11NO3	0.4
M182T376_pos	182.1170	376	3							HMDB0033868	beta-O-Methylynephrine	C10H15NO2	3.2
M182T753_pos	182.1178	753	3							HMDB0033868	beta-O-Methylynephrine	C10H15NO2	1.4
M182T113_pos	182.1653	113	3							HMDB0255811	4-Octyl-2H-triazole	C10H19N3	0.5
M183T696_pos	183.1009	696	3							HMDB0029456	Amyl 2-furoate	C10H14O3	3.5
M183T698_pos	183.1015	698	3							HMDB0029456	Amyl 2-furoate	C10H14O3	0.5
M184T344_pos	184.0606	344	3							HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.9
M184T730_pos	184.0968	730	3							HMDB0000068	Epinephrine	C9H13NO3	0.3
M184T644_pos	184.0970	644	3							HMDB0000068	Epinephrine	C9H13NO3	1.2
M186T364_pos	186.1129	364	3							HMDB0006348	Pseudoecgonine	C9H15NO3	2.4
M187T511_pos	187.0602	511	3							HMDB0041026	Erinapyrone C	C8H10O5	0.7
M187T488_pos	187.1078	488	3							HMDB0028695	Alanylproline	C8H14N2O3	0.6
M187T353_pos	187.1081	353	3						Amino acids and Peptides	HMDB0028695	Alanylproline	C8H14N2O3	1.8
M187T659_1_pos	187.1330	659	3							HMDB0010724	3-Oxodecanoic acid	C10H18O3	0.6
M187T413_pos	187.1443	413	3							HMDB0033553	Methylbutyl)nitrosoamino]-2-buta	C9H18N2O2	0.9
M187T560_pos	187.1443	560	3							HMDB0033553	Methylbutyl)nitrosoamino]-2-buta	C9H18N2O2	0.9
M188T398_pos	188.0918	398	3							HMDB0012150	2-Keto-6-acetamidocaproate	C8H13NO4	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M176T174_pos	176.0920	174	3	2.30E-11	0.60	TRUE	1.36E-01	0.90	FALSE	3.09E-09	1.47	FALSE	2.88E-02	0.83	FALSE
M178T652_pos	178.0500	652	3	6.06E-01	1.04	FALSE	5.31E-01	1.05	FALSE	7.48E-10	1.52	TRUE	3.76E-02	0.83	FALSE
M178T434_pos	178.0724	434	3	1.45E-03	1.29	FALSE	1.25E-01	0.88	FALSE	4.13E-23	2.29	TRUE	2.88E-01	0.85	FALSE
M178T403_pos	178.0865	403	3	4.14E-06	0.67	FALSE	1.98E-01	0.89	FALSE	2.28E-10	1.65	TRUE	1.82E-01	1.11	FALSE
M179T462_pos	179.0914	462	3	2.89E-10	1.53	TRUE	9.51E-02	1.12	FALSE	2.03E-01	1.07	FALSE	9.36E-01	0.99	FALSE
M179T953_pos	179.1431	953	3	5.82E-02	0.89	FALSE	6.05E-02	0.88	FALSE	1.62E-03	1.19	FALSE	9.66E-03	0.56	TRUE
M180T433_pos	180.0657	433	3	1.77E-02	0.46	TRUE	8.52E-01	1.06	FALSE	2.71E-01	0.74	FALSE	1.99E-01	0.81	FALSE
M180T362_pos	180.1366	362	3	5.03E-16	0.43	TRUE	7.95E-03	1.28	FALSE	7.64E-02	1.15	FALSE	3.41E-01	1.09	FALSE
M181T616_pos	180.9819	616	3	2.96E-09	1.65	TRUE	3.96E-01	0.93	FALSE	8.57E-01	1.01	FALSE	5.25E-01	0.92	FALSE
M181T658_pos	181.0496	658	3	2.75E-10	0.72	FALSE	5.81E-02	1.10	FALSE	2.67E-33	1.89	TRUE	4.71E-01	1.06	FALSE
M181T597_pos	181.0607	597	3	4.97E-04	0.70	FALSE	7.68E-01	0.97	FALSE	1.80E-08	1.67	TRUE	9.55E-01	0.99	FALSE
M181T397_pos	181.0975	397	3	5.12E-02	1.18	FALSE	6.98E-04	1.34	FALSE	9.98E-11	1.65	TRUE	2.89E-01	0.90	FALSE
M181T523_pos	181.1336	523	3	5.07E-03	0.45	TRUE	8.12E-01	1.07	FALSE	1.11E-01	0.69	FALSE	8.02E-01	1.03	FALSE
M181T822_pos	181.1223	822	3	3.21E-09	1.74	TRUE	2.41E-01	0.89	FALSE	1.55E-04	0.74	FALSE	5.20E-01	0.94	FALSE
M182T135_pos	182.0578	135	3	1.83E-02	0.80	FALSE	8.29E-01	1.02	FALSE	4.56E-11	1.79	TRUE	4.51E-01	0.88	FALSE
M182T267_pos	182.0813	267	3	1.81E-04	0.74	FALSE	3.10E-01	1.09	FALSE	7.15E-21	2.10	TRUE	9.70E-03	0.88	FALSE
M182T761_pos	182.0812	761	3	6.44E-06	1.39	FALSE	9.48E-15	0.48	TRUE	4.51E-04	1.24	FALSE	8.78E-01	0.97	FALSE
M182T536_pos	182.0812	536	3	2.12E-01	0.93	FALSE	1.69E-05	0.78	FALSE	4.77E-16	1.55	TRUE	7.01E-01	0.97	FALSE
M182T376_pos	182.1170	376	3	1.90E-04	0.61	TRUE	7.46E-01	1.04	FALSE	1.59E-02	1.31	FALSE	4.57E-01	1.12	FALSE
M182T753_pos	182.1178	753	3	7.07E-01	0.95	FALSE	1.52E-06	0.41	TRUE	3.22E-02	0.76	FALSE	9.09E-01	1.07	FALSE
M182T113_pos	182.1653	113	3	3.74E-11	0.58	TRUE	1.18E-01	0.88	FALSE	3.36E-08	0.68	FALSE	4.64E-01	1.10	FALSE
M183T696_pos	183.1009	696	3	3.53E-06	2.08	TRUE	7.29E-01	0.95	FALSE	2.53E-02	0.75	FALSE	1.14E-01	0.75	FALSE
M183T698_pos	183.1015	698	3	9.89E-05	1.88	TRUE	4.46E-01	0.88	FALSE	7.65E-02	0.79	FALSE	2.71E-01	0.81	FALSE
M184T344_pos	184.0606	344	3	1.70E-05	0.84	FALSE	9.99E-01	1.00	FALSE	8.74E-24	1.50	TRUE	7.44E-01	1.01	FALSE
M184T730_pos	184.0968	730	3	5.25E-14	1.79	TRUE	1.16E-05	0.75	FALSE	1.72E-05	0.76	FALSE	9.02E-01	1.02	FALSE
M184T644_pos	184.0970	644	3	3.83E-01	1.05	FALSE	1.41E-02	1.15	FALSE	8.39E-18	1.54	TRUE	2.50E-01	0.90	FALSE
M186T364_pos	186.1129	364	3	1.73E-08	1.48	FALSE	1.07E-01	1.12	FALSE	5.10E-14	1.61	TRUE	9.51E-02	0.80	FALSE
M187T511_pos	187.0602	511	3	3.68E-01	0.90	FALSE	3.26E-01	0.88	FALSE	4.49E-01	0.93	FALSE	9.72E-03	0.57	TRUE
M187T488_pos	187.1078	488	3	2.72E-34	0.23	TRUE	8.48E-01	1.02	FALSE	5.53E-06	1.41	FALSE	1.75E-01	0.75	FALSE
M187T353_pos	187.1081	353	3	2.13E-49	0.25	TRUE	6.34E-02	1.12	FALSE	7.40E-10	1.40	FALSE	3.65E-01	1.21	FALSE
M187T659_1_pos	187.1330	659	3	5.48E-25	1.68	TRUE	6.37E-01	1.02	FALSE	6.55E-01	1.02	FALSE	3.34E-01	1.06	FALSE
M187T413_pos	187.1443	413	3	1.89E-29	0.19	TRUE	4.28E-01	1.09	FALSE	5.93E-01	0.95	FALSE	2.56E-01	0.61	FALSE
M187T560_pos	187.1443	560	3	2.09E-03	0.64	TRUE	9.84E-02	1.28	FALSE	1.81E-02	1.34	FALSE	8.30E-01	0.95	FALSE
M188T398_pos	188.0918	398	3	2.63E-19	1.54	TRUE	7.77E-01	0.99	FALSE	6.98E-04	1.13	FALSE	7.35E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M188T357_pos	188.1028	357	3							HMDB0247067	6-Guanidino-2-oxocaproic acid	C7H13N3O3	0.9
M188T393_pos	188.1281	393	3							HMDB0013010	N-Heptanoylglycine	C9H17NO3	0.1
M188T600_pos	188.1282	600	3							HMDB0013010	N-Heptanoylglycine	C9H17NO3	0.3
M188T104_pos	188.1759	104	3							HMDB0001276	N1-Acetylspermidine	C9H21N3O	0.6
M189T387_pos	189.1236	387	3						Amino acids and Peptides	HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	1.1
M189T442_pos	189.1234	442	3							HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.3
M189T139_pos	189.1235	139	3						Amino acids and Peptides	HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.6
M189T178_pos	189.1235	178	3						Amino acids and Peptides	HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.8
M189T365_pos	189.1599	365	3							HMDB0001325	N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	0.9
M190T321_pos	190.0711	321	3							HMDB0000590	Glutarylglycine	C7H11NO5	0.7
M190T349_pos	190.1075	349	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.5
M190T239_pos	190.1075	239	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.7
M190T455_pos	190.1266	455	3							HMDB0251894	S-Ethyl dipropylthiocarbamate	C9H19NOS	3.1
M191T309_pos	191.0745	309	3							HMDB0032259	Ethyl 4-(acetylthio)butyrate	C8H14O3S	4.3
M191T431_pos	191.0912	431	3							HMDB0000325	3-Hydroxysuberic acid	C8H14O5	1.0
M191T125_pos	191.1027	125	3							HMDB0001370	Diaminopimelic acid	C7H14N2O4	0.5
M192T657_pos	192.1023	657	3							HMDB0001896	5-Methoxytryptophol	C11H13NO2	1.9
M193T987_pos	193.0133	987	3							HMDB0259233	TRIMELLITIC ANHYDRIDE	C9H4O5	0.6
M193T764_pos	193.1225	764	3							HMDB0031571	Methyl-1-phenyl-2-propanyl aceta	C12H16O2	0.9
M193T669_pos	193.1224	669	3							HMDB0031571	Methyl-1-phenyl-2-propanyl aceta	C12H16O2	0.4
M193T1034_pos	193.1951	1034	3							HMDB0061832	1-Acetyl-2-methylcyclopentene	C14H24	0.2
M194T761_pos	194.1177	761	3						Alkaloids	HMDB0003626	(R)-N-Methylsalsolinol	C11H15NO2	0.6
M195T712_pos	195.0644	712	3							HMDB0000954	Ferulic acid	C10H10O4	4.0
M195T409_pos	195.0766	409	3							HMDB0001867	4-Aminohippuric acid	C9H10N2O3	1.1
M195T585_pos	195.0877	585	3							HMDB0001847	Caffeine	C8H10N4O2	0.1
M195T412_pos	195.1232	412	3							HMDB0094708	Tetraethylene glycol	C8H18O5	2.4
M195T488_pos	195.1494	488	3							HMDB0244534	N-(1-Adamantyl)urea	C11H18N2O	0.9
M196T785_pos	196.0969	785	3							HMDB0014903	Metyrosine	C10H13NO3	0.4
M196T464_pos	196.0970	464	3							HMDB0014903	Metyrosine	C10H13NO3	0.8
M196T150_pos	196.0963	150	3							HMDB0014903	Metyrosine	C10H13NO3	2.5
M197T664_pos	197.0446	664	3							HMDB0030800	ethoxy-4,5-methylenedioxybenzoic	C9H8O5	0.8
M197T442_pos	197.0669	442	3							HMDB0001857	1,3-Dimethyluric acid	C7H8N4O3	0.1
M197T488_pos	197.0922	488	3							HMDB0032852	Ethylamino)-4,5-dihydroxybenzam	C9H12N2O3	0.9
M197T356_pos	197.0925	356	3							HMDB0032852	Ethylamino)-4,5-dihydroxybenzam	C9H12N2O3	2.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M188T357_pos	188.1028	357	3	1.33E-04	0.72	FALSE	1.34E-02	1.23	FALSE	1.35E-08	1.55	TRUE	7.46E-01	0.96	FALSE
M188T393_pos	188.1281	393	3	9.96E-04	0.52	TRUE	2.52E-01	1.26	FALSE	4.50E-02	1.40	FALSE	3.76E-01	0.91	FALSE
M188T600_pos	188.1282	600	3	7.11E-09	1.46	FALSE	2.29E-01	1.08	FALSE	1.41E-05	1.27	FALSE	3.53E-02	1.59	TRUE
M188T104_pos	188.1759	104	3	3.76E-05	1.46	FALSE	1.55E-05	1.49	FALSE	6.75E-11	1.73	TRUE	5.17E-01	0.93	FALSE
M189T387_pos	189.1236	387	3	1.40E-33	0.22	TRUE	2.40E-01	1.11	FALSE	8.40E-04	1.29	FALSE	8.54E-01	0.96	FALSE
M189T442_pos	189.1234	442	3	1.65E-50	0.10	TRUE	1.52E-01	1.13	FALSE	3.33E-07	1.44	FALSE	3.65E-01	0.77	FALSE
M189T139_pos	189.1235	139	3	2.92E-03	0.87	FALSE	5.06E-02	1.10	FALSE	2.64E-33	1.79	TRUE	7.03E-01	1.02	FALSE
M189T178_pos	189.1235	178	3	5.75E-02	0.82	FALSE	7.43E-01	0.97	FALSE	4.48E-06	1.53	TRUE	1.58E-02	0.72	FALSE
M189T365_pos	189.1599	365	3	2.58E-22	1.88	TRUE	2.63E-01	0.94	FALSE	6.04E-01	1.03	FALSE	2.13E-01	0.93	FALSE
M190T321_pos	190.0711	321	3	3.71E-03	0.73	FALSE	6.97E-02	0.82	FALSE	2.31E-08	1.74	TRUE	1.55E-01	0.49	FALSE
M190T349_pos	190.1075	349	3	4.24E-08	0.70	FALSE	7.64E-01	1.02	FALSE	2.61E-14	1.57	TRUE	6.42E-01	1.06	FALSE
M190T239_pos	190.1075	239	3	3.30E-06	0.73	FALSE	4.63E-01	1.05	FALSE	1.16E-23	2.00	TRUE	2.79E-02	0.88	FALSE
M190T455_pos	190.1266	455	3	1.02E-14	0.42	TRUE	4.04E-01	1.09	FALSE	7.25E-01	0.97	FALSE	3.99E-01	0.70	FALSE
M191T309_pos	191.0745	309	3	4.54E-08	0.68	FALSE	6.57E-02	1.14	FALSE	8.02E-18	1.78	TRUE	8.50E-01	0.97	FALSE
M191T431_pos	191.0912	431	3	3.50E-01	1.09	FALSE	9.69E-01	1.00	FALSE	2.56E-08	1.57	TRUE	3.24E-01	1.14	FALSE
M191T125_pos	191.1027	125	3	6.75E-37	0.18	TRUE	5.24E-01	1.06	FALSE	4.17E-05	1.38	FALSE	2.83E-01	0.78	FALSE
M192T657_pos	192.1023	657	3	1.67E-01	0.92	FALSE	3.65E-05	1.32	FALSE	1.77E-13	1.55	TRUE	1.39E-01	0.86	FALSE
M193T987_pos	193.0133	987	3	7.53E-01	0.97	FALSE	4.31E-01	1.08	FALSE	1.60E-01	1.12	FALSE	6.12E-05	0.47	TRUE
M193T764_pos	193.1225	764	3	2.43E-02	1.19	FALSE	2.11E-01	1.11	FALSE	2.46E-15	1.79	TRUE	1.84E-01	0.92	FALSE
M193T669_pos	193.1224	669	3	1.19E-35	1.61	TRUE	2.00E-01	1.04	FALSE	3.63E-02	1.06	FALSE	4.99E-02	0.88	FALSE
M193T1034_pos	193.1951	1034	3	3.02E-05	1.59	TRUE	8.51E-02	0.83	FALSE	7.97E-01	1.02	FALSE	6.83E-01	1.04	FALSE
M194T761_pos	194.1177	761	3	6.75E-02	0.79	FALSE	1.94E-03	1.53	TRUE	2.65E-02	1.28	FALSE	2.22E-01	1.37	FALSE
M195T712_pos	195.0644	712	3	4.57E-01	1.05	FALSE	3.40E-02	1.15	FALSE	9.66E-05	1.24	FALSE	7.94E-03	0.63	TRUE
M195T409_pos	195.0766	409	3	5.19E-06	0.60	TRUE	1.30E-01	1.19	FALSE	1.63E-01	1.14	FALSE	8.08E-01	1.05	FALSE
M195T585_pos	195.0877	585	3	8.24E-18	1.89	TRUE	1.28E-01	0.90	FALSE	3.37E-01	1.06	FALSE	3.64E-02	0.81	FALSE
M195T412_pos	195.1232	412	3	1.65E-34	0.31	TRUE	6.93E-01	1.03	FALSE	3.86E-01	0.95	FALSE	4.49E-01	1.15	FALSE
M195T488_pos	195.1494	488	3	9.25E-01	1.01	FALSE	3.02E-02	1.23	FALSE	2.09E-04	1.36	FALSE	8.83E-03	0.53	TRUE
M196T785_pos	196.0969	785	3	3.62E-12	1.46	FALSE	3.67E-18	0.63	TRUE	4.03E-01	0.96	FALSE	9.87E-01	1.00	FALSE
M196T464_pos	196.0970	464	3	1.43E-02	1.12	FALSE	4.29E-01	1.04	FALSE	1.35E-19	1.52	TRUE	2.24E-01	0.93	FALSE
M196T150_pos	196.0963	150	3	4.20E-16	0.33	TRUE	9.56E-01	0.99	FALSE	1.97E-02	1.26	FALSE	1.83E-01	0.42	FALSE
M197T664_pos	197.0446	664	3	2.80E-03	0.73	FALSE	5.85E-01	1.06	FALSE	9.05E-12	1.98	TRUE	2.81E-01	1.13	FALSE
M197T442_pos	197.0669	442	3	2.51E-01	1.12	FALSE	8.57E-01	1.02	FALSE	2.40E-06	1.51	TRUE	8.99E-01	0.99	FALSE
M197T488_pos	197.0922	488	3	4.10E-01	1.05	FALSE	2.10E-01	1.08	FALSE	2.13E-16	1.62	TRUE	1.23E-01	0.84	FALSE
M197T356_pos	197.0925	356	3	6.40E-01	0.97	FALSE	7.38E-01	1.02	FALSE	2.39E-12	1.53	TRUE	2.05E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M197T466_pos	197.0994	466	3							HMDB0040241	1-(2-Thienyl)-1-heptanone	C11H16OS	0.1
M197T691_pos	197.1174	691	3							HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	0.7
M198T706_pos	198.0529	706	3							HMDB0304531	vanillyl mandelate	C9H9O5	0.2
M198T514_pos	198.0763	514	3							HMDB0000181	L-Dopa	C9H11NO4	1.1
M198T378_pos	198.0871	378	3							HMDB0032055	N-Acetylhistidine	C8H11N3O3	1.1
M199T436_pos	199.1079	436	3							HMDB0014606	Metharbital	C9H14N2O3	0.7
M199T428_pos	199.1442	428	3							HMDB0243523	(-)-Slaframine	C10H18N2O2	0.7
M199T552_pos	199.1442	552	3							HMDB0243523	(-)-Slaframine	C10H18N2O2	0.5
M200T670_pos	200.0920	670	3							HMDB0035177	ahydro-6-hydroxy-7-(hydroxymeth	C9H13NO4	1.3
M201T525_pos	201.0610	525	3							HMDB0257302	ronidazole	C6H8N4O4	4.4
M201T450_pos	201.1235	450	3							HMDB0304430	N-alpha-acetyl lysine methyl ester	C9H16N2O3	3.2
M201T865_pos	201.1486	865	3						Fatty acids	HMDB0032662	(S)-9-Hydroxy-10-undecenoic acid	C11H20O3	0.6
M202T769_pos	202.1439	769	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.7
M203T154_pos	203.1129	154	3							HMDB0244741	itro-3-((tetrahydrofuran-3-yl)meth	C7H14N4O3	4.9
M203T207_pos	203.1392	207	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	1.0
M203T1025_pos	203.1795	1025	3							HMDB0035707	7alpha,10alpha)-1(5),3-Aromaden	C15H22	0.5
M203T297_pos	203.1837	297	3							HMDB0243867	1-Dodecanethiol	C12H26S	4.2
M204T486_pos	204.0272	486	3							HMDB0303970	(2R,3S)-2-methylisocitrate	C7H7O7	4.6
M204T411_pos	204.0868	411	3							HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	0.6
M204T516_pos	204.1018	516	3							HMDB0002096	3-Indolebutyric acid	C12H13NO2	0.6
M204T747_pos	204.1020	747	3							HMDB0002096	3-Indolebutyric acid	C12H13NO2	0.6
M204T346_pos	204.1233	346	3							HMDB0062176	N-Lactoylleucine	C9H17NO4	1.5
M205T609_pos	205.0497	609	3							HMDB0244212	1,4-Dihydroxy-2-naphthoic acid	C11H8O4	1.0
M205T900_pos	205.0860	900	3							HMDB0033303	Anofinic acid	C12H12O3	0.5
M205T252_pos	205.1185	252	3							HMDB0029052	Serylvaline	C8H16N2O4	0.9
M206T568_pos	206.0449	568	3							HMDB0000881	Xanthurenic acid	C10H7NO4	0.8
M206T173_pos	206.1025	173	3							HMDB0036394	N-Methylcalystegine C1	C8H15NO5	0.8
M207T714_pos	207.1001	714	3							HMDB0244930	Arginine chloromethyl ketone	C7H15ClN4O	3.2
M207T659_pos	207.1017	659	3							HMDB0030762	Ethyl trans-p-methoxycinnamate	C12H14O3	0.4
M208T421_2_pos	208.1334	421	3							HMDB0015319	Ciclopirox	C12H17NO2	0.9
M209T473_2_pos	209.1019	473	3							HMDB0029968	Ethyl beta-D-glucopyranoside	C8H16O6	0.3
M209T757_pos	209.1173	757	3							HMDB0029867	Isoelemicin	C12H16O3	0.4
M209T370_pos	209.1286	370	3							HMDB0015217	Pilocarpine	C11H16N2O2	0.8
M209T554_pos	209.1377	554	3							HMDB0062236	5S,6S-epoxy-15R-hydroxy-ETE	C9H20O5	3.1
M210T383_pos	210.0764	383	3							HMDB0000735	Hydroxyphenylacetylglycine	C10H11NO4	1.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M197T466_pos	197.0994	466	3	6.88E-03	1.16	FALSE	9.03E-01	0.99	FALSE	3.09E-18	1.61	TRUE	2.27E-01	0.92	FALSE
M197T691_pos	197.1174	691	3	9.45E-15	1.83	TRUE	4.06E-07	0.68	FALSE	5.28E-08	0.71	FALSE	1.73E-01	0.89	FALSE
M198T706_pos	198.0529	706	3	1.03E-05	1.78	TRUE	7.01E-01	1.05	FALSE	2.43E-02	0.78	FALSE	6.21E-01	0.92	FALSE
M198T514_pos	198.0763	514	3	1.30E-02	0.86	FALSE	3.46E-01	1.06	FALSE	5.03E-16	1.58	TRUE	4.33E-01	1.07	FALSE
M198T378_pos	198.0871	378	3	7.12E-03	0.86	FALSE	7.86E-02	1.11	FALSE	5.19E-25	1.77	TRUE	5.98E-02	0.90	FALSE
M199T436_pos	199.1079	436	3	2.93E-31	1.74	TRUE	3.72E-02	0.92	FALSE	9.36E-04	0.89	FALSE	2.76E-01	0.92	FALSE
M199T428_pos	199.1442	428	3	1.26E-17	0.53	TRUE	2.08E-01	1.09	FALSE	6.55E-01	1.03	FALSE	3.00E-01	1.44	FALSE
M199T552_pos	199.1442	552	3	2.75E-48	0.39	TRUE	3.54E-01	1.04	FALSE	1.97E-08	1.25	FALSE	8.93E-03	0.83	FALSE
M200T670_pos	200.0920	670	3	1.86E-07	1.43	FALSE	4.22E-12	0.62	TRUE	5.66E-02	0.90	FALSE	1.77E-02	0.84	FALSE
M201T525_pos	201.0610	525	3	6.17E-09	1.93	TRUE	4.56E-02	0.82	FALSE	8.09E-01	1.02	FALSE	1.24E-03	0.76	FALSE
M201T450_pos	201.1235	450	3	2.11E-41	0.32	TRUE	1.11E-01	1.11	FALSE	2.48E-04	1.21	FALSE	6.04E-01	0.89	FALSE
M201T865_pos	201.1486	865	3	1.23E-01	1.61	FALSE	8.36E-02	0.48	FALSE	1.18E-01	1.52	FALSE	5.23E-03	0.31	TRUE
M202T769_pos	202.1439	769	3	9.33E-01	0.99	FALSE	2.92E-03	1.70	TRUE	1.31E-02	1.42	FALSE	6.94E-01	0.95	FALSE
M203T154_pos	203.1129	154	3	1.08E-02	0.80	FALSE	1.18E-01	1.15	FALSE	6.22E-10	1.63	TRUE	5.76E-01	1.13	FALSE
M203T207_pos	203.1392	207	3	1.05E-04	1.22	FALSE	4.91E-02	1.11	FALSE	5.09E-19	1.55	TRUE	7.41E-01	0.96	FALSE
M203T1025_pos	203.1795	1025	3	1.12E-13	1.94	TRUE	7.76E-03	0.81	FALSE	2.79E-01	1.08	FALSE	7.11E-01	0.95	FALSE
M203T297_pos	203.1837	297	3	1.36E-07	2.18	TRUE	9.03E-01	0.98	FALSE	2.63E-02	1.30	FALSE	7.62E-11	-36.49	FALSE
M204T486_pos	204.0272	486	3	5.04E-04	0.70	FALSE	6.82E-01	1.04	FALSE	2.77E-08	1.68	TRUE	2.58E-01	0.88	FALSE
M204T411_pos	204.0868	411	3	9.67E-03	0.85	FALSE	6.56E-04	1.24	FALSE	3.12E-28	2.04	TRUE	9.16E-01	0.99	FALSE
M204T516_pos	204.1018	516	3	9.88E-01	1.00	FALSE	4.44E-01	1.04	FALSE	1.25E-24	1.73	TRUE	5.89E-03	0.87	FALSE
M204T747_pos	204.1020	747	3	3.40E-06	1.50	FALSE	8.30E-02	1.18	FALSE	6.50E-15	1.89	TRUE	6.01E-01	0.94	FALSE
M204T346_pos	204.1233	346	3	3.04E-01	0.92	FALSE	3.68E-01	0.93	FALSE	2.45E-13	1.71	TRUE	7.76E-01	0.95	FALSE
M205T609_pos	205.0497	609	3	2.33E-09	0.79	FALSE	9.24E-02	1.07	FALSE	1.55E-32	1.61	TRUE	3.92E-01	0.96	FALSE
M205T900_pos	205.0860	900	3	2.30E-02	0.87	FALSE	4.63E-01	0.95	FALSE	8.96E-01	0.99	FALSE	7.61E-03	0.56	TRUE
M205T252_pos	205.1185	252	3	3.75E-41	0.12	TRUE	3.54E-01	1.09	FALSE	3.27E-03	1.27	FALSE	4.10E-01	0.79	FALSE
M206T568_pos	206.0449	568	3	9.88E-01	1.00	FALSE	9.81E-01	1.00	FALSE	7.85E-10	1.59	TRUE	7.08E-01	0.96	FALSE
M206T173_pos	206.1025	173	3	3.10E-42	0.32	TRUE	2.58E-01	0.94	FALSE	1.12E-05	1.26	FALSE	1.34E-01	0.84	FALSE
M207T714_pos	207.1001	714	3	1.28E-08	1.74	TRUE	7.65E-01	0.97	FALSE	2.43E-02	0.83	FALSE	4.05E-01	0.91	FALSE
M207T659_pos	207.1017	659	3	4.34E-01	1.03	FALSE	6.60E-02	1.07	FALSE	6.33E-34	1.63	TRUE	4.71E-03	0.87	FALSE
M208T421_2_pos	208.1334	421	3	5.44E-01	1.03	FALSE	2.10E-01	1.06	FALSE	1.56E-25	1.56	TRUE	1.16E-03	0.85	FALSE
M209T473_2_pos	209.1019	473	3	5.17E-37	1.55	TRUE	4.25E-01	0.98	FALSE	1.00E-08	1.15	FALSE	7.70E-01	0.98	FALSE
M209T757_pos	209.1173	757	3	2.78E-06	0.85	FALSE	8.50E-03	1.10	FALSE	4.71E-37	1.62	TRUE	4.84E-02	0.88	FALSE
M209T370_pos	209.1286	370	3	3.25E-02	0.89	FALSE	8.08E-02	1.10	FALSE	3.99E-20	1.63	TRUE	1.04E-02	0.85	FALSE
M209T554_pos	209.1377	554	3	3.49E-08	0.14	TRUE	7.31E-01	0.91	FALSE	2.25E-01	1.32	FALSE	2.93E-01	0.67	FALSE
M210T383_pos	210.0764	383	3	3.03E-01	0.96	FALSE	2.01E-02	1.10	FALSE	7.22E-25	1.53	TRUE	3.42E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M210T413_pos	210.1126	413	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.8
M211T641_pos	211.0966	641	3							HMDB0013070	Sinapyl alcohol	C11H14O4	0.3
M211T764_pos	211.1330	764	3							HMDB0032797	Jasmonic acid	C12H18O3	0.4
M211T467_pos	211.1442	467	3							HMDB0034276	L,L-Cyclo(leucylprolyl)	C11H18N2O2	0.6
M212T491_pos	212.0920	491	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	1.4
M212T327_pos	212.0919	327	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	1.0
M212T403_pos	212.1026	403	3							HMDB0015078	Zalcitabine	C9H13N3O3	1.7
M213T970_pos	213.2214	970	3							HMDB0030924	2-Tetradecanone	C14H28O	0.4
M214T822_pos	214.0897	822	3							HMDB0032418	4-Methyl-5-thiazolyl)ethyl butano	C10H15NO2S	0.3
M215T547_pos	215.1391	547	3						Amino acids and Peptides	HMDB0003581	Dethiobiotin	C10H18N2O3	0.2
M215T350_pos	215.1392	350	3						Amino acids and Peptides	HMDB0003581	Dethiobiotin	C10H18N2O3	0.7
M216T159_pos	216.0979	159	3							HMDB0242267	yl-2-[(E)-hydroxyimino]-5-nitro-3-h	C8H13N3O4	0.0
M216T562_pos	216.1232	562	3							HMDB0013124	Propenoylcarnitine	C10H17NO4	0.6
M216T692_pos	216.1594	692	3							HMDB0013279	N-Nonanoylglycine	C11H21NO3	0.1
M217T557_pos	217.0973	557	3							HMDB0035665	Tetrahydro-beta-carboline-3-carbo	C12H12N2O2	0.5
M217T472_pos	217.1045	472	3							HMDB0259242	Trimethylolmelamine	C6H12N6O3	0.5
M217T155_pos	217.1185	155	3							HMDB0029027	Prolyl-Threonine	C9H16N2O4	0.9
M217T185_pos	217.1296	185	3							HMDB0004620	N-a-Acetyl-L-arginine	C8H16N4O3	0.3
M218T366_pos	218.1136	366	3							HMDB0000856	N-alpha-Acetyl-L-citrulline	C8H15N3O4	0.2
M218T405_pos	218.1580	405	3							HMDB0249477	Butylate	C11H23NOS	2.9
M219T649_pos	219.0655	649	3							HMDB0029518	Liqcoumarin	C12H10O4	1.3
M219T596_pos	219.0766	596	3							HMDB0034911	nophenylmethyl)amino]-3-oxopro	C11H10N2O3	0.8
M219T194_pos	219.0802	194	3							HMDB0013139	1-Hydroxypyrene	C16H10O	1.0
M219T645_pos	219.1223	645	3							HMDB0000350	3-Hydroxysebacic acid	C10H18O5	2.0
M219T880_2_pos	219.1744	880	3							HMDB0013687	Nookatone	C15H22O	0.5
M220T421_pos	220.0969	421	3							HMDB0013988	N-Deschlorobenzoyl indomethacin	C12H13NO3	0.2
M221T334_pos	221.1020	334	3							HMDB0242729	2-O-Isopropylidene-D-glucofurano	C9H16O6	0.3
M221T522_pos	221.1650	522	3							HMDB0014888	Prilocaine	C13H20N2O	0.7
M222T574_pos	222.0763	574	3							HMDB0038990	Methyl 5-hydroxyoxindole-3-acetat	C11H11NO4	0.9
M222T486_pos	222.1126	486	3							HMDB0014798	Metaxalone	C12H15NO3	0.7
M222T151_pos	222.1337	151	3							HMDB0254995	N-(2,3,4-Trihydroxybutyl)-L-valine	C9H19NO5	0.6
M223T235_pos	223.1079	235	3							HMDB0028848	Glycyl-Phenylalanine	C11H14N2O3	1.0
M223T397_pos	223.1442	397	3							HMDB0060678	-Hydroxymonoethylglycinexylidid	C12H18N2O2	0.6
M224T234_pos	224.1110	234	3							HMDB0259091	TILETAMINE	C12H17NOS	2.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M210T413_pos	210.1126	413	3	1.59E-05	0.82	FALSE	6.76E-02	1.09	FALSE	2.18E-26	1.64	TRUE	2.31E-01	0.95	FALSE
M211T641_pos	211.0966	641	3	8.29E-06	1.56	TRUE	7.03E-01	1.04	FALSE	3.94E-02	1.19	FALSE	7.55E-02	0.82	FALSE
M211T764_pos	211.1330	764	3	4.03E-01	0.97	FALSE	2.84E-03	1.13	FALSE	1.64E-30	1.61	TRUE	2.00E-01	0.93	FALSE
M211T467_pos	211.1442	467	3	1.67E-01	1.08	FALSE	3.52E-03	1.18	FALSE	7.94E-17	1.56	TRUE	4.19E-02	0.86	FALSE
M212T491_pos	212.0920	491	3	4.48E-06	1.52	TRUE	3.59E-05	0.71	FALSE	3.22E-02	1.18	FALSE	2.46E-02	0.74	FALSE
M212T327_pos	212.0919	327	3	1.02E-02	0.85	FALSE	3.23E-01	1.07	FALSE	1.11E-20	1.83	TRUE	3.86E-02	1.18	FALSE
M212T403_pos	212.1026	403	3	9.20E-01	1.01	FALSE	5.18E-01	1.04	FALSE	3.35E-14	1.57	TRUE	2.00E-02	0.88	FALSE
M213T970_pos	213.2214	970	3	2.36E-01	0.92	FALSE	8.10E-01	1.02	FALSE	2.79E-01	1.07	FALSE	2.57E-02	0.62	TRUE
M214T822_pos	214.0897	822	3	1.18E-01	1.22	FALSE	9.18E-01	0.99	FALSE	7.68E-14	0.39	TRUE	3.28E-01	1.08	FALSE
M215T547_pos	215.1391	547	3	9.33E-16	0.52	TRUE	8.13E-01	1.02	FALSE	2.03E-03	1.22	FALSE	6.84E-01	1.09	FALSE
M215T350_pos	215.1392	350	3	1.23E-38	0.32	TRUE	8.61E-01	0.99	FALSE	1.94E-09	1.42	FALSE	1.74E-02	0.77	FALSE
M216T159_pos	216.0979	159	3	2.53E-01	0.90	FALSE	2.38E-01	0.89	FALSE	4.72E-11	1.77	TRUE	9.59E-01	1.01	FALSE
M216T562_pos	216.1232	562	3	4.09E-13	1.54	TRUE	8.11E-01	0.99	FALSE	1.05E-06	1.27	FALSE	5.50E-03	0.71	FALSE
M216T692_pos	216.1594	692	3	1.35E-09	1.51	TRUE	6.59E-02	1.13	FALSE	5.75E-02	1.11	FALSE	1.92E-01	0.78	FALSE
M217T557_pos	217.0973	557	3	1.13E-02	0.84	FALSE	1.43E-01	1.11	FALSE	5.30E-26	2.11	TRUE	2.94E-03	0.88	FALSE
M217T472_pos	217.1045	472	3	9.70E-09	1.53	TRUE	1.17E-01	0.89	FALSE	2.57E-03	0.83	FALSE	2.01E-01	1.19	FALSE
M217T155_pos	217.1185	155	3	2.67E-09	0.64	TRUE	4.92E-01	0.95	FALSE	7.83E-05	1.28	FALSE	8.63E-01	1.04	FALSE
M217T185_pos	217.1296	185	3	8.17E-02	1.11	FALSE	3.13E-01	0.94	FALSE	5.08E-23	1.87	TRUE	1.00E+00	1.00	FALSE
M218T366_pos	218.1136	366	3	2.59E-05	0.77	FALSE	2.87E-01	1.07	FALSE	2.77E-14	1.56	TRUE	5.46E-01	1.05	FALSE
M218T405_pos	218.1580	405	3	2.72E-39	0.14	TRUE	1.59E-01	1.14	FALSE	1.49E-03	1.29	FALSE	2.26E-01	0.66	FALSE
M219T649_pos	219.0655	649	3	1.04E-01	0.91	FALSE	3.18E-01	1.06	FALSE	8.16E-19	1.66	TRUE	4.73E-01	1.04	FALSE
M219T596_pos	219.0766	596	3	1.90E-05	0.81	FALSE	8.20E-01	0.99	FALSE	2.33E-27	1.71	TRUE	3.67E-01	1.06	FALSE
M219T194_pos	219.0802	194	3	7.33E-04	0.75	FALSE	6.91E-01	0.97	FALSE	5.14E-09	1.57	TRUE	7.80E-01	1.03	FALSE
M219T645_pos	219.1223	645	3	1.52E-01	1.10	FALSE	8.65E-04	1.27	FALSE	1.10E-10	1.51	TRUE	2.82E-01	1.08	FALSE
M219T880_2_pos	219.1744	880	3	2.76E-01	1.59	FALSE	5.79E-01	0.74	FALSE	2.36E-01	1.55	FALSE	5.11E-03	0.37	TRUE
M220T421_pos	220.0969	421	3	4.09E-08	0.40	TRUE	7.02E-01	1.06	FALSE	1.05E-01	1.24	FALSE	6.67E-01	0.90	FALSE
M221T334_pos	221.1020	334	3	8.37E-06	1.66	TRUE	5.45E-01	0.93	FALSE	7.97E-01	0.98	FALSE	8.21E-01	1.06	FALSE
M221T522_pos	221.1650	522	3	1.18E-11	1.87	TRUE	7.49E-01	0.97	FALSE	7.84E-05	1.35	FALSE	1.10E-03	0.67	FALSE
M222T574_pos	222.0763	574	3	1.26E-20	1.52	TRUE	3.87E-01	0.97	FALSE	1.90E-06	0.84	FALSE	4.05E-01	0.96	FALSE
M222T486_pos	222.1126	486	3	1.17E-05	0.49	TRUE	9.96E-01	1.00	FALSE	7.53E-01	1.04	FALSE	9.03E-01	1.01	FALSE
M222T151_pos	222.1337	151	3	1.67E-04	0.76	FALSE	1.76E-01	1.11	FALSE	6.69E-18	1.84	TRUE	6.82E-01	0.97	FALSE
M223T235_pos	223.1079	235	3	7.89E-08	0.71	FALSE	1.34E-01	1.10	FALSE	4.99E-27	2.02	TRUE	5.51E-01	0.97	FALSE
M223T397_pos	223.1442	397	3	7.02E-01	0.97	FALSE	3.89E-01	1.08	FALSE	6.64E-09	1.63	TRUE	2.95E-02	0.78	FALSE
M224T234_pos	224.1110	234	3	1.15E-06	0.70	FALSE	5.13E-01	1.05	FALSE	9.16E-17	1.78	TRUE	2.88E-01	0.93	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M225T558_pos	225.1235	558	3							HMDB0014386	Butalbital	C11H16N2O3	0.6
M225T597_pos	225.1420	597	3							HMDB0040005	rimethyl-6-[4-(methylthio)butyl]p	C12H20N2S	0.0
M226T667_pos	226.1077	667	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	1.4
M226T754_pos	226.1440	754	3							HMDB0015009	Terbutaline	C12H19NO3	1.1
M226T701_pos	226.1439	701	3							HMDB0015009	Terbutaline	C12H19NO3	0.8
M227T637_pos	227.0820	637	3							HMDB0247633	yl-2-(2-furyl)-1,8-naphthyridine-4(	C13H10N2O2	2.3
M227T354_pos	227.1135	354	3							HMDB0000033	Carnosine	C9H14N4O3	1.4
M227T710_pos	227.1646	710	3							HMDB0031740	Methyl dihydrojasmonate	C13H22O3	1.9
M227T1038_pos	227.2007	1038	3							HMDB0000499	5-Tetradecenoic acid	C14H26O2	0.6
M228T307_pos	228.0273	307	3							HMDB0001228	L-Glutamic acid 5-phosphate	C5H10NO7P	2.1
M228T250_pos	228.0327	250	3							HMDB0304937	6-Hydroxyindoxyl sulfate	C9H9NO4S	1.0
M228T348_pos	228.0872	348	3							HMDB0304809	Pretyrosine	C10H13NO5	2.4
M228T878_1_pos	228.1023	878	3							HMDB0033452	Koenoline	C14H13NO2	1.8
M228T878_2_pos	228.1234	878	3							HMDB0032928	3,4,8-trimethyl-3H-imidazo[4,5-f]q	C12H13N5	4.3
M228T931_pos	228.2687	931	3							HMDB0243828	Pentadecylamine	C15H33N	0.6
M229T594_pos	229.0974	594	3							HMDB0245302	midazolylmethyl)phenyl]-2-proper	C13H12N2O2	1.1
M229T390_pos	229.1187	390	3							HMDB0006695	Prolylhydroxyproline	C10H16N2O4	1.8
M229T954_pos	229.1800	954	3							HMDB0035881	11-Hydroxy-9-tridecenoic acid	C13H24O3	0.7
M229T1066_pos	229.2164	1066	3							HMDB0000806	Myristic acid	C14H28O2	1.0
M230T495_pos	230.1389	495	3							HMDB0013126	Butenylcarnitine	C11H19NO4	0.8
M230T407_pos	230.1390	407	3							HMDB0013126	Butenylcarnitine	C11H19NO4	1.2
M231T575_pos	231.1129	575	3							HMDB0037942	etrahydro-1-methyl-beta-carboline	C13H14N2O2	0.5
M232T617_pos	232.1544	617	3							HMDB0002013	Butyrylcarnitine	C11H21NO4	0.4
M233T487_pos	233.0957	487	3							HMDB0060324	1-Methoxypyrene	C17H12O	1.6
M233T184_pos	233.1140	184	3							HMDB0001199	N2-Succinyl-L-ornithine	C9H16N2O5	3.3
M234T622_pos	234.0763	622	3							HMDB0033349	Casimiroin	C12H11NO4	1.1
M235T86_pos	234.9614	86	3							HMDB0062252	-mannosyl-diacetylchitobiosyl-L-as	C7H7IO	0.2
M236T526_pos	236.1283	526	3							HMDB0033610	Pandamarilactam 3x	C13H17NO3	0.9
M237T649_pos	237.0758	649	3						Shikimates and Phenylpropanoids	HMDB0030582	Dillapional	C12H12O5	0.3
M237T554_pos	237.1237	554	3							HMDB0015444	Hexobarbital	C12H16N2O3	1.5
M237T485_pos	237.1236	485	3							HMDB0015444	Hexobarbital	C12H16N2O3	1.0
M237T562_pos	237.1599	562	3							HMDB0014859	Procaine	C13H20N2O2	0.5
M238T444_pos	238.0942	444	3							HMDB0000238	Sepiapterin	C9H11N5O3	2.9
M238T516_pos	238.1075	516	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M225T558_pos	225.1235	558	3	6.38E-09	0.15	TRUE	9.76E-01	1.01	FALSE	5.72E-02	1.51	FALSE	8.68E-01	0.99	FALSE
M225T597_pos	225.1420	597	3	4.90E-03	0.77	FALSE	4.62E-03	0.79	FALSE	5.25E-08	1.58	TRUE	6.63E-02	1.29	FALSE
M226T667_pos	226.1077	667	3	2.85E-08	1.51	TRUE	4.04E-01	0.94	FALSE	2.22E-01	0.93	FALSE	2.34E-01	0.79	FALSE
M226T754_pos	226.1440	754	3	9.28E-01	1.01	FALSE	1.28E-04	1.39	FALSE	7.58E-12	1.69	TRUE	3.53E-01	1.20	FALSE
M226T701_pos	226.1439	701	3	7.98E-02	1.13	FALSE	1.39E-10	1.59	TRUE	5.68E-07	1.36	FALSE	5.44E-01	0.94	FALSE
M227T637_pos	227.0820	637	3	5.70E-10	1.41	FALSE	6.79E-04	0.84	FALSE	1.78E-22	1.68	TRUE	5.45E-01	0.97	FALSE
M227T354_pos	227.1135	354	3	4.68E-07	0.57	TRUE	8.09E-01	1.03	FALSE	8.03E-05	1.46	FALSE	9.63E-01	0.99	FALSE
M227T710_pos	227.1646	710	3	8.32E-19	1.81	TRUE	7.18E-01	0.98	FALSE	5.35E-01	0.97	FALSE	4.69E-01	0.88	FALSE
M227T1038_pos	227.2007	1038	3	9.72E-13	1.53	TRUE	2.01E-07	0.74	FALSE	2.99E-01	0.95	FALSE	2.85E-06	1.30	FALSE
M228T307_pos	228.0273	307	3	4.02E-01	1.08	FALSE	4.73E-01	0.94	FALSE	1.86E-15	1.99	TRUE	3.08E-01	0.90	FALSE
M228T250_pos	228.0327	250	3	6.19E-01	0.96	FALSE	1.82E-04	1.33	FALSE	3.91E-12	1.62	TRUE	1.18E-01	1.25	FALSE
M228T348_pos	228.0872	348	3	6.36E-14	0.72	FALSE	1.55E-01	1.06	FALSE	6.42E-35	1.74	TRUE	8.47E-01	0.99	FALSE
M228T878_1_pos	228.1023	878	3	7.61E-06	0.25	TRUE	7.16E-01	1.10	FALSE	1.62E-01	1.38	FALSE	3.03E-01	1.23	FALSE
M228T878_2_pos	228.1234	878	3	1.28E-04	0.33	TRUE	7.51E-01	1.09	FALSE	4.90E-01	1.17	FALSE	8.25E-01	0.97	FALSE
M228T931_pos	228.2687	931	3	4.59E-04	2.04	TRUE	5.70E-02	0.71	FALSE	1.26E-01	1.30	FALSE	5.99E-01	0.93	FALSE
M229T594_pos	229.0974	594	3	1.29E-03	1.20	FALSE	4.70E-03	1.18	FALSE	2.48E-16	1.57	TRUE	6.79E-01	1.05	FALSE
M229T390_pos	229.1187	390	3	1.48E-06	0.35	TRUE	3.72E-01	1.20	FALSE	7.53E-02	1.36	FALSE	7.24E-01	0.87	FALSE
M229T954_pos	229.1800	954	3	4.14E-01	1.74	FALSE	8.20E-01	0.83	FALSE	7.74E-02	3.08	FALSE	4.08E-03	0.20	TRUE
M229T1066_pos	229.2164	1066	3	1.92E-02	1.30	FALSE	2.12E-04	0.66	TRUE	8.70E-03	0.77	FALSE	8.25E-01	1.04	FALSE
M230T495_pos	230.1389	495	3	5.90E-08	0.69	FALSE	1.02E-01	1.12	FALSE	7.85E-24	1.99	TRUE	9.69E-01	1.00	FALSE
M230T407_pos	230.1390	407	3	4.49E-01	0.94	FALSE	6.36E-04	1.34	FALSE	9.39E-12	1.70	TRUE	8.49E-02	1.21	FALSE
M231T575_pos	231.1129	575	3	1.20E-03	1.24	FALSE	1.91E-03	1.24	FALSE	1.06E-12	1.56	TRUE	1.61E-02	1.24	FALSE
M232T617_pos	232.1544	617	3	6.60E-02	0.87	FALSE	6.56E-01	1.04	FALSE	3.94E-16	1.86	TRUE	3.35E-02	0.80	FALSE
M233T487_pos	233.0957	487	3	6.68E-10	0.50	TRUE	9.75E-01	1.00	FALSE	7.22E-04	1.37	FALSE	1.25E-01	1.28	FALSE
M233T184_pos	233.1140	184	3	8.14E-34	0.19	TRUE	7.24E-01	1.03	FALSE	3.16E-02	1.19	FALSE	2.42E-01	0.91	FALSE
M234T622_pos	234.0763	622	3	1.85E-05	1.50	TRUE	4.38E-01	1.08	FALSE	3.67E-03	1.26	FALSE	8.80E-01	0.98	FALSE
M235T86_pos	234.9614	86	3	1.37E-04	0.61	TRUE	8.57E-01	0.98	FALSE	8.55E-01	0.98	FALSE	5.54E-01	0.86	FALSE
M236T526_pos	236.1283	526	3	6.39E-11	0.51	TRUE	8.43E-02	1.19	FALSE	2.42E-04	1.36	FALSE	3.12E-01	0.89	FALSE
M237T649_pos	237.0758	649	3	6.45E-04	0.80	FALSE	4.87E-01	1.05	FALSE	5.03E-22	1.86	TRUE	3.65E-01	0.95	FALSE
M237T554_pos	237.1237	554	3	2.79E-25	0.17	TRUE	8.97E-01	1.02	FALSE	2.50E-03	1.37	FALSE	4.18E-01	1.15	FALSE
M237T485_pos	237.1236	485	3	1.01E-01	0.86	FALSE	4.01E-01	0.93	FALSE	1.05E-10	1.71	TRUE	1.62E-02	0.72	FALSE
M237T562_pos	237.1599	562	3	3.58E-01	0.92	FALSE	1.82E-05	1.50	FALSE	2.64E-08	1.56	TRUE	7.69E-02	1.25	FALSE
M238T444_pos	238.0942	444	3	2.34E-02	0.86	FALSE	8.80E-01	0.99	FALSE	4.12E-22	1.93	TRUE	2.72E-01	0.93	FALSE
M238T516_pos	238.1075	516	3	4.50E-01	0.96	FALSE	3.71E-01	1.04	FALSE	2.96E-23	1.62	TRUE	5.61E-02	0.90	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M239T648_pos	239.1066	648	3							HMDB0029700	Cinnamyl benzoate	C16H14O2	0.1
M239T406_pos	239.1131	406	3							HMDB0033065	2-Propanediol 1-O-b-D-glucopyran	C9H18O7	2.3
M239T361_pos	239.1394	361	3							HMDB0014562	Secobarbital	C12H18N2O3	1.4
M239T955_pos	239.2007	955	3							HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	0.6
M239T1073_pos	239.2369	1073	3							HMDB0034181	3-Methylcyclopentadecanone	C16H30O	0.2
M240T571_pos	240.0691	571	3							HMDB0042011	S-Phenylmercapturic acid	C11H13NO3S	0.8
M240T680_pos	240.0691	680	3							HMDB0042011	S-Phenylmercapturic acid	C11H13NO3S	0.9
M240T373_pos	240.0869	373	3							HMDB0250058	(3s)-3-(Benzyloxy)-L-Aspartic Acid	C11H13NO5	1.1
M240T413_pos	240.1010	413	3							HMDB0257651	2-(2-Chlorophenyl)ethylbiguanide	C10H14ClN5	0.3
M240T551_pos	240.1233	551	3							HMDB0254628	Methyldopate	C12H17NO4	1.3
M241T390_pos	241.1217	390	3							HMDB0030672	Obtustyrene	C16H16O2	2.6
M242T466_pos	242.0666	466	3							HMDB0037548	y-6,7-dimethoxy-2H-1,4-benzoxaz	C10H11NO6	2.7
M242T499_pos	242.0849	499	3							HMDB0040289	lsulfinylmethyl)phenyl methylcarb	C11H15NO3S	1.4
M242T385_pos	242.1130	385	3							HMDB0002224	5-Methyldeoxycytidine	C10H15N3O4	2.1
M242T462_pos	242.1131	462	3							HMDB0002224	5-Methyldeoxycytidine	C10H15N3O4	2.0
M242T792_pos	242.1393	792	3							HMDB0242338	ethylpropyl]-4-propyl-6-oxa-2-aza	C12H19NO4	2.5
M243T757_pos	243.0878	757	3							HMDB0254199	Lumichrome	C12H10N4O2	0.6
M243T399_pos	243.1079	399	3							HMDB0029953	D-erythro-D-galacto-octitol	C8H18O8	1.9
M243T445_pos	243.1339	445	3							HMDB0246097	Pueraria glycoside	C11H18N2O4	0.1
M243T377_pos	243.1343	377	3							HMDB0246097	Pueraria glycoside	C11H18N2O4	1.4
M244T487_1_pos	244.0821	487	3							HMDB0243807	ydroxymethyl)oxolan-2-yl]-4-hydro	C10H13NO6	2.1
M244T180_pos	244.0930	180	3							HMDB0000089	Cytidine	C9H13N3O5	0.7
M244T648_pos	244.1546	648	3							HMDB0002366	Tiglylcarnitine	C12H21NO4	1.0
M245T602_pos	245.0956	602	3							HMDB0248297	Amidephrine	C10H16N2O3S	0.8
M245T658_pos	245.1295	658	3							HMDB0014437	Etomidate	C14H16N2O2	4.1
M245T601_pos	245.1290	601	3							HMDB0014437	Etomidate	C14H16N2O2	2.1
M245T418_pos	245.1498	418	3							HMDB0028866	Hydroxyprolyl-Isoleucine	C11H20N2O4	0.8
M245T570_pos	245.1861	570	3						Amino acids and Peptides	HMDB0028910	Isoleucyl-Isoleucine	C12H24N2O3	0.6
M246T345_pos	246.0877	345	3							HMDB0244305	phenyl beta-D-glucopyranosiduro	C9H12FN3O4	2.9
M247T595_pos	247.1111	595	3							HMDB0028981	Methionyl-Proline	C10H18N2O3S	0.0
M247T472_pos	247.1112	472	3							HMDB0028981	Methionyl-Proline	C10H18N2O3S	0.3
M247T348_pos	247.1292	348	3							HMDB0011166	L-beta-aspartyl-L-leucine	C10H18N2O5	1.4
M247T456_pos	247.1292	456	3							HMDB0011166	L-beta-aspartyl-L-leucine	C10H18N2O5	1.5
M247T894_pos	247.1325	894	3							HMDB0030911	Oxo-5,11(13)-eudesmadien-12,8-o	C15H18O3	1.7
M247T955_pos	247.1903	955	3							HMDB0072866	MG(10:0/0:0/0:0)	C13H26O4	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M239T648_pos	239.1066	648	3	1.24E-16	1.95	TRUE	8.44E-01	1.01	FALSE	4.70E-01	1.05	FALSE	1.44E-01	1.14	FALSE
M239T406_pos	239.1131	406	3	9.59E-03	0.79	FALSE	7.68E-01	1.03	FALSE	3.90E-09	1.62	TRUE	9.31E-01	0.99	FALSE
M239T361_pos	239.1394	361	3	9.80E-01	1.00	FALSE	3.75E-02	1.13	FALSE	1.36E-20	1.66	TRUE	1.56E-02	0.89	FALSE
M239T955_pos	239.2007	955	3	2.22E-01	1.06	FALSE	2.12E-01	0.94	FALSE	8.05E-05	1.17	FALSE	1.18E-03	0.66	TRUE
M239T1073_pos	239.2369	1073	3	2.18E-03	1.50	FALSE	2.93E-04	0.60	TRUE	3.60E-02	1.27	FALSE	6.52E-01	0.92	FALSE
M240T571_pos	240.0691	571	3	6.83E-01	1.04	FALSE	9.72E-01	1.00	FALSE	5.13E-08	1.58	TRUE	1.55E-01	0.83	FALSE
M240T680_pos	240.0691	680	3	1.65E-03	0.85	FALSE	6.20E-02	1.11	FALSE	4.12E-18	1.55	TRUE	8.80E-01	1.01	FALSE
M240T373_pos	240.0869	373	3	9.15E-09	0.72	FALSE	6.29E-01	1.03	FALSE	1.07E-22	1.71	TRUE	9.22E-01	1.02	FALSE
M240T413_pos	240.1010	413	3	6.32E-01	1.05	FALSE	1.81E-01	0.86	FALSE	2.09E-05	1.52	TRUE	2.37E-01	0.77	FALSE
M240T551_pos	240.1233	551	3	6.13E-03	1.27	FALSE	2.35E-01	1.11	FALSE	1.53E-08	1.58	TRUE	1.40E-01	0.75	FALSE
M241T390_pos	241.1217	390	3	5.15E-01	1.10	FALSE	3.82E-01	1.14	FALSE	9.53E-13	3.00	TRUE	1.96E-01	0.76	FALSE
M242T466_pos	242.0666	466	3	1.99E-12	0.55	TRUE	8.74E-01	0.99	FALSE	3.87E-06	1.38	FALSE	3.33E-01	1.22	FALSE
M242T499_pos	242.0849	499	3	6.05E-02	0.91	FALSE	1.20E-01	1.09	FALSE	1.62E-17	1.54	TRUE	2.70E-01	0.91	FALSE
M242T385_pos	242.1130	385	3	2.51E-01	0.90	FALSE	8.65E-01	0.98	FALSE	5.91E-09	1.66	TRUE	2.23E-01	0.82	FALSE
M242T462_pos	242.1131	462	3	4.95E-01	1.05	FALSE	8.74E-01	1.01	FALSE	4.06E-11	1.54	TRUE	3.43E-01	0.79	FALSE
M242T792_pos	242.1393	792	3	2.12E-02	0.47	TRUE	3.02E-01	1.39	FALSE	8.01E-01	1.07	FALSE	5.88E-01	1.09	FALSE
M243T757_pos	243.0878	757	3	7.40E-03	0.92	FALSE	4.36E-04	0.88	FALSE	1.17E-54	1.78	TRUE	4.25E-01	1.05	FALSE
M243T399_pos	243.1079	399	3	1.52E-05	0.72	FALSE	4.38E-01	1.06	FALSE	6.85E-11	1.56	TRUE	5.05E-01	0.93	FALSE
M243T445_pos	243.1339	445	3	8.10E-69	0.12	TRUE	1.86E-01	1.08	FALSE	1.61E-11	1.43	FALSE	5.59E-01	1.11	FALSE
M243T377_pos	243.1343	377	3	7.03E-06	0.65	TRUE	4.81E-01	1.07	FALSE	6.48E-06	1.45	FALSE	2.15E-01	0.90	FALSE
M244T487_1_pos	244.0821	487	3	7.58E-11	0.35	TRUE	7.40E-01	1.05	FALSE	1.80E-02	1.34	FALSE	5.54E-02	0.89	FALSE
M244T180_pos	244.0930	180	3	4.31E-14	0.26	TRUE	5.42E-01	0.91	FALSE	4.49E-01	1.10	FALSE	3.01E-01	0.89	FALSE
M244T648_pos	244.1546	648	3	8.52E-11	1.86	TRUE	2.25E-02	1.24	FALSE	3.13E-02	1.18	FALSE	7.75E-01	0.95	FALSE
M245T602_pos	245.0956	602	3	1.99E-04	1.18	FALSE	1.20E-01	1.07	FALSE	3.33E-21	1.51	TRUE	1.09E-03	1.23	FALSE
M245T658_pos	245.1295	658	3	4.17E-01	1.09	FALSE	6.17E-01	1.06	FALSE	4.69E-07	1.67	TRUE	3.12E-01	1.48	FALSE
M245T601_pos	245.1290	601	3	6.88E-01	0.97	FALSE	4.79E-01	0.94	FALSE	7.99E-08	1.51	TRUE	1.24E-01	1.38	FALSE
M245T418_pos	245.1498	418	3	6.74E-07	0.75	FALSE	2.28E-01	1.07	FALSE	1.22E-28	1.94	TRUE	8.43E-03	0.87	FALSE
M245T570_pos	245.1861	570	3	7.81E-17	0.25	TRUE	4.53E-01	1.11	FALSE	9.04E-03	1.35	FALSE	1.02E-01	0.68	FALSE
M246T345_pos	246.0877	345	3	4.19E-01	1.10	FALSE	7.75E-01	1.03	FALSE	2.04E-10	1.98	TRUE	5.50E-01	1.06	FALSE
M247T595_pos	247.1111	595	3	9.78E-01	1.00	FALSE	5.90E-02	1.11	FALSE	3.24E-21	1.68	TRUE	3.87E-02	0.75	FALSE
M247T472_pos	247.1112	472	3	1.09E-13	0.36	TRUE	8.48E-01	1.02	FALSE	1.80E-01	1.15	FALSE	2.87E-03	0.85	FALSE
M247T348_pos	247.1292	348	3	2.98E-28	0.16	TRUE	9.31E-01	0.99	FALSE	2.80E-03	1.35	FALSE	8.89E-03	0.69	FALSE
M247T456_pos	247.1292	456	3	7.30E-71	0.05	TRUE	2.45E-01	1.08	FALSE	4.18E-02	1.12	FALSE	8.61E-01	1.09	FALSE
M247T894_pos	247.1325	894	3	2.22E-05	1.29	FALSE	4.65E-01	1.05	FALSE	1.29E-07	0.76	FALSE	2.78E-02	0.66	TRUE
M247T955_pos	247.1903	955	3	4.70E-01	1.75	FALSE	8.78E-01	0.86	FALSE	9.75E-02	3.40	FALSE	7.19E-03	0.23	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M247T1039_pos	247.2421	1039	3						Fatty acids	HMDB0251572	Dodecylbenzene	C18H30	0.2
M248T592_pos	248.0589	592	3							HMDB0252436	Forchlorfenuron	C12H10ClN3O	1.4
M248T477_pos	248.1388	477	3							HMDB0256126	Parbendazole	C13H17N3O2	2.1
M248T367_2_pos	248.1494	367	3							HMDB0013127	3-Hydroxybutyrylcarnitine	C11H21NO5	0.7
M249T702_pos	249.0914	702	3							HMDB0060321	1-Hydroxy-6-methoxypyrene	C17H12O2	1.8
M250T429_pos	250.1295	429	3							HMDB0243858	1-Deoxy-1-morpholino-D-fructose	C10H19NO6	3.8
M251T358_pos	251.1057	358	3							HMDB0028983	Methionyl-Threonine	C9H18N2O4S	1.2
M251T923_pos	251.1256	923	3							HMDB0250896	Dda-tetracycline	C10H14N6O2	2.0
M251T668_pos	251.1258	668	3							HMDB0250896	Dda-tetracycline	C10H14N6O2	2.6
M252T368_pos	252.1494	368	3							HMDB0060956	N-desmethylmirtazapine	C16H17N3	0.3
M253T377_1_pos	253.1186	377	3							HMDB0013940	N-Desmethylpromazine	C12H16N2O4	1.1
M253T685_pos	253.1414	685	3						Fatty acids				
M253T377_2_pos	253.1547	377	3							HMDB0014451	Talbutal	C13H20N2O3	0.3
M253T1038_pos	253.2525	1038	3						Fatty acids	HMDB0013813	13-Heptadecyn-1-ol	C17H32O	0.3
M254T650_pos	254.0484	650	3							HMDB0250934	Deferitrin	C11H11NO4S	0.8
M254T535_pos	254.1026	535	3							HMDB0011716	N-Acetylvanilalanine	C12H15NO5	1.0
M255T770_pos	255.0654	770	3							HMDB0003312	Daidzein	C15H10O4	0.8
M255T618_pos	255.0978	618	3							HMDB0029445	L-Agaridoxin	C11H14N2O5	0.9
M255T485_pos	255.1342	485	3							HMDB0014356	Midodrine	C12H18N2O4	1.1
M255T972_pos	255.2109	972	3							HMDB0041371	8-Nor-4(19),8,11,13-abietatetraen	C19H26	0.5
M255T1018_pos	255.2323	1018	3							HMDB0002186	Hypogeic acid	C16H30O2	1.6
M256T183_pos	256.0820	183	3							HMDB0304540	beta-D-ribosylnicotinate	C11H13NO6	1.6
M256T395_pos	256.0820	395	3							HMDB0304540	beta-D-ribosylnicotinate	C11H13NO6	1.8
M256T528_pos	256.1330	528	3							HMDB0040381	N-Methylschinifoline	C16H17NO2	0.9
M256T917_pos	256.2637	917	3							HMDB0012273	Palmitic amide	C16H33NO	0.9
M257T721_pos	257.0811	721	3							HMDB0005760	Dihydrodaidzein	C15H12O4	1.1
M257T793_pos	257.0811	793	3							HMDB0005760	Dihydrodaidzein	C15H12O4	0.9
M257T357_pos	257.1138	357	3							HMDB0011648	D-Ribofuranosyl)-1,4-dihydronicot	C11H16N2O5	2.3
M257T432_pos	257.1242	432	3							HMDB0011655	3-Carboxy-3-aminopropyl)-L-histid	C10H16N4O4	0.9
M257T146_pos	257.2478	146	3							HMDB0000220	Palmitic acid	C16H32O2	1.1
M259T357_pos	259.0962	357	3							HMDB0004629	O-Desmethylangolensin	C15H14O4	1.0
M259T418_pos	259.1292	418	3							HMDB0038614	gamma-L-Glutamyl-L-pipecolic acid	C11H18N2O5	1.3
M259T635_pos	259.2019	635	3						Fatty acids	HMDB0248073	Leucylleucine methyl ester	C13H26N2O3	1.2
M260T445_pos	260.0921	445	3							HMDB0258333	Skimmianine	C14H13NO4	1.4
M260T534_pos	260.1128	534	3							HMDB0013134	Fumarycarnitine	C11H17NO6	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M247T1039_pos	247.2421	1039	3	2.04E-13	1.78	TRUE	1.84E-07	0.67	FALSE	7.86E-01	0.98	FALSE	1.04E-04	1.31	FALSE
M248T592_pos	248.0589	592	3	1.42E-40	0.29	TRUE	3.89E-01	1.06	FALSE	2.64E-06	1.31	FALSE	9.70E-01	1.00	FALSE
M248T477_pos	248.1388	477	3	2.17E-02	8.94	TRUE	5.77E-07	-3.32	FALSE	2.24E-05	-7.49	FALSE	9.84E-01	1.01	FALSE
M248T367_2_pos	248.1494	367	3	7.28E-11	0.29	TRUE	9.65E-01	1.01	FALSE	1.24E-02	1.43	FALSE	6.96E-02	1.29	FALSE
M249T702_pos	249.0914	702	3	4.36E-10	0.72	FALSE	3.01E-01	1.05	FALSE	4.39E-22	1.61	TRUE	4.77E-01	0.97	FALSE
M250T429_pos	250.1295	429	3	1.19E-14	0.19	TRUE	6.91E-01	1.07	FALSE	4.38E-02	0.75	FALSE	1.78E-01	0.91	FALSE
M251T358_pos	251.1057	358	3	1.31E-27	0.36	TRUE	6.00E-01	1.04	FALSE	9.39E-04	1.24	FALSE	9.57E-01	1.01	FALSE
M251T923_pos	251.1256	923	3	1.05E-12	0.35	TRUE	7.90E-01	1.04	FALSE	1.09E-03	1.45	FALSE	9.71E-01	0.99	FALSE
M251T668_pos	251.1258	668	3	5.89E-48	2.07	TRUE	6.49E-01	1.02	FALSE	6.51E-14	0.78	FALSE	2.34E-01	0.93	FALSE
M252T368_pos	252.1494	368	3	1.32E-05	0.23	TRUE	7.10E-01	1.12	FALSE	7.88E-01	0.94	FALSE	2.13E-01	0.94	FALSE
M253T377_1_pos	253.1186	377	3	8.27E-09	0.44	TRUE	8.04E-01	1.04	FALSE	1.36E-03	1.45	FALSE	2.79E-01	1.25	FALSE
M253T685_pos	253.1414	685	3	7.27E-14	1.53	TRUE	8.85E-01	0.99	FALSE	9.20E-09	0.76	FALSE	2.19E-01	1.18	FALSE
M253T377_2_pos	253.1547	377	3	3.64E-02	1.16	FALSE	1.18E-01	1.12	FALSE	2.65E-13	1.64	TRUE	1.65E-01	0.88	FALSE
M253T1038_pos	253.2525	1038	3	3.16E-06	1.51	TRUE	6.05E-05	0.71	FALSE	4.91E-03	1.24	FALSE	3.48E-01	1.09	FALSE
M254T650_pos	254.0484	650	3	1.85E-01	1.07	FALSE	7.70E-01	1.02	FALSE	2.40E-17	1.52	TRUE	7.24E-01	1.05	FALSE
M254T535_pos	254.1026	535	3	2.64E-05	0.75	FALSE	9.22E-01	0.99	FALSE	1.76E-13	1.58	TRUE	9.81E-01	1.00	FALSE
M255T770_pos	255.0654	770	3	2.83E-14	2.13	TRUE	5.48E-02	0.83	FALSE	1.49E-02	1.21	FALSE	8.88E-01	1.02	FALSE
M255T618_pos	255.0978	618	3	5.77E-07	0.77	FALSE	1.17E-01	1.09	FALSE	7.11E-32	1.90	TRUE	2.11E-01	0.92	FALSE
M255T485_pos	255.1342	485	3	1.00E-01	0.87	FALSE	7.41E-01	1.03	FALSE	7.97E-09	1.58	TRUE	9.22E-01	0.98	FALSE
M255T972_pos	255.2109	972	3	6.52E-10	1.53	TRUE	9.57E-02	0.90	FALSE	2.33E-03	1.19	FALSE	8.26E-01	1.02	FALSE
M255T1018_pos	255.2323	1018	3	1.21E-03	1.25	FALSE	1.99E-03	0.81	FALSE	2.71E-01	1.07	FALSE	1.69E-03	1.81	TRUE
M256T183_pos	256.0820	183	3	2.91E-06	0.44	TRUE	1.62E-01	0.77	FALSE	2.46E-01	1.18	FALSE	1.83E-01	1.39	FALSE
M256T395_pos	256.0820	395	3	6.73E-05	0.73	FALSE	4.16E-01	1.07	FALSE	9.91E-15	1.78	TRUE	5.99E-01	0.96	FALSE
M256T528_pos	256.1330	528	3	2.86E-01	1.10	FALSE	9.90E-01	1.00	FALSE	1.02E-13	1.90	TRUE	1.63E-01	0.88	FALSE
M256T917_pos	256.2637	917	3	1.80E-05	3.12	TRUE	6.77E-02	0.68	FALSE	2.97E-01	1.24	FALSE	7.13E-01	0.94	FALSE
M257T721_pos	257.0811	721	3	2.29E-03	0.82	FALSE	1.19E-01	1.11	FALSE	4.79E-16	1.65	TRUE	6.78E-01	1.03	FALSE
M257T793_pos	257.0811	793	3	8.54E-02	0.93	FALSE	5.56E-01	1.03	FALSE	8.01E-22	1.50	TRUE	1.23E-03	0.83	FALSE
M257T357_pos	257.1138	357	3	2.29E-04	0.74	FALSE	1.43E-01	1.13	FALSE	1.68E-13	1.77	TRUE	3.78E-01	1.13	FALSE
M257T432_pos	257.1242	432	3	6.22E-02	0.87	FALSE	3.23E-01	1.08	FALSE	1.72E-19	1.94	TRUE	3.52E-03	0.78	FALSE
M257T146_pos	257.2478	146	3	8.21E-01	0.99	FALSE	2.17E-01	0.93	FALSE	2.63E-01	1.06	FALSE	1.41E-02	0.65	TRUE
M259T357_pos	259.0962	357	3	4.79E-04	0.72	FALSE	1.70E-01	0.88	FALSE	5.00E-07	1.52	TRUE	1.95E-01	0.88	FALSE
M259T418_pos	259.1292	418	3	5.42E-05	0.75	FALSE	6.61E-01	1.03	FALSE	1.73E-15	1.70	TRUE	8.50E-01	0.97	FALSE
M259T635_pos	259.2019	635	3	5.45E-05	1.37	FALSE	5.26E-07	1.49	FALSE	9.27E-17	1.85	TRUE	8.48E-01	1.01	FALSE
M260T445_pos	260.0921	445	3	5.24E-02	1.10	FALSE	7.89E-01	0.99	FALSE	8.30E-21	1.56	TRUE	2.00E-01	0.89	FALSE
M260T534_pos	260.1128	534	3	6.14E-02	0.83	FALSE	5.67E-04	1.47	FALSE	4.42E-15	2.20	TRUE	3.74E-01	0.87	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M260T471_pos	260.1503	471	3							HMDB0241663	3-Oxopentanoylcarnitine	C12H21NO5	4.0
M260T347_pos	260.1605	347	3							HMDB0028800	Glutaminylisoleucine	C11H21N3O4	0.2
M260T401_pos	260.1968	401	3							HMDB0028912	Isoleucyl-Lysine	C12H25N3O3	0.1
M260T366_pos	260.1971	366	3							HMDB0028912	Isoleucyl-Lysine	C12H25N3O3	1.1
M260T257_pos	260.1972	257	3							HMDB0028912	Isoleucyl-Lysine	C12H25N3O3	1.3
M260T164_pos	260.1971	164	3							HMDB0028912	Isoleucyl-Lysine	C12H25N3O3	1.1
M260T875_pos	260.2585	875	3						Fatty acids				
M261T599_pos	261.0875	599	3							HMDB0032102	etrahydro-b-carboline-1,3-dicarbo	C13H12N2O4	2.0
M261T463_pos	261.1445	463	3							HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	0.1
M261T375_pos	261.1447	375	3							HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	0.8
M261T778_pos	261.1596	778	3							HMDB0033481	Baptifoline	C15H20N2O2	0.5
M261T1045_pos	261.2214	1045	3						Terpenoids	HMDB0245878	3-Gonal	C18H28O	0.4
M262T491_pos	262.1192	491	3							HMDB0028852	Glycyl-Tryptophan	C13H15N3O3	2.4
M262T523_pos	262.1288	523	3							HMDB0033865	Lotaustralin	C11H19NO6	1.0
M262T291_pos	262.1288	291	3							HMDB0033865	Lotaustralin	C11H19NO6	1.1
M262T571_pos	262.1648	571	3							HMDB0061189	3-Hydroxyisovalerylcarnitine	C12H23NO5	0.3
M263T436_pos	263.1393	436	3							HMDB0014617	Methohexital	C14H18N2O3	1.2
M263T652_pos	263.1424	652	3							HMDB0028913	Isoleucyl-Methionine	C11H22N2O3S	0.1
M264T313_pos	264.1274	313	3							HMDB0249267	Didesethyl Chloroquine	C14H18ClN3	4.6
M265T837_pos	265.1072	837	3							HMDB0036544	Heliantriol A1	C14H16O5	0.7
M265T769_pos	265.1072	769	3							HMDB0036544	Heliantriol A1	C14H16O5	0.5
M265T680_pos	265.1221	680	3							HMDB0033832	Cinnamyl cinnamate	C18H16O2	0.7
M265T654_pos	265.1548	654	3							HMDB0015568	Vorinostat	C14H20N2O3	0.5
M265T86_pos	265.1760	86	3						Carbohydrates				
M266T465_pos	266.1391	465	3							HMDB0243530	diol, 2-(p-methoxybenzyl)-, 3-aceta	C14H19NO4	1.4
M267T384_pos	267.0979	384	3							HMDB0255007	N-(4-Aminobenzoyl)-L-glutamic aci	C12H14N2O5	1.4
M267T794_pos	267.1228	794	3							HMDB0040891	bis(4-hydroxyphenyl)-1,4,6-heptat	C14H18O5	0.4
M267T470_pos	267.1348	470	3							HMDB0029005	Phenylalanylthreonine	C13H18N2O4	3.1
M267T569_pos	267.1392	569	3							HMDB0015027	Dienestrol	C18H18O2	4.8
M268T375_pos	268.0921	375	3							HMDB0247328	-5-((4-nitrophenyl)amino)-5-oxope	C11H13N3O5	2.8
M268T413_pos	268.1655	413	3							HMDB0249665	Carbuterol	C13H21N3O3	0.1
M269T182_pos	269.0366	182	3							HMDB0254681	Metoprine	C11H10Cl2N4	3.8
M269T576_pos	269.1141	576	3							HMDB0029051	Seryltyrosine	C12H16N2O5	3.3
M269T465_pos	269.1499	465	3							HMDB0247322	(2-hydroxyethyl)amino-L-phenylal	C13H20N2O4	1.2
M269T633_pos	269.1748	633	3						Terpenoids	HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M260T471_pos	260.1503	471	3	4.20E-05	0.09	TRUE	9.61E-01	1.02	FALSE	2.80E-01	1.46	FALSE	2.74E-01	1.19	FALSE
M260T347_pos	260.1605	347	3	3.33E-07	0.62	TRUE	6.75E-01	0.96	FALSE	1.54E-01	1.12	FALSE	7.60E-01	0.95	FALSE
M260T401_pos	260.1968	401	3	2.34E-31	0.35	TRUE	8.71E-02	1.13	FALSE	9.24E-03	1.17	FALSE	2.66E-01	0.89	FALSE
M260T366_pos	260.1971	366	3	6.71E-14	0.50	TRUE	3.04E-02	1.21	FALSE	7.39E-07	1.44	FALSE	3.63E-01	1.13	FALSE
M260T257_pos	260.1972	257	3	5.16E-19	0.29	TRUE	3.86E-01	1.11	FALSE	2.78E-03	1.34	FALSE	9.87E-01	1.00	FALSE
M260T164_pos	260.1971	164	3	1.24E-16	0.16	TRUE	4.49E-01	1.14	FALSE	5.44E-01	0.92	FALSE	6.90E-01	0.95	FALSE
M260T875_pos	260.2585	875	3	2.32E-05	6.24	TRUE	1.83E-01	0.65	FALSE	1.32E-01	1.56	FALSE	4.55E-01	0.91	FALSE
M261T599_pos	261.0875	599	3	8.64E-08	0.36	TRUE	8.86E-01	1.03	FALSE	4.77E-01	1.11	FALSE	2.46E-01	0.82	FALSE
M261T463_pos	261.1445	463	3	1.07E-55	0.15	TRUE	4.16E-02	1.15	FALSE	2.81E-05	1.28	FALSE	4.50E-01	0.74	FALSE
M261T375_pos	261.1447	375	3	1.95E-33	0.28	TRUE	3.87E-01	1.07	FALSE	1.85E-07	1.44	FALSE	4.26E-01	0.91	FALSE
M261T778_pos	261.1596	778	3	4.54E-14	1.63	TRUE	2.37E-01	1.08	FALSE	9.20E-05	1.23	FALSE	3.05E-01	1.14	FALSE
M261T1045_pos	261.2214	1045	3	7.94E-01	1.09	FALSE	6.80E-02	0.40	FALSE	1.38E-03	2.58	TRUE	2.46E-01	0.84	FALSE
M262T491_pos	262.1192	491	3	1.49E-30	0.23	TRUE	8.77E-01	1.01	FALSE	4.70E-04	1.33	FALSE	7.00E-01	1.11	FALSE
M262T523_pos	262.1288	523	3	9.75E-03	0.79	FALSE	4.68E-01	1.07	FALSE	4.11E-14	1.97	TRUE	6.38E-02	0.58	FALSE
M262T291_pos	262.1288	291	3	1.70E-04	0.72	FALSE	2.43E-01	0.90	FALSE	7.85E-17	2.01	TRUE	5.48E-02	0.83	FALSE
M262T571_pos	262.1648	571	3	1.87E-08	0.68	FALSE	1.84E-01	1.09	FALSE	1.09E-19	1.79	TRUE	5.54E-01	0.95	FALSE
M263T436_pos	263.1393	436	3	1.22E-04	1.34	FALSE	3.53E-01	0.93	FALSE	9.32E-11	1.58	TRUE	4.10E-01	0.91	FALSE
M263T652_pos	263.1424	652	3	1.36E-23	0.13	TRUE	7.68E-01	0.96	FALSE	4.59E-02	1.27	FALSE	1.67E-01	0.78	FALSE
M264T313_pos	264.1274	313	3	1.66E-21	0.37	TRUE	6.77E-01	0.96	FALSE	5.37E-07	1.47	FALSE	6.76E-01	1.08	FALSE
M265T837_pos	265.1072	837	3	1.45E-06	1.43	FALSE	1.09E-05	0.73	FALSE	3.31E-04	1.26	FALSE	1.70E-02	0.65	TRUE
M265T769_pos	265.1072	769	3	4.73E-03	0.85	FALSE	7.23E-03	1.17	FALSE	1.92E-14	1.50	TRUE	2.16E-01	0.95	FALSE
M265T680_pos	265.1221	680	3	5.82E-17	1.55	TRUE	1.01E-01	0.92	FALSE	9.57E-02	1.07	FALSE	2.79E-02	0.85	FALSE
M265T654_pos	265.1548	654	3	1.18E-51	0.05	TRUE	1.92E-01	1.12	FALSE	8.55E-07	1.47	FALSE	1.65E-01	0.55	FALSE
M265T86_pos	265.1760	86	3	2.68E-13	0.02	TRUE	8.13E-01	1.06	FALSE	8.31E-01	1.05	FALSE	2.06E-01	0.58	FALSE
M266T465_pos	266.1391	465	3	6.65E-01	0.96	FALSE	5.23E-01	1.07	FALSE	9.55E-14	2.07	TRUE	1.96E-01	0.86	FALSE
M267T384_pos	267.0979	384	3	5.96E-01	0.98	FALSE	1.16E-03	1.13	FALSE	1.45E-27	1.50	TRUE	5.31E-01	0.98	FALSE
M267T794_pos	267.1228	794	3	5.60E-09	0.76	FALSE	1.35E-09	1.32	FALSE	1.24E-25	1.61	TRUE	2.50E-01	0.95	FALSE
M267T470_pos	267.1348	470	3	4.51E-01	1.06	FALSE	1.99E-02	1.21	FALSE	2.13E-12	1.69	TRUE	8.85E-01	1.01	FALSE
M267T569_pos	267.1392	569	3	2.04E-27	0.12	TRUE	8.92E-01	1.02	FALSE	5.70E-03	1.35	FALSE	7.80E-02	0.79	FALSE
M268T375_pos	268.0921	375	3	3.39E-03	0.68	FALSE	6.02E-01	0.93	FALSE	8.82E-08	1.89	TRUE	3.37E-01	1.19	FALSE
M268T413_pos	268.1655	413	3	2.05E-21	0.25	TRUE	4.77E-03	1.39	FALSE	1.14E-03	1.38	FALSE	8.54E-01	0.96	FALSE
M269T182_pos	269.0366	182	3	4.62E-23	0.15	TRUE	6.51E-01	1.06	FALSE	2.06E-03	0.70	FALSE	4.75E-01	0.87	FALSE
M269T576_pos	269.1141	576	3	1.51E-26	0.06	TRUE	7.78E-01	0.96	FALSE	2.26E-03	1.48	FALSE	3.20E-01	0.87	FALSE
M269T465_pos	269.1499	465	3	7.30E-04	1.33	FALSE	2.72E-01	1.10	FALSE	2.34E-28	2.82	TRUE	2.29E-03	0.72	FALSE
M269T633_pos	269.1748	633	3	3.24E-01	1.23	FALSE	2.84E-03	0.47	TRUE	9.34E-01	1.01	FALSE	6.96E-01	0.91	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M270T379_pos	270.1351	379	3							HMDB0251804	Endralazine	C14H15N5O	0.7
M270T597_pos	270.1338	597	3							HMDB0251804	Endralazine	C14H15N5O	4.2
M270T454_pos	270.1450	454	3							HMDB0260136	ine-2-carbonyl]amino]acetyl]pyrro	C12H19N3O4	0.7
M270T922_pos	270.2794	922	3							HMDB0040940	Capsiamide	C17H35NO	0.9
M271T444_pos	271.1389	444	3							HMDB0254886	Morinidazole	C11H18N4O4	4.2
M271T953_pos	271.2057	953	3							HMDB0248405	Androsta-4,16-dien-3-one	C19H26O	0.2
M272T564_pos	272.0492	564	3							HMDB0248349	Amoscanate	C13H9N3O2S	1.4
M272T618_pos	272.0921	618	3							HMDB0032109	Koeniginequinone B	C15H13NO4	1.3
M272T649_pos	272.1133	649	3							HMDB0246178	4-Aminophenylmannoside	C12H17NO6	1.6
M273T87_pos	272.9445	87	3							HMDB0245499	5-Diisothiocyanatobenzenesulfona	C8H4N2O3S3	4.3
M273T580_pos	273.1237	580	3							HMDB0035191	9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-t	C15H16N2O3	1.4
M273T821_pos	273.1311	821	3							HMDB0033663	Decarbamoylneosaxitoxin	C9H16N6O4	2.0
M273T1039_pos	273.2579	1039	3							HMDB0035394	ent-16-Kaurene	C20H32	0.8
M274T658_pos	274.1078	658	3							HMDB0000667	L-Thyronine	C15H15NO4	1.6
M274T800_pos	274.1440	800	3							HMDB0030187	(E,E)-Piperlonguminine	C16H19NO3	0.8
M274T547_pos	274.1543	547	3							HMDB0061158	N-Acetyl desmethyl frovatriptan	C15H19N3O2	2.7
M274T156_pos	274.1875	156	3							HMDB0028722	Arginylvaline	C11H23N5O3	0.7
M275T656_pos	275.1393	656	3							HMDB0034885	Imazamethabenz	C15H18N2O3	1.0
M275T134_pos	275.1968	134	3						Amino acids and Peptides	HMDB0248003	Adelmidrol	C13H26N2O4	1.0
M275T970_pos	275.2370	970	3							HMDB0005935	Androstenol	C19H30O	0.3
M276T140_pos	276.1192	140	3							HMDB0005766	Norophthalmic acid	C10H17N3O6	0.7
M276T382_pos	276.1442	382	3							HMDB0240779	O-Glutarylcarnitine	C12H21NO6	0.0
M277T396_pos	277.0872	396	3							HMDB0246110	Pound feminine-Methoxy Puerari	C15H13FO4	0.5
M277T517_pos	277.1060	517	3							HMDB0030145	Ascochitine	C15H16O5	3.8
M277T511_pos	277.1189	511	3							HMDB0062178	N-lactoyl-Tryptophan	C14H16N2O4	2.2
M277T431_pos	277.1283	431	3							HMDB0034263	Triethyl citrate	C12H20O7	0.5
M277T135_pos	277.1223	135	3							HMDB0252103	Etintidine	C12H16N6S	2.4
M277T955_pos	277.1800	955	3							HMDB0015586	Cyclandelate	C17H24O3	0.6
M278T808_pos	278.1753	808	3							HMDB0036325	Dinorcapsaicin	C16H23NO3	0.7
M278T907_pos	278.1860	907	3							HMDB0041944	N-Acetylprocainamide	C15H23N3O2	1.1
M279T702_pos	279.1704	702	3							HMDB0013243	Leucylphenylalanine	C15H22N2O3	0.1
M279T499_pos	279.1866	499	3							HMDB0014571	Triprolidine	C19H22N2	3.6
M280T626_pos	280.1182	626	3							HMDB0032807	Niazirin	C14H17NO5	1.0
M280T502_pos	280.1293	502	3							HMDB0028738	Asparaginyl-Phenylalanine	C13H17N3O4	0.3
M280T286_pos	280.1393	286	3							HMDB0037844	N-(1-Deoxy-1-fructosyl)valine	C11H21NO7	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M270T379_pos	270.1351	379	3	6.16E-01	1.06	FALSE	1.42E-01	1.20	FALSE	1.08E-04	1.51	TRUE	8.06E-01	1.10	FALSE
M270T597_pos	270.1338	597	3	6.83E-02	1.21	FALSE	2.50E-01	1.13	FALSE	3.79E-07	1.61	TRUE	1.04E-02	0.67	FALSE
M270T454_pos	270.1450	454	3	3.58E-01	0.95	FALSE	4.22E-01	1.04	FALSE	7.91E-23	1.65	TRUE	9.80E-02	0.91	FALSE
M270T922_pos	270.2794	922	3	3.53E-05	4.88	TRUE	1.76E-01	0.70	FALSE	4.62E-01	1.22	FALSE	8.90E-01	0.95	FALSE
M271T444_pos	271.1389	444	3	3.15E-02	0.83	FALSE	3.91E-01	1.08	FALSE	5.12E-17	2.03	TRUE	1.17E-01	0.87	FALSE
M271T953_pos	271.2057	953	3	3.56E-06	1.30	FALSE	3.52E-01	0.95	FALSE	1.35E-14	1.50	TRUE	3.87E-01	0.93	FALSE
M272T564_pos	272.0492	564	3	4.02E-02	1.29	FALSE	7.68E-01	0.96	FALSE	1.67E-05	1.62	TRUE	9.05E-01	0.99	FALSE
M272T618_pos	272.0921	618	3	6.94E-01	1.02	FALSE	7.50E-01	1.02	FALSE	2.10E-18	1.63	TRUE	3.34E-01	0.91	FALSE
M272T649_pos	272.1133	649	3	3.31E-02	1.12	FALSE	2.10E-01	1.07	FALSE	9.56E-16	1.50	TRUE	7.72E-01	1.02	FALSE
M273T87_pos	272.9445	87	3	4.65E-01	1.05	FALSE	2.69E-02	1.15	FALSE	2.29E-05	1.26	FALSE	8.49E-03	2.09	TRUE
M273T580_pos	273.1237	580	3	1.30E-01	0.93	FALSE	8.27E-01	1.01	FALSE	7.65E-23	1.56	TRUE	3.87E-02	0.88	FALSE
M273T821_pos	273.1311	821	3	9.40E-01	0.99	FALSE	3.67E-02	1.38	FALSE	1.36E-03	1.51	TRUE	9.01E-01	1.01	FALSE
M273T1039_pos	273.2579	1039	3	2.93E-06	3.04	TRUE	6.54E-02	0.70	FALSE	7.74E-01	1.05	FALSE	8.07E-01	0.94	FALSE
M274T658_pos	274.1078	658	3	3.12E-06	0.76	FALSE	6.03E-01	0.97	FALSE	2.88E-19	1.65	TRUE	8.56E-01	1.02	FALSE
M274T800_pos	274.1440	800	3	7.54E-05	2.27	TRUE	5.73E-01	0.90	FALSE	3.56E-01	0.86	FALSE	5.72E-01	0.68	FALSE
M274T547_pos	274.1543	547	3	1.75E-07	1.73	TRUE	7.07E-01	1.04	FALSE	1.87E-04	1.39	FALSE	6.82E-01	1.12	FALSE
M274T156_pos	274.1875	156	3	5.28E-24	0.17	TRUE	4.89E-01	1.10	FALSE	8.30E-01	0.98	FALSE	3.13E-01	0.82	FALSE
M275T656_pos	275.1393	656	3	1.96E-10	0.52	TRUE	5.81E-01	1.06	FALSE	3.71E-05	1.41	FALSE	4.77E-01	1.19	FALSE
M275T134_pos	275.1968	134	3	3.87E-07	0.70	FALSE	1.42E-02	1.19	FALSE	2.84E-13	1.61	TRUE	1.28E-01	1.12	FALSE
M275T970_pos	275.2370	970	3	1.72E-06	1.75	TRUE	4.86E-02	0.81	FALSE	4.03E-01	1.08	FALSE	8.60E-01	0.98	FALSE
M276T140_pos	276.1192	140	3	2.04E-01	0.82	FALSE	1.52E-01	0.80	FALSE	3.09E-05	1.78	TRUE	3.81E-01	0.78	FALSE
M276T382_pos	276.1442	382	3	5.44E-08	0.01	TRUE	9.54E-01	1.02	FALSE	6.67E-01	1.14	FALSE	5.88E-01	1.30	FALSE
M277T396_pos	277.0872	396	3	7.30E-02	1.21	FALSE	1.68E-06	0.52	TRUE	2.00E-02	1.24	FALSE	6.80E-01	1.07	FALSE
M277T517_pos	277.1060	517	3	5.88E-13	0.60	TRUE	4.92E-01	0.95	FALSE	7.11E-06	1.30	FALSE	2.14E-02	1.47	FALSE
M277T511_pos	277.1189	511	3	5.73E-57	0.13	TRUE	5.03E-01	0.95	FALSE	3.78E-03	1.19	FALSE	2.79E-02	0.72	FALSE
M277T431_pos	277.1283	431	3	5.49E-01	1.05	FALSE	9.10E-01	1.01	FALSE	1.65E-10	1.56	TRUE	1.58E-01	1.15	FALSE
M277T135_pos	277.1223	135	3	1.77E-04	0.66	TRUE	5.15E-01	0.93	FALSE	3.02E-05	1.50	FALSE	6.88E-01	0.90	FALSE
M277T955_pos	277.1800	955	3	1.01E-04	1.45	FALSE	3.95E-12	0.43	TRUE	6.25E-02	0.86	FALSE	7.23E-01	1.09	FALSE
M278T808_pos	278.1753	808	3	3.28E-15	-5.05	FALSE	9.82E-02	1.57	FALSE	2.16E-05	0.20	TRUE	1.35E-01	0.61	FALSE
M278T907_pos	278.1860	907	3	1.95E-25	2.63	TRUE	3.91E-06	0.70	FALSE	1.18E-01	1.11	FALSE	2.61E-02	0.79	FALSE
M279T702_pos	279.1704	702	3	4.07E-39	0.10	TRUE	1.50E-01	1.16	FALSE	5.43E-03	1.27	FALSE	8.15E-02	0.54	FALSE
M279T499_pos	279.1866	499	3	1.58E-34	0.13	TRUE	5.94E-01	1.06	FALSE	3.02E-02	0.82	FALSE	9.01E-01	0.98	FALSE
M280T626_pos	280.1182	626	3	1.20E-03	0.87	FALSE	5.18E-01	1.03	FALSE	4.05E-22	1.53	TRUE	8.06E-03	0.86	FALSE
M280T502_pos	280.1293	502	3	1.42E-23	0.18	TRUE	8.09E-01	1.03	FALSE	1.43E-01	1.17	FALSE	6.60E-01	0.87	FALSE
M280T286_pos	280.1393	286	3	3.76E-06	0.37	TRUE	7.16E-01	1.08	FALSE	8.92E-02	1.33	FALSE	9.02E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M280T209_pos	280.1393	209	3							HMDB0037844	N-(1-Deoxy-1-fructosyl)valine	C11H21NO7	0.9
M280T953_pos	280.2637	953	3							HMDB0062656	Linoleamide	C18H33NO	0.6
M281T787_pos	281.1024	787	3							HMDB0033884	Gravolenic acid	C14H16O6	1.5
M281T518_pos	281.1133	518	3							HMDB0000706	Aspartylphenylalanine	C13H16N2O5	0.3
M281T420_pos	281.1138	420	3							HMDB0000706	Aspartylphenylalanine	C13H16N2O5	2.0
M281T758_pos	281.1494	758	3							HMDB0029118	Tyrosyl-Valine	C14H20N2O4	0.7
M281T428_pos	281.1499	428	3							HMDB0029118	Tyrosyl-Valine	C14H20N2O4	1.3
M281T506_pos	281.1501	506	3							HMDB0029118	Tyrosyl-Valine	C14H20N2O4	1.9
M282T629_pos	282.1086	629	3							HMDB0040693	nma-Glutamyl)-4-carboxyphenylhy	C12H15N3O5	0.6
M282T397_pos	282.1345	397	3							HMDB0255476	3-Hydroxy-4-pivaloyloxyphenyl)ala	C14H19NO5	3.3
M283T575_pos	283.1079	575	3							HMDB0245789	rmethyl)-5,5-diphenylimidazolidine	C16H14N2O3	0.6
M283T521_pos	283.1437	521	3							HMDB0244561	zol-2-yl)ethyl)-5-ethyl-6-methylpyr	C17H18N2O2	1.6
M283T926_pos	283.2827	926	3						Terpenoids				
M284T616_pos	284.1283	616	3							HMDB0002372	N-Phenylacetylphenylalanine	C17H17NO3	0.6
M285T792_pos	285.1334	792	3							HMDB0029819	Phenylethyl beta-D-glucopyranosi	C14H20O6	0.4
M285T617_pos	285.1809	617	3							HMDB0247560	ycarbonyl)piperidin-4-yl)azetidine-	C14H24N2O4	0.1
M286T516_pos	286.1292	516	3							HMDB0241034	dimethylidenebutanedioylcarnitine	C13H19NO6	2.3
M286T362_pos	286.1394	362	3							HMDB0002171	Glycylprolylhydroxyproline	C12H19N3O5	1.3
M287T517_pos	287.1031	517	3							HMDB0013895	S-4-Hydroxymephenytoin	C15H14N2O4	1.7
M287T434_pos	287.1034	434	3							HMDB0013895	S-4-Hydroxymephenytoin	C15H14N2O4	2.6
M287T803_2_pos	287.1348	803	3							HMDB0255034	piperazino)propyl]-N-(2-amino-2-c	C11H18N4O5	0.6
M287T375_pos	287.1604	375	3							HMDB0015182	Abacavir	C14H18N6O	3.8
M287T462_pos	287.1606	462	3							HMDB0015182	Abacavir	C14H18N6O	3.2
M289T899_pos	289.2163	899	3						Terpenoids	HMDB0000077	Dehydroepiandrosterone	C19H28O2	0.5
M289T1017_pos	289.2528	1017	3						Terpenoids	HMDB0034736	Abietinol	C20H32O	0.7
M291T159_pos	291.2282	159	3							HMDB0014347	Succinylcholine	C14H30N2O4	1.2
M291T1033_2_pos	291.2317	1033	3							HMDB0000031	Androsterone	C19H30O2	0.4
M291T1031_pos	291.2682	1031	3							HMDB0035083	,6E,10E)-1,6,10,14-Phytatetraen-3	C20H34O	0.3
M292T527_pos	292.1295	527	3							HMDB0029050	Seryltryptophan	C14H17N3O4	0.9
M292T647_pos	292.1910	647	3							HMDB0015114	Cyclopentolate	C17H25NO3	1.0
M293T411_pos	293.1138	411	3						Amino acids and Peptides	HMDB0041309	(2S,4S)-Monatin	C14H16N2O5	1.9
M293T823_pos	293.1860	823	3							HMDB0014662	Carteolol	C16H24N2O3	0.3
M293T1002_pos	293.2098	1002	3						Fatty acids	HMDB0030996	yltetrahydro-2-oxo-3-furancarboxy	C18H28O3	4.6
M293T1039_pos	293.2841	1039	3							HMDB0032147	Geranylcitronellol	C20H36O	0.7
M295T520_pos	295.1654	520	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M280T209_pos	280.1393	209	3	4.88E-06	0.04	TRUE	8.88E-01	1.06	FALSE	9.29E-01	1.03	FALSE	5.29E-02	0.80	FALSE
M280T953_pos	280.2637	953	3	7.15E-01	1.06	FALSE	2.27E-01	0.81	FALSE	6.20E-01	1.07	FALSE	1.70E-02	120.07	TRUE
M281T787_pos	281.1024	787	3	5.46E-38	0.46	TRUE	4.44E-01	0.96	FALSE	7.67E-04	1.15	FALSE	1.13E-02	0.76	FALSE
M281T518_pos	281.1133	518	3	5.08E-36	0.22	TRUE	2.40E-02	1.21	FALSE	8.51E-02	1.13	FALSE	2.41E-01	0.82	FALSE
M281T420_pos	281.1138	420	3	2.58E-23	0.37	TRUE	8.54E-01	0.98	FALSE	2.38E-05	1.36	FALSE	6.72E-01	1.06	FALSE
M281T758_pos	281.1494	758	3	1.80E-09	0.56	TRUE	7.26E-02	1.19	FALSE	1.42E-06	1.49	FALSE	8.52E-01	0.98	FALSE
M281T428_pos	281.1499	428	3	1.39E-13	0.34	TRUE	7.76E-01	1.04	FALSE	2.89E-02	1.27	FALSE	2.73E-01	1.25	FALSE
M281T506_pos	281.1501	506	3	1.68E-51	0.14	TRUE	2.07E-01	1.10	FALSE	3.15E-09	1.48	FALSE	6.68E-01	0.94	FALSE
M282T629_pos	282.1086	629	3	2.51E-01	0.93	FALSE	8.76E-04	1.26	FALSE	7.00E-17	1.73	TRUE	6.20E-01	0.96	FALSE
M282T397_pos	282.1345	397	3	2.43E-01	0.92	FALSE	3.83E-01	1.07	FALSE	2.16E-19	1.94	TRUE	4.86E-01	0.96	FALSE
M283T575_pos	283.1079	575	3	8.76E-01	1.01	FALSE	8.12E-01	1.01	FALSE	4.07E-19	1.68	TRUE	1.11E-01	0.84	FALSE
M283T521_pos	283.1437	521	3	1.43E-11	1.78	TRUE	9.09E-01	0.99	FALSE	3.56E-07	1.44	FALSE	4.57E-01	0.92	FALSE
M283T926_pos	283.2827	926	3	2.64E-04	2.12	TRUE	1.90E-01	0.78	FALSE	7.57E-01	1.05	FALSE	7.80E-01	0.95	FALSE
M284T616_pos	284.1283	616	3	4.95E-06	1.59	TRUE	4.63E-01	0.93	FALSE	1.00E-01	0.87	FALSE	3.67E-01	0.82	FALSE
M285T792_pos	285.1334	792	3	1.00E-11	0.74	FALSE	2.88E-11	1.33	FALSE	1.17E-23	1.52	TRUE	2.03E-01	0.94	FALSE
M285T617_pos	285.1809	617	3	3.36E-01	0.94	FALSE	6.85E-02	1.13	FALSE	1.39E-14	1.60	TRUE	5.33E-01	0.92	FALSE
M286T516_pos	286.1292	516	3	3.86E-04	0.82	FALSE	1.98E-01	1.08	FALSE	1.54E-18	1.62	TRUE	7.41E-02	0.84	FALSE
M286T362_pos	286.1394	362	3	1.14E-04	0.68	FALSE	2.40E-01	1.13	FALSE	6.69E-15	2.10	TRUE	8.75E-01	1.03	FALSE
M287T517_pos	287.1031	517	3	2.87E-04	0.64	TRUE	9.24E-01	1.01	FALSE	7.63E-03	1.32	FALSE	7.64E-02	1.25	FALSE
M287T434_pos	287.1034	434	3	4.36E-06	0.68	FALSE	4.69E-01	0.94	FALSE	8.60E-12	1.68	TRUE	6.11E-01	1.07	FALSE
M287T803_2_pos	287.1348	803	3	7.22E-13	1.76	TRUE	3.09E-01	0.93	FALSE	7.13E-01	0.98	FALSE	2.56E-02	1.19	FALSE
M287T375_pos	287.1604	375	3	8.09E-01	1.02	FALSE	9.33E-02	1.12	FALSE	4.56E-15	1.61	TRUE	2.38E-01	1.21	FALSE
M287T462_pos	287.1606	462	3	3.67E-04	0.75	FALSE	9.19E-01	1.01	FALSE	8.69E-16	1.87	TRUE	7.54E-01	1.06	FALSE
M289T899_pos	289.2163	899	3	1.57E-11	1.57	TRUE	2.08E-03	0.82	FALSE	4.57E-01	0.96	FALSE	7.00E-01	1.04	FALSE
M289T1017_pos	289.2528	1017	3	9.40E-05	3.05	TRUE	3.23E-01	0.79	FALSE	5.42E-02	1.54	FALSE	8.95E-01	1.03	FALSE
M291T159_pos	291.2282	159	3	7.72E-02	1.16	FALSE	2.31E-03	1.30	FALSE	4.19E-13	1.78	TRUE	4.99E-01	0.95	FALSE
M291T1033_2_pos	291.2317	1033	3	6.88E-01	1.09	FALSE	6.87E-02	0.57	FALSE	6.36E-04	2.03	TRUE	6.62E-02	0.76	FALSE
M291T1031_pos	291.2682	1031	3	1.01E-04	2.00	TRUE	1.01E-02	0.67	FALSE	5.51E-01	0.92	FALSE	7.33E-01	1.15	FALSE
M292T527_pos	292.1295	527	3	3.08E-19	0.34	TRUE	4.73E-01	1.08	FALSE	3.08E-05	1.45	FALSE	2.12E-01	0.84	FALSE
M292T647_pos	292.1910	647	3	1.28E-01	1.19	FALSE	8.59E-01	0.98	FALSE	2.31E-08	1.79	TRUE	1.31E-01	1.32	FALSE
M293T411_pos	293.1138	411	3	1.62E-52	0.35	TRUE	7.17E-01	1.02	FALSE	6.98E-17	1.44	FALSE	7.83E-01	1.01	FALSE
M293T823_pos	293.1860	823	3	2.10E-20	0.66	TRUE	8.90E-01	1.01	FALSE	3.79E-17	1.38	FALSE	4.86E-01	1.03	FALSE
M293T1002_pos	293.2098	1002	3	3.78E-10	1.63	TRUE	2.60E-03	0.80	FALSE	2.30E-04	1.27	FALSE	1.23E-01	0.85	FALSE
M293T1039_pos	293.2841	1039	3	1.11E-03	2.65	TRUE	9.77E-02	0.66	FALSE	6.59E-01	0.90	FALSE	6.72E-01	1.12	FALSE
M295T520_pos	295.1654	520	3	2.77E-13	0.34	TRUE	9.91E-01	1.00	FALSE	6.31E-01	1.05	FALSE	1.06E-01	0.69	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M295T464_pos	295.1655	464	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.7
M296T396_pos	296.1214	396	3							HMDB0246982	Norquetiapine	C17H17N3S	0.7
M296T1067_pos	296.2590	1067	3						Fatty acids				
M297T487_pos	297.1810	487	3							HMDB0248879	Batelapine	C16H20N6	4.1
M298T915_pos	298.2743	915	3							HMDB0013648	Palmitoleoylethanolamde	C18H35NO2	0.7
M299T436_2_pos	299.1608	436	3							HMDB0035233	Olomoucine	C15H18N6O	2.2
M299T311_pos	299.1605	311	3							HMDB0035233	Olomoucine	C15H18N6O	3.4
M299T1038_2_pos	299.2582	1038	3						Fatty acids	HMDB0010736	3-Oxooctadecanoic acid	C18H34O3	0.4
M300T367_pos	300.1447	367	3							HMDB0241039	-dimethylidenepentanedioylcarnit	C14H21NO6	1.8
M303T473_pos	303.1673	473	3							HMDB0013016	Neuromedin B (1-3)	C12H22N4O5	3.2
M304T803_pos	304.1550	803	3							HMDB0003573	Scopolamine	C17H21NO4	2.1
M304T688_pos	304.1582	688	3							HMDB0255339	n-4-yl (2R)-2-acetamido-3-sulfanyl	C14H25NO4S	1.6
M304T564_pos	304.1659	564	3							HMDB0029096	Tryptophyl-Valine	C16H21N3O3	0.9
M305T746_pos	305.1498	746	3							HMDB0244641	-4-methyl-3-(4-methylpiperazin-1-	C16H20N2O4	0.9
M305T612_pos	305.1861	612	3							HMDB0259093	Tilisolol	C17H24N2O3	0.4
M305T1016_pos	305.2473	1016	3							HMDB0001043	Arachidonic acid	C20H32O2	0.5
M306T156_pos	306.0489	156	3						Carbohydrates	HMDB0250240	Cifostodine	C9H12N3O7P	1.1
M306T542_pos	306.1450	542	3							HMDB0029072	Threonyltryptophan	C15H19N3O4	0.4
M306T459_pos	306.1483	459	3							HMDB0031930	Benzosimuline	C20H19NO2	1.8
M306T388_pos	306.1660	388	3							HMDB0039161	Syndesine	C12H23N3O6	0.0
M306T350_pos	306.1657	350	3							HMDB0039161	Syndesine	C12H23N3O6	0.7
M306T881_pos	306.1844	881	3							HMDB0038173	Halocins	C21H23NO	2.7
M306T556_pos	306.1898	556	3							HMDB0248335	Therafectin	C14H27NO6	4.1
M307T497_pos	307.1025	497	3							HMDB0029891	Starch acetate	C12H18O9	0.4
M307T443_pos	307.1655	443	3							HMDB0253499	Inproquone	C16H22N2O4	0.7
M307T1032_pos	307.2625	1032	3							HMDB0002925	Dihomo-gamma-linolenic acid	C20H34O2	2.3
M307T958_pos	307.2629	958	3						Fatty acids	HMDB0002925	Dihomo-gamma-linolenic acid	C20H34O2	1.0
M308T91_pos	308.0136	91	3							HMDB0250364	Laromustine	C6H14ClN3O5S2	0.1
M308T677_pos	308.1497	677	3							HMDB0038582	oxy-4-methoxy-1-oxobutyl)-2,2-di	C16H21NO5	1.4
M309T91_2_pos	309.1659	91	3							HMDB0034879	no-5-carboxypentyl)amino]-1-deox	C12H24N2O7	0.8
M309T518_pos	309.1811	518	3							HMDB0060990	8-Hydroxycarteolol	C16H24N2O4	0.8
M310T375_pos	310.1391	375	3							HMDB0028809	Glutaminyltyrosine	C14H19N3O5	2.2
M311T410_pos	311.1244	410	3							HMDB0011741	gamma-Glutamyltyrosine	C14H18N2O6	2.2
M311T713_pos	311.1251	713	3							HMDB0011741	gamma-Glutamyltyrosine	C14H18N2O6	4.3
M311T497_pos	311.1965	497	3							HMDB0249829	Cetamolol	C16H26N2O4	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M295T464_pos	295.1655	464	3	9.56E-07	0.73	FALSE	2.27E-01	1.08	FALSE	3.96E-26	1.99	TRUE	2.83E-01	0.93	FALSE
M296T396_pos	296.1214	396	3	3.85E-20	0.21	TRUE	9.64E-01	1.01	FALSE	3.70E-03	1.39	FALSE	4.53E-01	0.82	FALSE
M296T1067_pos	296.2590	1067	3	8.68E-02	1.40	FALSE	3.20E-02	0.62	TRUE	2.84E-02	1.46	FALSE	6.09E-01	1.19	FALSE
M297T487_pos	297.1810	487	3	3.53E-04	0.78	FALSE	2.05E-01	1.09	FALSE	1.46E-21	1.93	TRUE	1.34E-01	0.91	FALSE
M298T915_pos	298.2743	915	3	8.44E-06	2.19	TRUE	6.09E-02	0.75	FALSE	1.28E-01	1.24	FALSE	7.09E-01	0.93	FALSE
M299T436_2_pos	299.1608	436	3	3.50E-03	0.75	FALSE	8.01E-02	1.20	FALSE	8.78E-08	1.61	TRUE	4.12E-01	0.91	FALSE
M299T311_pos	299.1605	311	3	8.03E-01	1.02	FALSE	5.51E-01	0.96	FALSE	3.09E-15	1.75	TRUE	5.11E-02	0.80	FALSE
M299T1038_2_pos	299.2582	1038	3	1.29E-06	1.55	TRUE	2.26E-05	0.69	FALSE	2.11E-03	1.27	FALSE	1.90E-01	1.13	FALSE
M300T367_pos	300.1447	367	3	3.62E-09	0.73	FALSE	3.07E-01	1.06	FALSE	3.93E-27	1.78	TRUE	4.15E-02	0.88	FALSE
M303T473_pos	303.1673	473	3	1.85E-31	0.22	TRUE	5.23E-01	1.06	FALSE	7.20E-04	1.31	FALSE	9.80E-01	1.00	FALSE
M304T803_pos	304.1550	803	3	2.36E-34	1.63	TRUE	6.00E-01	0.98	FALSE	4.08E-02	0.94	FALSE	6.07E-01	1.03	FALSE
M304T688_pos	304.1582	688	3	3.12E-10	0.70	FALSE	1.14E-02	1.15	FALSE	5.89E-34	2.08	TRUE	8.33E-02	0.95	FALSE
M304T564_pos	304.1659	564	3	5.95E-14	0.35	TRUE	3.72E-01	1.13	FALSE	1.07E-02	1.31	FALSE	7.51E-01	1.13	FALSE
M305T746_pos	305.1498	746	3	1.92E-07	0.62	TRUE	6.15E-01	0.95	FALSE	9.15E-02	1.14	FALSE	7.73E-02	1.37	FALSE
M305T612_pos	305.1861	612	3	1.03E-03	0.76	FALSE	2.82E-01	1.10	FALSE	1.17E-08	1.55	TRUE	8.28E-01	0.97	FALSE
M305T1016_pos	305.2473	1016	3	5.62E-11	1.87	TRUE	5.87E-04	0.73	FALSE	8.58E-01	1.01	FALSE	2.18E-02	1.13	FALSE
M306T156_pos	306.0489	156	3	2.34E-20	0.01	TRUE	9.64E-01	1.01	FALSE	6.33E-01	0.92	FALSE	9.62E-01	1.02	FALSE
M306T542_pos	306.1450	542	3	7.40E-27	0.44	TRUE	6.19E-02	1.13	FALSE	2.55E-07	1.34	FALSE	3.35E-01	1.14	FALSE
M306T459_pos	306.1483	459	3	5.02E-26	0.27	TRUE	6.75E-01	1.04	FALSE	1.32E-03	1.31	FALSE	5.70E-01	0.91	FALSE
M306T388_pos	306.1660	388	3	5.12E-50	0.11	TRUE	7.09E-01	1.03	FALSE	3.39E-01	1.07	FALSE	9.86E-01	0.99	FALSE
M306T350_pos	306.1657	350	3	4.71E-73	0.12	TRUE	4.22E-01	1.05	FALSE	2.98E-08	1.31	FALSE	5.39E-01	1.11	FALSE
M306T881_pos	306.1844	881	3	6.16E-01	0.93	FALSE	3.70E-03	1.51	TRUE	3.62E-02	1.29	FALSE	6.17E-01	1.19	FALSE
M306T556_pos	306.1898	556	3	7.69E-05	0.72	FALSE	3.06E-01	1.09	FALSE	1.45E-08	1.51	TRUE	7.99E-01	1.06	FALSE
M307T497_pos	307.1025	497	3	2.24E-02	0.80	FALSE	5.80E-03	1.33	FALSE	1.03E-11	1.88	TRUE	8.29E-01	1.02	FALSE
M307T443_pos	307.1655	443	3	4.81E-06	0.70	FALSE	1.36E-02	1.21	FALSE	1.16E-14	1.75	TRUE	8.07E-02	0.83	FALSE
M307T1032_pos	307.2625	1032	3	1.24E-04	1.69	TRUE	3.73E-02	0.76	FALSE	1.86E-01	0.86	FALSE	1.18E-03	1.39	FALSE
M307T958_pos	307.2629	958	3	5.09E-09	3.14	TRUE	4.30E-02	0.73	FALSE	5.68E-02	0.75	FALSE	5.98E-01	0.93	FALSE
M308T91_pos	308.0136	91	3	5.08E-21	0.56	TRUE	2.53E-01	1.07	FALSE	9.75E-04	1.17	FALSE	3.03E-01	0.84	FALSE
M308T677_pos	308.1497	677	3	8.04E-01	1.04	FALSE	1.51E-01	1.27	FALSE	2.94E-03	1.53	TRUE	2.75E-01	0.87	FALSE
M309T91_2_pos	309.1659	91	3	3.96E-13	0.02	TRUE	9.82E-01	1.01	FALSE	2.18E-01	1.30	FALSE	1.31E-01	1.14	FALSE
M309T518_pos	309.1811	518	3	1.03E-08	0.69	FALSE	1.34E-01	1.10	FALSE	6.31E-25	1.96	TRUE	8.49E-02	0.92	FALSE
M310T375_pos	310.1391	375	3	1.25E-04	0.60	TRUE	1.79E-02	1.37	FALSE	2.10E-02	1.29	FALSE	6.48E-03	1.30	FALSE
M311T410_pos	311.1244	410	3	1.00E-70	0.12	TRUE	9.26E-01	0.99	FALSE	1.24E-03	1.17	FALSE	2.57E-01	0.80	FALSE
M311T713_pos	311.1251	713	3	1.38E-08	0.59	TRUE	8.23E-01	0.98	FALSE	1.39E-01	1.12	FALSE	3.56E-01	0.87	FALSE
M311T497_pos	311.1965	497	3	2.41E-02	0.87	FALSE	2.89E-01	1.07	FALSE	2.21E-19	1.76	TRUE	1.30E-01	0.91	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M312T496_pos	312.1810	496	3							HMDB0255678	Noberastine	C17H21N5O	2.7
M312T491_pos	312.2171	491	3							HMDB0013325	2-trans,4-cis-Decadienoylcarnitine	C17H29NO4	0.7
M313T468_pos	313.1038	468	3							HMDB0256914	Pteroic acid	C14H12N6O3	1.8
M313T758_pos	313.1073	758	3							HMDB0030679	Cabreuvin	C18H16O5	0.9
M313T411_pos	313.1481	411	3							HMDB0005012	Olanzapine	C17H20N4S	0.0
M313T640_pos	313.1551	640	3							HMDB0013302	Phenylalanylphenylalanine	C18H20N2O3	1.2
M313T1015_pos	313.2359	1015	3						Fatty acids	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	4.5
M314T123_pos	314.0751	123	3							HMDB0246946	L-Chlorozotocin	C9H16ClN3O7	0.6
M314T438_pos	314.1063	438	3							HMDB0014683	Amoxapine	C17H16ClN3O	2.6
M314T730_pos	314.1600	730	3							HMDB0241045	1-dimethylidenehexanedioylcarniti	C15H23NO6	0.6
M314T941_pos	314.3056	941	3						Fatty acids				
M315T718_pos	315.1138	718	3							HMDB0252203	Fenleuton	C17H15FN2O3	0.4
M315T479_pos	315.1612	479	3							HMDB0240243	Homochlorcyclizine	C19H23ClN2	3.4
M316T539_pos	316.2232	539	3						Amino acids and Peptides	HMDB0094676	Val-Val-Val	C15H29N3O4	0.3
M316T964_pos	316.2849	964	3							HMDB0038057	Dehydrophytosphingosine	C18H37NO3	0.7
M316T908_pos	316.2848	908	3						Fatty acids	HMDB0038057	Dehydrophytosphingosine	C18H37NO3	0.7
M317T1005_pos	317.2097	1005	3							HMDB0000344	2-Methoxyestradiol-3-methylethe	C20H28O3	4.6
M319T1009_pos	319.2630	1009	3							HMDB0001449	Allopregnanolone	C21H34O2	0.6
M321T484_pos	321.1537	484	3							HMDB0000901	Valproic acid glucuronide	C14H24O8	2.1
M321T944_pos	321.2425	944	3						Fatty acids	HMDB0002190	16-Epoxy-8,11,14-eicosatrienoic ac	C20H32O3	0.3
M322T529_pos	322.0753	529	3							HMDB0251206	Diclofensine	C17H17Cl2NO	2.1
M322T443_pos	322.1402	443	3							HMDB0249646	Carboquone	C15H19N3O5	1.5
M322T398_pos	322.1864	398	3							HMDB0028716	Arginylphenylalanine	C15H23N5O3	2.8
M322T601_pos	322.1765	601	3							HMDB0252569	Gabexate	C16H23N3O4	1.2
M323T622_pos	323.1605	622	3							HMDB0247525	-(Phosphonooxy)decyl methacryla	C14H27O6P	4.0
M323T992_pos	323.2582	992	3							HMDB0005045	15(S)-Hydroxyeicosatrienoic acid	C20H34O3	0.3
M325T368_pos	325.1401	368	3							HMDB0011675	DHAP(10:0)	C13H25O7P	2.8
M325T559_pos	325.1548	559	3							HMDB0014895	Dolasetron	C19H20N2O3	0.5
M325T479_pos	325.1760	479	3							HMDB0255924	p-Hydroxyubenimex	C16H24N2O5	0.6
M325T972_pos	325.2374	972	3							HMDB0031007	etoxy-2-hydroxy-16-heptadecyn-4	C19H32O4	0.3
M325T960_pos	325.2528	960	3						Terpenoids				
M325T1027_pos	325.2736	1027	3						Fatty acids	HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	0.5
M325T957_pos	325.2737	957	3							HMDB0029797	(Z)-15-Oxo-11-eicosenoic acid	C20H36O3	0.2
M326T1072_pos	326.3057	1072	3							HMDB0002088	Oleoylethanolamide	C20H39NO2	1.0
M328T457_pos	328.1394	457	3							HMDB0037846	-(1-Deoxy-1-fructosyl)phenylalanir	C15H21NO7	0.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M312T496_pos	312.1810	496	3	9.76E-01	1.01	FALSE	3.41E-01	1.25	FALSE	4.51E-02	1.51	TRUE	2.31E-01	1.13	FALSE
M312T491_pos	312.2171	491	3	4.97E-11	1.94	TRUE	3.20E-02	1.22	FALSE	4.98E-01	1.06	FALSE	6.06E-01	0.91	FALSE
M313T468_pos	313.1038	468	3	2.37E-03	0.82	FALSE	5.01E-01	1.05	FALSE	1.78E-17	1.72	TRUE	3.88E-01	0.92	FALSE
M313T758_pos	313.1073	758	3	1.22E-08	0.68	FALSE	5.06E-02	1.14	FALSE	1.63E-21	1.84	TRUE	2.08E-02	0.86	FALSE
M313T411_pos	313.1481	411	3	1.97E-03	0.66	TRUE	3.95E-01	0.90	FALSE	7.50E-02	1.22	FALSE	9.90E-02	1.61	FALSE
M313T640_pos	313.1551	640	3	1.27E-01	0.86	FALSE	6.65E-01	1.05	FALSE	5.98E-18	2.39	TRUE	5.30E-02	0.67	FALSE
M313T1015_pos	313.2359	1015	3	7.11E-01	0.99	FALSE	1.51E-01	0.95	FALSE	8.62E-01	1.01	FALSE	1.69E-06	2.83	TRUE
M314T123_pos	314.0751	123	3	3.50E-01	0.88	FALSE	7.13E-01	0.95	FALSE	4.20E-04	1.53	TRUE	7.39E-01	0.85	FALSE
M314T438_pos	314.1063	438	3	9.49E-05	0.83	FALSE	5.17E-03	1.15	FALSE	2.15E-35	1.91	TRUE	1.07E-01	1.07	FALSE
M314T730_pos	314.1600	730	3	5.31E-02	0.80	FALSE	1.27E-08	2.03	TRUE	1.81E-01	0.87	FALSE	4.48E-01	1.11	FALSE
M314T941_pos	314.3056	941	3	1.54E-03	7.63	TRUE	4.34E-01	1.40	FALSE	6.06E-02	2.30	FALSE	8.07E-01	0.90	FALSE
M315T718_pos	315.1138	718	3	2.87E-12	0.70	FALSE	5.19E-02	1.10	FALSE	3.69E-26	1.70	TRUE	5.15E-01	1.06	FALSE
M315T479_pos	315.1612	479	3	5.81E-01	0.96	FALSE	4.83E-01	0.94	FALSE	5.87E-09	1.56	TRUE	3.35E-01	0.93	FALSE
M316T539_pos	316.2232	539	3	2.64E-32	0.30	TRUE	6.75E-01	0.97	FALSE	1.89E-04	1.28	FALSE	2.75E-01	3.03	FALSE
M316T964_pos	316.2849	964	3	1.59E-02	2.90	TRUE	6.80E-01	0.86	FALSE	6.10E-01	0.84	FALSE	9.39E-01	1.05	FALSE
M316T908_pos	316.2848	908	3	3.92E-02	5.31	TRUE	3.03E-01	1.96	FALSE	1.61E-01	0.42	FALSE	5.76E-01	0.86	FALSE
M317T1005_pos	317.2097	1005	3	4.99E-01	0.88	FALSE	1.24E-01	0.72	FALSE	4.33E-04	1.84	TRUE	6.45E-01	1.14	FALSE
M319T1009_pos	319.2630	1009	3	2.19E-03	1.70	TRUE	4.08E-02	0.71	FALSE	1.21E-01	1.26	FALSE	8.41E-01	0.97	FALSE
M321T484_pos	321.1537	484	3	1.67E-01	0.85	FALSE	9.14E-01	0.99	FALSE	9.28E-01	0.99	FALSE	2.53E-02	0.57	TRUE
M321T944_pos	321.2425	944	3	7.31E-11	2.69	TRUE	2.74E-01	0.86	FALSE	2.94E-03	1.42	FALSE	9.19E-01	0.98	FALSE
M322T529_pos	322.0753	529	3	6.58E-14	0.28	TRUE	6.42E-01	1.07	FALSE	9.81E-03	1.38	FALSE	4.27E-02	1.14	FALSE
M322T443_pos	322.1402	443	3	6.59E-03	0.81	FALSE	2.18E-01	1.11	FALSE	5.04E-10	1.58	TRUE	8.21E-01	1.02	FALSE
M322T398_pos	322.1864	398	3	1.26E-12	0.42	TRUE	1.30E-01	1.19	FALSE	2.71E-04	1.43	FALSE	6.27E-01	0.91	FALSE
M322T601_pos	322.1765	601	3	2.30E-26	0.31	TRUE	9.18E-01	0.99	FALSE	5.15E-04	1.30	FALSE	8.38E-01	1.03	FALSE
M323T622_pos	323.1605	622	3	7.06E-08	1.46	FALSE	5.17E-11	0.63	TRUE	6.42E-01	0.97	FALSE	2.09E-03	0.73	FALSE
M323T992_pos	323.2582	992	3	3.18E-05	2.78	TRUE	1.58E-01	0.74	FALSE	1.08E-01	1.37	FALSE	6.71E-01	1.09	FALSE
M325T368_pos	325.1401	368	3	5.61E-05	0.62	TRUE	9.88E-01	1.00	FALSE	6.29E-04	1.41	FALSE	9.90E-01	1.00	FALSE
M325T559_pos	325.1548	559	3	1.22E-03	1.32	FALSE	3.11E-01	1.09	FALSE	1.30E-12	1.77	TRUE	1.03E-01	0.90	FALSE
M325T479_pos	325.1760	479	3	6.35E-06	0.68	FALSE	7.55E-02	1.17	FALSE	1.39E-13	1.80	TRUE	6.52E-02	0.95	FALSE
M325T972_pos	325.2374	972	3	9.24E-23	3.87	TRUE	4.29E-01	0.92	FALSE	5.36E-02	1.20	FALSE	4.81E-02	0.69	FALSE
M325T960_pos	325.2528	960	3	3.40E-13	1.40	FALSE	9.67E-04	1.16	FALSE	1.46E-29	1.66	TRUE	4.00E-02	0.83	FALSE
M325T1027_pos	325.2736	1027	3	7.03E-05	1.83	TRUE	4.75E-01	0.90	FALSE	8.54E-02	1.24	FALSE	8.93E-03	1.31	FALSE
M325T957_pos	325.2737	957	3	4.99E-07	1.55	TRUE	6.64E-01	1.04	FALSE	5.43E-02	1.15	FALSE	1.47E-01	1.37	FALSE
M326T1072_pos	326.3057	1072	3	3.09E-04	1.99	TRUE	4.99E-02	0.70	FALSE	4.54E-01	1.13	FALSE	5.49E-01	0.89	FALSE
M328T457_pos	328.1394	457	3	8.30E-07	0.01	TRUE	9.17E-01	1.04	FALSE	8.83E-01	1.05	FALSE	7.23E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M329T596_pos	329.1860	596	3							HMDB0014736	Labetalol	C19H24N2O3	0.0
M330T972_pos	330.2272	972	3							HMDB0013202	6-Keto-decanoylcarnitine	C17H31NO5	0.8
M330T604_pos	330.2388	604	3							HMDB0304801	Ile-Val-Val	C16H31N3O4	0.1
M331T519_pos	331.0964	519	3							HMDB0245264	Dipropylsulfamoyl)-2-nitrobenzoic	C13H18N2O6S	1.6
M331T778_pos	331.1178	778	3							HMDB0011672	Aflatoxin B1 dialcohol	C18H18O6	0.6
M331T717_pos	331.1181	717	3							HMDB0011672	Aflatoxin B1 dialcohol	C18H18O6	1.6
M332T718_pos	332.1209	718	3							HMDB0014723	Nizatidine	C12H21N5O2S2	0.2
M332T565_pos	332.2182	565	3							HMDB0014924	Marimastat	C15H29N3O5	0.5
M332T621_pos	332.2181	621	3							HMDB0014924	Marimastat	C15H29N3O5	0.2
M332T487_pos	332.2181	487	3							HMDB0014924	Marimastat	C15H29N3O5	0.2
M333T462_pos	333.1088	462	3							HMDB0251046	Desidustat	C16H16N2O6	2.0
M333T460_pos	333.1343	460	3							HMDB0030664	3-Galloylcatechin	C18H20O6	3.2
M334T700_pos	334.1653	700	3							HMDB0256290	Pentopril	C18H23NO5	1.2
M334T461_pos	334.1869	461	3							HMDB0241734	4-Hydroxyoctanedioylcarnitine	C15H27NO7	2.6
M335T763_pos	335.1606	763	3							HMDB0037499	1-Ethenylhexyl butanoate	C17H22N2O5	1.3
M335T1020_pos	335.2801	1020	3						Fatty acids				
M336T700_pos	336.1669	700	3							HMDB0242692	N6-Cyclopentyladenosine	C15H21N5O4	0.8
M336T1062_pos	336.2902	1062	3							HMDB0246264	1-methylethyl)amino)-3-(2,4,6-trip	C21H37NO2	1.3
M337T665_pos	337.1397	665	3							HMDB0033107	Semilepidinoside A	C16H20N2O6	0.7
M339T996_pos	339.2527	996	3							HMDB0002265	14,15-DiHETrE	C20H34O4	0.8
M341T1016_pos	341.1993	1016	3							HMDB0015075	Methantheline	C21H26NO3	2.1
M342T781_pos	342.1817	781	3							HMDB0032382	thylbenzyl)-n2-(2-(5-methylpyridin	C19H23N3O3	1.5
M342T609_pos	342.2388	609	3							HMDB0251473	Diprotin A	C17H31N3O4	0.2
M346T704_pos	346.1803	704	3							HMDB0030224	Murrayacinine	C23H23NO2	0.4
M347T609_pos	347.1241	609	3							HMDB0015247	Nifedipine	C17H18N2O6	0.9
M348T231_pos	348.0707	231	3						Carbohydrates	HMDB0245974	3-Phosphoadenosine	C10H14N5O7P	1.1
M348T384_pos	348.1599	384	3							HMDB0252478	zylbenzoyl)-2,5-dimethyl-1H-pyrro	C22H21NO3	1.5
M348T622_pos	348.1595	622	3							HMDB0252478	zylbenzoyl)-2,5-dimethyl-1H-pyrro	C22H21NO3	0.2
M349T434_pos	349.1509	434	3							HMDB0256703	Porfiromycin	C16H20N4O5	0.6
M349T994_pos	349.2371	994	3							HMDB0000353	3b,15b,17a-Trihydroxy-pregnenon	C21H32O4	0.8
M350T787_pos	350.2073	787	3							HMDB0029225	Coutaric acid	C18H27N3O4	0.5
M351T931_pos	351.2151	931	3							HMDB0002341	8-iso-15-keto-PGE2	C20H30O5	4.4
M352T522_pos	352.1502	522	3							HMDB0248949	benfluorex	C19H20F3NO2	4.7
M353T810_pos	353.1530	810	3							HMDB0250043	henyl)-1H-pyrazol-4-yl)methyl]-4-p	C20H21ClN4	0.7
M355T428_pos	355.1867	428	3							HMDB0251077	-4-yn-2-yl]amino]-4-methyl-1-oxop	C17H26N2O6	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M329T596_pos	329.1860	596	3	5.60E-06	1.82	TRUE	7.58E-01	1.04	FALSE	1.01E-01	1.20	FALSE	3.40E-01	1.13	FALSE
M330T972_pos	330.2272	972	3	4.34E-16	0.58	TRUE	1.63E-01	0.92	FALSE	1.06E-05	1.27	FALSE	7.81E-01	0.94	FALSE
M330T604_pos	330.2388	604	3	1.91E-47	0.17	TRUE	9.03E-01	1.01	FALSE	5.03E-06	1.35	FALSE	1.02E-01	0.48	FALSE
M331T519_pos	331.0964	519	3	5.70E-11	0.63	TRUE	8.76E-01	1.01	FALSE	9.43E-11	1.49	FALSE	5.60E-01	0.92	FALSE
M331T778_pos	331.1178	778	3	4.53E-09	0.72	FALSE	1.44E-01	1.08	FALSE	1.62E-16	1.52	TRUE	8.67E-01	0.99	FALSE
M331T717_pos	331.1181	717	3	3.16E-09	0.72	FALSE	1.89E-01	1.08	FALSE	2.11E-26	1.78	TRUE	8.17E-02	1.11	FALSE
M332T718_pos	332.1209	718	3	1.25E-09	0.73	FALSE	1.65E-01	1.08	FALSE	5.95E-27	1.75	TRUE	4.76E-01	1.06	FALSE
M332T565_pos	332.2182	565	3	5.27E-53	0.12	TRUE	5.07E-01	1.05	FALSE	1.25E-03	1.23	FALSE	3.35E-01	0.76	FALSE
M332T621_pos	332.2181	621	3	3.48E-49	0.15	TRUE	8.20E-01	1.02	FALSE	5.41E-04	1.26	FALSE	3.48E-02	0.67	FALSE
M332T487_pos	332.2181	487	3	6.20E-63	0.13	TRUE	2.99E-01	1.07	FALSE	1.71E-02	1.14	FALSE	8.35E-01	1.05	FALSE
M333T462_pos	333.1088	462	3	3.77E-01	0.91	FALSE	7.50E-01	1.04	FALSE	1.19E-08	1.79	TRUE	8.97E-01	1.02	FALSE
M333T460_pos	333.1343	460	3	1.80E-01	1.25	FALSE	6.09E-01	1.10	FALSE	5.66E-04	1.69	TRUE	1.84E-01	1.89	FALSE
M334T700_pos	334.1653	700	3	1.73E-52	1.68	TRUE	7.48E-02	1.05	FALSE	1.99E-11	0.86	FALSE	4.79E-01	0.97	FALSE
M334T461_pos	334.1869	461	3	5.37E-10	0.46	TRUE	8.43E-01	0.98	FALSE	1.76E-04	1.47	FALSE	1.22E-01	0.75	FALSE
M335T763_pos	335.1606	763	3	2.40E-01	0.91	FALSE	6.79E-01	0.96	FALSE	6.33E-13	1.74	TRUE	9.47E-01	1.01	FALSE
M335T1020_pos	335.2801	1020	3	8.95E-01	1.02	FALSE	1.09E-01	1.22	FALSE	6.05E-01	1.05	FALSE	8.89E-08	10.01	TRUE
M336T700_pos	336.1669	700	3	1.73E-02	1.36	FALSE	1.29E-01	0.83	FALSE	4.26E-13	2.51	TRUE	1.70E-01	1.26	FALSE
M336T1062_pos	336.2902	1062	3	2.80E-04	1.68	TRUE	2.37E-02	0.74	FALSE	2.00E-01	1.17	FALSE	3.53E-01	1.23	FALSE
M337T665_pos	337.1397	665	3	1.20E-03	0.83	FALSE	1.41E-02	1.16	FALSE	2.26E-19	1.67	TRUE	7.47E-01	0.96	FALSE
M339T996_pos	339.2527	996	3	4.01E-13	2.10	TRUE	2.43E-01	0.89	FALSE	7.59E-02	1.15	FALSE	8.90E-01	0.98	FALSE
M341T1016_pos	341.1993	1016	3	2.15E-01	1.18	FALSE	5.27E-05	0.56	TRUE	9.15E-01	1.01	FALSE	1.75E-01	0.73	FALSE
M342T781_pos	342.1817	781	3	7.50E-01	0.98	FALSE	6.16E-02	1.16	FALSE	4.09E-12	1.60	TRUE	6.21E-01	0.95	FALSE
M342T609_pos	342.2388	609	3	5.51E-22	0.33	TRUE	1.99E-02	1.26	FALSE	4.90E-05	1.40	FALSE	2.60E-01	1.24	FALSE
M346T704_pos	346.1803	704	3	6.42E-04	1.30	FALSE	4.14E-01	0.94	FALSE	7.30E-09	1.50	TRUE	4.67E-01	0.90	FALSE
M347T609_pos	347.1241	609	3	5.58E-04	0.82	FALSE	2.14E-01	0.93	FALSE	3.95E-16	1.56	TRUE	1.61E-02	0.68	FALSE
M348T231_pos	348.0707	231	3	4.75E-02	0.77	FALSE	1.03E-01	1.25	FALSE	3.19E-06	1.75	TRUE	6.03E-02	1.69	FALSE
M348T384_pos	348.1599	384	3	6.53E-03	0.76	FALSE	8.94E-01	1.01	FALSE	8.29E-18	2.40	TRUE	1.75E-01	0.82	FALSE
M348T622_pos	348.1595	622	3	1.08E-01	1.15	FALSE	4.60E-03	0.78	FALSE	2.38E-07	1.49	FALSE	4.79E-03	0.51	TRUE
M349T434_pos	349.1509	434	3	4.08E-01	0.95	FALSE	8.92E-02	1.12	FALSE	1.55E-16	1.68	TRUE	7.43E-01	1.02	FALSE
M349T994_pos	349.2371	994	3	5.27E-12	1.61	TRUE	1.30E-04	0.76	FALSE	1.38E-10	1.47	FALSE	4.47E-01	1.05	FALSE
M350T787_pos	350.2073	787	3	1.88E-19	0.56	TRUE	4.93E-10	1.44	FALSE	8.22E-11	1.41	FALSE	7.38E-01	0.97	FALSE
M351T931_pos	351.2151	931	3	1.44E-09	0.61	TRUE	6.05E-02	1.17	FALSE	2.68E-08	1.48	FALSE	9.76E-01	1.00	FALSE
M352T522_pos	352.1502	522	3	8.63E-25	0.40	TRUE	6.78E-02	1.15	FALSE	9.42E-07	1.37	FALSE	8.92E-01	1.06	FALSE
M353T810_pos	353.1530	810	3	1.55E-07	1.52	TRUE	1.05E-04	0.75	FALSE	6.33E-04	1.26	FALSE	1.36E-01	0.85	FALSE
M355T428_pos	355.1867	428	3	1.57E-06	0.73	FALSE	2.99E-01	1.07	FALSE	5.59E-22	1.84	TRUE	9.75E-01	1.00	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M355T1069_pos	355.2835	1069	3							HMDB0011538	MG(0:0/18:2(9Z,12Z)/0:0)	C21H38O4	2.1
M357T686_pos	357.1337	686	3							HMDB0029459	Xanthoxylol	C20H20O6	1.3
M357T1039_pos	357.1936	1039	3							HMDB0033356	Xanthoplanine	C21H26NO4	0.4
M357T1075_pos	357.2790	1075	3							HMDB0002007	Tetracosahexaenoic acid	C24H36O2	0.5
M359T432_pos	359.1458	432	3							HMDB0001069	2-Phenylaminoadenosine	C16H18N6O4	1.2
M361T942_pos	361.2371	942	3							HMDB0003689	Neuroprotectin D1	C22H32O4	0.7
M362T364_pos	362.1457	364	3							HMDB0041208	De-O-methylsimmondsin	C15H23NO9	3.0
M362T705_pos	362.2079	705	3							HMDB0258218	Semagacestat	C19H27N3O4	1.2
M364T968_pos	364.2469	968	3							HMDB0242043	N-Lauroyl Tyrosine	C21H33NO4	3.7
M365T1010_pos	365.2685	1010	3							HMDB0036803	6-O-Acetylaustroinulin	C22H36O4	0.5
M366T846_pos	366.2752	846	3							HMDB0242052	N-Myristoyl Histidine	C20H35N3O3	0.2
M367T505_pos	367.1506	505	3							HMDB0012492	ypent-1-yl)-1,2,3,4-tetrahydro-bet	C17H22N2O7	1.6
M367T508_pos	367.1653	508	3							HMDB0061725	Rilpivirine	C22H18N6	3.5
M367T950_pos	367.3685	950	3						Fatty acids				
M369T515_pos	369.2023	515	3							HMDB0247527	yphenyl)amino]pyrrolo[2,1-f][1,2,4	C19H24N6O2	2.9
M370T552_pos	370.1499	552	3							HMDB0031947	Niazicinin	C17H23NO8	0.8
M371T638_pos	371.1275	638	3							HMDB0245794	trazol-5-YL)-3-pyridinyl]phenyl]-5-	C17H15FN6O3	3.3
M373T602_pos	373.1763	602	3							HMDB0251133	Diamfenetide	C20H24N2O5	1.3
M373T1054_pos	373.3102	1054	3							HMDB0035584	1-Phenyl-1,3-nonadecanedione	C25H40O2	0.2
M375T686_pos	375.1447	686	3							HMDB0030598	(-)-Wikstromol	C20H22O7	2.2
M375T647_pos	375.2060	647	3							HMDB0249686	Carmoxirole	C24H26N2O2	1.9
M377T1008_pos	377.1472	1008	3							HMDB0000244	Riboflavin	C17H20N4O6	4.2
M381T685_pos	381.1909	685	3							HMDB0030760	Pteroside B	C20H28O7	0.4
M381T797_pos	381.2019	797	3							HMDB0062311	Z-tetradecenoyl)-glycero-3-phospl	C17H33O7P	4.7
M382T577_pos	382.1979	577	3							HMDB0248690	holinomethyl)-1H-benzo[d]imidaz	C19H23N7O2	1.8
M382T1055_pos	382.2377	1055	3							HMDB0244414	dryloxy)ethyl]piperidine-4-acetic ac	C24H31NO3	0.0
M383T1032_pos	383.3307	1032	3							HMDB0001093	5a-Cholesta-8,24-dien-3-one	C27H42O	0.3
M384T493_pos	384.1156	493	3							HMDB0000912	Succinyladenosine	C14H17N5O8	1.7
M384T1047_2_pos	384.2532	1047	3							HMDB0030186	(E,E,E)-Sylvatine	C24H33NO3	0.3
M385T840_pos	385.2137	840	3							HMDB0061005	repaglinide aromatic amine	C22H28N2O4	4.0
M386T478_pos	386.1392	478	3							HMDB0244410	kopyrrolidin-1-YL 4-(pyren-1-YL)bu	C24H19NO4	1.4
M387T463_pos	387.2715	463	3						Amino acids and Peptides				
M389T493_pos	389.2030	493	3							HMDB0257936	yl-9-(10-methyl-1H-acridin-9-yl)-1H	C28H24N2	4.6
M390T938_pos	390.3004	938	3							HMDB0062330	N-Arachidonoyl GABA	C24H39NO3	0.4
M393T663_pos	393.2137	663	3							HMDB0252827	Glycylphenylalanylleucylglycine	C19H28N4O5	1.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M355T1069_pos	355.2835	1069	3	1.15E-01	1.40	FALSE	1.49E-01	0.68	FALSE	6.68E-05	2.18	TRUE	6.22E-01	0.83	FALSE
M357T686_pos	357.1337	686	3	6.57E-01	0.97	FALSE	7.63E-01	1.02	FALSE	2.02E-13	1.56	TRUE	7.27E-01	1.07	FALSE
M357T1039_pos	357.1936	1039	3	4.31E-12	1.61	TRUE	8.09E-08	0.70	FALSE	1.02E-01	0.91	FALSE	1.45E-04	1.26	FALSE
M357T1075_pos	357.2790	1075	3	4.49E-01	1.08	FALSE	1.51E-01	1.18	FALSE	1.25E-03	1.36	FALSE	3.13E-02	0.56	TRUE
M359T432_pos	359.1458	432	3	1.08E-17	0.27	TRUE	5.90E-01	1.07	FALSE	8.24E-03	1.33	FALSE	9.61E-01	1.01	FALSE
M361T942_pos	361.2371	942	3	5.05E-07	1.59	TRUE	3.21E-03	0.76	FALSE	5.17E-02	1.16	FALSE	8.13E-01	0.96	FALSE
M362T364_pos	362.1457	364	3	3.86E-01	1.09	FALSE	4.33E-02	1.24	FALSE	1.27E-08	1.72	TRUE	3.30E-01	1.17	FALSE
M362T705_pos	362.2079	705	3	8.40E-08	0.71	FALSE	3.09E-05	1.31	FALSE	1.26E-14	1.58	TRUE	1.95E-01	1.25	FALSE
M364T968_pos	364.2469	968	3	3.71E-06	0.81	FALSE	2.74E-01	1.05	FALSE	8.57E-23	0.64	TRUE	8.03E-02	1.17	FALSE
M365T1010_pos	365.2685	1010	3	1.59E-19	2.00	TRUE	5.85E-05	0.78	FALSE	1.97E-02	1.14	FALSE	5.64E-03	0.70	FALSE
M366T846_pos	366.2752	846	3	4.97E-07	0.66	TRUE	1.10E-05	1.44	FALSE	1.15E-04	1.32	FALSE	1.33E-01	1.15	FALSE
M367T505_pos	367.1506	505	3	1.14E-08	0.10	TRUE	9.41E-01	1.02	FALSE	5.91E-01	1.14	FALSE	5.18E-02	0.81	FALSE
M367T508_pos	367.1653	508	3	5.06E-06	0.12	TRUE	7.71E-01	1.11	FALSE	3.93E-01	0.78	FALSE	7.28E-01	1.02	FALSE
M367T950_pos	367.3685	950	3	1.60E-03	5.10	TRUE	1.79E-01	0.56	FALSE	1.23E-01	1.79	FALSE	7.74E-01	0.93	FALSE
M369T515_pos	369.2023	515	3	2.07E-10	0.65	TRUE	2.33E-01	1.08	FALSE	5.61E-11	1.46	FALSE	3.62E-01	0.94	FALSE
M370T552_pos	370.1499	552	3	1.59E-02	1.18	FALSE	2.50E-02	1.18	FALSE	1.87E-11	1.55	TRUE	7.04E-01	1.04	FALSE
M371T638_pos	371.1275	638	3	9.46E-03	0.79	FALSE	9.93E-01	1.00	FALSE	3.83E-08	1.56	TRUE	2.77E-01	0.80	FALSE
M373T602_pos	373.1763	602	3	5.43E-05	0.64	TRUE	5.86E-01	1.06	FALSE	3.15E-01	1.10	FALSE	2.94E-01	1.09	FALSE
M373T1054_pos	373.3102	1054	3	2.73E-04	1.43	FALSE	2.02E-05	0.65	TRUE	5.97E-01	1.04	FALSE	2.02E-01	1.09	FALSE
M375T686_pos	375.1447	686	3	3.91E-03	0.85	FALSE	2.12E-01	1.07	FALSE	2.17E-16	1.54	TRUE	2.23E-01	1.20	FALSE
M375T647_pos	375.2060	647	3	8.68E-16	0.41	TRUE	6.25E-01	1.05	FALSE	1.96E-01	1.11	FALSE	9.23E-01	1.02	FALSE
M377T1008_pos	377.1472	1008	3	6.05E-02	1.68	FALSE	1.01E-01	0.58	FALSE	3.77E-02	1.65	TRUE	6.45E-01	0.73	FALSE
M381T685_pos	381.1909	685	3	3.93E-05	0.81	FALSE	1.01E-03	1.19	FALSE	1.11E-23	1.67	TRUE	1.72E-01	1.09	FALSE
M381T797_pos	381.2019	797	3	5.16E-19	0.56	TRUE	8.30E-01	1.01	FALSE	2.21E-06	1.27	FALSE	1.73E-01	1.10	FALSE
M382T577_pos	382.1979	577	3	7.62E-28	0.19	TRUE	8.66E-01	0.98	FALSE	1.05E-01	1.16	FALSE	9.61E-01	0.99	FALSE
M382T1055_pos	382.2377	1055	3	1.67E-01	1.43	FALSE	1.06E-02	0.48	TRUE	8.00E-01	0.94	FALSE	5.63E-01	2.09	FALSE
M383T1032_pos	383.3307	1032	3	1.27E-01	1.68	FALSE	3.51E-02	0.55	TRUE	7.60E-01	0.92	FALSE	1.40E-01	0.25	FALSE
M384T493_pos	384.1156	493	3	2.60E-20	0.26	TRUE	9.28E-01	0.99	FALSE	1.81E-03	1.37	FALSE	3.80E-01	1.18	FALSE
M384T1047_2_pos	384.2532	1047	3	6.90E-01	1.16	FALSE	3.45E-02	0.41	TRUE	2.69E-01	0.70	FALSE	6.10E-01	1.98	FALSE
M385T840_pos	385.2137	840	3	3.70E-04	0.76	FALSE	2.34E-09	1.62	TRUE	5.21E-03	1.21	FALSE	1.24E-03	1.35	FALSE
M386T478_pos	386.1392	478	3	1.61E-07	0.77	FALSE	9.74E-02	1.09	FALSE	7.76E-24	1.64	TRUE	8.78E-01	1.01	FALSE
M387T463_pos	387.2715	463	3	2.15E-28	0.19	TRUE	7.55E-02	1.22	FALSE	3.57E-02	1.21	FALSE	4.74E-01	0.78	FALSE
M389T493_pos	389.2030	493	3	2.27E-39	0.18	TRUE	9.25E-01	1.01	FALSE	1.59E-05	1.38	FALSE	2.34E-01	1.24	FALSE
M390T938_pos	390.3004	938	3	8.20E-18	2.23	TRUE	1.22E-05	0.71	FALSE	4.30E-02	1.15	FALSE	5.27E-01	1.05	FALSE
M393T663_pos	393.2137	663	3	5.51E-34	0.20	TRUE	4.36E-01	1.08	FALSE	8.44E-01	1.02	FALSE	8.33E-01	0.92	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M393T999_pos	393.2626	999	3							HMDB0060730	20, 22-Dihydrodigoxigenin	C23H36O5	2.5
M393T1056_1_pos	393.3007	1056	3							HMDB0000348	b,12a-Dihydroxy-5a-cholanoic aci	C24H40O4	2.1
M399T617_pos	399.1702	617	3							HMDB0249303	ohexylamino)-N-(((1,1-dimethylet	C17H26N4O5S	1.2
M399T569_pos	399.1698	569	3							HMDB0249303	ohexylamino)-N-(((1,1-dimethylet	C17H26N4O5S	0.4
M399T1030_2_pos	399.3620	1030	3						Terpenoids	HMDB0001217	4alpha-Methylzymosterol	C28H46O	0.4
M400T951_pos	400.3421	951	3							HMDB0240774	L-Palmitoylcarnitine	C23H45NO4	0.1
M401T1004_pos	401.2690	1004	3							HMDB0012518	10-HETE	C25H36O4	1.0
M401T535_pos	401.2873	535	3						Amino acids and Peptides				
M403T1015_pos	403.2846	1015	3							HMDB0000541	b-Hydroxy-3-oxo-5b-cholanoic aci	C25H38O4	0.7
M406T779_pos	406.2337	779	3							HMDB0001938	Lisinopril	C21H31N3O5	0.1
M407T654_pos	407.2290	654	3							HMDB0038691	Kiwiionoside	C19H34O9	3.7
M407T569_pos	407.2382	569	3							HMDB0258096	nosine, 8-(butylamino)-N-cyclope	C19H30N6O4	4.7
M409T992_pos	409.2958	992	3							HMDB0000312	pha,12beta-Trihydroxy-5beta-cho	C24H40O5	2.3
M410T909_pos	410.2905	909	3							HMDB0241845	ethyl-5-pentylfuran-2-yl)pentano	C23H39NO5	1.0
M411T122_pos	411.0986	122	3							HMDB0248961	BENSULFURON-METHYL	C16H18N4O7S	4.2
M411T1029_pos	411.3610	1029	3							HMDB0001023	,4-Dimethylcholesta-8,14,24-trien	C29H46O	2.7
M413T119_pos	413.0981	119	3							HMDB0037098	Patientoside A	C19H21ClO8	4.1
M415T932_pos	415.2118	932	3							HMDB0014838	Eplerenone	C24H30O6	0.6
M415T951_pos	415.3208	951	3						Terpenoids	HMDB0036941	Smilagenone	C27H42O3	0.3
M416T783_pos	416.1821	783	3							HMDB0257434	Sabeluzole	C22H26FN3O2S	4.5
M417T881_pos	417.2024	881	3							HMDB0254818	Mmp inhibitor V	C22H28N2O6	0.9
M417T411_pos	417.2455	411	3							HMDB0252758	Glutamylleucylarginine	C17H32N6O6	0.2
M418T711_pos	418.2125	711	3							HMDB0246118	3(2H)-Pyridazinone	C25H27N3O3	0.1
M419T518_pos	419.2114	518	3							HMDB0244422	phenyl)pyrrolidin-1-yl)Methyl)phe	C26H27FN2O2	3.6
M421T972_pos	421.3315	972	3							HMDB0247056	6-Ethylchenodeoxycholic acid	C26H44O4	0.6
M422T714_pos	422.1750	714	3							HMDB0249980	(4-fluorophenyl)quinolin-3-yl]-3,5-	C25H24FNO4	2.9
M424T1026_pos	424.3423	1026	3							HMDB0240780	O-Linoleoylcarnitine	C25H45NO4	0.3
M427T601_pos	427.1577	601	3							HMDB0003556	Chitobiose	C15H26N2O12	4.4
M428T787_pos	428.3158	787	3							HMDB0241982	N-Linoleoyl Phenylalanine	C27H41NO3	0.3
M429T956_pos	429.2407	956	3							HMDB0015163	Irbesartan	C25H28N6O	2.1
M429T853_pos	429.2410	853	3							HMDB0015163	Irbesartan	C25H28N6O	2.9
M429T166_pos	429.2460	166	3						Amino acids and Peptides				
M429T1028_pos	429.3728	1028	3						Terpenoids	HMDB0003822	Cholesteryl acetate	C29H48O2	0.3
M431T782_pos	431.2790	782	3							HMDB0040994	thyl-2E-pentenoyl)-2b,9a-dihydrox	C26H38O5	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M393T999_pos	393.2626	999	3	1.59E-01	1.25	FALSE	1.36E-01	0.76	FALSE	8.45E-04	1.59	TRUE	1.96E-01	0.80	FALSE
M393T1056_1_pos	393.3007	1056	3	4.81E-02	1.17	FALSE	3.75E-01	1.08	FALSE	3.05E-09	1.56	TRUE	1.56E-01	1.27	FALSE
M399T617_pos	399.1702	617	3	2.73E-05	0.67	FALSE	7.81E-01	1.03	FALSE	7.26E-08	1.59	TRUE	1.80E-01	0.80	FALSE
M399T569_pos	399.1698	569	3	3.86E-03	0.73	FALSE	8.75E-01	1.02	FALSE	2.96E-06	1.58	TRUE	2.54E-01	0.80	FALSE
M399T1030_2_pos	399.3620	1030	3	7.55E-02	1.27	FALSE	7.78E-01	1.04	FALSE	1.66E-01	1.17	FALSE	2.75E-02	0.62	TRUE
M400T951_pos	400.3421	951	3	6.64E-04	3.46	TRUE	1.07E-01	0.59	FALSE	3.25E-01	1.32	FALSE	5.98E-01	0.95	FALSE
M401T1004_pos	401.2690	1004	3	8.14E-02	1.11	FALSE	3.29E-01	1.06	FALSE	1.37E-22	1.77	TRUE	1.50E-01	0.86	FALSE
M401T535_pos	401.2873	535	3	5.96E-20	0.26	TRUE	5.22E-02	1.27	FALSE	8.71E-03	1.30	FALSE	4.03E-01	0.83	FALSE
M403T1015_pos	403.2846	1015	3	1.00E-08	1.48	FALSE	7.05E-04	1.26	FALSE	3.53E-24	1.99	TRUE	2.29E-01	0.82	FALSE
M406T779_pos	406.2337	779	3	4.88E-07	0.60	TRUE	2.44E-01	1.13	FALSE	2.56E-04	1.38	FALSE	8.91E-01	0.97	FALSE
M407T654_pos	407.2290	654	3	7.32E-27	0.22	TRUE	9.42E-01	1.01	FALSE	4.00E-02	1.20	FALSE	8.58E-01	1.02	FALSE
M407T569_pos	407.2382	569	3	5.94E-12	0.63	TRUE	5.89E-01	1.04	FALSE	1.37E-03	1.19	FALSE	3.19E-02	1.25	FALSE
M409T992_pos	409.2958	992	3	1.33E-02	1.25	FALSE	3.94E-01	1.08	FALSE	1.28E-09	1.64	TRUE	6.43E-01	0.90	FALSE
M410T909_pos	410.2905	909	3	4.37E-02	0.72	FALSE	8.15E-02	1.30	FALSE	1.96E-04	1.73	TRUE	4.79E-01	0.89	FALSE
M411T122_pos	411.0986	122	3	3.34E-22	0.31	TRUE	5.85E-02	1.21	FALSE	1.38E-03	1.31	FALSE	1.34E-01	1.88	FALSE
M411T1029_pos	411.3610	1029	3	4.68E-04	1.77	TRUE	2.50E-01	0.84	FALSE	8.21E-01	1.03	FALSE	3.82E-01	0.81	FALSE
M413T119_pos	413.0981	119	3	2.01E-18	0.35	TRUE	2.83E-02	1.26	FALSE	6.90E-05	1.43	FALSE	9.79E-01	0.99	FALSE
M415T932_pos	415.2118	932	3	1.30E-01	1.16	FALSE	4.86E-01	0.93	FALSE	9.07E-01	1.01	FALSE	3.73E-10	25.94	TRUE
M415T951_pos	415.3208	951	3	8.05E-10	1.77	TRUE	3.40E-02	0.83	FALSE	1.98E-01	1.10	FALSE	9.68E-01	1.01	FALSE
M416T783_pos	416.1821	783	3	4.62E-04	0.58	TRUE	2.66E-01	1.20	FALSE	4.70E-02	1.30	FALSE	8.87E-01	0.99	FALSE
M417T881_pos	417.2024	881	3	1.09E-12	0.32	TRUE	7.49E-01	1.05	FALSE	7.04E-03	1.38	FALSE	6.95E-01	1.03	FALSE
M417T411_pos	417.2455	411	3	1.57E-34	0.15	TRUE	6.84E-01	0.96	FALSE	2.15E-01	1.11	FALSE	6.51E-01	0.81	FALSE
M418T711_pos	418.2125	711	3	2.69E-01	0.93	FALSE	5.24E-01	1.04	FALSE	9.52E-16	1.61	TRUE	8.81E-01	1.02	FALSE
M419T518_pos	419.2114	518	3	5.13E-25	0.30	TRUE	7.15E-01	1.04	FALSE	2.81E-02	1.19	FALSE	7.50E-01	1.02	FALSE
M421T972_pos	421.3315	972	3	1.27E-10	1.69	TRUE	5.88E-05	0.74	FALSE	4.96E-01	1.05	FALSE	8.36E-02	1.16	FALSE
M422T714_pos	422.1750	714	3	1.14E-10	0.72	FALSE	1.71E-02	1.13	FALSE	1.40E-22	1.60	TRUE	5.08E-01	0.97	FALSE
M424T1026_pos	424.3423	1026	3	8.25E-21	1.50	TRUE	1.52E-08	0.79	FALSE	3.12E-01	0.97	FALSE	7.83E-01	0.97	FALSE
M427T601_pos	427.1577	601	3	1.07E-13	0.37	TRUE	2.03E-01	1.17	FALSE	3.55E-03	1.35	FALSE	6.24E-01	0.93	FALSE
M428T787_pos	428.3158	787	3	5.83E-04	1.62	TRUE	4.32E-02	0.75	FALSE	8.84E-03	1.37	FALSE	7.84E-01	1.06	FALSE
M429T956_pos	429.2407	956	3	2.99E-07	0.64	TRUE	9.72E-01	1.00	FALSE	7.08E-02	0.88	FALSE	3.23E-02	0.81	FALSE
M429T853_pos	429.2410	853	3	7.64E-02	1.39	FALSE	8.96E-06	0.42	TRUE	7.33E-01	0.95	FALSE	2.65E-01	1.06	FALSE
M429T166_pos	429.2460	166	3	2.37E-10	0.11	TRUE	9.60E-01	0.99	FALSE	9.82E-01	1.00	FALSE	6.12E-01	0.92	FALSE
M429T1028_pos	429.3728	1028	3	9.07E-01	1.02	FALSE	6.59E-01	1.08	FALSE	2.44E-03	0.67	FALSE	4.28E-02	3.29	TRUE
M431T782_pos	431.2790	782	3	4.31E-06	1.50	TRUE	9.27E-01	0.99	FALSE	1.11E-01	1.13	FALSE	7.28E-01	1.11	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M432T774_pos	432.3471	774	3						Alkaloids	HMDB0038836	Solanocardinol	C27H45NO3	0.2
M433T822_pos	433.1972	822	3							HMDB0259867	Vofopitant	C21H23F3N6O	3.2
M433T748_pos	433.2100	748	3							HMDB0060897	Diphenhydramine N-glucuronide	C23H30NO7	1.2
M435T744_pos	435.2515	744	3							HMDB0007852	LysoPA(0:0/18:2(9Z,12Z))	C21H39O7P	2.0
M441T642_pos	441.2139	642	3							HMDB0249824	Ceranapril	C21H33N2O6P	2.3
M448T747_pos	448.3423	747	3							HMDB0062343	N-Stearoyl tyrosine	C27H45NO4	0.4
M448T817_pos	448.3423	817	3							HMDB0062343	N-Stearoyl tyrosine	C27H45NO4	0.5
M449T781_pos	449.2899	781	3							HMDB0040993	4)-oplopen-3-one 2-(2-methylbut	C26H40O6	0.3
M449T876_pos	449.3262	876	3							HMDB0032783	Porrigenin A	C27H44O5	0.2
M453T827_pos	453.2959	827	3							HMDB0062322	-nonadecanoyl-glycero-3-phospha	C22H45O7P	3.7
M453T805_pos	453.3158	805	3							HMDB0242645	Difluoro-1alpha,25-dihydroxyvitar	C27H42F2O3	3.8
M455T608_pos	455.1933	608	3							HMDB0260290	henylethylamino)-1-[4-(trifluorome	C26H25F3N2O2	1.8
M455T556_pos	455.2138	556	3							HMDB0039214	hydroxybutyrate [arabinosyl-(1->6	C19H34O12	3.3
M457T1059_pos	457.3666	1059	3							HMDB0002364	Oleanolic acid	C30H48O3	2.3
M460T670_pos	460.2555	670	3							HMDB0248539	Apstatin	C23H33N5O5	0.1
M461T684_pos	461.3088	684	3						Amino acids and Peptides				
M461T993_pos	461.3271	993	3							HMDB0032690	pha,22E,24R)-3,5,9,14-Tetrahydro	C28H44O5	2.0
M462T171_pos	462.2199	171	3						Amino acids and Peptides				
M463T738_pos	463.2549	738	3							HMDB0029349	Neryl rhamnosyl-glucoside	C22H38O10	2.4
M463T1037_pos	463.3760	1037	3							HMDB0034430	6-Deoxohomodolichosterone	C29H50O4	4.8
M464T1067_pos	464.3141	1067	3							HMDB0240599	LysoPE(P-18:1(9Z)/0:0)	C23H46NO6P	1.1
M465T843_pos	465.2235	843	3							HMDB0039501	Na-Hexanoyl-Nb-inosityltryptopha	C23H32N2O8	0.7
M468T745_pos	468.3069	745	3							HMDB0010379	LysoPC(14:0/0:0)	C22H46NO7P	3.4
M470T885_pos	470.2651	885	3							HMDB0253814	xaldehyde, 3-(1,3-benzodioxol-5-y	C26H35N3O5	0.4
M471T980_pos	471.3462	980	3						Terpenoids	HMDB0011628	Glycyrrhetinic acid	C30H46O4	1.5
M473T1034_2_pos	473.3250	1034	3							HMDB0035112	23-Epoxy-3,29-dihydroxy-27-norla	C29H44O5	2.5
M475T705_pos	475.2553	705	3							HMDB0254939	mTOR-IN-1	C25H30N8O2	2.5
M477T810_pos	477.2483	810	3							HMDB0003141	Retinoyl b-glucuronide	C26H36O8	0.1
M477T716_pos	477.2488	716	3							HMDB0003141	Retinoyl b-glucuronide	C26H36O8	1.1
M478T899_pos	478.2926	899	3							HMDB0011477	LysoPE(0:0/18:2(9Z,12Z))	C23H44NO7P	0.4
M479T762_pos	479.2506	762	3							HMDB0258351	xy)benzyl]-4-piperidinyl}-4-methyl	C29H32F2N2O2	0.3
M481T1067_pos	481.3137	1067	3							HMDB0030180	Crustecdysone	C27H44O7	4.7
M484T804_pos	484.3059	804	3							HMDB0060547	Hydroxybuprenorphine	C29H41NO5	0.3
M488T1047_2_pos	488.3354	1047	3							HMDB0241616	Z)-17-Hydroxydocosa-4,7,10,13,15	C29H45NO5	3.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M432T774_pos	432.3471	774	3	3.92E-02	3.23	TRUE	5.35E-02	3.08	FALSE	6.29E-01	0.81	FALSE	8.56E-01	1.11	FALSE
M433T822_pos	433.1972	822	3	2.93E-02	0.82	FALSE	1.51E-06	1.59	TRUE	1.44E-03	1.30	FALSE	2.18E-01	1.24	FALSE
M433T748_pos	433.2100	748	3	2.31E-03	0.82	FALSE	5.58E-02	1.13	FALSE	2.11E-22	1.86	TRUE	5.37E-01	0.95	FALSE
M435T744_pos	435.2515	744	3	9.63E-01	1.00	FALSE	3.77E-02	1.16	FALSE	1.15E-11	1.54	TRUE	1.16E-01	1.25	FALSE
M441T642_pos	441.2139	642	3	1.30E-01	0.85	FALSE	5.79E-03	1.36	FALSE	9.94E-06	1.54	TRUE	5.61E-03	1.38	FALSE
M448T747_pos	448.3423	747	3	1.61E-02	4.40	TRUE	2.01E-01	1.78	FALSE	3.71E-01	1.51	FALSE	9.08E-01	0.96	FALSE
M448T817_pos	448.3423	817	3	1.64E-03	2.32	TRUE	1.03E-01	1.51	FALSE	5.25E-01	1.15	FALSE	5.76E-01	0.79	FALSE
M449T781_pos	449.2899	781	3	6.95E-04	1.92	TRUE	2.20E-01	0.81	FALSE	2.09E-01	1.22	FALSE	9.03E-01	1.05	FALSE
M449T876_pos	449.3262	876	3	1.88E-06	1.60	TRUE	6.78E-01	0.96	FALSE	7.82E-02	1.16	FALSE	5.49E-01	1.13	FALSE
M453T827_pos	453.2959	827	3	7.73E-01	0.98	FALSE	8.35E-01	1.02	FALSE	1.76E-12	1.74	TRUE	3.86E-01	0.91	FALSE
M453T805_pos	453.3158	805	3	6.58E-01	1.06	FALSE	6.08E-01	0.93	FALSE	4.20E-07	1.91	TRUE	3.14E-01	0.80	FALSE
M455T608_pos	455.1933	608	3	8.54E-53	0.21	TRUE	1.31E-01	1.10	FALSE	1.15E-04	1.23	FALSE	3.15E-01	0.89	FALSE
M455T556_pos	455.2138	556	3	2.88E-05	0.76	FALSE	7.20E-01	1.02	FALSE	1.00E-23	1.91	TRUE	1.08E-01	0.92	FALSE
M457T1059_pos	457.3666	1059	3	1.46E-04	1.97	TRUE	9.94E-02	0.76	FALSE	3.84E-01	1.14	FALSE	2.91E-01	1.58	FALSE
M460T670_pos	460.2555	670	3	2.55E-08	0.68	FALSE	3.63E-02	1.15	FALSE	1.17E-18	1.76	TRUE	1.13E-01	1.13	FALSE
M461T684_pos	461.3088	684	3	1.45E-09	2.18	TRUE	1.44E-01	0.85	FALSE	3.21E-01	0.90	FALSE	5.24E-01	0.88	FALSE
M461T993_pos	461.3271	993	3	2.55E-07	1.60	TRUE	4.30E-04	0.74	FALSE	9.86E-01	1.00	FALSE	8.56E-01	1.02	FALSE
M462T171_pos	462.2199	171	3	2.53E-60	0.02	TRUE	9.64E-01	1.00	FALSE	3.50E-03	1.23	FALSE	1.10E-02	1.38	FALSE
M463T738_pos	463.2549	738	3	3.61E-01	0.93	FALSE	5.14E-01	0.95	FALSE	5.58E-10	1.55	TRUE	7.85E-01	0.98	FALSE
M463T1037_pos	463.3760	1037	3	8.77E-06	1.73	TRUE	2.23E-02	0.78	FALSE	3.80E-01	0.91	FALSE	6.74E-01	0.94	FALSE
M464T1067_pos	464.3141	1067	3	2.67E-02	1.48	FALSE	3.21E-01	0.81	FALSE	2.28E-04	1.80	TRUE	3.83E-01	1.18	FALSE
M465T843_pos	465.2235	843	3	1.55E-02	0.82	FALSE	7.51E-06	1.47	FALSE	1.67E-05	1.37	FALSE	9.86E-03	1.54	TRUE
M468T745_pos	468.3069	745	3	7.61E-04	0.73	FALSE	5.31E-01	0.94	FALSE	3.56E-09	1.64	TRUE	2.71E-01	0.88	FALSE
M470T885_pos	470.2651	885	3	1.87E-03	1.43	FALSE	4.72E-05	1.63	TRUE	2.50E-01	0.89	FALSE	3.59E-01	1.19	FALSE
M471T980_pos	471.3462	980	3	5.06E-06	1.67	TRUE	6.29E-01	1.06	FALSE	2.95E-01	1.10	FALSE	7.51E-02	1.16	FALSE
M473T1034_2_pos	473.3250	1034	3	1.81E-13	1.62	TRUE	6.18E-07	0.73	FALSE	6.25E-02	0.91	FALSE	3.80E-01	1.08	FALSE
M475T705_pos	475.2553	705	3	1.43E-07	0.61	TRUE	1.63E-01	1.14	FALSE	1.57E-05	1.42	FALSE	5.38E-02	1.22	FALSE
M477T810_pos	477.2483	810	3	1.16E-03	0.82	FALSE	5.67E-03	1.19	FALSE	2.02E-17	1.65	TRUE	8.85E-01	1.02	FALSE
M477T716_pos	477.2488	716	3	5.37E-01	0.96	FALSE	1.86E-01	1.09	FALSE	1.13E-03	1.19	FALSE	3.96E-04	1.78	TRUE
M478T899_pos	478.2926	899	3	2.14E-01	0.93	FALSE	7.93E-01	1.02	FALSE	7.57E-16	1.54	TRUE	8.15E-01	0.99	FALSE
M479T762_pos	479.2506	762	3	1.02E-10	0.27	TRUE	3.88E-01	1.17	FALSE	2.72E-01	1.18	FALSE	8.92E-01	1.02	FALSE
M481T1067_pos	481.3137	1067	3	1.76E-02	1.50	FALSE	6.80E-02	0.71	FALSE	7.85E-05	1.82	TRUE	9.12E-01	1.02	FALSE
M484T804_pos	484.3059	804	3	6.84E-04	0.20	TRUE	3.44E-01	1.48	FALSE	1.72E-01	1.60	FALSE	8.55E-01	0.95	FALSE
M488T1047_2_pos	488.3354	1047	3	1.04E-04	1.27	FALSE	2.82E-01	1.07	FALSE	8.19E-01	0.99	FALSE	4.90E-02	0.66	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M491T744_pos	491.3232	744	3							HMDB0257481	Sapacitabine	C26H42N4O5	0.7
M493T1048_pos	493.3290	1048	3							HMDB0062304	11Z-docosenoyl)-glycero-3-phosph	C25H49O7P	0.3
M494T446_pos	494.1984	446	3						Carbohydrates				
M504T927_pos	504.3333	927	3							HMDB0241613	9Z)-7,17-Dihydroxydocosa-5,8,10,	C29H45NO6	2.7
M506T811_pos	506.3486	811	3							HMDB0241611	9,20-Dihydroxydocosa-4,7,10,13,1	C29H47NO6	1.9
M507T987_pos	507.3682	987	3							HMDB0034519	Theasapogenol A	C30H50O6	0.4
M512T765_pos	512.3039	765	3							HMDB0242372	Cholylcysteine	C27H45NO6S	0.2
M512T816_pos	512.3042	816	3							HMDB0242372	Cholylcysteine	C27H45NO6S	0.3
M522T974_pos	522.3445	974	3							HMDB0242405	Chenodeoxycholylglutamic acid	C29H47NO7	3.8
M528T812_pos	528.2991	812	3							HMDB0251587	Doramapimod	C31H37N5O3	4.2
M542T644_pos	542.3241	644	3							HMDB0010397	ysoPC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0	C28H48NO7P	0.0
M543T623_pos	543.3143	623	3							HMDB0302594	PL	C28H46O10	3.9
M564T879_pos	564.3074	879	3							HMDB0014635	Fosinopril	C30H46NO7P	2.0
M584T912_pos	584.2892	912	3							HMDB0251330	Dihydrostreptomycin	C21H41N7O12	1.0
M593T727_2_pos	593.3334	727	3						Alkaloids	HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.1
M593T760_pos	593.3336	760	3							HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.3
M608T881_pos	608.3163	881	3							HMDB0242696	Chymostatin	C31H41N7O6	4.6
M635T879_pos	635.3417	879	3							HMDB0033573	27-Trihydroxy-1-oxowitha-5,24-die	C34H50O11	1.4
M649T678_pos	649.3447	678	3						Amino acids and Peptides				
M681T868_pos	681.3478	868	3							HMDB0035433	genin 3-[glucosyl-(1->4)-6-deoxy-a	C35H52O13	0.3
M97T604_neg	97.0659	604	3							HMDB0003315	Cyclohexanone	C6H10O	0.0
M101T518_neg	101.0608	518	3							HMDB0000718	Isovaleric acid	C5H10O2	0.3
M115T604_neg	115.0765	604	3							HMDB0000535	Caproic acid	C6H12O2	0.6
M124T553_neg	124.0405	553	3						Alkaloids	HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.6
M125T753_neg	125.0973	753	3						Fatty acids	HMDB0013809	(E)-2-octenal	C8H14O	0.7
M127T518_neg	127.0402	518	3							HMDB0031303	Osmundalactone	C6H8O3	0.8
M141T604_neg	141.0558	604	3							HMDB0033551	hyl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.6
M153T485_neg	153.0195	485	3						Shikimates and Phenylpropanoids	HMDB0000152	Gentisic acid	C7H6O4	0.8
M158T465_neg	158.0824	465	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.7
M159T604_neg	159.0663	604	3						Fatty acids	HMDB0000555	3-Methyladipic acid	C7H12O4	0.3
M165T635_neg	165.0194	635	3						Shikimates and Phenylpropanoids	HMDB0002107	Phthalic acid	C8H6O4	0.6
M169T753_neg	169.0871	753	3						Fatty acids	HMDB0030471	1,4-Ipomeadiol	C9H14O3	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M491T744_pos	491.3232	744	3	4.30E-01	1.07	FALSE	3.42E-02	0.82	FALSE	4.92E-05	1.38	FALSE	9.95E-03	0.59	TRUE
M493T1048_pos	493.3290	1048	3	4.21E-08	1.78	TRUE	2.98E-02	0.80	FALSE	3.22E-01	0.92	FALSE	7.62E-03	1.28	FALSE
M494T446_pos	494.1984	446	3	9.42E-01	1.01	FALSE	3.75E-04	0.67	FALSE	3.30E-09	1.75	TRUE	8.50E-03	1.32	FALSE
M504T927_pos	504.3333	927	3	3.36E-13	1.53	TRUE	1.29E-03	0.84	FALSE	2.01E-08	1.32	FALSE	4.67E-04	1.35	FALSE
M506T811_pos	506.3486	811	3	3.25E-09	1.78	TRUE	6.89E-03	0.79	FALSE	2.48E-02	1.20	FALSE	9.55E-01	1.00	FALSE
M507T987_pos	507.3682	987	3	8.46E-15	1.63	TRUE	4.69E-02	0.89	FALSE	1.10E-07	1.32	FALSE	2.86E-01	0.88	FALSE
M512T765_pos	512.3039	765	3	2.77E-18	1.71	TRUE	2.06E-03	0.84	FALSE	2.61E-12	1.43	FALSE	1.94E-01	0.93	FALSE
M512T816_pos	512.3042	816	3	3.06E-08	1.69	TRUE	1.13E-02	0.79	FALSE	5.50E-03	1.24	FALSE	8.25E-01	0.98	FALSE
M522T974_pos	522.3445	974	3	9.16E-01	1.01	FALSE	4.43E-01	1.04	FALSE	1.35E-22	1.70	TRUE	1.43E-01	0.93	FALSE
M528T812_pos	528.2991	812	3	1.47E-18	2.20	TRUE	5.64E-01	0.95	FALSE	6.15E-07	1.42	FALSE	7.88E-01	0.98	FALSE
M542T644_pos	542.3241	644	3	2.38E-39	0.10	TRUE	2.45E-01	1.13	FALSE	8.29E-01	1.02	FALSE	3.86E-01	1.19	FALSE
M543T623_pos	543.3143	623	3	3.66E-56	0.06	TRUE	4.44E-01	1.06	FALSE	4.08E-02	1.15	FALSE	5.88E-01	1.09	FALSE
M564T879_pos	564.3074	879	3	1.35E-03	1.90	TRUE	2.54E-01	1.24	FALSE	7.21E-02	1.35	FALSE	6.38E-01	0.95	FALSE
M584T912_pos	584.2892	912	3	5.41E-02	1.12	FALSE	8.34E-01	1.01	FALSE	1.16E-15	1.58	TRUE	6.04E-01	1.09	FALSE
M593T727_2_pos	593.3334	727	3	9.70E-01	1.00	FALSE	2.66E-04	1.21	FALSE	5.91E-22	1.62	TRUE	5.19E-02	0.87	FALSE
M593T760_pos	593.3336	760	3	3.70E-04	1.35	FALSE	2.33E-01	1.10	FALSE	1.84E-13	1.80	TRUE	4.57E-01	1.10	FALSE
M608T881_pos	608.3163	881	3	1.13E-01	1.15	FALSE	4.61E-02	1.19	FALSE	5.29E-11	1.71	TRUE	1.33E-01	0.75	FALSE
M635T879_pos	635.3417	879	3	2.31E-13	0.65	TRUE	3.74E-06	1.30	FALSE	1.14E-06	1.26	FALSE	8.63E-01	1.02	FALSE
M649T678_pos	649.3447	678	3	1.98E-08	1.96	TRUE	1.52E-01	0.84	FALSE	8.47E-01	0.98	FALSE	1.04E-01	0.79	FALSE
M681T868_pos	681.3478	868	3	1.60E-22	0.59	TRUE	7.15E-04	1.18	FALSE	3.21E-09	1.29	FALSE	5.57E-01	0.94	FALSE
M97T604_neg	97.0659	604	3	2.91E-06	0.81	FALSE	5.24E-03	1.14	FALSE	2.84E-34	1.82	TRUE	4.40E-01	1.05	FALSE
M101T518_neg	101.0608	518	3	8.58E-11	0.74	FALSE	3.45E-02	1.10	FALSE	1.19E-38	1.90	TRUE	2.41E-01	0.94	FALSE
M115T604_neg	115.0765	604	3	1.85E-06	0.80	FALSE	6.75E-03	1.14	FALSE	1.55E-35	1.87	TRUE	9.20E-01	1.01	FALSE
M124T553_neg	124.0405	553	3	8.59E-01	0.98	FALSE	6.39E-01	0.96	FALSE	2.69E-08	1.58	TRUE	2.62E-01	0.79	FALSE
M125T753_neg	125.0973	753	3	2.28E-04	0.87	FALSE	3.53E-02	1.09	FALSE	1.10E-31	1.60	TRUE	8.78E-01	0.99	FALSE
M127T518_neg	127.0402	518	3	1.35E-10	0.74	FALSE	7.42E-02	1.09	FALSE	6.59E-36	1.87	TRUE	2.39E-01	0.94	FALSE
M141T604_neg	141.0558	604	3	4.88E-06	0.81	FALSE	1.64E-02	1.12	FALSE	1.50E-33	1.82	TRUE	9.87E-01	1.00	FALSE
M153T485_neg	153.0195	485	3	1.74E-06	0.76	FALSE	4.25E-01	1.05	FALSE	4.23E-25	1.82	TRUE	5.69E-01	1.04	FALSE
M158T465_neg	158.0824	465	3	2.58E-22	1.50	TRUE	9.69E-01	1.00	FALSE	5.98E-03	1.09	FALSE	3.19E-03	0.83	FALSE
M159T604_neg	159.0663	604	3	3.81E-06	0.80	FALSE	6.88E-03	1.14	FALSE	4.85E-35	1.87	TRUE	9.18E-01	1.01	FALSE
M165T635_neg	165.0194	635	3	2.89E-04	0.79	FALSE	4.45E-02	1.14	FALSE	1.38E-21	1.85	TRUE	1.23E-01	1.11	FALSE
M169T753_neg	169.0871	753	3	1.21E-04	0.86	FALSE	1.72E-02	1.10	FALSE	3.89E-30	1.57	TRUE	2.74E-01	1.09	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M171T707_neg	171.0664	707	3						Fatty acids	HMDB0000341	2-Octenedioic acid	C8H12O4	0.5
M171T987_neg	171.1391	987	3						Fatty acids	HMDB0000511	Capric acid	C10H20O2	0.3
M172T526_neg	172.0980	526	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.6
M173T686_neg	173.0820	686	3						Fatty acids	HMDB0000893	Suberic acid	C8H14O4	0.2
M174T200_neg	174.0408	200	3						Amino acids and Peptides	HMDB0000812	N-Acetyl-L-aspartic acid	C6H9NO5	0.2
M175T332_neg	175.0249	332	3						Fatty acids	HMDB0000044	Ascorbic acid	C6H8O6	0.3
M179T657_neg	179.0351	657	3							HMDB0000707	4-Hydroxyphenylpyruvic acid	C9H8O4	0.8
M182T508_neg	181.9918	508	3							HMDB0029723	Saccharin	C7H5NO3S	0.3
M184T675_neg	184.0980	675	3							HMDB0006348	Pseudoecgonine	C9H15NO3	0.3
M186T397_neg	186.0773	397	3							HMDB0012150	2-Keto-6-acetamidocaproate	C8H13NO4	0.4
M187T753_neg	187.0976	753	3						Fatty acids	HMDB0000784	Azelaic acid	C9H16O4	0.0
M189T422_neg	189.0405	422	3						Fatty acids	HMDB0012710	3-Dehydroquinic acid	C7H10O6	0.2
M189T501_neg	189.0769	501	3							HMDB0000325	3-Hydroxysuberic acid	C8H14O5	0.5
M193T495_neg	193.0983	495	3							HMDB0041440	Laccarin	C10H14N2O2	0.5
M195T664_neg	195.0300	664	3						Shikimates and Phenylpropanoids	HMDB0030800	ethoxy-4,5-methylenedioxybenzoic	C9H8O5	0.4
M197T651_neg	197.0819	651	3							HMDB0004998	Guaifenesin	C10H14O4	0.0
M201T499_neg	201.0769	499	3						Fatty acids	HMDB0032306	Diethyl oxalpropionate	C9H14O5	0.4
M202T411_neg	202.0722	411	3						Amino acids and Peptides	HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	0.3
M204T808_neg	204.0666	808	3							HMDB0000671	Indolelactic acid	C11H11NO3	0.1
M205T545_neg	205.0619	545	3							HMDB0248299	Amidinophenylpyruvic acid	C10H10N2O3	0.1
M209T553_neg	209.0680	553	3						Alkaloids	HMDB0002123	1,3,7-Trimethyluric acid	C8H10N4O3	0.1
M210T720_neg	210.0772	720	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	0.3
M215T565_neg	215.0925	565	3							HMDB0301824	Isoketocamphoric acid	C10H16O5	0.1
M215T946_neg	215.1653	946	3						Fatty acids	HMDB0000387	3-Hydroxydodecanoic acid	C12H24O3	0.1
M216T383_neg	216.1242	383	3							HMDB0240784	O-Propanoyl-D-carnitine	C10H19NO4	0.4
M217T644_neg	217.1082	644	3							HMDB0000350	3-Hydroxysebacic acid	C10H18O5	0.2
M218T354_neg	218.1047	354	3							HMDB0012204	Zeatin	C10H13N5O	0.1
M221T609_neg	221.0456	609	3						Shikimates and Phenylpropanoids	HMDB0253642	Isofraxidin	C11H10O5	0.1
M222T422_neg	222.0408	422	3							HMDB0004083	no-3-hydroxyphenyl)-2,4-dioxobuta	C10H9NO5	0.1
M224T477_neg	224.0565	477	3							HMDB0037264	-4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	0.2
M224T369_neg	224.0929	369	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.3
M225T640_neg	225.1132	640	3							HMDB0040705	Allixin	C12H18O4	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M171T707_neg	171.0664	707	3	3.36E-28	1.38	FALSE	2.92E-01	0.97	FALSE	1.18E-12	0.85	FALSE	9.20E-06	1.62	TRUE
M171T987_neg	171.1391	987	3	8.44E-03	2.60	TRUE	4.22E-01	0.76	FALSE	1.01E-01	1.63	FALSE	7.92E-02	0.40	FALSE
M172T526_neg	172.0980	526	3	2.56E-23	1.61	TRUE	8.11E-01	1.01	FALSE	5.08E-01	1.02	FALSE	9.95E-02	0.92	FALSE
M173T686_neg	173.0820	686	3	5.02E-04	0.88	FALSE	3.69E-02	1.08	FALSE	3.55E-35	1.65	TRUE	6.91E-01	0.97	FALSE
M174T200_neg	174.0408	200	3	1.87E-04	0.68	FALSE	5.56E-03	0.74	FALSE	7.41E-11	1.88	TRUE	2.71E-01	0.88	FALSE
M175T332_neg	175.0249	332	3	4.21E-56	0.09	TRUE	8.14E-01	1.02	FALSE	2.76E-02	1.16	FALSE	1.08E-02	0.71	FALSE
M179T657_neg	179.0351	657	3	3.52E-12	0.69	FALSE	3.25E-01	1.05	FALSE	1.90E-25	1.71	TRUE	3.91E-01	1.10	FALSE
M182T508_neg	181.9918	508	3	2.96E-10	1.66	TRUE	1.90E-01	1.11	FALSE	1.34E-03	1.24	FALSE	9.51E-01	0.99	FALSE
M184T675_neg	184.0980	675	3	1.39E-02	0.87	FALSE	1.34E-04	1.26	FALSE	9.83E-15	1.50	TRUE	6.03E-02	1.18	FALSE
M186T397_neg	186.0773	397	3	2.13E-20	1.59	TRUE	6.79E-02	1.09	FALSE	9.08E-04	1.14	FALSE	1.05E-01	1.13	FALSE
M187T753_neg	187.0976	753	3	8.68E-05	0.86	FALSE	1.67E-02	1.10	FALSE	2.86E-31	1.60	TRUE	9.45E-01	1.00	FALSE
M189T422_neg	189.0405	422	3	6.19E-60	0.17	TRUE	6.50E-01	1.03	FALSE	2.75E-06	1.28	FALSE	7.47E-02	0.85	FALSE
M189T501_neg	189.0769	501	3	4.52E-06	0.82	FALSE	3.23E-02	1.10	FALSE	4.32E-36	1.83	TRUE	9.21E-01	0.99	FALSE
M193T495_neg	193.0983	495	3	6.98E-08	0.77	FALSE	8.58E-02	1.09	FALSE	2.87E-33	1.87	TRUE	7.44E-01	0.98	FALSE
M195T664_neg	195.0300	664	3	8.89E-03	0.70	FALSE	5.15E-01	1.09	FALSE	9.22E-10	2.18	TRUE	2.32E-01	1.35	FALSE
M197T651_neg	197.0819	651	3	9.45E-13	1.73	TRUE	8.90E-01	1.01	FALSE	6.81E-01	1.03	FALSE	7.77E-01	0.96	FALSE
M201T499_neg	201.0769	499	3	1.72E-01	0.90	FALSE	3.12E-01	1.08	FALSE	4.09E-16	1.83	TRUE	4.76E-01	0.92	FALSE
M202T411_neg	202.0722	411	3	4.96E-05	0.79	FALSE	6.58E-05	1.27	FALSE	2.73E-32	2.13	TRUE	5.12E-01	1.05	FALSE
M204T808_neg	204.0666	808	3	8.57E-01	0.99	FALSE	5.18E-01	0.95	FALSE	6.77E-13	1.63	TRUE	6.49E-01	1.09	FALSE
M205T545_neg	205.0619	545	3	3.69E-02	1.09	FALSE	8.93E-02	1.08	FALSE	3.60E-39	1.85	TRUE	6.02E-01	1.03	FALSE
M209T553_neg	209.0680	553	3	1.00E-20	1.67	TRUE	1.09E-03	1.18	FALSE	2.66E-01	1.05	FALSE	7.21E-01	1.03	FALSE
M210T720_neg	210.0772	720	3	3.82E-07	0.77	FALSE	3.06E-02	1.12	FALSE	5.91E-22	1.61	TRUE	3.04E-01	0.93	FALSE
M215T565_neg	215.0925	565	3	6.17E-01	1.05	FALSE	4.88E-01	1.07	FALSE	6.63E-10	1.68	TRUE	1.72E-01	0.82	FALSE
M215T946_neg	215.1653	946	3	2.42E-14	1.62	TRUE	1.09E-04	0.80	FALSE	3.94E-07	1.30	FALSE	4.57E-01	0.92	FALSE
M216T383_neg	216.1242	383	3	5.11E-03	0.83	FALSE	4.75E-01	1.05	FALSE	4.00E-22	1.91	TRUE	2.99E-01	0.96	FALSE
M217T644_neg	217.1082	644	3	4.83E-01	0.96	FALSE	7.87E-03	1.19	FALSE	2.58E-20	1.78	TRUE	3.97E-01	1.08	FALSE
M218T354_neg	218.1047	354	3	1.10E-09	1.86	TRUE	2.71E-01	1.11	FALSE	2.13E-01	1.11	FALSE	4.05E-01	1.18	FALSE
M221T609_neg	221.0456	609	3	2.19E-13	0.72	FALSE	1.65E-02	1.11	FALSE	1.24E-35	1.77	TRUE	7.42E-01	1.02	FALSE
M222T422_neg	222.0408	422	3	1.70E-03	0.73	FALSE	3.06E-01	1.11	FALSE	4.09E-19	2.53	TRUE	5.99E-02	0.62	FALSE
M224T477_neg	224.0565	477	3	4.27E-05	0.82	FALSE	3.26E-01	1.05	FALSE	5.92E-26	1.67	TRUE	8.16E-01	0.98	FALSE
M224T369_neg	224.0929	369	3	1.64E-04	0.82	FALSE	1.68E-01	1.08	FALSE	2.47E-27	1.83	TRUE	5.57E-01	0.96	FALSE
M225T640_neg	225.1132	640	3	2.25E-16	1.76	TRUE	2.19E-01	1.08	FALSE	3.76E-03	1.17	FALSE	9.42E-01	0.99	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M227T668_neg	227.1289	668	3							HMDB0000933	Traumatic acid	C12H20O4	0.1
M229T545_1_neg	229.0718	545	3							HMDB0246021	lactitol, 1,2:5,6-dianhydro-, diacet	C10H14O6	0.2
M229T492_neg	229.1558	492	3						Amino acids and Peptides	HMDB0028920	Isoleucyl-Valine	C11H22N2O3	0.3
M232T474_neg	232.0285	474	3							HMDB0258566	Sulbactam	C8H11NO5S	0.0
M237T575_neg	237.0880	575	3							HMDB0015084	Felbamate	C11H14N2O4	0.1
M238T374_neg	238.0722	374	3							HMDB0250058	(3s)-3-(Benzyloxy)-L-Aspartic Acid	C11H13NO5	0.3
M239T411_neg	239.0674	411	3						Carbohydrates	HMDB0032559	b1)-2-(1-Methylpropyl)-4,6-dinitro	C10H12N2O5	0.2
M240T623_neg	240.0878	623	3						Alkaloids	HMDB0014567	Methocarbamol	C11H15NO5	0.2
M241T658_neg	241.1081	658	3							HMDB0251246	Diethylene glycol dimethacrylate	C12H18O5	0.1
M242T868_neg	242.1762	868	3						Amino acids and Peptides	HMDB0013286	N-Undecanoylglycine	C13H25NO3	0.1
M243T510_neg	243.1351	510	3							HMDB0028866	Hydroxyprolyl-Isoleucine	C11H20N2O4	0.2
M243T419_neg	243.1351	419	3							HMDB0028866	Hydroxyprolyl-Isoleucine	C11H20N2O4	0.1
M243T565_neg	243.1715	565	3						Amino acids and Peptides	HMDB0028910	Isoleucyl-Isoleucine	C12H24N2O3	0.3
M245T764_neg	245.1394	764	3						Fatty acids	HMDB0000413	3-Hydroxydodecanedioic acid	C12H22O5	0.0
M253T649_neg	253.0718	649	3							HMDB0249245	Bis(2-hydroxyethyl) terephthalate	C12H14O6	0.1
M253T427_neg	253.0831	427	3						Carbohydrates	HMDB0029445	L-Agaridoxin	C11H14N2O5	0.3
M254T451_neg	254.0671	451	3							HMDB0304540	beta-D-ribosylnicotinate	C11H13NO6	0.3
M255T508_neg	255.0455	508	3						Amino acids and Peptides	HMDB0256765	Preparation 11	C8H17O5PS	2.5
M255T620_neg	255.0885	620	3						Alkaloids	HMDB0247463	8-Phenyltheophylline	C13H12N4O2	1.0
M257T686_neg	257.1396	686	3						Fatty acids				
M267T399_neg	267.0734	399	3						Carbohydrates	HMDB0000195	Inosine	C10H12N4O5	0.2
M271T480_neg	271.0935	480	3						Amino acids and Peptides				
M271T1015_neg	271.2278	1015	3						Fatty acids	HMDB0006294	16-Hydroxyhexadecanoic acid	C16H32O3	0.1
M271T1062_neg	271.2279	1062	3						Fatty acids	HMDB0006294	16-Hydroxyhexadecanoic acid	C16H32O3	0.0
M272T770_neg	272.0928	770	3							HMDB0000667	L-Thyronine	C15H15NO4	0.0
M273T648_neg	273.1133	648	3							HMDB0033921	2-propenyl)-7,8-dimethoxy-2H-1-b	C16H18O4	0.3
M279T978_neg	279.2330	978	3							HMDB0000673	Linoleic acid	C18H32O2	0.0
M281T770_neg	281.1030	770	3						Terpenoids	HMDB0249246	Bis(2-methoxyethyl) phthalate	C14H18O6	0.2
M282T398_neg	282.0844	398	3						Carbohydrates	HMDB0000133	Guanosine	C10H13N5O5	0.1
M283T793_neg	283.1187	793	3							HMDB0029819	Phenylethyl beta-D-glucopyranosi	C14H20O6	0.1
M285T803_neg	285.1132	803	3						Shikimates and Phenylpropanoids	HMDB0030152	beta-Sitosterol acetate	C17H18O4	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M227T668_neg	227.1289	668	3	1.12E-24	1.54	TRUE	9.20E-01	1.00	FALSE	5.87E-01	1.02	FALSE	4.52E-01	0.95	FALSE
M229T545_1_neg	229.0718	545	3	1.53E-01	0.90	FALSE	7.11E-02	1.15	FALSE	2.15E-16	1.84	TRUE	1.69E-01	0.89	FALSE
M229T492_neg	229.1558	492	3	6.20E-29	0.17	TRUE	2.29E-01	1.15	FALSE	2.15E-02	1.24	FALSE	1.91E-01	0.68	FALSE
M232T474_neg	232.0285	474	3	1.19E-01	0.87	FALSE	4.27E-01	1.07	FALSE	7.54E-11	1.69	TRUE	6.68E-01	0.94	FALSE
M237T575_neg	237.0880	575	3	1.79E-04	0.71	FALSE	5.31E-01	0.94	FALSE	5.23E-15	2.00	TRUE	4.62E-01	0.92	FALSE
M238T374_neg	238.0722	374	3	2.59E-13	0.77	FALSE	7.19E-03	1.10	FALSE	3.55E-37	1.60	TRUE	4.02E-01	1.04	FALSE
M239T411_neg	239.0674	411	3	7.41E-03	0.86	FALSE	1.75E-01	1.08	FALSE	2.32E-26	1.90	TRUE	6.97E-01	1.02	FALSE
M240T623_neg	240.0878	623	3	2.67E-03	0.85	FALSE	1.19E-02	1.15	FALSE	7.83E-18	1.56	TRUE	2.00E-02	1.12	FALSE
M241T658_neg	241.1081	658	3	6.27E-01	0.98	FALSE	5.15E-02	1.09	FALSE	4.64E-28	1.61	TRUE	3.36E-01	0.94	FALSE
M242T868_neg	242.1762	868	3	3.82E-01	1.09	FALSE	8.75E-01	0.98	FALSE	7.69E-02	1.17	FALSE	8.47E-03	1.67	TRUE
M243T510_neg	243.1351	510	3	9.91E-22	1.72	TRUE	9.83E-01	1.00	FALSE	8.73E-01	0.99	FALSE	1.69E-02	0.88	FALSE
M243T419_neg	243.1351	419	3	5.51E-02	0.91	FALSE	3.58E-01	1.05	FALSE	1.10E-24	1.67	TRUE	5.83E-01	0.98	FALSE
M243T565_neg	243.1715	565	3	1.49E-17	0.25	TRUE	5.27E-01	1.09	FALSE	2.49E-02	1.29	FALSE	1.37E-01	0.71	FALSE
M245T764_neg	245.1394	764	3	8.11E-04	0.87	FALSE	3.11E-02	1.09	FALSE	3.55E-32	1.66	TRUE	8.97E-01	0.99	FALSE
M253T649_neg	253.0718	649	3	2.97E-05	0.72	FALSE	3.66E-01	1.08	FALSE	1.94E-19	2.01	TRUE	7.55E-01	1.02	FALSE
M253T427_neg	253.0831	427	3	6.57E-02	0.83	FALSE	8.07E-01	1.03	FALSE	2.44E-11	1.88	TRUE	3.15E-01	0.85	FALSE
M254T451_neg	254.0671	451	3	2.83E-01	0.93	FALSE	5.95E-01	0.96	FALSE	1.63E-11	1.54	TRUE	8.62E-01	0.98	FALSE
M255T508_neg	255.0455	508	3	9.64E-01	1.00	FALSE	3.51E-01	0.91	FALSE	6.53E-08	1.61	TRUE	2.72E-01	0.80	FALSE
M255T620_neg	255.0885	620	3	3.45E-03	0.82	FALSE	1.09E-02	1.20	FALSE	8.73E-19	1.80	TRUE	4.91E-01	0.91	FALSE
M257T686_neg	257.1396	686	3	1.24E-24	1.80	TRUE	5.56E-02	1.10	FALSE	9.08E-01	1.00	FALSE	7.27E-01	1.04	FALSE
M267T399_neg	267.0734	399	3	8.00E-62	0.14	TRUE	1.63E-01	1.09	FALSE	1.30E-02	1.14	FALSE	3.37E-01	1.38	FALSE
M271T480_neg	271.0935	480	3	3.04E-07	0.77	FALSE	2.36E-01	1.06	FALSE	2.09E-25	1.69	TRUE	7.33E-02	1.09	FALSE
M271T1015_neg	271.2278	1015	3	1.46E-07	1.56	TRUE	1.03E-04	0.72	FALSE	1.99E-01	0.91	FALSE	1.34E-01	1.26	FALSE
M271T1062_neg	271.2279	1062	3	1.49E-01	1.35	FALSE	1.31E-02	0.60	TRUE	3.96E-01	0.86	FALSE	9.18E-01	0.97	FALSE
M272T770_neg	272.0928	770	3	1.85E-01	1.08	FALSE	4.09E-01	1.05	FALSE	1.01E-14	1.51	TRUE	6.37E-01	0.95	FALSE
M273T648_neg	273.1133	648	3	7.21E-10	1.64	TRUE	5.85E-01	1.04	FALSE	8.37E-01	0.99	FALSE	2.70E-02	1.34	FALSE
M279T978_neg	279.2330	978	3	1.31E-04	1.26	FALSE	4.91E-01	0.96	FALSE	4.42E-12	1.48	FALSE	1.15E-05	1.60	TRUE
M281T770_neg	281.1030	770	3	8.41E-07	0.79	FALSE	3.46E-06	1.26	FALSE	3.23E-23	1.60	TRUE	2.01E-01	1.07	FALSE
M282T398_neg	282.0844	398	3	2.64E-30	0.24	TRUE	5.49E-01	1.06	FALSE	8.88E-05	1.37	FALSE	3.12E-01	1.27	FALSE
M283T793_neg	283.1187	793	3	3.77E-07	0.77	FALSE	2.24E-08	1.33	FALSE	1.07E-22	1.62	TRUE	6.94E-01	0.98	FALSE
M285T803_neg	285.1132	803	3	5.95E-22	1.65	TRUE	7.79E-01	1.01	FALSE	8.04E-07	1.22	FALSE	2.21E-02	1.20	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M285T718_neg	285.1132	718	3						Shikimates and Phenylpropanoids	HMDB0030152	beta-Sitosterol acetate	C17H18O4	0.1
M285T633_neg	285.1708	633	3						Fatty acids	HMDB0240222	Thonzylamine	C16H22N4O	4.6
M291T889_neg	291.1603	889	3							HMDB0034658	9-Acetoxyfukinanolide	C17H24O4	0.4
M295T544_neg	295.1663	544	3							HMDB0248879	Batelapine	C16H20N6	4.5
M297T787_neg	297.0983	787	3							HMDB0010350	2-Phenylethanol glucuronide	C14H18O7	1.0
M297T491_neg	297.1093	491	3							HMDB0001107	7-Methylguanosine	C11H16N5O5	4.8
M301T761_neg	301.1447	761	3							HMDB0000530	6-Ketoestriol	C18H22O4	0.4
M305T846_neg	305.1871	846	3						Alkaloids	HMDB0255251	N,N-Diallylpentobarbital	C17H26N2O3	0.1
M309T913_neg	309.1709	913	3							HMDB0040756	6,8-dimethoxy-7(11)-eremophilen	C17H26O5	0.4
M310T808_neg	310.1085	808	3							HMDB0030217	Launobine	C18H17NO4	0.0
M311T432_neg	311.1348	432	3							HMDB0005012	Olanzapine	C17H20N4S	3.9
M311T911_neg	311.1863	911	3							HMDB0242731	Arteether	C17H28O5	0.3
M313T700_neg	313.1082	700	3							HMDB0030567	(-)-3,4,9-Trimethoxypterocarpan	C18H18O5	0.0
M317T389_neg	317.0990	389	3						Amino acids and Peptides				
M317T926_neg	317.1759	926	3							HMDB0006709	Ubiquinone-2	C19H26O4	0.1
M317T1014_neg	317.2122	1014	3							HMDB0001337	Leukotriene A4	C20H30O3	0.0
M319T737_neg	319.1299	737	3							HMDB0038970	Formylfusarochromanone	C16H20N2O5	0.0
M323T491_neg	323.1615	491	3							HMDB0255924	p-Hydroxyubenimex	C16H24N2O5	0.8
M323T680_neg	323.1612	680	3							HMDB0255924	p-Hydroxyubenimex	C16H24N2O5	0.0
M324T542_neg	324.0231	542	3							HMDB0002377	Urothion	C11H11N5O3S2	0.1
M325T435_neg	325.1074	435	3							HMDB0030605	ihydroxy-3-methoxy-2-prenylxant	C19H18O5	2.3
M325T954_neg	325.2020	954	3						Fatty acids	HMDB0031963	2-Epoxy-7(11)-eremophilene-6,8,	C18H30O5	0.1
M329T717_neg	329.1031	717	3							HMDB0011672	Aflatoxin B1 dialcohol	C18H18O6	0.1
M329T756_neg	329.1031	756	3							HMDB0011672	Aflatoxin B1 dialcohol	C18H18O6	0.1
M333T784_neg	333.0901	784	3							HMDB0015186	Penicillin G	C16H18N2O4S	3.9
M335T665_neg	335.1248	665	3							HMDB0033107	Semilepidinoside A	C16H20N2O6	0.0
M337T945_neg	337.2384	945	3						Terpenoids	HMDB0002265	14,15-DiHETrE	C20H34O4	0.0
M347T994_neg	347.2228	994	3							HMDB0000353	3b,15b,17a-Trihydroxy-pregnenon	C21H32O4	0.1
M352T595_2_neg	352.1767	595	3							HMDB0241202	7E)-Undeca-2,5,7-trienedioylcarni	C18H27NO6	0.3
M361T664_neg	361.1407	664	3						Alkaloids				
M361T994_neg	361.2021	994	3						Terpenoids	HMDB0000063	Cortisol	C21H30O5	0.1
M363T1014_neg	363.2176	1014	3							HMDB0000903	Tetrahydrocortisone	C21H32O5	0.1
M365T586_neg	365.1354	586	3							HMDB0012492	ypent-1-yl)-1,2,3,4-tetrahydro-bet	C17H22N2O7	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M285T718_neg	285.1132	718	3	4.12E-12	0.69	FALSE	7.33E-02	1.10	FALSE	1.78E-24	1.67	TRUE	1.68E-01	1.11	FALSE
M285T633_neg	285.1708	633	3	5.46E-01	1.15	FALSE	3.77E-03	0.43	TRUE	8.27E-01	1.04	FALSE	7.34E-01	0.92	FALSE
M291T889_neg	291.1603	889	3	1.14E-20	1.68	TRUE	2.76E-01	0.95	FALSE	2.80E-01	0.96	FALSE	6.45E-01	0.95	FALSE
M295T544_neg	295.1663	544	3	6.20E-02	0.90	FALSE	6.76E-03	1.17	FALSE	1.06E-25	1.84	TRUE	1.94E-01	0.96	FALSE
M297T787_neg	297.0983	787	3	2.61E-01	0.91	FALSE	9.45E-03	0.80	FALSE	6.43E-21	0.46	TRUE	9.99E-02	0.75	FALSE
M297T491_neg	297.1093	491	3	1.11E-02	0.85	FALSE	2.31E-02	1.16	FALSE	7.65E-22	1.82	TRUE	3.40E-01	1.08	FALSE
M301T761_neg	301.1447	761	3	5.92E-44	2.18	TRUE	9.98E-05	0.85	FALSE	2.73E-02	0.92	FALSE	5.81E-01	0.97	FALSE
M305T846_neg	305.1871	846	3	7.73E-04	0.76	FALSE	9.60E-08	1.57	TRUE	1.11E-02	1.20	FALSE	2.25E-02	1.26	FALSE
M309T913_neg	309.1709	913	3	1.97E-02	0.88	FALSE	6.99E-01	0.98	FALSE	9.35E-01	1.00	FALSE	5.08E-04	1.58	TRUE
M310T808_neg	310.1085	808	3	9.69E-01	1.00	FALSE	4.94E-01	0.95	FALSE	1.50E-12	1.67	TRUE	4.66E-01	1.14	FALSE
M311T432_neg	311.1348	432	3	9.63E-01	1.00	FALSE	8.43E-01	1.02	FALSE	4.02E-08	1.55	TRUE	6.39E-01	1.09	FALSE
M311T911_neg	311.1863	911	3	3.71E-04	1.38	FALSE	7.08E-03	1.28	FALSE	9.64E-11	1.71	TRUE	1.00E-01	0.76	FALSE
M313T700_neg	313.1082	700	3	2.57E-52	3.23	TRUE	2.66E-03	0.85	FALSE	5.08E-01	0.97	FALSE	4.90E-01	0.92	FALSE
M317T389_neg	317.0990	389	3	3.22E-21	0.40	TRUE	5.80E-01	0.95	FALSE	2.57E-05	1.35	FALSE	6.78E-01	0.95	FALSE
M317T926_neg	317.1759	926	3	1.07E-33	2.21	TRUE	2.86E-08	0.75	FALSE	1.26E-03	1.16	FALSE	5.47E-01	0.95	FALSE
M317T1014_neg	317.2122	1014	3	4.73E-03	1.35	FALSE	3.15E-04	0.66	TRUE	9.58E-01	1.00	FALSE	7.22E-01	0.94	FALSE
M319T737_neg	319.1299	737	3	2.62E-03	0.80	FALSE	1.48E-03	1.26	FALSE	1.03E-12	1.63	TRUE	9.70E-04	0.67	FALSE
M323T491_neg	323.1615	491	3	2.91E-04	0.81	FALSE	2.51E-02	1.15	FALSE	1.14E-26	1.92	TRUE	5.95E-01	0.91	FALSE
M323T680_neg	323.1612	680	3	2.56E-06	1.54	TRUE	3.27E-01	0.91	FALSE	2.79E-01	0.92	FALSE	4.78E-01	0.86	FALSE
M324T542_neg	324.0231	542	3	1.32E-02	1.19	FALSE	1.12E-01	1.12	FALSE	5.61E-20	1.91	TRUE	8.82E-01	0.99	FALSE
M325T435_neg	325.1074	435	3	1.61E-20	0.26	TRUE	2.39E-01	1.15	FALSE	9.77E-02	1.18	FALSE	1.91E-01	1.35	FALSE
M325T954_neg	325.2020	954	3	3.55E-04	1.50	FALSE	4.45E-07	0.48	TRUE	2.68E-02	0.81	FALSE	5.89E-01	1.10	FALSE
M329T717_neg	329.1031	717	3	2.15E-13	0.67	FALSE	6.32E-02	1.10	FALSE	9.93E-26	1.71	TRUE	3.65E-01	1.08	FALSE
M329T756_neg	329.1031	756	3	7.21E-05	0.74	FALSE	1.32E-01	1.12	FALSE	1.94E-19	1.94	TRUE	5.88E-02	0.85	FALSE
M333T784_neg	333.0901	784	3	3.42E-40	2.97	TRUE	5.35E-06	0.75	FALSE	3.35E-12	0.68	FALSE	3.00E-01	0.89	FALSE
M335T665_neg	335.1248	665	3	9.25E-03	0.85	FALSE	2.54E-02	1.15	FALSE	5.35E-21	1.77	TRUE	8.13E-01	0.98	FALSE
M337T945_neg	337.2384	945	3	2.64E-15	3.69	TRUE	8.10E-02	0.79	FALSE	1.19E-02	1.35	FALSE	3.02E-01	0.85	FALSE
M347T994_neg	347.2228	994	3	1.07E-18	2.20	TRUE	4.49E-04	0.76	FALSE	9.26E-06	1.36	FALSE	5.44E-01	1.06	FALSE
M352T595_2_neg	352.1767	595	3	4.62E-12	1.68	TRUE	9.97E-01	1.00	FALSE	1.13E-01	0.91	FALSE	1.38E-01	1.26	FALSE
M361T664_neg	361.1407	664	3	5.64E-01	1.04	FALSE	2.32E-01	0.91	FALSE	2.46E-15	1.79	TRUE	1.69E-02	1.22	FALSE
M361T994_neg	361.2021	994	3	1.79E-11	1.61	TRUE	3.71E-02	0.87	FALSE	5.04E-04	1.23	FALSE	9.06E-01	1.01	FALSE
M363T1014_neg	363.2176	1014	3	1.74E-04	1.36	FALSE	1.63E-06	0.65	TRUE	3.43E-01	1.07	FALSE	9.69E-01	1.00	FALSE
M365T586_neg	365.1354	586	3	1.86E-01	0.91	FALSE	1.66E-02	1.20	FALSE	3.46E-13	1.67	TRUE	6.32E-01	1.04	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M365T866_neg	365.1971	866	3							HMDB0006059	20-Carboxy-leukotriene B4	C20H30O6	0.3
M373T1056_neg	373.2749	1056	3							HMDB0000308	3b-Hydroxy-5-cholenoic acid	C24H38O3	0.3
M375T1054_neg	375.2905	1054	3						Terpenoids	HMDB0000381	Allolithocholic acid	C24H40O3	0.1
M377T127_neg	377.0857	127	3							HMDB0249301	hloro-12-(4-chlorophenyl)dodecan	C18H25Cl3O2	2.4
M378T634_neg	378.1560	634	3						Alkaloids				
M397T688_neg	397.1869	688	3						Terpenoids	HMDB0034575	Apotrichodiol	C20H30O8	0.4
M417T1004_neg	417.2649	1004	3							HMDB0005007	Simvastatin	C25H38O5	0.5
M419T1056_neg	419.2804	1056	3							HMDB0248372	dodecyloxy)hydroxyphosphinyl)oxy	C21H43NO5P	0.4
M421T1053_neg	421.2960	1053	3						Terpenoids	HMDB0244296	7-Methyl-cholic acid	C25H42O5	0.2
M432T395_neg	432.1747	395	3							HMDB0249379	Brexpiprazole	C25H27N3O2S	0.9
M445T334_neg	445.1566	334	3						Carbohydrates				
M449T1034_neg	449.3274	1034	3							HMDB0000601	Coprocholic acid	C27H46O5	0.3
M466T895_neg	466.1985	895	3							HMDB0244824	rbonyl-Val-Ala-Asp(OMe)-fluorom	C22H30FN3O7	2.1
M469T1048_neg	469.3325	1048	3						Terpenoids	HMDB0011628	Glycyrrhetinic acid	C30H46O4	0.3
M471T669_neg	471.2602	669	3						Polyketides				
M475T714_neg	475.2341	714	3							HMDB0003141	Retinoyl b-glucuronide	C26H36O8	0.7
M475T811_neg	475.2338	811	3						Terpenoids	HMDB0003141	Retinoyl b-glucuronide	C26H36O8	0.1
M477T832_neg	477.2496	832	3						Terpenoids				
M483T658_neg	483.2239	658	3							HMDB0038238	Plantaricin BN	C24H36O10	0.6
M485T998_neg	485.3274	998	3						Terpenoids	HMDB0034526	Bassic acid	C30H46O5	0.3
M487T669_neg	487.2551	669	3						Polyketides	HMDB0038732	a-Ionol O-[arabinosyl-(1->6)-gluco	C24H40O10	0.5
M493T727_neg	493.2444	727	3						Terpenoids	HMDB0033655	7-(3-methylpentanoate) 11-(3-hyd	C26H38O9	0.2
M494T760_neg	494.2948	760	3							HMDB0242393	Chenodeoxycholylcysteine	C27H45NO5S	0.5
M515T1048_neg	515.3380	1048	3						Terpenoids	HMDB0015570	Fusidic Acid	C31H48O6	0.4
M535T398_neg	535.1546	398	3						Carbohydrates				
M582T921_neg	582.2746	921	3							HMDB0251330	Dihydrostreptomycin	C21H41N7O12	0.9
M593T940_neg	593.3345	940	3							HMDB0240259	Stercobilin	C33H46N4O6	0.0
M593T733_neg	593.3347	733	3							HMDB0240259	Stercobilin	C33H46N4O6	0.3
M595T947_neg	595.3501	947	3							HMDB0004157	Stercobilinogen	C33H48N4O6	0.1
M603T789_neg	603.2922	789	3						Terpenoids	HMDB0251363	Dilazep	C31H44N2O10	0.2
M607T349_neg	607.2094	349	3						Carbohydrates				
M609T696_neg	609.1827	696	3						Shikimates and Phenylpropanoids	HMDB0003265	Hesperidin	C28H34O15	0.3
M626T862_neg	626.3009	862	3							HMDB0260201	nyl)amino)phenyl)methyl)-2,5-dio	C35H41N5O6	3.9
M653T722_neg	653.2718	722	3						Polyketides				

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M365T866_neg	365.1971	866	3	8.17E-09	0.72	FALSE	2.15E-02	1.14	FALSE	8.36E-16	1.53	TRUE	1.01E-01	1.19	FALSE
M373T1056_neg	373.2749	1056	3	5.31E-04	1.26	FALSE	8.44E-01	0.99	FALSE	2.86E-13	1.59	TRUE	9.46E-02	1.16	FALSE
M375T1054_neg	375.2905	1054	3	5.69E-09	1.45	FALSE	1.25E-12	0.64	TRUE	6.20E-03	0.86	FALSE	8.18E-02	1.17	FALSE
M377T127_neg	377.0857	127	3	2.99E-14	0.28	TRUE	3.72E-01	1.14	FALSE	2.10E-02	1.33	FALSE	9.49E-01	1.04	FALSE
M378T634_neg	378.1560	634	3	1.46E-19	2.51	TRUE	7.72E-01	0.97	FALSE	1.37E-06	0.69	FALSE	2.40E-01	0.80	FALSE
M397T688_neg	397.1869	688	3	4.63E-02	0.87	FALSE	1.53E-04	1.33	FALSE	6.35E-19	1.90	TRUE	5.23E-02	1.19	FALSE
M417T1004_neg	417.2649	1004	3	1.52E-02	0.90	FALSE	4.70E-01	1.03	FALSE	8.38E-28	1.62	TRUE	2.77E-01	1.07	FALSE
M419T1056_neg	419.2804	1056	3	1.95E-04	1.29	FALSE	7.41E-01	0.98	FALSE	1.50E-13	1.61	TRUE	2.99E-02	1.22	FALSE
M421T1053_neg	421.2960	1053	3	7.84E-09	1.43	FALSE	3.17E-13	0.64	TRUE	1.03E-02	0.88	FALSE	8.30E-02	1.16	FALSE
M432T395_neg	432.1747	395	3	1.66E-54	2.45	TRUE	2.54E-02	0.91	FALSE	1.83E-03	0.90	FALSE	5.09E-01	1.04	FALSE
M445T334_neg	445.1566	334	3	4.92E-03	1.90	TRUE	7.40E-01	1.09	FALSE	7.00E-02	0.70	FALSE	2.13E-01	0.34	FALSE
M449T1034_neg	449.3274	1034	3	5.68E-16	1.72	TRUE	1.26E-07	0.72	FALSE	2.42E-01	0.94	FALSE	6.14E-01	1.05	FALSE
M466T895_neg	466.1985	895	3	1.29E-06	1.49	FALSE	9.04E-01	1.01	FALSE	3.31E-13	1.73	TRUE	9.67E-04	0.69	FALSE
M469T1048_neg	469.3325	1048	3	2.35E-08	1.99	TRUE	1.75E-01	0.85	FALSE	9.64E-01	1.00	FALSE	6.68E-02	1.38	FALSE
M471T669_neg	471.2602	669	3	2.40E-25	1.92	TRUE	9.70E-01	1.00	FALSE	7.83E-01	1.01	FALSE	7.97E-01	1.02	FALSE
M475T714_neg	475.2341	714	3	8.56E-02	1.12	FALSE	8.85E-07	1.45	FALSE	2.14E-06	1.34	FALSE	8.75E-04	2.11	TRUE
M475T811_neg	475.2338	811	3	1.24E-02	0.81	FALSE	1.59E-02	1.24	FALSE	6.55E-09	1.57	TRUE	4.02E-01	1.18	FALSE
M477T832_neg	477.2496	832	3	1.81E-04	0.73	FALSE	1.89E-02	1.22	FALSE	4.29E-09	1.56	TRUE	5.90E-01	1.08	FALSE
M483T658_neg	483.2239	658	3	2.02E-02	1.15	FALSE	2.35E-01	1.08	FALSE	6.69E-23	1.84	TRUE	3.02E-01	0.88	FALSE
M485T998_neg	485.3274	998	3	6.72E-17	2.86	TRUE	1.97E-02	0.77	FALSE	2.33E-02	1.23	FALSE	1.54E-01	1.48	FALSE
M487T669_neg	487.2551	669	3	7.26E-07	1.33	FALSE	5.16E-01	1.04	FALSE	1.54E-17	1.59	TRUE	2.72E-01	0.92	FALSE
M493T727_neg	493.2444	727	3	4.20E-06	0.75	FALSE	1.30E-01	1.11	FALSE	1.01E-13	1.55	TRUE	1.92E-01	1.18	FALSE
M494T760_neg	494.2948	760	3	3.72E-29	2.70	TRUE	2.23E-01	0.92	FALSE	3.18E-10	1.50	FALSE	1.86E-02	0.83	FALSE
M515T1048_neg	515.3380	1048	3	8.11E-05	1.66	TRUE	4.74E-01	0.91	FALSE	9.67E-01	1.00	FALSE	7.17E-02	1.45	FALSE
M535T398_neg	535.1546	398	3	1.46E-38	0.04	TRUE	4.36E-01	1.09	FALSE	2.97E-01	0.90	FALSE	1.67E-01	2.77	FALSE
M582T921_neg	582.2746	921	3	7.80E-05	1.34	FALSE	6.03E-01	1.04	FALSE	2.81E-12	1.62	TRUE	9.29E-01	0.99	FALSE
M593T940_neg	593.3345	940	3	6.21E-08	0.62	TRUE	7.70E-05	1.41	FALSE	1.95E-02	0.84	FALSE	6.09E-01	0.94	FALSE
M593T733_neg	593.3347	733	3	2.62E-23	1.52	TRUE	5.37E-01	1.02	FALSE	2.58E-01	1.04	FALSE	1.16E-02	0.90	FALSE
M595T947_neg	595.3501	947	3	9.91E-02	0.85	FALSE	1.42E-06	1.66	TRUE	6.94E-02	0.85	FALSE	6.79E-01	1.07	FALSE
M603T789_neg	603.2922	789	3	6.58E-01	0.96	FALSE	2.53E-01	1.12	FALSE	2.78E-12	1.95	TRUE	3.66E-02	1.19	FALSE
M607T349_neg	607.2094	349	3	4.48E-05	2.07	TRUE	4.04E-01	0.86	FALSE	1.24E-01	0.80	FALSE	3.55E-01	0.69	FALSE
M609T696_neg	609.1827	696	3	1.05E-01	2.10	FALSE	9.76E-01	1.02	FALSE	9.36E-02	1.94	FALSE	9.91E-03	6.13	TRUE
M626T862_neg	626.3009	862	3	2.99E-02	1.19	FALSE	3.20E-01	1.09	FALSE	8.17E-17	1.93	TRUE	7.74E-01	1.05	FALSE
M653T722_neg	653.2718	722	3	2.91E-01	0.91	FALSE	4.58E-03	1.30	FALSE	1.52E-18	2.20	TRUE	2.41E-01	1.16	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M673T774_neg	673.3592	774	3							HMDB0250252	Cimicifugoside	C37H54O11	0.2
M686T1008_neg	685.5048	1008	3							HMDB0116371	DG(11D3/11M3/0:0)	C42H70O7	0.2
M699T983_neg	699.4840	983	3						Polyketides				
M733T785_neg	733.3820	785	3						Amino acids and Peptides				
M785T783_neg	785.4596	783	3							HMDB0263917	PA(18:2(9Z,11Z)/6 keto-PGF1alpha	C41H71O12P	1.9
M794T958_neg	793.5260	958	3							HMDB0270792	PG(a-17:0/18:1(12Z)-2OH(9,10))	C41H79O12P	2.9
M798T982_neg	797.5570	982	3						Terpenoids				
M799T783_neg	799.4388	783	3						Amino acids and Peptides				
M812T1007_neg	811.5729	1007	3						Terpenoids				
M827T419_neg	827.3041	419	3						Carbohydrates				
M883T805_neg	883.4976	805	3							HMDB0269934	20:4(5Z,8Z,11Z,14Z)/6 keto-PGF1al	C46H77O14P	0.2
M942T856_neg	941.5178	856	3							HMDB0274621	PGP(a-21:0/5-iso PGF2VI)	C45H84O16P2	1.8
M960T777_neg	959.5375	777	3							HMDB0274653	21:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-	C49H86O14P2	4.7
M960T853_neg	959.5374	853	3							HMDB0274653	21:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-	C49H86O14P2	4.8
M81T518_neg	81.0346	518	3							HMDB0013749	2-Methylfuran	C5H6O	0.3
M82T475_neg	82.0298	475	3							HMDB0255970	Oxazine	C4H5NO	0.4
M83T518_neg	83.0502	518	3							HMDB0001184	Methyl propenyl ketone	C5H8O	0.1
M93T745_neg	93.0346	745	3							HMDB0000228	Phenol	C6H6O	0.2
M93T454_neg	93.0346	454	3							HMDB0000228	Phenol	C6H6O	0.1
M94T637_neg	94.0298	637	3							HMDB0013751	2-Hydroxypyridine	C5H5NO	0.1
M94T365_neg	94.0298	365	3							HMDB0013751	2-Hydroxypyridine	C5H5NO	0.1
M94T554_neg	94.0299	554	3							HMDB0013751	2-Hydroxypyridine	C5H5NO	0.2
M95T604_neg	95.0502	604	3							HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.2
M97T753_neg	97.0659	753	3							HMDB0003315	Cyclohexanone	C6H10O	0.0
M99T536_neg	99.0452	536	3							HMDB0000509	Senecioic acid	C5H8O2	0.2
M102T371_neg	102.0561	371	3							HMDB0000092	Dimethylglycine	C4H9NO2	0.5
M108T562_neg	108.0217	562	3							HMDB0256033	p-Benzosemiquinone	C6H5O2	0.0
M108T657_neg	108.0455	657	3							HMDB0245309	Piconol	C6H7NO	0.0
M108T576_neg	108.0456	576	3							HMDB0001169	4-Aminophenol	C6H7NO	0.8
M109T562_neg	109.0295	562	3							HMDB0000957	Pyrocatechol	C6H6O2	0.0
M109T401_neg	109.0408	401	3							HMDB0003905	Imidazole-4-acetaldehyde	C5H6N2O	0.5
M111T686_neg	111.0816	686	3							HMDB0031483	(Z)-4-Heptenal	C7H12O	0.3
M112T479_neg	112.0227	479	3							HMDB0302343	Butenyl isothiocyanate	C5H7NS	0.9
M113T578_neg	113.0609	578	3							HMDB0000453	delta-Hexanolactone	C6H10O2	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M673T774_neg	673.3592	774	3	2.06E-01	1.14	FALSE	3.78E-01	1.10	FALSE	1.72E-07	1.64	TRUE	7.17E-01	0.92	FALSE
M686T1008_neg	685.5048	1008	3	7.27E-02	1.79	FALSE	1.21E-01	0.54	FALSE	3.19E-03	2.39	TRUE	5.68E-01	0.84	FALSE
M699T983_neg	699.4840	983	3	4.23E-10	2.35	TRUE	5.17E-02	0.77	FALSE	1.78E-02	1.29	FALSE	9.11E-02	1.43	FALSE
M733T785_neg	733.3820	785	3	1.34E-01	0.74	FALSE	4.14E-02	1.55	TRUE	5.80E-02	1.40	FALSE	5.11E-01	1.27	FALSE
M785T783_neg	785.4596	783	3	8.87E-07	2.30	TRUE	5.66E-01	0.92	FALSE	5.67E-02	1.30	FALSE	1.14E-02	1.47	FALSE
M794T958_neg	793.5260	958	3	1.06E-07	1.45	FALSE	1.68E-02	1.18	FALSE	1.68E-30	2.32	TRUE	3.92E-02	0.81	FALSE
M798T982_neg	797.5570	982	3	2.51E-02	1.73	TRUE	1.79E-01	0.67	FALSE	4.66E-01	0.86	FALSE	5.70E-01	0.63	FALSE
M799T783_neg	799.4388	783	3	3.81E-02	1.41	FALSE	8.84E-01	1.02	FALSE	3.78E-07	2.18	TRUE	4.47E-02	1.35	FALSE
M812T1007_neg	811.5729	1007	3	1.01E-04	1.39	FALSE	7.51E-01	0.97	FALSE	2.32E-12	1.72	TRUE	2.72E-01	0.89	FALSE
M827T419_neg	827.3041	419	3	8.29E-10	2.04	TRUE	7.98E-01	0.97	FALSE	9.73E-02	0.86	FALSE	5.05E-01	0.76	FALSE
M883T805_neg	883.4976	805	3	1.78E-08	1.50	TRUE	1.09E-03	0.80	FALSE	5.54E-08	1.41	FALSE	1.45E-01	1.16	FALSE
M942T856_neg	941.5178	856	3	2.82E-01	0.91	FALSE	8.46E-03	1.29	FALSE	1.87E-10	1.71	TRUE	8.23E-02	1.17	FALSE
M960T777_neg	959.5375	777	3	7.39E-01	1.04	FALSE	2.27E-02	1.37	FALSE	4.24E-11	2.32	TRUE	6.08E-01	1.11	FALSE
M960T853_neg	959.5374	853	3	1.91E-02	0.78	FALSE	1.99E-01	1.15	FALSE	9.05E-11	1.92	TRUE	9.12E-01	0.98	FALSE
M81T518_neg	81.0346	518	3	2.96E-04	0.80	FALSE	5.82E-02	1.13	FALSE	1.41E-27	2.02	TRUE	1.61E-01	0.90	FALSE
M82T475_neg	82.0298	475	3	2.14E-02	0.81	FALSE	3.35E-01	1.09	FALSE	4.29E-12	1.80	TRUE	7.43E-01	0.95	FALSE
M83T518_neg	83.0502	518	3	1.39E-10	0.73	FALSE	4.75E-02	1.10	FALSE	6.43E-37	1.91	TRUE	3.45E-01	0.94	FALSE
M93T745_neg	93.0346	745	3	4.07E-02	1.71	TRUE	1.41E-01	0.64	FALSE	5.81E-01	0.88	FALSE	1.84E-01	1.74	FALSE
M93T454_neg	93.0346	454	3	2.68E-03	1.27	FALSE	4.37E-03	1.26	FALSE	2.65E-17	1.93	TRUE	2.75E-01	0.90	FALSE
M94T637_neg	94.0298	637	3	8.73E-09	1.68	TRUE	3.77E-02	1.20	FALSE	4.34E-07	1.47	FALSE	6.33E-01	1.05	FALSE
M94T365_neg	94.0298	365	3	9.46E-01	1.00	FALSE	9.05E-01	1.01	FALSE	1.27E-17	1.63	TRUE	1.46E-01	0.82	FALSE
M94T554_neg	94.0299	554	3	1.83E-11	0.27	TRUE	4.14E-01	1.15	FALSE	2.19E-02	1.39	FALSE	2.63E-01	0.88	FALSE
M95T604_neg	95.0502	604	3	1.73E-06	0.79	FALSE	2.02E-03	1.17	FALSE	2.25E-33	1.91	TRUE	6.31E-01	1.03	FALSE
M97T753_neg	97.0659	753	3	2.29E-02	0.87	FALSE	3.03E-02	1.15	FALSE	3.94E-22	1.80	TRUE	2.80E-01	0.89	FALSE
M99T536_neg	99.0452	536	3	6.10E-07	0.79	FALSE	7.66E-02	1.09	FALSE	3.64E-32	1.80	TRUE	1.28E-01	0.90	FALSE
M102T371_neg	102.0561	371	3	1.61E-13	1.65	TRUE	5.00E-01	0.96	FALSE	6.61E-01	0.98	FALSE	9.71E-01	1.00	FALSE
M108T562_neg	108.0217	562	3	5.05E-07	1.63	TRUE	7.22E-01	1.03	FALSE	9.51E-01	1.00	FALSE	7.86E-01	1.03	FALSE
M108T657_neg	108.0455	657	3	1.36E-07	0.12	TRUE	9.51E-01	0.98	FALSE	7.91E-01	1.07	FALSE	2.25E-01	1.22	FALSE
M108T576_neg	108.0456	576	3	1.93E-11	0.51	TRUE	1.57E-01	0.87	FALSE	1.43E-01	1.13	FALSE	7.44E-01	1.05	FALSE
M109T562_neg	109.0295	562	3	1.83E-07	1.72	TRUE	6.55E-01	0.96	FALSE	5.26E-01	1.06	FALSE	3.45E-01	0.89	FALSE
M109T401_neg	109.0408	401	3	4.47E-03	1.27	FALSE	5.61E-01	0.95	FALSE	6.38E-08	1.51	TRUE	1.08E-01	0.76	FALSE
M111T686_neg	111.0816	686	3	2.32E-04	0.88	FALSE	1.10E-01	1.06	FALSE	7.77E-34	1.58	TRUE	5.89E-01	0.97	FALSE
M112T479_neg	112.0227	479	3	3.47E-01	1.04	FALSE	8.97E-01	0.99	FALSE	1.25E-19	1.51	TRUE	5.17E-01	1.04	FALSE
M113T578_neg	113.0609	578	3	5.00E-12	0.70	FALSE	1.31E-01	1.08	FALSE	1.87E-22	1.59	TRUE	9.61E-01	1.00	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M114T411_neg	114.0198	411	3							HMDB0246560	4-Oxo-2-azetidinecarboxylic acid	C4H5NO3	1.2
M114T197_neg	114.0197	197	3							HMDB0246560	4-Oxo-2-azetidinecarboxylic acid	C4H5NO3	0.5
M114T403_neg	114.0561	403	3							HMDB0000162	L-Proline	C5H9NO2	0.8
M115T149_neg	115.0037	149	3							HMDB0000134	Fumaric acid	C4H4O4	0.3
M115T267_neg	115.0038	267	3							HMDB0000134	Fumaric acid	C4H4O4	0.6
M115T453_neg	115.0402	453	3							HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	0.7
M116T475_neg	116.0176	475	3							HMDB0002287	Homocysteine thiolactone	C4H7NOS	0.7
M116T508_neg	116.0506	508	3							HMDB0000738	Indole	C8H7N	0.5
M116T407_neg	116.0718	407	3							HMDB0000883	L-Valine	C5H11NO2	0.9
M119T554_neg	119.0173	554	3							HMDB0112255	Allyl methyl sulfone	C4H8O2S	0.9
M120T688_neg	120.0456	688	3							HMDB0004461	Benzamide	C7H7NO	0.6
M120T460_neg	120.0456	460	3							HMDB0004461	Benzamide	C7H7NO	0.7
M121T1029_neg	120.9965	1029	3							HMDB0244180	1,3-Propane sultone	C3H6O3S	0.4
M121T505_neg	121.0408	505	3							HMDB0001406	Niacinamide	C6H6N2O	0.8
M122T547_neg	122.0612	547	3							HMDB0029300	p-Anisidine	C7H9NO	0.8
M123T526_neg	123.0566	526	3							HMDB0004181	Methylimidazole acetaldehyde	C6H8N2O	2.0
M123T753_neg	123.0816	753	3							HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.6
M124T369_neg	124.0405	369	3						Alkaloids	HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.9
M124T411_neg	124.0405	411	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	1.1
M124T570_neg	124.0769	570	3							HMDB0030345	6-Acetyl-1,2,3,4-tetrahydropyridine	C7H11NO	0.7
M127T540_neg	126.9860	540	3							HMDB0259027	THIOPHENE-2-CARBOXYLIC ACID	C5H4O2S	0.9
M127T707_neg	127.0766	707	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.9
M127T656_neg	127.0766	656	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.8
M128T475_neg	128.0177	475	3							HMDB0251849	Epigoitrin	C5H7NOS	0.9
M128T412_neg	128.0354	412	3							HMDB0000267	Pyroglutamic acid	C5H7NO3	0.9
M128T526_neg	128.1082	526	3							HMDB0246589	4-Trimethylaminobutyraldehyde	C7H15NO	1.0
M129T526_neg	129.0558	526	3							HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	0.9
M130T382_neg	130.0875	382	3							HMDB0000172	L-Isoleucine	C6H13NO2	0.8
M132T643_neg	132.0455	643	3						Alkaloids	HMDB0004094	Indoxyl	C8H7NO	0.4
M133T405_neg	133.0508	405	3							HMDB0000421	2,3-Dihydroxyvaleric acid	C5H10O4	0.9
M133T609_neg	133.0660	609	3							HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	0.8
M134T422_neg	134.0612	422	3							HMDB0001250	N-Acetylarylamine	C8H9NO	0.6
M135T261_neg	135.0313	261	3						Alkaloids	HMDB0000157	Hypoxanthine	C5H4N4O	0.4
M138T395_neg	138.0198	395	3							HMDB0001232	4-Nitrophenol	C6H5NO3	0.8
M138T703_neg	138.0198	703	3							HMDB0001232	4-Nitrophenol	C6H5NO3	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M114T411_neg	114.0198	411	3	6.27E-01	0.97	FALSE	4.26E-01	1.04	FALSE	3.75E-16	1.51	TRUE	2.89E-01	1.07	FALSE
M114T197_neg	114.0197	197	3	1.32E-02	0.81	FALSE	1.13E-01	0.87	FALSE	1.86E-08	1.55	TRUE	8.73E-01	0.98	FALSE
M114T403_neg	114.0561	403	3	6.02E-01	1.02	FALSE	9.99E-01	1.00	FALSE	1.49E-23	1.54	TRUE	2.74E-01	0.93	FALSE
M115T149_neg	115.0037	149	3	2.19E-22	0.10	TRUE	7.33E-01	1.05	FALSE	5.96E-02	1.28	FALSE	4.70E-03	0.74	FALSE
M115T267_neg	115.0038	267	3	1.56E-51	0.07	TRUE	8.76E-01	1.01	FALSE	6.03E-02	1.15	FALSE	1.85E-02	1.38	FALSE
M115T453_neg	115.0402	453	3	3.23E-03	0.20	TRUE	5.72E-01	1.32	FALSE	8.65E-01	0.94	FALSE	5.35E-01	1.11	FALSE
M116T475_neg	116.0176	475	3	5.62E-03	0.80	FALSE	4.20E-01	1.07	FALSE	8.32E-13	1.70	TRUE	8.09E-01	0.97	FALSE
M116T508_neg	116.0506	508	3	3.99E-40	0.41	TRUE	3.43E-01	1.05	FALSE	3.63E-14	1.43	FALSE	6.80E-01	0.95	FALSE
M116T407_neg	116.0718	407	3	5.70E-01	0.98	FALSE	5.00E-01	1.03	FALSE	3.19E-21	1.52	TRUE	5.37E-01	1.05	FALSE
M119T554_neg	119.0173	554	3	1.40E-02	0.87	FALSE	8.96E-14	1.56	TRUE	3.62E-09	1.36	FALSE	4.68E-01	1.09	FALSE
M120T688_neg	120.0456	688	3	3.88E-10	1.89	TRUE	2.58E-03	1.43	FALSE	2.02E-01	0.90	FALSE	9.89E-01	1.00	FALSE
M120T460_neg	120.0456	460	3	1.05E-02	0.86	FALSE	3.49E-01	1.06	FALSE	2.91E-19	1.67	TRUE	5.06E-02	0.86	FALSE
M121T1029_neg	120.9965	1029	3	1.26E-24	0.60	TRUE	2.89E-06	1.23	FALSE	4.37E-02	0.93	FALSE	3.62E-01	0.89	FALSE
M121T505_neg	121.0408	505	3	1.23E-02	0.69	FALSE	4.91E-01	0.90	FALSE	2.12E-06	1.88	TRUE	6.27E-01	1.05	FALSE
M122T547_neg	122.0612	547	3	8.51E-01	0.99	FALSE	3.53E-01	1.06	FALSE	3.55E-13	1.54	TRUE	5.87E-01	0.94	FALSE
M123T526_neg	123.0566	526	3	2.28E-01	1.11	FALSE	5.36E-02	1.19	FALSE	4.66E-21	2.36	TRUE	6.00E-01	1.06	FALSE
M123T753_neg	123.0816	753	3	1.57E-02	0.85	FALSE	8.11E-03	1.19	FALSE	5.19E-20	1.81	TRUE	2.04E-01	0.88	FALSE
M124T369_neg	124.0405	369	3	1.86E-02	0.90	FALSE	9.91E-02	1.08	FALSE	5.15E-30	1.68	TRUE	5.47E-01	1.05	FALSE
M124T411_neg	124.0405	411	3	1.05E-02	0.87	FALSE	2.51E-01	1.06	FALSE	1.09E-27	1.82	TRUE	7.22E-01	1.02	FALSE
M124T570_neg	124.0769	570	3	4.80E-03	0.83	FALSE	5.77E-01	0.96	FALSE	2.21E-11	1.51	TRUE	5.99E-01	1.09	FALSE
M127T540_neg	126.9860	540	3	7.08E-01	1.03	FALSE	2.27E-06	1.45	FALSE	2.55E-10	1.56	TRUE	5.64E-02	0.74	FALSE
M127T707_neg	127.0766	707	3	2.30E-19	1.33	FALSE	9.76E-01	1.00	FALSE	3.58E-06	0.89	FALSE	9.42E-05	1.63	TRUE
M127T656_neg	127.0766	656	3	6.51E-04	0.84	FALSE	1.73E-01	1.07	FALSE	7.86E-19	1.53	TRUE	7.46E-01	0.96	FALSE
M128T475_neg	128.0177	475	3	4.91E-03	0.81	FALSE	4.76E-01	1.06	FALSE	1.46E-12	1.66	TRUE	8.55E-01	0.98	FALSE
M128T412_neg	128.0354	412	3	7.44E-04	0.84	FALSE	3.11E-03	1.17	FALSE	3.11E-29	1.85	TRUE	6.12E-01	1.03	FALSE
M128T526_neg	128.1082	526	3	8.31E-18	2.04	TRUE	6.30E-01	0.97	FALSE	4.14E-02	1.14	FALSE	5.50E-01	0.94	FALSE
M129T526_neg	129.0558	526	3	8.75E-09	1.51	TRUE	2.09E-01	1.09	FALSE	2.77E-02	1.14	FALSE	4.23E-01	0.88	FALSE
M130T382_neg	130.0875	382	3	6.17E-10	0.09	TRUE	6.79E-01	1.12	FALSE	1.01E-01	1.45	FALSE	9.25E-01	1.00	FALSE
M132T643_neg	132.0455	643	3	5.27E-01	1.07	FALSE	6.22E-01	1.05	FALSE	1.30E-06	1.58	TRUE	7.74E-01	1.06	FALSE
M133T405_neg	133.0508	405	3	6.54E-01	0.97	FALSE	9.07E-01	0.99	FALSE	4.52E-12	1.68	TRUE	7.52E-01	1.04	FALSE
M133T609_neg	133.0660	609	3	7.89E-13	0.73	FALSE	1.29E-02	1.11	FALSE	1.19E-36	1.80	TRUE	9.97E-01	1.00	FALSE
M134T422_neg	134.0612	422	3	4.28E-04	0.69	FALSE	1.69E-01	1.16	FALSE	4.81E-20	2.66	TRUE	1.04E-01	0.70	FALSE
M135T261_neg	135.0313	261	3	2.19E-46	0.06	TRUE	1.00E-02	1.29	FALSE	1.01E-03	1.31	FALSE	5.52E-02	1.55	FALSE
M138T395_neg	138.0198	395	3	1.54E-01	1.11	FALSE	3.74E-05	1.38	FALSE	7.76E-26	2.31	TRUE	2.69E-01	1.16	FALSE
M138T703_neg	138.0198	703	3	4.86E-02	1.19	FALSE	2.53E-02	0.80	FALSE	2.44E-37	0.24	TRUE	9.45E-02	1.47	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M140T469_neg	140.0354	469	3							HMDB0001280	-Aminomuconic acid semialdehyd	C6H7NO3	0.9
M140T676_neg	140.1082	676	3							HMDB0030324	(R)-Pelletierine	C8H15NO	0.9
M142T406_neg	142.0511	406	3							HMDB0000894	Vinylacetylglycine	C6H9NO3	0.9
M142T508_neg	142.0662	508	3							HMDB0033115	6-Methylquinoline	C10H9N	0.0
M143T536_neg	143.0351	536	3							HMDB0000393	3-Hexenedioic acid	C6H8O4	0.7
M143T438_neg	143.1191	438	3							HMDB0002284	N-Acetylcadaverine	C7H16N2O	0.7
M144T750_neg	144.0455	750	3							HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.3
M144T519_neg	144.0668	519	3							HMDB0000730	Isobutyrylglycine	C6H11NO3	1.3
M144T308_neg	144.0667	308	3							HMDB0000730	Isobutyrylglycine	C6H11NO3	0.8
M145T467_neg	145.0143	467	3							HMDB0000208	Oxoglutaric acid	C5H6O5	0.4
M145T365_neg	145.0410	365	3							HMDB0244250	1,8-Naphthyridin-2(1H)-one	C8H6N2O	2.0
M145T762_neg	145.0871	762	3							HMDB0002207	3-Hydroxyisoheptanoic acid	C7H14O3	0.7
M146T160_neg	146.0459	160	3							HMDB0000148	L-Glutamic acid	C5H9NO4	0.4
M147T723_neg	147.0486	723	3							HMDB0303256	(+/-)-3-Mercapto-1-butyl acetate	C6H12O2S	0.2
M149T363_neg	148.9915	363	3							HMDB0247921	Acetyloxysulfanyl acetate	C4H6O4S	0.7
M149T502_neg	149.0093	502	3							HMDB0000956	Tartaric acid	C4H6O6	0.7
M149T360_neg	149.0279	360	3							HMDB0037115	1)-2-Hydroxy-4-(methylthio)butar	C5H10O3S	0.9
M149T713_neg	149.0609	713	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.7
M150T397_neg	150.0421	397	3							HMDB0000132	Guanine	C5H5N5O	0.2
M150T281_neg	150.0422	281	3							HMDB0000132	Guanine	C5H5N5O	0.5
M150T422_neg	150.0561	422	3							HMDB0001859	Acetaminophen	C8H9NO2	0.6
M150T692_neg	150.0925	692	3							HMDB0001387	N-Methylphenylethanolamine	C9H13NO	0.5
M151T664_neg	151.0402	664	3						Shikimates and Phenylpropanoids	HMDB0000020	p-Hydroxyphenylacetic acid	C8H8O3	0.6
M152T657_neg	152.0356	657	3							HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	1.5
M152T546_neg	152.0719	546	3							HMDB0000073	Dopamine	C8H11NO2	1.6
M153T562_neg	153.0195	562	3						Shikimates and Phenylpropanoids	HMDB0000152	Gentisic acid	C7H6O4	0.9
M153T459_neg	153.0307	459	3							HMDB0244990	2-Amino-4-nitrophenol	C6H6N2O3	1.0
M153T420_neg	153.0321	420	3							HMDB0012209	Diethylphosphate	C4H11O4P	1.1
M153T651_neg	153.0922	651	3							HMDB0031302	Methyl 2-octynoate	C9H14O2	0.6
M155T383_neg	155.0463	383	3							HMDB0000544	5-Hydroxymethyl-4-methyluracil	C6H8N2O3	0.7
M155T398_neg	155.0827	398	3							HMDB0242468	(2-Ethylcrotonoyl)urea	C7H12N2O2	0.8
M157T403_neg	157.0620	403	3							HMDB0031670	methyl)-5,5-dimethyl-2,4-imidazo	C6H10N2O3	0.7
M157T562_neg	157.0872	562	3							HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M140T469_neg	140.0354	469	3	1.25E-02	0.85	FALSE	4.97E-03	1.21	FALSE	4.88E-18	1.72	TRUE	3.05E-02	1.19	FALSE
M140T676_neg	140.1082	676	3	3.92E-03	0.84	FALSE	2.14E-06	1.36	FALSE	5.53E-15	1.56	TRUE	2.03E-02	1.25	FALSE
M142T406_neg	142.0511	406	3	5.05E-11	0.61	TRUE	1.29E-02	1.20	FALSE	2.62E-06	1.35	FALSE	8.95E-03	1.24	FALSE
M142T508_neg	142.0662	508	3	7.00E-40	0.37	TRUE	1.07E-01	1.10	FALSE	3.20E-14	1.49	FALSE	1.44E-01	1.19	FALSE
M143T536_neg	143.0351	536	3	1.92E-01	1.06	FALSE	1.88E-01	1.06	FALSE	1.07E-30	1.75	TRUE	2.23E-01	1.10	FALSE
M143T438_neg	143.1191	438	3	1.20E-31	0.30	TRUE	9.00E-01	0.99	FALSE	2.46E-06	1.39	FALSE	6.24E-01	1.08	FALSE
M144T750_neg	144.0455	750	3	2.02E-03	0.86	FALSE	2.16E-01	1.07	FALSE	5.14E-31	1.86	TRUE	8.36E-02	0.86	FALSE
M144T519_neg	144.0668	519	3	6.38E-07	0.62	TRUE	4.88E-01	1.07	FALSE	1.28E-01	1.13	FALSE	2.06E-01	0.94	FALSE
M144T308_neg	144.0667	308	3	1.40E-05	0.71	FALSE	1.74E-01	1.12	FALSE	2.52E-18	1.96	TRUE	7.11E-01	0.94	FALSE
M145T467_neg	145.0143	467	3	3.42E-03	0.10	TRUE	5.35E-01	1.46	FALSE	4.80E-01	0.71	FALSE	2.78E-01	1.50	FALSE
M145T365_neg	145.0410	365	3	7.25E-01	1.02	FALSE	3.94E-01	1.04	FALSE	9.28E-30	1.78	TRUE	5.88E-01	0.96	FALSE
M145T762_neg	145.0871	762	3	5.00E-01	0.95	FALSE	6.65E-01	1.04	FALSE	1.72E-03	0.81	FALSE	8.08E-10	6.40	TRUE
M146T160_neg	146.0459	160	3	2.94E-02	0.84	FALSE	1.11E-01	1.14	FALSE	1.57E-18	1.99	TRUE	7.35E-01	1.06	FALSE
M147T723_neg	147.0486	723	3	7.23E-01	1.03	FALSE	4.33E-06	1.59	TRUE	6.16E-02	1.16	FALSE	6.69E-01	1.11	FALSE
M149T363_neg	148.9915	363	3	8.68E-05	1.50	TRUE	1.81E-04	0.68	FALSE	1.69E-01	0.89	FALSE	5.29E-01	1.13	FALSE
M149T502_neg	149.0093	502	3	1.37E-01	1.97	FALSE	8.95E-01	1.08	FALSE	3.58E-04	5.50	TRUE	2.45E-01	0.23	FALSE
M149T360_neg	149.0279	360	3	2.70E-11	1.64	TRUE	1.75E-03	0.80	FALSE	2.69E-01	1.07	FALSE	3.72E-01	0.93	FALSE
M149T713_neg	149.0609	713	3	1.31E-07	0.71	FALSE	3.77E-01	1.06	FALSE	1.16E-16	1.65	TRUE	1.22E-01	0.84	FALSE
M150T397_neg	150.0421	397	3	3.43E-21	0.29	TRUE	5.04E-01	1.08	FALSE	2.68E-04	1.40	FALSE	5.01E-01	1.26	FALSE
M150T281_neg	150.0422	281	3	1.26E-03	1.42	FALSE	8.68E-04	1.46	FALSE	2.26E-11	1.99	TRUE	8.43E-01	0.95	FALSE
M150T422_neg	150.0561	422	3	2.12E-04	0.75	FALSE	1.22E-01	1.13	FALSE	7.45E-26	2.34	TRUE	5.78E-02	0.74	FALSE
M150T692_neg	150.0925	692	3	6.94E-01	1.04	FALSE	3.00E-01	1.11	FALSE	1.21E-14	2.14	TRUE	3.36E-01	0.88	FALSE
M151T664_neg	151.0402	664	3	1.99E-03	0.71	FALSE	6.16E-01	1.06	FALSE	1.32E-11	2.02	TRUE	2.33E-01	1.23	FALSE
M152T657_neg	152.0356	657	3	7.73E-10	0.07	TRUE	8.81E-01	1.04	FALSE	4.15E-01	1.21	FALSE	1.73E-01	1.33	FALSE
M152T546_neg	152.0719	546	3	1.08E-03	1.29	FALSE	5.19E-01	1.05	FALSE	1.87E-14	1.76	TRUE	8.99E-01	0.99	FALSE
M153T562_neg	153.0195	562	3	4.16E-08	1.81	TRUE	6.96E-01	0.96	FALSE	8.46E-01	1.02	FALSE	8.74E-01	1.02	FALSE
M153T459_neg	153.0307	459	3	6.55E-03	0.83	FALSE	1.20E-01	1.12	FALSE	1.06E-23	2.04	TRUE	4.00E-01	0.91	FALSE
M153T420_neg	153.0321	420	3	2.07E-11	1.52	TRUE	3.21E-01	0.94	FALSE	6.61E-02	1.10	FALSE	1.61E-02	1.33	FALSE
M153T651_neg	153.0922	651	3	2.36E-11	1.56	TRUE	6.81E-01	0.97	FALSE	3.19E-02	1.12	FALSE	5.86E-01	0.94	FALSE
M155T383_neg	155.0463	383	3	7.51E-01	1.02	FALSE	2.47E-03	0.85	FALSE	1.16E-17	1.50	TRUE	1.28E-01	0.92	FALSE
M155T398_neg	155.0827	398	3	1.15E-07	0.72	FALSE	8.24E-01	0.99	FALSE	1.23E-26	1.95	TRUE	8.13E-01	0.98	FALSE
M157T403_neg	157.0620	403	3	3.29E-01	1.06	FALSE	8.48E-01	0.99	FALSE	7.54E-20	1.70	TRUE	7.06E-01	0.94	FALSE
M157T562_neg	157.0872	562	3	8.57E-25	1.56	TRUE	8.59E-01	1.01	FALSE	1.43E-01	1.05	FALSE	3.82E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M158T632_neg	158.0824	632	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.7
M158T412_neg	158.0824	412	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.9
M159T447_neg	159.0122	447	3							HMDB0035901	Thiacremonone	C6H8O3S	0.5
M159T407_neg	159.0776	407	3						Amino acids and Peptides	HMDB0003459	D-Alanyl-D-alanine	C6H12N2O3	0.7
M159T118_neg	159.0776	118	3							HMDB0003459	D-Alanyl-D-alanine	C6H12N2O3	0.4
M159T831_neg	159.1028	831	3							HMDB0000486	7-Hydroxyoctanoic acid	C8H16O3	0.7
M160T422_neg	160.0405	422	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.5
M160T484_neg	160.0405	484	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.7
M162T409_neg	161.9868	409	3							HMDB0033585	Acesulfame	C4H5NO4S	0.7
M162T486_neg	162.0561	486	3						Alkaloids	HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.5
M163T656_neg	163.0402	656	3							HMDB0000205	Phenylpyruvic acid	C9H8O3	1.0
M163T380_neg	163.0613	380	3							HMDB0000174	L-Fucose	C6H12O5	0.6
M164T688_neg	164.0354	688	3						Alkaloids	HMDB0003454	4-Pyridoxolactone	C8H7NO3	0.6
M165T589_neg	165.0194	589	3						Shikimates and Phenylpropanoids	HMDB0002107	Phthalic acid	C8H6O4	0.5
M166T293_neg	166.0371	293	3							HMDB0000401	2,8-Dihydroxyadenine	C5H5N5O2	0.5
M166T720_neg	166.0874	720	3							HMDB0000022	3-Methoxytyramine	C9H13NO2	0.5
M167T526_neg	167.0464	526	3							HMDB0013159	2,3-Diaminosalicylic acid	C7H8N2O3	1.0
M168T569_neg	168.0667	569	3							HMDB0000216	Norepinephrine	C8H11NO3	0.6
M169T517_neg	169.0143	517	3							HMDB0005807	Gallic acid	C7H6O5	0.2
M169T562_neg	169.0143	562	3							HMDB0005807	Gallic acid	C7H6O5	0.6
M169T365_neg	169.0368	365	3						Alkaloids				
M169T845_neg	169.0871	845	3							HMDB0030471	1,4-Ipomeadiol	C9H14O3	0.5
M169T947_neg	169.1599	947	3							HMDB0030941	Undecanal	C11H22O	0.4
M171T656_neg	171.0663	656	3						Fatty acids	HMDB0000341	2-Octenedioic acid	C8H12O4	0.4
M171T565_neg	171.1028	565	3							HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	0.5
M172T475_neg	172.0075	475	3							HMDB0258581	Sulfanilic acid	C6H7NO3S	0.5
M172T397_neg	172.0616	397	3							HMDB0006488	-Acetyl-L-glutamate 5-semialdehyd	C7H11NO4	0.6
M173T817_neg	173.1184	817	3						Fatty acids	HMDB0031513	\xc2\xb1)-3-Hydroxynonanoic acid	C9H18O3	0.4
M173T882_neg	173.1184	882	3							HMDB0031513	\xc2\xb1)-3-Hydroxynonanoic acid	C9H18O3	0.4
M174T652_neg	174.0561	652	3							HMDB0000197	Indoleacetic acid	C10H9NO2	0.5
M174T401_neg	174.0773	401	3							HMDB0002201	N-Carboxyethyl-g-aminobutyric acid	C7H13NO4	0.7
M175T86_neg	174.9561	86	3							HMDB0254641	Methylenediphosphonic acid	CH6O6P2	3.1
M176T444_neg	176.0387	444	3							HMDB0240544	N-Acetyl-S-methylcysteine	C6H11NO3S	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M158T632_neg	158.0824	632	3	2.34E-07	0.60	TRUE	4.15E-01	1.08	FALSE	9.28E-02	1.15	FALSE	5.81E-01	0.97	FALSE
M158T412_neg	158.0824	412	3	1.09E-04	0.81	FALSE	1.79E-04	1.23	FALSE	2.80E-32	1.96	TRUE	9.35E-01	1.01	FALSE
M159T447_neg	159.0122	447	3	7.15E-50	0.37	TRUE	8.56E-01	1.01	FALSE	1.62E-17	1.46	FALSE	1.36E-01	0.89	FALSE
M159T407_neg	159.0776	407	3	3.08E-02	1.14	FALSE	2.32E-01	1.08	FALSE	1.41E-18	1.70	TRUE	9.65E-01	1.00	FALSE
M159T118_neg	159.0776	118	3	5.63E-08	1.52	TRUE	5.69E-01	1.04	FALSE	1.43E-08	1.47	FALSE	1.59E-02	0.74	FALSE
M159T831_neg	159.1028	831	3	7.93E-03	1.13	FALSE	9.59E-01	1.00	FALSE	9.26E-01	1.00	FALSE	4.03E-08	2.52	TRUE
M160T422_neg	160.0405	422	3	2.91E-04	0.72	FALSE	3.51E-01	1.09	FALSE	1.79E-20	2.38	TRUE	5.67E-02	0.65	FALSE
M160T484_neg	160.0405	484	3	7.65E-01	1.03	FALSE	1.92E-01	0.88	FALSE	1.78E-10	1.80	TRUE	2.45E-01	0.82	FALSE
M162T409_neg	161.9868	409	3	3.31E-03	1.57	TRUE	5.19E-01	0.91	FALSE	4.66E-02	1.30	FALSE	5.34E-01	0.85	FALSE
M162T486_neg	162.0561	486	3	1.28E-01	0.91	FALSE	8.30E-01	0.99	FALSE	3.04E-23	1.91	TRUE	2.75E-03	0.68	FALSE
M163T656_neg	163.0402	656	3	1.03E-03	0.65	TRUE	1.53E-01	1.22	FALSE	3.73E-03	1.39	FALSE	8.38E-01	1.04	FALSE
M163T380_neg	163.0613	380	3	5.43E-01	0.95	FALSE	6.41E-01	1.04	FALSE	1.38E-11	1.71	TRUE	6.78E-01	1.08	FALSE
M164T688_neg	164.0354	688	3	1.98E-10	1.61	TRUE	1.26E-03	1.32	FALSE	3.14E-02	0.88	FALSE	6.72E-01	0.97	FALSE
M165T589_neg	165.0194	589	3	6.64E-12	0.63	TRUE	1.63E-01	1.10	FALSE	2.32E-04	1.23	FALSE	3.55E-02	1.21	FALSE
M166T293_neg	166.0371	293	3	7.91E-02	0.86	FALSE	3.37E-02	1.21	FALSE	4.40E-23	2.49	TRUE	2.39E-01	0.73	FALSE
M166T720_neg	166.0874	720	3	9.57E-11	0.74	FALSE	1.64E-02	1.12	FALSE	7.55E-24	1.56	TRUE	2.34E-01	0.92	FALSE
M167T526_neg	167.0464	526	3	1.43E-01	1.07	FALSE	2.19E-02	1.12	FALSE	2.34E-27	1.75	TRUE	1.78E-01	0.93	FALSE
M168T569_neg	168.0667	569	3	1.27E-07	0.55	TRUE	9.02E-01	0.99	FALSE	4.38E-04	1.39	FALSE	6.78E-01	1.05	FALSE
M169T517_neg	169.0143	517	3	7.99E-06	0.73	FALSE	1.46E-01	1.11	FALSE	4.39E-22	1.98	TRUE	5.63E-01	0.94	FALSE
M169T562_neg	169.0143	562	3	6.52E-05	1.74	TRUE	2.93E-01	1.16	FALSE	1.96E-02	1.32	FALSE	9.90E-01	1.00	FALSE
M169T365_neg	169.0368	365	3	1.57E-03	0.79	FALSE	3.59E-01	1.07	FALSE	1.34E-19	1.96	TRUE	6.13E-01	1.05	FALSE
M169T845_neg	169.0871	845	3	3.08E-15	2.19	TRUE	3.98E-01	0.93	FALSE	7.89E-01	1.02	FALSE	1.17E-01	0.84	FALSE
M169T947_neg	169.1599	947	3	5.62E-11	1.72	TRUE	7.95E-04	0.76	FALSE	5.02E-06	1.37	FALSE	7.64E-01	0.96	FALSE
M171T656_neg	171.0663	656	3	2.84E-02	0.90	FALSE	4.04E-01	1.04	FALSE	2.84E-22	1.60	TRUE	1.94E-01	0.85	FALSE
M171T565_neg	171.1028	565	3	4.88E-01	1.06	FALSE	4.88E-01	1.06	FALSE	4.40E-09	1.52	TRUE	2.84E-01	0.87	FALSE
M172T475_neg	172.0075	475	3	5.58E-04	0.73	FALSE	1.71E-01	1.13	FALSE	1.25E-13	1.91	TRUE	9.03E-01	0.98	FALSE
M172T397_neg	172.0616	397	3	6.07E-02	0.90	FALSE	1.19E-02	1.15	FALSE	2.17E-27	1.84	TRUE	1.50E-01	0.82	FALSE
M173T817_neg	173.1184	817	3	1.32E-05	1.15	FALSE	7.95E-01	1.01	FALSE	2.15E-02	0.94	FALSE	9.39E-10	15.54	TRUE
M173T882_neg	173.1184	882	3	9.52E-01	1.00	FALSE	3.27E-01	1.09	FALSE	3.78E-01	1.06	FALSE	6.76E-06	2.32	TRUE
M174T652_neg	174.0561	652	3	2.04E-03	0.25	TRUE	4.07E-01	1.42	FALSE	9.41E-01	1.03	FALSE	1.04E-01	0.77	FALSE
M174T401_neg	174.0773	401	3	3.97E-02	1.17	FALSE	3.49E-07	1.50	FALSE	7.22E-13	1.68	TRUE	1.12E-01	1.15	FALSE
M175T86_neg	174.9561	86	3	1.59E-05	0.52	TRUE	9.10E-01	0.98	FALSE	1.93E-01	1.17	FALSE	4.24E-01	1.15	FALSE
M176T444_neg	176.0387	444	3	6.53E-33	1.66	TRUE	2.61E-03	1.12	FALSE	7.85E-03	0.92	FALSE	6.33E-01	0.97	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M176T643_neg	176.0354	643	3						Alkaloids	HMDB0040612	4-Acetyl-2(3H)-benzoxazolone	C9H7NO3	0.4
M176T435_neg	176.0583	435	3							HMDB0247091	1H)-Pteridinone, 2-amino-6-meth	C7H7N5O	2.9
M177T422_neg	177.0228	422	3							HMDB0240388	ihydroxy-5-methylthio-4-pentenoi	C6H10O4S	0.7
M177T609_neg	177.0561	609	3							HMDB0002040	4-Methoxycinnamic acid	C10H10O3	2.0
M178T422_neg	178.0510	422	3							HMDB0000714	Hippuric acid	C9H9NO3	0.4
M179T433_neg	179.0456	433	3							HMDB0003269	Nicotinuric acid	C8H8N2O3	3.4
M179T427_neg	179.0827	427	3							HMDB0004076	5-Hydroxykynurenamine	C9H12N2O2	0.5
M181T297_neg	181.0177	297	3							HMDB0032825	Dipropyl trisulfide	C6H14S3	4.5
M181T406_neg	181.0368	406	3							HMDB0001970	3-Methyluric acid	C6H6N4O3	0.5
M181T659_neg	181.0871	659	3							HMDB0029456	Amyl 2-furoate	C10H14O3	0.4
M181T452_neg	181.0983	452	3							HMDB0244796	opyranosyloxy)-4-methyl-2H-1-be	C9H14N2O2	0.5
M182T478_neg	182.0459	478	3						Alkaloids	HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.4
M183T460_neg	183.0488	460	3							HMDB0032401	-3-[(2-methyl-3-furyl)thio]-2-butar	C9H12O2S	1.6
M183T611_neg	183.0778	611	3							HMDB0248870	Barbital	C8H12N2O3	1.3
M183T514_neg	183.0776	514	3							HMDB0248870	Barbital	C8H12N2O3	0.6
M183T696_neg	183.1027	696	3						Fatty acids	HMDB0036117	(-)-3-Thujene	C10H16O3	0.3
M185T185_neg	185.0456	185	3							HMDB0041026	Erinapyrone C	C8H10O5	0.2
M185T512_neg	185.0456	512	3							HMDB0041026	Erinapyrone C	C8H10O5	0.4
M187T506_neg	187.0612	506	3							HMDB0059767	Tetrahydro-2,5-furan-diacetic acid	C8H12O5	0.3
M187T189_neg	187.0725	189	3							HMDB0006029	N-Acetylglutamine	C7H12N2O4	0.2
M187T454_neg	187.1089	454	3						Amino acids and Peptides	HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.3
M187T386_neg	187.1088	386	3							HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.1
M187T850_neg	187.1340	850	3							HMDB0002203	3-Hydroxycapric acid	C10H20O3	0.2
M188T484_neg	188.0356	484	3							HMDB0000715	Kynurenic acid	C10H7NO3	1.3
M188T685_neg	188.0354	685	3							HMDB0000715	Kynurenic acid	C10H7NO3	0.3
M188T508_neg	188.0574	508	3							HMDB0031574	sothiocyanato-6-(methylthio)hexa	C8H15NS2	0.5
M188T438_neg	188.1121	438	3							HMDB0251894	S-Ethyl dipropylthiocarbamate	C9H19NOS	3.3
M189T365_neg	189.0308	365	3							HMDB0015491	Nitroxoline	C9H6N2O3	1.2
M189T610_neg	189.0769	610	3							HMDB0000325	3-Hydroxysuberic acid	C8H14O5	0.2
M190T542_neg	190.0180	542	3							HMDB0244750	Thiazolidinedicarboxylic acid, 2-me	C6H9NO4S	0.4
M191T241_neg	191.0197	241	3							HMDB0000094	Citric acid	C6H8O7	0.0
M192T657_neg	192.0664	657	3							HMDB0000821	Phenylacetylglycine	C10H11NO3	1.2
M192T389_neg	192.0778	389	3							HMDB0062376	trosoamino)-1-(3-pyridinyl)-1-buta	C9H11N3O2	0.1
M193T566_neg	193.0359	566	3							HMDB0000127	D-Glucuronic acid	C6H10O7	2.7
M193T124_neg	193.0354	124	3						Carbohydrates	HMDB0000127	D-Glucuronic acid	C6H10O7	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M176T643_neg	176.0354	643	3	4.07E-01	1.09	FALSE	9.93E-01	1.00	FALSE	7.13E-07	1.62	TRUE	7.59E-01	1.08	FALSE
M176T435_neg	176.0583	435	3	9.77E-02	1.12	FALSE	9.35E-01	1.01	FALSE	4.99E-30	2.30	TRUE	3.71E-01	0.87	FALSE
M177T422_neg	177.0228	422	3	1.97E-02	0.85	FALSE	7.85E-01	1.02	FALSE	1.02E-13	1.62	TRUE	3.51E-01	0.89	FALSE
M177T609_neg	177.0561	609	3	2.19E-07	0.74	FALSE	8.18E-03	1.16	FALSE	3.46E-24	1.78	TRUE	6.75E-01	1.04	FALSE
M178T422_neg	178.0510	422	3	7.31E-05	0.73	FALSE	4.81E-01	1.06	FALSE	2.72E-25	2.32	TRUE	9.49E-02	0.73	FALSE
M179T433_neg	179.0456	433	3	5.23E-01	0.94	FALSE	8.65E-01	0.98	FALSE	1.10E-08	1.75	TRUE	5.75E-01	0.93	FALSE
M179T427_neg	179.0827	427	3	4.04E-03	0.80	FALSE	9.37E-01	1.01	FALSE	4.37E-16	1.85	TRUE	3.68E-01	0.89	FALSE
M181T297_neg	181.0177	297	3	5.31E-01	1.21	FALSE	4.39E-01	1.26	FALSE	2.09E-03	2.43	TRUE	1.70E-01	0.45	FALSE
M181T406_neg	181.0368	406	3	5.06E-02	0.58	FALSE	2.22E-01	1.40	FALSE	1.49E-02	1.81	TRUE	7.42E-01	1.10	FALSE
M181T659_neg	181.0871	659	3	8.74E-01	1.01	FALSE	2.50E-02	1.10	FALSE	1.30E-27	1.56	TRUE	2.24E-01	0.93	FALSE
M181T452_neg	181.0983	452	3	2.63E-01	0.94	FALSE	1.08E-01	1.09	FALSE	1.35E-18	1.59	TRUE	8.74E-01	1.02	FALSE
M182T478_neg	182.0459	478	3	6.84E-01	1.02	FALSE	4.25E-01	1.05	FALSE	4.40E-21	1.76	TRUE	5.32E-01	0.89	FALSE
M183T460_neg	183.0488	460	3	1.66E-01	0.89	FALSE	4.59E-01	1.07	FALSE	1.07E-12	1.78	TRUE	5.60E-01	1.09	FALSE
M183T611_neg	183.0778	611	3	6.18E-01	1.05	FALSE	7.86E-02	1.20	FALSE	3.28E-07	1.62	TRUE	6.09E-01	0.89	FALSE
M183T514_neg	183.0776	514	3	1.14E-01	1.08	FALSE	1.10E-01	1.08	FALSE	2.90E-20	1.52	TRUE	1.88E-01	0.93	FALSE
M183T696_neg	183.1027	696	3	1.15E-02	1.56	TRUE	5.98E-01	0.90	FALSE	1.26E-01	0.79	FALSE	3.50E-01	0.85	FALSE
M185T185_neg	185.0456	185	3	2.09E-01	1.08	FALSE	5.12E-01	0.96	FALSE	1.74E-13	1.54	TRUE	4.24E-01	0.90	FALSE
M185T512_neg	185.0456	512	3	5.68E-16	0.61	TRUE	4.64E-03	1.17	FALSE	2.07E-09	1.35	FALSE	1.10E-01	0.83	FALSE
M187T506_neg	187.0612	506	3	9.28E-03	0.87	FALSE	6.41E-02	1.11	FALSE	6.34E-19	1.59	TRUE	8.88E-01	1.01	FALSE
M187T189_neg	187.0725	189	3	2.44E-01	0.95	FALSE	1.50E-02	1.12	FALSE	1.43E-22	1.53	TRUE	3.85E-01	0.93	FALSE
M187T454_neg	187.1089	454	3	8.44E-44	0.15	TRUE	3.37E-01	1.09	FALSE	6.32E-05	1.34	FALSE	5.32E-02	0.66	FALSE
M187T386_neg	187.1088	386	3	8.89E-31	0.25	TRUE	2.96E-01	1.10	FALSE	5.90E-04	1.30	FALSE	5.95E-01	1.11	FALSE
M187T850_neg	187.1340	850	3	1.45E-01	1.18	FALSE	8.91E-01	0.98	FALSE	3.90E-01	0.92	FALSE	7.70E-05	3.34	TRUE
M188T484_neg	188.0356	484	3	1.82E-03	0.80	FALSE	6.33E-01	0.96	FALSE	1.32E-25	2.20	TRUE	1.00E-01	0.80	FALSE
M188T685_neg	188.0354	685	3	5.41E-02	1.22	FALSE	9.90E-03	0.73	FALSE	5.76E-10	1.84	TRUE	4.27E-01	1.17	FALSE
M188T508_neg	188.0574	508	3	2.27E-26	0.35	TRUE	6.53E-02	1.16	FALSE	1.84E-03	1.24	FALSE	8.61E-01	0.95	FALSE
M188T438_neg	188.1121	438	3	4.70E-29	0.36	TRUE	3.38E-01	1.07	FALSE	1.61E-03	1.22	FALSE	9.68E-01	1.01	FALSE
M189T365_neg	189.0308	365	3	1.47E-02	1.11	FALSE	1.61E-01	1.06	FALSE	1.28E-34	1.76	TRUE	5.92E-01	1.04	FALSE
M189T610_neg	189.0769	610	3	2.97E-09	0.71	FALSE	1.65E-01	1.08	FALSE	1.23E-23	1.76	TRUE	5.41E-02	0.82	FALSE
M190T542_neg	190.0180	542	3	5.09E-01	1.08	FALSE	6.07E-01	0.94	FALSE	5.87E-09	1.89	TRUE	4.06E-01	0.85	FALSE
M191T241_neg	191.0197	241	3	9.19E-23	0.16	TRUE	9.50E-01	1.01	FALSE	6.19E-03	1.37	FALSE	4.21E-01	0.85	FALSE
M192T657_neg	192.0664	657	3	7.13E-21	0.37	TRUE	4.13E-01	1.08	FALSE	2.78E-04	1.33	FALSE	6.59E-01	0.97	FALSE
M192T389_neg	192.0778	389	3	5.15E-01	0.96	FALSE	4.54E-01	1.05	FALSE	5.35E-15	1.66	TRUE	8.48E-02	0.79	FALSE
M193T566_neg	193.0359	566	3	6.77E-01	0.96	FALSE	3.93E-02	1.25	FALSE	7.29E-15	2.24	TRUE	7.34E-01	1.05	FALSE
M193T124_neg	193.0354	124	3	5.54E-21	0.16	TRUE	2.23E-01	1.19	FALSE	1.18E-02	1.36	FALSE	7.45E-01	1.08	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M193T711_neg	193.0507	711	3							HMDB0000954	Ferulic acid	C10H10O4	0.4
M193T519_neg	193.0610	519	3							HMDB0001867	4-Aminohippuric acid	C9H10N2O3	4.5
M193T941_neg	193.0903	941	3							HMDB0243978	1-Octanesulfonic acid	C8H18O3S	0.6
M194T410_neg	194.0683	410	3							HMDB0247221	7-(2-Hydroxyethyl)guanine	C7H9N5O2	0.0
M194T365_neg	194.0824	365	3							HMDB0014903	Metyrosine	C10H13NO3	0.5
M194T414_neg	194.0936	414	3							HMDB0062443	(Nitrosoamino)propyl]-3-pyridiner	C9H13N3O2	0.3
M195T442_1_neg	195.0278	442	3							HMDB0247453	8-Nitroguanine	C5H4N6O3	2.9
M195T479_neg	195.0523	479	3							HMDB0001857	1,3-Dimethyluric acid	C7H8N4O3	0.1
M195T675_neg	195.0663	675	3						Shikimates and Phenylpropanoids	HMDB0000434	Homoveratric acid	C10H12O4	0.2
M195T365_neg	195.0854	365	3							HMDB0040241	1-(2-Thienyl)-1-heptanone	C11H16OS	2.4
M195T629_neg	195.1027	629	3							HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	0.4
M195T915_neg	195.1391	915	3							HMDB0030867	ihydro-5-(2-octenyl)-2(3H)-furanor	C12H20O2	0.2
M196T554_neg	196.0616	554	3							HMDB0000181	L-Dopa	C9H11NO4	0.4
M196T378_neg	196.0727	378	3							HMDB0032055	N-Acetylhistidine	C8H11N3O3	0.2
M197T457_neg	197.0093	457	3							HMDB0304184	4-maleyl-acetoacetate	C8H6O6	4.8
M197T484_neg	197.0567	484	3							HMDB0015188	Mimosine	C8H10N2O4	0.4
M199T465_neg	199.0079	465	3							HMDB0062775	4-Vinylphenol sulfate	C8H8O4S	4.1
M200T566_neg	200.0387	566	3							HMDB0256227	Penicillanic acid	C8H11NO3S	0.3
M201T543_neg	201.0769	543	3							HMDB0032306	Diethyl oxalpropionate	C9H14O5	0.3
M201T528_neg	201.1244	528	3						Amino acids and Peptides	HMDB0028690	Alanylisoleucine	C9H18N2O3	0.3
M201T387_neg	201.1246	387	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.5
M201T959_neg	201.1497	959	3							HMDB0032443	3-Hydroxynonyl acetate	C11H22O3	0.3
M202T513_neg	202.0179	513	3							HMDB0002015	Cystathionine ketimine	C7H9NO4S	0.2
M202T352_neg	202.0721	352	3							HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	0.1
M202T250_neg	202.0721	250	3							HMDB0062715	N-acetyl-L-2-aminoadipate(2-)	C8H13NO5	0.2
M202T690_neg	202.1089	690	3							HMDB0062176	N-Lactoylleucine	C9H17NO4	2.2
M203T379_neg	203.0562	379	3							HMDB0041031	-5-(hydroxymethyl)-2-methoxy-2-c	C8H12O6	0.4
M203T568_neg	203.0925	568	3						Alkaloids	HMDB0303910	2-Hydroxyglutaric acid diethyl este	C9H16O5	0.0
M203T369_neg	203.1040	369	3							HMDB0029052	Serylvaline	C8H16N2O4	1.1
M203T248_neg	203.1038	248	3							HMDB0029052	Serylvaline	C8H16N2O4	0.1
M204T661_neg	204.0304	661	3							HMDB0000881	Xanthurenic acid	C10H7NO4	0.8
M204T599_neg	204.0305	599	3							HMDB0000881	Xanthurenic acid	C10H7NO4	1.2
M204T520_neg	204.0305	520	3							HMDB0000881	Xanthurenic acid	C10H7NO4	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M193T711_neg	193.0507	711	3	8.99E-11	0.71	FALSE	1.09E-01	1.09	FALSE	2.25E-26	1.74	TRUE	9.54E-01	1.00	FALSE
M193T519_neg	193.0610	519	3	4.04E-03	2.07	TRUE	8.62E-01	0.95	FALSE	1.43E-01	1.36	FALSE	3.30E-01	1.41	FALSE
M193T941_neg	193.0903	941	3	2.94E-01	1.10	FALSE	2.08E-01	0.89	FALSE	3.76E-01	1.08	FALSE	3.90E-06	2.63	TRUE
M194T410_neg	194.0683	410	3	5.83E-01	0.94	FALSE	2.10E-01	1.15	FALSE	1.91E-05	1.56	TRUE	2.20E-01	1.24	FALSE
M194T365_neg	194.0824	365	3	9.27E-01	1.01	FALSE	8.27E-01	1.02	FALSE	6.05E-16	1.70	TRUE	1.42E-01	0.81	FALSE
M194T414_neg	194.0936	414	3	9.76E-01	1.00	FALSE	8.07E-01	0.98	FALSE	9.46E-08	1.54	TRUE	8.51E-01	0.97	FALSE
M195T442_1_neg	195.0278	442	3	2.31E-04	0.78	FALSE	3.81E-01	1.06	FALSE	3.14E-11	1.51	TRUE	4.67E-01	1.15	FALSE
M195T479_neg	195.0523	479	3	4.37E-01	0.95	FALSE	4.09E-03	1.21	FALSE	7.94E-20	1.81	TRUE	5.86E-01	1.03	FALSE
M195T675_neg	195.0663	675	3	6.45E-01	1.11	FALSE	1.04E-02	0.50	TRUE	4.68E-01	1.15	FALSE	9.75E-01	1.00	FALSE
M195T365_neg	195.0854	365	3	9.46E-01	1.00	FALSE	6.76E-01	1.03	FALSE	1.02E-14	1.70	TRUE	2.10E-01	0.83	FALSE
M195T629_neg	195.1027	629	3	2.60E-02	1.19	FALSE	4.68E-01	1.06	FALSE	9.43E-18	1.94	TRUE	3.24E-01	0.94	FALSE
M195T915_neg	195.1391	915	3	6.75E-01	1.04	FALSE	2.60E-01	1.11	FALSE	5.04E-05	0.74	FALSE	1.36E-02	1.87	TRUE
M196T554_neg	196.0616	554	3	4.25E-02	1.17	FALSE	4.22E-01	1.06	FALSE	1.33E-09	1.53	TRUE	6.21E-01	0.92	FALSE
M196T378_neg	196.0727	378	3	3.37E-03	0.85	FALSE	6.86E-01	1.02	FALSE	5.76E-22	1.71	TRUE	1.22E-01	0.91	FALSE
M197T457_neg	197.0093	457	3	5.13E-07	0.31	TRUE	7.33E-01	1.08	FALSE	7.74E-02	1.37	FALSE	2.57E-01	0.85	FALSE
M197T484_neg	197.0567	484	3	1.41E-01	0.93	FALSE	3.70E-03	1.17	FALSE	2.60E-26	1.76	TRUE	7.23E-01	1.03	FALSE
M199T465_neg	199.0079	465	3	2.11E-01	0.91	FALSE	9.58E-01	1.00	FALSE	3.08E-14	1.75	TRUE	1.18E-01	0.72	FALSE
M200T566_neg	200.0387	566	3	1.22E-02	1.40	FALSE	4.79E-01	1.10	FALSE	4.93E-05	1.63	TRUE	4.69E-01	1.15	FALSE
M201T543_neg	201.0769	543	3	2.61E-05	0.74	FALSE	6.71E-02	1.14	FALSE	6.73E-20	1.87	TRUE	8.81E-02	0.82	FALSE
M201T528_neg	201.1244	528	3	2.51E-14	0.26	TRUE	7.12E-01	1.06	FALSE	2.43E-03	1.47	FALSE	3.76E-01	0.86	FALSE
M201T387_neg	201.1246	387	3	1.12E-05	0.63	TRUE	5.78E-01	1.06	FALSE	3.98E-04	1.37	FALSE	1.13E-01	0.79	FALSE
M201T959_neg	201.1497	959	3	9.37E-05	1.54	TRUE	5.83E-02	0.82	FALSE	4.79E-02	1.20	FALSE	3.97E-02	1.29	FALSE
M202T513_neg	202.0179	513	3	8.65E-01	1.02	FALSE	9.12E-01	1.01	FALSE	1.97E-07	1.57	TRUE	2.85E-01	0.85	FALSE
M202T352_neg	202.0721	352	3	9.89E-01	1.00	FALSE	6.16E-01	1.04	FALSE	4.35E-12	1.63	TRUE	3.77E-01	0.87	FALSE
M202T250_neg	202.0721	250	3	8.10E-01	1.03	FALSE	5.34E-01	0.93	FALSE	1.28E-07	1.69	TRUE	9.81E-01	1.00	FALSE
M202T690_neg	202.1089	690	3	2.86E-31	0.27	TRUE	9.25E-02	1.16	FALSE	4.77E-07	1.46	FALSE	3.62E-01	0.79	FALSE
M203T379_neg	203.0562	379	3	1.61E-09	0.76	FALSE	5.07E-01	1.03	FALSE	1.67E-25	1.60	TRUE	4.69E-01	0.93	FALSE
M203T568_neg	203.0925	568	3	4.34E-02	0.89	FALSE	8.34E-02	1.11	FALSE	9.16E-19	1.65	TRUE	7.26E-01	0.93	FALSE
M203T369_neg	203.1040	369	3	1.11E-07	0.67	FALSE	7.66E-01	0.98	FALSE	1.09E-15	1.76	TRUE	3.76E-01	0.87	FALSE
M203T248_neg	203.1038	248	3	1.78E-26	0.25	TRUE	4.16E-01	1.09	FALSE	1.58E-03	1.31	FALSE	4.22E-01	1.07	FALSE
M204T661_neg	204.0304	661	3	6.96E-01	0.94	FALSE	6.25E-01	1.08	FALSE	1.34E-05	1.82	TRUE	1.16E-01	0.58	FALSE
M204T599_neg	204.0305	599	3	2.28E-03	0.71	FALSE	5.79E-01	1.07	FALSE	4.84E-11	1.98	TRUE	5.25E-01	1.12	FALSE
M204T520_neg	204.0305	520	3	2.29E-01	0.94	FALSE	1.11E-01	1.08	FALSE	2.16E-36	1.95	TRUE	8.39E-01	0.99	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M204T422_neg	204.0312	422	3							HMDB0000881	Xanthurenic acid	C10H7NO4	4.8
M204T380_neg	204.0878	380	3							HMDB0036394	N-Methylcalystegine C1	C8H15NO5	0.4
M205T672_neg	205.0539	672	3							HMDB0245244	3-Mercaptopropyl)pentanedioic a	C8H14O4S	0.5
M205T1010_neg	205.1599	1010	3							HMDB0013816	2,4-Di-tert-butylphenol	C14H22O	0.4
M207T374_neg	206.9970	374	3							HMDB0032653	thylsulfinyl)-1-propenyl] 2-propen	C7H12OS3	3.8
M207T422_neg	206.9969	422	3							HMDB0032653	thylsulfinyl)-1-propenyl] 2-propen	C7H12OS3	4.1
M207T692_neg	207.0122	692	3							HMDB0243955	1-Naphthalenesulfonic acid	C10H8O3S	0.3
M207T414_neg	207.0873	414	3							HMDB0029968	Ethyl beta-D-glucopyranoside	C8H16O6	0.5
M208T417_neg	208.0979	417	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.0
M208T823_neg	208.0980	823	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.2
M209T717_neg	209.0456	717	3							HMDB0011714	Vanilpyruvic acid	C10H10O5	0.1
M209T417_1_neg	209.0460	417	3							HMDB0011714	Vanilpyruvic acid	C10H10O5	2.1
M209T434_neg	209.0568	434	3							HMDB0031813	oyl-2-amino-2-(4-hydroxyphenyl)a	C9H10N2O4	0.2
M209T923_neg	209.1184	923	3							HMDB0032797	Jasmonic acid	C12H18O3	0.2
M210T400_neg	210.0875	400	3							HMDB0015078	Zalcitabine	C9H13N3O3	4.5
M211T743_neg	211.0977	743	3							HMDB0059744	3,4-Methyleneazelaic acid	C11H16O4	0.3
M212T740_neg	212.1293	740	3							HMDB0094807	2-nonenoylglycine	C11H19NO3	0.5
M213T348_neg	213.1245	348	3							HMDB0003581	Dethiobiotin	C10H18N2O3	0.4
M213T944_neg	213.1496	944	3							HMDB0010727	3-Oxododecanoic acid	C12H22O3	0.1
M214T491_neg	214.0722	491	3							HMDB0255166	N-Methacryloyl-L-glutamic acid	C9H13NO5	0.7
M214T172_neg	214.0833	172	3							HMDB0242267	yl-2-[(E)-hydroxyimino]-5-nitro-3-h	C8H13N3O4	0.3
M215T556_neg	215.0828	556	3							HMDB0035665	Tetrahydro-beta-carboline-3-carbo	C12H12N2O2	1.1
M215T637_neg	215.0925	637	3							HMDB0301824	Isoketocamphoric acid	C10H16O5	0.1
M216T596_neg	216.0336	596	3							HMDB0006409	Tyramine-O-sulfate	C8H11NO4S	0.0
M217T805_neg	217.0503	805	3							HMDB0029518	Liqcoumarin	C12H10O4	1.3
M217T500_neg	217.0913	500	3							HMDB0037764	2-(Acetyloxy)ethyl]butyl] ethaneth	C10H18O3S	4.3
M218T519_neg	218.0491	519	3							HMDB0242184	N-Acetylalliin	C8H13NO4S	0.6
M220T489_neg	220.0977	489	3							HMDB0249479	Butylone	C12H15NO3	0.9
M220T539_neg	220.0980	539	3							HMDB0014798	Metaxalone	C12H15NO3	0.2
M221T442_neg	221.0491	442	3							HMDB0033041	1-Propenylthio)propyl propyl disul	C9H18S3	2.9
M221T915_neg	221.1547	915	3							HMDB0035593	Rishitin	C14H22O2	0.1
M221T988_neg	221.1547	988	3							HMDB0035593	Rishitin	C14H22O2	0.2
M223T629_neg	223.0717	629	3							HMDB0000732	Hydroxykynurenine	C10H12N2O4	3.1
M223T555_neg	223.1088	555	3							HMDB0014386	Butalbital	C11H16N2O3	0.0
M224T374_neg	224.0565	374	3							HMDB0037264	4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M204T422_neg	204.0312	422	3	1.13E-05	0.69	FALSE	2.32E-02	1.22	FALSE	8.56E-22	2.26	TRUE	9.15E-01	0.98	FALSE
M204T380_neg	204.0878	380	3	1.47E-02	1.18	FALSE	1.08E-01	1.12	FALSE	3.33E-13	1.59	TRUE	1.85E-01	1.17	FALSE
M205T672_neg	205.0539	672	3	6.22E-11	0.69	FALSE	2.77E-05	1.26	FALSE	1.33E-24	1.73	TRUE	9.12E-01	1.01	FALSE
M205T1010_neg	205.1599	1010	3	8.29E-05	0.71	FALSE	3.71E-03	1.30	FALSE	2.01E-09	0.62	TRUE	9.46E-01	0.99	FALSE
M207T374_neg	206.9970	374	3	5.13E-01	0.94	FALSE	2.72E-02	1.22	FALSE	3.06E-09	1.62	TRUE	1.29E-01	1.20	FALSE
M207T422_neg	206.9969	422	3	3.26E-60	0.07	TRUE	5.78E-01	1.04	FALSE	3.84E-02	1.14	FALSE	6.04E-02	0.63	FALSE
M207T692_neg	207.0122	692	3	1.90E-02	1.26	FALSE	7.14E-01	1.04	FALSE	1.57E-07	1.59	TRUE	9.77E-02	0.63	FALSE
M207T414_neg	207.0873	414	3	1.94E-03	1.72	TRUE	4.13E-02	0.69	FALSE	2.54E-01	1.18	FALSE	1.65E-01	0.24	FALSE
M208T417_neg	208.0979	417	3	9.52E-13	2.32	TRUE	9.92E-01	1.00	FALSE	8.26E-02	0.85	FALSE	3.54E-01	1.17	FALSE
M208T823_neg	208.0980	823	3	9.06E-13	0.11	TRUE	9.38E-01	1.02	FALSE	9.91E-02	1.36	FALSE	9.21E-01	1.03	FALSE
M209T717_neg	209.0456	717	3	8.42E-09	0.72	FALSE	3.92E-02	1.13	FALSE	7.49E-33	2.07	TRUE	7.87E-01	1.02	FALSE
M209T417_1_neg	209.0460	417	3	8.56E-01	0.97	FALSE	7.09E-01	1.06	FALSE	1.07E-04	1.67	TRUE	5.89E-01	0.80	FALSE
M209T434_neg	209.0568	434	3	3.98E-02	0.85	FALSE	2.35E-02	1.20	FALSE	2.52E-22	2.16	TRUE	1.87E-01	1.10	FALSE
M209T923_neg	209.1184	923	3	1.08E-03	0.65	TRUE	5.54E-01	1.08	FALSE	3.94E-02	1.26	FALSE	6.38E-01	0.90	FALSE
M210T400_neg	210.0875	400	3	1.48E-02	1.29	FALSE	7.00E-01	1.04	FALSE	2.29E-01	1.11	FALSE	2.33E-02	0.61	TRUE
M211T743_neg	211.0977	743	3	8.65E-07	1.44	FALSE	3.86E-07	1.46	FALSE	1.03E-18	1.88	TRUE	8.25E-02	1.16	FALSE
M212T740_neg	212.1293	740	3	1.51E-01	2.74	FALSE	1.86E-03	-11.78	FALSE	1.37E-02	0.18	TRUE	7.47E-01	0.90	FALSE
M213T348_neg	213.1245	348	3	5.33E-23	0.46	TRUE	9.90E-01	1.00	FALSE	3.36E-08	1.39	FALSE	1.10E-01	0.86	FALSE
M213T944_neg	213.1496	944	3	5.53E-07	1.42	FALSE	7.16E-02	0.88	FALSE	2.20E-01	1.07	FALSE	1.22E-02	1.66	TRUE
M214T491_neg	214.0722	491	3	7.90E-02	0.90	FALSE	1.53E-04	1.26	FALSE	6.98E-18	1.62	TRUE	9.17E-03	1.31	FALSE
M214T172_neg	214.0833	172	3	8.35E-01	1.02	FALSE	4.02E-01	0.92	FALSE	1.25E-07	1.62	TRUE	5.69E-02	0.62	FALSE
M215T556_neg	215.0828	556	3	2.27E-03	0.83	FALSE	1.41E-01	1.09	FALSE	4.93E-29	2.03	TRUE	1.61E-01	0.92	FALSE
M215T637_neg	215.0925	637	3	3.23E-03	0.89	FALSE	3.13E-02	1.09	FALSE	9.21E-32	1.66	TRUE	6.76E-01	0.98	FALSE
M216T596_neg	216.0336	596	3	9.89E-03	1.15	FALSE	2.35E-01	1.07	FALSE	3.47E-15	1.52	TRUE	1.76E-01	0.92	FALSE
M217T805_neg	217.0503	805	3	5.50E-07	0.62	TRUE	2.12E-02	1.25	FALSE	2.76E-02	1.19	FALSE	7.05E-01	1.05	FALSE
M217T500_neg	217.0913	500	3	8.86E-01	1.01	FALSE	8.24E-02	1.14	FALSE	1.31E-11	1.60	TRUE	4.45E-01	1.09	FALSE
M218T519_neg	218.0491	519	3	3.61E-01	0.91	FALSE	4.23E-02	1.25	FALSE	3.04E-09	1.78	TRUE	8.13E-01	0.96	FALSE
M220T489_neg	220.0977	489	3	9.48E-03	0.53	TRUE	9.32E-01	1.02	FALSE	7.03E-01	0.93	FALSE	2.07E-01	0.40	FALSE
M220T539_neg	220.0980	539	3	1.34E-01	1.09	FALSE	3.77E-13	1.56	TRUE	5.02E-06	1.27	FALSE	1.90E-02	1.19	FALSE
M221T442_neg	221.0491	442	3	3.62E-01	1.08	FALSE	7.57E-01	1.03	FALSE	1.90E-18	2.07	TRUE	9.63E-01	0.99	FALSE
M221T915_neg	221.1547	915	3	3.35E-01	0.93	FALSE	4.47E-01	1.06	FALSE	2.09E-10	1.59	TRUE	3.72E-01	0.87	FALSE
M221T988_neg	221.1547	988	3	3.61E-03	0.88	FALSE	2.58E-01	1.05	FALSE	3.73E-01	1.03	FALSE	4.23E-03	0.65	TRUE
M223T629_neg	223.0717	629	3	7.19E-01	0.95	FALSE	9.89E-01	1.00	FALSE	1.41E-05	1.85	TRUE	6.36E-01	1.19	FALSE
M223T555_neg	223.1088	555	3	5.10E-13	0.12	TRUE	7.84E-01	1.06	FALSE	2.84E-02	1.48	FALSE	9.01E-01	0.98	FALSE
M224T374_neg	224.0565	374	3	3.91E-01	0.92	FALSE	8.77E-04	1.40	FALSE	1.99E-07	1.59	TRUE	6.46E-01	1.12	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M224T825_neg	224.0931	825	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	1.1
M224T674_neg	224.0929	674	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.4
M225T561_neg	225.0440	561	3							HMDB0254851	Monochlorobimane	C10H11ClN2O2	1.6
M225T684_neg	225.1133	684	3							HMDB0040705	Allixin	C12H18O4	0.2
M225T1045_neg	225.1860	1045	3							HMDB0000499	5-Tetradecenoic acid	C14H26O2	0.0
M225T1063_neg	225.2224	1063	3							HMDB0031078	Pentadecanal	C15H30O	0.0
M226T563_neg	226.0446	563	3						Alkaloids				
M226T348_neg	226.0722	348	3							HMDB0304809	Pretyrosine	C10H13NO5	0.5
M227T523_neg	227.1037	523	3						Amino acids and Peptides	HMDB0006695	Prolylhydroxyproline	C10H16N2O4	0.1
M228T738_neg	228.1243	738	3							HMDB0013126	Butenylcarnitine	C11H19NO4	0.6
M228T497_neg	228.1242	497	3							HMDB0013126	Butenylcarnitine	C11H19NO4	0.3
M228T827_neg	228.1605	827	3						Fatty acids	HMDB0013267	N-Decanoylglycine	C12H23NO3	0.0
M229T87_neg	228.9666	87	3							HMDB0246068	3,5-Dinitrobenzoyl chloride	C7H3ClN2O5	3.5
M229T439_neg	229.0718	439	3							HMDB0246021	lactitol, 1,2:5,6-dianhydro-, diacet	C10H14O6	0.2
M229T574_neg	229.0983	574	3						Amino acids and Peptides	HMDB0037942	etrahydro-1-methyl-beta-carboline	C13H14N2O2	0.2
M230T264_neg	230.1146	264	3						Amino acids and Peptides	HMDB0028744	Asparaginyl-Valine	C9H17N3O4	0.0
M231T708_neg	231.1238	708	3							HMDB0304007	1,2-dibutyrin	C11H20O5	0.0
M231T442_neg	231.1351	442	3						Amino acids and Peptides	HMDB0013075	Spermic acid 2	C10H20N2O4	0.3
M231T355_neg	231.1351	355	3						Amino acids and Peptides	HMDB0013075	Spermic acid 2	C10H20N2O4	0.4
M232T381_neg	232.0738	381	3							HMDB0246289	idin-2-yl-[1,2,4]oxadiazol-5-yl)-but	C11H11N3O3	4.6
M232T344_neg	232.1191	344	3							HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	0.3
M233T484_neg	232.9762	484	3							HMDB0124993	Protocatechuic acid 3-O-sulfate	C7H6O7S	0.2
M233T576_neg	233.1031	576	3							HMDB0260291	4-Carboxybutylperoxy)pentanoic a	C10H18O6	0.0
M233T509_neg	233.1030	509	3							HMDB0260291	4-Carboxybutylperoxy)pentanoic a	C10H18O6	0.2
M235T654_neg	235.0361	654	3							HMDB0033350	Brassinin	C11H12N2S2	3.6
M235T500_neg	235.1090	500	3							HMDB0015444	Hexobarbital	C12H16N2O3	0.7
M236T389_neg	236.0672	389	3						Amino acids and Peptides				
M236T481_neg	236.0565	481	3							HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	0.3
M236T458_neg	236.0928	458	3						Amino acids and Peptides	HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.0
M236T400_neg	236.1292	400	3							HMDB0259807	viloxazine	C13H19NO3	0.1
M237T624_neg	237.0435	624	3							HMDB0030400	L-4-Chlorotryptophan	C11H11ClN2O2	0.3
M237T520_neg	237.0522	520	3							HMDB0256529	Picartamide	C11H14N2S2	1.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M224T825_neg	224.0931	825	3	7.69E-12	0.66	TRUE	1.37E-01	1.09	FALSE	1.56E-11	1.42	FALSE	1.62E-02	0.86	FALSE
M224T674_neg	224.0929	674	3	4.41E-03	1.28	FALSE	3.51E-01	1.09	FALSE	1.00E-09	1.63	TRUE	7.75E-01	0.94	FALSE
M225T561_neg	225.0440	561	3	2.91E-01	0.90	FALSE	2.54E-01	1.13	FALSE	3.03E-11	1.93	TRUE	1.84E-01	1.18	FALSE
M225T684_neg	225.1133	684	3	1.03E-16	1.54	TRUE	3.94E-01	0.96	FALSE	4.92E-01	1.03	FALSE	8.96E-01	0.99	FALSE
M225T1045_neg	225.1860	1045	3	1.37E-03	0.71	FALSE	2.43E-01	0.88	FALSE	4.71E-02	1.20	FALSE	1.16E-02	1.69	TRUE
M225T1063_neg	225.2224	1063	3	3.93E-02	1.86	TRUE	6.12E-02	0.59	FALSE	7.80E-01	0.93	FALSE	9.04E-01	0.96	FALSE
M226T563_neg	226.0446	563	3	1.74E-01	1.19	FALSE	3.71E-01	1.14	FALSE	3.68E-04	1.52	TRUE	9.23E-01	0.92	FALSE
M226T348_neg	226.0722	348	3	5.61E-01	1.03	FALSE	1.03E-02	1.16	FALSE	6.07E-23	1.72	TRUE	9.70E-01	1.00	FALSE
M227T523_neg	227.1037	523	3	7.90E-04	0.60	TRUE	4.23E-01	1.13	FALSE	5.78E-01	1.07	FALSE	1.45E-01	1.55	FALSE
M228T738_neg	228.1243	738	3	4.20E-02	1.41	FALSE	9.21E-05	2.08	TRUE	2.28E-01	1.19	FALSE	7.79E-01	1.06	FALSE
M228T497_neg	228.1242	497	3	4.54E-06	0.74	FALSE	4.43E-01	1.05	FALSE	3.74E-16	1.66	TRUE	8.70E-01	0.98	FALSE
M228T827_neg	228.1605	827	3	1.23E-01	1.98	FALSE	4.89E-01	1.33	FALSE	7.48E-02	0.50	FALSE	1.80E-04	2.78	TRUE
M229T87_neg	228.9666	87	3	3.89E-01	0.92	FALSE	6.36E-01	1.05	FALSE	3.33E-01	0.92	FALSE	1.72E-02	3.12	TRUE
M229T439_neg	229.0718	439	3	5.81E-01	1.03	FALSE	5.64E-01	1.03	FALSE	8.88E-17	1.57	TRUE	5.86E-01	0.95	FALSE
M229T574_neg	229.0983	574	3	6.60E-01	1.04	FALSE	8.11E-02	0.85	FALSE	9.12E-01	1.01	FALSE	8.04E-03	1.65	TRUE
M230T264_neg	230.1146	264	3	1.32E-39	0.09	TRUE	6.84E-01	1.04	FALSE	7.50E-03	1.26	FALSE	5.07E-01	0.92	FALSE
M231T708_neg	231.1238	708	3	5.96E-01	0.94	FALSE	9.06E-03	1.40	FALSE	3.57E-06	1.66	TRUE	7.21E-01	1.04	FALSE
M231T442_neg	231.1351	442	3	9.16E-40	0.12	TRUE	2.84E-01	1.11	FALSE	2.12E-03	1.29	FALSE	1.80E-01	0.66	FALSE
M231T355_neg	231.1351	355	3	1.59E-25	0.18	TRUE	4.77E-01	1.09	FALSE	2.57E-02	1.25	FALSE	4.60E-01	0.82	FALSE
M232T381_neg	232.0738	381	3	3.27E-03	0.68	FALSE	6.57E-01	1.06	FALSE	1.01E-04	1.56	TRUE	1.14E-01	0.89	FALSE
M232T344_neg	232.1191	344	3	7.71E-03	0.40	TRUE	6.57E-01	1.16	FALSE	5.88E-01	1.16	FALSE	2.62E-01	0.83	FALSE
M233T484_neg	232.9762	484	3	2.52E-13	0.42	TRUE	5.87E-01	0.94	FALSE	1.49E-02	1.25	FALSE	2.14E-01	1.26	FALSE
M233T576_neg	233.1031	576	3	4.26E-29	0.46	TRUE	8.66E-01	0.99	FALSE	3.97E-12	1.44	FALSE	7.66E-01	1.05	FALSE
M233T509_neg	233.1030	509	3	1.03E-03	0.84	FALSE	2.86E-02	1.13	FALSE	3.85E-26	1.82	TRUE	6.49E-01	1.04	FALSE
M235T654_neg	235.0361	654	3	6.07E-01	1.07	FALSE	3.86E-01	1.12	FALSE	1.03E-05	1.65	TRUE	2.01E-01	0.76	FALSE
M235T500_neg	235.1090	500	3	1.97E-01	0.88	FALSE	6.98E-01	1.04	FALSE	4.21E-24	2.90	TRUE	1.69E-01	0.82	FALSE
M236T389_neg	236.0672	389	3	5.48E-01	0.95	FALSE	9.06E-01	1.01	FALSE	1.70E-12	1.71	TRUE	4.88E-01	0.90	FALSE
M236T481_neg	236.0565	481	3	1.49E-01	0.88	FALSE	3.00E-01	0.91	FALSE	5.25E-16	1.97	TRUE	6.45E-01	0.94	FALSE
M236T458_neg	236.0928	458	3	1.38E-08	0.02	TRUE	9.64E-01	1.02	FALSE	3.67E-01	1.29	FALSE	6.28E-01	0.96	FALSE
M236T400_neg	236.1292	400	3	3.28E-02	1.18	FALSE	6.86E-01	0.97	FALSE	5.15E-13	1.69	TRUE	6.11E-01	1.06	FALSE
M237T624_neg	237.0435	624	3	8.34E-01	1.02	FALSE	1.55E-01	1.15	FALSE	9.97E-18	2.27	TRUE	5.04E-01	1.10	FALSE
M237T520_neg	237.0522	520	3	6.38E-01	1.04	FALSE	8.55E-01	0.99	FALSE	2.92E-10	1.58	TRUE	4.79E-02	0.75	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M237T470_neg	237.0437	470	3							HMDB0030400	L-4-Chlorotryptophan	C11H11ClN2O2	0.1
M237T752_neg	237.0921	752	3							HMDB0029700	Cinnamyl benzoate	C16H14O2	0.1
M238T724_neg	238.0722	724	3							HMDB0250058	(3s)-3-(Benzyloxy)-L-Aspartic Acid	C11H13NO5	0.5
M238T648_neg	238.0722	648	3							HMDB0250058	(3s)-3-(Benzyloxy)-L-Aspartic Acid	C11H13NO5	0.3
M238T414_neg	238.0829	414	3							HMDB0245533	2-Acetylacteoside	C10H13N3O4	1.9
M239T423_neg	239.1402	423	3							HMDB0015407	Pirbuterol	C12H20N2O3	0.3
M239T761_neg	239.1653	761	3							HMDB0032369	L-Menthyl acetoacetate	C14H24O3	0.1
M240T655_neg	240.0515	655	3							HMDB0037548	y-6,7-dimethoxy-2H-1,4-benzoxaz	C10H11NO6	0.6
M241T564_neg	241.0625	564	3							HMDB0240720	mino-7-methoxy-3H-phenoxazin-3-	C13H10N2O3	2.6
M242T707_neg	242.0440	707	3							HMDB0062185	yl-2-acylglycerophosphoethanolar	C6H14NO7P	2.1
M242T652_neg	242.0493	652	3							HMDB0258050	thyl-8-oxo-5-thia-1-azabicyclo[4.2.	C10H13NO4S	0.4
M242T179_neg	242.0782	179	3							HMDB0000089	Cytidine	C9H13N3O5	0.1
M243T699_neg	243.1604	699	3							HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	0.9
M243T988_neg	243.1966	988	3						Fatty acids	HMDB0002261	2-Hydroxymyristic acid	C14H28O3	0.0
M244T428_neg	244.1303	428	3						Amino acids and Peptides	HMDB0028734	Asparaginylisoleucine	C10H19N3O4	0.1
M244T469_neg	244.1194	469	3							HMDB0241651	3-Oxobutanoylcarnitine	C11H19NO5	1.3
M244T290_neg	244.1303	290	3							HMDB0028734	Asparaginylisoleucine	C10H19N3O4	0.1
M244T645_neg	244.1555	645	3						Fatty acids	HMDB0000378	2-Methylbutyroylcarnitine	C12H23NO4	0.1
M245T561_neg	245.0125	561	3							HMDB0094710	-[3-(Sulfooxy)phenyl]propanoic ac	C9H10O6S	0.0
M245T634_neg	245.0125	634	3							HMDB0094710	-[3-(Sulfooxy)phenyl]propanoic ac	C9H10O6S	0.0
M245T673_neg	245.0936	673	3							HMDB0013713	N-Acetyltryptophan	C13H14N2O3	1.9
M245T548_neg	245.0936	548	3						Amino acids and Peptides	HMDB0013713	N-Acetyltryptophan	C13H14N2O3	1.7
M245T431_neg	245.0933	431	3							HMDB0013713	N-Acetyltryptophan	C13H14N2O3	0.6
M246T593_neg	246.0437	593	3							HMDB0252436	Forchlorfenuron	C12H10ClN3O	1.3
M247T414_neg	247.1300	414	3						Amino acids and Peptides				
M247T675_neg	247.1187	675	3							HMDB0031876	Prenyl glucoside	C11H20O6	0.0
M248T387_neg	248.0776	387	3							HMDB0001526	S-Acetyldihydrolipoamide	C10H19NO2S2	3.4
M248T462_neg	248.1040	462	3							HMDB0255983	Oxibendazole	C12H15N3O3	0.5
M249T630_neg	249.0807	630	3							HMDB0244922	eridin-1-yl)[1,3]thiazolo[4,5-d]pyri	C11H14N4OS	3.6
M249T796_neg	249.1133	796	3							HMDB0002012	Ubiquinone-1	C14H18O4	0.4
M249T1044_neg	249.1497	1044	3							HMDB0015371	Gemfibrozil	C15H22O3	0.4
M250T1011_neg	250.1452	1011	3							HMDB0245262	2-Nitrophenyl octyl ether	C14H21NO3	1.3
M252T386_neg	252.0987	386	3							HMDB0256959	Pyricarbate	C11H15N3O4	1.2
M253T770_neg	253.0507	770	3							HMDB0003312	Daidzein	C15H10O4	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M237T470_neg	237.0437	470	3	1.38E-43	0.17	TRUE	6.40E-01	1.04	FALSE	6.06E-05	1.32	FALSE	7.35E-03	1.36	FALSE
M237T752_neg	237.0921	752	3	1.17E-05	2.71	TRUE	5.29E-01	0.87	FALSE	1.23E-01	1.32	FALSE	5.04E-01	0.87	FALSE
M238T724_neg	238.0722	724	3	1.17E-26	0.26	TRUE	7.27E-01	1.03	FALSE	9.21E-06	1.45	FALSE	6.89E-02	1.20	FALSE
M238T648_neg	238.0722	648	3	3.69E-04	1.34	FALSE	7.50E-01	1.03	FALSE	2.57E-09	1.56	TRUE	8.16E-01	0.98	FALSE
M238T414_neg	238.0829	414	3	8.89E-01	1.01	FALSE	6.92E-01	0.96	FALSE	3.22E-11	1.75	TRUE	7.97E-02	0.75	FALSE
M239T423_neg	239.1402	423	3	7.14E-08	1.57	TRUE	2.74E-01	1.09	FALSE	4.08E-01	1.06	FALSE	2.13E-01	1.20	FALSE
M239T761_neg	239.1653	761	3	1.32E-01	0.83	FALSE	2.38E-01	1.17	FALSE	1.33E-04	1.53	TRUE	9.84E-01	0.99	FALSE
M240T655_neg	240.0515	655	3	9.19E-42	0.36	TRUE	5.89E-01	1.03	FALSE	3.67E-05	1.22	FALSE	9.70E-02	0.67	FALSE
M241T564_neg	241.0625	564	3	1.93E-13	1.75	TRUE	7.30E-01	0.98	FALSE	6.21E-06	1.33	FALSE	4.55E-01	1.09	FALSE
M242T707_neg	242.0440	707	3	1.46E-02	1.48	FALSE	8.30E-01	0.96	FALSE	3.79E-03	0.67	TRUE	5.83E-01	1.14	FALSE
M242T652_neg	242.0493	652	3	9.27E-01	0.99	FALSE	2.95E-01	1.19	FALSE	4.93E-04	1.62	TRUE	7.41E-01	0.87	FALSE
M242T179_neg	242.0782	179	3	4.32E-10	0.49	TRUE	1.56E-02	0.76	FALSE	7.50E-05	1.45	FALSE	6.28E-01	1.06	FALSE
M243T699_neg	243.1604	699	3	3.05E-08	0.48	TRUE	9.02E-01	0.98	FALSE	8.29E-01	1.02	FALSE	1.48E-01	1.72	FALSE
M243T988_neg	243.1966	988	3	4.47E-11	1.75	TRUE	4.14E-03	0.80	FALSE	6.78E-02	1.13	FALSE	8.47E-01	1.03	FALSE
M244T428_neg	244.1303	428	3	9.39E-36	0.14	TRUE	2.49E-01	1.13	FALSE	1.99E-03	1.30	FALSE	4.76E-01	1.12	FALSE
M244T469_neg	244.1194	469	3	4.25E-18	1.70	TRUE	6.16E-01	1.03	FALSE	4.47E-07	1.28	FALSE	1.01E-01	0.92	FALSE
M244T290_neg	244.1303	290	3	2.99E-53	0.07	TRUE	3.92E-01	1.08	FALSE	2.80E-03	1.24	FALSE	8.29E-01	0.95	FALSE
M244T645_neg	244.1555	645	3	1.20E-09	1.62	TRUE	5.39E-01	1.05	FALSE	9.31E-01	1.01	FALSE	5.73E-01	0.94	FALSE
M245T561_neg	245.0125	561	3	9.00E-02	1.22	FALSE	2.03E-01	0.86	FALSE	3.68E-07	1.72	TRUE	5.20E-01	0.90	FALSE
M245T634_neg	245.0125	634	3	1.30E-01	0.83	FALSE	2.17E-01	0.85	FALSE	1.36E-08	1.92	TRUE	1.58E-01	1.37	FALSE
M245T673_neg	245.0936	673	3	2.16E-01	1.12	FALSE	2.56E-01	0.89	FALSE	9.10E-04	1.31	FALSE	3.31E-02	0.52	TRUE
M245T548_neg	245.0936	548	3	1.94E-12	0.70	FALSE	7.52E-02	1.09	FALSE	1.76E-35	1.94	TRUE	4.52E-01	0.95	FALSE
M245T431_neg	245.0933	431	3	7.46E-06	0.56	TRUE	6.95E-01	1.05	FALSE	2.44E-04	1.49	FALSE	1.28E-01	0.91	FALSE
M246T593_neg	246.0437	593	3	6.42E-33	0.33	TRUE	7.16E-01	1.03	FALSE	5.28E-02	1.12	FALSE	7.51E-01	0.96	FALSE
M247T414_neg	247.1300	414	3	5.35E-15	1.74	TRUE	1.31E-01	0.90	FALSE	4.52E-05	0.79	FALSE	2.33E-01	1.09	FALSE
M247T675_neg	247.1187	675	3	3.57E-20	0.50	TRUE	4.14E-01	0.94	FALSE	2.36E-10	1.47	FALSE	6.87E-01	0.95	FALSE
M248T387_neg	248.0776	387	3	1.46E-30	0.17	TRUE	7.27E-01	1.04	FALSE	3.04E-04	1.40	FALSE	8.19E-01	1.05	FALSE
M248T462_neg	248.1040	462	3	3.01E-02	0.81	FALSE	5.14E-01	1.07	FALSE	2.03E-10	1.79	TRUE	1.88E-02	1.44	FALSE
M249T630_neg	249.0807	630	3	1.33E-10	1.58	TRUE	4.83E-02	1.14	FALSE	2.72E-03	1.19	FALSE	1.11E-01	1.19	FALSE
M249T796_neg	249.1133	796	3	3.62E-10	1.54	TRUE	7.95E-01	1.02	FALSE	1.60E-01	0.92	FALSE	4.40E-01	0.89	FALSE
M249T1044_neg	249.1497	1044	3	5.25E-04	0.84	FALSE	2.36E-02	1.13	FALSE	3.98E-03	0.88	FALSE	4.86E-06	2.73	TRUE
M250T1011_neg	250.1452	1011	3	5.56E-02	0.88	FALSE	4.95E-01	1.05	FALSE	2.23E-11	0.65	TRUE	4.05E-01	1.09	FALSE
M252T386_neg	252.0987	386	3	4.63E-04	0.78	FALSE	9.00E-01	0.99	FALSE	7.88E-17	1.76	TRUE	2.17E-01	0.93	FALSE
M253T770_neg	253.0507	770	3	3.71E-14	2.23	TRUE	1.24E-01	0.86	FALSE	4.56E-01	1.06	FALSE	5.67E-01	0.93	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M253T799_neg	253.0751	799	3							HMDB0255529	Neosalacinol	C9H18O6S	0.1
M253T618_neg	253.0829	618	3							HMDB0029445	L-Agaridoxin	C11H14N2O5	0.4
M253T361_neg	253.0839	361	3							HMDB0245609	acid, [(diethoxyphosphinyl)oxy]me	C9H19O6P	3.0
M253T486_neg	253.1194	486	3							HMDB0014356	Midodrine	C12H18N2O4	0.0
M253T877_neg	253.1445	877	3							HMDB0249518	C75 trans	C14H22O4	0.1
M255T419_neg	255.1053	419	3							HMDB0015190	Echothiophate	C9H23NO3PS	4.3
M255T358_neg	255.0989	358	3							HMDB0011648	D-Ribofuranosyl)-1,4-dihydronicot	C11H16N2O5	0.8
M255T561_neg	255.1240	561	3							HMDB0031772	oxy-1-(2,4,5-trimethoxyphenyl)-2-p	C13H20O5	0.8
M255T656_neg	255.1238	656	3							HMDB0031772	oxy-1-(2,4,5-trimethoxyphenyl)-2-p	C13H20O5	0.0
M256T405_neg	256.0827	405	3							HMDB0257806	enyl(ethoxycarbonyl)amino]-2-met	C11H15NO6	0.3
M256T505_neg	256.0926	505	3						Amino acids and Peptides				
M256T600_neg	256.1918	600	3							HMDB0013272	N-Lauroylglycine	C14H27NO3	0.1
M257T722_neg	257.0822	722	3							HMDB0004629	O-Desmethylangolensin	C15H14O4	0.9
M257T758_neg	257.1304	758	3							HMDB0246654	hylaminomethyl-gamma-aminobut	C15H18N2O2	3.1
M258T627_neg	258.0387	627	3							HMDB0250754	D-Glucosamine-6-phosphate	C6H14NO8P	1.2
M258T482_neg	258.0983	482	3							HMDB0013134	Fumarycarnitine	C11H17NO6	0.1
M259T464_neg	259.1299	464	3						Amino acids and Peptides	HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	0.3
M259T385_neg	259.1300	385	3							HMDB0011170	gamma-Glutamylisoleucine	C11H20N2O5	0.2
M259T748_neg	259.1456	748	3							HMDB0033481	Baptifoline	C15H20N2O2	1.7
M260T557_neg	260.0234	557	3							HMDB0062550	2-Methoxyacetaminophen sulfate	C9H11NO6S	0.0
M260T721_neg	260.0565	721	3							HMDB0251110	Dehydroxymethylepoxyquinomicin	C13H11NO5	0.3
M260T569_neg	260.0596	569	3							HMDB0257905	ylamino 2,5-dihydroxybenzenesulf	C10H15NO5S	0.7
M260T357_neg	260.0776	357	3							HMDB0030277	Dihydromaleimide beta-D-glucosid	C10H15NO7	0.3
M260T550_neg	260.1140	550	3							HMDB0033865	Lotaustralin	C11H19NO6	0.3
M261T644_neg	261.0591	644	3							HMDB0303207	arboxymethyl cellulose, sodium sa	C8H15NaO8	0.3
M261T770_neg	261.1609	770	3							HMDB0253250	Hydrogenated MDI	C15H22N2O2	0.0
M262T342_neg	262.0836	342	3							HMDB0255930	Olaquindox	C12H13N3O4	1.2
M262T554_neg	262.0944	554	3							HMDB0255538	Neplanocin A	C11H13N5O3	0.6
M262T774_neg	262.1449	774	3							HMDB0032305	n-4-yl)benzo[d][1,3]dioxole-5-carb	C15H21NO3	0.1
M262T770_neg	262.1642	770	3							HMDB0252571	Gacyclidine	C16H25NS	2.5
M263T695_neg	263.0592	695	3							HMDB0253829	ydroxyethyl)-3-(2-nitro-1h-imidazo	C8H10F2N4O4	2.0
M263T773_neg	263.0565	773	3							HMDB0260006	Zilascor	C13H12O6	1.4
M263T817_neg	263.0956	817	3							HMDB0256659	, N-(3R)-1-azabicyclo[2.2.2]oct-3-y	C14H17ClN2O	0.3
M263T651_neg	263.1403	651	3						Amino acids and Peptides	HMDB0015568	Vorinostat	C14H20N2O3	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M253T799_neg	253.0751	799	3	3.64E-01	0.88	FALSE	7.32E-01	0.95	FALSE	2.03E-04	1.61	TRUE	8.57E-01	0.99	FALSE
M253T618_neg	253.0829	618	3	1.19E-07	0.70	FALSE	3.95E-02	1.15	FALSE	3.85E-27	2.09	TRUE	8.10E-01	1.02	FALSE
M253T361_neg	253.0839	361	3	2.75E-02	0.74	FALSE	8.73E-02	1.28	FALSE	2.28E-08	2.06	TRUE	7.29E-01	0.91	FALSE
M253T486_neg	253.1194	486	3	5.87E-01	0.94	FALSE	4.98E-01	1.08	FALSE	5.77E-06	1.54	TRUE	3.95E-01	0.88	FALSE
M253T877_neg	253.1445	877	3	6.00E-01	1.04	FALSE	6.95E-01	0.97	FALSE	6.37E-05	1.33	FALSE	3.51E-03	0.49	TRUE
M255T419_neg	255.1053	419	3	1.36E-02	0.86	FALSE	5.68E-01	1.04	FALSE	6.60E-16	1.62	TRUE	2.98E-01	0.90	FALSE
M255T358_neg	255.0989	358	3	2.64E-02	0.80	FALSE	6.34E-02	1.22	FALSE	4.45E-11	1.85	TRUE	2.17E-01	1.22	FALSE
M255T561_neg	255.1240	561	3	1.95E-10	1.71	TRUE	2.99E-02	1.19	FALSE	1.49E-02	1.18	FALSE	1.07E-01	1.21	FALSE
M255T656_neg	255.1238	656	3	1.77E-22	1.78	TRUE	5.18E-01	1.03	FALSE	7.31E-01	1.02	FALSE	6.98E-01	0.94	FALSE
M256T405_neg	256.0827	405	3	2.98E-01	0.92	FALSE	6.25E-01	1.04	FALSE	1.99E-14	1.86	TRUE	6.89E-01	0.95	FALSE
M256T505_neg	256.0926	505	3	9.35E-01	0.99	FALSE	7.79E-01	1.03	FALSE	4.79E-07	1.66	TRUE	6.64E-01	1.08	FALSE
M256T600_neg	256.1918	600	3	1.37E-24	2.00	TRUE	9.82E-01	1.00	FALSE	2.15E-04	0.83	FALSE	9.75E-01	1.00	FALSE
M257T722_neg	257.0822	722	3	5.31E-01	1.19	FALSE	3.40E-02	1.92	TRUE	4.35E-01	0.83	FALSE	1.86E-02	1.42	FALSE
M257T758_neg	257.1304	758	3	5.38E-02	1.23	FALSE	2.14E-01	0.86	FALSE	2.93E-08	1.74	TRUE	7.06E-01	0.91	FALSE
M258T627_neg	258.0387	627	3	5.96E-29	2.32	TRUE	1.03E-01	0.91	FALSE	1.80E-12	0.67	FALSE	6.77E-01	1.04	FALSE
M258T482_neg	258.0983	482	3	1.33E-12	0.70	FALSE	7.19E-01	1.02	FALSE	2.59E-26	1.68	TRUE	8.97E-02	1.11	FALSE
M259T464_neg	259.1299	464	3	2.73E-51	0.15	TRUE	6.11E-01	1.04	FALSE	8.57E-03	1.18	FALSE	7.26E-01	0.91	FALSE
M259T385_neg	259.1300	385	3	5.85E-32	0.41	TRUE	5.74E-01	1.04	FALSE	3.96E-11	1.43	FALSE	5.45E-01	0.94	FALSE
M259T748_neg	259.1456	748	3	9.48E-04	1.26	FALSE	1.58E-11	0.58	TRUE	3.53E-01	1.06	FALSE	9.74E-01	1.00	FALSE
M260T557_neg	260.0234	557	3	5.01E-35	0.15	TRUE	6.60E-01	1.05	FALSE	4.19E-06	1.50	FALSE	6.74E-01	1.05	FALSE
M260T721_neg	260.0565	721	3	5.60E-04	1.24	FALSE	5.30E-01	1.04	FALSE	1.10E-13	1.55	TRUE	7.42E-01	0.95	FALSE
M260T569_neg	260.0596	569	3	2.84E-03	0.81	FALSE	7.24E-03	1.22	FALSE	3.51E-15	1.73	TRUE	3.46E-01	0.85	FALSE
M260T357_neg	260.0776	357	3	2.82E-03	0.83	FALSE	5.97E-01	1.04	FALSE	6.98E-18	1.70	TRUE	4.20E-01	0.93	FALSE
M260T550_neg	260.1140	550	3	1.49E-06	0.68	FALSE	7.36E-02	1.16	FALSE	1.04E-21	2.15	TRUE	3.45E-01	0.92	FALSE
M261T644_neg	261.0591	644	3	7.24E-02	1.61	FALSE	2.37E-02	0.54	TRUE	9.08E-02	0.68	FALSE	8.51E-01	0.89	FALSE
M261T770_neg	261.1609	770	3	2.77E-05	1.37	FALSE	1.14E-11	0.56	TRUE	5.66E-07	1.39	FALSE	7.37E-01	1.03	FALSE
M262T342_neg	262.0836	342	3	5.38E-01	1.06	FALSE	4.66E-01	1.07	FALSE	2.70E-11	1.77	TRUE	5.34E-01	1.09	FALSE
M262T554_neg	262.0944	554	3	1.85E-01	0.93	FALSE	1.48E-09	1.43	FALSE	2.09E-21	1.71	TRUE	1.22E-02	1.15	FALSE
M262T774_neg	262.1449	774	3	2.54E-16	2.27	TRUE	3.07E-03	0.72	FALSE	2.55E-01	0.92	FALSE	1.40E-01	0.77	FALSE
M262T770_neg	262.1642	770	3	7.30E-06	1.37	FALSE	2.84E-12	0.59	TRUE	7.38E-07	1.35	FALSE	3.98E-01	1.12	FALSE
M263T695_neg	263.0592	695	3	3.92E-01	1.14	FALSE	7.37E-01	0.95	FALSE	1.70E-06	1.95	TRUE	8.38E-01	1.05	FALSE
M263T773_neg	263.0565	773	3	1.00E-04	0.73	FALSE	9.87E-01	1.00	FALSE	1.81E-11	1.66	TRUE	5.09E-01	1.12	FALSE
M263T817_neg	263.0956	817	3	1.12E-01	0.88	FALSE	3.80E-01	1.07	FALSE	1.40E-13	1.75	TRUE	6.74E-01	0.93	FALSE
M263T651_neg	263.1403	651	3	2.50E-49	0.11	TRUE	7.50E-01	1.03	FALSE	1.44E-04	1.31	FALSE	6.90E-02	0.70	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M264T472_neg	264.0515	472	3						Alkaloids	HMDB0041949	Nitecapone	C12H11NO6	0.7
M264T539_neg	264.0879	539	3							HMDB0059732	-(2-Phenylacetoxy)propionylglycin	C13H15NO5	0.7
M264T466_neg	264.1243	466	3							HMDB0243530	diol, 2-(p-methoxybenzyl)-, 3-aceta	C14H19NO4	0.5
M265T416_neg	265.1195	416	3							HMDB0029005	Phenylalanylthreonine	C13H18N2O4	0.4
M266T375_neg	266.0783	375	3							HMDB0247328	-5-((4-nitrophenyl)amino)-5-oxope	C11H13N3O5	0.1
M267T800_neg	267.0907	800	3							HMDB0015302	Moclobemide	C13H17ClN2O2	0.4
M267T743_neg	267.0985	743	3							HMDB0029051	Seryltyrosine	C12H16N2O5	0.5
M267T413_neg	267.1352	413	3							HMDB0247322	(2-hydroxyethyl)amino-L-phenylala	C13H20N2O4	0.5
M268T372_neg	268.1302	372	3							HMDB0260136	ine-2-carbonyl]amino]acetyl]pyrro	C12H19N3O4	0.4
M268T417_neg	268.1192	417	3							HMDB0251804	Endralazine	C14H15N5O	4.4
M269T503_neg	269.0667	503	3							HMDB0059806	Phenylglucuronide	C12H14O7	0.2
M269T379_neg	269.0669	379	3							HMDB0059806	Phenylglucuronide	C12H14O7	1.0
M269T458_neg	269.0668	458	3							HMDB0059806	Phenylglucuronide	C12H14O7	0.3
M269T949_neg	269.1299	949	3							HMDB0250271	Ciproxifan	C16H18N2O2	1.2
M270T457_neg	270.0986	457	3							HMDB0246178	4-Aminophenylmannoside	C12H17NO6	0.9
M271T655_neg	271.0473	655	3							HMDB0029496	Fukiic acid	C11H12O8	4.9
M271T412_neg	271.0461	412	3							HMDB0029496	Fukiic acid	C11H12O8	0.5
M271T986_neg	271.0642	986	3							HMDB0258522	,5-dimethyl-1H-pyrrol-2-yl)methyl	C15H13ClN2O	0.7
M271T964_neg	271.1453	964	3							HMDB0258470	-cyano-3-(4-hydroxy-3,5-bis(1-me	C16H20N2O2	0.3
M271T565_neg	271.1774	565	3							HMDB0258266	methyl)amino)-1-oxohexyl)amino)p	C12H24N4O3	0.6
M272T380_neg	272.0777	380	3							HMDB0242493	olidin-1-yl) 5-(2-hydroxyethoxy)-4-	C11H15NO7	0.3
M272T658_neg	272.0958	658	3							HMDB0255133	l-N-(2-hydroxy-3-sulfopropyl)-3-to	C12H19NO4S	1.6
M272T569_neg	272.1140	569	3							HMDB0013129	Glutaconylcarnitine	C12H19NO6	0.1
M273T650_neg	273.0881	650	3							HMDB0035115	rahydro-1-methyl-beta-carboline-1	C14H14N2O4	0.0
M273T678_neg	273.0977	678	3							HMDB0244610	minoethylamino)ethylamino]ethy	C12H18O7	1.1
M274T498_neg	274.0933	498	3							HMDB0030697	Sarmentosin	C11H17NO7	0.2
M274T132_neg	274.1044	132	3							HMDB0005766	Norophthalmic acid	C10H17N3O6	0.3
M274T356_neg	274.1408	356	3							HMDB0003869	epsilon-(gamma-Glutamyl)lysine	C11H21N3O5	0.2
M275T532_neg	275.0674	532	3							HMDB0257088	racemic mixture	C15H17OPS	3.3
M275T706_neg	275.1500	706	3						Fatty acids	HMDB0250877	Daumone	C13H24O6	0.1
M275T894_neg	275.1760	894	3						Alkaloids	HMDB0015555	Molindone	C16H24N2O2	1.8
M276T415_neg	276.0295	415	3							HMDB0015128	Azathioprine	C9H7N7O2S	5.0
M276T906_neg	276.1716	906	3							HMDB0041944	N-Acetylprocainamide	C15H23N3O2	0.4
M277T345_neg	277.0501	345	3							HMDB0252357	Fluorescamine	C17H10O4	1.9
M277T432_neg	277.0863	432	3						Amino acids and Peptides	HMDB0028825	Glutamylmethionine	C10H18N2O5S	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M264T472_neg	264.0515	472	3	1.65E-06	0.69	FALSE	3.47E-01	1.08	FALSE	1.22E-22	2.11	TRUE	3.71E-01	0.93	FALSE
M264T539_neg	264.0879	539	3	4.48E-02	0.87	FALSE	4.35E-08	1.49	FALSE	1.93E-10	1.50	TRUE	6.04E-01	1.06	FALSE
M264T466_neg	264.1243	466	3	8.73E-05	0.71	FALSE	9.20E-01	0.99	FALSE	3.46E-08	1.53	TRUE	5.53E-01	0.92	FALSE
M265T416_neg	265.1195	416	3	1.43E-13	0.27	TRUE	6.63E-01	1.07	FALSE	6.31E-03	1.43	FALSE	2.68E-01	0.77	FALSE
M266T375_neg	266.0783	375	3	1.07E-02	0.70	FALSE	7.85E-01	1.04	FALSE	1.86E-08	2.07	TRUE	1.49E-01	1.48	FALSE
M267T800_neg	267.0907	800	3	9.80E-01	1.00	FALSE	1.90E-02	1.17	FALSE	4.57E-13	1.54	TRUE	9.24E-01	0.99	FALSE
M267T743_neg	267.0985	743	3	2.68E-02	0.85	FALSE	7.48E-01	1.02	FALSE	8.69E-05	1.29	FALSE	2.34E-02	0.61	TRUE
M267T413_neg	267.1352	413	3	1.21E-02	0.79	FALSE	5.49E-01	1.06	FALSE	8.12E-08	1.59	TRUE	2.86E-01	0.94	FALSE
M268T372_neg	268.1302	372	3	1.49E-02	0.78	FALSE	8.72E-01	0.98	FALSE	2.21E-06	1.54	TRUE	7.04E-01	0.94	FALSE
M268T417_neg	268.1192	417	3	2.80E-10	2.14	TRUE	8.26E-01	1.03	FALSE	9.24E-02	0.85	FALSE	5.17E-01	1.14	FALSE
M269T503_neg	269.0667	503	3	9.08E-09	1.52	TRUE	4.92E-01	1.05	FALSE	1.65E-02	1.16	FALSE	9.85E-01	1.00	FALSE
M269T379_neg	269.0669	379	3	2.94E-02	0.86	FALSE	6.21E-01	1.04	FALSE	3.35E-16	1.75	TRUE	4.69E-01	0.86	FALSE
M269T458_neg	269.0668	458	3	3.29E-11	1.64	TRUE	6.45E-01	0.97	FALSE	1.56E-03	1.21	FALSE	8.42E-01	1.03	FALSE
M269T949_neg	269.1299	949	3	1.31E-05	0.65	TRUE	1.72E-03	1.38	FALSE	5.19E-04	1.34	FALSE	4.08E-01	1.15	FALSE
M270T457_neg	270.0986	457	3	1.42E-02	0.86	FALSE	5.54E-03	1.19	FALSE	2.14E-19	1.71	TRUE	6.01E-02	0.86	FALSE
M271T655_neg	271.0473	655	3	2.61E-06	0.76	FALSE	2.34E-01	1.07	FALSE	2.62E-28	1.95	TRUE	7.32E-01	0.97	FALSE
M271T412_neg	271.0461	412	3	2.64E-04	0.71	FALSE	6.63E-01	1.04	FALSE	1.47E-15	2.05	TRUE	2.53E-01	1.15	FALSE
M271T986_neg	271.0642	986	3	2.14E-04	2.35	TRUE	1.27E-01	0.70	FALSE	2.99E-01	1.21	FALSE	9.36E-02	0.53	FALSE
M271T964_neg	271.1453	964	3	1.89E-06	1.91	TRUE	2.10E-04	0.67	FALSE	5.07E-01	1.08	FALSE	7.78E-01	0.95	FALSE
M271T565_neg	271.1774	565	3	4.07E-07	1.62	TRUE	5.84E-01	1.06	FALSE	2.45E-03	1.27	FALSE	4.16E-01	1.13	FALSE
M272T380_neg	272.0777	380	3	3.99E-01	1.06	FALSE	8.08E-01	0.98	FALSE	2.10E-11	1.54	TRUE	1.61E-01	0.83	FALSE
M272T658_neg	272.0958	658	3	1.60E-01	0.87	FALSE	6.66E-01	0.96	FALSE	5.53E-07	1.57	TRUE	4.82E-01	1.08	FALSE
M272T569_neg	272.1140	569	3	8.06E-11	0.69	FALSE	6.84E-01	1.02	FALSE	4.72E-22	1.67	TRUE	5.63E-01	1.05	FALSE
M273T650_neg	273.0881	650	3	3.04E-18	0.44	TRUE	3.62E-01	1.08	FALSE	3.35E-03	1.23	FALSE	2.75E-02	0.79	FALSE
M273T678_neg	273.0977	678	3	8.14E-05	1.37	FALSE	3.00E-09	1.63	TRUE	2.43E-01	1.08	FALSE	4.67E-01	1.08	FALSE
M274T498_neg	274.0933	498	3	7.86E-07	0.71	FALSE	2.88E-02	1.17	FALSE	1.04E-28	2.25	TRUE	1.07E-01	0.86	FALSE
M274T132_neg	274.1044	132	3	3.38E-01	0.90	FALSE	4.66E-01	0.92	FALSE	1.27E-09	1.89	TRUE	1.56E-01	0.79	FALSE
M274T356_neg	274.1408	356	3	7.04E-26	0.48	TRUE	8.15E-01	0.99	FALSE	1.42E-03	1.17	FALSE	8.58E-01	1.03	FALSE
M275T532_neg	275.0674	532	3	3.23E-11	0.19	TRUE	7.51E-01	1.06	FALSE	1.30E-01	1.29	FALSE	1.05E-01	1.43	FALSE
M275T706_neg	275.1500	706	3	5.52E-04	0.85	FALSE	3.03E-03	1.16	FALSE	3.28E-29	1.76	TRUE	8.60E-01	0.99	FALSE
M275T894_neg	275.1760	894	3	3.76E-10	1.84	TRUE	2.24E-02	0.82	FALSE	9.40E-04	1.30	FALSE	3.86E-02	1.22	FALSE
M276T415_neg	276.0295	415	3	8.01E-01	1.03	FALSE	9.95E-01	1.00	FALSE	2.45E-06	1.69	TRUE	4.47E-01	1.22	FALSE
M276T906_neg	276.1716	906	3	4.86E-12	4.64	TRUE	3.59E-01	0.85	FALSE	6.60E-01	1.07	FALSE	1.66E-01	1.31	FALSE
M277T345_neg	277.0501	345	3	7.61E-01	1.03	FALSE	3.53E-03	1.39	FALSE	1.94E-09	1.84	TRUE	6.01E-02	1.48	FALSE
M277T432_neg	277.0863	432	3	1.02E-04	0.65	TRUE	1.37E-01	1.19	FALSE	1.75E-02	1.25	FALSE	7.14E-01	0.95	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M277T787_neg	277.1082	787	3						Terpenoids	HMDB0030766	-Hydroxy-12-methoxydihydrokawa	C15H18O5	0.2
M278T485_neg	278.1145	485	3							HMDB0028738	Asparaginyl-Phenylalanine	C13H17N3O4	0.5
M279T422_neg	279.0988	422	3						Amino acids and Peptides	HMDB0000706	Aspartylphenylalanine	C13H16N2O5	0.7
M279T833_neg	279.1705	833	3							HMDB0245010	2-Aminobenzylstatine	C15H24N2O3	3.3
M280T472_neg	280.0591	472	3							HMDB0252331	Flufenamic acid	C14H10F3NO2	0.2
M280T520_neg	280.0935	520	3							HMDB0040693	nma-Glutamyl)-4-carboxyphenylhy	C12H15N3O5	1.5
M280T629_neg	280.0936	629	3							HMDB0040693	nma-Glutamyl)-4-carboxyphenylhy	C12H15N3O5	1.2
M280T831_neg	280.0977	831	3							HMDB0247920	Acetoxyacetylaminofluorene	C17H15NO3	0.6
M280T484_neg	280.1191	484	3							HMDB0255476	3-Hydroxy-4-pivaloyloxyphenyl)ala	C14H19NO5	0.1
M280T400_neg	280.1191	400	3							HMDB0255476	3-Hydroxy-4-pivaloyloxyphenyl)ala	C14H19NO5	0.4
M281T405_neg	281.1148	405	3							HMDB0029073	Threonyltyrosine	C13H18N2O5	1.8
M283T454_neg	283.0936	454	3						Carbohydrates	HMDB0061067	arabinofuranosylguanine	C10H14N5O5	4.8
M284T398_neg	284.0886	398	3							HMDB0005923	N4-Acetylcytidine	C11H15N3O6	0.9
M284T533_neg	284.1140	533	3							HMDB0241034	dimethylidenebutanedioylcarnitine	C13H19NO6	0.1
M285T637_neg	285.0614	637	3							HMDB0029498	Dimethyl fukiic acid	C12H14O8	0.6
M285T743_neg	285.0772	743	3							HMDB0029527	Melilotocarpan B	C16H14O5	1.2
M285T574_neg	285.0894	574	3							HMDB0013895	S-4-Hydroxymephenytoin	C15H14N2O4	4.8
M286T565_neg	286.1773	565	3						Amino acids and Peptides				
M287T560_neg	287.0232	560	3							HMDB0240473	4-Methylumbelliferone sulfate	C11H12O7S	0.5
M288T190_neg	288.1200	190	3							HMDB0005765	Ophthalmic acid	C11H19N3O6	0.5
M289T502_neg	289.0502	502	3							HMDB0041121	-Hydroxyphenyl)naphthalic anhyd	C18H10O4	1.4
M289T551_neg	289.1085	551	3							HMDB0038722	5,6-Dihydro-11-methoxyyangonin	C16H18O5	1.1
M289T609_neg	289.1232	609	3							HMDB0040916	(4-Methyl-3-pentenyl)anthraquino	C20H18O2	0.9
M289T746_neg	289.1656	746	3							HMDB0032959	1-Octen-3-yl glucoside	C14H26O6	0.2
M290T575_neg	290.0704	575	3							HMDB0002354	Hawkinsin	C11H17NO6S	0.1
M290T753_neg	290.1066	753	3							HMDB0250696	Cyproconazole	C15H18ClN3O	0.2
M291T867_neg	291.1240	867	3							HMDB0030767	11,12-Dimethoxydihydrokawain	C16H20O5	0.6
M293T510_neg	293.1145	510	3						Amino acids and Peptides	HMDB0000594	gamma-Glutamylphenylalanine	C14H18N2O5	0.7
M293T442_neg	293.1145	442	3						Amino acids and Peptides	HMDB0000594	gamma-Glutamylphenylalanine	C14H18N2O5	0.9
M293T494_neg	293.1508	494	3							HMDB0028919	Isoleucyl-Tyrosine	C15H22N2O4	0.3
M293T1004_neg	293.2122	1004	3							HMDB0004668	13-OxoODE	C18H30O3	0.0
M294T773_neg	294.1712	773	3							HMDB0014333	Esmolol	C16H25NO4	0.4
M295T1019_neg	295.2278	1019	3							HMDB0004667	13-HODE	C18H32O3	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M277T787_neg	277.1082	787	3	3.87E-04	0.80	FALSE	3.59E-03	1.21	FALSE	1.96E-18	1.72	TRUE	6.04E-01	0.93	FALSE
M278T485_neg	278.1145	485	3	3.96E-34	0.14	TRUE	6.96E-01	1.04	FALSE	2.21E-03	1.32	FALSE	7.39E-01	0.90	FALSE
M279T422_neg	279.0988	422	3	4.14E-25	0.37	TRUE	5.42E-01	1.05	FALSE	1.16E-07	1.45	FALSE	7.90E-01	0.97	FALSE
M279T833_neg	279.1705	833	3	7.52E-01	1.03	FALSE	9.22E-01	1.01	FALSE	5.50E-02	1.20	FALSE	2.56E-03	1.53	TRUE
M280T472_neg	280.0591	472	3	5.12E-03	0.86	FALSE	1.39E-01	1.09	FALSE	2.64E-28	1.91	TRUE	8.06E-01	1.02	FALSE
M280T520_neg	280.0935	520	3	1.16E-02	0.83	FALSE	6.19E-02	1.16	FALSE	1.36E-19	1.97	TRUE	5.96E-01	0.93	FALSE
M280T629_neg	280.0936	629	3	2.27E-01	0.91	FALSE	2.37E-04	1.36	FALSE	2.12E-17	1.96	TRUE	6.96E-01	1.03	FALSE
M280T831_neg	280.0977	831	3	1.10E-03	1.35	FALSE	3.33E-02	1.22	FALSE	3.50E-08	1.58	TRUE	8.82E-01	1.02	FALSE
M280T484_neg	280.1191	484	3	1.88E-05	0.68	FALSE	2.48E-01	1.11	FALSE	3.61E-18	2.15	TRUE	4.48E-01	1.07	FALSE
M280T400_neg	280.1191	400	3	3.45E-01	1.08	FALSE	5.42E-01	1.05	FALSE	6.17E-19	2.00	TRUE	8.55E-01	1.02	FALSE
M281T405_neg	281.1148	405	3	4.71E-32	0.25	TRUE	3.27E-01	1.09	FALSE	1.25E-02	1.20	FALSE	7.25E-01	1.05	FALSE
M283T454_neg	283.0936	454	3	4.13E-02	0.79	FALSE	7.12E-01	1.04	FALSE	2.78E-10	1.98	TRUE	2.02E-01	0.75	FALSE
M284T398_neg	284.0886	398	3	6.21E-05	0.69	FALSE	4.06E-01	1.08	FALSE	5.07E-10	1.68	TRUE	1.26E-02	0.72	FALSE
M284T533_neg	284.1140	533	3	7.43E-01	0.98	FALSE	2.66E-01	1.07	FALSE	5.20E-17	1.58	TRUE	6.26E-01	1.02	FALSE
M285T637_neg	285.0614	637	3	6.74E-11	1.51	TRUE	4.77E-03	0.84	FALSE	3.82E-02	0.90	FALSE	5.18E-01	1.09	FALSE
M285T743_neg	285.0772	743	3	2.73E-05	0.76	FALSE	4.06E-01	1.06	FALSE	9.03E-20	1.80	TRUE	7.32E-01	0.96	FALSE
M285T574_neg	285.0894	574	3	3.06E-04	0.74	FALSE	8.74E-01	1.01	FALSE	1.37E-07	1.47	FALSE	8.29E-03	1.84	TRUE
M286T565_neg	286.1773	565	3	5.95E-49	0.10	TRUE	3.42E-01	1.09	FALSE	2.67E-05	1.36	FALSE	5.52E-02	0.62	FALSE
M287T560_neg	287.0232	560	3	8.13E-03	0.74	FALSE	4.32E-03	1.41	FALSE	7.10E-14	2.31	TRUE	8.84E-03	1.47	FALSE
M288T190_neg	288.1200	190	3	2.09E-01	0.91	FALSE	5.65E-02	1.16	FALSE	9.91E-10	1.54	TRUE	7.59E-01	0.95	FALSE
M289T502_neg	289.0502	502	3	3.54E-05	0.68	FALSE	6.72E-01	0.96	FALSE	2.88E-07	1.54	TRUE	5.22E-01	0.93	FALSE
M289T551_neg	289.1085	551	3	6.21E-12	1.67	TRUE	5.68E-01	1.04	FALSE	4.29E-01	0.95	FALSE	2.90E-01	1.12	FALSE
M289T609_neg	289.1232	609	3	4.69E-22	1.69	TRUE	4.30E-02	1.11	FALSE	9.05E-03	0.90	FALSE	5.76E-01	0.94	FALSE
M289T746_neg	289.1656	746	3	6.55E-05	0.82	FALSE	2.20E-01	1.07	FALSE	4.21E-22	1.62	TRUE	4.60E-01	0.95	FALSE
M290T575_neg	290.0704	575	3	6.93E-05	0.73	FALSE	1.35E-01	1.13	FALSE	1.23E-14	1.79	TRUE	1.71E-01	0.83	FALSE
M290T753_neg	290.1066	753	3	2.35E-04	0.78	FALSE	1.69E-03	1.24	FALSE	1.97E-21	1.87	TRUE	2.51E-01	1.17	FALSE
M291T867_neg	291.1240	867	3	4.62E-09	0.74	FALSE	2.86E-01	1.06	FALSE	6.40E-22	1.60	TRUE	5.70E-01	0.95	FALSE
M293T510_neg	293.1145	510	3	2.04E-56	0.11	TRUE	5.81E-01	1.04	FALSE	8.33E-04	1.23	FALSE	7.88E-01	0.97	FALSE
M293T442_neg	293.1145	442	3	7.81E-37	0.14	TRUE	4.12E-01	1.09	FALSE	2.59E-04	1.36	FALSE	1.82E-01	0.79	FALSE
M293T494_neg	293.1508	494	3	3.64E-10	0.69	FALSE	6.63E-02	1.11	FALSE	6.80E-26	1.84	TRUE	6.63E-01	1.03	FALSE
M293T1004_neg	293.2122	1004	3	3.03E-02	1.62	TRUE	7.55E-01	0.93	FALSE	7.64E-01	1.06	FALSE	3.49E-01	0.78	FALSE
M294T773_neg	294.1712	773	3	1.50E-03	3.21	TRUE	6.89E-01	0.85	FALSE	1.99E-01	0.69	FALSE	8.65E-02	0.54	FALSE
M295T1019_neg	295.2278	1019	3	4.77E-01	1.28	FALSE	8.63E-01	0.92	FALSE	3.33E-02	1.96	TRUE	9.55E-01	1.02	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M298T575_neg	298.0932	575	3							HMDB0041517	eta-D-Glucopyranosyl anthranilat	C13H17NO7	0.1
M298T368_neg	298.1298	368	3							HMDB0241039	-dimethylidenepentanedioylcarnit	C14H21NO6	0.5
M299T499_neg	299.0722	499	3							HMDB0041849	Carboxytolbutamide	C12H16N2O5S	5.0
M299T878_neg	299.1864	878	3						Fatty acids				
M300T556_neg	300.0738	556	3							HMDB0244855	-Nitrophenyl a-D-galactopyranosic	C12H15NO8	4.5
M301T356_neg	301.1510	356	3							HMDB0013016	Neuromedin B (1-3)	C12H22N4O5	2.6
M302T562_neg	302.1511	562	3							HMDB0029096	Tryptophyl-Valine	C16H21N3O3	0.1
M302T666_neg	302.1615	666	3							HMDB0013328	Pimelylcarnitine	C14H25NO6	1.9
M302T488_neg	302.1722	488	3						Amino acids and Peptides				
M303T746_neg	303.1352	746	3							HMDB0244641	-4-methyl-3-(4-methylpiperazin-1-	C16H20N2O4	0.5
M303T805_neg	303.1349	805	3							HMDB0244641	-4-methyl-3-(4-methylpiperazin-1-	C16H20N2O4	0.3
M304T155_neg	304.0340	155	3							HMDB0250240	Cifostodine	C9H12N3O7P	0.1
M304T480_neg	304.1194	480	3							HMDB0031929	Zanthodioline	C16H19NO5	1.0
M304T542_neg	304.1304	542	3							HMDB0029072	Threonyltryptophan	C15H19N3O4	0.3
M304T461_neg	304.1513	461	3							HMDB0039161	Syndesine	C12H23N3O6	0.3
M304T386_neg	304.1515	386	3							HMDB0039161	Syndesine	C12H23N3O6	0.2
M305T78_neg	304.9091	78	3							HMDB0244389	DE-beta-Cyd	C12H6Cl4O	2.9
M305T401_neg	305.0181	401	3							HMDB0011640	Topaquinone	C9H11N2O8P	0.1
M305T273_neg	305.0180	273	3							HMDB0011640	Topaquinone	C9H11N2O8P	0.0
M305T610_neg	305.0700	610	3							HMDB0255296	N4-Acetylsulfamonomethoxine	C13H14N4O3S	4.6
M305T992_neg	305.2122	992	3							HMDB0000523	5-Androstene-3b,16b,17a-triol	C19H30O3	0.1
M306T678_neg	306.1349	678	3						Alkaloids	HMDB0038582	oxy-4-methoxy-1-oxobutyl)-2,2-di	C16H21NO5	0.6
M307T823_neg	307.0725	823	3						Alkaloids	HMDB0033459	Flazine	C17H12N2O4	0.2
M307T915_neg	307.1190	915	3							HMDB0037772	8-Acetylegelolide	C16H20O6	1.1
M307T518_neg	307.1678	518	3							HMDB0248865	Baquiloprim	C17H20N6	0.5
M308T126_neg	308.0986	126	3						Carbohydrates	HMDB0000230	N-Acetylneuraminic acid	C11H19NO9	0.2
M309T715_neg	309.1081	715	3							HMDB0011741	gamma-Glutamyltyrosine	C14H18N2O6	3.7
M309T919_neg	309.1014	919	3							HMDB0242124	Dibutyl sulfosuccinate	C12H22O7S	0.1
M309T411_neg	309.1095	411	3						Amino acids and Peptides	HMDB0011741	gamma-Glutamyltyrosine	C14H18N2O6	0.9
M309T696_neg	309.1249	696	3							HMDB0258528	2-dihydroindol-3-ylidenemethyl)-1	C18H18N2O3	1.3
M309T455_neg	309.1458	455	3							HMDB0250969	Delgocitini	C16H18N6O	3.8
M310T739_neg	310.1084	739	3							HMDB0030217	Launobine	C18H17NO4	0.2
M310T774_neg	310.1198	774	3							HMDB0249842	-7,8-dimethoxy-3,5-dihydro-2,3-be	C17H17N3O3	0.4
M310T475_neg	310.1297	475	3							HMDB0033939	Domoic acid	C15H21NO6	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M298T575_neg	298.0932	575	3	1.66E-12	0.38	TRUE	3.06E-01	1.14	FALSE	1.09E-03	1.42	FALSE	4.62E-01	0.91	FALSE
M298T368_neg	298.1298	368	3	1.44E-02	0.86	FALSE	5.55E-02	1.13	FALSE	7.07E-27	1.98	TRUE	1.90E-01	0.92	FALSE
M299T499_neg	299.0722	499	3	1.90E-01	1.32	FALSE	8.19E-01	1.06	FALSE	8.30E-04	1.90	TRUE	3.75E-01	1.34	FALSE
M299T878_neg	299.1864	878	3	2.79E-01	0.95	FALSE	6.10E-03	1.16	FALSE	1.67E-19	1.58	TRUE	6.58E-01	1.05	FALSE
M300T556_neg	300.0738	556	3	5.77E-01	0.96	FALSE	7.81E-01	1.02	FALSE	5.46E-14	1.73	TRUE	7.31E-01	0.97	FALSE
M301T356_neg	301.1510	356	3	4.52E-35	0.24	TRUE	5.33E-01	1.05	FALSE	2.70E-04	1.30	FALSE	4.37E-01	0.91	FALSE
M302T562_neg	302.1511	562	3	1.04E-18	0.29	TRUE	7.15E-01	1.05	FALSE	2.11E-04	1.46	FALSE	5.95E-02	0.66	FALSE
M302T666_neg	302.1615	666	3	1.67E-01	0.85	FALSE	1.87E-02	0.72	FALSE	2.39E-06	1.68	TRUE	8.50E-01	1.02	FALSE
M302T488_neg	302.1722	488	3	3.68E-60	0.13	TRUE	4.61E-01	1.05	FALSE	1.42E-06	1.32	FALSE	2.11E-01	0.73	FALSE
M303T746_neg	303.1352	746	3	8.60E-10	1.52	TRUE	2.24E-08	0.69	FALSE	1.29E-03	1.20	FALSE	8.51E-02	0.84	FALSE
M303T805_neg	303.1349	805	3	4.14E-05	2.10	TRUE	2.28E-01	0.82	FALSE	1.10E-01	1.27	FALSE	7.45E-01	0.96	FALSE
M304T155_neg	304.0340	155	3	1.96E-14	0.02	TRUE	9.96E-01	1.00	FALSE	5.22E-01	0.88	FALSE	9.55E-01	1.08	FALSE
M304T480_neg	304.1194	480	3	3.67E-02	0.86	FALSE	5.76E-01	1.04	FALSE	2.43E-12	1.62	TRUE	6.18E-01	1.05	FALSE
M304T542_neg	304.1304	542	3	1.35E-18	0.50	TRUE	5.69E-02	1.15	FALSE	4.40E-07	1.36	FALSE	2.25E-01	1.07	FALSE
M304T461_neg	304.1513	461	3	1.03E-27	0.13	TRUE	9.28E-01	1.01	FALSE	4.06E-02	1.24	FALSE	7.55E-02	0.34	FALSE
M304T386_neg	304.1515	386	3	2.66E-54	0.08	TRUE	6.72E-01	1.04	FALSE	1.77E-01	1.10	FALSE	8.61E-01	1.07	FALSE
M305T78_neg	304.9091	78	3	3.68E-02	0.61	TRUE	7.15E-01	1.09	FALSE	1.93E-01	0.77	FALSE	1.54E-01	1.29	FALSE
M305T401_neg	305.0181	401	3	2.59E-12	0.02	TRUE	9.76E-01	0.99	FALSE	8.82E-01	0.97	FALSE	9.60E-01	1.07	FALSE
M305T273_neg	305.0180	273	3	7.93E-16	0.00	TRUE	8.47E-01	0.95	FALSE	4.00E-01	1.18	FALSE	9.34E-01	0.89	FALSE
M305T610_neg	305.0700	610	3	6.69E-01	0.95	FALSE	7.80E-01	1.04	FALSE	1.05E-09	1.98	TRUE	4.31E-01	1.28	FALSE
M305T992_neg	305.2122	992	3	4.80E-09	1.60	TRUE	1.62E-02	0.83	FALSE	4.35E-02	1.14	FALSE	1.04E-01	0.72	FALSE
M306T678_neg	306.1349	678	3	6.63E-08	2.23	TRUE	9.86E-02	1.25	FALSE	3.40E-01	0.89	FALSE	2.91E-01	0.86	FALSE
M307T823_neg	307.0725	823	3	3.78E-03	1.28	FALSE	7.09E-01	1.03	FALSE	1.51E-20	2.24	TRUE	1.68E-01	0.92	FALSE
M307T915_neg	307.1190	915	3	4.92E-11	0.68	FALSE	2.30E-01	1.07	FALSE	8.25E-16	1.54	TRUE	9.20E-01	1.01	FALSE
M307T518_neg	307.1678	518	3	1.29E-01	0.90	FALSE	9.28E-01	1.01	FALSE	2.75E-17	1.73	TRUE	5.13E-01	0.95	FALSE
M308T126_neg	308.0986	126	3	4.93E-11	0.11	TRUE	3.23E-01	1.27	FALSE	7.47E-02	1.43	FALSE	1.92E-01	1.12	FALSE
M309T715_neg	309.1081	715	3	4.88E-11	0.47	TRUE	5.18E-01	0.93	FALSE	2.80E-04	1.40	FALSE	8.14E-01	1.01	FALSE
M309T919_neg	309.1014	919	3	4.85E-03	0.80	FALSE	8.15E-01	0.98	FALSE	5.16E-03	1.21	FALSE	1.34E-05	2.30	TRUE
M309T411_neg	309.1095	411	3	1.49E-73	0.08	TRUE	8.67E-01	1.01	FALSE	1.56E-04	1.22	FALSE	8.24E-01	0.97	FALSE
M309T696_neg	309.1249	696	3	3.02E-02	1.28	FALSE	2.15E-01	1.16	FALSE	1.94E-05	1.55	TRUE	5.13E-01	0.90	FALSE
M309T455_neg	309.1458	455	3	4.10E-06	0.76	FALSE	2.26E-01	1.08	FALSE	7.08E-24	1.84	TRUE	4.06E-03	0.80	FALSE
M310T739_neg	310.1084	739	3	4.70E-03	0.85	FALSE	7.48E-01	0.98	FALSE	2.90E-14	1.53	TRUE	1.71E-01	1.22	FALSE
M310T774_neg	310.1198	774	3	2.13E-02	0.63	TRUE	4.13E-01	1.19	FALSE	3.48E-01	1.17	FALSE	8.89E-01	0.99	FALSE
M310T475_neg	310.1297	475	3	1.55E-11	0.47	TRUE	4.30E-01	1.09	FALSE	5.24E-05	1.44	FALSE	5.56E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M311T502_neg	311.0409	502	3						Shikimates and Phenylpropanoids	HMDB0013680	Caftaric acid	C13H12O9	0.0
M311T470_neg	311.0884	470	3							HMDB0256914	Pteroic acid	C14H12N6O3	4.4
M311T708_neg	311.1041	708	3							HMDB0040435	Dictyoquinazol A	C17H16N2O4	1.1
M311T638_neg	311.1403	638	3							HMDB0013302	Phenylalanylphenylalanine	C18H20N2O3	0.6
M312T433_1_neg	312.0346	433	3							HMDB0253594	Isazofos	C9H17ClN3O3PS	0.8
M312T612_neg	312.0778	612	3							HMDB0245242	2-Methylthioadenosine	C11H15N5O4S	1.9
M312T759_neg	312.1455	759	3							HMDB0241045	4-dimethylidenehexanedioylcarniti	C15H23NO6	0.6
M312T1031_neg	312.2545	1031	3							HMDB0013034	Palmitoylglycine	C18H35NO3	0.4
M314T495_neg	314.1246	495	3							HMDB0245634	9-benzyl-2-(2-methoxyethoxy)-9H-	C15H17N5O3	3.9
M315T520_neg	315.0855	520	3						Fatty acids				
M316T577_neg	316.1192	577	3							HMDB0030341	Piplartine	C17H19NO5	0.5
M316T564_neg	316.1878	564	3						Amino acids and Peptides				
M317T675_neg	317.1396	675	3							HMDB0031752	(S,E)-Zearalenone	C18H22O5	0.5
M319T648_neg	319.1199	648	3							HMDB0015159	Mycophenolic acid	C17H20O6	3.8
M319T948_neg	319.1915	948	3						Terpenoids	HMDB0012798	4-Oxoretinal	C19H28O4	0.1
M319T946_neg	319.2279	946	3							HMDB0002190	6-Epoxy-8,11,14-eicosatrienoic ac	C20H32O3	0.1
M320T532_neg	320.0604	532	3							HMDB0251206	Diclofensine	C17H17Cl2NO	3.2
M320T601_neg	320.1616	601	3							HMDB0252569	Gabexate	C16H23N3O4	0.2
M321T528_neg	321.0287	528	3							HMDB0303547	Sodium sulfate decahydrate	H20Na2O14S	2.8
M321T708_neg	321.1013	708	3							HMDB0030266	Berberrubine	C19H16NO4	2.1
M321T1019_neg	321.2435	1019	3							HMDB0005045	15(S)-Hydroxyeicosatrienoic acid	C20H34O3	0.0
M322T709_neg	322.1044	709	3							HMDB0258233	Senicapoc	C20H15F2NO	1.5
M323T995_neg	323.2228	995	3							HMDB0031007	etoxy-2-hydroxy-16-heptadecyn-4	C19H32O4	0.0
M324T932_2_neg	324.1239	932	3							HMDB0030245	Nornantenine	C19H19NO4	0.7
M325T569_neg	325.0566	569	3						Shikimates and Phenylpropanoids	HMDB0029199	Fertaric acid	C14H14O9	0.4
M326T458_neg	326.1246	458	3							HMDB0037846	-(1-Deoxy-1-fructosyl)phenylalanir	C15H21NO7	0.3
M327T702_neg	327.1021	702	3						Amino acids and Peptides	HMDB0259320	Tubulin Polymerization Inhibitor	C22H16O3	1.6
M327T1067_neg	327.1269	1067	3							HMDB0257012	PZXDYQVSAFZTBI-UHFFFAOYSA-N	C19H21ClN2O	0.1
M328T639_neg	328.0863	639	3							HMDB0060799	7-Hydroxyamoxapine	C17H16ClN3O2	1.4
M328T1034_neg	328.2495	1034	3							HMDB0006202	4,8 Dimethylnonanoyl carnitine	C18H35NO4	0.6
M329T521_neg	329.0817	521	3							HMDB0245264	ipropylsulfamoyl)-2-nitrobenzoic	C13H18N2O6S	1.4
M329T625_neg	329.1031	625	3							HMDB0011672	Aflatoxin B1 dialcohol	C18H18O6	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M311T502_neg	311.0409	502	3	1.66E-01	2.15	FALSE	8.75E-01	1.12	FALSE	1.15E-03	7.16	TRUE	1.90E-01	0.05	FALSE
M311T470_neg	311.0884	470	3	9.20E-04	0.79	FALSE	5.06E-01	1.05	FALSE	5.68E-24	2.09	TRUE	2.92E-01	0.93	FALSE
M311T708_neg	311.1041	708	3	2.91E-01	0.93	FALSE	4.37E-01	1.06	FALSE	5.51E-17	1.79	TRUE	2.47E-01	0.89	FALSE
M311T638_neg	311.1403	638	3	3.91E-01	0.91	FALSE	7.19E-01	1.05	FALSE	1.77E-17	2.57	TRUE	5.45E-02	0.69	FALSE
M312T433_1_neg	312.0346	433	3	1.21E-09	0.00	TRUE	9.09E-01	0.96	FALSE	4.90E-01	1.21	FALSE	1.49E-01	0.09	FALSE
M312T612_neg	312.0778	612	3	1.01E-02	0.85	FALSE	6.38E-01	1.03	FALSE	4.85E-21	1.82	TRUE	2.60E-01	0.86	FALSE
M312T759_neg	312.1455	759	3	1.03E-04	1.92	TRUE	1.39E-01	1.28	FALSE	7.27E-03	0.68	FALSE	3.17E-01	0.75	FALSE
M312T1031_neg	312.2545	1031	3	1.65E-03	3.09	TRUE	2.33E-01	0.68	FALSE	8.81E-01	1.04	FALSE	9.18E-01	1.11	FALSE
M314T495_neg	314.1246	495	3	3.82E-04	0.84	FALSE	7.60E-01	1.02	FALSE	1.26E-25	1.67	TRUE	7.22E-01	0.97	FALSE
M315T520_neg	315.0855	520	3	6.85E-01	1.11	FALSE	9.56E-02	0.58	FALSE	1.66E-04	2.44	TRUE	3.91E-01	0.81	FALSE
M316T577_neg	316.1192	577	3	1.15E-10	2.51	TRUE	3.29E-01	0.88	FALSE	8.79E-03	0.75	FALSE	4.71E-01	0.91	FALSE
M316T564_neg	316.1878	564	3	8.66E-40	0.13	TRUE	4.28E-01	1.08	FALSE	6.59E-03	1.24	FALSE	6.99E-01	0.91	FALSE
M317T675_neg	317.1396	675	3	3.50E-12	1.61	TRUE	4.15E-01	0.95	FALSE	6.05E-01	0.97	FALSE	7.55E-01	0.97	FALSE
M319T648_neg	319.1199	648	3	7.12E-20	1.83	TRUE	4.28E-01	1.05	FALSE	3.77E-02	0.90	FALSE	1.68E-02	1.37	FALSE
M319T948_neg	319.1915	948	3	2.29E-05	1.68	TRUE	7.67E-02	0.80	FALSE	3.51E-01	0.91	FALSE	2.26E-01	0.84	FALSE
M319T946_neg	319.2279	946	3	6.78E-05	1.59	TRUE	8.89E-02	0.82	FALSE	7.43E-01	0.97	FALSE	6.56E-02	0.69	FALSE
M320T532_neg	320.0604	532	3	2.91E-11	0.20	TRUE	7.34E-01	1.07	FALSE	7.27E-02	1.35	FALSE	2.93E-01	1.27	FALSE
M320T601_neg	320.1616	601	3	5.76E-54	0.08	TRUE	3.59E-01	1.08	FALSE	3.04E-04	1.29	FALSE	4.76E-01	0.60	FALSE
M321T528_neg	321.0287	528	3	2.87E-02	0.76	FALSE	2.95E-01	1.15	FALSE	5.66E-16	2.83	TRUE	7.21E-03	1.47	FALSE
M321T708_neg	321.1013	708	3	1.76E-01	1.18	FALSE	5.17E-02	1.29	FALSE	1.50E-08	1.94	TRUE	7.77E-01	0.95	FALSE
M321T1019_neg	321.2435	1019	3	5.75E-04	1.52	TRUE	2.28E-01	0.87	FALSE	9.32E-01	1.01	FALSE	2.71E-01	1.41	FALSE
M322T709_neg	322.1044	709	3	3.46E-01	1.11	FALSE	4.54E-02	1.26	FALSE	3.26E-10	1.92	TRUE	7.68E-01	0.95	FALSE
M323T995_neg	323.2228	995	3	1.16E-18	1.77	TRUE	4.90E-02	0.88	FALSE	4.43E-07	1.30	FALSE	7.41E-01	1.04	FALSE
M324T932_2_neg	324.1239	932	3	5.26E-03	1.30	FALSE	8.63E-01	1.02	FALSE	2.53E-17	2.18	TRUE	6.95E-01	0.96	FALSE
M325T569_neg	325.0566	569	3	2.26E-01	1.73	FALSE	7.23E-01	0.82	FALSE	2.82E-03	3.77	TRUE	9.83E-01	1.01	FALSE
M326T458_neg	326.1246	458	3	8.85E-07	0.01	TRUE	9.29E-01	1.04	FALSE	7.95E-01	1.09	FALSE	8.45E-01	1.05	FALSE
M327T702_neg	327.1021	702	3	1.12E-01	1.23	FALSE	1.44E-01	0.83	FALSE	2.09E-04	1.54	TRUE	1.77E-01	0.79	FALSE
M327T1067_neg	327.1269	1067	3	2.47E-01	1.22	FALSE	1.61E-03	0.53	TRUE	4.40E-02	0.74	FALSE	7.46E-01	1.12	FALSE
M328T639_neg	328.0863	639	3	1.47E-03	0.72	FALSE	3.24E-01	1.11	FALSE	8.88E-11	1.84	TRUE	2.77E-01	0.78	FALSE
M328T1034_neg	328.2495	1034	3	1.89E-03	0.49	TRUE	9.20E-01	1.02	FALSE	8.97E-01	1.03	FALSE	9.69E-01	0.98	FALSE
M329T521_neg	329.0817	521	3	1.40E-02	0.85	FALSE	4.43E-01	1.05	FALSE	9.68E-15	1.64	TRUE	4.21E-01	1.08	FALSE
M329T625_neg	329.1031	625	3	4.94E-11	2.39	TRUE	1.71E-01	0.84	FALSE	8.93E-01	1.01	FALSE	3.07E-01	0.74	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M329T705_neg	329.1606	705	3							HMDB0005796	Picrocrocin	C16H26O7	0.1
M329T1001_neg	329.2698	1001	3							HMDB0011533	MG(0:0/16:0/0:0)	C19H38O4	0.3
M330T510_neg	330.1671	510	3						Amino acids and Peptides				
M330T564_neg	330.2034	564	3							HMDB0014924	Marimastat	C15H29N3O5	0.2
M330T630_neg	330.2035	630	3						Amino acids and Peptides	HMDB0014924	Marimastat	C15H29N3O5	0.0
M331T462_neg	331.1187	462	3							HMDB0030664	3-Galloylcatechin	C18H20O6	0.1
M333T410_neg	333.0767	410	3							HMDB0252365	Fluorescin	C20H14O5	0.4
M333T666_neg	333.0993	666	3							HMDB0060479	Glutathione episulfonium ion	C12H20N3O6S	2.0
M333T607_neg	333.1342	607	3							HMDB0250411	Combretastatin	C18H22O6	0.5
M333T798_neg	333.1820	798	3							HMDB0256796	Proglumide	C18H26N2O4	0.1
M334T666_neg	334.1014	666	3							HMDB0248950	benfluralin	C13H16F3N3O4	1.9
M334T657_neg	334.1668	657	3							HMDB0242680	Integerrimine	C18H25NO5	2.5
M335T421_neg	335.0444	421	3							HMDB0059977	hydroxyphenyl)-valeric acid-O-me	C12H16O9S	0.6
M335T721_neg	335.1171	721	3							HMDB0003409	Berberine	C20H18NO4	2.4
M335T985_neg	335.2228	985	3						Terpenoids	HMDB0001085	Leukotriene B4	C20H32O4	0.2
M336T407_neg	336.0425	407	3							HMDB0249723	itro-alpha-((2,2,2-trifluoro-1-(triflu	C9H9F6N3O4	0.2
M336T655_neg	336.1817	655	3							HMDB0029325	3,6-Ditigloyloxytropan-7-ol	C18H27NO5	0.2
M339T468_neg	339.0724	468	3							HMDB0030820	Aesculin	C15H16O9	0.8
M339T439_neg	339.0933	439	3							HMDB0001030	25-Azacholesterol	C12H20O11	0.1
M339T840_neg	339.1020	840	3							HMDB0251443	Diphacinone	C23H16O3	1.9
M341T757_neg	341.1189	757	3							HMDB0060900	Clozapine N-oxide	C18H19ClN4O	4.2
M341T466_neg	341.1454	466	3						Carbohydrates				
M341T1002_neg	341.1760	1002	3							HMDB0029525	methoxyphenyl)-5-methoxy-1-phe	C21H26O4	0.5
M342T517_neg	342.0880	517	3							HMDB0259831	Violacein	C20H13N3O3	1.1
M342T355_neg	342.1195	355	3						Amino acids and Peptides	HMDB0037845	N-(1-Deoxy-1-fructosyl)tyrosine	C15H21NO8	0.3
M342T714_neg	342.1348	714	3							HMDB0039755	trans-Feruloyl-4-O-methyldopami	C19H21NO5	0.4
M342T773_neg	342.1709	773	3							HMDB0030211	(R)-Laudanidine	C20H25NO4	0.6
M342T1045_neg	342.2653	1045	3							HMDB0240804	8-Methylundecanoylcarnitine	C19H37NO4	0.9
M343T499_neg	343.0608	499	3							HMDB0257614	hoxy-1H-indol-3-yl)ethyl]amino]oxy	C13H16N2O7S	0.8
M343T703_neg	343.1189	703	3							HMDB0035029	Dehydrocyanaropicrin	C19H20O6	0.5
M343T784_neg	343.1191	784	3							HMDB0035029	Dehydrocyanaropicrin	C19H20O6	1.0
M343T1038_neg	343.2489	1038	3							HMDB0092900	DG(8:0/0:0/8:0)	C19H36O5	0.4
M344T386_1_neg	344.0403	386	3						Carbohydrates	HMDB0011683	Molybdopterin precursor Z	C10H12N5O7P	0.4
M345T388_neg	345.1416	388	3							HMDB0253972	Laninamivir	C13H22N4O7	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M329T705_neg	329.1606	705	3	3.60E-02	0.90	FALSE	1.69E-01	1.08	FALSE	1.05E-22	1.67	TRUE	4.12E-01	0.92	FALSE
M329T1001_neg	329.2698	1001	3	2.05E-10	2.28	TRUE	5.83E-02	0.80	FALSE	7.51E-01	0.97	FALSE	4.01E-02	1.35	FALSE
M330T510_neg	330.1671	510	3	8.92E-50	0.07	TRUE	8.37E-01	1.02	FALSE	1.13E-02	1.21	FALSE	7.83E-01	0.92	FALSE
M330T564_neg	330.2034	564	3	3.56E-48	0.14	TRUE	4.76E-01	1.06	FALSE	6.32E-05	1.32	FALSE	5.83E-01	0.85	FALSE
M330T630_neg	330.2035	630	3	3.92E-33	0.15	TRUE	5.39E-01	1.07	FALSE	9.26E-02	1.16	FALSE	1.07E-01	0.69	FALSE
M331T462_neg	331.1187	462	3	2.59E-27	2.13	TRUE	7.93E-01	1.02	FALSE	2.85E-03	0.86	FALSE	6.62E-01	0.95	FALSE
M333T410_neg	333.0767	410	3	7.49E-01	1.02	FALSE	4.94E-02	1.16	FALSE	1.85E-13	1.67	TRUE	3.63E-03	1.28	FALSE
M333T666_neg	333.0993	666	3	6.09E-05	0.78	FALSE	8.63E-01	1.01	FALSE	1.17E-15	1.58	TRUE	3.79E-02	1.38	FALSE
M333T607_neg	333.1342	607	3	2.43E-41	3.39	TRUE	2.47E-01	1.08	FALSE	8.15E-07	0.76	FALSE	5.14E-01	1.09	FALSE
M333T798_neg	333.1820	798	3	2.22E-01	1.12	FALSE	5.09E-10	0.53	TRUE	5.26E-01	0.95	FALSE	2.42E-02	1.33	FALSE
M334T666_neg	334.1014	666	3	3.32E-05	0.77	FALSE	5.08E-01	1.04	FALSE	4.41E-18	1.69	TRUE	2.20E-01	1.17	FALSE
M334T657_neg	334.1668	657	3	6.72E-09	0.55	TRUE	6.90E-01	1.04	FALSE	3.70E-03	0.78	FALSE	6.74E-01	0.82	FALSE
M335T421_neg	335.0444	421	3	7.84E-01	0.97	FALSE	1.55E-03	1.37	FALSE	1.60E-11	1.83	TRUE	3.95E-03	1.46	FALSE
M335T721_neg	335.1171	721	3	1.87E-03	0.85	FALSE	4.78E-01	1.04	FALSE	2.92E-17	1.53	TRUE	6.81E-01	0.95	FALSE
M335T985_neg	335.2228	985	3	8.65E-05	1.85	TRUE	6.49E-01	1.07	FALSE	1.92E-01	1.19	FALSE	9.19E-01	0.99	FALSE
M336T407_neg	336.0425	407	3	1.24E-05	0.18	TRUE	4.16E-01	1.32	FALSE	8.13E-01	1.07	FALSE	9.07E-01	1.16	FALSE
M336T655_neg	336.1817	655	3	2.29E-19	2.10	TRUE	9.35E-01	1.01	FALSE	1.16E-05	0.76	FALSE	3.30E-01	1.19	FALSE
M339T468_neg	339.0724	468	3	5.42E-06	0.67	FALSE	9.65E-01	1.00	FALSE	9.87E-18	2.07	TRUE	7.65E-01	1.05	FALSE
M339T439_neg	339.0933	439	3	1.01E-11	0.09	TRUE	9.88E-01	1.00	FALSE	1.60E-01	1.33	FALSE	3.16E-02	1.41	FALSE
M339T840_neg	339.1020	840	3	5.02E-03	0.67	FALSE	6.10E-01	0.93	FALSE	3.17E-05	1.69	TRUE	6.32E-02	1.66	FALSE
M341T757_neg	341.1189	757	3	1.17E-01	1.27	FALSE	4.46E-01	0.89	FALSE	2.61E-03	1.51	TRUE	4.18E-01	0.87	FALSE
M341T466_neg	341.1454	466	3	3.18E-10	1.95	TRUE	2.13E-01	0.88	FALSE	1.71E-03	0.76	FALSE	2.82E-01	0.73	FALSE
M341T1002_neg	341.1760	1002	3	4.85E-05	17.60	TRUE	3.05E-01	0.68	FALSE	1.29E-01	1.80	FALSE	7.09E-01	0.95	FALSE
M342T517_neg	342.0880	517	3	7.23E-01	0.96	FALSE	3.48E-01	0.88	FALSE	8.27E-03	0.78	FALSE	5.44E-04	1.65	TRUE
M342T355_neg	342.1195	355	3	3.39E-07	0.02	TRUE	9.25E-01	1.04	FALSE	7.48E-01	1.11	FALSE	9.29E-01	0.98	FALSE
M342T714_neg	342.1348	714	3	1.43E-28	2.43	TRUE	2.47E-01	0.93	FALSE	7.91E-01	1.01	FALSE	2.83E-02	0.77	FALSE
M342T773_neg	342.1709	773	3	1.35E-04	0.81	FALSE	6.03E-01	1.03	FALSE	5.34E-17	1.55	TRUE	4.40E-02	0.85	FALSE
M342T1045_neg	342.2653	1045	3	2.06E-05	0.46	TRUE	3.90E-01	0.86	FALSE	5.85E-01	0.92	FALSE	5.42E-01	1.21	FALSE
M343T499_neg	343.0608	499	3	6.63E-01	0.94	FALSE	4.92E-01	1.10	FALSE	8.81E-09	2.14	TRUE	8.80E-01	0.98	FALSE
M343T703_neg	343.1189	703	3	7.02E-32	2.14	TRUE	4.96E-01	0.96	FALSE	5.55E-01	1.03	FALSE	7.31E-01	0.96	FALSE
M343T784_neg	343.1191	784	3	5.12E-32	7.12	TRUE	2.76E-01	1.12	FALSE	1.79E-02	0.80	FALSE	4.41E-01	0.84	FALSE
M343T1038_neg	343.2489	1038	3	6.21E-01	1.05	FALSE	1.93E-04	0.67	TRUE	9.38E-01	0.99	FALSE	7.42E-01	0.93	FALSE
M344T386_1_neg	344.0403	386	3	3.27E-23	0.02	TRUE	8.51E-01	1.03	FALSE	7.35E-01	0.95	FALSE	7.16E-01	1.45	FALSE
M345T388_neg	345.1416	388	3	2.50E-05	0.72	FALSE	3.06E-01	1.08	FALSE	2.46E-22	2.14	TRUE	7.41E-02	0.78	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M345T953_neg	345.1708	953	3							HMDB0032819	Gibberellin A113	C20H26O5	0.1
M345T448_neg	345.1782	448	3						Amino acids and Peptides				
M346T801_neg	346.1298	801	3							HMDB0255456	Naproxcinod	C18H21NO6	0.4
M347T435_neg	347.1368	435	3							HMDB0256703	Porfiromycin	C16H20N4O5	2.0
M348T787_neg	348.1926	787	3							HMDB0029225	Coutaric acid	C18H27N3O4	0.7
M349T602_neg	349.0598	602	3						Shikimates and Phenylpropanoids	HMDB0256891	propyl-3,7-dihydropurin-8-yl)benze	C14H14N4O5S	4.1
M349T613_neg	349.1405	613	3						Alkaloids				
M351T810_neg	351.1389	810	3							HMDB0244814	,4,5,5-tetramethylimidazoline-1-o	C25H20O2	0.3
M352T576_neg	352.1038	576	3							HMDB0035502	Licoagrochalcone B	C16H19NO8	0.0
M354T417_neg	354.1561	417	3							HMDB0253057	,3,6-tetrahydro-7H-purin-7-yl)-N-(	C18H21N5O3	3.0
M355T676_neg	355.1045	676	3							HMDB0254997	4-Dinitrophenyl)-5-methoxytrypta	C17H16N4O5	0.8
M356T885_neg	356.2079	885	3							HMDB0241173	Undec-5-enedioylcarnitine	C18H31NO6	0.2
M357T482_neg	357.0802	482	3							HMDB0244735	iphenyl-1H-imidazol-2-yl)benzoyl (	C22H15ClN2O	0.4
M357T719_neg	357.0982	719	3							HMDB0034218	Chrysoobtusin	C19H18O7	0.7
M357T955_neg	357.1740	955	3							HMDB0257242	Rislenemdaz	C19H23FN4O2	2.1
M358T971_neg	358.1766	971	3							HMDB0253741	droxyacetyl)pyrrolidine-1-carbonyl	C19H25N3O4	1.6
M360T784_neg	360.1091	784	3							HMDB0029297	Avenanthramide A2	C18H19NO7	0.6
M360T361_neg	360.1303	361	3							HMDB0041208	De-O-methylsimmondsin	C15H23NO9	0.9
M361T834_neg	361.1661	834	3							HMDB0013692	Secoisolariciresinol	C20H26O6	1.1
M362T774_neg	362.1722	774	3							HMDB0254077	Libenzapril	C18H25N3O5	0.0
M363T823_neg	363.1450	823	3							HMDB0033420	Gibberellin A55	C19H24O7	0.3
M365T913_neg	365.1970	913	3						Terpenoids	HMDB0006059	20-Carboxy-leukotriene B4	C20H30O6	0.2
M367T979_neg	367.1585	979	3							HMDB0247812	racyclo[8.7.0.0^{2,7}.0^{11,15}]he	C19H28O5S	0.2
M369T638_neg	369.1129	638	3							HMDB0245794	trazol-5-YL)-3-pyridinyl]phenyl]-5-	C17H15FN6O3	3.2
M369T422_neg	369.1404	422	3						Carbohydrates	HMDB0032197	Cellulose, microcrystalline	C14H26O11	0.5
M370T639_neg	370.1158	639	3							HMDB0062374	hydroxyphenyl)-4-oxobutanoic aci	C16H21NO9	4.0
M370T604_neg	370.1615	604	3							HMDB0254009	Lenperone	C22H23F2NO2	2.5
M370T1072_neg	370.2968	1072	3							HMDB0240823	4-Methyltridecanoylcarnitine	C21H41NO4	1.3
M371T706_neg	371.0774	706	3							HMDB0060620	Sulindac sulfone	C20H17FO4S	4.1
M371T772_neg	371.1284	772	3							HMDB0259582	,4-difluorophenyl)methyl)-4-piper	C17H17F5N4	4.6
M372T625_neg	372.2141	625	3						Amino acids and Peptides				
M372T1042_neg	372.2755	1042	3							HMDB0061639	3-hydroxytridecanoyl carnitine	C20H39NO5	0.2
M373T1033_neg	373.1271	1033	3							HMDB0040912	-Hydroxy-2-pyridinyl)methyl]aden	C16H18N6O5	1.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M345T953_neg	345.1708	953	3	5.58E-03	1.34	FALSE	5.11E-01	0.93	FALSE	5.83E-13	2.09	TRUE	7.30E-01	0.96	FALSE
M345T448_neg	345.1782	448	3	1.71E-36	0.09	TRUE	8.13E-01	1.03	FALSE	1.34E-01	1.15	FALSE	4.57E-01	0.75	FALSE
M346T801_neg	346.1298	801	3	4.94E-08	0.67	FALSE	9.60E-01	1.00	FALSE	4.25E-16	1.73	TRUE	3.75E-01	1.14	FALSE
M347T435_neg	347.1368	435	3	9.16E-01	1.01	FALSE	1.25E-02	1.19	FALSE	5.11E-15	1.64	TRUE	8.26E-01	1.02	FALSE
M348T787_neg	348.1926	787	3	2.34E-17	0.60	TRUE	4.02E-11	1.45	FALSE	6.85E-07	1.27	FALSE	6.27E-01	1.05	FALSE
M349T602_neg	349.0598	602	3	3.47E-02	0.83	FALSE	7.31E-01	1.03	FALSE	1.38E-09	1.65	TRUE	1.77E-01	1.41	FALSE
M349T613_neg	349.1405	613	3	1.37E-01	0.88	FALSE	2.49E-01	0.90	FALSE	7.80E-11	1.69	TRUE	9.84E-02	1.30	FALSE
M351T810_neg	351.1389	810	3	4.11E-10	1.92	TRUE	1.43E-05	0.67	FALSE	3.90E-06	1.50	FALSE	3.65E-01	0.90	FALSE
M352T576_neg	352.1038	576	3	3.78E-06	0.71	FALSE	5.82E-01	1.04	FALSE	4.83E-10	1.52	TRUE	3.72E-01	0.87	FALSE
M354T417_neg	354.1561	417	3	6.24E-01	1.09	FALSE	9.82E-01	1.00	FALSE	1.50E-07	2.53	TRUE	1.75E-01	0.70	FALSE
M355T676_neg	355.1045	676	3	6.92E-01	1.04	FALSE	8.13E-01	1.02	FALSE	2.33E-06	1.52	TRUE	6.58E-01	1.04	FALSE
M356T885_neg	356.2079	885	3	6.76E-01	0.94	FALSE	5.55E-02	1.33	FALSE	1.71E-06	1.86	TRUE	7.56E-01	1.05	FALSE
M357T482_neg	357.0802	482	3	4.75E-11	0.44	TRUE	2.85E-01	1.13	FALSE	4.13E-03	1.33	FALSE	1.37E-01	1.19	FALSE
M357T719_neg	357.0982	719	3	1.38E-06	0.72	FALSE	6.33E-02	1.14	FALSE	1.15E-24	2.00	TRUE	3.78E-01	1.10	FALSE
M357T955_neg	357.1740	955	3	6.98E-03	2.15	TRUE	3.76E-01	1.24	FALSE	2.61E-01	1.30	FALSE	2.90E-01	0.60	FALSE
M358T971_neg	358.1766	971	3	1.89E-03	5.08	TRUE	7.32E-01	1.13	FALSE	5.60E-02	2.11	FALSE	1.22E-01	0.33	FALSE
M360T784_neg	360.1091	784	3	2.05E-48	2.91	TRUE	4.41E-13	0.68	FALSE	3.12E-07	0.80	FALSE	4.62E-01	0.93	FALSE
M360T361_neg	360.1303	361	3	9.85E-01	1.00	FALSE	2.76E-01	1.12	FALSE	8.04E-11	1.84	TRUE	3.92E-02	1.18	FALSE
M361T834_neg	361.1661	834	3	3.79E-01	0.94	FALSE	5.54E-04	1.30	FALSE	4.03E-11	1.56	TRUE	9.10E-01	1.02	FALSE
M362T774_neg	362.1722	774	3	5.27E-05	0.73	FALSE	6.79E-01	0.96	FALSE	5.61E-11	1.60	TRUE	3.96E-01	0.76	FALSE
M363T823_neg	363.1450	823	3	1.24E-04	0.75	FALSE	3.17E-01	1.08	FALSE	2.56E-18	1.90	TRUE	7.38E-02	0.83	FALSE
M365T913_neg	365.1970	913	3	7.08E-07	0.71	FALSE	2.50E-01	1.08	FALSE	3.72E-14	1.62	TRUE	4.69E-01	0.95	FALSE
M367T979_neg	367.1585	979	3	5.38E-02	2.17	FALSE	5.93E-01	0.76	FALSE	4.15E-02	0.49	TRUE	9.28E-01	1.08	FALSE
M369T638_neg	369.1129	638	3	1.44E-01	0.85	FALSE	5.66E-01	1.07	FALSE	1.24E-06	1.67	TRUE	2.90E-01	0.77	FALSE
M369T422_neg	369.1404	422	3	1.53E-04	1.60	TRUE	3.22E-01	0.88	FALSE	5.68E-01	0.94	FALSE	3.45E-01	0.72	FALSE
M370T639_neg	370.1158	639	3	5.65E-02	0.82	FALSE	9.45E-01	1.01	FALSE	1.25E-07	1.68	TRUE	3.52E-01	0.78	FALSE
M370T604_neg	370.1615	604	3	1.81E-01	1.11	FALSE	7.37E-04	1.32	FALSE	4.10E-10	1.58	TRUE	7.52E-01	1.04	FALSE
M370T1072_neg	370.2968	1072	3	1.14E-02	1.96	TRUE	9.91E-02	0.62	FALSE	7.54E-01	0.93	FALSE	6.98E-01	1.12	FALSE
M371T706_neg	371.0774	706	3	1.04E-01	1.17	FALSE	8.62E-01	1.02	FALSE	1.42E-04	1.39	FALSE	2.63E-02	0.41	TRUE
M371T772_neg	371.1284	772	3	1.64E-22	0.28	TRUE	1.83E-01	1.15	FALSE	7.89E-04	1.35	FALSE	6.06E-01	1.06	FALSE
M372T625_neg	372.2141	625	3	3.85E-61	0.06	TRUE	2.77E-01	1.09	FALSE	8.60E-04	1.24	FALSE	4.18E-01	0.68	FALSE
M372T1042_neg	372.2755	1042	3	1.96E-13	0.63	TRUE	1.43E-09	1.44	FALSE	6.60E-04	0.84	FALSE	6.14E-02	0.77	FALSE
M373T1033_neg	373.1271	1033	3	1.00E-01	1.30	FALSE	1.42E-03	0.56	TRUE	2.53E-01	0.85	FALSE	8.73E-01	0.94	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M377T751_neg	377.0817	751	3							HMDB0014717	Carbenicillin	C17H18N2O6S	1.1
M377T462_neg	377.1245	462	3							HMDB0029304	3,4-DHPEA-EA	C19H22O8	0.8
M377T564_neg	377.1248	564	3							HMDB0029304	3,4-DHPEA-EA	C19H22O8	1.7
M377T844_neg	377.1608	844	3							HMDB0030657	Carinol	C20H26O7	0.6
M379T587_neg	379.0983	587	3							HMDB0015541	Meticillin	C17H20N2O6S	3.7
M381T867_neg	381.1921	867	3							HMDB0012553	2-Oxo-20-trihydroxy-leukotriene B	C20H30O7	0.7
M382T495_neg	382.1008	495	3						Carbohydrates	HMDB0000912	Succinyladenosine	C14H17N5O8	1.0
M382T867_neg	382.1954	867	3							HMDB0254167	Losmapimod	C22H26FN3O2	4.7
M383T1001_neg	383.3280	1001	3							HMDB0241929	N-Palmitoyl Lysine	C22H44N2O3	0.3
M385T803_1_neg	385.0386	803	3							HMDB0247239	hydroxy-5-(2-fluorophenyl)-1,3-dih	C17H11ClF4N2O2	3.5
M387T364_neg	387.1559	364	3							HMDB0014545	Nisoldipine	C20H24N2O6	0.6
M387T603_neg	387.1662	603	3						Fatty acids	HMDB0039964	-Glucopyranosyl-11-hydroxyjasmo	C18H28O9	0.5
M387T772_neg	387.1816	772	3							HMDB0030711	Cyclomammein	C22H28O6	0.7
M388T604_neg	388.1695	604	3							HMDB0255769	Ilginatini	C21H20FN7	1.0
M388T510_neg	388.1726	510	3						Amino acids and Peptides				
M389T760_neg	389.1245	760	3							HMDB0030564	trans-Piceid	C20H22O8	0.7
M391T1034_neg	391.2129	1034	3							HMDB0034662	Dihydrofukinolide	C22H32O6	0.6
M391T984_neg	391.2854	984	3						Terpenoids	HMDB0000348	3b,12a-Dihydroxy-5a-cholanoic aci	C24H40O4	0.1
M392T504_neg	392.1200	504	3							HMDB0249089	Besifloxacin	C19H21ClFN3O3	4.4
M393T919_neg	393.1951	919	3						Fatty acids	HMDB0247300	l-7H-pyrimido[4,5-b][1,4]oxazin-6-	C22H26N4O3	4.9
M397T558_neg	397.1553	558	3							HMDB0249303	lohexylamino)-N-(((1,1-dimethylet	C17H26N4O5S	0.5
M398T701_neg	398.2186	701	3							HMDB0249582	Candoxatrilat	C20H33NO7	0.5
M401T662_neg	401.1818	662	3							HMDB0031763	yl 7-epi-12-hydroxyjasmonate gluc	C19H30O9	0.2
M401T1079_neg	401.2911	1079	3							HMDB0029887	Sorbitan palmitate	C22H42O6	0.5
M403T841_1_neg	403.1005	841	3							HMDB0253567	Ipragliflozin	C21H21FO5S	3.9
M403T841_2_neg	403.2488	841	3							HMDB0000447	12a-Dihydroxy-3-oxo-4-cholenoic a	C24H36O5	0.5
M407T984_neg	407.2804	984	3						Terpenoids	HMDB0000312	pha,12beta-Trihydroxy-5beta-cho	C24H40O5	0.3
M408T434_neg	408.1514	434	3							HMDB0060454	Chondroitin D-glucuronate	C16H27NO11	0.5
M409T846_neg	409.1408	846	3							HMDB0250871	Darusentan	C22H22N2O6	0.8
M409T805_neg	409.1777	805	3							HMDB0042005	Quinaprilat	C23H26N2O5	2.1
M410T805_neg	410.1806	805	3							HMDB0253755	enyl)amino]-5,6-dihydro-8,8-dime	C22H23F2N5O	2.1
M411T809_neg	411.1935	809	3							HMDB0256185	9-ethoxy-8-methoxy-1,2,3,4,4a,10b	C23H28N2O5	2.4
M411T745_neg	411.1930	745	3							HMDB0256185	9-ethoxy-8-methoxy-1,2,3,4,4a,10b	C23H28N2O5	1.2
M413T1062_neg	413.1591	1062	3							HMDB0029511	Garcinone C	C23H26O7	3.6
M413T770_neg	413.2085	770	3							HMDB0247263	7-Hydroxymitragynine	C23H30N2O5	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M377T751_neg	377.0817	751	3	3.71E-04	0.68	FALSE	4.24E-01	0.91	FALSE	6.68E-10	1.84	TRUE	1.77E-01	1.50	FALSE
M377T462_neg	377.1245	462	3	1.91E-18	3.10	TRUE	7.05E-01	0.96	FALSE	2.11E-02	0.81	FALSE	9.21E-01	1.02	FALSE
M377T564_neg	377.1248	564	3	1.37E-40	2.77	TRUE	2.95E-01	1.06	FALSE	1.45E-01	0.93	FALSE	3.45E-01	0.90	FALSE
M377T844_neg	377.1608	844	3	4.07E-08	0.76	FALSE	3.82E-02	1.11	FALSE	7.00E-23	1.60	TRUE	8.80E-02	0.89	FALSE
M379T587_neg	379.0983	587	3	4.42E-04	1.50	FALSE	6.23E-01	0.94	FALSE	1.61E-04	0.68	FALSE	8.51E-03	1.71	TRUE
M381T867_neg	381.1921	867	3	7.09E-04	0.82	FALSE	5.84E-02	1.12	FALSE	3.21E-23	1.80	TRUE	6.76E-01	0.97	FALSE
M382T495_neg	382.1008	495	3	1.36E-18	0.26	TRUE	8.82E-01	0.98	FALSE	1.68E-03	1.40	FALSE	5.15E-01	1.13	FALSE
M382T867_neg	382.1954	867	3	3.13E-06	0.74	FALSE	1.13E-01	1.11	FALSE	2.64E-24	1.92	TRUE	5.86E-01	1.04	FALSE
M383T1001_neg	383.3280	1001	3	7.11E-10	2.19	TRUE	1.51E-03	0.70	FALSE	1.09E-03	1.40	FALSE	8.11E-01	0.97	FALSE
M385T803_1_neg	385.0386	803	3	1.84E-17	2.17	TRUE	5.58E-01	1.05	FALSE	3.90E-01	0.94	FALSE	2.26E-01	1.20	FALSE
M387T364_neg	387.1559	364	3	9.84E-02	0.76	FALSE	5.68E-01	0.90	FALSE	7.21E-06	1.96	TRUE	6.46E-01	0.91	FALSE
M387T603_neg	387.1662	603	3	1.29E-01	1.85	FALSE	7.58E-01	0.86	FALSE	4.45E-02	2.05	TRUE	1.54E-01	4.06	FALSE
M387T772_neg	387.1816	772	3	9.84E-09	2.81	TRUE	4.75E-01	1.12	FALSE	5.57E-01	1.08	FALSE	9.99E-01	1.00	FALSE
M388T604_neg	388.1695	604	3	1.38E-01	1.74	FALSE	8.59E-01	0.92	FALSE	2.99E-02	2.06	TRUE	1.23E-01	4.15	FALSE
M388T510_neg	388.1726	510	3	5.35E-69	0.04	TRUE	8.66E-01	0.99	FALSE	4.64E-10	1.47	FALSE	6.61E-01	1.13	FALSE
M389T760_neg	389.1245	760	3	9.76E-02	0.87	FALSE	4.50E-01	1.07	FALSE	2.83E-12	1.72	TRUE	5.56E-01	0.94	FALSE
M391T1034_neg	391.2129	1034	3	2.98E-02	1.28	FALSE	8.42E-01	1.02	FALSE	3.67E-09	1.88	TRUE	2.72E-01	0.85	FALSE
M391T984_neg	391.2854	984	3	7.22E-14	1.67	TRUE	2.72E-07	0.71	FALSE	3.36E-02	0.89	FALSE	7.45E-01	0.95	FALSE
M392T504_neg	392.1200	504	3	2.29E-29	0.26	TRUE	8.46E-01	1.02	FALSE	2.63E-01	1.09	FALSE	3.18E-01	1.15	FALSE
M393T919_neg	393.1951	919	3	1.31E-03	0.77	FALSE	4.97E-02	1.18	FALSE	1.58E-11	1.64	TRUE	4.05E-01	0.89	FALSE
M397T558_neg	397.1553	558	3	2.29E-01	0.89	FALSE	4.23E-01	1.09	FALSE	1.87E-07	1.62	TRUE	5.20E-01	0.83	FALSE
M398T701_neg	398.2186	701	3	5.97E-06	1.53	TRUE	1.08E-01	1.16	FALSE	7.50E-01	1.03	FALSE	3.72E-01	1.13	FALSE
M401T662_neg	401.1818	662	3	2.65E-07	0.71	FALSE	2.48E-01	1.08	FALSE	1.16E-23	1.95	TRUE	4.78E-03	0.71	FALSE
M401T1079_neg	401.2911	1079	3	1.01E-01	1.59	FALSE	1.92E-01	0.59	FALSE	1.04E-05	3.39	TRUE	2.42E-01	0.79	FALSE
M403T841_1_neg	403.1005	841	3	1.21E-46	0.05	TRUE	1.72E-01	1.14	FALSE	6.38E-04	1.33	FALSE	8.46E-01	1.10	FALSE
M403T841_2_neg	403.2488	841	3	3.62E-03	1.22	FALSE	1.54E-03	1.25	FALSE	5.17E-12	1.55	TRUE	2.29E-01	0.88	FALSE
M407T984_neg	407.2804	984	3	1.62E-02	1.54	TRUE	3.75E-01	0.83	FALSE	1.73E-01	0.81	FALSE	7.35E-01	0.84	FALSE
M408T434_neg	408.1514	434	3	9.63E-01	1.01	FALSE	4.82E-02	1.33	FALSE	6.34E-12	2.50	TRUE	4.91E-03	1.47	FALSE
M409T846_neg	409.1408	846	3	7.85E-07	0.68	FALSE	3.37E-01	1.08	FALSE	5.84E-19	1.97	TRUE	8.00E-01	0.98	FALSE
M409T805_neg	409.1777	805	3	1.22E-04	1.81	TRUE	3.73E-01	0.88	FALSE	6.26E-02	1.27	FALSE	6.66E-01	1.04	FALSE
M410T805_neg	410.1806	805	3	7.47E-05	2.01	TRUE	2.98E-01	0.85	FALSE	3.21E-02	1.37	FALSE	8.63E-01	0.98	FALSE
M411T809_neg	411.1935	809	3	1.80E-03	1.47	FALSE	6.83E-04	0.66	TRUE	4.18E-03	0.74	FALSE	5.08E-01	0.91	FALSE
M411T745_neg	411.1930	745	3	5.86E-02	0.70	FALSE	2.37E-03	1.86	TRUE	8.43E-02	1.33	FALSE	8.89E-01	1.04	FALSE
M413T1062_neg	413.1591	1062	3	7.62E-02	1.44	FALSE	2.42E-01	0.78	FALSE	1.31E-02	1.56	TRUE	9.56E-02	1.98	FALSE
M413T770_neg	413.2085	770	3	4.58E-01	0.90	FALSE	1.57E-04	1.86	TRUE	5.12E-02	1.29	FALSE	9.08E-01	1.06	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M414T1077_neg	414.1714	1077	3							HMDB0244387	ic acid, 2-(((2-methoxyphenyl)acet	C26H25NO4	0.7
M414T783_neg	414.1672	783	3							HMDB0257434	Sabeluzole	C22H26FN3O2S	3.7
M419T656_neg	419.1712	656	3						Polyketides	HMDB0034876	Castaneiolide	C22H28O8	0.2
M419T1048_neg	419.3168	1048	3							HMDB0247056	6-Ethylchenodeoxycholic acid	C26H44O4	0.3
M425T1007_neg	425.2472	1007	3							HMDB0251636	Dual-release hydrocortisone	C22H38N2O4S	1.7
M429T784_neg	429.0649	784	3							HMDB0248294	ifluoromethyl)phenyl)-4-pyrimidin	C20H13F3N4O2S	2.5
M431T821_neg	431.1823	821	3							HMDB0259867	Vofopitant	C21H23F3N6O	2.4
M433T608_neg	433.1652	608	3							HMDB0041166	Cycloartocarpin	C26H26O6	1.0
M436T836_neg	436.2244	836	3							HMDB0033469	N1,N10-Dicoumaroylspermidine	C25H31N3O4	0.5
M438T946_neg	438.1662	946	3							HMDB0254003	Lefradafibanum	C23H25N3O6	1.9
M450T1068_neg	450.1718	1068	3							HMDB0259671	phenyl)methylcarbamoyl)-4-meth	C26H26FNO5	0.9
M453T708_neg	453.1671	708	3							HMDB0257679	-phenylbutan-2-yl]amino]-2-oxo-4	C24H26N2O7	0.9
M453T984_neg	453.2859	984	3						Terpenoids	HMDB0296939	(2:0/20:3(8Z,11Z,14Z)-2OH(5,6)/0	C25H42O7	0.3
M462T1000_neg	462.3245	1000	3							HMDB0240765	3-Hydroxyarachidonoylcarnitine	C27H45NO5	4.3
M464T1068_neg	464.1511	1068	3							HMDB0015540	Bacampicillin	C21H27N3O7S	3.0
M466T1062_neg	466.2946	1062	3						Fatty acids	HMDB0010379	LysoPC(14:0/0:0)	C22H46NO7P	1.4
M477T827_neg	477.1704	827	3						Alkaloids				
M477T762_neg	477.2360	762	3							HMDB0258351	xy)benzyl]-4-piperidinyl}-4-methyl	C29H32F2N2O2	0.2
M479T1013_neg	479.3379	1013	3							HMDB0034081	Brassinolide	C28H48O6	0.1
M487T985_neg	487.3428	985	3							HMDB0034036	Pitheduloside I	C30H48O5	0.2
M487T930_neg	487.3429	930	3							HMDB0034036	Pitheduloside I	C30H48O5	0.0
M491T705_neg	491.2288	705	3							HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.4
M493T569_neg	493.2307	569	3							HMDB0041054	Ustiloxin D	C23H34N4O8	0.6
M493T834_neg	493.2445	834	3							HMDB0033655	7-(3-methylpentanoate) 11-(3-hyd	C26H38O9	0.4
M495T709_neg	495.2238	709	3							HMDB0035626	Glaucarubin	C25H36O10	0.5
M497T999_neg	497.3485	999	3						Terpenoids				
M498T866_neg	498.2610	866	3							HMDB0248778	Osimertini	C28H33N7O2	2.7
M502T874_neg	502.3179	874	3							HMDB0241613	9Z)-7,17-Dihydroxydocosa-5,8,10,	C29H45NO6	1.0
M503T456_neg	503.1985	456	3						Carbohydrates				
M503T1007_neg	503.2625	1007	3							HMDB0246702	Phorbol-12,13-dibutyrate	C28H40O8	5.0
M505T714_neg	505.1356	714	3							HMDB0037352	Caryatin glucoside	C24H26O12	0.9
M507T1073_neg	507.3328	1073	3							HMDB0250439	Contignasterol	C29H48O7	0.2
M515T834_neg	515.2289	834	3							HMDB0030005	Austalide A	C28H36O9	0.6
M517T313_neg	517.1777	313	3							HMDB0032777	Ciceritol	C19H34O16	0.7
M520T1049_neg	520.2658	1049	3							HMDB0240604	LysoPS(18:2(9Z,12Z)/0:0)	C24H44NO9P	4.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M414T1077_neg	414.1714	1077	3	2.79E-03	0.63	TRUE	9.44E-01	0.99	FALSE	5.20E-01	1.09	FALSE	9.55E-02	1.73	FALSE
M414T783_neg	414.1672	783	3	2.65E-03	0.63	TRUE	5.89E-01	1.09	FALSE	2.55E-01	1.16	FALSE	7.04E-01	0.91	FALSE
M419T656_neg	419.1712	656	3	3.23E-05	3.26	TRUE	5.03E-01	0.85	FALSE	3.11E-01	1.25	FALSE	4.97E-01	0.82	FALSE
M419T1048_neg	419.3168	1048	3	8.60E-11	1.88	TRUE	1.40E-03	0.74	FALSE	2.58E-04	1.34	FALSE	5.73E-01	1.12	FALSE
M425T1007_neg	425.2472	1007	3	2.52E-01	1.17	FALSE	4.87E-01	0.90	FALSE	6.18E-05	1.66	TRUE	8.57E-01	0.94	FALSE
M429T784_neg	429.0649	784	3	1.57E-31	3.02	TRUE	2.54E-03	0.80	FALSE	1.06E-01	0.90	FALSE	9.40E-01	0.99	FALSE
M431T821_neg	431.1823	821	3	9.35E-01	0.99	FALSE	1.77E-08	1.58	TRUE	1.53E-01	1.10	FALSE	3.33E-02	1.42	FALSE
M433T608_neg	433.1652	608	3	9.28E-02	1.26	FALSE	7.08E-01	0.95	FALSE	2.35E-11	2.48	TRUE	9.02E-01	1.02	FALSE
M436T836_neg	436.2244	836	3	3.68E-03	1.37	FALSE	1.17E-04	1.52	TRUE	7.38E-02	1.18	FALSE	1.98E-01	0.77	FALSE
M438T946_neg	438.1662	946	3	1.40E-15	2.85	TRUE	1.13E-01	0.84	FALSE	1.98E-01	1.13	FALSE	6.14E-01	0.93	FALSE
M450T1068_neg	450.1718	1068	3	3.51E-02	1.49	FALSE	4.17E-05	0.35	TRUE	1.81E-01	1.25	FALSE	1.91E-01	2.38	FALSE
M453T708_neg	453.1671	708	3	4.63E-01	0.94	FALSE	7.07E-01	1.03	FALSE	8.20E-15	1.83	TRUE	9.24E-01	1.02	FALSE
M453T984_neg	453.2859	984	3	1.06E-01	1.57	FALSE	3.34E-01	0.71	FALSE	4.07E-02	0.61	TRUE	8.17E-01	0.82	FALSE
M462T1000_neg	462.3245	1000	3	1.75E-12	2.86	TRUE	6.31E-01	0.94	FALSE	9.40E-02	1.21	FALSE	2.65E-01	1.21	FALSE
M464T1068_neg	464.1511	1068	3	3.30E-01	1.16	FALSE	1.73E-03	0.55	TRUE	4.26E-01	1.11	FALSE	1.20E-01	2.62	FALSE
M466T1062_neg	466.2946	1062	3	7.56E-01	0.94	FALSE	5.89E-01	0.89	FALSE	3.43E-05	2.14	TRUE	4.73E-01	0.89	FALSE
M477T827_neg	477.1704	827	3	1.41E-03	0.63	TRUE	2.29E-02	0.72	FALSE	1.34E-01	1.20	FALSE	2.40E-01	1.37	FALSE
M477T762_neg	477.2360	762	3	1.01E-08	0.17	TRUE	3.71E-01	1.25	FALSE	5.18E-01	1.14	FALSE	8.11E-01	0.97	FALSE
M479T1013_neg	479.3379	1013	3	8.99E-12	1.98	TRUE	6.71E-04	0.74	FALSE	1.77E-03	1.29	FALSE	4.81E-01	0.87	FALSE
M487T985_neg	487.3428	985	3	1.70E-07	1.52	TRUE	9.40E-03	0.81	FALSE	5.75E-02	1.13	FALSE	6.18E-02	3.02	FALSE
M487T930_neg	487.3429	930	3	1.07E-15	1.56	TRUE	1.66E-05	0.79	FALSE	1.01E-02	1.12	FALSE	1.57E-01	1.18	FALSE
M491T705_neg	491.2288	705	3	1.04E-07	-3.30	FALSE	1.75E-04	0.30	TRUE	4.24E-04	-0.03	FALSE	6.54E-01	1.10	FALSE
M493T569_neg	493.2307	569	3	3.57E-36	0.13	TRUE	1.82E-01	1.15	FALSE	9.71E-04	1.33	FALSE	6.32E-01	1.23	FALSE
M493T834_neg	493.2445	834	3	1.81E-01	0.88	FALSE	3.51E-01	1.10	FALSE	1.76E-08	1.62	TRUE	9.94E-01	1.00	FALSE
M495T709_neg	495.2238	709	3	1.97E-02	0.83	FALSE	6.99E-01	1.03	FALSE	1.15E-08	1.52	TRUE	9.02E-01	1.02	FALSE
M497T999_neg	497.3485	999	3	1.00E-08	2.07	TRUE	3.54E-02	0.78	FALSE	6.67E-01	1.04	FALSE	1.68E-02	0.68	FALSE
M498T866_neg	498.2610	866	3	1.49E-03	0.60	TRUE	5.65E-01	1.09	FALSE	3.20E-01	1.14	FALSE	3.53E-02	1.29	FALSE
M502T874_neg	502.3179	874	3	6.04E-02	1.24	FALSE	4.59E-05	0.63	TRUE	2.10E-03	0.73	FALSE	3.47E-01	1.23	FALSE
M503T456_neg	503.1985	456	3	4.18E-08	1.90	TRUE	1.51E-01	1.19	FALSE	5.41E-02	0.83	FALSE	7.42E-01	0.86	FALSE
M503T1007_neg	503.2625	1007	3	1.66E-04	1.45	FALSE	2.28E-01	1.13	FALSE	2.67E-07	1.57	TRUE	9.00E-01	0.97	FALSE
M505T714_neg	505.1356	714	3	2.74E-01	1.98	FALSE	9.46E-01	0.94	FALSE	9.07E-03	5.40	TRUE	9.90E-01	1.01	FALSE
M507T1073_neg	507.3328	1073	3	2.92E-02	1.94	TRUE	3.14E-01	0.74	FALSE	1.93E-01	1.40	FALSE	9.43E-01	0.98	FALSE
M515T834_neg	515.2289	834	3	8.57E-01	0.95	FALSE	1.36E-02	0.36	TRUE	1.76E-01	1.43	FALSE	1.67E-01	1.21	FALSE
M517T313_neg	517.1777	313	3	7.94E-02	0.69	FALSE	5.70E-01	1.14	FALSE	6.25E-04	1.94	TRUE	2.02E-01	0.37	FALSE
M520T1049_neg	520.2658	1049	3	9.14E-01	0.99	FALSE	1.09E-01	0.79	FALSE	3.32E-02	1.28	FALSE	2.42E-02	0.39	TRUE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M520T975_neg	520.3288	975	3						Terpenoids	HMDB0242405	Chenodeoxycholylglutamic acid	C29H47NO7	1.6
M523T745_neg	523.2546	745	3							HMDB0250421	phenylpropyl)-N6-((4-hydroxyphe	C28H36N4O6	3.0
M523T808_neg	523.2551	808	3							HMDB0250421	phenylpropyl)-N6-((4-hydroxyphe	C28H36N4O6	2.2
M526T740_neg	526.2846	740	3							HMDB0251587	Doramapimod	C31H37N5O3	4.3
M526T812_neg	526.2847	812	3							HMDB0251587	Doramapimod	C31H37N5O3	4.4
M527T1002_neg	527.3381	1002	3							HMDB0033079	Ganoderic acid V	C32H48O6	0.5
M531T594_neg	531.1923	594	3							HMDB0256642	Plevitrexed	C26H25FN8O4	2.4
M532T773_neg	532.2560	773	3							HMDB0251917	Ergovaline	C29H35N5O5	1.0
M532T718_neg	532.2555	718	3							HMDB0251917	Ergovaline	C29H35N5O5	2.0
M533T931_neg	533.3485	931	3							HMDB0297127	DG(8:0/PGJ2/0:0)	C31H50O7	0.1
M539T420_neg	539.1413	420	3						Carbohydrates				
M545T677_neg	545.2066	677	3							HMDB0252167	Farglitazar	C34H30N2O5	3.0
M548T407_neg	548.1039	407	3						Carbohydrates				
M549T442_neg	549.0878	442	3							HMDB0037368	Quercetin 3-(2-galloylglucoside)	C24H22O15	1.4
M549T790_neg	549.3447	790	3							HMDB0297203	20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,	C31H50O8	2.5
M551T820_neg	551.3591	820	3							HMDB0036298	Cyclopassifloic acid E	C31H52O8	0.2
M560T912_neg	560.2797	912	3							HMDB0250860	Dapitant	C37H39NO4	1.7
M563T453_neg	563.1527	453	3						Carbohydrates				
M566T602_neg	566.2279	602	3							HMDB0257349	methyl-17-prop-1-ynyl-9,11,12,14,	C33H33N3O6	3.1
M567T673_neg	567.2924	673	3							HMDB0244970	Enkephalinamide-Leu, Ala(2)-	C29H40N6O6	2.3
M567T784_neg	567.2967	784	3							HMDB0001097	Protoporphyrinogen IX	C34H40N4O4	1.8
M570T878_neg	570.2788	878	3							HMDB0012986	Kinetensin 4-7	C26H37N9O6	1.1
M572T445_neg	572.1151	445	3						Carbohydrates				
M572T700_neg	572.2863	700	3							HMDB0249052	Benzoylhypaconine	C31H43NO9	0.3
M579T450_neg	579.1474	450	3						Carbohydrates				
M579T679_neg	579.1722	679	3						Shikimates and Phenylpropanoids	HMDB0002927	Naringin	C27H32O14	0.5
M587T424_neg	587.1259	424	3							HMDB0245649	Bioadykinin Fragment 1-5	C19H25N8O12P	0.5
M588T453_neg	588.1100	453	3						Carbohydrates				
M589T725_neg	589.3035	725	3							HMDB0004158	Urobilinogen	C33H42N4O6	0.5
M633T922_neg	633.4008	922	3							HMDB0029606	Maslinic acid 3-O-b-D-glucoside	C36H58O9	0.0
M635T919_neg	635.4161	919	3							HMDB0036438	Fasciculic acid B	C36H60O9	0.5
M661T440_2_neg	661.2301	440	3							HMDB0040318	Blumeatin	C36H38O12	1.5
M663T785_neg	663.3858	785	3							HMDB0262739	PA(10:0/PGF1alpha)	C33H61O11P	3.1
M665T447_neg	665.2513	447	3						Carbohydrates				

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M520T975_neg	520.3288	975	3	2.93E-02	1.13	FALSE	2.96E-01	1.06	FALSE	8.98E-31	2.03	TRUE	3.33E-01	0.94	FALSE
M523T745_neg	523.2546	745	3	5.39E-01	1.04	FALSE	2.32E-02	1.18	FALSE	3.76E-11	1.52	TRUE	4.74E-01	1.09	FALSE
M523T808_neg	523.2551	808	3	1.56E-01	0.88	FALSE	8.50E-01	1.02	FALSE	2.03E-09	1.67	TRUE	2.07E-01	1.21	FALSE
M526T740_neg	526.2846	740	3	4.91E-12	1.92	TRUE	2.67E-03	0.76	FALSE	5.50E-05	1.36	FALSE	6.35E-01	0.92	FALSE
M526T812_neg	526.2847	812	3	3.79E-04	6.37	TRUE	2.15E-01	0.64	FALSE	6.40E-01	0.85	FALSE	7.91E-01	0.97	FALSE
M527T1002_neg	527.3381	1002	3	5.39E-12	1.90	TRUE	4.32E-05	0.70	FALSE	3.55E-01	1.07	FALSE	5.77E-01	1.05	FALSE
M531T594_neg	531.1923	594	3	1.15E-01	1.21	FALSE	2.90E-01	1.15	FALSE	1.27E-04	1.53	TRUE	7.22E-01	1.05	FALSE
M532T773_neg	532.2560	773	3	1.22E-06	2.94	TRUE	1.64E-01	0.69	FALSE	2.94E-01	0.83	FALSE	6.22E-01	1.19	FALSE
M532T718_neg	532.2555	718	3	1.60E-01	1.23	FALSE	5.85E-01	0.92	FALSE	1.16E-09	2.36	TRUE	5.84E-02	0.37	FALSE
M533T931_neg	533.3485	931	3	8.05E-17	1.50	TRUE	7.73E-06	0.81	FALSE	2.22E-03	1.13	FALSE	9.57E-02	1.16	FALSE
M539T420_neg	539.1413	420	3	1.28E-21	0.00	FALSE	8.82E-01	0.97	FALSE	7.52E-05	1.97	TRUE	8.97E-01	1.10	FALSE
M545T677_neg	545.2066	677	3	1.97E-08	1.61	TRUE	7.89E-01	0.98	FALSE	6.87E-01	0.97	FALSE	6.38E-02	0.79	FALSE
M548T407_neg	548.1039	407	3	1.50E-34	0.01	TRUE	8.42E-01	1.03	FALSE	9.54E-01	0.99	FALSE	3.32E-01	1.92	FALSE
M549T442_neg	549.0878	442	3	1.80E-34	0.02	TRUE	8.29E-01	1.03	FALSE	3.79E-01	0.91	FALSE	5.91E-01	0.62	FALSE
M549T790_neg	549.3447	790	3	2.87E-14	2.65	TRUE	1.10E-02	1.35	FALSE	4.09E-01	0.92	FALSE	5.43E-01	1.09	FALSE
M551T820_neg	551.3591	820	3	6.68E-25	2.36	TRUE	1.23E-02	0.83	FALSE	1.56E-02	0.87	FALSE	4.68E-01	1.12	FALSE
M560T912_neg	560.2797	912	3	3.49E-03	0.83	FALSE	2.71E-01	1.07	FALSE	1.06E-18	1.72	TRUE	1.39E-01	1.30	FALSE
M563T453_neg	563.1527	453	3	5.10E-13	0.00	FALSE	8.99E-01	0.97	FALSE	3.19E-03	2.01	TRUE	2.37E-01	2.07	FALSE
M566T602_neg	566.2279	602	3	4.81E-02	2.44	TRUE	4.82E-01	0.67	FALSE	7.17E-02	1.99	FALSE	7.89E-02	3.83	FALSE
M567T673_neg	567.2924	673	3	6.77E-11	1.63	TRUE	2.80E-02	0.85	FALSE	1.49E-07	1.40	FALSE	1.69E-01	1.20	FALSE
M567T784_neg	567.2967	784	3	5.42E-22	4.90	TRUE	2.25E-01	0.85	FALSE	1.13E-03	0.70	FALSE	3.44E-01	1.25	FALSE
M570T878_neg	570.2788	878	3	1.40E-02	5.90	TRUE	9.23E-02	0.32	FALSE	3.47E-01	0.62	FALSE	9.37E-02	-0.11	FALSE
M572T445_neg	572.1151	445	3	1.90E-21	0.01	TRUE	8.09E-01	1.05	FALSE	3.58E-01	0.86	FALSE	3.80E-01	0.32	FALSE
M572T700_neg	572.2863	700	3	1.99E-24	2.60	TRUE	2.30E-01	1.10	FALSE	3.87E-01	0.94	FALSE	3.05E-01	0.89	FALSE
M579T450_neg	579.1474	450	3	1.65E-08	-0.01	FALSE	7.82E-01	0.90	FALSE	1.41E-02	2.20	TRUE			#VALUE!
M579T679_neg	579.1722	679	3	4.81E-01	1.45	FALSE	7.22E-01	0.80	FALSE	4.80E-02	2.65	TRUE	3.94E-01	2.03	FALSE
M587T424_neg	587.1259	424	3	2.35E-18	0.00	TRUE	8.41E-01	1.04	FALSE	1.57E-01	0.78	FALSE	1.00E+00	1.00	FALSE
M588T453_neg	588.1100	453	3	8.40E-11	0.02	TRUE	9.47E-01	1.02	FALSE	1.80E-01	0.72	FALSE	3.59E-01	3.80	FALSE
M589T725_neg	589.3035	725	3	8.27E-09	1.79	TRUE	7.93E-01	0.98	FALSE	8.84E-02	1.15	FALSE	6.36E-01	0.95	FALSE
M633T922_neg	633.4008	922	3	1.49E-03	0.48	TRUE	3.64E-01	1.25	FALSE	1.11E-01	1.36	FALSE	4.73E-01	0.74	FALSE
M635T919_neg	635.4161	919	3	1.66E-02	0.72	FALSE	2.14E-01	1.19	FALSE	1.19E-06	1.84	TRUE	5.47E-01	0.88	FALSE
M661T440_2_neg	661.2301	440	3	1.75E-30	1.78	TRUE	6.44E-01	0.98	FALSE	6.55E-01	1.02	FALSE	6.12E-01	0.95	FALSE
M663T785_neg	663.3858	785	3	2.49E-13	1.89	TRUE	6.04E-05	0.73	FALSE	3.34E-01	1.07	FALSE	1.46E-01	1.15	FALSE
M665T447_neg	665.2513	447	3	8.49E-06	1.98	TRUE	2.99E-01	0.85	FALSE	5.01E-01	0.92	FALSE	3.07E-01	1.49	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M665T751_neg	665.3543	751	3							HMDB0033703	Coroloside	C35H54O12	0.0
M679T779_neg	679.3700	779	3							HMDB0258821	Tenuifolin	C36H56O12	0.1
M695T853_neg	695.4014	853	3							HMDB0035697	Momordicoside E	C37H60O12	0.3
M716T1026_neg	715.5518	1026	3						Terpenoids	HMDB0296503	DG(21:0/PGJ2/0:0)	C44H76O7	0.1
M781T419_neg	781.2988	419	3						Carbohydrates				
M808T1006_neg	807.5416	1006	3							HMDB0268817	PG(18:0/18:1(12Z)-2OH(9,10))	C42H81O12P	2.8
M868T89_neg	867.7848	89	3							HMDB0042720	G(14:0/22:4(7Z,10Z,13Z,16Z)/O-18:	C57H104O5	4.2
M923T92_neg	922.7258	92	3							HMDB0008618	PC(22:2(13Z,16Z)/24:1(15Z))	C54H102NO8P	1.3
M946T82_neg	945.8316	82	3							HMDB0050850	(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	C63H110O5	3.8
M71T581_pos	71.0489	581	3							HMDB0034233	2-Butenal	C4H6O	3.0
M75T554_pos	75.0261	554	3							HMDB0031635	2-Propene-1-thiol	C3H6S	2.6
M75T712_pos	75.0439	712	3							HMDB0244090	1,2-Dioxolane	C3H6O2	2.6
M87T804_pos	87.0439	804	3							HMDB0245045	2-Butyne-1,4-diol	C4H6O2	1.6
M89T868_pos	89.0596	868	3							HMDB0000039	Butyric acid	C4H8O2	0.6
M99T803_pos	99.0805	803	3							HMDB0003315	Cyclohexanone	C6H10O	0.4
M103T581_pos	103.0754	581	3							HMDB0000718	Isovaleric acid	C5H10O2	0.2
M104T108_pos	104.1070	108	3							HMDB0244984	2-Amino-3-methyl-1-butanol	C5H13NO	0.4
M105T784_pos	105.0699	784	3							HMDB0034240	Styrene	C8H8	0.0
M111T687_pos	111.0805	687	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.5
M114T584_pos	114.0914	584	3							HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	0.2
M117T804_pos	117.0910	804	3						Fatty acids	HMDB0000535	Caproic acid	C6H12O2	0.1
M119T714_pos	119.0492	714	3							HMDB0030968	2,4,6-Octatriyn-1-ol	C8H6O	0.2
M127T916_pos	127.1118	916	3							HMDB0013809	(E)-2-octenal	C8H14O	0.3
M129T1022_pos	129.0182	1022	3							HMDB0059784	5-Hydroxy-2-furoic acid	C5H4O4	0.1
M131T868_pos	131.1067	868	3						Fatty acids	HMDB0000666	Heptanoic acid	C7H14O2	0.2
M132T127_pos	132.1019	127	3						Amino acids and Peptides	HMDB0000172	L-Isoleucine	C6H13NO2	0.0
M137T714_pos	137.0597	714	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.1
M138T462_pos	138.0550	462	3						Amino acids and Peptides	HMDB0000875	Trigonelline	C7H7NO2	0.1
M138T556_pos	138.0550	556	3							HMDB0000875	Trigonelline	C7H7NO2	0.2
M139T608_pos	139.0390	608	3							HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.2
M139T803_2_pos	139.1118	803	3						Fatty acids	HMDB0013824	2-Pentylfuran	C9H14O	0.2
M140T708_pos	140.1070	708	3							HMDB0029613	9-Azabicyclo[3.3.1]nonan-3-one	C8H13NO	0.3
M141T128_pos	141.0659	128	3							HMDB0002144	1,3-Dimethyluracil	C6H8N2O2	0.0
M142T618_pos	142.0863	618	3							HMDB0014731	Ethosuximide	C7H11NO2	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M665T751_neg	665.3543	751	3	8.66E-02	1.26	FALSE	1.35E-01	1.23	FALSE	5.61E-10	2.22	TRUE	1.50E-01	0.76	FALSE
M679T779_neg	679.3700	779	3	7.81E-01	0.96	FALSE	4.40E-01	1.11	FALSE	9.13E-11	2.26	TRUE	3.38E-01	0.87	FALSE
M695T853_neg	695.4014	853	3	9.61E-05	0.73	FALSE	2.03E-01	1.11	FALSE	6.26E-18	1.99	TRUE	1.89E-01	0.89	FALSE
M716T1026_neg	715.5518	1026	3	4.61E-04	2.03	TRUE	1.78E-01	0.76	FALSE	3.45E-01	1.17	FALSE	1.04E-01	1.39	FALSE
M781T419_neg	781.2988	419	3	8.26E-11	2.00	TRUE	8.87E-01	1.01	FALSE	5.38E-02	0.85	FALSE	6.12E-01	1.17	FALSE
M808T1006_neg	807.5416	1006	3	1.14E-01	1.16	FALSE	4.17E-01	1.08	FALSE	5.87E-26	2.96	TRUE	9.23E-01	0.99	FALSE
M868T89_neg	867.7848	89	3	3.19E-04	1.21	FALSE	4.55E-02	1.12	FALSE	5.50E-09	1.32	FALSE	1.88E-06	0.42	TRUE
M923T92_neg	922.7258	92	3	2.94E-07	1.40	FALSE	1.43E-01	1.10	FALSE	8.75E-01	1.01	FALSE	1.98E-10	0.21	TRUE
M946T82_neg	945.8316	82	3	6.47E-05	1.43	FALSE	4.63E-02	1.19	FALSE	2.37E-05	1.39	FALSE	3.18E-02	0.61	TRUE
M71T581_pos	71.0489	581	3	3.73E-16	1.43	FALSE	3.35E-01	0.96	FALSE	1.77E-01	1.05	FALSE	6.86E-01	1.03	FALSE
M75T554_pos	75.0261	554	3	4.89E-01	1.03	FALSE	2.33E-13	1.43	FALSE	5.84E-18	1.48	FALSE	1.97E-01	1.12	FALSE
M75T712_pos	75.0439	712	3	2.60E-19	1.33	FALSE	3.45E-01	1.03	FALSE	8.57E-02	0.96	FALSE	7.43E-01	1.01	FALSE
M87T804_pos	87.0439	804	3	9.65E-17	1.21	FALSE	1.36E-01	1.03	FALSE	6.03E-03	0.95	FALSE	9.40E-01	1.00	FALSE
M89T868_pos	89.0596	868	3	1.19E-13	1.20	FALSE	3.85E-01	1.02	FALSE	5.26E-02	0.96	FALSE	3.21E-01	0.94	FALSE
M99T803_pos	99.0805	803	3	3.63E-20	1.34	FALSE	1.95E-02	1.07	FALSE	2.23E-03	0.93	FALSE	8.28E-01	0.99	FALSE
M103T581_pos	103.0754	581	3	2.88E-22	1.46	FALSE	4.14E-01	0.97	FALSE	4.94E-01	1.02	FALSE	6.88E-01	1.02	FALSE
M104T108_pos	104.1070	108	3	7.76E-02	1.31	FALSE	2.91E-01	0.83	FALSE	1.00E-01	1.24	FALSE	4.16E-01	1.47	FALSE
M105T784_pos	105.0699	784	3	1.11E-10	1.18	FALSE	1.29E-01	1.04	FALSE	3.42E-02	1.04	FALSE	4.40E-01	0.95	FALSE
M111T687_pos	111.0805	687	3	5.16E-01	1.02	FALSE	1.67E-03	1.10	FALSE	1.96E-35	1.48	FALSE	8.24E-02	0.93	FALSE
M114T584_pos	114.0914	584	3	5.57E-06	1.46	FALSE	4.97E-01	0.95	FALSE	4.29E-03	1.23	FALSE	2.63E-01	1.17	FALSE
M117T804_pos	117.0910	804	3	4.82E-16	1.23	FALSE	1.72E-01	1.03	FALSE	5.14E-02	0.96	FALSE	6.66E-01	0.98	FALSE
M119T714_pos	119.0492	714	3	3.21E-26	1.35	FALSE	6.72E-04	1.09	FALSE	1.53E-02	1.05	FALSE	8.79E-01	0.99	FALSE
M127T916_pos	127.1118	916	3	8.97E-02	1.30	FALSE	8.02E-01	1.04	FALSE	1.43E-01	1.22	FALSE	1.11E-01	0.62	FALSE
M129T1022_pos	129.0182	1022	3	3.57E-16	0.88	FALSE	2.07E-07	1.08	FALSE	4.28E-02	0.98	FALSE	4.81E-01	0.98	FALSE
M131T868_pos	131.1067	868	3	2.09E-13	1.22	FALSE	3.49E-01	1.03	FALSE	8.40E-02	0.96	FALSE	6.69E-01	0.97	FALSE
M132T127_pos	132.1019	127	3	7.36E-05	1.15	FALSE	8.12E-02	1.07	FALSE	2.34E-09	1.21	FALSE	7.82E-01	0.99	FALSE
M137T714_pos	137.0597	714	3	3.48E-22	1.36	FALSE	3.70E-03	1.09	FALSE	1.57E-04	1.10	FALSE	4.50E-01	0.95	FALSE
M138T462_pos	138.0550	462	3	1.58E-09	0.71	FALSE	9.20E-01	0.99	FALSE	6.53E-15	1.48	FALSE	4.15E-02	0.82	FALSE
M138T556_pos	138.0550	556	3	7.83E-03	0.68	FALSE	3.83E-01	0.88	FALSE	1.12E-01	1.22	FALSE	6.33E-01	1.04	FALSE
M139T608_pos	139.0390	608	3	4.20E-24	1.49	FALSE	4.75E-01	1.03	FALSE	1.85E-08	1.19	FALSE	8.05E-01	0.98	FALSE
M139T803_2_pos	139.1118	803	3	7.15E-01	0.99	FALSE	2.64E-02	1.08	FALSE	2.62E-18	1.34	FALSE	1.73E-04	0.83	FALSE
M140T708_pos	140.1070	708	3	8.44E-12	1.34	FALSE	1.82E-05	1.20	FALSE	4.42E-02	1.07	FALSE	6.22E-02	0.87	FALSE
M141T128_pos	141.0659	128	3	3.84E-01	0.96	FALSE	1.20E-02	1.12	FALSE	6.59E-15	1.39	FALSE	4.34E-01	1.06	FALSE
M142T618_pos	142.0863	618	3	3.94E-10	1.39	FALSE	4.44E-09	0.68	FALSE	1.32E-02	0.90	FALSE	4.12E-01	0.97	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M142T766_pos	142.1227	766	3							HMDB0030324	(R)-Pelletierine	C8H15NO	0.3
M145T767_pos	145.1223	767	3							HMDB0000482	Caprylic acid	C8H16O2	0.3
M145T868_pos	145.1223	868	3						Fatty acids	HMDB0000482	Caprylic acid	C8H16O2	0.2
M145T916_pos	145.1223	916	3						Fatty acids	HMDB0000482	Caprylic acid	C8H16O2	0.2
M146T627_pos	146.0601	627	3						Alkaloids	HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.1
M146T85_pos	146.1652	85	3							HMDB0001257	Spermidine	C7H19N3	0.5
M149T588_pos	149.0234	588	3							HMDB0256501	Phthalic anhydride	C8H4O3	0.4
M149T933_pos	149.0598	933	3							HMDB0000567	Cinnamic acid	C9H8O2	0.5
M149T1044_pos	149.0961	1044	3							HMDB0002214	Cuminaldehyde	C10H12O	0.3
M149T883_pos	149.1325	883	3						Terpenoids	HMDB0059834	Pentylbenzene	C11H16	0.2
M151T767_pos	151.0965	767	3						Fatty acids	HMDB0259193	TRIETHYLENE GLYCOL	C6H14O4	0.2
M154T469_pos	154.0499	469	3							HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	0.1
M157T1023_pos	157.0132	1023	3							HMDB0004812	2,5-Furandicarboxylic acid	C6H4O5	0.3
M157T802_pos	157.1224	802	3						Fatty acids	HMDB0004362	4-Hydroxynonenal	C9H16O2	0.3
M158T877_pos	158.1540	877	3							HMDB0245344	2,2,6,6-Tetramethyl-4-piperidinol	C9H19NO	0.2
M159T917_2_pos	159.1380	917	3						Fatty acids	HMDB0000798	Oenanthic ether	C9H18O2	0.3
M161T970_pos	161.0961	970	3							HMDB0031567	3-Methyl-4-phenyl-3-buten-2-one	C11H12O	0.2
M162T569_pos	162.0550	569	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.5
M163T987_pos	163.0754	987	3							HMDB0029714	,5-Dihydro-1-benzoxepin-3(2H)-on	C10H10O2	0.2
M163T846_pos	163.0754	846	3							HMDB0029714	,5-Dihydro-1-benzoxepin-3(2H)-on	C10H10O2	0.3
M163T670_2_pos	163.1118	670	3							HMDB0031208	1-Phenyl-1-pentanone	C11H14O	0.4
M163T917_pos	163.1330	917	3							HMDB0033625	(3R,7R)-1,3,7-Octanetriol	C8H18O3	0.5
M164T677_pos	164.0707	677	3							HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.4
M166T555_pos	166.0499	555	3							HMDB0003454	4-Pyridoxolactone	C8H7NO3	0.5
M167T934_pos	167.0703	934	3						Shikimates and Phenylpropanoids	HMDB0000375	3-(3-Hydroxyphenyl)propanoic acid	C9H10O3	0.2
M167T632_pos	167.1179	632	3						Alkaloids	HMDB0029742	opropyl-2-methoxy-5-methylpyraz	C9H14N2O	0.0
M167T882_pos	167.1431	882	3						Fatty acids	HMDB0030002	(-)-Nopol	C11H18O	0.2
M168T486_pos	168.0656	486	3							HMDB0001545	Pyridoxal	C8H9NO3	0.4
M170T115_pos	170.0578	115	3							HMDB0060244	Phosphodimethylethanolamine	C4H12NO4P	0.9
M171T758_pos	171.1492	758	3							HMDB0246938	o-3-methyl-1-pyrrolidin-1-YL-butar	C9H18N2O	0.1
M172T659_pos	172.1332	659	3							HMDB0005015	Gabapentin	C9H17NO2	0.2
M173T785_pos	173.0574	785	3						Fatty acids				
M173T1074_pos	173.1172	1074	3							HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	0.1
M174T627_pos	174.0550	627	3						Alkaloids	HMDB0000842	Quinaldic acid	C10H7NO2	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M142T766_pos	142.1227	766	3	2.22E-13	0.67	FALSE	2.64E-04	1.21	FALSE	4.08E-03	1.14	FALSE	5.88E-02	0.83	FALSE
M145T767_pos	145.1223	767	3	2.87E-01	1.08	FALSE	5.71E-01	1.05	FALSE	8.76E-01	1.01	FALSE	8.49E-01	1.05	FALSE
M145T868_pos	145.1223	868	3	4.52E-14	1.20	FALSE	5.33E-01	1.01	FALSE	2.00E-01	0.98	FALSE	9.64E-01	1.00	FALSE
M145T916_pos	145.1223	916	3	2.29E-01	1.13	FALSE	9.30E-01	0.99	FALSE	4.23E-02	1.21	FALSE	2.55E-01	0.77	FALSE
M146T627_pos	146.0601	627	3	4.58E-06	1.23	FALSE	4.56E-01	1.03	FALSE	4.26E-10	1.28	FALSE	1.80E-01	1.07	FALSE
M146T85_pos	146.1652	85	3	2.60E-01	0.90	FALSE	1.41E-01	0.86	FALSE	3.21E-04	1.34	FALSE	7.63E-01	0.96	FALSE
M149T588_pos	149.0234	588	3	5.80E-11	0.71	FALSE	9.67E-02	1.09	FALSE	1.71E-08	1.28	FALSE	4.02E-02	1.21	FALSE
M149T933_pos	149.0598	933	3	5.81E-04	0.94	FALSE	9.71E-02	0.97	FALSE	2.25E-17	0.86	FALSE	2.43E-01	1.45	FALSE
M149T1044_pos	149.0961	1044	3	8.73E-09	1.42	FALSE	3.18E-05	0.78	FALSE	1.14E-02	1.14	FALSE	2.20E-03	1.31	FALSE
M149T883_pos	149.1325	883	3	1.25E-01	0.96	FALSE	3.71E-02	1.06	FALSE	1.92E-14	1.22	FALSE	4.68E-01	1.06	FALSE
M151T767_pos	151.0965	767	3	2.64E-01	1.08	FALSE	5.31E-01	1.05	FALSE	9.23E-01	1.01	FALSE	9.59E-01	1.01	FALSE
M154T469_pos	154.0499	469	3	1.68E-20	1.44	FALSE	2.98E-01	1.04	FALSE	2.34E-17	1.33	FALSE	6.39E-01	1.04	FALSE
M157T1023_pos	157.0132	1023	3	6.68E-21	0.87	FALSE	1.06E-08	1.08	FALSE	5.64E-02	0.98	FALSE	1.95E-01	0.95	FALSE
M157T802_pos	157.1224	802	3	1.09E-01	1.05	FALSE	6.72E-02	1.07	FALSE	5.47E-10	1.21	FALSE	1.53E-01	0.92	FALSE
M158T877_pos	158.1540	877	3	5.04E-13	1.17	FALSE	7.76E-01	1.01	FALSE	1.43E-25	0.81	FALSE	8.25E-03	0.92	FALSE
M159T917_2_pos	159.1380	917	3	2.56E-01	1.12	FALSE	9.85E-01	1.00	FALSE	4.37E-02	1.19	FALSE	2.55E-01	0.78	FALSE
M161T970_pos	161.0961	970	3	5.77E-01	0.96	FALSE	9.40E-02	1.14	FALSE	1.52E-05	0.75	FALSE	6.78E-01	1.02	FALSE
M162T569_pos	162.0550	569	3	5.14E-01	1.04	FALSE	5.10E-01	1.04	FALSE	4.38E-12	1.42	FALSE	9.55E-02	1.11	FALSE
M163T987_pos	163.0754	987	3	2.27E-08	0.94	FALSE	9.02E-02	1.02	FALSE	6.11E-07	0.95	FALSE	8.87E-01	1.00	FALSE
M163T846_pos	163.0754	846	3	2.08E-09	1.14	FALSE	3.60E-02	0.95	FALSE	5.60E-24	0.81	FALSE	1.08E-01	1.11	FALSE
M163T670_2_pos	163.1118	670	3	3.90E-03	1.09	FALSE	2.02E-01	1.04	FALSE	4.19E-28	1.42	FALSE	7.94E-02	0.93	FALSE
M163T917_pos	163.1330	917	3	2.67E-01	1.10	FALSE	9.65E-01	1.00	FALSE	2.63E-01	1.09	FALSE	3.83E-01	0.86	FALSE
M164T677_pos	164.0707	677	3	6.84E-01	1.03	FALSE	7.70E-01	1.02	FALSE	2.94E-07	1.34	FALSE	3.01E-01	0.84	FALSE
M166T555_pos	166.0499	555	3	4.97E-04	1.16	FALSE	6.40E-05	0.83	FALSE	6.21E-14	1.34	FALSE	5.93E-01	1.05	FALSE
M167T934_pos	167.0703	934	3	8.21E-01	1.00	FALSE	2.48E-01	1.02	FALSE	4.01E-13	0.90	FALSE	7.94E-01	1.01	FALSE
M167T632_pos	167.1179	632	3	1.22E-01	1.08	FALSE	1.14E-07	1.31	FALSE	3.81E-09	1.29	FALSE	1.10E-01	0.86	FALSE
M167T882_pos	167.1431	882	3	1.00E-01	0.95	FALSE	3.11E-02	1.07	FALSE	3.17E-14	1.23	FALSE	4.88E-01	1.06	FALSE
M168T486_pos	168.0656	486	3	2.69E-27	1.44	FALSE	2.59E-01	1.03	FALSE	6.89E-20	1.29	FALSE	9.87E-01	1.00	FALSE
M170T115_pos	170.0578	115	3	1.08E-01	1.11	FALSE	3.93E-01	1.06	FALSE	7.42E-09	1.41	FALSE	1.59E-01	0.88	FALSE
M171T758_pos	171.1492	758	3	5.53E-10	1.29	FALSE	9.33E-01	1.00	FALSE	4.31E-21	0.70	FALSE	8.39E-03	1.16	FALSE
M172T659_pos	172.1332	659	3	2.37E-27	1.46	FALSE	4.09E-01	0.98	FALSE	1.68E-10	0.84	FALSE	9.80E-01	1.00	FALSE
M173T785_pos	173.0574	785	3	7.02E-18	1.29	FALSE	4.92E-03	1.08	FALSE	2.24E-13	0.83	FALSE	4.15E-01	0.94	FALSE
M173T1074_pos	173.1172	1074	3	2.91E-01	1.99	FALSE	4.60E-01	1.59	FALSE	4.31E-01	1.55	FALSE	8.15E-01	0.86	FALSE
M174T627_pos	174.0550	627	3	1.48E-04	1.21	FALSE	2.98E-01	1.05	FALSE	1.39E-11	1.36	FALSE	6.77E-02	1.10	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M174T697_pos	174.1853	697	3						Fatty acids				
M175T687_pos	175.0966	687	3						Fatty acids	HMDB0000893	Suberic acid	C8H14O4	0.5
M176T706_pos	176.0706	706	3						Alkaloids	HMDB0000197	Indoleacetic acid	C10H9NO2	0.2
M177T772_pos	177.0910	772	3							HMDB0029699	Cinnamyl acetate	C11H12O2	0.0
M181T670_pos	181.1224	670	3						Terpenoids	HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.5
M182T678_pos	182.0812	678	3							HMDB0000158	L-Tyrosine	C9H11NO3	0.3
M183T903_pos	183.0805	903	3							HMDB0013163	2-Hydroxyfluorene	C13H10O	0.5
M183T778_pos	183.1016	778	3							HMDB0029456	Amyl 2-furoate	C10H14O3	0.2
M184T401_pos	184.0605	401	3							HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.3
M185T583_pos	185.1285	583	3							HMDB0061384	(3-acetamidopropyl)pyrrolidin-2-o	C9H16N2O2	0.2
M186T385_pos	186.0762	385	3							HMDB0244794	bicyclo[3.1.0]hexane-2,6-dicarbox	C8H11NO4	0.9
M186T741_pos	186.1126	741	3							HMDB0006348	Pseudoecgonine	C9H15NO3	0.7
M186T726_pos	186.1490	726	3							HMDB0243943	1-Methylpiperidin-4-yl butanoate	C10H19NO2	0.5
M186T659_pos	186.1490	659	3							HMDB0243943	1-Methylpiperidin-4-yl butanoate	C10H19NO2	0.5
M189T984_pos	189.1275	984	3							HMDB0031855	5-Methyl-2-phenyl-2-hexenal	C13H16O	0.5
M190T572_pos	190.0499	572	3							HMDB0000715	Kynurenic acid	C10H7NO3	0.4
M190T759_pos	190.0864	759	3							HMDB0002302	Indole-3-propionic acid	C11H11NO2	0.5
M190T362_pos	190.1438	362	3						Fatty acids				
M191T756_pos	191.1069	756	3							HMDB0030905	(4-Methoxyphenyl)-1-penten-3-or	C12H14O2	1.3
M192T627_pos	192.0656	627	3						Alkaloids	HMDB0000763	5-Hydroxyindoleacetic acid	C10H9NO3	0.3
M194T361_pos	194.0813	361	3							HMDB0000821	Phenylacetylglycine	C10H11NO3	0.9
M194T367_pos	194.1177	367	3						Alkaloids	HMDB0003626	(R)-N-Methylsalsolinol	C11H15NO2	0.7
M195T934_pos	195.1016	934	3							HMDB0031517	)-3-Hydroxy-5-phenylpentanoic ac	C11H14O3	0.1
M195T1066_pos	195.1228	1066	3							HMDB0094708	Tetraethylene glycol	C8H18O5	0.3
M195T1001_pos	195.1744	1001	3							HMDB0031846	Geranylacetone	C13H22O	0.5
M198T617_pos	198.1278	617	3							HMDB0036173	2-(3-Phenylpropyl)pyridine	C14H15N	0.1
M199T854_pos	199.1329	854	3							HMDB0253742	-Methylcyclohexyl)-4-oxobutanoic	C11H18O3	0.3
M200T785_pos	200.1646	785	3							HMDB0062669	11-nitro-1-undecene	C11H21NO2	0.5
M200T992_pos	200.2010	992	3						Fatty acids	HMDB0251566	Dodecanamide	C12H25NO	0.6
M201T645_pos	201.1125	645	3							HMDB0000603	cis-4-Decenedioic acid	C10H16O4	2.0
M201T552_pos	201.1599	552	3							HMDB0013076	Spermine dialdehyde	C10H20N2O2	0.5
M203T970_pos	203.1068	970	3							HMDB0030816	cetyl-2,2-dimethyl-2H-1-benzopyr	C13H14O2	0.6
M203T997_pos	203.1431	997	3							HMDB0030572	(\xc2\xb1)-Anisoxide	C14H18O	0.3
M204T345_pos	204.0827	345	3							HMDB0245559	Fluorofenidone	C12H10FNO	4.0
M205T700_pos	205.0861	700	3							HMDB0033303	Anofinic acid	C12H12O3	0.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M174T697_pos	174.1853	697	3	4.02E-01	1.12	FALSE	4.99E-03	1.50	FALSE	2.26E-01	1.15	FALSE	6.53E-01	1.13	FALSE
M175T687_pos	175.0966	687	3	5.02E-01	1.02	FALSE	1.69E-01	1.04	FALSE	1.99E-34	1.42	FALSE	4.68E-01	0.97	FALSE
M176T706_pos	176.0706	706	3	2.35E-02	1.26	FALSE	6.99E-01	1.04	FALSE	7.01E-02	1.18	FALSE	4.01E-02	0.79	FALSE
M177T772_pos	177.0910	772	3	1.97E-08	1.27	FALSE	9.94E-01	1.00	FALSE	1.84E-02	1.09	FALSE	3.96E-02	0.76	FALSE
M181T670_pos	181.1224	670	3	1.22E-04	1.11	FALSE	6.97E-02	1.05	FALSE	5.41E-28	1.37	FALSE	7.48E-02	0.93	FALSE
M182T678_pos	182.0812	678	3	8.61E-01	1.01	FALSE	5.19E-01	1.05	FALSE	2.65E-06	1.36	FALSE	9.83E-01	1.01	FALSE
M183T903_pos	183.0805	903	3	1.10E-05	1.07	FALSE	4.19E-01	1.01	FALSE	8.45E-19	0.88	FALSE	4.36E-01	0.98	FALSE
M183T778_pos	183.1016	778	3	1.23E-01	0.94	FALSE	3.29E-01	1.04	FALSE	1.70E-02	1.08	FALSE	1.60E-02	0.83	FALSE
M184T401_pos	184.0605	401	3	6.51E-18	1.39	FALSE	9.27E-01	1.00	FALSE	1.39E-15	1.30	FALSE	7.49E-01	0.98	FALSE
M185T583_pos	185.1285	583	3	5.01E-04	1.17	FALSE	2.16E-01	1.07	FALSE	6.42E-03	1.11	FALSE	8.85E-01	1.01	FALSE
M186T385_pos	186.0762	385	3	9.27E-03	1.09	FALSE	1.03E-06	1.19	FALSE	1.12E-12	1.26	FALSE	3.68E-02	0.93	FALSE
M186T741_pos	186.1126	741	3	1.90E-02	0.76	FALSE	2.87E-01	0.87	FALSE	1.57E-01	1.16	FALSE	9.08E-01	0.98	FALSE
M186T726_pos	186.1490	726	3	1.02E-05	1.13	FALSE	8.85E-01	1.00	FALSE	1.05E-10	0.85	FALSE	9.91E-01	1.00	FALSE
M186T659_pos	186.1490	659	3	3.92E-25	1.41	FALSE	5.84E-01	0.98	FALSE	5.14E-06	0.89	FALSE	8.14E-01	0.99	FALSE
M189T984_pos	189.1275	984	3	1.82E-04	0.95	FALSE	3.13E-01	1.02	FALSE	3.55E-05	0.95	FALSE	5.41E-01	0.98	FALSE
M190T572_pos	190.0499	572	3	5.86E-01	1.03	FALSE	4.63E-01	1.04	FALSE	5.28E-14	1.47	FALSE	4.94E-02	1.11	FALSE
M190T759_pos	190.0864	759	3	5.86E-05	1.20	FALSE	6.27E-01	0.98	FALSE	3.90E-03	1.12	FALSE	2.86E-01	0.94	FALSE
M190T362_pos	190.1438	362	3	1.55E-04	1.27	FALSE	7.41E-01	0.98	FALSE	9.53E-04	1.20	FALSE	3.10E-01	1.13	FALSE
M191T756_pos	191.1069	756	3	5.33E-01	1.04	FALSE	8.89E-01	1.01	FALSE	2.12E-10	1.45	FALSE	2.71E-01	0.95	FALSE
M192T627_pos	192.0656	627	3	1.50E-04	1.20	FALSE	4.17E-01	1.04	FALSE	6.92E-11	1.33	FALSE	5.74E-02	1.10	FALSE
M194T361_pos	194.0813	361	3	3.10E-01	0.92	FALSE	4.74E-01	1.07	FALSE	1.75E-05	1.40	FALSE	8.26E-01	1.03	FALSE
M194T367_pos	194.1177	367	3	4.97E-02	1.07	FALSE	6.47E-01	0.98	FALSE	1.13E-06	1.17	FALSE	4.20E-03	0.89	FALSE
M195T934_pos	195.1016	934	3	5.88E-01	1.01	FALSE	2.72E-01	1.02	FALSE	1.00E-14	0.89	FALSE	3.82E-01	0.98	FALSE
M195T1066_pos	195.1228	1066	3	8.27E-02	0.98	FALSE	4.13E-01	0.99	FALSE	6.11E-01	1.01	FALSE	2.37E-01	0.94	FALSE
M195T1001_pos	195.1744	1001	3	2.38E-01	0.96	FALSE	5.55E-01	0.98	FALSE	2.32E-01	0.96	FALSE	9.86E-01	1.00	FALSE
M198T617_pos	198.1278	617	3	1.68E-42	1.22	FALSE	2.97E-01	0.99	FALSE	6.86E-20	0.91	FALSE	6.56E-01	1.01	FALSE
M199T854_pos	199.1329	854	3	2.67E-02	0.93	FALSE	4.63E-01	1.03	FALSE	2.12E-24	1.43	FALSE	7.13E-06	0.79	FALSE
M200T785_pos	200.1646	785	3	1.21E-05	1.09	FALSE	3.42E-04	1.07	FALSE	3.82E-08	0.91	FALSE	4.88E-02	0.92	FALSE
M200T992_pos	200.2010	992	3	3.16E-08	0.91	FALSE	6.15E-01	1.01	FALSE	3.59E-10	0.91	FALSE	4.32E-01	0.98	FALSE
M201T645_pos	201.1125	645	3	3.33E-04	1.25	FALSE	9.31E-02	1.11	FALSE	2.02E-08	1.37	FALSE	2.60E-01	1.11	FALSE
M201T552_pos	201.1599	552	3	3.30E-05	1.39	FALSE	6.76E-02	0.86	FALSE	3.33E-01	0.94	FALSE	1.42E-01	0.77	FALSE
M203T970_pos	203.1068	970	3	3.54E-01	0.94	FALSE	1.21E-01	1.11	FALSE	7.90E-06	0.77	FALSE	8.85E-01	0.99	FALSE
M203T997_pos	203.1431	997	3	1.99E-01	0.99	FALSE	9.00E-02	1.02	FALSE	2.87E-07	0.95	FALSE	5.65E-01	1.02	FALSE
M204T345_pos	204.0827	345	3	7.43E-01	1.02	FALSE	1.54E-03	1.26	FALSE	1.00E-08	1.44	FALSE	7.13E-01	1.04	FALSE
M205T700_pos	205.0861	700	3	1.46E-02	1.36	FALSE	6.87E-01	0.94	FALSE	7.53E-02	1.21	FALSE	2.66E-01	1.14	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M206T609_pos	206.0821	609	3							HMDB0000671	Indolelactic acid	C11H11NO3	4.7
M208T569_pos	208.0605	569	3						Alkaloids	HMDB0000978	-Aminophenyl)-2,4-dioxobutanoic	C10H9NO4	0.3
M208T404_pos	208.0970	404	3							HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	1.0
M209T1025_pos	209.1901	1025	3							HMDB0032215	2-Decylfuran	C14H24O	0.5
M211T563_pos	211.1082	563	3							HMDB0015441	Aprobarbital	C10H14N2O3	2.1
M211T992_pos	211.1095	992	3							HMDB0303275	Potassium caprate	C10H19KO2	0.2
M211T875_pos	211.1693	875	3							HMDB0030425	Linalyl propionate	C13H22O2	0.4
M211T1062_pos	211.2057	1062	3							HMDB0032525	Tetradec-2-enal	C14H26O	0.4
M212T497_pos	212.1030	497	3							HMDB0015078	Zalcitabine	C9H13N3O3	0.0
M213T1023_pos	213.0758	1023	3							HMDB0000913	Vanillactic acid	C10H12O5	0.1
M213T398_pos	213.1342	398	3						Amino acids and Peptides				
M214T834_pos	214.1803	834	3						Fatty acids				
M214T1005_pos	214.2167	1005	3						Fatty acids				
M215T469_pos	215.0487	469	3							HMDB0246327	4-Acetamidobenzenesulfonamide	C8H10N2O3S	1.1
M215T769_pos	215.1643	769	3							HMDB0010727	3-Oxododecanoic acid	C12H22O3	0.5
M217T1022_pos	217.0344	1022	3							HMDB0242250	(+)-Diacetyl-L-tartaric anhydride	C8H8O7	0.3
M217T492_pos	217.0647	492	3							HMDB0255060	-Acetyl-S-(2-cyanoethyl)-L-cystein	C8H12N2O3S	2.6
M217T916_pos	217.1228	916	3							HMDB0040833	xy-3-(3-methyl-2-butenyl)phenyl]-	C14H16O2	2.1
M217T854_pos	217.1436	854	3						Fatty acids	HMDB0000888	Undecanedioic acid	C11H20O4	0.6
M217T465_pos	217.1548	465	3							HMDB0029140	Valylvaline	C10H20N2O3	0.7
M218T581_pos	218.0249	581	3							HMDB0303276	Potassium cyclamate	C6H12KNO3S	0.4
M219T797_pos	219.0477	797	3							HMDB0303730	Sodium gluconate	C6H11NaO7	0.9
M219T924_pos	219.1381	924	3							HMDB0030759	(R)-Pterosin B	C14H18O2	0.5
M219T1033_pos	219.1956	1033	3							HMDB0040219	8-Dimethoxy-2,6-dimethyl-2-octar	C12H26O3	0.8
M220T352_pos	220.1194	352	3							HMDB0012204	Zeatin	C10H13N5O	0.4
M222T468_2_pos	222.1490	468	3							HMDB0030305	Dioscorine	C13H19NO2	0.8
M223T1033_pos	223.1691	1033	3							HMDB0035593	Rishitin	C14H22O2	0.5
M223T1034_pos	223.2057	1034	3							HMDB0004305	Farnesol	C15H26O	0.4
M224T677_pos	224.0377	677	3							HMDB0255449	Naphthionic acid	C10H9NO3S	0.7
M224T394_pos	224.1030	394	3							HMDB0062375	trosamino)-1-(1-oxido-3-pyridinyl)-	C10H13N3O3	0.2
M224T783_pos	224.1283	783	3							HMDB0015168	Cerulenin	C12H17NO3	0.7
M224T973_pos	224.2011	973	3							HMDB0030951	E,E)-2,4-Decadienoic isobutylamid	C14H25NO	0.7
M225T802_pos	225.1100	802	3							HMDB0246998	amino-9-(2-hydroxyethoxymethyl)-	C8H12N6O2	2.6
M225T997_pos	225.1253	997	3							HMDB0259269	Tripropyl phosphate	C9H21O4P	1.2
M225T894_pos	225.1484	894	3							HMDB0029670	Epoxyeremopetasinorol	C13H20O3	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M206T609_pos	206.0821	609	3	2.13E-05	1.27	FALSE	1.48E-02	1.15	FALSE	5.94E-09	1.34	FALSE	9.12E-01	1.02	FALSE
M208T569_pos	208.0605	569	3	7.08E-01	0.98	FALSE	6.27E-01	1.03	FALSE	2.29E-12	1.42	FALSE	1.09E-01	1.11	FALSE
M208T404_pos	208.0970	404	3	1.84E-04	1.17	FALSE	2.22E-02	1.10	FALSE	5.38E-19	1.42	FALSE	2.11E-01	1.05	FALSE
M209T1025_pos	209.1901	1025	3	5.82E-03	0.87	FALSE	4.01E-01	1.05	FALSE	7.01E-02	0.92	FALSE	3.57E-01	0.91	FALSE
M211T563_pos	211.1082	563	3	7.67E-09	1.24	FALSE	1.73E-02	1.09	FALSE	8.41E-19	1.36	FALSE	2.64E-02	0.87	FALSE
M211T992_pos	211.1095	992	3	7.88E-01	1.00	FALSE	1.74E-01	1.01	FALSE	4.43E-03	0.98	FALSE	3.06E-01	1.02	FALSE
M211T875_pos	211.1693	875	3	4.86E-01	1.03	FALSE	9.97E-02	0.94	FALSE	1.94E-02	0.93	FALSE	4.35E-01	1.05	FALSE
M211T1062_pos	211.2057	1062	3	9.44E-03	0.91	FALSE	8.26E-03	1.11	FALSE	2.73E-01	0.96	FALSE	9.36E-01	1.01	FALSE
M212T497_pos	212.1030	497	3	9.60E-02	1.10	FALSE	4.95E-01	1.04	FALSE	2.87E-13	1.46	FALSE	1.70E-03	0.83	FALSE
M213T1023_pos	213.0758	1023	3	1.80E-21	0.85	FALSE	1.47E-09	1.09	FALSE	3.61E-02	0.97	FALSE	7.20E-02	0.93	FALSE
M213T398_pos	213.1342	398	3	5.11E-02	1.16	FALSE	2.39E-01	1.10	FALSE	3.89E-08	1.46	FALSE	1.32E-01	0.87	FALSE
M214T834_pos	214.1803	834	3	1.37E-04	1.06	FALSE	2.43E-01	0.98	FALSE	1.68E-07	0.93	FALSE	1.83E-01	0.94	FALSE
M214T1005_pos	214.2167	1005	3	8.04E-02	0.90	FALSE	1.10E-01	0.90	FALSE	5.39E-05	0.80	FALSE	9.24E-01	1.00	FALSE
M215T469_pos	215.0487	469	3	2.13E-07	1.24	FALSE	4.51E-01	0.97	FALSE	7.13E-16	1.36	FALSE	1.89E-01	0.90	FALSE
M215T769_pos	215.1643	769	3	1.58E-07	1.21	FALSE	6.60E-01	0.98	FALSE	4.81E-04	0.90	FALSE	3.71E-01	1.08	FALSE
M217T1022_pos	217.0344	1022	3	8.59E-19	0.87	FALSE	9.21E-09	1.09	FALSE	4.48E-02	0.97	FALSE	2.23E-01	0.96	FALSE
M217T492_pos	217.0647	492	3	9.25E-02	1.13	FALSE	8.42E-01	0.99	FALSE	1.51E-09	1.50	FALSE	2.94E-01	0.87	FALSE
M217T916_pos	217.1228	916	3	8.20E-01	1.00	FALSE	9.55E-01	1.00	FALSE	1.28E-11	0.91	FALSE	2.07E-01	0.96	FALSE
M217T854_pos	217.1436	854	3	2.60E-11	0.79	FALSE	7.84E-01	1.01	FALSE	6.42E-18	1.33	FALSE	1.52E-02	0.88	FALSE
M217T465_pos	217.1548	465	3	7.34E-05	1.24	FALSE	9.26E-01	1.01	FALSE	7.57E-02	0.92	FALSE	2.76E-01	0.96	FALSE
M218T581_pos	218.0249	581	3	1.94E-03	1.24	FALSE	2.90E-02	0.85	FALSE	1.00E-09	1.46	FALSE	1.78E-01	0.89	FALSE
M219T797_pos	219.0477	797	3	5.35E-23	1.20	FALSE	9.46E-01	1.00	FALSE	3.28E-28	0.83	FALSE	1.14E-03	0.92	FALSE
M219T924_pos	219.1381	924	3	3.79E-03	1.05	FALSE	5.50E-01	1.01	FALSE	4.02E-08	0.92	FALSE	9.42E-01	1.00	FALSE
M219T1033_pos	219.1956	1033	3	2.11E-06	1.48	FALSE	2.31E-04	0.73	FALSE	5.67E-01	1.04	FALSE	3.91E-01	1.13	FALSE
M220T352_pos	220.1194	352	3	1.14E-07	1.33	FALSE	3.58E-02	1.12	FALSE	5.77E-04	1.17	FALSE	2.49E-01	1.15	FALSE
M222T468_2_pos	222.1490	468	3	3.96E-01	1.13	FALSE	1.83E-01	0.80	FALSE	8.15E-03	1.41	FALSE	3.15E-02	1.11	FALSE
M223T1033_pos	223.1691	1033	3	4.04E-01	1.18	FALSE	7.85E-01	0.94	FALSE	6.59E-01	1.08	FALSE	1.32E-01	1.14	FALSE
M223T1034_pos	223.2057	1034	3	6.48E-04	0.94	FALSE	4.33E-02	1.04	FALSE	1.14E-03	0.95	FALSE	3.70E-01	1.03	FALSE
M224T677_pos	224.0377	677	3	7.53E-01	1.02	FALSE	5.58E-01	0.96	FALSE	5.16E-11	1.49	FALSE	6.03E-01	1.08	FALSE
M224T394_pos	224.1030	394	3	4.54E-03	1.20	FALSE	6.71E-01	1.03	FALSE	4.75E-05	1.26	FALSE	3.17E-02	0.75	FALSE
M224T783_pos	224.1283	783	3	5.14E-07	1.25	FALSE	3.19E-02	1.11	FALSE	9.79E-01	1.00	FALSE	8.43E-03	1.24	FALSE
M224T973_pos	224.2011	973	3	2.93E-01	1.52	FALSE	1.12E-01	0.38	FALSE	6.72E-01	0.86	FALSE	2.50E-01	-7.87	FALSE
M225T802_pos	225.1100	802	3	2.52E-02	1.07	FALSE	6.48E-02	1.06	FALSE	6.64E-02	1.05	FALSE	9.14E-03	0.80	FALSE
M225T997_pos	225.1253	997	3	4.96E-06	0.91	FALSE	1.87E-02	1.05	FALSE	4.90E-12	0.88	FALSE	9.93E-01	1.00	FALSE
M225T894_pos	225.1484	894	3	2.92E-01	1.01	FALSE	9.62E-01	1.00	FALSE	3.98E-14	0.91	FALSE	5.57E-02	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M226T1010_pos	226.2168	1010	3						Fatty acids				
M228T1035_pos	228.2323	1035	3						Fatty acids				
M229T768_2_pos	229.1424	768	3							HMDB0000933	Traumatic acid	C12H20O4	4.3
M229T669_pos	229.1435	669	3							HMDB0000933	Traumatic acid	C12H20O4	0.2
M229T859_pos	229.1435	859	3							HMDB0000933	Traumatic acid	C12H20O4	0.4
M230T346_pos	230.1865	346	3							HMDB0041947	N1,N8-Diacetylspermidine	C11H23N3O2	0.8
M231T581_pos	231.0315	581	3							HMDB0240372	3-Phenylpropionic acid sulfate	C9H10O5S	2.7
M231T892_pos	231.1592	892	3						Fatty acids	HMDB0000623	Dodecanedioic acid	C12H22O4	0.4
M233T525_pos	233.0108	525	3						Amino acids and Peptides	HMDB0041646	4-Dihydroxyacetophenone 5-sulfa	C8H8O6S	2.7
M235T815_pos	235.1329	815	3							HMDB0030763	(10S,11S)-Pterosin C	C14H18O3	0.3
M237T879_pos	237.1850	879	3							HMDB0002352	Capsidiol	C15H24O2	0.5
M237T1006_pos	237.2215	1006	3							HMDB0031851	rimethylbicyclo[2.2.1]hept-1-yl)cyc	C16H28O	0.7
M239T848_pos	239.1278	848	3							HMDB0033191	methyl-6-(1-oxopropyl)-1,3,5-cyclo	C13H18O4	0.1
M239T714_pos	239.1391	714	3							HMDB0014562	Secobarbital	C12H18N2O3	0.3
M239T517_pos	239.1487	517	3							HMDB0256256	Pentaethylene glycol	C10H22O6	0.8
M240T499_pos	240.1233	499	3							HMDB0254628	Methyldopate	C12H17NO4	1.2
M241T942_pos	241.1799	942	3							HMDB0032369	L-Menthyl acetoacetate	C14H24O3	0.4
M242T362_pos	242.1029	362	3							HMDB0014567	Methocarbamol	C11H15NO5	2.4
M242T1048_pos	242.2480	1048	3						Fatty acids				
M243T968_1_pos	243.1592	968	3							HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	0.7
M245T669_pos	245.1385	669	3							HMDB0032472	Polyethylene, oxidized	C12H20O5	0.5
M245T403_pos	245.1607	403	3							HMDB0252056	Ethyl N2-acetyl-L-argininate	C10H20N4O3	0.4
M245T882_pos	245.1749	882	3						Fatty acids	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	0.8
M245T926_pos	245.1750	926	3							HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	1.0
M248T522_pos	248.1143	522	3							HMDB0242235	(+-)-Carbovir	C11H13N5O2	0.3
M249T581_pos	249.0420	581	3							HMDB0240528	Homovanillyl alcohol sulfate	C9H12O6S	2.8
M249T917_2_pos	249.2062	917	3						Fatty acids	HMDB0032181	ega-hydroxypoly(oxyethylene) poly	C13H28O4	0.6
M251T1042_pos	251.0469	1042	3							HMDB0251449	Diphenyl phosphate	C12H11O4P	0.5
M251T917_pos	251.0791	917	3							HMDB0250519	Cppene	C8H15N2O5P	0.3
M251T1071_pos	251.2370	1071	3							HMDB0031336	(Z)-9-Cycloheptadecen-1-one	C17H30O	0.4
M253T680_pos	253.1185	680	3							HMDB0013940	N-Desmethylpromazine	C12H16N2O4	0.9
M253T757_pos	253.1188	757	3							HMDB0013940	N-Desmethylpromazine	C12H16N2O4	2.1
M253T518_pos	253.1278	518	3							HMDB0040822	2,3-Butanediol glucoside	C10H20O7	1.7
M253T815_pos	253.1436	815	3							HMDB0033197	methyl-6-(1-oxobutyl)-1,3,5-cyclo	C14H20O4	0.5
M255T726_pos	255.1956	726	3							HMDB0029604	Lubiminol	C15H26O3	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M226T1010_pos	226.2168	1010	3	2.00E-02	0.95	FALSE	6.29E-02	1.05	FALSE	2.87E-07	0.90	FALSE	3.85E-01	1.03	FALSE
M228T1035_pos	228.2323	1035	3	3.64E-06	0.90	FALSE	1.95E-01	1.03	FALSE	1.16E-06	0.90	FALSE	8.61E-01	1.01	FALSE
M229T768_2_pos	229.1424	768	3	1.15E-01	1.09	FALSE	3.69E-01	1.06	FALSE	8.42E-01	1.01	FALSE	8.37E-01	1.04	FALSE
M229T669_pos	229.1435	669	3	2.78E-18	1.49	FALSE	8.51E-01	0.99	FALSE	1.39E-02	1.09	FALSE	6.79E-02	0.90	FALSE
M229T859_pos	229.1435	859	3	5.11E-04	0.89	FALSE	1.15E-01	0.94	FALSE	2.38E-08	1.19	FALSE	1.56E-01	0.91	FALSE
M230T346_pos	230.1865	346	3	7.26E-11	1.45	FALSE	3.63E-02	1.12	FALSE	6.78E-06	1.24	FALSE	9.08E-01	1.01	FALSE
M231T581_pos	231.0315	581	3	2.10E-09	1.41	FALSE	2.62E-01	0.94	FALSE	9.86E-01	1.00	FALSE	5.63E-01	1.07	FALSE
M231T892_pos	231.1592	892	3	7.95E-14	0.79	FALSE	8.21E-02	1.06	FALSE	4.11E-21	1.32	FALSE	8.69E-01	0.99	FALSE
M233T525_pos	233.0108	525	3	1.11E-31	1.44	FALSE	4.51E-02	0.95	FALSE	9.18E-02	0.96	FALSE	7.83E-01	1.02	FALSE
M235T815_pos	235.1329	815	3	9.22E-15	1.35	FALSE	9.65E-01	1.00	FALSE	1.00E-01	1.05	FALSE	6.56E-01	1.03	FALSE
M237T879_pos	237.1850	879	3	1.86E-01	0.94	FALSE	2.28E-04	1.19	FALSE	2.73E-19	1.50	FALSE	9.80E-01	1.00	FALSE
M237T1006_pos	237.2215	1006	3	4.58E-04	1.14	FALSE	5.96E-03	0.90	FALSE	1.13E-02	0.92	FALSE	2.01E-06	1.40	FALSE
M239T848_pos	239.1278	848	3	6.46E-04	1.08	FALSE	2.07E-02	0.95	FALSE	3.79E-14	0.85	FALSE	3.35E-01	1.06	FALSE
M239T714_pos	239.1391	714	3	3.61E-07	1.29	FALSE	6.65E-01	1.03	FALSE	3.52E-01	1.04	FALSE	7.82E-01	1.01	FALSE
M239T517_pos	239.1487	517	3	9.10E-07	1.19	FALSE	4.84E-01	0.98	FALSE	6.71E-01	0.99	FALSE	2.09E-03	1.46	FALSE
M240T499_pos	240.1233	499	3	7.63E-03	1.12	FALSE	4.01E-02	1.09	FALSE	2.27E-14	1.34	FALSE	3.34E-01	0.96	FALSE
M241T942_pos	241.1799	942	3	7.31E-01	1.02	FALSE	7.65E-01	0.99	FALSE	2.54E-17	1.48	FALSE	2.98E-01	0.89	FALSE
M242T362_pos	242.1029	362	3	1.92E-07	0.81	FALSE	2.97E-01	1.04	FALSE	1.13E-22	1.46	FALSE	6.96E-02	1.11	FALSE
M242T1048_pos	242.2480	1048	3	1.72E-05	0.90	FALSE	2.53E-03	1.08	FALSE	1.43E-07	0.89	FALSE	3.26E-01	1.04	FALSE
M243T968_1_pos	243.1592	968	3	1.68E-02	0.97	FALSE	3.92E-01	1.01	FALSE	1.10E-05	0.96	FALSE	5.19E-01	0.98	FALSE
M245T669_pos	245.1385	669	3	4.61E-03	1.09	FALSE	1.57E-01	1.05	FALSE	1.07E-27	1.43	FALSE	2.98E-02	0.93	FALSE
M245T403_pos	245.1607	403	3	2.56E-05	1.22	FALSE	9.50E-01	1.00	FALSE	3.77E-15	1.41	FALSE	5.42E-02	1.17	FALSE
M245T882_pos	245.1749	882	3	6.10E-03	0.92	FALSE	7.44E-02	1.06	FALSE	8.11E-11	1.19	FALSE	4.82E-01	1.06	FALSE
M245T926_pos	245.1750	926	3	5.99E-07	0.84	FALSE	2.39E-02	1.09	FALSE	3.18E-07	1.17	FALSE	4.43E-02	1.19	FALSE
M248T522_pos	248.1143	522	3	1.18E-12	1.40	FALSE	4.07E-09	1.31	FALSE	1.94E-13	1.36	FALSE	1.12E-01	1.04	FALSE
M249T581_pos	249.0420	581	3	1.48E-04	1.34	FALSE	6.73E-02	0.87	FALSE	4.53E-01	0.95	FALSE	7.29E-01	1.06	FALSE
M249T917_2_pos	249.2062	917	3	4.36E-01	1.02	FALSE	6.51E-01	1.01	FALSE	1.04E-06	0.90	FALSE	1.91E-08	-33.97	FALSE
M251T1042_pos	251.0469	1042	3	4.22E-07	0.93	FALSE	1.18E-02	1.04	FALSE	7.20E-02	0.98	FALSE	3.92E-02	0.95	FALSE
M251T917_pos	251.0791	917	3	1.70E-01	1.07	FALSE	5.65E-01	1.03	FALSE	8.10E-01	1.01	FALSE	2.21E-01	0.86	FALSE
M251T1071_pos	251.2370	1071	3	2.05E-02	0.96	FALSE	7.30E-01	1.01	FALSE	5.38E-01	0.99	FALSE	9.71E-01	1.00	FALSE
M253T680_pos	253.1185	680	3	9.23E-01	1.01	FALSE	6.16E-01	1.03	FALSE	2.10E-11	1.47	FALSE	1.64E-02	0.82	FALSE
M253T757_pos	253.1188	757	3	1.61E-02	1.09	FALSE	2.72E-01	1.04	FALSE	1.84E-13	1.29	FALSE	4.63E-03	0.85	FALSE
M253T518_pos	253.1278	518	3	5.32E-35	1.46	FALSE	2.63E-01	1.03	FALSE	1.92E-12	1.17	FALSE	4.45E-01	0.96	FALSE
M253T815_pos	253.1436	815	3	1.94E-13	1.37	FALSE	5.95E-01	1.02	FALSE	2.03E-01	1.04	FALSE	5.33E-01	0.94	FALSE
M255T726_pos	255.1956	726	3	2.47E-14	1.42	FALSE	2.10E-01	1.06	FALSE	2.63E-02	0.92	FALSE	3.22E-01	1.12	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M256T1067_pos	256.2635	1067	3						Fatty acids	HMDB0012273	Palmitic amide	C16H33NO	0.0
M257T1033_pos	257.1045	1033	3							HMDB0247463	8-Phenyltheophylline	C13H12N4O2	4.8
M257T920_pos	257.1749	920	3							HMDB0030993	ltetrahydro-2-oxo-3-furancarboxy	C14H24O4	0.6
M258T606_pos	258.1704	606	3							HMDB0013161	2-Hexenoylcarnitine	C13H23NO4	1.7
M258T603_pos	258.2066	603	3							HMDB0013272	N-Lauroylglycine	C14H27NO3	0.7
M259T942_pos	259.1905	942	3							HMDB0000872	Tetradecanedioic acid	C14H26O4	0.4
M263T793_pos	263.1280	793	3							HMDB0030549	thoxy-6-[2-(4-methoxyphenyl)ethy	C15H18O4	0.7
M263T1038_pos	263.2371	1038	3						Fatty acids	HMDB0034495	4-Trimethyl-5,9,13-pentadecatrien	C18H30O	0.5
M267T670_pos	267.1206	670	3							HMDB0246876	beta-Pregnane-3alpha,20alpha-di	C10H14N6O3	2.4
M267T664_pos	267.1340	664	3							HMDB0029005	Phenylalanylthreonine	C13H18N2O4	0.1
M267T992_pos	267.1720	992	3							HMDB0303280	Potassium myristate	C14H27KO2	0.2
M267T891_pos	267.1957	891	3						Fatty acids	HMDB0033917	roxy-3-methoxy-2,10-bisaboladien	C16H26O3	0.7
M268T501_pos	268.1656	501	3							HMDB0249665	Carbuterol	C13H21N3O3	0.0
M269T1016_pos	269.2098	1016	3						Fatty acids				
M270T521_pos	270.2064	521	3							HMDB0032255	carbonyl)methyl)-p-menthane-3-ca	C15H27NO3	0.1
M270T1078_pos	270.2793	1078	3						Fatty acids	HMDB0040940	Capsiamide	C17H35NO	0.4
M271T632_pos	271.0751	632	3							HMDB0240217	3-(Cystein-S-yl)acetaminophen	C11H14N2O4S	1.5
M271T772_pos	271.1079	772	3							HMDB0060568	10,11-Dihydroxycarbamazepine	C15H14N2O3	0.8
M271T1002_pos	271.2270	1002	3						Fatty acids	HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	0.7
M272T764_pos	272.1859	764	3							HMDB0241681	Hept-3-enoylcarnitine	C14H25NO4	0.8
M272T973_pos	272.2586	973	3						Fatty acids	HMDB0242181	Hexadecasphingosine	C16H33NO2	0.8
M273T1022_pos	273.0969	1022	3							HMDB0029943	Arbutin	C12H16O7	0.2
M273T1017_pos	273.2064	1017	3							HMDB0035918	7(14)-Bisabolene-2,3,10,11-tetrol	C15H28O4	1.4
M276T619_pos	276.1807	619	3							HMDB0013131	3-Hydroxyhexanoylcarnitine	C13H25NO5	0.5
M277T580_pos	277.0524	580	3							HMDB0060924	Suprofen S-oxide	C14H12O4S	1.8
M278T1002_pos	278.2480	1002	3							HMDB0256035	4-(Dodecylamino)Phenol	C18H31NO	0.5
M279T997_pos	279.1592	997	3							HMDB0001518	alpha-CEHC	C16H22O4	0.5
M281T700_pos	281.1173	700	3							HMDB0015081	Phenprocoumon	C18H16O3	0.4
M281T793_pos	281.1385	793	3							HMDB0035620	Artabsinolide A	C15H20O5	0.5
M282T1075_pos	282.2791	1075	3						Fatty acids	HMDB0002117	Oleamide	C18H35NO	0.1
M283T1065_pos	283.1752	1065	3							HMDB0061822	Hexaethylene glycol	C12H26O7	0.3
M283T553_pos	283.1752	553	3							HMDB0061822	Hexaethylene glycol	C12H26O7	0.1
M283T878_pos	283.1905	878	3							HMDB0033630	Lactapiperanol C	C16H26O4	0.6
M285T891_pos	285.2062	891	3							HMDB0258926	Tetranorprostanedioic acid	C16H28O4	0.5
M285T1033_pos	285.2427	1033	3							HMDB0035473	Avocadyne	C17H32O3	0.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M256T1067_pos	256.2635	1067	3	3.30E-01	0.97	FALSE	6.54E-01	0.99	FALSE	8.39E-01	0.99	FALSE	4.04E-01	1.08	FALSE
M257T1033_pos	257.1045	1033	3	3.33E-02	1.11	FALSE	8.62E-02	0.92	FALSE	8.51E-01	1.01	FALSE	4.51E-01	1.06	FALSE
M257T920_pos	257.1749	920	3	4.23E-04	0.89	FALSE	1.33E-01	1.06	FALSE	3.04E-14	1.27	FALSE	8.38E-01	0.98	FALSE
M258T606_pos	258.1704	606	3	3.85E-06	1.30	FALSE	3.94E-01	0.95	FALSE	1.50E-06	1.27	FALSE	6.77E-01	0.93	FALSE
M258T603_pos	258.2066	603	3	6.55E-16	1.36	FALSE	7.13E-01	1.01	FALSE	2.55E-09	1.21	FALSE	2.14E-02	0.90	FALSE
M259T942_pos	259.1905	942	3	2.49E-02	0.91	FALSE	3.76E-01	0.96	FALSE	5.41E-20	1.46	FALSE	1.09E-01	0.89	FALSE
M263T793_pos	263.1280	793	3	1.39E-06	1.26	FALSE	1.13E-02	1.13	FALSE	2.60E-03	1.13	FALSE	4.88E-01	1.08	FALSE
M263T1038_pos	263.2371	1038	3	2.95E-02	1.24	FALSE	7.39E-03	0.75	FALSE	1.58E-02	1.23	FALSE	6.31E-01	1.06	FALSE
M267T670_pos	267.1206	670	3	2.28E-40	1.46	FALSE	4.76E-03	1.07	FALSE	3.68E-10	1.14	FALSE	9.29E-01	1.00	FALSE
M267T664_pos	267.1340	664	3	7.08E-03	1.20	FALSE	4.36E-01	0.95	FALSE	5.27E-03	1.18	FALSE	4.03E-01	1.06	FALSE
M267T992_pos	267.1720	992	3	3.25E-02	0.98	FALSE	3.82E-01	1.01	FALSE	1.31E-03	0.98	FALSE	4.80E-01	0.99	FALSE
M267T891_pos	267.1957	891	3	3.39E-01	0.97	FALSE	5.26E-02	1.08	FALSE	1.89E-17	1.34	FALSE	6.52E-01	1.04	FALSE
M268T501_pos	268.1656	501	3	4.29E-04	1.21	FALSE	5.84E-01	1.03	FALSE	2.83E-09	1.34	FALSE	1.47E-02	0.82	FALSE
M269T1016_pos	269.2098	1016	3	1.62E-01	0.96	FALSE	2.36E-01	1.04	FALSE	9.63E-01	1.00	FALSE	9.23E-03	1.26	FALSE
M270T521_pos	270.2064	521	3	3.14E-10	1.43	FALSE	2.57E-01	1.07	FALSE	6.90E-06	1.24	FALSE	6.12E-01	1.05	FALSE
M270T1078_pos	270.2793	1078	3	7.15E-02	1.06	FALSE	4.51E-01	0.97	FALSE	3.87E-02	0.94	FALSE	4.26E-01	1.06	FALSE
M271T632_pos	271.0751	632	3	4.00E-09	1.29	FALSE	4.57E-01	1.03	FALSE	3.77E-10	1.27	FALSE	9.12E-04	0.82	FALSE
M271T772_pos	271.1079	772	3	4.03E-03	1.14	FALSE	3.57E-01	1.04	FALSE	2.88E-14	1.37	FALSE	8.14E-04	0.79	FALSE
M271T1002_pos	271.2270	1002	3	9.45E-05	1.13	FALSE	9.43E-04	0.90	FALSE	4.83E-04	1.10	FALSE	1.55E-04	1.32	FALSE
M272T764_pos	272.1859	764	3	8.38E-11	1.31	FALSE	2.01E-01	1.05	FALSE	3.09E-03	1.11	FALSE	3.52E-04	0.77	FALSE
M272T973_pos	272.2586	973	3	9.65E-01	1.00	FALSE	9.40E-01	1.00	FALSE	1.77E-05	1.06	FALSE	5.40E-01	0.98	FALSE
M273T1022_pos	273.0969	1022	3	2.11E-19	0.86	FALSE	9.97E-09	1.09	FALSE	2.35E-02	0.97	FALSE	1.41E-01	0.95	FALSE
M273T1017_pos	273.2064	1017	3	1.13E-02	0.96	FALSE	6.28E-04	1.05	FALSE	8.77E-03	0.97	FALSE	2.47E-01	1.03	FALSE
M276T619_pos	276.1807	619	3	1.19E-06	1.29	FALSE	4.63E-01	0.96	FALSE	2.88E-04	1.18	FALSE	2.31E-02	0.76	FALSE
M277T580_pos	277.0524	580	3	9.75E-06	1.45	FALSE	4.94E-01	0.94	FALSE	1.39E-02	1.19	FALSE	6.94E-01	1.09	FALSE
M278T1002_pos	278.2480	1002	3	8.83E-06	0.93	FALSE	9.37E-02	1.03	FALSE	5.68E-04	0.95	FALSE	3.67E-01	1.03	FALSE
M279T997_pos	279.1592	997	3	1.71E-01	0.97	FALSE	1.52E-01	1.04	FALSE	1.71E-07	0.89	FALSE	3.69E-01	1.02	FALSE
M281T700_pos	281.1173	700	3	5.45E-24	1.37	FALSE	8.84E-02	1.05	FALSE	7.24E-15	1.22	FALSE	3.65E-01	1.04	FALSE
M281T793_pos	281.1385	793	3	1.93E-06	0.78	FALSE	4.60E-02	1.11	FALSE	1.88E-02	1.11	FALSE	5.01E-01	0.96	FALSE
M282T1075_pos	282.2791	1075	3	3.56E-03	0.95	FALSE	1.93E-02	1.05	FALSE	1.08E-01	0.97	FALSE	1.03E-01	1.06	FALSE
M283T1065_pos	283.1752	1065	3	9.90E-01	1.00	FALSE	3.34E-01	0.98	FALSE	5.23E-01	1.01	FALSE	1.03E-01	0.92	FALSE
M283T553_pos	283.1752	553	3	1.78E-06	1.16	FALSE	4.47E-01	0.98	FALSE	4.45E-01	1.02	FALSE	4.37E-04	1.48	FALSE
M283T878_pos	283.1905	878	3	5.37E-02	0.93	FALSE	1.07E-03	1.14	FALSE	8.84E-23	1.47	FALSE	6.57E-01	0.96	FALSE
M285T891_pos	285.2062	891	3	3.50E-01	0.97	FALSE	4.02E-02	1.08	FALSE	3.30E-17	1.33	FALSE	6.43E-01	1.04	FALSE
M285T1033_pos	285.2427	1033	3	9.67E-02	1.39	FALSE	5.32E-01	0.88	FALSE	4.54E-01	1.14	FALSE	9.58E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M287T803_1_pos	287.0944	803	3							HMDB0252019	Ethofumesate	C13H18O5S	1.1
M287T690_pos	287.1859	690	3							HMDB0240222	Thonzylamine	C16H22N4O	2.4
M287T890_pos	287.2215	890	3						Fatty acids	HMDB0000672	Hexadecanedioic acid	C16H30O4	0.5
M287T858_pos	287.2696	858	3							HMDB0250199	yl hexyl(2-(hexylamino)ethyl)carba	C16H34N2O2	0.9
M289T1033_pos	289.1309	1033	3							HMDB0251156	Diazoxon	C12H21N2O4P	0.9
M289T822_pos	289.1549	822	3							HMDB0034913	Imazamethabenz-methyl	C16H20N2O3	1.0
M289T992_pos	289.1541	992	3							HMDB0034913	Imazamethabenz-methyl	C16H20N2O3	1.9
M291T608_pos	291.1374	608	3							HMDB0040916	(4-Methyl-3-pentenyl)anthraquino	C20H18O2	1.9
M291T888_pos	291.2168	888	3						Fatty acids	HMDB0040168	Glycerol 1-(5-hydroxydodecanoate	C15H30O5	0.5
M297T1071_pos	297.2789	1071	3						Fatty acids	HMDB0013622	10Z-Nonadecenoic acid	C19H36O2	0.4
M298T990_pos	298.2742	990	3						Fatty acids	HMDB0013648	Palmitoleoylethanolamde	C18H35NO2	0.5
M299T700_pos	299.1281	700	3							HMDB0004808	7C-aglycone	C18H18O4	0.9
M300T1006_pos	300.2535	1006	3							HMDB0013300	Pentadecanoylglycine	C17H33NO3	0.5
M300T1015_pos	300.2898	1015	3						Fatty acids	HMDB0000252	Sphingosine	C18H37NO2	0.2
M301T807_pos	301.1184	807	3							HMDB0243809	no]-2-oxoethyl}-6-oxo-1,6-dihydro	C16H16N2O4	0.5
M303T905_pos	303.1206	905	3							HMDB0304380	indole-3-acetyl-glutamine	C15H16N3O4	4.2
M303T785_pos	303.1704	785	3							HMDB0251775	Emivirine	C17H22N2O3	0.2
M303T891_pos	303.2169	891	3						Fatty acids	HMDB0037830	xi-7-Hydroxyhexadecanedioic acid	C16H30O5	1.1
M304T1074_pos	304.2610	1074	3						Fatty acids				
M305T904_pos	305.2113	904	3						Terpenoids	HMDB0000309	lpha,16beta-Dihydroxyandrosteno	C19H28O3	0.4
M307T992_pos	307.1650	992	3							HMDB0253499	Inproquone	C16H22N2O4	0.8
M307T701_pos	307.1655	701	3							HMDB0253499	Inproquone	C16H22N2O4	0.7
M309T801_pos	309.2272	801	3							HMDB0037162	1,2,3-Tris(1-ethoxyethoxy)propane	C15H32O6	0.2
M309T978_pos	309.2578	978	3						Terpenoids				
M311T714_pos	311.0592	714	3							HMDB0240500	Dihydroresveratrol 3-sulfate	C14H14O6S	2.6
M311T914_pos	311.1855	914	3							HMDB0040756	-6,8-dimethoxy-7(11)-eremophilen	C17H26O5	0.6
M312T962_pos	312.1596	962	3							HMDB0029378	(-)-Thebaine	C19H21NO3	0.4
M313T1075_2_pos	313.3214	1075	3							HMDB0255793	1,2 Dipalmitoylphosphatidylcholine	C19H40N2O	0.1
M314T1027_pos	314.2693	1027	3							HMDB0013034	Palmitoylglycine	C18H35NO3	1.2
M314T1060_pos	314.3056	1060	3						Fatty acids				
M315T932_pos	315.1230	932	3							HMDB0030567	(-)-3,4,9-Trimethoxypterocarpan	C18H18O5	0.9
M315T858_pos	315.1957	858	3							HMDB0006285	4-oxo-Retinoic acid	C20H26O3	0.6
M315T1063_pos	315.2533	1063	3							HMDB0000782	Octadecanedioic acid	C18H34O4	0.8
M316T1038_pos	316.2847	1038	3						Fatty acids	HMDB0038057	Dehydrophytosphingosine	C18H37NO3	0.4
M317T948_pos	317.1748	948	3							HMDB0029566	Isopulegone caffeate	C19H24O4	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M287T803_1_pos	287.0944	803	3	8.90E-04	1.10	FALSE	2.39E-01	1.04	FALSE	7.42E-01	0.99	FALSE	3.38E-01	1.06	FALSE
M287T690_pos	287.1859	690	3	1.55E-04	1.28	FALSE	9.40E-01	1.01	FALSE	2.76E-02	1.13	FALSE	4.31E-01	1.16	FALSE
M287T890_pos	287.2215	890	3	1.16E-03	1.23	FALSE	9.12E-02	0.89	FALSE	8.93E-01	1.01	FALSE	2.12E-01	0.90	FALSE
M287T858_pos	287.2696	858	3	5.45E-07	0.81	FALSE	2.70E-01	0.96	FALSE	6.74E-01	0.99	FALSE	1.94E-01	0.89	FALSE
M289T1033_pos	289.1309	1033	3	7.83E-03	1.14	FALSE	1.84E-01	0.94	FALSE	6.33E-01	1.02	FALSE	4.40E-01	1.07	FALSE
M289T822_pos	289.1549	822	3	2.79E-01	1.04	FALSE	7.64E-01	0.99	FALSE	2.39E-21	1.39	FALSE	3.97E-02	0.91	FALSE
M289T992_pos	289.1541	992	3	8.95E-02	0.97	FALSE	5.89E-01	1.01	FALSE	4.24E-04	0.94	FALSE	1.43E-01	0.91	FALSE
M291T608_pos	291.1374	608	3	2.97E-09	1.22	FALSE	7.90E-01	1.01	FALSE	1.79E-13	1.25	FALSE	1.85E-02	0.92	FALSE
M291T888_pos	291.2168	888	3	4.65E-01	0.95	FALSE	2.74E-01	1.09	FALSE	7.92E-02	1.11	FALSE	9.90E-01	1.00	FALSE
M297T1071_pos	297.2789	1071	3	8.75E-01	1.05	FALSE	4.40E-01	1.30	FALSE	2.35E-01	1.38	FALSE	9.78E-01	1.02	FALSE
M298T990_pos	298.2742	990	3	2.82E-03	0.96	FALSE	3.98E-01	1.01	FALSE	1.07E-02	1.03	FALSE	8.84E-01	0.99	FALSE
M299T700_pos	299.1281	700	3	7.04E-20	1.31	FALSE	1.44E-01	1.04	FALSE	9.11E-16	1.22	FALSE	1.87E-01	1.05	FALSE
M300T1006_pos	300.2535	1006	3	5.74E-04	0.96	FALSE	2.81E-02	1.03	FALSE	8.38E-03	0.97	FALSE	1.53E-01	1.04	FALSE
M300T1015_pos	300.2898	1015	3	1.20E-04	1.05	FALSE	1.02E-01	0.98	FALSE	3.87E-02	1.02	FALSE	5.73E-01	0.99	FALSE
M301T807_pos	301.1184	807	3	2.42E-01	1.05	FALSE	7.40E-01	1.02	FALSE	1.84E-10	1.30	FALSE	2.64E-02	0.89	FALSE
M303T905_pos	303.1206	905	3	1.34E-03	1.06	FALSE	8.49E-01	1.00	FALSE	1.38E-18	0.87	FALSE	2.96E-01	1.03	FALSE
M303T785_pos	303.1704	785	3	2.79E-04	1.19	FALSE	3.10E-06	0.81	FALSE	8.20E-09	1.28	FALSE	4.73E-01	0.96	FALSE
M303T891_pos	303.2169	891	3	4.50E-01	0.97	FALSE	8.90E-02	1.07	FALSE	1.96E-13	1.28	FALSE	5.00E-01	1.06	FALSE
M304T1074_pos	304.2610	1074	3	3.96E-03	0.86	FALSE	2.82E-02	1.13	FALSE	8.29E-03	0.89	FALSE	1.19E-01	1.26	FALSE
M305T904_pos	305.2113	904	3	4.68E-18	1.29	FALSE	4.85E-01	0.98	FALSE	7.31E-01	0.99	FALSE	3.49E-01	1.11	FALSE
M307T992_pos	307.1650	992	3	6.12E-05	0.91	FALSE	8.19E-01	1.01	FALSE	2.62E-05	0.91	FALSE	7.90E-01	0.99	FALSE
M307T701_pos	307.1655	701	3	1.68E-05	1.20	FALSE	3.39E-06	0.83	FALSE	3.59E-06	1.19	FALSE	5.49E-02	0.90	FALSE
M309T801_pos	309.2272	801	3	1.65E-02	0.91	FALSE	7.71E-02	1.07	FALSE	4.34E-01	0.97	FALSE	7.62E-01	1.03	FALSE
M309T978_pos	309.2578	978	3	1.22E-10	1.15	FALSE	1.20E-01	0.97	FALSE	7.27E-11	1.13	FALSE	2.81E-01	0.97	FALSE
M311T714_pos	311.0592	714	3	4.38E-28	1.37	FALSE	4.67E-02	1.05	FALSE	3.58E-01	0.98	FALSE	2.00E-01	0.94	FALSE
M311T914_pos	311.1855	914	3	2.30E-01	1.02	FALSE	1.05E-01	1.03	FALSE	3.85E-11	0.91	FALSE	7.95E-04	1.10	FALSE
M312T962_pos	312.1596	962	3	4.38E-01	1.57	FALSE	4.02E-01	0.47	FALSE	8.84E-02	2.48	FALSE	3.89E-01	0.40	FALSE
M313T1075_2_pos	313.3214	1075	3	2.83E-01	0.95	FALSE	1.42E-02	1.12	FALSE	2.06E-03	0.88	FALSE	1.94E-01	1.18	FALSE
M314T1027_pos	314.2693	1027	3	1.70E-01	1.04	FALSE	4.31E-01	0.97	FALSE	4.38E-01	0.98	FALSE	7.22E-01	1.03	FALSE
M314T1060_pos	314.3056	1060	3	7.21E-01	1.14	FALSE	8.81E-01	1.05	FALSE	6.52E-01	0.87	FALSE	4.08E-01	0.67	FALSE
M315T932_pos	315.1230	932	3	2.47E-07	0.87	FALSE	3.01E-02	0.95	FALSE	3.17E-14	0.84	FALSE	2.09E-01	1.74	FALSE
M315T858_pos	315.1957	858	3	3.78E-02	1.07	FALSE	5.25E-02	1.07	FALSE	2.93E-08	1.18	FALSE	9.01E-01	0.99	FALSE
M315T1063_pos	315.2533	1063	3	5.47E-01	1.05	FALSE	2.04E-01	1.11	FALSE	2.24E-01	1.08	FALSE	4.09E-01	0.96	FALSE
M316T1038_pos	316.2847	1038	3	1.65E-05	1.39	FALSE	4.91E-07	0.69	FALSE	3.13E-02	1.15	FALSE	1.01E-01	1.19	FALSE
M317T948_pos	317.1748	948	3	4.51E-02	0.93	FALSE	7.09E-03	0.91	FALSE	3.45E-16	1.31	FALSE	4.45E-02	0.87	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M319T1029_pos	319.1913	1029	3							HMDB0006709	Ubiquinone-2	C19H26O4	2.9
M319T858_pos	319.2111	858	3							HMDB0029850	L-Citronellol glucoside	C16H30O6	1.4
M321T793_pos	321.1312	793	3							HMDB0242669	urin-9-yl)-N-cyclopropyl-3,4-dihydr	C13H16N6O4	1.9
M321T1037_pos	321.2417	1037	3						Fatty acids	HMDB0002190	6-Epoxy-8,11,14-eicosatrienoic ac	C20H32O3	2.3
M323T678_pos	323.1604	678	3							HMDB0247525	-(Phosphonooxy)decyl methacryla	C14H27O6P	4.4
M325T684_pos	325.1094	684	3							HMDB0015527	Prazepam	C19H17ClN2O	2.6
M325T891_pos	325.1992	891	3						Fatty acids				
M327T903_pos	327.0083	903	3							HMDB0259277	Tris(2-chloropropyl) phosphate	C9H18Cl3O4P	0.6
M327T963_pos	327.0782	963	3							HMDB0259262	TRIPHENYL PHOSPHATE	C18H15O4P	0.5
M327T582_pos	327.2013	582	3							HMDB0061835	Heptaethylene glycol	C14H30O8	0.2
M328T897_pos	328.2121	897	3							HMDB0241110	Z)-3-Hydroxydeca-4,6-dienoylcarn	C17H29NO5	0.9
M328T1042_2_pos	328.2847	1042	3						Fatty acids	HMDB0013246	Margaroylglycine	C19H37NO3	0.1
M329T701_pos	329.1166	701	3							HMDB0259320	Tubulin Polymerization Inhibitor	C22H16O3	2.0
M329T1022_pos	329.1594	1022	3							HMDB0029777	Cymorcin monoglucoside	C16H24O7	0.2
M329T932_pos	329.2322	932	3							HMDB0035919	Corchorifatty acid F	C18H32O5	0.1
M332T424_pos	332.1492	424	3							HMDB0302721	Pretazettine	C18H21NO5	0.2
M333T613_pos	333.1338	613	3							HMDB0030664	3-Galloylcatechin	C18H20O6	1.5
M333T1034_pos	333.2774	1034	3							HMDB0002226	Adrenic acid	C22H36O2	4.1
M335T896_pos	335.1955	896	3							HMDB0256796	Proglumide	C18H26N2O4	3.2
M336T1046_pos	336.3253	1046	3							HMDB0031678	Pipericine	C22H41NO	2.2
M339T784_pos	339.0906	784	3							HMDB0253873	L-Ascorbic acid 2-glucoside	C12H18O11	4.7
M339T883_pos	339.2313	883	3							HMDB0032502	Santalyl phenylacetate	C23H30O2	1.6
M341T1014_pos	341.2084	1014	3							HMDB0256359	Pexacerfont	C18H24N6O	0.2
M343T986_pos	343.1542	986	3							HMDB0030859	Austrobailignan 7	C20H22O5	0.6
M343T1043_pos	343.2118	1043	3							HMDB0002277	2,3-Dinor-6-keto-prostaglandin F1	C18H30O6	0.8
M346T454_pos	346.1651	454	3							HMDB0242457	-yl)-2-methoxyphenyl)amino)pyrin	C19H23NO5	0.5
M346T769_pos	346.1652	769	3							HMDB0242457	-yl)-2-methoxyphenyl)amino)pyrin	C19H23NO5	0.7
M347T921_pos	347.1705	921	3							HMDB0033222	R)-6,9-Dihydroxyfenchone 6-O-b-D	C16H26O8	1.2
M348T717_pos	348.1447	717	3							HMDB0255456	Naproxcinod	C18H21NO6	1.7
M349T866_pos	349.2011	866	3							HMDB0032010	Gibberellin A110	C20H28O5	0.4
M349T824_pos	349.2109	824	3							HMDB0015695	Roxatidine acetate	C19H28N2O4	3.7
M355T857_pos	355.2268	857	3							HMDB0252122	Etretinate	C23H30O3	0.2
M355T866_pos	355.2625	866	3							HMDB0039760	empferol 3-(2G-apiosylrobinobiosi	C24H34O2	1.9
M355T979_pos	355.2631	979	3							HMDB0039760	empferol 3-(2G-apiosylrobinobiosi	C24H34O2	0.2
M355T916_pos	355.2631	916	3							HMDB0039760	empferol 3-(2G-apiosylrobinobiosi	C24H34O2	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M319T1029_pos	319.1913	1029	3	9.48E-01	1.01	FALSE	2.27E-01	1.22	FALSE	8.25E-01	1.03	FALSE	6.18E-01	0.97	FALSE
M319T858_pos	319.2111	858	3	3.53E-01	0.96	FALSE	1.83E-02	1.11	FALSE	2.90E-18	1.44	FALSE	8.85E-01	0.99	FALSE
M321T793_pos	321.1312	793	3	4.49E-05	1.18	FALSE	2.02E-02	1.10	FALSE	8.76E-01	0.99	FALSE	3.60E-01	1.12	FALSE
M321T1037_pos	321.2417	1037	3	1.25E-04	1.31	FALSE	2.20E-06	0.72	FALSE	3.07E-03	1.20	FALSE	4.71E-01	1.06	FALSE
M323T678_pos	323.1604	678	3	1.35E-02	1.11	FALSE	7.74E-02	1.08	FALSE	7.50E-16	1.38	FALSE	1.18E-03	0.81	FALSE
M325T684_pos	325.1094	684	3	2.80E-01	1.48	FALSE	1.84E-01	0.56	FALSE	7.60E-01	0.91	FALSE	5.75E-01	0.76	FALSE
M325T891_pos	325.1992	891	3	6.35E-05	0.87	FALSE	1.90E-01	1.05	FALSE	6.97E-07	1.16	FALSE	8.81E-01	1.01	FALSE
M327T903_pos	327.0083	903	3	2.51E-03	0.93	FALSE	7.11E-04	0.92	FALSE	9.51E-23	0.79	FALSE	2.73E-01	0.94	FALSE
M327T963_pos	327.0782	963	3	5.28E-13	0.90	FALSE	9.26E-01	1.00	FALSE	2.13E-25	0.87	FALSE	1.57E-01	1.04	FALSE
M327T582_pos	327.2013	582	3	5.38E-25	1.16	FALSE	3.79E-01	0.99	FALSE	8.28E-01	1.00	FALSE	4.33E-08	1.45	FALSE
M328T897_pos	328.2121	897	3	3.61E-01	1.08	FALSE	1.93E-03	1.30	FALSE	4.40E-06	1.40	FALSE	1.14E-01	1.26	FALSE
M328T1042_2_pos	328.2847	1042	3	1.24E-01	0.98	FALSE	2.11E-01	1.02	FALSE	4.47E-03	0.97	FALSE	6.72E-01	1.01	FALSE
M329T701_pos	329.1166	701	3	5.90E-02	1.22	FALSE	3.82E-02	0.81	FALSE	4.17E-05	1.48	FALSE	1.84E-01	0.77	FALSE
M329T1022_pos	329.1594	1022	3	3.47E-18	0.87	FALSE	1.65E-07	1.08	FALSE	2.85E-02	0.97	FALSE	1.53E-01	0.95	FALSE
M329T932_pos	329.2322	932	3	2.02E-03	0.89	FALSE	1.47E-02	1.10	FALSE	1.48E-19	1.40	FALSE	2.57E-01	0.90	FALSE
M332T424_pos	332.1492	424	3	4.24E-05	0.79	FALSE	7.50E-01	1.02	FALSE	8.58E-14	1.49	FALSE	6.85E-01	1.04	FALSE
M333T613_pos	333.1338	613	3	2.59E-13	1.31	FALSE	5.75E-02	1.07	FALSE	1.06E-13	1.27	FALSE	6.18E-03	1.18	FALSE
M333T1034_pos	333.2774	1034	3	1.64E-01	0.85	FALSE	1.40E-01	0.84	FALSE	7.87E-01	0.97	FALSE	6.34E-01	0.86	FALSE
M335T896_pos	335.1955	896	3	2.29E-04	0.73	FALSE	1.06E-02	0.81	FALSE	1.37E-05	1.38	FALSE	7.94E-02	1.36	FALSE
M336T1046_pos	336.3253	1046	3	9.65E-01	1.00	FALSE	5.57E-01	0.97	FALSE	9.97E-01	1.00	FALSE	1.91E-01	1.26	FALSE
M339T784_pos	339.0906	784	3	2.24E-08	1.18	FALSE	1.51E-03	1.10	FALSE	7.31E-04	0.92	FALSE	5.15E-01	0.95	FALSE
M339T883_pos	339.2313	883	3	7.16E-07	1.18	FALSE	9.69E-01	1.00	FALSE	2.04E-01	1.04	FALSE	5.17E-01	0.96	FALSE
M341T1014_pos	341.2084	1014	3	1.14E-01	1.12	FALSE	6.92E-05	0.74	FALSE	8.08E-01	0.99	FALSE	7.28E-01	0.96	FALSE
M343T986_pos	343.1542	986	3	6.62E-21	0.90	FALSE	2.19E-01	1.01	FALSE	7.35E-12	0.94	FALSE	6.93E-01	0.99	FALSE
M343T1043_pos	343.2118	1043	3	3.32E-05	0.93	FALSE	1.81E-04	1.06	FALSE	1.60E-04	0.95	FALSE	7.69E-01	0.99	FALSE
M346T454_pos	346.1651	454	3	2.41E-01	1.04	FALSE	7.74E-01	1.01	FALSE	9.92E-25	1.46	FALSE	6.73E-02	0.93	FALSE
M346T769_pos	346.1652	769	3	4.26E-04	0.86	FALSE	2.28E-08	1.29	FALSE	4.85E-20	1.48	FALSE	3.67E-02	0.90	FALSE
M347T921_pos	347.1705	921	3	3.99E-05	0.90	FALSE	4.58E-01	0.98	FALSE	7.64E-01	0.99	FALSE	2.42E-01	1.12	FALSE
M348T717_pos	348.1447	717	3	1.08E-06	0.85	FALSE	3.70E-01	1.03	FALSE	4.65E-23	1.38	FALSE	5.68E-01	1.03	FALSE
M349T866_pos	349.2011	866	3	1.71E-08	0.77	FALSE	1.28E-02	1.12	FALSE	1.10E-19	1.48	FALSE	4.77E-01	1.05	FALSE
M349T824_pos	349.2109	824	3	2.59E-04	0.81	FALSE	1.28E-03	1.21	FALSE	2.21E-11	1.43	FALSE	1.73E-01	1.10	FALSE
M355T857_pos	355.2268	857	3	2.93E-02	1.08	FALSE	1.42E-04	1.16	FALSE	1.09E-08	1.21	FALSE	4.97E-02	1.13	FALSE
M355T866_pos	355.2625	866	3	2.65E-11	1.37	FALSE	4.79E-04	0.85	FALSE	1.46E-01	0.95	FALSE	3.94E-02	0.89	FALSE
M355T979_pos	355.2631	979	3	5.59E-11	1.32	FALSE	9.13E-01	1.00	FALSE	5.71E-05	1.15	FALSE	4.16E-01	0.90	FALSE
M355T916_pos	355.2631	916	3	1.12E-17	1.30	FALSE	7.99E-02	0.95	FALSE	2.17E-04	1.10	FALSE	3.59E-02	0.92	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M356T1065_pos	356.3160	1065	3							HMDB0013303	Pristanoylglycine	C21H41NO3	0.2
M356T1061_pos	356.3526	1061	3							HMDB0248559	Arachidoyl Ethanolamide	C22H45NO2	0.7
M357T677_pos	357.1191	677	3							HMDB0254997	4-Dinitrophenyl)-5-methoxytrypta	C17H16N4O5	0.7
M359T970_pos	359.2409	970	3							HMDB0012983	Kinetensin 1-3	C15H30N6O4	2.2
M360T987_pos	360.1809	987	3							HMDB0246188	,16,17-octahydro-7H-cyclopenta[a	C20H25NO5	0.9
M363T1042_pos	363.1721	1042	3							HMDB0250103	Chlormadinone	C21H27ClO3	0.2
M363T839_pos	363.2264	839	3							HMDB0249563	Calpeptin	C20H30N2O4	3.9
M363T1052_pos	363.3106	1052	3							HMDB0246913	raethylene glycol monododecyl et	C20H42O5	0.4
M365T1044_pos	365.1938	1044	3							HMDB0255318	o)-8-(methylamino)purin-9-yl]-5-(h	C16H24N6O4	1.6
M367T857_pos	367.1907	857	3							HMDB0304620	Clusiaphenone B	C23H26O4	0.8
M371T606_pos	371.2276	606	3							HMDB0094680	Octaethylene glycol	C16H34O9	0.2
M373T857_pos	373.2374	857	3							HMDB0012869	7-Hydroxy-D4-neuroprostane	C23H32O4	0.1
M373T916_pos	373.2738	916	3						Terpenoids	HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.3
M373T813_pos	373.2738	813	3						Terpenoids	HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.2
M375T883_pos	375.2531	883	3							HMDB0006472	Calcitroic acid	C23H34O4	0.4
M377T1068_pos	377.3262	1068	3						Fatty acids				
M380T1052_pos	380.3372	1052	3						Fatty acids				
M383T999_pos	383.2041	999	3							HMDB0258626	Sumarotene	C24H30O2S	0.4
M383T753_pos	383.2069	753	3							HMDB0012553	2-Oxo-20-trihydroxy-leukotriene B	C20H30O7	1.3
M385T506_pos	385.1760	506	3							HMDB0257548	(N-(1-carboxy-2-phenylethyl)-L-ph	C21H24N2O5	0.5
M385T857_pos	385.2012	857	3							HMDB0031380	3beta)-7-Hydroxy-11,16-dioxo-8,1	C23H28O5	0.6
M385T1052_2_pos	385.2927	1052	3						Fatty acids				
M389T959_pos	389.2686	959	3						Terpenoids	HMDB0030366	Cavipetin C	C24H36O4	0.0
M391T813_pos	391.2844	813	3							HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	0.2
M391T956_pos	391.2844	956	3						Terpenoids	HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	0.4
M394T1068_pos	394.3527	1068	3						Fatty acids				
M395T1019_pos	395.2427	1019	3							HMDB0031964	xy-7(11)-eremophilene-6-angeloyl	C22H34O6	0.4
M395T993_pos	395.2943	993	3							HMDB0038506	8-Dehydro-beta-micropteroxanth	C27H38O2	0.3
M397T1056_pos	397.2714	1056	3							HMDB0062325	1-hexadecyl-glycero-3-phosphate	C19H41O6P	0.0
M398T826_pos	398.2159	826	3							HMDB0247323	Comfrey	C20H31NO7	3.6
M399T999_1_pos	399.1782	999	3							HMDB0249046	BENZOYLARGININE NITROANILIDE	C19H22N6O4	1.8
M399T840_pos	399.2279	840	3							HMDB0041933	Mitragynine	C23H30N2O4	0.2
M403T1023_2_pos	403.2327	1023	3							HMDB0034159	Acetyl tributyl citrate	C20H34O8	0.2
M405T832_pos	405.2384	832	3							HMDB0014905	Benzquinamide	C22H32N2O5	0.1
M405T869_pos	405.2637	869	3						Terpenoids	HMDB0000447	12a-Dihydroxy-3-oxo-4-cholenoic a	C24H36O5	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M356T1065_pos	356.3160	1065	3	4.75E-02	0.95	FALSE	9.05E-02	1.05	FALSE	1.09E-03	0.93	FALSE	3.51E-01	1.05	FALSE
M356T1061_pos	356.3526	1061	3	2.65E-01	0.97	FALSE	2.28E-02	1.07	FALSE	1.73E-03	0.93	FALSE	6.55E-01	1.03	FALSE
M357T677_pos	357.1191	677	3	1.30E-01	1.10	FALSE	2.01E-01	1.09	FALSE	1.64E-10	1.44	FALSE	5.52E-02	0.87	FALSE
M359T970_pos	359.2409	970	3	3.23E-01	1.02	FALSE	2.39E-01	0.97	FALSE	6.33E-02	0.97	FALSE	1.30E-01	1.05	FALSE
M360T987_pos	360.1809	987	3	1.03E-15	0.90	FALSE	1.18E-01	1.02	FALSE	1.53E-06	0.95	FALSE	7.53E-01	1.01	FALSE
M363T1042_pos	363.1721	1042	3	8.30E-01	1.00	FALSE	4.21E-01	0.99	FALSE	5.24E-01	0.99	FALSE	4.10E-01	0.98	FALSE
M363T839_pos	363.2264	839	3	2.12E-01	1.23	FALSE	2.98E-02	0.71	FALSE	3.96E-01	0.89	FALSE	9.79E-01	1.01	FALSE
M363T1052_pos	363.3106	1052	3	2.21E-04	0.95	FALSE	6.11E-01	1.01	FALSE	5.01E-03	0.97	FALSE	5.04E-01	0.98	FALSE
M365T1044_pos	365.1938	1044	3	2.28E-07	0.86	FALSE	3.15E-04	1.11	FALSE	3.99E-05	0.90	FALSE	6.26E-01	1.02	FALSE
M367T857_pos	367.1907	857	3	7.49E-01	1.01	FALSE	5.94E-03	1.12	FALSE	3.53E-08	1.21	FALSE	1.99E-02	1.15	FALSE
M371T606_pos	371.2276	606	3	7.90E-13	1.15	FALSE	9.35E-01	1.00	FALSE	1.57E-01	1.02	FALSE	1.96E-06	1.33	FALSE
M373T857_pos	373.2374	857	3	1.92E-01	1.04	FALSE	1.60E-04	1.15	FALSE	1.42E-08	1.19	FALSE	1.03E-02	1.17	FALSE
M373T916_pos	373.2738	916	3	4.55E-14	1.30	FALSE	1.32E-01	0.95	FALSE	3.87E-03	1.08	FALSE	1.05E-02	0.91	FALSE
M373T813_pos	373.2738	813	3	4.02E-15	1.35	FALSE	7.18E-02	0.94	FALSE	9.95E-02	1.05	FALSE	6.44E-01	0.97	FALSE
M375T883_pos	375.2531	883	3	2.07E-05	1.15	FALSE	9.08E-01	1.00	FALSE	8.15E-04	1.10	FALSE	6.60E-01	0.96	FALSE
M377T1068_pos	377.3262	1068	3	3.99E-02	0.96	FALSE	3.07E-02	1.05	FALSE	1.86E-06	0.91	FALSE	4.64E-01	1.04	FALSE
M380T1052_pos	380.3372	1052	3	2.47E-03	0.96	FALSE	1.28E-01	0.98	FALSE	2.43E-03	0.97	FALSE	5.65E-01	1.02	FALSE
M383T999_pos	383.2041	999	3	2.59E-01	0.98	FALSE	6.21E-01	1.01	FALSE	1.90E-01	0.98	FALSE	9.31E-01	1.00	FALSE
M383T753_pos	383.2069	753	3	7.21E-03	1.21	FALSE	4.50E-04	0.78	FALSE	6.53E-02	1.12	FALSE	4.76E-02	0.86	FALSE
M385T506_pos	385.1760	506	3	3.05E-01	1.04	FALSE	8.13E-01	1.01	FALSE	1.65E-25	1.49	FALSE	3.34E-01	0.95	FALSE
M385T857_pos	385.2012	857	3	1.56E-01	1.05	FALSE	1.12E-04	1.15	FALSE	2.71E-10	1.22	FALSE	4.05E-02	1.13	FALSE
M385T1052_2_pos	385.2927	1052	3	2.93E-04	0.92	FALSE	9.38E-01	1.00	FALSE	7.88E-02	0.97	FALSE	4.53E-01	1.02	FALSE
M389T959_pos	389.2686	959	3	7.00E-15	1.26	FALSE	7.70E-03	1.08	FALSE	1.89E-32	1.42	FALSE	1.71E-01	0.93	FALSE
M391T813_pos	391.2844	813	3	3.23E-19	1.31	FALSE	2.19E-01	0.97	FALSE	2.26E-01	1.03	FALSE	8.14E-02	0.95	FALSE
M391T956_pos	391.2844	956	3	2.47E-09	1.15	FALSE	1.40E-02	0.94	FALSE	1.18E-09	1.13	FALSE	8.03E-01	0.99	FALSE
M394T1068_pos	394.3527	1068	3	4.30E-02	0.96	FALSE	8.28E-01	1.00	FALSE	7.52E-04	0.94	FALSE	6.30E-01	1.03	FALSE
M395T1019_pos	395.2427	1019	3	3.82E-01	1.04	FALSE	3.41E-03	0.88	FALSE	3.87E-01	1.03	FALSE	4.18E-01	0.91	FALSE
M395T993_pos	395.2943	993	3	6.52E-10	1.32	FALSE	7.73E-04	0.87	FALSE	1.71E-01	1.05	FALSE	2.07E-01	0.89	FALSE
M397T1056_pos	397.2714	1056	3	1.40E-02	1.17	FALSE	4.16E-01	0.95	FALSE	1.50E-09	1.42	FALSE	2.22E-02	1.26	FALSE
M398T826_pos	398.2159	826	3	7.20E-01	1.04	FALSE	2.55E-01	1.14	FALSE	2.32E-04	1.43	FALSE	2.30E-01	1.17	FALSE
M399T999_1_pos	399.1782	999	3	4.31E-05	0.92	FALSE	4.84E-01	1.02	FALSE	3.24E-07	1.10	FALSE	5.49E-01	0.97	FALSE
M399T840_pos	399.2279	840	3	3.76E-01	0.92	FALSE	3.03E-03	1.37	FALSE	3.33E-03	1.30	FALSE	5.42E-01	1.13	FALSE
M403T1023_2_pos	403.2327	1023	3	7.07E-01	0.99	FALSE	3.49E-01	1.01	FALSE	5.07E-01	0.99	FALSE	5.01E-01	0.98	FALSE
M405T832_pos	405.2384	832	3	3.39E-01	0.93	FALSE	2.27E-06	1.44	FALSE	9.62E-02	1.11	FALSE	2.04E-01	1.11	FALSE
M405T869_pos	405.2637	869	3	7.98E-01	1.02	FALSE	2.21E-01	1.08	FALSE	4.11E-01	1.04	FALSE	1.35E-01	1.20	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M406T960_pos	406.2952	960	3						Terpenoids	HMDB0242004	N-Arachidonoyl Threonine	C24H39NO4	0.0
M407T857_2_pos	407.2216	857	3							HMDB0256110	Panduratin A	C26H30O4	0.3
M407T872_pos	407.2793	872	3							HMDB0000391	7-Ketodeoxycholic acid	C24H38O5	0.3
M411T961_pos	411.2508	961	3						Terpenoids	HMDB0007849	LysoPA(0:0/16:0)	C19H39O7P	0.3
M420T726_pos	420.2284	726	3							HMDB0248012	Adimolol	C25H29N3O3	0.5
M420T891_pos	420.2286	891	3							HMDB0248012	Adimolol	C25H29N3O3	1.1
M420T960_pos	420.3113	960	3							HMDB0006463	Stearidonyl carnitine	C25H41NO4	1.1
M421T1067_pos	421.3524	1067	3						Fatty acids				
M425T857_pos	425.2324	857	3							HMDB0034183	Licoricidin	C26H32O5	0.4
M427T961_2_pos	427.2248	961	3							HMDB0256736	Pratosartan	C25H26N6O	1.7
M429T1007_pos	429.2401	1007	3							HMDB0015163	Irbesartan	C25H28N6O	0.9
M429T818_pos	429.2637	818	3							HMDB0034064	E-pentenoyl)-2b,9a-dihydroxy-4Z,	C26H36O5	0.3
M430T1042_pos	430.2101	1042	3							HMDB0253176	Hippuryl-histidyl-leucine	C21H27N5O5	3.7
M430T718_pos	430.3317	718	3							HMDB0062336	N-Oleoyl phenylalanine	C27H43NO3	0.2
M431T993_pos	431.3157	993	3						Terpenoids	HMDB0011590	(24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0/	C27H42O4	0.3
M431T1039_pos	431.3521	1039	3							HMDB0012166	-Carboxy-5alpha-cholesta-8-en-3b	C28H46O3	0.3
M433T969_pos	433.2950	969	3						Terpenoids	HMDB0014792	Latanoprost	C26H40O5	0.3
M434T395_pos	434.1891	395	3							HMDB0249379	Brexpiprazole	C25H27N3O2S	1.3
M436T978_pos	436.3429	978	3						Fatty acids				
M437T931_2_pos	437.3265	931	3							HMDB0002195	Varanic acid	C26H44O5	0.8
M441T1023_pos	441.1886	1023	3							HMDB0039914	(3-methyl-2-butenyl)-8-(3-hydroxy	C25H28O7	4.9
M441T592_pos	441.2384	592	3							HMDB0247885	,3-oxazol-2-yl]-7-oxabicyclo[2.2.1]	C25H32N2O5	0.1
M443T857_pos	443.2429	857	3							HMDB0031958	3-O-Acetylepisamarcandin	C26H34O6	0.3
M443T1067_pos	443.3343	1067	3						Fatty acids				
M447T1007_pos	447.2042	1007	3							HMDB0247861	enyl)methyl]-3-[[4-(1-oxidopyridin	C25H26N4O4	3.5
M447T1046_pos	447.3109	1046	3							HMDB0030913	Cepagenin	C27H42O5	0.9
M450T979_pos	450.3580	979	3							HMDB0241578	Icosa-8,11,14-trienoylcarnitine	C27H47NO4	0.5
M452T1080_pos	452.3946	1080	3						Fatty acids				
M452T1060_2_pos	452.4829	1060	3							HMDB0038842	Longamide	C30H61NO	0.7
M459T825_pos	459.2379	825	3							HMDB0034760	Hydroxystrobilurin D	C26H34O7	0.4
M461T1034_pos	461.3627	1034	3							HMDB0012555	2-Oxo-20-trihydroxy-leukotriene B	C29H48O4	0.3
M465T1054_pos	465.2507	1054	3							HMDB0255880	Obelin	C26H32N4O4	2.3
M465T1067_pos	465.3787	1067	3						Fatty acids				
M466T994_pos	466.3533	994	3							HMDB0006482	LysoSM(d18:1)	C23H50N2O5P	0.6
M470T713_pos	470.2649	713	3							HMDB0253814	xaldehyde, 3-(1,3-benzodioxol-5-y	C26H35N3O5	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M406T960_pos	406.2952	960	3	1.05E-05	1.10	FALSE	1.17E-04	1.09	FALSE	7.69E-14	1.16	FALSE	2.23E-01	0.94	FALSE
M407T857_2_pos	407.2216	857	3	2.11E-01	1.05	FALSE	6.69E-04	1.14	FALSE	4.32E-11	1.25	FALSE	4.82E-02	1.11	FALSE
M407T872_pos	407.2793	872	3	3.42E-03	1.19	FALSE	4.41E-01	1.05	FALSE	1.71E-02	1.13	FALSE	3.27E-01	0.91	FALSE
M411T961_pos	411.2508	961	3	2.38E-01	1.02	FALSE	3.11E-05	1.08	FALSE	4.05E-02	1.03	FALSE	4.53E-01	1.02	FALSE
M420T726_pos	420.2284	726	3	6.15E-07	1.36	FALSE	2.81E-09	0.70	FALSE	7.64E-01	0.98	FALSE	3.08E-01	1.17	FALSE
M420T891_pos	420.2286	891	3	9.00E-01	0.99	FALSE	9.96E-02	1.18	FALSE	3.03E-01	1.09	FALSE	2.87E-01	0.83	FALSE
M420T960_pos	420.3113	960	3	2.92E-10	1.23	FALSE	1.20E-05	1.15	FALSE	8.55E-23	1.35	FALSE	5.61E-03	0.81	FALSE
M421T1067_pos	421.3524	1067	3	3.20E-01	0.98	FALSE	7.67E-01	0.99	FALSE	4.86E-01	1.01	FALSE	1.39E-01	0.92	FALSE
M425T857_pos	425.2324	857	3	4.74E-02	1.08	FALSE	1.86E-04	1.16	FALSE	1.53E-08	1.21	FALSE	2.75E-02	1.14	FALSE
M427T961_2_pos	427.2248	961	3	3.98E-02	0.95	FALSE	3.42E-01	1.03	FALSE	7.17E-17	1.23	FALSE	8.38E-01	0.98	FALSE
M429T1007_pos	429.2401	1007	3	3.52E-03	0.90	FALSE	6.73E-01	0.98	FALSE	3.12E-07	1.17	FALSE	9.69E-02	0.85	FALSE
M429T818_pos	429.2637	818	3	6.04E-01	0.96	FALSE	4.75E-03	1.23	FALSE	1.69E-08	1.44	FALSE	4.12E-01	1.14	FALSE
M430T1042_pos	430.2101	1042	3	6.98E-15	0.69	FALSE	8.20E-10	1.32	FALSE	7.42E-05	0.86	FALSE	3.24E-01	0.93	FALSE
M430T718_pos	430.3317	718	3	9.52E-01	1.01	FALSE	4.19E-02	0.82	FALSE	4.76E-02	1.17	FALSE	1.64E-01	1.24	FALSE
M431T993_pos	431.3157	993	3	4.05E-14	1.45	FALSE	3.50E-04	0.85	FALSE	1.41E-04	1.16	FALSE	8.74E-02	0.84	FALSE
M431T1039_pos	431.3521	1039	3	3.10E-03	1.45	FALSE	1.34E-02	0.74	FALSE	4.22E-01	0.92	FALSE	6.63E-01	1.05	FALSE
M433T969_pos	433.2950	969	3	1.67E-09	1.34	FALSE	8.68E-01	1.01	FALSE	1.70E-14	1.40	FALSE	3.05E-01	0.93	FALSE
M434T395_pos	434.1891	395	3	4.85E-17	1.34	FALSE	2.40E-01	0.96	FALSE	9.65E-07	1.15	FALSE	7.82E-01	1.01	FALSE
M436T978_pos	436.3429	978	3	2.17E-08	1.26	FALSE	6.93E-02	0.93	FALSE	5.16E-09	1.24	FALSE	7.83E-03	0.86	FALSE
M437T931_2_pos	437.3265	931	3	5.45E-08	1.37	FALSE	6.56E-03	0.86	FALSE	5.94E-02	1.10	FALSE	2.01E-01	0.90	FALSE
M441T1023_pos	441.1886	1023	3	3.95E-10	0.86	FALSE	1.43E-01	1.04	FALSE	3.57E-05	1.09	FALSE	2.20E-02	0.89	FALSE
M441T592_pos	441.2384	592	3	3.13E-02	1.14	FALSE	1.35E-01	1.10	FALSE	1.44E-08	1.38	FALSE	1.48E-01	1.11	FALSE
M443T857_pos	443.2429	857	3	4.50E-02	1.07	FALSE	6.36E-04	1.13	FALSE	3.72E-08	1.19	FALSE	3.55E-02	1.14	FALSE
M443T1067_pos	443.3343	1067	3	8.11E-01	1.00	FALSE	3.87E-01	1.01	FALSE	1.19E-01	0.98	FALSE	3.19E-01	1.04	FALSE
M447T1007_pos	447.2042	1007	3	1.09E-03	0.89	FALSE	6.29E-02	1.07	FALSE	1.01E-03	1.11	FALSE	5.85E-01	0.97	FALSE
M447T1046_pos	447.3109	1046	3	4.52E-01	1.09	FALSE	7.22E-01	1.04	FALSE	7.68E-01	0.97	FALSE	1.47E-01	1.20	FALSE
M450T979_pos	450.3580	979	3	2.79E-05	1.19	FALSE	4.05E-01	1.04	FALSE	5.80E-11	1.29	FALSE	7.03E-03	0.81	FALSE
M452T1080_pos	452.3946	1080	3	4.74E-01	1.01	FALSE	6.37E-01	1.01	FALSE	6.79E-01	0.99	FALSE	1.75E-01	1.04	FALSE
M452T1060_2_pos	452.4829	1060	3	1.16E-05	0.80	FALSE	1.98E-03	1.18	FALSE	4.85E-03	0.88	FALSE	1.51E-01	1.20	FALSE
M459T825_pos	459.2379	825	3	2.23E-01	1.06	FALSE	3.63E-02	1.12	FALSE	3.27E-09	1.31	FALSE	8.24E-01	1.02	FALSE
M461T1034_pos	461.3627	1034	3	4.17E-01	0.98	FALSE	9.80E-01	1.00	FALSE	1.32E-03	0.94	FALSE	7.70E-01	1.02	FALSE
M465T1054_pos	465.2507	1054	3	4.01E-01	0.97	FALSE	6.75E-05	0.84	FALSE	1.07E-10	0.78	FALSE	1.63E-01	1.16	FALSE
M465T1067_pos	465.3787	1067	3	9.26E-01	1.00	FALSE	5.47E-02	0.97	FALSE	1.11E-01	1.02	FALSE	5.12E-01	0.97	FALSE
M466T994_pos	466.3533	994	3	2.95E-04	1.13	FALSE	3.42E-01	0.97	FALSE	3.67E-01	0.97	FALSE	2.90E-01	0.94	FALSE
M470T713_pos	470.2649	713	3	1.03E-05	1.40	FALSE	1.28E-03	1.29	FALSE	4.31E-06	1.35	FALSE	9.47E-02	1.28	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M471T994_pos	471.3086	994	3							HMDB0035113	-29-hydroxy-27-norlanost-8-ene-3,	C29H42O5	4.0
M474T757_pos	474.2709	757	3							HMDB0015603	Ximelagatran	C24H35N5O5	0.5
M476T645_pos	476.3066	645	3							HMDB0015090	Netilmicin	C21H41N5O7	2.7
M478T691_pos	478.3165	691	3							HMDB0241797	oxyoct-1-en-1-yl]-5-oxocyclopent-2	C27H43NO6	0.3
M481T854_2_pos	481.2796	854	3							HMDB0255516	Neoandrographolide	C26H40O8	0.0
M482T1066_pos	482.4052	1066	3						Fatty acids				
M483T1033_pos	483.3448	1033	3							HMDB0032111	Adlupone	C31H46O4	4.3
M486T738_pos	486.2713	738	3							HMDB0242427	-13-(methoxymethyl)-11-methyl-1	C24H39NO9	3.1
M487T1066_pos	487.3606	1066	3						Fatty acids				
M492T758_2_pos	492.3686	758	3							HMDB0241607	)-3-Hydroxydocosa-7,10,13,16-tet	C29H49NO5	0.5
M496T1079_pos	496.4209	1079	3						Fatty acids				
M500T703_pos	500.2755	703	3							HMDB0248778	Osimertini	C28H33N7O2	2.8
M501T994_pos	501.3207	994	3							HMDB0033234	Ganoderic acid beta	C30H44O6	0.8
M503T1066_pos	503.3350	1066	3							HMDB0034551	Medicagenic acid	C30H46O6	3.5
M504T873_pos	504.3324	873	3							HMDB0241613	9Z)-7,17-Dihydroxydocosa-5,8,10,	C29H45NO6	0.9
M506T722_pos	506.3480	722	3							HMDB0241611	9,20-Dihydroxydocosa-4,7,10,13,1	C29H47NO6	0.8
M508T979_pos	508.3645	979	3							HMDB0242380	Cholylvaline	C29H49NO6	2.3
M509T1066_pos	509.4050	1066	3						Fatty acids				
M510T675_pos	510.2812	675	3							HMDB0253969	Landiolol	C25H39N3O8	0.4
M525T661_pos	525.2879	661	3							HMDB0258550	Sucrose laurate	C24H44O12	5.0
M526T1065_pos	526.4314	1065	3						Fatty acids				
M526T1037_pos	526.4835	1037	3							HMDB0240987	19-Methyltetracosanoylcarnitine	C32H63NO4	1.0
M531T1066_pos	531.3869	1066	3						Fatty acids				
M540T1079_pos	540.4471	1079	3						Fatty acids				
M547T1066_pos	547.3610	1066	3							HMDB0041547	Hovenidulcigenin B	C32H50O7	3.6
M556T1051_pos	556.4420	1051	3						Fatty acids				
M562T1051_pos	562.4011	1051	3							HMDB0304100	hydroxy-5-all-trans-hexaprenylber	C37H53O4	2.0
M567T1047_pos	567.2977	1047	3							HMDB0002379	Mesoporphyrin IX	C34H38N4O4	2.0
M570T1065_pos	570.4576	1065	3						Fatty acids				
M575T1065_pos	575.4130	1065	3						Fatty acids				
M591T1066_pos	591.3875	1066	3							HMDB0037956	-Epidioxyergosta-6,22E-dien-3b-ol	C34H54O8	2.9
M597T947_pos	597.3647	947	3							HMDB0004157	Stercobilinogen	C33H48N4O6	0.0
M600T1050_pos	600.4683	1050	3						Fatty acids				
M605T1080_pos	605.4051	1080	3							HMDB0040498	3-Epipapyriferic acid	C35H56O8	0.5
M608T688_pos	608.3857	688	3						Amino acids and Peptides				

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M471T994_pos	471.3086	994	3	3.56E-08	1.20	FALSE	2.45E-02	0.93	FALSE	2.48E-01	1.03	FALSE	1.15E-01	0.89	FALSE
M474T757_pos	474.2709	757	3	9.65E-01	1.01	FALSE	4.23E-02	1.36	FALSE	1.27E-02	1.40	FALSE	8.69E-01	1.03	FALSE
M476T645_pos	476.3066	645	3	3.77E-12	1.24	FALSE	3.06E-01	0.97	FALSE	1.08E-07	1.15	FALSE	2.51E-02	1.15	FALSE
M478T691_pos	478.3165	691	3	7.72E-09	1.46	FALSE	3.58E-02	1.15	FALSE	2.21E-04	1.23	FALSE	9.59E-01	1.00	FALSE
M481T854_2_pos	481.2796	854	3	1.98E-05	0.82	FALSE	2.55E-01	1.05	FALSE	6.63E-16	1.41	FALSE	9.81E-01	1.00	FALSE
M482T1066_pos	482.4052	1066	3	8.32E-01	1.00	FALSE	7.68E-01	1.00	FALSE	6.30E-02	0.98	FALSE	6.52E-01	1.02	FALSE
M483T1033_pos	483.3448	1033	3	9.85E-01	1.00	FALSE	6.80E-01	1.02	FALSE	1.04E-01	0.93	FALSE	4.51E-01	1.08	FALSE
M486T738_pos	486.2713	738	3	3.64E-03	1.15	FALSE	2.24E-01	0.94	FALSE	1.08E-16	1.47	FALSE	7.22E-01	1.03	FALSE
M487T1066_pos	487.3606	1066	3	9.68E-01	1.00	FALSE	1.21E-01	1.02	FALSE	8.25E-02	0.98	FALSE	2.74E-01	1.03	FALSE
M492T758_2_pos	492.3686	758	3	5.28E-05	1.43	FALSE	3.50E-05	0.70	FALSE	4.94E-02	1.16	FALSE	1.06E-01	1.17	FALSE
M496T1079_pos	496.4209	1079	3	6.52E-01	0.99	FALSE	8.34E-01	1.00	FALSE	2.15E-01	0.99	FALSE	3.20E-01	1.04	FALSE
M500T703_pos	500.2755	703	3	5.09E-01	0.95	FALSE	9.84E-02	0.88	FALSE	2.93E-05	1.31	FALSE	9.45E-02	0.91	FALSE
M501T994_pos	501.3207	994	3	1.59E-06	1.23	FALSE	1.36E-01	1.07	FALSE	1.08E-18	1.43	FALSE	1.30E-01	0.95	FALSE
M503T1066_pos	503.3350	1066	3	7.38E-01	0.99	FALSE	4.86E-01	1.02	FALSE	8.72E-08	1.16	FALSE	2.34E-01	0.94	FALSE
M504T873_pos	504.3324	873	3	3.52E-02	1.20	FALSE	4.34E-04	0.73	FALSE	6.45E-01	0.97	FALSE	1.19E-01	1.47	FALSE
M506T722_pos	506.3480	722	3	1.00E-08	1.32	FALSE	4.83E-02	0.91	FALSE	5.94E-03	1.12	FALSE	6.55E-01	1.04	FALSE
M508T979_pos	508.3645	979	3	1.13E-09	1.25	FALSE	9.95E-01	1.00	FALSE	5.33E-09	1.20	FALSE	1.23E-03	0.77	FALSE
M509T1066_pos	509.4050	1066	3	6.42E-01	1.01	FALSE	9.25E-02	0.97	FALSE	4.36E-01	1.01	FALSE	1.03E-01	0.92	FALSE
M510T675_pos	510.2812	675	3	8.78E-02	1.09	FALSE	6.15E-01	0.97	FALSE	3.92E-12	1.38	FALSE	1.46E-01	0.85	FALSE
M525T661_pos	525.2879	661	3	1.42E-02	1.09	FALSE	6.88E-01	0.99	FALSE	1.83E-08	1.19	FALSE	4.06E-02	1.14	FALSE
M526T1065_pos	526.4314	1065	3	6.32E-01	1.00	FALSE	8.32E-01	1.00	FALSE	6.80E-02	0.99	FALSE	5.15E-01	1.01	FALSE
M526T1037_pos	526.4835	1037	3	4.98E-06	1.44	FALSE	4.53E-06	0.70	FALSE	7.84E-02	1.13	FALSE	1.12E-01	1.14	FALSE
M531T1066_pos	531.3869	1066	3	1.93E-01	0.99	FALSE	5.53E-01	1.00	FALSE	4.57E-01	1.01	FALSE	8.10E-01	1.01	FALSE
M540T1079_pos	540.4471	1079	3	3.53E-01	0.99	FALSE	8.99E-01	1.00	FALSE	9.21E-02	0.99	FALSE	6.22E-01	1.02	FALSE
M547T1066_pos	547.3610	1066	3	8.94E-01	1.00	FALSE	2.51E-01	0.96	FALSE	4.29E-10	1.19	FALSE	1.21E-01	0.93	FALSE
M556T1051_pos	556.4420	1051	3	3.85E-02	0.98	FALSE	2.13E-01	0.99	FALSE	3.97E-03	0.98	FALSE	6.98E-01	1.01	FALSE
M562T1051_pos	562.4011	1051	3	9.46E-01	1.00	FALSE	5.14E-01	0.99	FALSE	8.49E-01	1.00	FALSE	8.34E-01	1.00	FALSE
M567T1047_pos	567.2977	1047	3	8.35E-01	1.05	FALSE	7.58E-01	1.06	FALSE	1.18E-01	1.34	FALSE	4.77E-01	0.85	FALSE
M570T1065_pos	570.4576	1065	3	8.15E-01	1.00	FALSE	6.59E-01	1.00	FALSE	9.82E-01	1.00	FALSE	7.40E-01	0.99	FALSE
M575T1065_pos	575.4130	1065	3	7.19E-01	1.00	FALSE	7.21E-01	1.00	FALSE	2.23E-02	1.02	FALSE	7.36E-01	0.99	FALSE
M591T1066_pos	591.3875	1066	3	5.63E-01	1.02	FALSE	1.55E-01	0.95	FALSE	2.58E-12	1.25	FALSE	9.40E-03	0.83	FALSE
M597T947_pos	597.3647	947	3	5.57E-05	0.76	FALSE	2.72E-04	1.29	FALSE	2.28E-02	1.14	FALSE	2.66E-01	1.12	FALSE
M600T1050_pos	600.4683	1050	3	6.28E-01	1.00	FALSE	1.88E-01	0.99	FALSE	3.66E-01	1.01	FALSE	8.73E-01	1.00	FALSE
M605T1080_pos	605.4051	1080	3	3.43E-01	0.97	FALSE	2.31E-01	0.96	FALSE	9.35E-11	1.22	FALSE	8.82E-02	0.91	FALSE
M608T688_pos	608.3857	688	3	4.42E-03	1.14	FALSE	8.78E-02	0.92	FALSE	1.67E-04	1.16	FALSE	7.40E-01	1.02	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M616T1013_pos	616.4915	1013	3							HMDB0290009	Cer(d18:1/PGJ2)	C38H65NO5	3.3
M628T1078_pos	628.4996	1078	3						Fatty acids				
M632T1022_2_pos	632.3060	1022	3							HMDB0254473	Mesaconitine	C33H45NO11	0.8
M633T1078_pos	633.4550	1078	3						Fatty acids				
M635T1065_pos	635.4137	1065	3							HMDB0029606	Maslinic acid 3-O-b-D-glucoside	C36H58O9	2.6
M639T1079_pos	638.5724	1079	3						Fatty acids				
M644T1050_pos	644.4945	1050	3						Fatty acids				
M649T1039_pos	648.5178	1039	3						Fatty acids				
M649T1079_pos	649.4311	1079	3							HMDB0036430	Momordicoside K	C37H60O9	0.2
M652T700_pos	652.4105	700	3						Amino acids and Peptides				
M653T948_pos	653.2851	948	3							HMDB0041246	Secoisotetrandrine	C38H40N2O8	0.9
M659T1064_pos	658.5102	1064	3						Fatty acids				
M663T977_pos	662.5358	977	3							HMDB0290109	Cer(d20:1/PGE2)	C40H71NO6	0.7
M665T847_pos	665.3891	847	3							HMDB0034552	edicagenic acid 3-O-beta-D-glucosi	C36H56O11	0.7
M673T1078_pos	672.5259	1078	3						Fatty acids	HMDB0256098	2,3-Dipalmitoyl-S-glycerylcysteine	C38H73NO6S	4.1
M679T1065_pos	679.4400	1065	3							HMDB0060814	Descladinose roxithromycin	C33H62N2O12	3.6
M689T1050_pos	688.5210	1050	3						Fatty acids				
M693T1078_pos	693.4574	1078	3							HMDB0250429	Concanamycin	C39H64O10	0.3
M703T1021_pos	702.5159	1021	3							HMDB0258356	Soblidotin	C39H67N5O6	0.7
M703T840_pos	703.4071	840	3						Alkaloids				
M717T1077_pos	716.5523	1077	3						Fatty acids				
M737T1078_pos	737.4837	1078	3							HMDB0033886	drillasterol 3-[glucosyl-(1->4)-gluco	C41H68O11	0.4
M766T976_pos	765.5666	976	3							HMDB0116652	PG(a-13:0/i-22:0)	C41H81O10P	3.3
M767T1064_pos	767.4927	1064	3							HMDB0031830	Ginsenoside Rg5	C42H70O12	1.7
M782T979_pos	781.5614	979	3						Terpenoids				
M783T417_pos	783.3140	417	3						Carbohydrates				
M799T979_pos	798.5880	979	3						Terpenoids				
M800T960_pos	799.5123	960	3							HMDB0264686	:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5	C43H75O11P	0.3
M804T979_pos	803.5434	979	3						Terpenoids	HMDB0264646	PA(20:0/PGF2alpha)	C43H79O11P	0.1
M820T978_pos	819.5175	978	3							HMDB0116589	0:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z	C46H75O10P	0.5
M827T1023_pos	827.4400	1023	3							HMDB0034637	Phytolaccoside E	C42H66O16	2.9
M836T1062_pos	835.6187	1062	3							HMDB0115348	PA(22:4(7Z,10Z,13Z,16Z)/24:1(15Z)	C49H87O8P	2.9
M60T1024_pos	60.0805	1024	3							HMDB0000906	Trimethylamine	C3H9N	3.8
M69T803_pos	69.0697	803	3							HMDB0249189	Bicyclo[2.1.0]pentane	C5H8	2.7
M73T665_pos	73.0646	665	3							HMDB0000246	Tetrahydrofuran	C4H8O	2.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M616T1013_pos	616.4915	1013	3	7.85E-02	1.18	FALSE	4.92E-03	0.74	FALSE	2.47E-06	1.48	FALSE	2.23E-01	1.26	FALSE
M628T1078_pos	628.4996	1078	3	9.12E-03	1.03	FALSE	4.78E-01	0.99	FALSE	9.43E-01	1.00	FALSE	4.84E-01	1.02	FALSE
M632T1022_2_pos	632.3060	1022	3	2.92E-18	0.71	FALSE	4.19E-08	1.22	FALSE	5.61E-02	0.94	FALSE	2.41E-01	0.91	FALSE
M633T1078_pos	633.4550	1078	3	1.58E-01	0.99	FALSE	9.46E-01	1.00	FALSE	6.61E-01	1.00	FALSE	4.22E-02	1.07	FALSE
M635T1065_pos	635.4137	1065	3	6.97E-01	1.01	FALSE	5.28E-02	0.95	FALSE	2.77E-10	1.18	FALSE	2.08E-02	0.90	FALSE
M639T1079_pos	638.5724	1079	3	5.77E-02	3.45	FALSE	2.24E-01	0.51	FALSE	9.43E-01	1.04	FALSE	2.15E-01	1.78	FALSE
M644T1050_pos	644.4945	1050	3	5.10E-01	1.01	FALSE	1.50E-01	0.99	FALSE	4.50E-01	1.01	FALSE	1.03E-01	1.04	FALSE
M649T1039_pos	648.5178	1039	3	1.97E-03	1.24	FALSE	1.41E-07	0.69	FALSE	9.12E-02	1.10	FALSE	4.20E-02	1.24	FALSE
M649T1079_pos	649.4311	1079	3	2.43E-01	1.04	FALSE	1.14E-01	0.94	FALSE	3.05E-11	1.25	FALSE	5.76E-03	0.87	FALSE
M652T700_pos	652.4105	700	3	7.78E-04	1.20	FALSE	5.47E-01	0.97	FALSE	3.07E-06	1.26	FALSE	3.35E-01	1.09	FALSE
M653T948_pos	653.2851	948	3	3.67E-06	0.73	FALSE	1.44E-05	1.35	FALSE	3.60E-02	0.89	FALSE	5.20E-01	0.92	FALSE
M659T1064_pos	658.5102	1064	3	1.69E-01	1.01	FALSE	1.99E-01	0.99	FALSE	2.71E-01	0.99	FALSE	5.55E-01	1.01	FALSE
M663T977_pos	662.5358	977	3	2.00E-04	1.10	FALSE	8.61E-01	1.00	FALSE	4.53E-12	1.18	FALSE	3.19E-02	0.91	FALSE
M665T847_pos	665.3891	847	3	1.04E-02	0.86	FALSE	1.92E-01	1.09	FALSE	3.15E-01	1.05	FALSE	3.74E-02	1.35	FALSE
M673T1078_pos	672.5259	1078	3	9.39E-02	1.02	FALSE	3.26E-01	1.01	FALSE	9.08E-01	1.00	FALSE	4.11E-01	1.02	FALSE
M679T1065_pos	679.4400	1065	3	7.14E-01	1.01	FALSE	1.67E-02	0.93	FALSE	9.52E-12	1.21	FALSE	2.69E-02	0.89	FALSE
M689T1050_pos	688.5210	1050	3	6.68E-01	1.00	FALSE	9.56E-02	0.98	FALSE	4.46E-02	0.98	FALSE	2.10E-01	1.03	FALSE
M693T1078_pos	693.4574	1078	3	3.57E-01	1.03	FALSE	1.92E-02	0.92	FALSE	4.53E-11	1.24	FALSE	4.08E-03	0.88	FALSE
M703T1021_pos	702.5159	1021	3	3.05E-01	0.99	FALSE	5.60E-01	1.01	FALSE	7.75E-03	1.03	FALSE	4.71E-01	0.97	FALSE
M703T840_pos	703.4071	840	3	1.71E-03	0.75	FALSE	4.68E-01	1.07	FALSE	1.08E-05	1.43	FALSE	9.55E-02	1.30	FALSE
M717T1077_pos	716.5523	1077	3	4.16E-02	1.02	FALSE	8.06E-01	1.00	FALSE	6.12E-01	0.99	FALSE	5.08E-01	1.02	FALSE
M737T1078_pos	737.4837	1078	3	8.19E-02	1.07	FALSE	2.37E-01	0.95	FALSE	4.24E-10	1.26	FALSE	5.63E-02	0.90	FALSE
M766T976_pos	765.5666	976	3	2.26E-08	1.44	FALSE	5.14E-05	0.76	FALSE	7.21E-03	1.16	FALSE	8.72E-01	1.02	FALSE
M767T1064_pos	767.4927	1064	3	2.55E-01	1.04	FALSE	3.03E-01	0.97	FALSE	1.19E-08	1.19	FALSE	7.09E-02	0.90	FALSE
M782T979_pos	781.5614	979	3	3.88E-12	1.38	FALSE	6.23E-01	0.98	FALSE	1.71E-14	1.37	FALSE	2.74E-01	0.93	FALSE
M783T417_pos	783.3140	417	3	3.83E-05	1.39	FALSE	8.39E-01	0.98	FALSE	3.68E-01	1.06	FALSE	9.47E-01	0.99	FALSE
M799T979_pos	798.5880	979	3	5.76E-01	1.01	FALSE	9.52E-01	1.00	FALSE	1.20E-01	1.03	FALSE	5.12E-01	0.97	FALSE
M800T960_pos	799.5123	960	3	4.97E-12	1.29	FALSE	1.49E-04	1.15	FALSE	2.37E-25	1.44	FALSE	4.95E-02	0.85	FALSE
M804T979_pos	803.5434	979	3	1.43E-01	1.02	FALSE	7.22E-01	0.99	FALSE	5.02E-01	0.99	FALSE	8.15E-01	0.99	FALSE
M820T978_pos	819.5175	978	3	2.16E-06	0.89	FALSE	4.87E-01	1.02	FALSE	3.84E-05	1.09	FALSE	1.13E-01	0.94	FALSE
M827T1023_pos	827.4400	1023	3	7.45E-05	1.05	FALSE	3.22E-05	0.95	FALSE	7.96E-03	0.97	FALSE	3.36E-01	0.97	FALSE
M836T1062_pos	835.6187	1062	3	9.70E-03	1.04	FALSE	4.15E-01	0.99	FALSE	9.63E-01	1.00	FALSE	4.79E-01	1.02	FALSE
M60T1024_pos	60.0805	1024	3	2.48E-02	0.91	FALSE	9.07E-01	1.01	FALSE	4.32E-01	0.97	FALSE	5.11E-01	1.06	FALSE
M69T803_pos	69.0697	803	3	2.39E-01	1.04	FALSE	7.46E-01	0.99	FALSE	3.78E-04	1.10	FALSE	2.09E-02	0.84	FALSE
M73T665_pos	73.0646	665	3	7.36E-03	0.91	FALSE	2.79E-01	1.04	FALSE	5.48E-09	1.21	FALSE	3.89E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M73T604_pos	73.0646	604	3							HMDB0000246	Tetrahydrofuran	C4H8O	2.6
M75T804_pos	75.0439	804	3							HMDB0244090	1,2-Dioxolane	C3H6O2	2.4
M81T1038_pos	81.0697	1038	3							HMDB0251502	1,3,5-Hexatriene	C6H8	2.2
M83T580_pos	83.0853	580	3						Fatty acids	HMDB0031544	3-Methylcyclopentene	C6H10	2.3
M83T1038_pos	83.0854	1038	3							HMDB0031544	3-Methylcyclopentene	C6H10	1.8
M83T753_pos	83.0854	753	3							HMDB0031544	3-Methylcyclopentene	C6H10	1.9
M85T334_pos	85.0283	334	3							HMDB0032330	ydroxy-2-butenoic acid gamma-lac	C4H4O2	1.6
M85T704_pos	85.0646	704	3							HMDB0001184	Methyl propenyl ketone	C5H8O	1.7
M85T1039_pos	85.1010	1039	3							HMDB0029597	Cyclohexane	C6H12	1.8
M86T82_pos	86.0963	82	3							HMDB0034301	Piperidine	C5H11N	1.4
M87T700_pos	87.0439	700	3							HMDB0245045	2-Butyne-1,4-diol	C4H6O2	1.6
M87T1042_pos	87.0803	1042	3							HMDB0006478	Isovaleraldehyde	C5H10O	1.7
M88T118_pos	88.0392	118	3							HMDB0003609	2-Aminoacrylic acid	C3H5NO2	1.5
M89T987_pos	89.0596	987	3							HMDB0000039	Butyric acid	C4H8O2	0.7
M89T767_pos	89.0597	767	3							HMDB0000039	Butyric acid	C4H8O2	0.6
M89T804_pos	89.0596	804	3							HMDB0000039	Butyric acid	C4H8O2	0.7
M89T917_pos	89.0597	917	3							HMDB0000039	Butyric acid	C4H8O2	0.6
M95T165_pos	95.0162	165	3							HMDB0004983	Dimethyl sulfone	C2H6O2S	0.5
M95T1033_pos	95.0856	1033	3							HMDB0031532	1-Methyl-1,3-cyclohexadiene	C7H10	0.4
M97T770_pos	97.0648	770	3							HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.5
M97T883_pos	97.0648	883	3							HMDB0031545	2-Methyl-2-cyclopenten-1-one	C6H8O	0.5
M97T1038_pos	97.1012	1038	3							HMDB0254637	Methylenecyclohexane	C7H12	0.3
M97T797_pos	97.1012	797	3							HMDB0254637	Methylenecyclohexane	C7H12	0.5
M98T416_pos	98.0601	416	3							HMDB0031339	1-Cyano-2-hydroxy-3-butene	C5H7NO	0.6
M99T992_pos	98.9842	992	3							HMDB0001429	Phosphate	H3O4P	0.3
M99T409_pos	99.0441	409	3							HMDB0013742	2-Furanmethanol	C5H6O2	0.4
M100T444_pos	100.0757	444	3							HMDB0011749	2-Piperidinone	C5H9NO	0.2
M100T756_pos	100.0757	756	3							HMDB0011749	2-Piperidinone	C5H9NO	0.5
M100T897_pos	100.0757	897	3							HMDB0011749	2-Piperidinone	C5H9NO	0.4
M100T138_pos	100.0757	138	3							HMDB0011749	2-Piperidinone	C5H9NO	0.5
M100T345_pos	100.1122	345	3							HMDB0031404	Cyclohexylamine	C6H13N	0.8
M101T868_pos	101.0597	868	3							HMDB0000509	Senecioic acid	C5H8O2	0.4
M101T378_pos	101.0598	378	3							HMDB0000509	Senecioic acid	C5H8O2	0.6
M103T554_pos	103.0212	554	3							HMDB0031242	Dihydro-3(2H)-thiophenone	C4H6OS	0.4
M103T1033_pos	103.0754	1033	3							HMDB0000718	Isovaleric acid	C5H10O2	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M73T604_pos	73.0646	604	3	4.19E-04	1.14	FALSE	6.53E-02	1.07	FALSE	1.12E-01	1.05	FALSE	3.57E-01	1.04	FALSE
M75T804_pos	75.0439	804	3	1.40E-15	1.22	FALSE	4.50E-02	1.05	FALSE	2.97E-02	0.96	FALSE	8.64E-01	1.01	FALSE
M81T1038_pos	81.0697	1038	3	1.33E-06	1.28	FALSE	3.61E-03	0.86	FALSE	3.19E-01	1.04	FALSE	7.41E-02	1.19	FALSE
M83T580_pos	83.0853	580	3	2.04E-07	1.39	FALSE	1.80E-01	0.92	FALSE	9.41E-02	1.09	FALSE	7.14E-01	0.93	FALSE
M83T1038_pos	83.0854	1038	3	1.70E-05	0.77	FALSE	1.24E-02	1.17	FALSE	6.63E-01	0.98	FALSE	6.42E-01	1.12	FALSE
M83T753_pos	83.0854	753	3	7.16E-03	0.92	FALSE	5.55E-03	1.09	FALSE	2.75E-29	1.42	FALSE	8.92E-01	0.99	FALSE
M85T334_pos	85.0283	334	3	9.86E-11	0.67	FALSE	9.52E-02	0.90	FALSE	2.31E-01	0.94	FALSE	3.60E-01	0.81	FALSE
M85T704_pos	85.0646	704	3	2.44E-12	1.41	FALSE	4.77E-02	1.10	FALSE	1.17E-01	1.06	FALSE	8.07E-01	0.97	FALSE
M85T1039_pos	85.1010	1039	3	3.68E-01	1.03	FALSE	4.71E-02	0.93	FALSE	1.47E-01	0.96	FALSE	1.46E-02	1.17	FALSE
M86T82_pos	86.0963	82	3	7.55E-01	0.98	FALSE	2.51E-02	1.19	FALSE	1.81E-03	1.24	FALSE	1.59E-01	0.71	FALSE
M87T700_pos	87.0439	700	3	2.61E-19	1.34	FALSE	2.38E-01	1.04	FALSE	1.68E-01	0.97	FALSE	1.86E-01	0.90	FALSE
M87T1042_pos	87.0803	1042	3	6.24E-01	0.96	FALSE	3.87E-01	1.07	FALSE	3.02E-01	1.07	FALSE	6.51E-01	1.12	FALSE
M88T118_pos	88.0392	118	3	9.47E-01	0.99	FALSE	7.37E-01	1.03	FALSE	1.42E-04	0.76	FALSE	1.18E-01	0.54	FALSE
M89T987_pos	89.0596	987	3	4.16E-05	1.45	FALSE	1.23E-01	0.87	FALSE	4.68E-01	1.06	FALSE	1.38E-01	0.77	FALSE
M89T767_pos	89.0597	767	3	1.85E-01	1.09	FALSE	5.75E-01	1.04	FALSE	9.72E-01	1.00	FALSE	9.20E-01	1.02	FALSE
M89T804_pos	89.0596	804	3	1.50E-17	1.22	FALSE	2.88E-01	1.02	FALSE	8.69E-03	0.95	FALSE	7.72E-01	0.99	FALSE
M89T917_pos	89.0597	917	3	3.05E-01	1.10	FALSE	9.52E-01	1.01	FALSE	7.88E-02	1.15	FALSE	2.98E-01	0.80	FALSE
M95T165_pos	95.0162	165	3	1.82E-02	1.17	FALSE	4.12E-06	1.38	FALSE	5.26E-01	1.04	FALSE	5.15E-01	0.92	FALSE
M95T1033_pos	95.0856	1033	3	4.00E-03	1.18	FALSE	8.77E-02	0.90	FALSE	5.30E-01	0.97	FALSE	2.22E-01	1.15	FALSE
M97T770_pos	97.0648	770	3	4.91E-08	1.35	FALSE	2.08E-06	1.30	FALSE	6.01E-04	0.85	FALSE	3.78E-02	0.80	FALSE
M97T883_pos	97.0648	883	3	1.45E-01	0.95	FALSE	1.16E-02	1.10	FALSE	1.62E-01	1.04	FALSE	2.66E-01	1.09	FALSE
M97T1038_pos	97.1012	1038	3	9.03E-04	1.23	FALSE	7.76E-03	0.84	FALSE	4.39E-01	1.04	FALSE	3.50E-02	1.17	FALSE
M97T797_pos	97.1012	797	3	1.48E-03	1.11	FALSE	2.49E-01	1.04	FALSE	7.89E-07	1.16	FALSE	4.69E-03	0.84	FALSE
M98T416_pos	98.0601	416	3	3.42E-01	1.05	FALSE	3.15E-01	1.05	FALSE	6.91E-08	1.26	FALSE	4.20E-01	0.94	FALSE
M99T992_pos	98.9842	992	3	2.77E-03	0.97	FALSE	1.81E-01	1.01	FALSE	2.13E-03	0.97	FALSE	5.76E-02	1.04	FALSE
M99T409_pos	99.0441	409	3	9.16E-01	1.00	FALSE	1.60E-01	1.07	FALSE	2.13E-01	0.95	FALSE	7.29E-02	1.16	FALSE
M100T444_pos	100.0757	444	3	1.24E-04	1.27	FALSE	7.04E-04	1.24	FALSE	3.93E-08	1.36	FALSE	7.75E-01	0.99	FALSE
M100T756_pos	100.0757	756	3	4.70E-22	1.37	FALSE	5.77E-02	1.06	FALSE	4.90E-01	0.98	FALSE	5.34E-02	0.91	FALSE
M100T897_pos	100.0757	897	3	7.84E-01	1.02	FALSE	2.22E-03	1.22	FALSE	1.52E-03	1.19	FALSE	6.06E-02	1.24	FALSE
M100T138_pos	100.0757	138	3	1.14E-01	1.10	FALSE	1.87E-02	1.16	FALSE	8.47E-11	1.44	FALSE	4.41E-01	0.95	FALSE
M100T345_pos	100.1122	345	3	1.74E-07	1.40	FALSE	2.27E-01	0.93	FALSE	3.24E-02	1.12	FALSE	6.52E-01	0.97	FALSE
M101T868_pos	101.0597	868	3	5.95E-04	1.18	FALSE	2.03E-02	1.12	FALSE	1.24E-01	0.94	FALSE	4.07E-01	0.91	FALSE
M101T378_pos	101.0598	378	3	8.17E-01	0.98	FALSE	5.45E-01	1.04	FALSE	7.90E-08	1.39	FALSE	9.08E-01	0.99	FALSE
M103T554_pos	103.0212	554	3	1.71E-01	1.07	FALSE	4.12E-13	1.42	FALSE	9.49E-17	1.45	FALSE	2.25E-01	1.11	FALSE
M103T1033_pos	103.0754	1033	3	1.42E-03	1.12	FALSE	8.06E-03	0.90	FALSE	6.98E-01	0.99	FALSE	8.12E-01	1.02	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M103T987_pos	103.0754	987	3							HMDB0000718	Isovaleric acid	C5H10O2	0.3
M103T712_pos	103.0754	712	3							HMDB0000718	Isovaleric acid	C5H10O2	0.2
M103T917_pos	103.0754	917	3							HMDB0000718	Isovaleric acid	C5H10O2	0.5
M103T868_pos	103.0754	868	3							HMDB0000718	Isovaleric acid	C5H10O2	0.4
M105T446_pos	105.0699	446	3							HMDB0034240	Styrene	C8H8	0.1
M107T578_pos	107.0492	578	3							HMDB0006115	Benzaldehyde	C7H6O	0.2
M107T970_pos	107.0492	970	3							HMDB0006115	Benzaldehyde	C7H6O	0.5
M107T1014_pos	107.0492	1014	3							HMDB0006115	Benzaldehyde	C7H6O	0.6
M107T772_pos	107.0492	772	3							HMDB0006115	Benzaldehyde	C7H6O	0.4
M107T1017_pos	107.0703	1017	3							HMDB0034778	(2R*,3R*)-1,2,3-Butanetriol	C4H10O3	0.7
M107T1067_pos	107.0703	1067	3							HMDB0034778	(2R*,3R*)-1,2,3-Butanetriol	C4H10O3	0.6
M107T753_pos	107.0855	753	3							HMDB0059810	m-Xylene	C8H10	0.5
M107T882_pos	107.0856	882	3							HMDB0059810	m-Xylene	C8H10	0.4
M109T739_pos	109.0648	739	3							HMDB0001858	p-Cresol	C7H8O	0.2
M109T1033_pos	109.1012	1033	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.2
M109T779_pos	109.1012	779	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.3
M109T941_pos	109.1012	941	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.3
M109T729_pos	109.1012	729	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.3
M109T882_pos	109.1012	882	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.4
M109T659_pos	109.1012	659	3							HMDB0061897	(Z)-1,3-Octadiene	C8H12	0.3
M110T675_pos	110.0965	675	3							HMDB0029722	1,2,5-Trimethyl-1H-pyrrole	C7H11N	0.7
M111T1046_pos	111.0206	1046	3							HMDB0252085	Ethylphosphonic acid	C2H7O3P	0.1
M111T971_pos	111.0206	971	3							HMDB0252085	Ethylphosphonic acid	C2H7O3P	0.2
M111T865_pos	111.0206	865	3							HMDB0252085	Ethylphosphonic acid	C2H7O3P	0.2
M111T798_pos	111.0206	798	3							HMDB0252085	Ethylphosphonic acid	C2H7O3P	0.2
M111T393_pos	111.0441	393	3							HMDB0000957	Pyrocatechol	C6H6O2	0.4
M111T1039_pos	111.0805	1039	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.6
M111T882_pos	111.0805	882	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.4
M111T614_pos	111.0805	614	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.4
M111T809_pos	111.0805	809	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.3
M111T803_pos	111.1169	803	3							HMDB0244246	1,7-Octadiene	C8H14	0.4
M111T942_pos	111.1169	942	3							HMDB0244246	1,7-Octadiene	C8H14	0.4
M111T1030_pos	111.1169	1030	3							HMDB0244246	1,7-Octadiene	C8H14	0.2
M112T79_pos	112.1121	79	3							HMDB0247421	8-Azabicyclo[3.2.1]octane	C7H13N	0.6
M113T868_pos	113.0961	868	3							HMDB0031483	(Z)-4-Heptenal	C7H12O	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M103T987_pos	103.0754	987	3	4.19E-04	1.24	FALSE	1.27E-01	0.91	FALSE	2.01E-01	1.07	FALSE	1.51E-01	0.81	FALSE
M103T712_pos	103.0754	712	3	7.56E-04	1.18	FALSE	7.24E-01	1.02	FALSE	8.16E-02	0.93	FALSE	3.86E-01	1.10	FALSE
M103T917_pos	103.0754	917	3	2.28E-01	1.08	FALSE	9.24E-01	1.01	FALSE	1.68E-01	1.08	FALSE	2.41E-01	0.84	FALSE
M103T868_pos	103.0754	868	3	2.96E-02	1.07	FALSE	9.38E-01	1.00	FALSE	4.35E-02	0.95	FALSE	9.52E-01	1.01	FALSE
M105T446_pos	105.0699	446	3	7.97E-01	0.98	FALSE	1.91E-02	1.18	FALSE	1.42E-08	1.43	FALSE	2.84E-02	0.76	FALSE
M107T578_pos	107.0492	578	3	1.49E-03	1.14	FALSE	1.42E-02	1.11	FALSE	1.02E-14	1.36	FALSE	1.62E-01	0.91	FALSE
M107T970_pos	107.0492	970	3	8.92E-09	0.88	FALSE	7.02E-01	1.01	FALSE	2.49E-09	0.89	FALSE	5.06E-01	0.95	FALSE
M107T1014_pos	107.0492	1014	3	1.05E-05	0.90	FALSE	3.04E-01	1.03	FALSE	3.64E-04	0.93	FALSE	9.75E-01	1.00	FALSE
M107T772_pos	107.0492	772	3	1.65E-10	1.47	FALSE	8.88E-01	1.01	FALSE	4.38E-02	1.10	FALSE	8.49E-01	0.96	FALSE
M107T1017_pos	107.0703	1017	3	2.20E-01	0.97	FALSE	2.75E-01	1.03	FALSE	8.98E-01	1.00	FALSE	4.16E-01	1.07	FALSE
M107T1067_pos	107.0703	1067	3	7.06E-01	1.01	FALSE	6.19E-01	1.02	FALSE	2.04E-01	0.96	FALSE	4.81E-01	1.07	FALSE
M107T753_pos	107.0855	753	3	7.12E-01	0.99	FALSE	3.73E-03	1.11	FALSE	6.54E-24	1.43	FALSE	6.36E-02	0.85	FALSE
M107T882_pos	107.0856	882	3	6.99E-01	1.01	FALSE	7.34E-02	1.07	FALSE	5.01E-06	1.16	FALSE	1.90E-01	1.19	FALSE
M109T739_pos	109.0648	739	3	4.05E-03	1.20	FALSE	4.66E-01	0.95	FALSE	2.40E-02	0.89	FALSE	5.76E-02	0.61	FALSE
M109T1033_pos	109.1012	1033	3	2.48E-05	1.31	FALSE	4.21E-03	0.83	FALSE	8.84E-01	1.01	FALSE	2.40E-02	1.19	FALSE
M109T779_pos	109.1012	779	3	9.12E-01	1.01	FALSE	6.21E-01	1.03	FALSE	4.04E-01	0.95	FALSE	4.79E-01	0.90	FALSE
M109T941_pos	109.1012	941	3	2.39E-01	1.07	FALSE	5.88E-01	1.04	FALSE	7.03E-01	0.98	FALSE	5.79E-02	0.85	FALSE
M109T729_pos	109.1012	729	3	2.96E-01	1.05	FALSE	2.64E-01	1.07	FALSE	1.38E-02	0.90	FALSE	2.37E-01	1.21	FALSE
M109T882_pos	109.1012	882	3	6.21E-01	1.03	FALSE	9.69E-01	1.00	FALSE	1.09E-01	1.08	FALSE	6.14E-01	0.92	FALSE
M109T659_pos	109.1012	659	3	3.76E-28	1.47	FALSE	8.25E-01	1.01	FALSE	2.80E-11	0.84	FALSE	2.97E-01	0.96	FALSE
M110T675_pos	110.0965	675	3	2.94E-04	1.29	FALSE	1.54E-01	0.90	FALSE	2.71E-04	1.25	FALSE	6.94E-01	0.92	FALSE
M111T1046_pos	111.0206	1046	3	1.27E-01	0.88	FALSE	8.38E-01	0.98	FALSE	8.30E-01	0.98	FALSE	4.05E-01	1.28	FALSE
M111T971_pos	111.0206	971	3	3.22E-01	1.04	FALSE	1.75E-01	0.94	FALSE	1.87E-02	1.09	FALSE	3.64E-01	0.88	FALSE
M111T865_pos	111.0206	865	3	4.07E-01	1.04	FALSE	7.95E-01	1.01	FALSE	2.98E-05	0.84	FALSE	3.08E-01	0.92	FALSE
M111T798_pos	111.0206	798	3	3.35E-08	1.32	FALSE	2.13E-01	0.94	FALSE	3.64E-09	0.77	FALSE	2.18E-01	0.85	FALSE
M111T393_pos	111.0441	393	3	1.37E-08	1.27	FALSE	1.59E-01	1.06	FALSE	4.04E-13	1.32	FALSE	9.75E-02	0.93	FALSE
M111T1039_pos	111.0805	1039	3	8.67E-01	1.01	FALSE	3.39E-01	0.94	FALSE	4.10E-01	1.04	FALSE	1.27E-01	0.74	FALSE
M111T882_pos	111.0805	882	3	4.06E-01	0.97	FALSE	4.01E-03	1.11	FALSE	5.45E-07	1.17	FALSE	9.58E-01	1.01	FALSE
M111T614_pos	111.0805	614	3	9.30E-19	1.49	FALSE	2.05E-10	1.30	FALSE	3.01E-01	0.96	FALSE	1.66E-01	0.91	FALSE
M111T809_pos	111.0805	809	3	1.33E-02	0.85	FALSE	9.63E-01	1.00	FALSE	9.15E-04	1.21	FALSE	3.81E-01	0.89	FALSE
M111T803_pos	111.1169	803	3	1.76E-01	1.04	FALSE	7.64E-02	1.06	FALSE	1.45E-17	1.29	FALSE	1.12E-03	0.86	FALSE
M111T942_pos	111.1169	942	3	2.57E-01	1.03	FALSE	5.90E-01	1.02	FALSE	8.96E-05	0.90	FALSE	6.89E-02	1.09	FALSE
M111T1030_pos	111.1169	1030	3	3.18E-02	1.20	FALSE	4.17E-01	0.93	FALSE	9.58E-01	1.00	FALSE	4.88E-01	1.07	FALSE
M112T79_pos	112.1121	79	3	4.01E-01	0.93	FALSE	2.99E-01	0.90	FALSE	1.92E-03	1.27	FALSE	6.67E-01	1.05	FALSE
M113T868_pos	113.0961	868	3	3.69E-16	1.34	FALSE	2.06E-01	1.04	FALSE	6.59E-04	0.91	FALSE	7.36E-01	0.97	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M113T1039_pos	113.1325	1039	3							HMDB0032449	1-Octene	C8H16	0.4
M114T121_pos	114.0662	121	3						Alkaloids	HMDB0000562	Creatinine	C4H7N3O	0.5
M114T628_pos	114.0914	628	3							HMDB0031199	2,5-Dihydro-2,4,5-trimethyloxazole	C6H11NO	0.5
M115T84_pos	114.9876	84	3						Fatty acids				
M115T351_pos	115.0503	351	3							HMDB0000076	Dihydrouracil	C4H6N2O2	0.7
M115T883_pos	115.0754	883	3							HMDB0000453	delta-Hexanolactone	C6H10O2	0.4
M115T1039_pos	115.0754	1039	3							HMDB0000453	delta-Hexanolactone	C6H10O2	0.1
M116T518_pos	116.0707	518	3							HMDB0000162	L-Proline	C5H9NO2	1.0
M116T993_pos	116.0707	993	3							HMDB0000162	L-Proline	C5H9NO2	0.8
M116T754_pos	116.0707	754	3							HMDB0000162	L-Proline	C5H9NO2	0.7
M116T1041_pos	116.0707	1041	3							HMDB0000162	L-Proline	C5H9NO2	0.9
M116T674_2_pos	116.1070	674	3							HMDB0031651	N-(3-Methylbutyl)acetamide	C6H13NO	0.4
M117T650_pos	117.0369	650	3							HMDB0038556	Dihydro-2-methyl-3(2H)-thiophenc	C5H8OS	0.2
M117T709_pos	117.0910	709	3						Fatty acids	HMDB0000535	Caproic acid	C6H12O2	0.2
M117T849_pos	117.0910	849	3							HMDB0000535	Caproic acid	C6H12O2	0.4
M117T987_pos	117.0911	987	3							HMDB0000535	Caproic acid	C6H12O2	0.4
M120T615_pos	120.0557	615	3							HMDB0244873	1H-Benzotriazole	C6H5N3	0.6
M120T620_pos	120.0808	620	3							HMDB0253472	Indoline	C8H9N	0.5
M121T362_pos	121.0649	362	3							HMDB0004072	4-Hydroxystyrene	C8H8O	0.5
M121T1039_pos	121.1012	1039	3							HMDB0013733	1,2,4-Trimethylbenzene	C9H12	0.1
M121T769_pos	121.1012	769	3							HMDB0013733	1,2,4-Trimethylbenzene	C9H12	0.2
M121T882_pos	121.1012	882	3							HMDB0013733	1,2,4-Trimethylbenzene	C9H12	0.3
M121T808_pos	121.1012	808	3							HMDB0013733	1,2,4-Trimethylbenzene	C9H12	0.2
M121T687_pos	121.1012	687	3						Terpenoids	HMDB0013733	1,2,4-Trimethylbenzene	C9H12	0.3
M122T846_pos	122.0965	846	3							HMDB0001020	N,N-Dimethylaniline	C8H11N	0.7
M123T157_pos	123.0553	157	3						Alkaloids	HMDB0001406	Niacinamide	C6H6N2O	0.3
M123T488_pos	123.0441	488	3							HMDB0001870	Benzoic acid	C7H6O2	0.7
M123T1036_pos	123.1168	1036	3							HMDB0038140	Santene	C9H14	0.1
M123T744_pos	123.1168	744	3							HMDB0038140	Santene	C9H14	0.2
M123T882_pos	123.1169	882	3							HMDB0038140	Santene	C9H14	0.2
M125T615_pos	125.0961	615	3							HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.4
M125T1039_pos	125.0961	1039	3							HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.2
M125T699_pos	125.0961	699	3							HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.3
M125T883_pos	125.0961	883	3							HMDB0031414	2,3-Dimethyl-2-cyclohexen-1-one	C8H12O	0.3
M125T1038_pos	125.1325	1038	3							HMDB0031415	2,6-Dimethyl-2,4-heptadiene	C9H16	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M113T1039_pos	113.1325	1039	3	8.36E-13	1.47	FALSE	1.55E-07	0.76	FALSE	9.17E-01	1.00	FALSE	5.19E-02	1.17	FALSE
M114T121_pos	114.0662	121	3	3.46E-01	0.86	FALSE	4.03E-01	0.88	FALSE	1.34E-02	1.41	FALSE	3.58E-01	0.80	FALSE
M114T628_pos	114.0914	628	3	3.34E-03	0.81	FALSE	1.89E-01	0.90	FALSE	1.71E-02	1.16	FALSE	3.05E-01	1.30	FALSE
M115T84_pos	114.9876	84	3	5.10E-02	1.03	FALSE	5.38E-01	1.01	FALSE	1.48E-03	1.05	FALSE	5.79E-04	0.82	FALSE
M115T351_pos	115.0503	351	3	4.21E-04	1.22	FALSE	2.54E-01	0.94	FALSE	2.66E-01	1.06	FALSE	2.19E-01	0.81	FALSE
M115T883_pos	115.0754	883	3	5.39E-01	0.98	FALSE	2.44E-01	1.05	FALSE	6.12E-01	1.02	FALSE	6.07E-01	1.05	FALSE
M115T1039_pos	115.0754	1039	3	1.32E-09	1.22	FALSE	2.47E-06	0.86	FALSE	4.96E-01	0.98	FALSE	3.15E-01	1.07	FALSE
M116T518_pos	116.0707	518	3	1.45E-01	0.90	FALSE	2.61E-01	0.92	FALSE	9.40E-01	1.00	FALSE	7.87E-01	1.06	FALSE
M116T993_pos	116.0707	993	3	5.68E-01	0.98	FALSE	9.28E-01	1.00	FALSE	6.00E-01	1.02	FALSE	1.27E-01	0.89	FALSE
M116T754_pos	116.0707	754	3	4.15E-01	0.94	FALSE	8.85E-01	1.01	FALSE	3.56E-01	1.07	FALSE	5.82E-01	0.92	FALSE
M116T1041_pos	116.0707	1041	3	6.00E-01	1.02	FALSE	9.04E-02	1.08	FALSE	5.39E-02	0.93	FALSE	9.97E-01	1.00	FALSE
M116T674_2_pos	116.1070	674	3	1.51E-06	1.33	FALSE	1.54E-01	1.09	FALSE	2.49E-02	0.89	FALSE	3.47E-01	0.87	FALSE
M117T650_pos	117.0369	650	3	8.11E-03	1.16	FALSE	2.11E-04	1.25	FALSE	2.63E-06	1.26	FALSE	8.55E-01	0.99	FALSE
M117T709_pos	117.0910	709	3	6.19E-11	1.32	FALSE	6.05E-01	0.98	FALSE	1.50E-01	0.95	FALSE	2.79E-01	0.91	FALSE
M117T849_pos	117.0910	849	3	4.09E-01	1.06	FALSE	6.80E-01	1.03	FALSE	9.02E-02	0.90	FALSE	2.65E-01	1.08	FALSE
M117T987_pos	117.0911	987	3	7.72E-04	1.16	FALSE	1.17E-01	0.93	FALSE	4.08E-01	1.03	FALSE	2.71E-01	0.92	FALSE
M120T615_pos	120.0557	615	3	8.12E-01	1.01	FALSE	6.72E-01	0.97	FALSE	1.37E-01	1.08	FALSE	8.97E-02	0.85	FALSE
M120T620_pos	120.0808	620	3	1.72E-04	0.78	FALSE	8.10E-01	1.02	FALSE	7.92E-05	1.25	FALSE	8.94E-02	0.86	FALSE
M121T362_pos	121.0649	362	3	1.05E-03	1.48	FALSE	2.16E-02	0.75	FALSE	6.88E-01	1.04	FALSE	9.62E-01	0.99	FALSE
M121T1039_pos	121.1012	1039	3	3.32E-09	1.45	FALSE	1.33E-04	0.79	FALSE	8.90E-01	1.01	FALSE	3.14E-02	1.15	FALSE
M121T769_pos	121.1012	769	3	2.19E-02	1.19	FALSE	1.15E-01	1.13	FALSE	2.43E-01	0.93	FALSE	1.92E-01	0.76	FALSE
M121T882_pos	121.1012	882	3	7.85E-01	1.01	FALSE	4.08E-04	1.22	FALSE	1.30E-01	1.07	FALSE	7.79E-01	0.99	FALSE
M121T808_pos	121.1012	808	3	4.03E-01	0.97	FALSE	2.42E-01	1.04	FALSE	6.40E-12	1.22	FALSE	3.71E-02	0.86	FALSE
M121T687_pos	121.1012	687	3	2.92E-03	1.21	FALSE	4.01E-01	1.06	FALSE	2.46E-04	1.23	FALSE	1.03E-03	0.87	FALSE
M122T846_pos	122.0965	846	3	3.75E-01	1.06	FALSE	6.26E-01	1.03	FALSE	4.10E-02	0.89	FALSE	7.68E-01	1.04	FALSE
M123T157_pos	123.0553	157	3	4.15E-01	0.92	FALSE	7.31E-01	1.04	FALSE	2.79E-03	1.32	FALSE	3.25E-01	1.16	FALSE
M123T488_pos	123.0441	488	3	4.21E-03	1.18	FALSE	8.34E-01	0.99	FALSE	2.57E-06	1.27	FALSE	4.96E-01	0.97	FALSE
M123T1036_pos	123.1168	1036	3	6.85E-04	1.20	FALSE	4.94E-01	0.96	FALSE	4.92E-01	1.03	FALSE	4.02E-01	1.06	FALSE
M123T744_pos	123.1168	744	3	7.24E-09	1.37	FALSE	1.44E-05	1.27	FALSE	2.18E-04	0.84	FALSE	1.23E-01	0.90	FALSE
M123T882_pos	123.1169	882	3	4.21E-01	1.04	FALSE	2.03E-01	1.07	FALSE	8.38E-01	0.99	FALSE	5.58E-01	0.94	FALSE
M125T615_pos	125.0961	615	3	5.22E-01	0.92	FALSE	2.80E-01	1.17	FALSE	1.35E-02	1.34	FALSE	5.34E-01	0.71	FALSE
M125T1039_pos	125.0961	1039	3	4.62E-03	1.13	FALSE	1.57E-04	0.84	FALSE	6.65E-01	1.02	FALSE	2.78E-03	1.21	FALSE
M125T699_pos	125.0961	699	3	1.41E-05	1.48	FALSE	9.63E-01	1.00	FALSE	2.45E-02	0.84	FALSE	1.95E-01	0.68	FALSE
M125T883_pos	125.0961	883	3	5.93E-03	1.14	FALSE	3.43E-01	1.05	FALSE	1.70E-03	0.88	FALSE	3.49E-01	1.18	FALSE
M125T1038_pos	125.1325	1038	3	1.85E-02	1.15	FALSE	8.09E-02	0.90	FALSE	6.55E-01	0.98	FALSE	8.49E-01	1.02	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M126T647_pos	126.0914	647	3							HMDB0030345	6-Acetyl-1,2,3,4-tetrahydropyridine	C7H11NO	0.3
M126T743_pos	126.0914	743	3							HMDB0030345	6-Acetyl-1,2,3,4-tetrahydropyridine	C7H11NO	0.7
M126T584_pos	126.0914	584	3							HMDB0030345	6-Acetyl-1,2,3,4-tetrahydropyridine	C7H11NO	0.4
M127T144_pos	127.0390	144	3							HMDB0013674	1,2,3-Trihydroxybenzene	C6H6O3	0.5
M127T547_pos	127.0754	547	3							HMDB0029582	Methyl sorbate	C7H10O2	0.1
M127T1043_pos	127.1118	1043	3							HMDB0013809	(E)-2-octenal	C8H14O	0.3
M127T1039_pos	127.1482	1039	3							HMDB0031270	1-Nonene	C9H18	0.2
M128T432_pos	128.0707	432	3							HMDB0001084	1-Piperideine-2-carboxylic acid	C6H9NO2	0.4
M128T364_pos	128.0707	364	3						Amino acids and Peptides	HMDB0001084	1-Piperideine-2-carboxylic acid	C6H9NO2	0.5
M128T497_pos	128.1070	497	3							HMDB0031667	Nor-psi-tropine	C7H13NO	0.3
M128T206_pos	128.1071	206	3						Alkaloids	HMDB0031667	Nor-psi-tropine	C7H13NO	0.6
M129T378_pos	129.0547	378	3							HMDB0031303	Osmundalactone	C6H8O3	0.3
M129T575_pos	129.0546	575	3						Fatty acids	HMDB0031303	Osmundalactone	C6H8O3	0.1
M129T882_pos	129.0910	882	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.3
M129T687_pos	129.0911	687	3							HMDB0029165	1,3-Diacetylpropane	C7H12O2	0.5
M129T560_pos	129.1023	560	3							HMDB0256575	piperidine-1-carboxamide	C6H12N2O	0.3
M130T594_pos	130.0651	594	3							HMDB0011664	3-Methylene-indolenine	C9H7N	0.0
M130T891_pos	130.0651	891	3							HMDB0011664	3-Methylene-indolenine	C9H7N	0.1
M130T759_pos	130.0651	759	3						Alkaloids	HMDB0011664	3-Methylene-indolenine	C9H7N	0.2
M130T706_pos	130.0651	706	3							HMDB0011664	3-Methylene-indolenine	C9H7N	0.2
M130T173_pos	130.0863	173	3						Amino acids and Peptides	HMDB0000070	Pipecolic acid	C6H11NO2	0.7
M131T722_pos	131.0525	722	3							HMDB0031370	2-[(Methylthio)methyl]-2-butenal	C6H10OS	0.1
M131T803_pos	131.1067	803	3						Fatty acids	HMDB0000666	Heptanoic acid	C7H14O2	0.1
M132T67_pos	132.0656	67	3							HMDB0000725	4-Hydroxyproline	C5H9NO3	0.6
M133T359_pos	133.0319	359	3							HMDB0059667	3-Methyl sulfolene	C5H8O2S	0.6
M133T699_pos	133.0648	699	3							HMDB0003441	Cinnamaldehyde	C9H8O	0.2
M133T774_pos	133.0648	774	3							HMDB0003441	Cinnamaldehyde	C9H8O	0.2
M133T473_2_pos	133.0859	473	3							HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.2
M133T767_pos	133.0860	767	3							HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.2
M133T1066_pos	133.0859	1066	3							HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.1
M135T601_pos	135.0441	601	3							HMDB0032469	Phthalide	C8H6O2	0.2
M135T752_pos	135.0805	752	3							HMDB0029639	(4-Methylphenyl)acetaldehyde	C9H10O	0.4
M135T804_pos	135.1016	804	3							HMDB0032478	lypropylene glycol (m w 1,200-3,0	C6H14O3	0.6
M135T854_pos	135.1169	854	3							HMDB0005805	p-Cymene	C10H14	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M126T647_pos	126.0914	647	3	6.89E-01	0.97	FALSE	6.46E-01	1.04	FALSE	8.95E-05	1.30	FALSE	8.39E-01	1.04	FALSE
M126T743_pos	126.0914	743	3	5.09E-01	1.03	FALSE	1.24E-01	0.93	FALSE	6.50E-01	1.02	FALSE	7.77E-01	1.03	FALSE
M126T584_pos	126.0914	584	3	4.14E-06	1.28	FALSE	2.61E-04	0.79	FALSE	1.40E-06	1.26	FALSE	9.07E-01	0.98	FALSE
M127T144_pos	127.0390	144	3	1.29E-01	1.35	FALSE	1.57E-01	0.73	FALSE	3.13E-01	1.19	FALSE	9.90E-01	0.99	FALSE
M127T547_pos	127.0754	547	3	1.95E-16	1.46	FALSE	1.75E-02	0.90	FALSE	8.07E-01	1.01	FALSE	1.85E-01	0.83	FALSE
M127T1043_pos	127.1118	1043	3	3.83E-01	0.96	FALSE	3.14E-01	1.06	FALSE	1.92E-01	0.94	FALSE	5.97E-01	1.06	FALSE
M127T1039_pos	127.1482	1039	3	5.65E-01	0.96	FALSE	2.86E-01	0.92	FALSE	3.21E-01	0.94	FALSE	3.36E-01	1.08	FALSE
M128T432_pos	128.0707	432	3	1.55E-05	1.18	FALSE	6.91E-01	0.98	FALSE	2.75E-07	1.19	FALSE	2.71E-03	0.85	FALSE
M128T364_pos	128.0707	364	3	4.55E-02	0.86	FALSE	5.56E-01	1.05	FALSE	6.64E-08	1.45	FALSE	1.42E-01	0.78	FALSE
M128T497_pos	128.1070	497	3	1.00E-08	1.31	FALSE	3.50E-01	0.96	FALSE	3.01E-01	0.96	FALSE	6.59E-02	0.86	FALSE
M128T206_pos	128.1071	206	3	1.74E-01	0.89	FALSE	9.35E-01	1.01	FALSE	1.50E-04	1.35	FALSE	7.47E-02	0.76	FALSE
M129T378_pos	129.0547	378	3	3.95E-05	0.74	FALSE	2.05E-04	1.33	FALSE	2.49E-01	1.07	FALSE	4.20E-01	1.07	FALSE
M129T575_pos	129.0546	575	3	5.26E-01	0.96	FALSE	2.39E-01	1.08	FALSE	4.16E-02	1.12	FALSE	9.25E-02	1.45	FALSE
M129T882_pos	129.0910	882	3	3.16E-01	1.03	FALSE	6.02E-03	1.10	FALSE	3.78E-05	1.13	FALSE	2.89E-01	1.08	FALSE
M129T687_pos	129.0911	687	3	1.90E-02	1.06	FALSE	7.26E-05	1.11	FALSE	2.34E-31	1.37	FALSE	1.99E-01	0.95	FALSE
M129T560_pos	129.1023	560	3	9.48E-09	1.32	FALSE	9.98E-09	0.73	FALSE	1.30E-06	0.82	FALSE	2.81E-03	1.49	FALSE
M130T594_pos	130.0651	594	3	3.60E-02	0.89	FALSE	5.20E-01	1.04	FALSE	1.31E-05	1.25	FALSE	5.04E-01	0.95	FALSE
M130T891_pos	130.0651	891	3	9.54E-02	1.16	FALSE	7.68E-02	1.17	FALSE	1.10E-01	1.13	FALSE	1.31E-02	0.67	FALSE
M130T759_pos	130.0651	759	3	3.60E-06	1.22	FALSE	1.82E-01	0.94	FALSE	1.73E-02	1.09	FALSE	7.22E-02	0.90	FALSE
M130T706_pos	130.0651	706	3	3.56E-02	1.24	FALSE	7.40E-01	1.04	FALSE	4.93E-02	1.19	FALSE	4.52E-02	0.80	FALSE
M130T173_pos	130.0863	173	3	1.55E-02	0.85	FALSE	1.05E-01	1.11	FALSE	3.61E-10	1.46	FALSE	8.77E-03	0.76	FALSE
M131T722_pos	131.0525	722	3	1.30E-02	1.13	FALSE	5.27E-11	1.38	FALSE	1.15E-03	1.15	FALSE	1.87E-01	1.17	FALSE
M131T803_pos	131.1067	803	3	9.95E-16	1.20	FALSE	9.35E-02	1.04	FALSE	3.10E-02	0.96	FALSE	8.36E-01	1.01	FALSE
M132T67_pos	132.0656	67	3	5.43E-03	1.17	FALSE	4.81E-01	0.96	FALSE	4.42E-01	0.96	FALSE	1.86E-01	1.14	FALSE
M133T359_pos	133.0319	359	3	3.40E-01	0.94	FALSE	5.99E-04	0.81	FALSE	2.90E-01	1.06	FALSE	7.38E-03	0.75	FALSE
M133T699_pos	133.0648	699	3	3.52E-16	1.47	FALSE	2.69E-01	1.05	FALSE	1.44E-01	1.06	FALSE	7.94E-01	1.01	FALSE
M133T774_pos	133.0648	774	3	5.57E-01	1.06	FALSE	6.28E-01	1.05	FALSE	2.13E-01	0.90	FALSE	3.56E-01	0.92	FALSE
M133T473_2_pos	133.0859	473	3	1.07E-17	1.41	FALSE	5.30E-04	0.88	FALSE	1.28E-08	0.83	FALSE	7.08E-01	0.94	FALSE
M133T767_pos	133.0860	767	3	2.61E-01	1.08	FALSE	5.50E-01	1.05	FALSE	7.93E-01	1.02	FALSE	9.88E-01	1.00	FALSE
M133T1066_pos	133.0859	1066	3	2.33E-01	0.94	FALSE	4.13E-01	0.96	FALSE	2.40E-01	1.05	FALSE	4.92E-01	0.92	FALSE
M135T601_pos	135.0441	601	3	2.76E-25	1.47	FALSE	6.75E-01	0.99	FALSE	6.98E-08	1.17	FALSE	8.99E-01	1.00	FALSE
M135T752_pos	135.0805	752	3	2.13E-01	0.95	FALSE	3.16E-02	1.10	FALSE	6.05E-17	1.40	FALSE	1.29E-01	0.81	FALSE
M135T804_pos	135.1016	804	3	1.62E-08	1.16	FALSE	2.33E-01	1.03	FALSE	2.74E-04	0.92	FALSE	1.98E-01	1.07	FALSE
M135T854_pos	135.1169	854	3	3.21E-01	0.97	FALSE	3.57E-01	1.03	FALSE	2.38E-05	1.12	FALSE	5.48E-01	1.04	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M135T1039_pos	135.1169	1039	3							HMDB0005805	p-Cymene	C10H14	0.2
M135T971_pos	135.1169	971	3							HMDB0005805	p-Cymene	C10H14	0.2
M136T391_pos	136.0395	391	3							HMDB0032931	2-Benzoxazolol	C7H5NO2	1.5
M136T714_pos	136.0758	714	3							HMDB0001250	N-Acetylarylamine	C8H9NO	0.5
M137T815_pos	137.0597	815	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.2
M137T621_pos	137.0597	621	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.3
M137T926_pos	137.0597	926	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.3
M137T889_pos	137.0597	889	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.3
M137T769_pos	137.0961	769	3							HMDB0029667	2,3,6-Trimethylphenol	C9H12O	0.2
M137T659_pos	137.0961	659	3							HMDB0029667	2,3,6-Trimethylphenol	C9H12O	0.2
M137T1038_pos	137.1325	1038	3							HMDB0003375	(+)-Limonene	C10H16	0.1
M138T332_pos	138.0550	332	3							HMDB0000875	Trigonelline	C7H7NO2	0.1
M138T631_pos	138.0914	631	3							HMDB0000306	Tyramine	C8H11NO	0.3
M138T755_pos	138.0914	755	3							HMDB0000306	Tyramine	C8H11NO	0.8
M139T565_pos	139.0390	565	3							HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.1
M139T687_pos	139.0753	687	3							HMDB0004284	Tyrosol	C8H10O2	0.6
M139T768_pos	139.1118	768	3							HMDB0013824	2-Pentylfuran	C9H14O	0.2
M139T1038_1_pos	139.1118	1038	3							HMDB0013824	2-Pentylfuran	C9H14O	0.2
M139T854_pos	139.1118	854	3							HMDB0013824	2-Pentylfuran	C9H14O	0.3
M139T713_pos	139.1118	713	3							HMDB0013824	2-Pentylfuran	C9H14O	0.2
M139T1038_2_pos	139.1482	1038	3							HMDB0037213	xi-p-Menth-3-ene	C10H18	0.2
M140T250_pos	140.0343	250	3							HMDB0001232	4-Nitrophenol	C6H5NO3	0.3
M140T690_pos	140.0707	690	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.4
M140T631_pos	140.0706	631	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.1
M140T384_pos	140.0707	384	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.6
M140T136_pos	140.0707	136	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.5
M140T372_pos	140.0933	372	3							HMDB0251408	Dimethyltriazenoimidazole	C5H9N5	1.8
M141T1038_pos	141.1274	1038	3							HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	0.2
M141T1019_pos	141.1638	1019	3							HMDB0031455	p-Menthane	C10H20	0.3
M142T353_pos	142.0613	353	3							HMDB0251409	Dimetridazole	C5H7N3O2	1.3
M142T389_pos	142.0863	389	3							HMDB0014731	Ethosuximide	C7H11NO2	0.5
M142T346_pos	142.1227	346	3							HMDB0030324	(R)-Pelletierine	C8H15NO	0.5
M142T715_pos	142.1227	715	3							HMDB0030324	(R)-Pelletierine	C8H15NO	0.5
M143T742_pos	143.0703	742	3						Fatty acids	HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.2
M143T1039_pos	143.1067	1039	3							HMDB0000392	2-Octenoic acid	C8H14O2	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M135T1039_pos	135.1169	1039	3	1.01E-02	1.22	FALSE	7.94E-03	0.82	FALSE	6.12E-02	0.88	FALSE	5.66E-02	1.18	FALSE
M135T971_pos	135.1169	971	3	7.38E-01	0.98	FALSE	5.58E-01	0.97	FALSE	8.90E-01	1.01	FALSE	7.11E-01	0.98	FALSE
M136T391_pos	136.0395	391	3	1.65E-02	0.91	FALSE	1.68E-01	1.06	FALSE	1.51E-24	1.48	FALSE	7.25E-01	0.97	FALSE
M136T714_pos	136.0758	714	3	6.52E-03	0.76	FALSE	4.82E-02	1.23	FALSE	1.47E-03	1.32	FALSE	6.28E-01	1.11	FALSE
M137T815_pos	137.0597	815	3	1.76E-21	1.43	FALSE	7.72E-02	0.94	FALSE	2.49E-01	0.97	FALSE	4.40E-01	1.04	FALSE
M137T621_pos	137.0597	621	3	7.12E-09	1.36	FALSE	8.92E-01	1.01	FALSE	5.42E-07	1.25	FALSE	7.76E-01	1.02	FALSE
M137T926_pos	137.0597	926	3	1.31E-11	1.35	FALSE	3.24E-04	0.86	FALSE	1.21E-09	1.26	FALSE	7.38E-01	1.02	FALSE
M137T889_pos	137.0597	889	3	2.53E-17	1.30	FALSE	4.61E-01	1.02	FALSE	9.35E-01	1.00	FALSE	3.80E-01	0.93	FALSE
M137T769_pos	137.0961	769	3	7.56E-02	1.08	FALSE	1.25E-01	1.07	FALSE	5.89E-03	1.10	FALSE	7.38E-02	0.91	FALSE
M137T659_pos	137.0961	659	3	4.55E-07	1.19	FALSE	5.12E-02	1.07	FALSE	7.14E-13	1.25	FALSE	6.95E-01	0.96	FALSE
M137T1038_pos	137.1325	1038	3	3.46E-05	1.29	FALSE	7.69E-03	0.84	FALSE	3.99E-02	1.12	FALSE	2.69E-02	1.27	FALSE
M138T332_pos	138.0550	332	3	4.10E-07	1.43	FALSE	1.89E-01	0.91	FALSE	8.36E-07	1.35	FALSE	2.07E-01	0.90	FALSE
M138T631_pos	138.0914	631	3	1.64E-12	1.45	FALSE	5.84E-01	1.03	FALSE	1.14E-06	1.24	FALSE	1.58E-01	1.19	FALSE
M138T755_pos	138.0914	755	3	7.75E-01	1.01	FALSE	1.80E-02	0.88	FALSE	2.63E-03	1.14	FALSE	8.55E-02	0.74	FALSE
M139T565_pos	139.0390	565	3	4.87E-02	1.15	FALSE	9.54E-01	1.00	FALSE	6.45E-07	1.37	FALSE	9.13E-02	0.90	FALSE
M139T687_pos	139.0753	687	3	2.71E-03	1.10	FALSE	7.17E-01	1.01	FALSE	2.18E-18	1.32	FALSE	1.09E-01	0.91	FALSE
M139T768_pos	139.1118	768	3	2.22E-05	1.17	FALSE	3.01E-01	0.96	FALSE	4.21E-02	0.94	FALSE	2.92E-01	0.91	FALSE
M139T1038_1_pos	139.1118	1038	3	5.89E-08	1.47	FALSE	2.48E-06	0.72	FALSE	6.95E-01	0.98	FALSE	6.73E-04	1.22	FALSE
M139T854_pos	139.1118	854	3	3.83E-01	1.07	FALSE	2.85E-02	1.20	FALSE	7.77E-02	1.13	FALSE	9.33E-02	0.63	FALSE
M139T713_pos	139.1118	713	3	5.72E-09	1.44	FALSE	4.44E-01	1.05	FALSE	1.92E-05	0.80	FALSE	4.16E-01	0.89	FALSE
M139T1038_2_pos	139.1482	1038	3	9.27E-01	0.99	FALSE	6.36E-01	1.03	FALSE	3.32E-04	0.82	FALSE	3.66E-02	1.32	FALSE
M140T250_pos	140.0343	250	3	8.19E-03	0.78	FALSE	9.90E-01	1.00	FALSE	9.57E-06	1.44	FALSE	4.62E-01	1.14	FALSE
M140T690_pos	140.0707	690	3	1.47E-02	1.12	FALSE	9.57E-02	1.08	FALSE	3.87E-05	1.18	FALSE	1.20E-01	0.86	FALSE
M140T631_pos	140.0706	631	3	1.30E-01	0.89	FALSE	6.97E-01	0.97	FALSE	2.00E-03	1.22	FALSE	4.46E-01	1.10	FALSE
M140T384_pos	140.0707	384	3	1.41E-08	1.19	FALSE	9.46E-01	1.00	FALSE	1.49E-03	1.08	FALSE	5.64E-02	0.88	FALSE
M140T136_pos	140.0707	136	3	7.77E-01	0.98	FALSE	3.00E-01	0.94	FALSE	1.22E-08	1.34	FALSE	7.78E-01	1.03	FALSE
M140T372_pos	140.0933	372	3	6.38E-02	0.89	FALSE	5.02E-01	1.05	FALSE	3.63E-10	1.44	FALSE	1.46E-01	0.84	FALSE
M141T1038_pos	141.1274	1038	3	7.20E-06	1.32	FALSE	3.25E-02	0.88	FALSE	2.09E-01	1.07	FALSE	3.78E-01	1.08	FALSE
M141T1019_pos	141.1638	1019	3	5.95E-01	0.96	FALSE	2.06E-01	0.91	FALSE	4.32E-02	0.88	FALSE	8.98E-01	1.02	FALSE
M142T353_pos	142.0613	353	3	8.57E-01	1.04	FALSE	6.11E-01	0.90	FALSE	8.44E-01	1.03	FALSE	9.39E-01	1.03	FALSE
M142T389_pos	142.0863	389	3	4.31E-01	1.07	FALSE	5.23E-01	1.06	FALSE	7.44E-01	0.98	FALSE	5.68E-02	1.19	FALSE
M142T346_pos	142.1227	346	3	1.31E-02	1.36	FALSE	9.92E-01	1.00	FALSE	7.57E-01	0.97	FALSE	1.35E-01	0.74	FALSE
M142T715_pos	142.1227	715	3	6.14E-02	1.22	FALSE	1.50E-02	1.29	FALSE	3.50E-03	1.31	FALSE	9.14E-01	1.01	FALSE
M143T742_pos	143.0703	742	3	1.13E-16	1.47	FALSE	4.11E-01	0.96	FALSE	1.57E-04	0.87	FALSE	4.22E-01	0.90	FALSE
M143T1039_pos	143.1067	1039	3	6.31E-06	1.45	FALSE	2.96E-02	0.83	FALSE	4.35E-01	0.95	FALSE	6.75E-04	1.29	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M143T698_pos	143.1067	698	3							HMDB0000392	2-Octenoic acid	C8H14O2	0.3
M143T752_pos	143.1067	752	3						Fatty acids	HMDB0000392	2-Octenoic acid	C8H14O2	0.2
M143T810_pos	143.1067	810	3						Fatty acids	HMDB0000392	2-Octenoic acid	C8H14O2	0.2
M144T495_pos	144.0806	495	3							HMDB0033115	6-Methylquinoline	C10H9N	1.2
M144T611_pos	144.1020	611	3						Fatty acids	HMDB0004827	Proline betaine	C7H13NO2	0.4
M144T349_pos	144.1020	349	3							HMDB0004827	Proline betaine	C7H13NO2	0.5
M145T695_pos	145.0318	695	3							HMDB0246446	Hydroxy-2,4-dimethylthiophen-3-c	C6H8O2S	0.1
M146T432_2_pos	146.0813	432	3							HMDB0000730	Isobutyrylglycine	C6H11NO3	0.7
M146T121_pos	146.1176	121	3							HMDB0001161	4-Trimethylammoniobutanoic acid	C7H15NO2	0.1
M146T175_pos	146.1541	175	3							HMDB0253104	Heptaminol	C8H19NO	0.8
M147T161_pos	146.9962	161	3							HMDB0246772	5-Chlorouracil	C4H3ClN2O2	4.1
M147T76_pos	146.9962	76	3							HMDB0246772	5-Chlorouracil	C4H3ClN2O2	4.5
M147T659_pos	147.0802	659	3							HMDB0029602	4-Phenyl-2-butenal	C10H10O	1.4
M148T603_pos	148.0394	603	3							HMDB0006779	Indole-5,6-quinone	C8H5NO2	0.8
M148T663_pos	148.0758	663	3							HMDB0005785	Indole-3-carbinol	C9H9NO	0.4
M149T1032_pos	149.0233	1032	3							HMDB0256501	Phthalic anhydride	C8H4O3	0.1
M149T899_pos	149.0234	899	3							HMDB0256501	Phthalic anhydride	C8H4O3	0.3
M149T610_pos	149.0598	610	3							HMDB0000567	Cinnamic acid	C9H8O2	0.7
M149T946_pos	149.0961	946	3							HMDB0002214	Cuminaldehyde	C10H12O	0.4
M149T904_pos	149.0962	904	3							HMDB0002214	Cuminaldehyde	C10H12O	0.4
M149T808_pos	149.0962	808	3							HMDB0002214	Cuminaldehyde	C10H12O	0.5
M149T772_pos	149.0961	772	3							HMDB0002214	Cuminaldehyde	C10H12O	0.3
M149T714_pos	149.0961	714	3							HMDB0002214	Cuminaldehyde	C10H12O	0.3
M149T668_pos	149.0962	668	3							HMDB0002214	Cuminaldehyde	C10H12O	0.6
M149T868_pos	149.1173	868	3							HMDB0259190	Triethyl orthoformate	C7H16O3	0.8
M150T480_pos	150.0553	480	3							HMDB0004058	5,6-Dihydroxyindole	C8H7NO2	2.3
M150T674_pos	150.0915	674	3							HMDB0030175	Venoterpine	C9H11NO	0.9
M150T397_pos	150.0914	397	3							HMDB0030175	Venoterpine	C9H11NO	0.5
M150T719_pos	150.0914	719	3							HMDB0030175	Venoterpine	C9H11NO	0.5
M151T675_pos	151.0754	675	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.3
M151T811_pos	151.0754	811	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.0
M151T929_pos	151.0754	929	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.1
M151T724_pos	151.0754	724	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.4
M151T1067_pos	151.0965	1067	3							HMDB0259193	TRIETHYLENE GLYCOL	C6H14O4	0.2
M151T1039_pos	151.1481	1039	3							HMDB0030944	Cystophorene	C11H18	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M143T698_pos	143.1067	698	3	6.76E-09	1.46	FALSE	3.95E-01	1.06	FALSE	6.84E-01	0.98	FALSE	4.70E-01	0.90	FALSE
M143T752_pos	143.1067	752	3	1.35E-01	0.95	FALSE	7.15E-03	1.09	FALSE	1.58E-31	1.47	FALSE	6.32E-01	0.98	FALSE
M143T810_pos	143.1067	810	3	9.91E-01	1.00	FALSE	4.47E-02	0.76	FALSE	7.51E-01	0.97	FALSE	7.12E-01	1.08	FALSE
M144T495_pos	144.0806	495	3	7.19E-01	1.03	FALSE	5.19E-01	1.06	FALSE	1.24E-03	1.29	FALSE	9.44E-01	1.01	FALSE
M144T611_pos	144.1020	611	3	3.57E-04	1.19	FALSE	1.19E-01	0.92	FALSE	2.36E-01	0.95	FALSE	4.25E-01	0.92	FALSE
M144T349_pos	144.1020	349	3	6.29E-02	1.09	FALSE	8.92E-01	0.99	FALSE	2.25E-09	1.29	FALSE	6.62E-01	0.95	FALSE
M145T695_pos	145.0318	695	3	7.42E-02	1.34	FALSE	2.41E-01	0.80	FALSE	6.31E-01	0.93	FALSE	2.19E-01	0.69	FALSE
M146T432_2_pos	146.0813	432	3	2.45E-07	1.24	FALSE	6.56E-01	1.02	FALSE	2.14E-03	1.12	FALSE	7.11E-01	1.03	FALSE
M146T121_pos	146.1176	121	3	3.69E-04	0.87	FALSE	1.64E-01	1.06	FALSE	4.69E-19	1.38	FALSE	4.73E-01	0.95	FALSE
M146T175_pos	146.1541	175	3	9.77E-04	1.38	FALSE	2.88E-01	0.90	FALSE	3.73E-01	1.08	FALSE	2.14E-01	0.87	FALSE
M147T161_pos	146.9962	161	3	3.40E-01	1.11	FALSE	2.59E-01	1.13	FALSE	2.82E-03	0.75	FALSE	4.39E-01	0.81	FALSE
M147T76_pos	146.9962	76	3	4.59E-01	0.94	FALSE	9.68E-01	1.00	FALSE	7.56E-01	0.98	FALSE	6.37E-01	1.10	FALSE
M147T659_pos	147.0802	659	3	1.49E-01	0.91	FALSE	6.23E-01	0.96	FALSE	1.13E-01	1.10	FALSE	7.62E-02	0.90	FALSE
M148T603_pos	148.0394	603	3	6.07E-09	1.37	FALSE	4.19E-02	0.89	FALSE	6.11E-07	1.26	FALSE	5.17E-01	0.94	FALSE
M148T663_pos	148.0758	663	3	7.31E-12	1.45	FALSE	3.92E-01	1.05	FALSE	8.64E-01	1.01	FALSE	7.40E-01	1.07	FALSE
M149T1032_pos	149.0233	1032	3	1.10E-03	0.84	FALSE	1.46E-02	1.15	FALSE	3.85E-01	0.96	FALSE	9.24E-01	1.00	FALSE
M149T899_pos	149.0234	899	3	5.08E-01	0.96	FALSE	5.58E-01	0.96	FALSE	5.26E-01	0.97	FALSE	2.82E-01	1.16	FALSE
M149T610_pos	149.0598	610	3	3.10E-13	1.39	FALSE	9.86E-01	1.00	FALSE	1.49E-05	1.18	FALSE	2.84E-01	1.14	FALSE
M149T946_pos	149.0961	946	3	1.18E-05	1.19	FALSE	1.10E-04	0.85	FALSE	8.15E-01	0.99	FALSE	1.88E-01	1.20	FALSE
M149T904_pos	149.0962	904	3	1.90E-17	1.27	FALSE	4.90E-01	0.98	FALSE	5.92E-02	0.96	FALSE	2.39E-03	0.91	FALSE
M149T808_pos	149.0962	808	3	6.13E-01	1.02	FALSE	6.42E-02	1.08	FALSE	1.04E-05	1.18	FALSE	2.91E-02	0.82	FALSE
M149T772_pos	149.0961	772	3	1.17E-08	1.23	FALSE	4.70E-01	1.03	FALSE	1.72E-02	1.08	FALSE	2.14E-02	0.81	FALSE
M149T714_pos	149.0961	714	3	6.31E-04	1.49	FALSE	4.22E-01	0.90	FALSE	1.15E-01	0.86	FALSE	3.82E-01	0.88	FALSE
M149T668_pos	149.0962	668	3	7.09E-03	1.12	FALSE	6.78E-01	1.02	FALSE	5.49E-01	0.98	FALSE	2.35E-01	0.91	FALSE
M149T868_pos	149.1173	868	3	2.81E-06	1.11	FALSE	8.57E-01	1.00	FALSE	8.96E-02	0.97	FALSE	9.52E-01	1.00	FALSE
M150T480_pos	150.0553	480	3	2.03E-05	1.25	FALSE	5.76E-01	0.97	FALSE	1.06E-01	0.93	FALSE	4.74E-01	1.05	FALSE
M150T674_pos	150.0915	674	3	3.12E-07	1.19	FALSE	3.28E-01	1.03	FALSE	3.76E-14	1.27	FALSE	1.53E-01	0.95	FALSE
M150T397_pos	150.0914	397	3	2.21E-06	1.31	FALSE	4.64E-04	0.81	FALSE	6.62E-05	1.21	FALSE	4.84E-01	1.14	FALSE
M150T719_pos	150.0914	719	3	3.84E-07	0.82	FALSE	7.86E-02	1.07	FALSE	3.20E-25	1.50	FALSE	8.24E-02	0.87	FALSE
M151T675_pos	151.0754	675	3	1.47E-06	1.42	FALSE	1.14E-03	0.78	FALSE	4.92E-01	1.04	FALSE	6.18E-01	0.95	FALSE
M151T811_pos	151.0754	811	3	2.56E-02	1.09	FALSE	3.09E-01	0.96	FALSE	2.93E-02	0.93	FALSE	8.53E-01	0.99	FALSE
M151T929_pos	151.0754	929	3	9.99E-01	1.00	FALSE	9.03E-01	1.00	FALSE	2.49E-01	0.96	FALSE	4.47E-01	0.95	FALSE
M151T724_pos	151.0754	724	3	6.78E-01	0.98	FALSE	1.82E-01	1.07	FALSE	9.91E-01	1.00	FALSE	2.03E-01	1.14	FALSE
M151T1067_pos	151.0965	1067	3	3.47E-01	0.99	FALSE	4.63E-01	1.01	FALSE	1.17E-01	0.98	FALSE	4.12E-01	0.97	FALSE
M151T1039_pos	151.1481	1039	3	4.02E-03	1.17	FALSE	9.19E-01	0.99	FALSE	6.32E-01	0.98	FALSE	7.26E-02	1.20	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M152T81_pos	152.0100	81	3							HMDB0245086	-Cyanoethyl dihydrogen phosphat	C3H6NO4P	4.5
M152T113_pos	152.0221	113	3							HMDB0243777	1-(2-Chloroethyl)-1-nitrosourea	C3H6ClN3O2	0.0
M152T552_pos	152.0707	552	3							HMDB0001859	Acetaminophen	C8H9NO2	0.4
M153T868_pos	153.0891	868	3							HMDB0243749	(Trifluoromethyl)cyclohexane	C7H11F3	3.8
M153T604_pos	153.0911	604	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.3
M153T853_pos	153.1274	853	3							HMDB0003450	(-)-trans-Carveol	C10H16O	0.3
M153T955_pos	153.1274	955	3							HMDB0003450	(-)-trans-Carveol	C10H16O	0.3
M153T1038_pos	153.1638	1038	3							HMDB0032712	1,4-Undecadiene	C11H20	0.2
M154T391_pos	154.0499	391	3							HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	0.3
M154T424_pos	154.0865	424	3							HMDB0000073	Dopamine	C8H11NO2	1.6
M154T568_pos	154.0864	568	3							HMDB0000073	Dopamine	C8H11NO2	1.2
M155T1028_pos	154.9647	1028	3							HMDB0303644	Calcium fumarate	C4H2CaO4	2.9
M155T84_pos	154.9676	84	3							HMDB0031333	Chloropentafluoroethane	C2ClF5	3.2
M155T992_pos	155.0468	992	3						Fatty acids	HMDB0012209	Diethylphosphate	C4H11O4P	0.3
M155T659_pos	155.1067	659	3						Fatty acids	HMDB0031302	Methyl 2-octynoate	C9H14O2	0.3
M156T180_pos	156.0769	180	3							HMDB0000177	L-Histidine	C6H9N3O2	0.7
M156T506_pos	156.1020	506	3						Alkaloids	HMDB0030353	Arecoline	C8H13NO2	0.5
M157T382_pos	157.0609	382	3						Amino acids and Peptides	HMDB0000544	5-Hydroxymethyl-4-methyluracil	C6H8N2O3	0.7
M157T535_pos	157.0609	535	3							HMDB0000544	5-Hydroxymethyl-4-methyluracil	C6H8N2O3	0.7
M157T454_pos	157.0859	454	3							HMDB0031101	8-Hydroxy-5,6-octadienoic acid	C8H12O3	0.4
M157T768_pos	157.1224	768	3							HMDB0004362	4-Hydroxynonenal	C9H16O2	0.4
M158T694_pos	158.1176	694	3							HMDB0014447	Tranexamic Acid	C8H15NO2	0.4
M158T541_pos	158.1176	541	3							HMDB0014447	Tranexamic Acid	C8H15NO2	0.3
M158T254_pos	158.1540	254	3							HMDB0245344	2,2,6,6-Tetramethyl-4-piperidinol	C9H19NO	0.5
M159T402_pos	159.0764	402	3						Amino acids and Peptides	HMDB0031670	methyl)-5,5-dimethyl-2,4-imidazo	C6H10N2O3	0.1
M159T893_pos	159.1171	893	3							HMDB0243990	1-Phenyl-1-cyclohexene	C12H14	1.4
M159T955_pos	159.1380	955	3							HMDB0000798	Oenanthic ether	C9H18O2	0.5
M159T429_pos	159.1492	429	3							HMDB0254871	Monopropionylcadaverine	C8H18N2O	0.4
M160T126_pos	160.0969	126	3							HMDB0000339	2-Methylbutyrylglycine	C7H13NO3	0.4
M160T265_pos	160.1333	265	3							HMDB0000991	DL-2-Aminooctanoic acid	C8H17NO2	0.6
M161T82_pos	160.9932	82	3						Fatty acids				
M161T121_pos	161.0922	121	3							HMDB0003459	D-Alanyl-D-alanine	C6H12N2O3	1.0
M161T916_pos	161.0961	916	3							HMDB0031567	3-Methyl-4-phenyl-3-buten-2-one	C11H12O	0.0
M161T1037_pos	161.1324	1037	3							HMDB0061813	lethylethenyl)-4-(1-methylethyl)be	C12H16	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M152T81_pos	152.0100	81	3	5.82E-02	0.93	FALSE	3.63E-01	0.97	FALSE	2.01E-01	0.96	FALSE	2.94E-01	1.12	FALSE
M152T113_pos	152.0221	113	3	2.59E-01	1.14	FALSE	5.84E-01	0.93	FALSE	3.98E-01	0.92	FALSE	2.54E-02	1.47	FALSE
M152T552_pos	152.0707	552	3	9.07E-01	1.01	FALSE	6.31E-01	1.05	FALSE	5.12E-05	1.42	FALSE	5.34E-01	0.92	FALSE
M153T868_pos	153.0891	868	3	2.99E-18	1.33	FALSE	8.82E-02	1.05	FALSE	8.01E-09	0.86	FALSE	8.54E-01	0.98	FALSE
M153T604_pos	153.0911	604	3	6.61E-16	1.32	FALSE	1.20E-10	1.23	FALSE	9.78E-01	1.00	FALSE	9.06E-01	0.99	FALSE
M153T853_pos	153.1274	853	3	4.58E-03	0.92	FALSE	4.58E-01	1.02	FALSE	6.68E-17	1.25	FALSE	1.63E-01	1.07	FALSE
M153T955_pos	153.1274	955	3	4.75E-01	0.95	FALSE	8.40E-01	1.02	FALSE	2.80E-03	0.83	FALSE	7.63E-01	0.95	FALSE
M153T1038_pos	153.1638	1038	3	5.86E-01	0.95	FALSE	2.57E-01	0.88	FALSE	2.52E-01	0.90	FALSE	1.18E-02	1.20	FALSE
M154T391_pos	154.0499	391	3	4.77E-01	0.98	FALSE	3.49E-01	1.03	FALSE	6.87E-25	1.43	FALSE	5.71E-01	0.96	FALSE
M154T424_pos	154.0865	424	3	1.89E-01	1.12	FALSE	9.24E-01	0.99	FALSE	1.46E-02	1.20	FALSE	3.81E-01	0.80	FALSE
M154T568_pos	154.0864	568	3	1.84E-01	0.91	FALSE	7.14E-01	1.03	FALSE	1.03E-04	1.30	FALSE	5.32E-01	0.96	FALSE
M155T1028_pos	154.9647	1028	3	7.92E-04	0.69	FALSE	2.30E-02	1.30	FALSE	5.64E-01	0.95	FALSE	5.04E-01	1.09	FALSE
M155T84_pos	154.9676	84	3	9.84E-02	1.09	FALSE	9.74E-01	1.00	FALSE	8.97E-01	1.01	FALSE	1.38E-01	0.82	FALSE
M155T992_pos	155.0468	992	3	8.44E-01	1.00	FALSE	1.31E-01	1.02	FALSE	3.12E-03	0.97	FALSE	5.18E-01	1.01	FALSE
M155T659_pos	155.1067	659	3	4.75E-24	1.45	FALSE	8.38E-01	1.01	FALSE	1.16E-07	0.86	FALSE	8.34E-01	0.99	FALSE
M156T180_pos	156.0769	180	3	4.05E-01	1.16	FALSE	7.30E-02	1.38	FALSE	1.94E-01	0.82	FALSE	9.15E-01	1.05	FALSE
M156T506_pos	156.1020	506	3	7.65E-03	1.24	FALSE	5.94E-01	0.96	FALSE	6.01E-07	1.44	FALSE	1.73E-01	1.22	FALSE
M157T382_pos	157.0609	382	3	3.21E-01	1.05	FALSE	1.02E-04	0.82	FALSE	1.90E-03	1.14	FALSE	4.96E-03	0.85	FALSE
M157T535_pos	157.0609	535	3	4.33E-01	0.95	FALSE	9.57E-01	1.00	FALSE	7.81E-01	1.02	FALSE	4.27E-02	1.13	FALSE
M157T454_pos	157.0859	454	3	3.67E-06	1.43	FALSE	5.92E-01	1.04	FALSE	4.23E-02	1.14	FALSE	2.44E-01	0.89	FALSE
M157T768_pos	157.1224	768	3	2.84E-04	1.19	FALSE	4.35E-02	1.11	FALSE	2.03E-01	0.95	FALSE	6.58E-01	1.07	FALSE
M158T694_pos	158.1176	694	3	6.53E-09	1.48	FALSE	8.26E-06	0.68	FALSE	1.43E-01	1.09	FALSE	4.37E-02	0.68	FALSE
M158T541_pos	158.1176	541	3	1.72E-06	1.28	FALSE	3.92E-01	1.05	FALSE	8.95E-02	1.08	FALSE	6.26E-01	0.96	FALSE
M158T254_pos	158.1540	254	3	6.48E-01	1.06	FALSE	9.36E-01	1.01	FALSE	6.03E-02	1.25	FALSE	6.39E-11	-19.01	FALSE
M159T402_pos	159.0764	402	3	6.50E-01	1.02	FALSE	5.65E-01	1.03	FALSE	2.65E-19	1.46	FALSE	8.21E-02	0.91	FALSE
M159T893_pos	159.1171	893	3	2.77E-02	0.93	FALSE	2.78E-01	1.04	FALSE	4.75E-12	1.24	FALSE	6.69E-01	1.02	FALSE
M159T955_pos	159.1380	955	3	1.30E-01	1.30	FALSE	9.58E-01	0.99	FALSE	4.50E-01	0.89	FALSE	3.11E-01	0.53	FALSE
M159T429_pos	159.1492	429	3	1.52E-02	1.19	FALSE	9.01E-01	1.01	FALSE	3.16E-05	1.30	FALSE	8.31E-03	0.76	FALSE
M160T126_pos	160.0969	126	3	2.20E-02	1.26	FALSE	1.37E-01	0.86	FALSE	2.71E-01	1.10	FALSE	3.81E-01	0.78	FALSE
M160T265_pos	160.1333	265	3	1.38E-04	1.23	FALSE	2.72E-01	1.06	FALSE	3.80E-10	1.37	FALSE	7.76E-01	1.02	FALSE
M161T82_pos	160.9932	82	3	5.16E-01	1.02	FALSE	1.22E-01	0.95	FALSE	5.68E-01	1.01	FALSE	2.37E-04	0.83	FALSE
M161T121_pos	161.0922	121	3	5.49E-01	0.97	FALSE	6.31E-01	1.02	FALSE	8.11E-14	1.41	FALSE	7.41E-01	0.98	FALSE
M161T916_pos	161.0961	916	3	8.47E-07	1.26	FALSE	1.85E-01	1.06	FALSE	6.01E-02	1.08	FALSE	8.53E-01	1.02	FALSE
M161T1037_pos	161.1324	1037	3	2.39E-01	1.12	FALSE	3.94E-01	0.92	FALSE	4.76E-01	1.06	FALSE	4.68E-01	1.26	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M162T364_pos	162.0579	364	3							HMDB0029440	trans-S-(1-Propenyl)-L-cysteine	C6H11NO2S	2.9
M162T476_pos	162.0551	476	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.8
M162T644_pos	162.0551	644	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.9
M162T128_pos	162.0762	128	3							HMDB0000510	Aminoadipic acid	C6H11NO4	0.6
M162T115_pos	162.1125	115	3						Fatty acids	HMDB0244982	droxy-gamma-trimethylaminobut	C7H15NO3	0.4
M162T165_pos	162.1126	165	3							HMDB0244982	droxy-gamma-trimethylaminobut	C7H15NO3	0.6
M163T670_1_pos	163.0754	670	3							HMDB0029714	,5-Dihydro-1-benzoxepin-3(2H)-on	C10H10O2	0.3
M163T905_pos	163.0754	905	3							HMDB0029714	,5-Dihydro-1-benzoxepin-3(2H)-on	C10H10O2	0.3
M163T784_pos	163.0754	784	3							HMDB0029714	,5-Dihydro-1-benzoxepin-3(2H)-on	C10H10O2	0.0
M163T1039_pos	163.1482	1039	3							HMDB0013806	1,3-Diisopropylbenzene	C12H18	0.2
M164T608_pos	164.0708	608	3							HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.9
M164T154_pos	164.0917	154	3							HMDB0011727	Bicine	C6H13NO4	0.1
M165T779_pos	165.0911	779	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.3
M165T717_pos	165.0911	717	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.3
M165T1038_2_pos	165.1275	1038	3							HMDB0029653	ethoxy-1-methylethyl)-4-methylbe	C11H16O	0.4
M165T860_pos	165.1275	860	3							HMDB0029653	ethoxy-1-methylethyl)-4-methylbe	C11H16O	0.4
M166T401_pos	166.0500	401	3							HMDB0003454	4-Pyridoxolactone	C8H7NO3	0.7
M166T744_pos	166.0863	744	3							HMDB0000159	L-Phenylalanine	C9H11NO2	0.6
M166T699_pos	166.1228	699	3							HMDB0001943	Pseudoephedrine	C10H15NO	0.8
M167T1002_pos	167.0555	1002	3							HMDB0034394	S-Propyl 1-propanesulfinothioate	C6H14OS2	2.0
M167T513_pos	167.0818	513	3							HMDB0247540	3,4-Dihydroxyphenylacetamidine	C8H10N2O2	2.0
M167T911_pos	167.1065	911	3							HMDB0004586	Perillic acid	C10H14O2	0.9
M167T639_pos	167.1068	639	3							HMDB0004586	Perillic acid	C10H14O2	0.8
M168T785_pos	168.1021	785	3							HMDB0000022	3-Methoxytyramine	C9H13NO2	1.0
M169T515_pos	169.0498	515	3							HMDB0000130	Homogentisic acid	C8H8O4	1.5
M169T968_pos	169.0858	968	3							HMDB0244846	xahydro-4-methylphthalic anhydri	C9H12O3	0.7
M169T114_pos	169.0971	114	3							HMDB0001431	Pyridoxamine	C8H12N2O2	0.6
M169T660_pos	169.0859	660	3							HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	0.1
M169T713_pos	169.1223	713	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.2
M169T783_pos	169.1223	783	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.2
M169T1054_pos	169.1223	1054	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.2
M169T834_pos	169.1224	834	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.3
M169T973_pos	169.1223	973	3							HMDB0013105	trans-4,5-epoxy-2(E)-decenal	C10H16O2	0.2
M170T491_pos	170.0813	491	3							HMDB0000216	Norepinephrine	C8H11NO3	0.5
M170T268_pos	170.0818	268	3							HMDB0000216	Norepinephrine	C8H11NO3	3.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M162T364_pos	162.0579	364	3	3.25E-01	1.11	FALSE	1.77E-01	1.16	FALSE	1.26E-01	1.15	FALSE	4.39E-01	0.90	FALSE
M162T476_pos	162.0551	476	3	2.16E-07	1.46	FALSE	2.18E-01	0.92	FALSE	1.76E-03	1.21	FALSE	2.17E-01	0.84	FALSE
M162T644_pos	162.0551	644	3	1.21E-02	1.15	FALSE	9.53E-01	1.00	FALSE	2.30E-11	1.40	FALSE	7.68E-02	0.85	FALSE
M162T128_pos	162.0762	128	3	5.69E-06	0.75	FALSE	1.27E-01	0.91	FALSE	7.41E-01	1.02	FALSE	3.22E-01	0.93	FALSE
M162T115_pos	162.1125	115	3	2.70E-03	0.84	FALSE	4.73E-01	1.04	FALSE	8.20E-04	1.19	FALSE	1.46E-01	1.18	FALSE
M162T165_pos	162.1126	165	3	5.58E-02	1.10	FALSE	2.39E-01	1.06	FALSE	1.01E-14	1.45	FALSE	8.12E-02	0.92	FALSE
M163T670_1_pos	163.0754	670	3	8.50E-02	0.88	FALSE	7.07E-01	0.97	FALSE	7.29E-02	1.13	FALSE	7.64E-01	1.06	FALSE
M163T905_pos	163.0754	905	3	6.54E-01	0.99	FALSE	2.83E-02	0.93	FALSE	5.48E-01	0.98	FALSE	9.68E-01	1.00	FALSE
M163T784_pos	163.0754	784	3	9.38E-02	1.18	FALSE	2.00E-02	0.78	FALSE	6.63E-01	0.96	FALSE	3.03E-01	1.21	FALSE
M163T1039_pos	163.1482	1039	3	2.30E-06	1.49	FALSE	1.37E-04	0.72	FALSE	1.01E-01	1.12	FALSE	3.54E-01	1.07	FALSE
M164T608_pos	164.0708	608	3	6.63E-01	1.02	FALSE	7.84E-01	1.02	FALSE	8.67E-05	1.21	FALSE	5.09E-01	1.09	FALSE
M164T154_pos	164.0917	154	3	9.27E-01	0.99	FALSE	1.90E-01	1.09	FALSE	5.29E-07	1.33	FALSE	5.47E-01	1.06	FALSE
M165T779_pos	165.0911	779	3	2.43E-01	1.06	FALSE	2.68E-02	1.13	FALSE	1.13E-02	1.12	FALSE	2.04E-01	0.84	FALSE
M165T717_pos	165.0911	717	3	1.80E-03	1.40	FALSE	9.50E-01	1.01	FALSE	9.94E-01	1.00	FALSE	3.95E-01	0.89	FALSE
M165T1038_2_pos	165.1275	1038	3	3.18E-01	1.16	FALSE	5.42E-01	0.91	FALSE	9.28E-01	0.99	FALSE	9.03E-01	1.04	FALSE
M165T860_pos	165.1275	860	3	2.48E-03	1.11	FALSE	8.01E-01	0.99	FALSE	9.46E-06	1.14	FALSE	1.37E-02	0.81	FALSE
M166T401_pos	166.0500	401	3	1.77E-16	1.37	FALSE	9.01E-01	1.00	FALSE	5.98E-17	1.32	FALSE	6.47E-01	0.97	FALSE
M166T744_pos	166.0863	744	3	1.34E-01	1.14	FALSE	3.60E-02	0.84	FALSE	4.93E-01	1.05	FALSE	8.06E-01	1.05	FALSE
M166T699_pos	166.1228	699	3	7.78E-01	0.97	FALSE	2.82E-04	1.41	FALSE	8.44E-05	1.37	FALSE	3.38E-01	0.86	FALSE
M167T1002_pos	167.0555	1002	3	1.41E-01	0.94	FALSE	8.74E-01	0.99	FALSE	2.56E-01	0.96	FALSE	6.87E-01	1.02	FALSE
M167T513_pos	167.0818	513	3	6.75E-09	1.35	FALSE	3.96E-01	1.05	FALSE	4.81E-15	1.45	FALSE	5.46E-02	0.83	FALSE
M167T911_pos	167.1065	911	3	2.52E-01	1.11	FALSE	4.77E-02	0.83	FALSE	1.57E-01	0.90	FALSE	9.39E-01	0.99	FALSE
M167T639_pos	167.1068	639	3	7.51E-12	1.46	FALSE	2.78E-01	1.06	FALSE	2.85E-01	1.05	FALSE	1.36E-02	0.80	FALSE
M168T785_pos	168.1021	785	3	5.70E-08	1.18	FALSE	7.71E-09	0.85	FALSE	4.29E-04	1.10	FALSE	3.65E-02	0.90	FALSE
M169T515_pos	169.0498	515	3	1.27E-04	1.20	FALSE	7.58E-01	0.98	FALSE	1.09E-14	1.42	FALSE	2.45E-01	0.88	FALSE
M169T968_pos	169.0858	968	3	3.80E-01	0.99	FALSE	1.44E-02	1.04	FALSE	2.47E-04	0.95	FALSE	9.23E-01	1.00	FALSE
M169T114_pos	169.0971	114	3	3.69E-01	0.93	FALSE	5.13E-01	0.95	FALSE	4.55E-06	1.42	FALSE	9.98E-01	1.00	FALSE
M169T660_pos	169.0859	660	3	1.64E-08	1.44	FALSE	5.66E-09	1.45	FALSE	1.84E-01	1.07	FALSE	6.38E-02	0.77	FALSE
M169T713_pos	169.1223	713	3	1.65E-07	1.39	FALSE	5.04E-01	1.04	FALSE	4.00E-01	0.96	FALSE	3.51E-01	0.97	FALSE
M169T783_pos	169.1223	783	3	1.12E-06	1.23	FALSE	2.94E-01	1.05	FALSE	2.77E-03	0.90	FALSE	3.68E-01	1.11	FALSE
M169T1054_pos	169.1223	1054	3	2.28E-12	1.35	FALSE	1.15E-10	0.77	FALSE	4.54E-01	1.03	FALSE	9.49E-01	1.01	FALSE
M169T834_pos	169.1224	834	3	4.63E-01	1.05	FALSE	6.27E-01	1.03	FALSE	3.50E-01	0.95	FALSE	5.89E-01	0.92	FALSE
M169T973_pos	169.1223	973	3	8.58E-01	0.98	FALSE	9.88E-01	1.00	FALSE	3.01E-01	0.91	FALSE	5.97E-02	0.80	FALSE
M170T491_pos	170.0813	491	3	2.52E-01	1.10	FALSE	4.61E-01	0.93	FALSE	9.15E-01	0.99	FALSE	3.16E-04	0.79	FALSE
M170T268_pos	170.0818	268	3	2.41E-02	1.19	FALSE	2.10E-01	1.10	FALSE	7.53E-07	1.40	FALSE	8.04E-01	1.04	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M170T160_pos	170.0923	160	3							HMDB0000001	1-Methylhistidine	C7H11N3O2	0.5
M170T346_pos	170.0924	346	3							HMDB0000001	1-Methylhistidine	C7H11N3O2	0.3
M171T604_pos	171.1016	604	3							HMDB0030471	1,4-Ipomeadiol	C9H14O3	0.4
M171T496_1_pos	171.1126	496	3							HMDB0015333	Levetiracetam	C8H14N2O2	1.0
M171T803_pos	171.1380	803	3							HMDB0004980	cis-4-Decenoic acid	C10H18O2	0.5
M171T405_pos	171.1493	405	3							HMDB0246938	o-3-methyl-1-pyrrolidin-1-YL-butar	C9H18N2O	0.5
M171T349_pos	171.1493	349	3							HMDB0246938	o-3-methyl-1-pyrrolidin-1-YL-butar	C9H18N2O	0.7
M171T1011_pos	171.1744	1011	3							HMDB0030941	Undecanal	C11H22O	0.5
M172T758_1_pos	172.0757	758	3							HMDB0243957	1-Naphthamide	C11H9NO	0.1
M172T461_pos	172.0969	461	3							HMDB0247190	)-2-Oxotetrahydrofuran-3-Yl]butar	C8H13NO3	0.5
M172T496_pos	172.0970	496	3							HMDB0247190	)-2-Oxotetrahydrofuran-3-Yl]butar	C8H13NO3	1.1
M172T599_pos	172.0969	599	3							HMDB0247190	)-2-Oxotetrahydrofuran-3-Yl]butar	C8H13NO3	0.7
M172T347_pos	172.1117	347	3							HMDB0015454	Rasagiline	C12H13N	2.2
M172T340_pos	172.1333	340	3							HMDB0005015	Gabapentin	C9H17NO2	0.6
M173T415_pos	173.0806	415	3							HMDB0000341	2-Octenedioic acid	C8H12O4	1.1
M173T659_1_pos	173.1174	659	3							HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	0.8
M173T339_pos	173.1649	339	3							HMDB0246342	mino-2,2,6,6-tetramethylpiperidin-	C9H20N2O	0.4
M174T622_pos	174.1125	622	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.5
M174T349_pos	174.1128	349	3							HMDB0000701	Hexanoylglycine	C8H15NO3	1.7
M174T420_pos	174.1490	420	3							HMDB0243489	eridinol, 1-hydroxy-2,2,6,6-tetram	C9H19NO2	0.7
M175T742_pos	175.0965	742	3							HMDB0000893	Suberic acid	C8H14O4	0.3
M175T1072_pos	175.0965	1072	3							HMDB0000893	Suberic acid	C8H14O4	0.3
M175T1016_pos	175.0966	1016	3							HMDB0000893	Suberic acid	C8H14O4	0.4
M175T923_pos	175.1117	923	3							HMDB0031622	6-Phenyl-3-hexen-2-one	C12H14O	0.0
M175T485_pos	175.1224	485	3							HMDB0004370	N-Methyltryptamine	C11H14N2	3.5
M175T1025_pos	175.1482	1025	3							HMDB0036683	a-Dihydro-1,4,4,7a-tetramethyl-4H	C13H18	0.2
M175T973_pos	175.1481	973	3							HMDB0036683	a-Dihydro-1,4,4,7a-tetramethyl-4H	C13H18	0.1
M175T874_pos	175.1482	874	3							HMDB0036683	a-Dihydro-1,4,4,7a-tetramethyl-4H	C13H18	0.2
M176T371_pos	176.1282	371	3							HMDB0254992	N-(2-Hydroxypropyl)valine	C8H17NO3	0.3
M176T274_pos	176.1282	274	3							HMDB0254992	N-(2-Hydroxypropyl)valine	C8H17NO3	0.7
M177T893_pos	177.1275	893	3							HMDB0031569	4-Methyl-1-phenyl-2-pentanone	C12H16O	0.5
M177T941_pos	177.1639	941	3							HMDB0035180	(6E,8E)-4,6,8-Megastigmatriene	C13H20	0.4
M177T1002_pos	177.1638	1002	3							HMDB0035180	(6E,8E)-4,6,8-Megastigmatriene	C13H20	0.4
M177T1053_pos	177.1638	1053	3							HMDB0035180	(6E,8E)-4,6,8-Megastigmatriene	C13H20	0.2
M178T442_pos	178.0532	442	3							HMDB0001015	N-Formyl-L-methionine	C6H11NO3S	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M170T160_pos	170.0923	160	3	2.59E-03	1.21	FALSE	1.47E-02	0.85	FALSE	1.82E-01	1.08	FALSE	2.32E-01	0.86	FALSE
M170T346_pos	170.0924	346	3	2.20E-03	1.24	FALSE	7.85E-01	1.02	FALSE	1.55E-01	1.09	FALSE	7.13E-01	0.93	FALSE
M171T604_pos	171.1016	604	3	3.89E-10	1.30	FALSE	3.22E-05	1.19	FALSE	1.58E-05	0.86	FALSE	7.07E-01	0.98	FALSE
M171T496_1_pos	171.1126	496	3	6.40E-01	0.97	FALSE	4.27E-01	1.05	FALSE	5.42E-01	1.03	FALSE	3.16E-01	0.90	FALSE
M171T803_pos	171.1380	803	3	6.66E-03	1.10	FALSE	1.04E-03	1.13	FALSE	4.40E-04	1.12	FALSE	5.58E-01	0.97	FALSE
M171T405_pos	171.1493	405	3	9.49E-01	1.00	FALSE	2.67E-01	1.08	FALSE	2.38E-01	1.07	FALSE	1.31E-01	0.73	FALSE
M171T349_pos	171.1493	349	3	3.35E-09	1.46	FALSE	1.10E-01	0.90	FALSE	5.01E-01	1.04	FALSE	3.64E-01	0.95	FALSE
M171T1011_pos	171.1744	1011	3	2.52E-01	0.98	FALSE	8.36E-01	1.00	FALSE	2.09E-06	0.94	FALSE	6.60E-05	1.19	FALSE
M172T758_1_pos	172.0757	758	3	5.92E-05	1.20	FALSE	8.35E-01	0.99	FALSE	1.05E-03	1.14	FALSE	1.36E-01	0.92	FALSE
M172T461_pos	172.0969	461	3	4.82E-19	1.36	FALSE	3.12E-01	1.03	FALSE	8.13E-16	1.26	FALSE	1.69E-02	0.94	FALSE
M172T496_pos	172.0970	496	3	6.65E-14	1.32	FALSE	9.78E-01	1.00	FALSE	1.04E-20	1.37	FALSE	4.21E-03	0.88	FALSE
M172T599_pos	172.0969	599	3	6.29E-10	1.29	FALSE	1.72E-01	0.94	FALSE	5.50E-03	1.10	FALSE	2.05E-02	0.86	FALSE
M172T347_pos	172.1117	347	3	1.27E-03	0.71	FALSE	9.96E-01	1.00	FALSE	2.88E-02	1.22	FALSE	4.78E-01	0.91	FALSE
M172T340_pos	172.1333	340	3	8.67E-01	1.01	FALSE	4.08E-01	1.04	FALSE	1.18E-05	1.22	FALSE	1.78E-01	1.06	FALSE
M173T415_pos	173.0806	415	3	7.87E-01	0.97	FALSE	3.31E-01	1.11	FALSE	6.73E-01	1.04	FALSE	3.72E-01	0.65	FALSE
M173T659_1_pos	173.1174	659	3	2.30E-22	1.45	FALSE	1.16E-01	1.06	FALSE	1.64E-10	0.82	FALSE	2.67E-01	0.95	FALSE
M173T339_pos	173.1649	339	3	5.77E-07	1.45	FALSE	6.73E-02	0.87	FALSE	3.81E-02	1.14	FALSE	8.68E-01	1.01	FALSE
M174T622_pos	174.1125	622	3	5.86E-01	0.93	FALSE	2.60E-01	0.83	FALSE	3.84E-01	1.11	FALSE	6.72E-01	0.87	FALSE
M174T349_pos	174.1128	349	3	1.01E-01	0.91	FALSE	5.73E-01	0.97	FALSE	5.25E-07	1.30	FALSE	3.23E-01	0.96	FALSE
M174T420_pos	174.1490	420	3	1.01E-04	1.19	FALSE	6.09E-01	0.98	FALSE	2.66E-09	1.27	FALSE	2.24E-02	0.81	FALSE
M175T742_pos	175.0965	742	3	3.29E-12	1.37	FALSE	7.27E-01	0.98	FALSE	1.90E-18	0.70	FALSE	5.54E-02	0.84	FALSE
M175T1072_pos	175.0965	1072	3	1.11E-02	1.14	FALSE	7.08E-02	0.91	FALSE	4.49E-01	0.97	FALSE	2.80E-01	0.86	FALSE
M175T1016_pos	175.0966	1016	3	7.20E-01	1.02	FALSE	9.37E-01	1.01	FALSE	3.88E-01	0.96	FALSE	6.10E-01	1.09	FALSE
M175T923_pos	175.1117	923	3	1.38E-07	0.70	FALSE	4.63E-01	1.05	FALSE	1.09E-01	1.10	FALSE	5.93E-01	1.04	FALSE
M175T485_pos	175.1224	485	3	3.01E-01	0.91	FALSE	4.12E-01	1.08	FALSE	6.20E-06	1.46	FALSE	2.93E-01	0.87	FALSE
M175T1025_pos	175.1482	1025	3	2.10E-01	0.91	FALSE	4.20E-01	1.07	FALSE	4.49E-01	1.05	FALSE	2.84E-01	1.18	FALSE
M175T973_pos	175.1481	973	3	3.80E-01	0.93	FALSE	1.72E-02	0.80	FALSE	4.88E-01	0.95	FALSE	7.51E-01	1.08	FALSE
M175T874_pos	175.1482	874	3	1.99E-03	1.15	FALSE	6.56E-02	0.92	FALSE	2.26E-05	0.85	FALSE	9.17E-01	1.01	FALSE
M176T371_pos	176.1282	371	3	7.37E-01	1.02	FALSE	4.67E-01	1.04	FALSE	1.27E-12	1.36	FALSE	2.17E-02	0.92	FALSE
M176T274_pos	176.1282	274	3	1.37E-01	1.13	FALSE	3.65E-01	0.93	FALSE	1.39E-04	1.32	FALSE	5.87E-01	0.92	FALSE
M177T893_pos	177.1275	893	3	2.90E-01	0.95	FALSE	3.06E-01	1.06	FALSE	4.48E-06	1.23	FALSE	7.67E-01	0.96	FALSE
M177T941_pos	177.1639	941	3	3.99E-02	1.11	FALSE	2.44E-01	0.94	FALSE	7.06E-03	1.13	FALSE	8.63E-01	0.97	FALSE
M177T1002_pos	177.1638	1002	3	3.65E-01	1.02	FALSE	2.85E-02	0.96	FALSE	1.96E-01	0.98	FALSE	7.12E-01	0.96	FALSE
M177T1053_pos	177.1638	1053	3	5.30E-04	1.33	FALSE	1.78E-04	0.72	FALSE	9.97E-02	1.12	FALSE	7.62E-01	1.05	FALSE
M178T442_pos	178.0532	442	3	8.45E-12	1.25	FALSE	3.23E-02	1.07	FALSE	2.18E-17	1.28	FALSE	9.98E-01	1.00	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M178T535_pos	178.0501	535	3						Alkaloids	HMDB0040612	4-Acetyl-2(3H)-benzoxazolone	C9H7NO3	1.1
M178T533_pos	178.0864	533	3							HMDB0001855	5-Hydroxytryptophol	C10H11NO2	1.0
M179T890_pos	179.1067	890	3							HMDB0002043	5-Phenylvaleric acid	C11H14O2	0.4
M179T1038_pos	179.1431	1038	3							HMDB0014956	Propofol	C12H18O	0.4
M180T553_pos	180.0657	553	3							HMDB0000714	Hippuric acid	C9H9NO3	1.2
M180T365_pos	180.0658	365	3							HMDB0000714	Hippuric acid	C9H9NO3	1.4
M180T385_pos	180.1021	385	3							HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	1.0
M180T846_pos	180.1020	846	3							HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	0.6
M180T947_pos	180.1020	947	3							HMDB0001189	2(N)-Methyl-norsalsolinol	C10H13NO2	0.5
M181T481_pos	181.0720	481	3							HMDB0001860	Paraxanthine	C7H8N4O2	0.1
M181T414_pos	181.0723	414	3							HMDB0001860	Paraxanthine	C7H8N4O2	1.4
M181T759_pos	181.0712	759	3							HMDB0000122	D-Glucose	C6H12O6	2.9
M181T652_pos	181.0860	652	3							HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	0.6
M181T565_pos	181.0859	565	3							HMDB0062773	ydroxy-(2E,8E)-decadien-4-ynoic /	C10H12O3	0.1
M181T1014_pos	181.0856	1014	3							HMDB0062773	ydroxy-(2E,8E)-decadien-4-ynoic /	C10H12O3	1.6
M181T858_pos	181.1224	858	3							HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.3
M181T767_pos	181.1224	767	3							HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.4
M182T582_pos	182.0651	582	3							HMDB0256252	Pentaerythritol mononitrate	C5H11NO6	4.3
M183T475_pos	183.0767	475	3							HMDB0246019	3,4-Dephostatin, Ethyl-	C8H10N2O3	1.6
M183T645_pos	183.1018	645	3							HMDB0029456	Amyl 2-furoate	C10H14O3	1.4
M183T394_pos	183.1130	394	3							HMDB0244796	opyranosyloxy)-4-methyl-2H-1-be	C9H14N2O2	0.9
M183T861_pos	183.1379	861	3							HMDB0030006	Tetramethyl-1,6-dioxaspiro[4.4]no	C11H18O2	0.2
M183T785_pos	183.1380	785	3							HMDB0030006	Tetramethyl-1,6-dioxaspiro[4.4]no	C11H18O2	0.4
M183T1034_pos	183.1380	1034	3							HMDB0030006	Tetramethyl-1,6-dioxaspiro[4.4]no	C11H18O2	0.2
M183T1012_pos	183.1744	1012	3							HMDB0031020	2-Dodecenal	C12H22O	0.4
M184T555_pos	184.0606	555	3							HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.8
M184T567_pos	184.0969	567	3							HMDB0000068	Epinephrine	C9H13NO3	0.7
M184T481_pos	184.0969	481	3							HMDB0000068	Epinephrine	C9H13NO3	0.6
M184T956_pos	184.1121	956	3							HMDB0248313	Benzhydrylamine	C13H13N	0.3
M184T1017_1_pos	184.1121	1017	3							HMDB0248313	Benzhydrylamine	C13H13N	0.1
M184T684_pos	184.1333	684	3							HMDB0015239	Methyprylon	C10H17NO2	0.8
M184T360_pos	184.1334	360	3							HMDB0015239	Methyprylon	C10H17NO2	0.8
M185T462_pos	185.0810	462	3							HMDB0001490	Vanylglycol	C9H12O4	0.7
M185T382_2_pos	185.0922	382	3							HMDB0248870	Barbital	C8H12N2O3	0.5
M185T511_pos	185.0922	511	3							HMDB0248870	Barbital	C8H12N2O3	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M178T535_pos	178.0501	535	3	1.02E-02	1.21	FALSE	7.23E-01	0.97	FALSE	4.29E-05	1.31	FALSE	6.58E-01	0.96	FALSE
M178T533_pos	178.0864	533	3	6.64E-04	0.71	FALSE	5.63E-01	0.94	FALSE	8.06E-01	0.98	FALSE	9.70E-01	1.00	FALSE
M179T890_pos	179.1067	890	3	8.79E-05	1.07	FALSE	5.72E-02	1.03	FALSE	1.29E-11	0.90	FALSE	7.57E-01	0.99	FALSE
M179T1038_pos	179.1431	1038	3	1.40E-01	1.22	FALSE	2.85E-01	0.86	FALSE	3.53E-01	1.12	FALSE	3.29E-01	1.07	FALSE
M180T553_pos	180.0657	553	3	1.24E-02	1.46	FALSE	4.64E-01	0.90	FALSE	5.00E-02	1.29	FALSE	3.16E-01	0.84	FALSE
M180T365_pos	180.0658	365	3	3.15E-03	0.73	FALSE	3.14E-01	1.12	FALSE	3.90E-03	1.31	FALSE	9.70E-01	1.01	FALSE
M180T385_pos	180.1021	385	3	2.28E-12	1.39	FALSE	1.18E-05	1.22	FALSE	1.10E-11	1.32	FALSE	1.27E-01	1.08	FALSE
M180T846_pos	180.1020	846	3	6.22E-07	0.69	FALSE	7.88E-01	1.02	FALSE	2.09E-03	1.21	FALSE	5.62E-01	1.11	FALSE
M180T947_pos	180.1020	947	3	8.12E-07	0.75	FALSE	4.15E-04	1.23	FALSE	9.77E-02	1.08	FALSE	6.97E-01	1.04	FALSE
M181T481_pos	181.0720	481	3	3.73E-03	1.44	FALSE	1.21E-02	0.69	FALSE	4.28E-01	1.09	FALSE	9.21E-02	0.79	FALSE
M181T414_pos	181.0723	414	3	2.26E-02	1.23	FALSE	9.50E-01	0.99	FALSE	6.89E-02	1.15	FALSE	1.51E-01	0.88	FALSE
M181T759_pos	181.0712	759	3	3.86E-04	1.23	FALSE	1.39E-03	1.21	FALSE	4.78E-01	0.97	FALSE	6.80E-02	1.31	FALSE
M181T652_pos	181.0860	652	3	1.18E-05	1.43	FALSE	9.83E-01	1.00	FALSE	7.93E-01	0.98	FALSE	3.45E-01	0.83	FALSE
M181T565_pos	181.0859	565	3	7.13E-02	1.12	FALSE	6.69E-01	1.03	FALSE	2.18E-10	1.46	FALSE	1.65E-01	0.85	FALSE
M181T1014_pos	181.0856	1014	3	8.40E-03	0.86	FALSE	4.06E-01	1.05	FALSE	1.16E-01	1.08	FALSE	7.94E-01	1.02	FALSE
M181T858_pos	181.1224	858	3	5.92E-05	1.23	FALSE	1.29E-03	1.19	FALSE	9.05E-08	1.28	FALSE	2.33E-03	0.76	FALSE
M181T767_pos	181.1224	767	3	1.63E-04	1.22	FALSE	9.69E-05	1.23	FALSE	6.33E-02	0.92	FALSE	2.53E-01	0.81	FALSE
M182T582_pos	182.0651	582	3	2.58E-03	0.80	FALSE	9.18E-01	0.99	FALSE	2.21E-04	1.28	FALSE	8.42E-01	1.02	FALSE
M183T475_pos	183.0767	475	3	3.10E-05	1.40	FALSE	7.23E-03	1.25	FALSE	8.55E-07	1.42	FALSE	5.89E-01	0.94	FALSE
M183T645_pos	183.1018	645	3	2.92E-11	1.30	FALSE	2.23E-06	1.20	FALSE	1.65E-12	1.28	FALSE	7.49E-01	1.02	FALSE
M183T394_pos	183.1130	394	3	1.99E-02	1.12	FALSE	4.61E-01	1.04	FALSE	7.77E-16	1.44	FALSE	1.30E-02	0.85	FALSE
M183T861_pos	183.1379	861	3	3.03E-01	1.16	FALSE	3.79E-01	0.88	FALSE	9.98E-01	1.00	FALSE	6.86E-02	0.83	FALSE
M183T785_pos	183.1380	785	3	4.64E-01	0.94	FALSE	8.71E-01	0.98	FALSE	3.42E-01	1.08	FALSE	9.31E-01	0.98	FALSE
M183T1034_pos	183.1380	1034	3	8.31E-01	1.03	FALSE	5.74E-01	0.93	FALSE	4.72E-01	0.93	FALSE	9.77E-01	1.00	FALSE
M183T1012_pos	183.1744	1012	3	1.55E-01	2.38	FALSE	8.13E-01	0.85	FALSE	1.08E-01	2.35	FALSE	7.37E-01	0.84	FALSE
M184T555_pos	184.0606	555	3	3.26E-04	1.16	FALSE	6.67E-05	0.84	FALSE	1.07E-09	1.25	FALSE	9.33E-01	1.01	FALSE
M184T567_pos	184.0969	567	3	3.83E-21	1.49	FALSE	3.66E-01	0.97	FALSE	9.16E-07	1.18	FALSE	8.94E-02	0.89	FALSE
M184T481_pos	184.0969	481	3	3.74E-10	1.24	FALSE	4.65E-05	1.15	FALSE	7.15E-15	1.28	FALSE	5.92E-01	0.98	FALSE
M184T956_pos	184.1121	956	3	4.27E-06	0.93	FALSE	1.88E-01	0.98	FALSE	3.85E-18	0.88	FALSE	6.57E-01	0.98	FALSE
M184T1017_1_pos	184.1121	1017	3	3.86E-01	1.05	FALSE	3.36E-01	1.06	FALSE	2.26E-01	0.94	FALSE	5.33E-01	0.96	FALSE
M184T684_pos	184.1333	684	3	5.00E-05	1.47	FALSE	1.48E-01	1.15	FALSE	6.29E-01	0.96	FALSE	3.64E-02	0.82	FALSE
M184T360_pos	184.1334	360	3	6.80E-03	1.13	FALSE	8.29E-01	0.99	FALSE	3.51E-05	1.17	FALSE	9.13E-01	1.01	FALSE
M185T462_pos	185.0810	462	3	9.47E-01	1.01	FALSE	7.48E-01	0.97	FALSE	6.06E-01	0.97	FALSE	1.38E-01	0.62	FALSE
M185T382_2_pos	185.0922	382	3	3.90E-07	1.41	FALSE	1.16E-04	0.75	FALSE	1.07E-07	1.37	FALSE	2.28E-01	0.88	FALSE
M185T511_pos	185.0922	511	3	1.23E-01	1.08	FALSE	2.26E-01	1.07	FALSE	5.11E-15	1.46	FALSE	4.20E-02	0.85	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M185T998_pos	185.1169	998	3						Fatty acids	HMDB0036117	(-)-3-Thujene	C10H16O3	1.8
M185T807_pos	185.1173	807	3							HMDB0036117	(-)-3-Thujene	C10H16O3	0.2
M185T490_pos	185.1286	490	3							HMDB0061384	(3-acetamidopropyl)pyrrolidin-2-o	C9H16N2O2	0.5
M185T428_pos	185.1286	428	3						Amino acids and Peptides	HMDB0061384	(3-acetamidopropyl)pyrrolidin-2-o	C9H16N2O2	0.6
M185T882_pos	185.1537	882	3						Fatty acids	HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	0.3
M185T917_pos	185.1901	917	3							HMDB0031019	2-Dodecanone	C12H24O	0.5
M186T635_pos	186.1127	635	3							HMDB0006348	Pseudoecgonine	C9H15NO3	1.0
M186T379_pos	186.1490	379	3							HMDB0243943	1-Methylpiperidin-4-yl butanoate	C10H19NO2	0.7
M186T493_pos	186.1489	493	3							HMDB0243943	1-Methylpiperidin-4-yl butanoate	C10H19NO2	0.5
M186T772_pos	186.1489	772	3							HMDB0243943	1-Methylpiperidin-4-yl butanoate	C10H19NO2	0.5
M187T703_pos	187.0277	703	3							HMDB0303692	Calcium propionate	C6H10CaO4	0.5
M187T942_pos	187.1484	942	3							HMDB0035759	thyl-5,6-dihydro-1,4-dimethylazul	C14H18	1.3
M187T339_pos	187.1806	339	3							HMDB0247651	oxyethyl)piperidin-3-YL]-N-methyl	C10H22N2O	0.8
M188T578_2_pos	188.0707	578	3						Alkaloids	HMDB0000734	Indoleacrylic acid	C11H9NO2	0.7
M189T703_pos	189.0209	703	3							HMDB0245722	2-Chlorobenzylidenemalononitrile	C10H5ClN2	2.6
M189T478_pos	189.0407	478	3							HMDB0032289	Furfuryl propyl disulfide	C8H12OS2	2.6
M189T335_pos	189.0872	335	3							HMDB0006029	N-Acetylglutamine	C7H12N2O4	1.2
M189T973_pos	189.1639	973	3							HMDB0251132	Congressane	C14H20	0.5
M189T1026_pos	189.1638	1026	3							HMDB0251132	Congressane	C14H20	0.4
M190T163_pos	190.0171	163	3							HMDB0004823	Lanthionine ketimine	C6H7NO4S	1.1
M190T569_1_pos	190.1075	569	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.7
M190T461_pos	190.1075	461	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.6
M191T670_pos	191.1068	670	3							HMDB0030905	(4-Methoxyphenyl)-1-penten-3-or	C12H14O2	0.5
M191T957_pos	191.1795	957	3						Terpenoids	HMDB0013820	2-Methyl-2-phenyl-undecane	C14H22	0.4
M191T1054_pos	191.1795	1054	3							HMDB0013820	2-Methyl-2-phenyl-undecane	C14H22	0.3
M193T1035_pos	193.0472	1035	3							HMDB0243914	2-(Trifluoromethoxy)anisole	C8H7F3O2	0.8
M193T866_pos	193.1223	866	3							HMDB0031571	Methyl-1-phenyl-2-propanyl aceta	C12H16O2	0.2
M193T1038_pos	193.1587	1038	3							HMDB0029820	2,6-Diisopropyl-3-methylphenol	C13H20O	0.0
M193T874_pos	193.1588	874	3							HMDB0029820	2,6-Diisopropyl-3-methylphenol	C13H20O	0.5
M194T657_pos	194.0816	657	3							HMDB0000821	Phenylacetylglycine	C10H11NO3	2.4
M194T683_pos	194.1176	683	3						Alkaloids	HMDB0003626	(R)-N-Methylsalsolinol	C11H15NO2	0.3
M194T593_pos	194.1177	593	3							HMDB0003626	(R)-N-Methylsalsolinol	C11H15NO2	0.6
M195T670_pos	195.0652	670	3							HMDB0000954	Ferulic acid	C10H10O4	0.0
M195T772_pos	195.1016	772	3							HMDB0031517	)-3-Hydroxy-5-phenylpentanoic ac	C11H14O3	0.0
M195T453_pos	195.1135	453	3							HMDB0041440	Laccarin	C10H14N2O2	3.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M185T998_pos	185.1169	998	3	6.61E-01	0.99	FALSE	9.08E-03	1.08	FALSE	2.69E-02	0.94	FALSE	9.73E-01	1.00	FALSE
M185T807_pos	185.1173	807	3	9.87E-01	1.00	FALSE	2.34E-02	1.09	FALSE	1.18E-17	1.33	FALSE	1.33E-03	0.78	FALSE
M185T490_pos	185.1286	490	3	4.92E-15	1.30	FALSE	9.18E-01	1.00	FALSE	9.01E-01	1.00	FALSE	3.04E-02	0.89	FALSE
M185T428_pos	185.1286	428	3	3.12E-01	1.10	FALSE	7.55E-01	1.03	FALSE	5.22E-05	0.70	FALSE	3.61E-02	1.46	FALSE
M185T882_pos	185.1537	882	3	5.59E-02	0.95	FALSE	4.10E-02	1.07	FALSE	4.47E-15	1.24	FALSE	8.81E-01	1.01	FALSE
M185T917_pos	185.1901	917	3	2.80E-01	0.91	FALSE	3.66E-01	1.08	FALSE	8.74E-01	1.01	FALSE	5.80E-02	2.53	FALSE
M186T635_pos	186.1127	635	3	4.38E-06	1.26	FALSE	4.98E-03	0.85	FALSE	6.85E-01	1.02	FALSE	3.89E-02	1.42	FALSE
M186T379_pos	186.1490	379	3	2.13E-05	1.18	FALSE	4.80E-01	1.03	FALSE	5.61E-21	1.44	FALSE	8.66E-02	0.94	FALSE
M186T493_pos	186.1489	493	3	9.53E-02	0.91	FALSE	6.68E-01	1.03	FALSE	4.77E-04	1.20	FALSE	3.07E-01	0.88	FALSE
M186T772_pos	186.1489	772	3	1.50E-09	1.21	FALSE	8.39E-01	1.01	FALSE	1.76E-12	0.82	FALSE	4.67E-01	0.95	FALSE
M187T703_pos	187.0277	703	3	8.97E-01	0.99	FALSE	7.91E-01	1.01	FALSE	5.88E-02	0.92	FALSE	4.51E-01	0.92	FALSE
M187T942_pos	187.1484	942	3	1.80E-01	1.05	FALSE	3.52E-01	0.97	FALSE	1.78E-15	1.31	FALSE	2.87E-01	0.93	FALSE
M187T339_pos	187.1806	339	3	1.55E-08	1.47	FALSE	4.02E-01	0.95	FALSE	4.74E-04	1.22	FALSE	8.82E-01	1.02	FALSE
M188T578_2_pos	188.0707	578	3	6.96E-05	0.75	FALSE	8.79E-01	1.01	FALSE	4.82E-07	1.38	FALSE	9.92E-01	1.00	FALSE
M189T703_pos	189.0209	703	3	4.00E-01	0.96	FALSE	3.44E-01	1.05	FALSE	6.32E-02	0.92	FALSE	8.58E-01	1.02	FALSE
M189T478_pos	189.0407	478	3	4.31E-07	1.21	FALSE	7.53E-01	1.01	FALSE	4.65E-26	1.47	FALSE	4.09E-01	0.97	FALSE
M189T335_pos	189.0872	335	3	8.69E-01	0.99	FALSE	5.09E-01	0.95	FALSE	8.75E-02	1.11	FALSE	4.78E-01	0.87	FALSE
M189T973_pos	189.1639	973	3	2.06E-03	1.50	FALSE	2.95E-02	0.73	FALSE	1.01E-02	1.34	FALSE	4.74E-01	1.09	FALSE
M189T1026_pos	189.1638	1026	3	1.52E-07	1.43	FALSE	4.76E-02	0.88	FALSE	6.14E-01	0.97	FALSE	2.79E-01	1.12	FALSE
M190T163_pos	190.0171	163	3	1.69E-03	1.25	FALSE	4.96E-03	1.22	FALSE	6.29E-07	1.36	FALSE	3.15E-02	1.26	FALSE
M190T569_1_pos	190.1075	569	3	3.86E-01	0.86	FALSE	1.30E-01	1.35	FALSE	4.35E-02	1.36	FALSE	4.52E-01	1.36	FALSE
M190T461_pos	190.1075	461	3	4.57E-25	1.45	FALSE	4.05E-01	1.03	FALSE	3.76E-10	1.19	FALSE	2.51E-01	0.96	FALSE
M191T670_pos	191.1068	670	3	2.11E-02	1.07	FALSE	1.90E-01	1.04	FALSE	2.55E-29	1.41	FALSE	2.45E-02	0.94	FALSE
M191T957_pos	191.1795	957	3	1.00E-02	0.83	FALSE	7.35E-01	1.03	FALSE	4.73E-02	0.88	FALSE	4.10E-01	1.10	FALSE
M191T1054_pos	191.1795	1054	3	8.01E-01	0.97	FALSE	7.10E-01	0.95	FALSE	6.27E-01	0.94	FALSE	9.23E-01	0.99	FALSE
M193T1035_pos	193.0472	1035	3	6.65E-03	0.89	FALSE	3.62E-02	1.09	FALSE	5.12E-02	0.93	FALSE	9.15E-01	1.01	FALSE
M193T866_pos	193.1223	866	3	1.54E-02	0.92	FALSE	8.97E-02	1.06	FALSE	2.05E-12	1.25	FALSE	1.23E-02	0.82	FALSE
M193T1038_pos	193.1587	1038	3	4.85E-03	1.35	FALSE	6.70E-01	0.95	FALSE	7.27E-01	0.97	FALSE	5.86E-01	1.17	FALSE
M193T874_pos	193.1588	874	3	3.99E-02	1.08	FALSE	6.06E-02	0.93	FALSE	1.04E-04	0.88	FALSE	6.01E-02	0.82	FALSE
M194T657_pos	194.0816	657	3	2.18E-02	1.26	FALSE	5.13E-02	0.82	FALSE	1.90E-01	0.89	FALSE	1.90E-01	0.87	FALSE
M194T683_pos	194.1176	683	3	8.00E-02	1.11	FALSE	3.20E-10	1.45	FALSE	4.78E-06	1.26	FALSE	9.60E-01	1.01	FALSE
M194T593_pos	194.1177	593	3	2.45E-01	1.04	FALSE	4.57E-04	1.14	FALSE	3.31E-03	1.10	FALSE	2.25E-01	1.12	FALSE
M195T670_pos	195.0652	670	3	8.14E-02	1.26	FALSE	3.96E-02	1.33	FALSE	2.33E-01	0.87	FALSE	7.04E-02	0.30	FALSE
M195T772_pos	195.1016	772	3	1.40E-07	1.32	FALSE	2.13E-01	1.07	FALSE	5.77E-02	1.09	FALSE	9.13E-02	0.81	FALSE
M195T453_pos	195.1135	453	3	1.36E-01	0.81	FALSE	4.12E-01	1.12	FALSE	4.82E-02	1.27	FALSE	3.17E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M195T473_pos	195.1227	473	3							HMDB0094708	Tetraethylene glycol	C8H18O5	0.0
M195T893_pos	195.1380	893	3							HMDB0014018	4-Hydroxypropofol	C12H18O2	0.0
M195T986_pos	195.1363	986	3							HMDB0303292	Sodium caprate	C10H19NaO2	4.0
M195T1025_pos	195.1379	1025	3							HMDB0014018	4-Hydroxypropofol	C12H18O2	0.4
M196T581_pos	196.0607	581	3							HMDB0000840	Salicyluric acid	C9H9NO4	1.2
M196T523_pos	196.0965	523	3							HMDB0014903	Metyrosine	C10H13NO3	1.5
M196T681_pos	196.0969	681	3							HMDB0014903	Metyrosine	C10H13NO3	0.6
M197T430_pos	197.0923	430	3							HMDB0032852	Ethylamino)-4,5-dihydroxybenzam	C9H12N2O3	1.0
M197T803_pos	197.1172	803	3							HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	0.1
M197T659_pos	197.1174	659	3							HMDB0036226	2,6-Dimethoxy-4-propylphenol	C11H16O3	0.7
M197T418_pos	197.1286	418	3							HMDB0029741	propyl-3,5-dimethoxy-6-methylpyr	C10H16N2O2	0.6
M197T925_pos	197.1537	925	3							HMDB0030867	ihydro-5-(2-octenyl)-2(3H)-furanor	C12H20O2	0.6
M197T1033_pos	197.1537	1033	3							HMDB0030867	ihydro-5-(2-octenyl)-2(3H)-furanor	C12H20O2	0.4
M197T769_pos	197.1537	769	3							HMDB0030867	ihydro-5-(2-octenyl)-2(3H)-furanor	C12H20O2	0.5
M197T1034_pos	197.1900	1034	3							HMDB0032247	(Z)-4-Dodecenal	C13H24O	0.2
M197T987_pos	197.1901	987	3							HMDB0032247	(Z)-4-Dodecenal	C13H24O	0.5
M198T110_pos	198.0528	110	3							HMDB0304531	vanillyl mandelate	C9H9O5	0.0
M198T517_pos	198.0586	517	3							HMDB0257425	S-Phenyl-L-cysteine	C9H11NO2S	1.4
M198T540_pos	198.0871	540	3							HMDB0032055	N-Acetylhistidine	C8H11N3O3	1.1
M198T142_pos	198.0871	142	3							HMDB0032055	N-Acetylhistidine	C8H11N3O3	1.1
M198T475_pos	198.0875	475	3							HMDB0032055	N-Acetylhistidine	C8H11N3O3	1.1
M198T529_pos	198.1126	529	3							HMDB0004063	Metanephrine	C10H15NO3	0.7
M198T603_pos	198.1127	603	3							HMDB0004063	Metanephrine	C10H15NO3	1.1
M198T698_pos	198.1128	698	3							HMDB0004063	Metanephrine	C10H15NO3	1.8
M198T368_pos	198.1599	368	3							HMDB0249802	Centperazine	C10H19N3O	0.7
M199T373_pos	199.0828	373	3							HMDB0004400	Acetylamino-6-amino-3-methylura	C7H10N4O3	1.3
M199T371_pos	199.1124	371	3							HMDB0032078	Dibenzyl ether	C14H14O	3.5
M199T689_pos	199.1078	689	3							HMDB0014606	Metharbital	C9H14N2O3	0.5
M199T803_pos	199.1328	803	3							HMDB0253742	-Methylcyclohexyl)-4-oxobutanoic	C11H18O3	0.3
M199T883_pos	199.1694	883	3						Fatty acids	HMDB0000529	5Z-Dodecenoic acid	C12H22O2	0.5
M199T1029_pos	199.1693	1029	3							HMDB0000529	5Z-Dodecenoic acid	C12H22O2	0.5
M199T1039_pos	199.2057	1039	3							HMDB0030928	Tridecanal	C13H26O	0.5
M200T512_pos	200.0919	512	3							HMDB0035177	ahydro-6-hydroxy-7-(hydroxymeth	C9H13NO4	0.7
M200T462_pos	200.0919	462	3							HMDB0035177	ahydro-6-hydroxy-7-(hydroxymeth	C9H13NO4	0.7
M200T342_pos	200.1031	342	3							HMDB0060477	na-Glutamyl-beta-aminopropionor	C8H13N3O3	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M195T473_pos	195.1227	473	3	7.74E-19	1.44	FALSE	1.47E-04	0.87	FALSE	1.54E-07	0.84	FALSE	8.43E-01	0.97	FALSE
M195T893_pos	195.1380	893	3	3.03E-01	0.93	FALSE	9.39E-01	0.99	FALSE	8.78E-02	1.11	FALSE	2.88E-01	1.15	FALSE
M195T986_pos	195.1363	986	3	2.86E-02	1.17	FALSE	8.87E-02	0.88	FALSE	7.08E-01	1.02	FALSE	1.11E-01	0.80	FALSE
M195T1025_pos	195.1379	1025	3	8.81E-07	1.34	FALSE	3.11E-02	0.88	FALSE	3.94E-01	1.04	FALSE	9.70E-01	1.01	FALSE
M196T581_pos	196.0607	581	3	9.00E-01	1.01	FALSE	8.05E-01	1.03	FALSE	3.27E-01	1.09	FALSE	5.12E-01	0.85	FALSE
M196T523_pos	196.0965	523	3	1.04E-08	1.35	FALSE	7.27E-02	1.10	FALSE	5.87E-06	1.22	FALSE	6.04E-01	1.06	FALSE
M196T681_pos	196.0969	681	3	1.36E-11	1.39	FALSE	2.72E-04	0.83	FALSE	2.77E-03	1.13	FALSE	1.80E-01	0.88	FALSE
M197T430_pos	197.0923	430	3	4.62E-13	1.45	FALSE	2.74E-01	1.06	FALSE	7.78E-01	1.01	FALSE	1.08E-01	0.81	FALSE
M197T803_pos	197.1172	803	3	5.67E-01	0.96	FALSE	9.09E-01	0.99	FALSE	5.88E-02	0.90	FALSE	7.77E-01	0.95	FALSE
M197T659_pos	197.1174	659	3	8.16E-10	1.28	FALSE	2.42E-01	1.05	FALSE	6.85E-11	1.26	FALSE	7.62E-01	0.98	FALSE
M197T418_pos	197.1286	418	3	2.89E-01	1.06	FALSE	1.21E-02	1.15	FALSE	9.34E-11	1.39	FALSE	1.76E-02	0.83	FALSE
M197T925_pos	197.1537	925	3	8.79E-02	1.11	FALSE	6.14E-01	0.97	FALSE	5.52E-02	0.90	FALSE	9.69E-01	1.01	FALSE
M197T1033_pos	197.1537	1033	3	5.10E-01	1.07	FALSE	6.59E-01	0.95	FALSE	6.50E-01	1.04	FALSE	8.35E-01	0.98	FALSE
M197T769_pos	197.1537	769	3	7.01E-18	1.32	FALSE	4.75E-01	1.02	FALSE	2.44E-01	0.97	FALSE	2.35E-01	0.96	FALSE
M197T1034_pos	197.1900	1034	3	5.92E-06	1.37	FALSE	6.07E-03	0.83	FALSE	9.00E-02	1.11	FALSE	3.79E-01	1.10	FALSE
M197T987_pos	197.1901	987	3	7.21E-01	1.03	FALSE	6.04E-01	1.05	FALSE	8.21E-01	1.02	FALSE	4.83E-01	0.94	FALSE
M198T110_pos	198.0528	110	3	3.33E-01	0.92	FALSE	4.39E-01	0.94	FALSE	7.15E-03	1.22	FALSE	5.82E-01	1.08	FALSE
M198T517_pos	198.0586	517	3	3.09E-02	1.14	FALSE	1.24E-01	1.10	FALSE	1.29E-11	1.46	FALSE	1.44E-02	0.90	FALSE
M198T540_pos	198.0871	540	3	1.03E-03	1.24	FALSE	4.95E-01	0.95	FALSE	9.90E-08	1.37	FALSE	1.35E-03	0.79	FALSE
M198T142_pos	198.0871	142	3	4.91E-02	0.90	FALSE	9.92E-01	1.00	FALSE	2.85E-11	1.41	FALSE	2.54E-01	1.15	FALSE
M198T475_pos	198.0875	475	3	6.56E-04	1.23	FALSE	4.68E-01	0.96	FALSE	2.83E-06	1.29	FALSE	2.56E-01	0.85	FALSE
M198T529_pos	198.1126	529	3	1.17E-06	1.32	FALSE	5.98E-01	1.03	FALSE	4.17E-02	1.10	FALSE	9.09E-01	0.98	FALSE
M198T603_pos	198.1127	603	3	7.77E-03	1.25	FALSE	8.97E-01	0.99	FALSE	6.70E-01	0.97	FALSE	3.35E-01	0.88	FALSE
M198T698_pos	198.1128	698	3	6.37E-03	1.22	FALSE	1.44E-02	0.78	FALSE	6.49E-01	0.97	FALSE	9.46E-01	1.02	FALSE
M198T368_pos	198.1599	368	3	4.96E-02	1.25	FALSE	1.50E-02	1.34	FALSE	3.83E-04	1.43	FALSE	1.48E-03	1.28	FALSE
M199T373_pos	199.0828	373	3	1.51E-01	1.12	FALSE	2.21E-01	0.90	FALSE	1.34E-03	0.79	FALSE	3.34E-01	0.83	FALSE
M199T371_pos	199.1124	371	3	2.68E-01	0.89	FALSE	2.17E-01	0.85	FALSE	4.77E-04	1.40	FALSE	5.93E-01	0.88	FALSE
M199T689_pos	199.1078	689	3	1.10E-04	1.16	FALSE	2.98E-01	1.04	FALSE	1.25E-18	1.37	FALSE	1.98E-01	0.93	FALSE
M199T803_pos	199.1328	803	3	6.01E-01	1.01	FALSE	1.36E-02	1.06	FALSE	1.26E-04	1.08	FALSE	2.11E-01	0.96	FALSE
M199T883_pos	199.1694	883	3	4.47E-02	0.95	FALSE	1.78E-02	1.07	FALSE	1.40E-11	1.17	FALSE	4.63E-01	1.06	FALSE
M199T1029_pos	199.1693	1029	3	8.13E-01	1.02	FALSE	1.76E-02	1.23	FALSE	2.07E-01	0.91	FALSE	2.76E-01	0.95	FALSE
M199T1039_pos	199.2057	1039	3	8.40E-02	1.14	FALSE	3.00E-01	0.92	FALSE	1.32E-01	0.91	FALSE	3.05E-05	1.38	FALSE
M200T512_pos	200.0919	512	3	3.20E-12	1.39	FALSE	3.93E-03	1.14	FALSE	2.51E-07	1.23	FALSE	1.45E-01	0.88	FALSE
M200T462_pos	200.0919	462	3	1.10E-20	1.40	FALSE	1.47E-01	1.05	FALSE	8.06E-10	1.20	FALSE	3.40E-01	0.96	FALSE
M200T342_pos	200.1031	342	3	7.32E-01	1.02	FALSE	7.07E-02	0.91	FALSE	1.04E-17	1.50	FALSE	8.65E-02	0.83	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M200T625_pos	200.1288	625	3							HMDB0006406	Ecgonine methyl ester	C10H17NO3	3.5
M200T112_pos	200.1759	112	3							HMDB0014849	Diethylcarbamazine	C10H21N3O	0.6
M201T778_pos	201.1122	778	3							HMDB0000603	cis-4-Decenedioic acid	C10H16O4	0.4
M202T683_pos	202.1439	683	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.7
M202T444_pos	202.1439	444	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.6
M203T457_pos	203.0914	457	3							HMDB0032306	Diethyl oxalpropionate	C9H14O5	0.2
M203T411_pos	203.1175	411	3							HMDB0029835	Tetrahydroharmol	C12H14N2O	2.1
M203T753_pos	203.1280	753	3							HMDB0000792	Sebacic acid	C10H18O4	0.8
M203T128_pos	203.1502	128	3							HMDB0001539	Asymmetric dimethylarginine	C8H18N4O2	0.0
M204T445_pos	204.0691	445	3							HMDB0240543	N-Acetyl-S-allylcysteine	C8H13NO3S	1.1
M204T380_pos	204.0663	380	3							HMDB0060484	Indolepyruvate	C11H9NO3	3.8
M204T496_pos	204.1231	496	3							HMDB0062176	N-Lactoylleucine	C9H17NO4	0.1
M205T75_pos	205.0348	75	3							HMDB0031665	Daucic acid	C7H8O7	2.7
M205T682_pos	205.0796	682	3							HMDB0258111	Methyl-5-thiazolyl)-1-phenylmethyl	C11H12N2S	1.0
M205T1016_pos	205.0860	1016	3							HMDB0033303	Anofinic acid	C12H12O3	0.1
M205T1035_pos	205.1223	1035	3							HMDB0030770	oxy-3-(3-methyl-2-butenyl)acetopl	C13H16O2	0.2
M205T942_pos	205.1588	942	3							HMDB0031776	R,7S)-6,7-Epoxy-1,3-tetradecadiyn	C14H20O	0.6
M205T1054_pos	205.1588	1054	3							HMDB0031776	R,7S)-6,7-Epoxy-1,3-tetradecadiyn	C14H20O	0.5
M205T1040_pos	205.1951	1040	3							HMDB0030644	delta-Amorphene	C15H24	0.3
M206T393_pos	206.0851	393	3							HMDB0094704	N-Propionylmethionine	C8H15NO3S	2.5
M206T558_pos	206.0844	558	3							HMDB0094704	N-Propionylmethionine	C8H15NO3S	0.8
M206T753_pos	206.1388	753	3						Fatty acids	HMDB0004231	Panthenol	C9H19NO4	0.6
M207T831_pos	207.1014	831	3							HMDB0030762	Ethyl trans-p-methoxycinnamate	C12H14O3	0.8
M207T792_pos	207.1016	792	3							HMDB0030762	Ethyl trans-p-methoxycinnamate	C12H14O3	0.1
M207T728_pos	207.1381	728	3							HMDB0001925	Ibuprofen	C13H18O2	0.7
M207T903_pos	207.1380	903	3							HMDB0001925	Ibuprofen	C13H18O2	0.2
M207T987_pos	207.1744	987	3							HMDB0013816	2,4-Di-tert-butylphenol	C14H22O	0.4
M208T368_pos	208.0970	368	3							HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	1.0
M209T649_pos	209.0809	649	3							HMDB0012127	(R)-2-Benzylsuccinate	C11H12O4	0.3
M209T670_pos	209.1173	670	3							HMDB0029867	Isoelemicin	C12H16O3	0.5
M209T499_pos	209.1285	499	3							HMDB0015217	Pilocarpine	C11H16N2O2	0.4
M209T965_pos	209.1537	965	3							HMDB0029668	Eremopetasinorol	C13H20O2	0.5
M209T907_pos	209.1537	907	3							HMDB0029668	Eremopetasinorol	C13H20O2	0.4
M209T1054_pos	209.1537	1054	3							HMDB0029668	Eremopetasinorol	C13H20O2	0.4
M209T957_pos	209.1901	957	3							HMDB0032215	2-Decylfuran	C14H24O	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M200T625_pos	200.1288	625	3	8.15E-04	1.44	FALSE	9.53E-01	1.01	FALSE	7.16E-02	1.18	FALSE	4.79E-01	0.87	FALSE
M200T112_pos	200.1759	112	3	3.39E-03	0.83	FALSE	8.99E-01	1.01	FALSE	4.52E-02	1.12	FALSE	3.77E-02	1.28	FALSE
M201T778_pos	201.1122	778	3	4.12E-01	0.96	FALSE	1.10E-01	1.08	FALSE	6.07E-04	1.15	FALSE	2.82E-01	0.90	FALSE
M202T683_pos	202.1439	683	3	2.01E-15	1.48	FALSE	3.77E-01	1.04	FALSE	1.43E-02	1.10	FALSE	1.78E-03	0.81	FALSE
M202T444_pos	202.1439	444	3	4.82E-01	1.05	FALSE	5.83E-01	0.96	FALSE	8.87E-01	0.99	FALSE	2.86E-02	1.40	FALSE
M203T457_pos	203.0914	457	3	4.07E-01	0.86	FALSE	3.19E-01	0.82	FALSE	4.20E-01	0.88	FALSE	6.54E-01	0.84	FALSE
M203T411_pos	203.1175	411	3	1.04E-01	1.21	FALSE	9.01E-03	0.72	FALSE	9.20E-03	1.31	FALSE	3.23E-01	1.15	FALSE
M203T753_pos	203.1280	753	3	1.27E-01	0.96	FALSE	3.16E-02	1.06	FALSE	3.03E-22	1.31	FALSE	2.18E-01	0.93	FALSE
M203T128_pos	203.1502	128	3	5.67E-06	0.72	FALSE	3.85E-01	1.06	FALSE	4.81E-04	1.24	FALSE	8.84E-02	1.52	FALSE
M204T445_pos	204.0691	445	3	1.16E-12	1.34	FALSE	6.78E-01	0.98	FALSE	1.87E-11	1.27	FALSE	5.81E-01	1.02	FALSE
M204T380_pos	204.0663	380	3	5.50E-01	1.09	FALSE	1.32E-01	0.80	FALSE	8.07E-01	1.03	FALSE	6.40E-01	1.06	FALSE
M204T496_pos	204.1231	496	3	2.45E-02	1.09	FALSE	1.87E-01	1.06	FALSE	1.23E-04	1.15	FALSE	5.23E-01	0.93	FALSE
M205T75_pos	205.0348	75	3	1.78E-01	1.12	FALSE	6.73E-01	1.04	FALSE	9.69E-02	0.89	FALSE	2.78E-01	0.78	FALSE
M205T682_pos	205.0796	682	3	2.80E-08	0.69	FALSE	8.79E-01	0.99	FALSE	1.22E-08	1.39	FALSE	1.57E-10	-17.33	FALSE
M205T1016_pos	205.0860	1016	3	1.35E-01	0.69	FALSE	9.47E-02	1.58	FALSE	7.09E-01	0.92	FALSE	7.14E-01	1.15	FALSE
M205T1035_pos	205.1223	1035	3	2.31E-05	0.85	FALSE	4.02E-04	1.15	FALSE	3.59E-01	0.97	FALSE	9.36E-01	1.01	FALSE
M205T942_pos	205.1588	942	3	2.11E-01	0.95	FALSE	5.51E-02	0.92	FALSE	2.76E-11	1.28	FALSE	9.66E-01	1.00	FALSE
M205T1054_pos	205.1588	1054	3	1.16E-01	1.07	FALSE	2.21E-01	0.95	FALSE	7.61E-01	1.01	FALSE	8.86E-01	0.99	FALSE
M205T1040_pos	205.1951	1040	3	5.16E-06	1.42	FALSE	4.63E-01	0.95	FALSE	3.34E-01	0.94	FALSE	4.66E-02	1.41	FALSE
M206T393_pos	206.0851	393	3	6.29E-03	1.20	FALSE	6.36E-01	1.03	FALSE	2.35E-05	1.29	FALSE	4.15E-02	0.74	FALSE
M206T558_pos	206.0844	558	3	1.43E-04	1.21	FALSE	5.19E-02	1.11	FALSE	1.25E-05	1.21	FALSE	7.90E-01	0.98	FALSE
M206T753_pos	206.1388	753	3	1.75E-01	1.03	FALSE	5.75E-07	1.12	FALSE	1.96E-19	1.22	FALSE	1.56E-01	0.91	FALSE
M207T831_pos	207.1014	831	3	6.41E-02	1.11	FALSE	2.05E-01	1.08	FALSE	6.50E-02	1.10	FALSE	5.47E-02	0.70	FALSE
M207T792_pos	207.1016	792	3	6.12E-03	0.90	FALSE	2.47E-07	1.23	FALSE	1.32E-15	1.34	FALSE	1.01E-02	0.87	FALSE
M207T728_pos	207.1381	728	3	3.70E-04	1.19	FALSE	4.51E-01	1.04	FALSE	3.00E-01	0.96	FALSE	4.51E-01	0.93	FALSE
M207T903_pos	207.1380	903	3	3.91E-01	0.96	FALSE	7.98E-01	1.01	FALSE	1.44E-07	1.29	FALSE	7.32E-02	0.77	FALSE
M207T987_pos	207.1744	987	3	6.84E-01	0.97	FALSE	8.93E-01	1.01	FALSE	3.71E-01	1.07	FALSE	2.21E-01	0.86	FALSE
M208T368_pos	208.0970	368	3	5.81E-06	1.19	FALSE	1.49E-02	1.10	FALSE	1.34E-17	1.36	FALSE	3.52E-01	1.04	FALSE
M209T649_pos	209.0809	649	3	1.22E-02	1.14	FALSE	8.28E-01	1.01	FALSE	7.04E-05	1.21	FALSE	2.02E-01	0.95	FALSE
M209T670_pos	209.1173	670	3	2.36E-01	1.04	FALSE	1.99E-01	1.05	FALSE	5.57E-29	1.49	FALSE	5.40E-02	0.92	FALSE
M209T499_pos	209.1285	499	3	4.37E-02	0.79	FALSE	3.28E-01	1.13	FALSE	4.38E-03	1.34	FALSE	3.47E-01	0.94	FALSE
M209T965_pos	209.1537	965	3	2.17E-01	1.04	FALSE	8.64E-01	1.01	FALSE	1.14E-01	0.96	FALSE	4.30E-01	1.05	FALSE
M209T907_pos	209.1537	907	3	1.39E-04	1.08	FALSE	2.55E-01	0.97	FALSE	6.68E-03	0.95	FALSE	9.75E-01	1.00	FALSE
M209T1054_pos	209.1537	1054	3	2.12E-01	1.07	FALSE	1.97E-02	1.14	FALSE	8.11E-01	1.01	FALSE	5.44E-01	0.93	FALSE
M209T957_pos	209.1901	957	3	2.71E-01	0.93	FALSE	8.66E-01	0.99	FALSE	3.42E-02	0.89	FALSE	3.93E-01	1.17	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M210T443_pos	210.0762	443	3							HMDB0000735	Hydroxyphenylacetylglycine	C10H11NO4	0.7
M210T594_2_pos	210.1124	594	3							HMDB0248234	alpha-Methyltyrosine methyl este	C11H15NO3	0.2
M210T543_pos	210.1126	543	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.7
M210T757_pos	210.1130	757	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	2.7
M211T85_pos	210.9688	85	3							HMDB0303198	Calcium glycerophosphate	C3H7CaO6P	4.5
M211T985_pos	211.0238	985	3							HMDB0248978	Benzene-1,2,3-tricarboxylic acid	C9H6O6	0.5
M211T552_pos	211.0826	552	3							HMDB0002123	1,3,7-Trimethyluric acid	C8H10N4O3	0.3
M211T646_pos	211.1087	646	3							HMDB0303275	Potassium caprate	C10H19KO2	3.6
M211T398_pos	211.1084	398	3							HMDB0015441	Aprobarbital	C10H14N2O3	3.4
M211T859_pos	211.1330	859	3							HMDB0032797	Jasmonic acid	C12H18O3	0.4
M211T995_pos	211.1692	995	3							HMDB0030425	Linalyl propionate	C13H22O2	0.1
M212T716_pos	212.1284	716	3							HMDB0014861	Methoxamine	C11H17NO3	1.2
M213T107_pos	213.0749	107	3							HMDB0000913	Vanillactic acid	C10H12O5	3.9
M213T685_pos	213.0758	685	3							HMDB0000913	Vanillactic acid	C10H12O5	0.4
M213T368_pos	213.1236	368	3							HMDB0011180	Prolylproline	C10H16N2O3	1.3
M213T893_pos	213.1486	893	3						Fatty acids	HMDB0029388	Cucurbic acid	C12H20O3	0.2
M214T694_pos	214.1076	694	3							HMDB0253757	kainic acid	C10H15NO4	0.8
M215T581_2_pos	215.0591	581	3							HMDB0258573	Sulfaguanidine	C7H10N4O2S	3.0
M215T800_pos	215.1279	800	3							HMDB0030984	tetrahydro-2-oxo-3-furancarboxy	C11H18O4	0.5
M216T491_pos	216.0869	491	3							HMDB0255166	N-Methacryloyl-L-glutamic acid	C9H13NO5	1.1
M216T441_pos	216.1021	441	3							HMDB0032888	Acetyl vitamin K5	C13H13NO2	1.1
M216T513_pos	216.1232	513	3							HMDB0013124	Propenoylcarnitine	C10H17NO4	0.7
M216T382_pos	216.1596	382	3							HMDB0013279	N-Nonanoylglycine	C11H21NO3	0.8
M217T1057_pos	217.1049	1057	3							HMDB0259242	Trimethylolmelamine	C6H12N6O3	2.2
M217T945_pos	217.1800	945	3							HMDB0000387	3-Hydroxydodecanoic acid	C12H24O3	0.6
M217T1055_pos	217.1952	1055	3							HMDB0036578	Cyperotundone	C16H24	0.4
M218T432_pos	218.0820	432	3							HMDB0244957	2-(Quinolin-8-yloxy)propanoic acid	C12H11NO3	3.9
M218T352_pos	218.0849	352	3							HMDB0247169	Mercapto-2-methyl-1-oxopropyl)-L	C9H15NO3S	1.7
M218T525_2_pos	218.1210	525	3							HMDB0249401	c acid, 2-methyl-2-((piperidinomet	C10H19NO2S	0.2
M219T718_pos	219.1380	718	3							HMDB0030759	(R)-Pterosin B	C14H18O2	0.2
M219T884_pos	219.1381	884	3							HMDB0030759	(R)-Pterosin B	C14H18O2	0.6
M219T1035_pos	219.1744	1035	3							HMDB0013687	Nookatone	C15H22O	0.4
M219T931_pos	219.1745	931	3							HMDB0013687	Nookatone	C15H22O	0.9
M219T1008_pos	219.2109	1008	3							HMDB0034498	4,8,12-Trimethyl-1,3,7,11-tridecat	C16H26	0.6
M220T447_pos	220.0607	447	3							HMDB0039387	yl 2,6-dihydroxy-4-quinolinecarbox	C11H9NO4	1.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M210T443_pos	210.0762	443	3	3.52E-04	0.74	FALSE	3.36E-01	0.92	FALSE	2.72E-07	1.48	FALSE	3.18E-01	0.90	FALSE
M210T594_2_pos	210.1124	594	3	1.05E-04	1.34	FALSE	2.31E-01	1.09	FALSE	9.26E-07	1.39	FALSE	7.37E-01	0.96	FALSE
M210T543_pos	210.1126	543	3	2.65E-04	1.30	FALSE	9.94E-01	1.00	FALSE	2.96E-05	1.30	FALSE	9.52E-01	1.01	FALSE
M210T757_pos	210.1130	757	3	6.80E-02	0.90	FALSE	3.44E-01	0.94	FALSE	3.41E-01	0.95	FALSE	7.43E-01	1.01	FALSE
M211T85_pos	210.9688	85	3	1.02E-01	1.10	FALSE	8.85E-01	0.99	FALSE	2.00E-02	1.13	FALSE	4.08E-01	0.89	FALSE
M211T985_pos	211.0238	985	3	5.39E-03	0.82	FALSE	7.00E-02	1.14	FALSE	7.31E-07	1.37	FALSE	4.99E-02	0.75	FALSE
M211T552_pos	211.0826	552	3	3.09E-09	1.41	FALSE	1.59E-02	1.15	FALSE	1.59E-08	1.33	FALSE	6.25E-01	0.97	FALSE
M211T646_pos	211.1087	646	3	9.21E-01	0.99	FALSE	2.25E-02	1.19	FALSE	1.70E-09	1.47	FALSE	6.99E-01	1.09	FALSE
M211T398_pos	211.1084	398	3	1.36E-01	1.05	FALSE	2.46E-01	1.04	FALSE	1.76E-26	1.47	FALSE	6.71E-02	0.91	FALSE
M211T859_pos	211.1330	859	3	1.88E-03	0.89	FALSE	5.37E-01	1.02	FALSE	2.55E-13	1.29	FALSE	5.62E-02	0.81	FALSE
M211T995_pos	211.1692	995	3	3.04E-01	0.94	FALSE	8.38E-01	1.01	FALSE	6.70E-01	1.02	FALSE	8.76E-01	0.98	FALSE
M212T716_pos	212.1284	716	3	1.76E-02	0.84	FALSE	7.19E-08	1.50	FALSE	6.09E-09	1.46	FALSE	6.65E-01	0.95	FALSE
M213T107_pos	213.0749	107	3	8.61E-04	0.71	FALSE	2.90E-01	0.89	FALSE	2.09E-02	1.23	FALSE	2.69E-01	1.13	FALSE
M213T685_pos	213.0758	685	3	3.91E-01	1.13	FALSE	8.25E-01	0.97	FALSE	6.31E-02	0.80	FALSE	8.87E-01	0.96	FALSE
M213T368_pos	213.1236	368	3	1.89E-02	0.91	FALSE	1.82E-01	1.06	FALSE	9.61E-14	1.33	FALSE	3.41E-01	0.92	FALSE
M213T893_pos	213.1486	893	3	3.27E-07	0.83	FALSE	1.16E-01	1.06	FALSE	1.15E-16	1.33	FALSE	6.05E-01	0.96	FALSE
M214T694_pos	214.1076	694	3	1.07E-03	0.67	FALSE	3.61E-01	1.12	FALSE	1.31E-02	1.30	FALSE	5.04E-02	0.74	FALSE
M215T581_2_pos	215.0591	581	3	1.30E-01	0.88	FALSE	4.86E-01	1.06	FALSE	3.05E-01	1.07	FALSE	9.40E-01	1.02	FALSE
M215T800_pos	215.1279	800	3	1.07E-21	1.36	FALSE	5.46E-02	1.06	FALSE	9.50E-02	1.04	FALSE	3.39E-01	0.96	FALSE
M216T491_pos	216.0869	491	3	5.48E-01	0.96	FALSE	1.66E-01	0.91	FALSE	2.77E-02	1.13	FALSE	1.77E-01	0.79	FALSE
M216T441_pos	216.1021	441	3	3.15E-07	1.32	FALSE	5.50E-01	0.97	FALSE	5.22E-04	1.18	FALSE	8.96E-03	0.88	FALSE
M216T513_pos	216.1232	513	3	1.34E-27	1.41	FALSE	6.36E-01	1.01	FALSE	1.50E-06	1.12	FALSE	1.02E-02	0.91	FALSE
M216T382_pos	216.1596	382	3	2.32E-05	1.17	FALSE	5.21E-01	1.02	FALSE	2.23E-16	1.34	FALSE	3.54E-01	0.95	FALSE
M217T1057_pos	217.1049	1057	3	4.49E-01	1.03	FALSE	4.35E-02	1.09	FALSE	7.83E-01	0.99	FALSE	1.19E-01	0.91	FALSE
M217T945_pos	217.1800	945	3	1.25E-10	1.27	FALSE	5.70E-04	0.88	FALSE	5.01E-01	1.02	FALSE	4.17E-01	1.07	FALSE
M217T1055_pos	217.1952	1055	3	5.39E-01	1.06	FALSE	6.61E-01	1.04	FALSE	7.13E-01	1.03	FALSE	5.34E-01	1.11	FALSE
M218T432_pos	218.0820	432	3	5.45E-01	1.04	FALSE	1.35E-01	1.11	FALSE	8.74E-03	1.17	FALSE	1.86E-01	1.09	FALSE
M218T352_pos	218.0849	352	3	9.91E-03	1.19	FALSE	9.76E-02	1.12	FALSE	1.21E-06	1.33	FALSE	4.89E-02	1.11	FALSE
M218T525_2_pos	218.1210	525	3	1.54E-04	1.34	FALSE	4.01E-01	1.07	FALSE	7.96E-03	1.19	FALSE	4.82E-01	1.11	FALSE
M219T718_pos	219.1380	718	3	8.90E-02	1.11	FALSE	7.01E-01	1.03	FALSE	4.00E-01	0.96	FALSE	4.48E-01	0.97	FALSE
M219T884_pos	219.1381	884	3	9.52E-01	1.00	FALSE	3.58E-01	1.05	FALSE	4.47E-01	1.03	FALSE	1.83E-03	0.83	FALSE
M219T1035_pos	219.1744	1035	3	6.02E-01	1.03	FALSE	4.11E-01	0.95	FALSE	1.25E-01	0.93	FALSE	5.20E-01	0.90	FALSE
M219T931_pos	219.1745	931	3	1.66E-01	1.04	FALSE	5.48E-01	0.98	FALSE	7.81E-01	0.99	FALSE	2.65E-01	0.90	FALSE
M219T1008_pos	219.2109	1008	3	3.17E-01	0.94	FALSE	7.07E-01	0.98	FALSE	2.88E-01	0.95	FALSE	2.07E-02	1.29	FALSE
M220T447_pos	220.0607	447	3	6.26E-01	0.97	FALSE	5.33E-01	0.96	FALSE	2.39E-09	1.44	FALSE	4.06E-01	1.15	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M220T650_pos	220.0610	650	3							HMDB0039387	yl 2,6-dihydroxy-4-quinolinecarbox	C11H9NO4	2.6
M220T437_1_pos	220.1180	437	3							HMDB0000210	Pantothenic acid	C9H17NO5	0.2
M220T291_pos	220.1194	291	3							HMDB0012204	Zeatin	C10H13N5O	0.5
M220T803_pos	220.1545	803	3						Fatty acids	HMDB0014563	Miglustat	C10H21NO4	0.6
M221T401_pos	221.0950	401	3							HMDB0028788	Cysteinyl-Valine	C8H16N2O3S	2.0
M221T969_pos	221.1173	969	3							HMDB0032589	tyl-2-hydroxyphenyl)-3-methyl-1-b	C13H16O3	0.1
M221T992_pos	221.1536	992	3							HMDB0013817	2,6-Di-tert-butylbenzoquinone	C14H20O2	0.1
M221T839_pos	221.1538	839	3						Terpenoids	HMDB0013817	2,6-Di-tert-butylbenzoquinone	C14H20O2	0.8
M221T1015_pos	221.1901	1015	3							HMDB0013688	Nootkatol	C15H24O	0.4
M222T511_pos	222.0764	511	3							HMDB0038990	Methyl 5-hydroxyoxindole-3-acetat	C11H11NO4	1.6
M222T759_pos	222.1126	759	3							HMDB0014798	Metaxalone	C12H15NO3	0.6
M222T393_pos	222.1126	393	3							HMDB0014798	Metaxalone	C12H15NO3	0.6
M223T963_pos	223.0637	963	3							HMDB0033041	1-Propenylthio)propyl propyl disulf	C9H18S3	2.8
M223T907_pos	223.0638	907	3							HMDB0033041	1-Propenylthio)propyl propyl disulf	C9H18S3	2.6
M223T1001_pos	223.0635	1001	3							HMDB0033041	1-Propenylthio)propyl propyl disulf	C9H18S3	3.9
M223T878_pos	223.0965	878	3							HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	0.2
M223T779_pos	223.0945	779	3							HMDB0257744	1,3-Dioxolan-2-yl)purine-2,6-diam	C8H10N6O2	3.3
M223T110_pos	223.0964	110	3							HMDB0002056	Monoisobutyl phthalic acid	C12H14O4	0.2
M223T596_pos	223.1532	596	3							HMDB0258894	Tetraglyme	C10H22O5	3.7
M223T953_pos	223.1693	953	3							HMDB0035593	Rishitin	C14H22O2	0.3
M223T957_pos	223.2058	957	3						Terpenoids	HMDB0004305	Farnesol	C15H26O	0.6
M224T615_pos	224.0919	615	3							HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	0.7
M224T533_pos	224.0920	533	3							HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	1.2
M224T471_2_pos	224.0920	471	3							HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	1.1
M224T685_pos	224.1279	685	3							HMDB0015168	Cerulenin	C12H17NO3	0.9
M224T466_pos	224.1283	466	3							HMDB0015168	Cerulenin	C12H17NO3	1.0
M224T368_pos	224.1284	368	3							HMDB0015168	Cerulenin	C12H17NO3	1.1
M225T630_pos	225.0873	630	3							HMDB0000732	Hydroxykynurenine	C10H12N2O4	1.3
M225T925_pos	225.0912	925	3							HMDB0032584	4-Hydroxychalcone	C15H12O2	0.8
M225T704_pos	225.1236	704	3							HMDB0014386	Butalbital	C11H16N2O3	1.2
M225T607_pos	225.1236	607	3							HMDB0014386	Butalbital	C11H16N2O3	1.1
M225T399_pos	225.1238	399	3							HMDB0014386	Butalbital	C11H16N2O3	1.8
M225T490_pos	225.1236	490	3							HMDB0014386	Butalbital	C11H16N2O3	1.0
M225T645_pos	225.1234	645	3							HMDB0014386	Butalbital	C11H16N2O3	0.2
M225T448_pos	225.1239	448	3							HMDB0014386	Butalbital	C11H16N2O3	2.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M220T650_pos	220.0610	650	3	3.36E-10	1.27	FALSE	7.88E-02	0.93	FALSE	1.57E-24	1.45	FALSE	6.65E-01	0.98	FALSE
M220T437_1_pos	220.1180	437	3	4.26E-01	0.96	FALSE	3.57E-01	1.05	FALSE	3.42E-13	1.47	FALSE	2.79E-02	0.90	FALSE
M220T291_pos	220.1194	291	3	7.15E-04	1.32	FALSE	1.36E-01	1.14	FALSE	8.41E-03	1.21	FALSE	3.01E-01	1.18	FALSE
M220T803_pos	220.1545	803	3	1.06E-02	1.08	FALSE	5.34E-03	1.09	FALSE	3.52E-02	1.06	FALSE	8.25E-02	0.89	FALSE
M221T401_pos	221.0950	401	3	9.44E-01	1.01	FALSE	3.79E-01	1.11	FALSE	6.94E-02	1.18	FALSE	5.27E-02	1.26	FALSE
M221T969_pos	221.1173	969	3	8.87E-04	0.88	FALSE	2.49E-02	1.09	FALSE	9.81E-11	0.80	FALSE	5.39E-01	1.03	FALSE
M221T992_pos	221.1536	992	3	4.07E-03	1.22	FALSE	4.57E-01	0.95	FALSE	2.20E-05	1.29	FALSE	9.29E-01	1.02	FALSE
M221T839_pos	221.1538	839	3	4.05E-01	1.05	FALSE	4.08E-01	1.05	FALSE	4.11E-01	0.96	FALSE	7.07E-03	0.80	FALSE
M221T1015_pos	221.1901	1015	3	9.39E-01	1.00	FALSE	4.40E-01	0.98	FALSE	1.05E-01	1.04	FALSE	7.80E-01	1.01	FALSE
M222T511_pos	222.0764	511	3	6.14E-01	1.02	FALSE	4.84E-01	1.03	FALSE	2.09E-05	1.18	FALSE	1.77E-01	0.94	FALSE
M222T759_pos	222.1126	759	3	5.87E-01	1.02	FALSE	2.80E-01	1.05	FALSE	1.68E-01	1.05	FALSE	4.55E-01	0.91	FALSE
M222T393_pos	222.1126	393	3	1.57E-06	1.24	FALSE	9.55E-02	0.93	FALSE	3.26E-01	0.96	FALSE	1.43E-01	0.88	FALSE
M223T963_pos	223.0637	963	3	8.70E-01	1.01	FALSE	5.47E-01	1.02	FALSE	3.51E-01	0.97	FALSE	8.57E-01	1.02	FALSE
M223T907_pos	223.0638	907	3	6.54E-01	0.98	FALSE	4.12E-01	1.05	FALSE	4.08E-01	0.96	FALSE	1.05E-01	1.27	FALSE
M223T1001_pos	223.0635	1001	3	4.35E-01	1.04	FALSE	1.13E-01	1.09	FALSE	5.36E-01	1.03	FALSE	7.37E-01	1.07	FALSE
M223T878_pos	223.0965	878	3	6.61E-08	0.72	FALSE	3.17E-04	1.25	FALSE	1.55E-05	1.25	FALSE	1.38E-01	1.11	FALSE
M223T779_pos	223.0945	779	3	1.16E-02	1.11	FALSE	3.11E-02	1.10	FALSE	2.99E-02	0.93	FALSE	6.06E-02	0.78	FALSE
M223T110_pos	223.0964	110	3	7.91E-01	0.97	FALSE	4.96E-01	1.10	FALSE	6.08E-01	1.06	FALSE	6.81E-01	0.96	FALSE
M223T596_pos	223.1532	596	3	3.62E-01	1.07	FALSE	2.41E-01	1.09	FALSE	6.07E-05	1.29	FALSE	1.14E-01	0.85	FALSE
M223T953_pos	223.1693	953	3	5.46E-01	1.03	FALSE	6.31E-01	0.97	FALSE	4.90E-12	1.39	FALSE	2.57E-02	0.80	FALSE
M223T957_pos	223.2058	957	3	1.31E-01	0.90	FALSE	3.14E-01	1.07	FALSE	8.82E-01	0.99	FALSE	3.86E-01	1.18	FALSE
M224T615_pos	224.0919	615	3	3.21E-10	1.41	FALSE	5.31E-01	1.03	FALSE	8.93E-04	1.16	FALSE	5.95E-01	1.11	FALSE
M224T533_pos	224.0920	533	3	5.55E-04	1.15	FALSE	5.62E-01	1.02	FALSE	9.36E-10	1.25	FALSE	7.58E-01	1.02	FALSE
M224T471_2_pos	224.0920	471	3	9.50E-10	0.69	FALSE	8.21E-01	1.01	FALSE	1.24E-07	1.31	FALSE	1.97E-01	0.89	FALSE
M224T685_pos	224.1279	685	3	1.21E-06	1.24	FALSE	1.70E-01	1.06	FALSE	7.81E-01	1.01	FALSE	9.01E-01	0.99	FALSE
M224T466_pos	224.1283	466	3	2.93E-05	1.21	FALSE	5.05E-02	1.10	FALSE	2.36E-10	1.30	FALSE	1.59E-01	0.90	FALSE
M224T368_pos	224.1284	368	3	5.09E-01	1.03	FALSE	3.55E-01	1.04	FALSE	5.10E-16	1.42	FALSE	1.97E-02	0.88	FALSE
M225T630_pos	225.0873	630	3	1.79E-06	1.21	FALSE	4.77E-01	1.03	FALSE	6.39E-19	1.41	FALSE	2.69E-03	0.89	FALSE
M225T925_pos	225.0912	925	3	1.62E-01	0.90	FALSE	2.54E-01	1.10	FALSE	8.09E-01	0.98	FALSE	9.95E-01	1.00	FALSE
M225T704_pos	225.1236	704	3	8.57E-02	1.15	FALSE	4.47E-01	1.06	FALSE	5.21E-01	1.05	FALSE	3.88E-01	0.91	FALSE
M225T607_pos	225.1236	607	3	1.78E-01	1.15	FALSE	2.03E-01	0.88	FALSE	5.09E-04	1.37	FALSE	5.09E-01	1.16	FALSE
M225T399_pos	225.1238	399	3	8.85E-01	0.98	FALSE	4.74E-01	0.89	FALSE	1.88E-01	1.17	FALSE	3.26E-02	0.74	FALSE
M225T490_pos	225.1236	490	3	4.97E-04	1.14	FALSE	5.87E-01	1.02	FALSE	5.45E-18	1.37	FALSE	1.10E-03	0.85	FALSE
M225T645_pos	225.1234	645	3	5.07E-03	1.12	FALSE	1.83E-04	1.17	FALSE	1.09E-21	1.48	FALSE	1.14E-01	0.93	FALSE
M225T448_pos	225.1239	448	3	5.26E-01	1.03	FALSE	2.55E-02	1.11	FALSE	2.19E-09	1.28	FALSE	4.76E-01	0.94	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M225T974_pos	225.1850	974	3							HMDB0000560	Goshuyic acid	C14H24O2	0.4
M226T568_pos	226.0713	568	3							HMDB0037264	4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	1.2
M226T589_pos	226.1077	589	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	1.3
M226T519_pos	226.1077	519	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	1.6
M226T356_pos	226.1180	356	3							HMDB0041953	Nnal-N-oxide	C10H15N3O3	2.9
M226T890_pos	226.1227	890	3							HMDB0247971	cryloyl-2-dimethylaminonaphthal	C15H15NO	0.2
M227T560_pos	227.1032	560	3							HMDB0000245	Porphobilinogen	C10H14N2O4	2.5
M227T757_pos	227.1278	757	3							HMDB0040705	Allixin	C12H18O4	0.1
M227T669_pos	227.1279	669	3							HMDB0040705	Allixin	C12H18O4	0.6
M227T383_pos	227.1392	383	3							HMDB0014457	Pentobarbital	C11H18N2O3	0.9
M227T925_pos	227.1643	925	3							HMDB0031740	Methyl dihydrojasmonate	C13H22O3	0.5
M227T882_pos	227.1643	882	3							HMDB0031740	Methyl dihydrojasmonate	C13H22O3	0.7
M227T920_pos	227.2007	920	3							HMDB0000499	5-Tetradecenoic acid	C14H26O2	0.8
M227T981_pos	227.2007	981	3							HMDB0000499	5-Tetradecenoic acid	C14H26O2	0.6
M228T769_pos	228.1021	769	3							HMDB0033452	Koenoline	C14H13NO2	0.7
M228T550_pos	228.1233	550	3							HMDB0032928	3,4,8-trimethyl-3H-imidazo[4,5-f]q	C12H13N5	4.7
M228T874_pos	228.1959	874	3						Fatty acids				
M230T473_pos	230.0958	473	3							HMDB0003045	Ergothioneine	C9H15N3O2S	0.3
M230T509_pos	230.0974	509	3							HMDB0246755	Benzo[c]phenanthridine	C17H11N	4.4
M230T442_pos	230.1132	442	3							HMDB0028739	Asparaginyl-Proline	C9H15N3O4	1.4
M230T581_2_pos	230.1388	581	3							HMDB0013126	Butenylcarnitine	C11H19NO4	0.5
M230T868_pos	230.1753	868	3							HMDB0013267	N-Decanoylglycine	C12H23NO3	0.9
M230T873_pos	230.2480	873	3							HMDB0304813	Xestoaminol C	C14H31NO	0.7
M231T359_pos	231.0806	359	3							HMDB0244005	1-Pyrenecarboxaldehyde	C17H10O	0.9
M231T476_pos	231.1163	476	3							HMDB0244175	M-Terphenyl	C18H14	2.3
M231T1054_1_pos	231.2108	1054	3							HMDB0245136	2-Gonen	C17H26	0.4
M232T483_pos	232.1092	483	3							HMDB0015377	Isocarboxazid	C12H13N3O2	4.8
M232T666_pos	232.1181	666	3							HMDB0000726	Isovalerylglutamic acid	C10H17NO5	0.5
M232T491_pos	232.1545	491	3							HMDB0002013	Butyrylcarnitine	C11H21NO4	0.9
M233T378_pos	233.0956	378	3							HMDB0060324	1-Methoxypyrene	C17H12O	2.2
M233T527_pos	233.1286	527	3							HMDB0001389	Melatonin	C13H16N2O2	0.4
M233T1033_pos	233.2264	1033	3							HMDB0061857	6-Phenylundecane	C17H28	0.2
M234T803_pos	234.0575	803	3							HMDB0038592	Brassicanal B	C12H11NO2S	3.6
M234T461_pos	234.0795	461	3							HMDB0244631	ydroxy-2-(N-acetylcysteinyl)-3-but	C9H15NO4S	0.2
M234T475_pos	234.1327	475	3							HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	3.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M225T974_pos	225.1850	974	3	9.73E-01	1.00	FALSE	4.19E-01	0.92	FALSE	2.36E-01	1.11	FALSE	2.92E-01	1.14	FALSE
M226T568_pos	226.0713	568	3	4.95E-04	1.31	FALSE	3.80E-01	1.07	FALSE	7.50E-01	1.02	FALSE	9.89E-01	1.00	FALSE
M226T589_pos	226.1077	589	3	2.03E-02	0.89	FALSE	1.37E-02	1.14	FALSE	2.69E-13	1.41	FALSE	7.56E-01	0.96	FALSE
M226T519_pos	226.1077	519	3	5.01E-01	0.92	FALSE	8.50E-01	1.02	FALSE	1.07E-01	1.20	FALSE	5.41E-01	0.91	FALSE
M226T356_pos	226.1180	356	3	1.62E-01	0.88	FALSE	4.08E-01	0.93	FALSE	3.07E-06	1.46	FALSE	8.16E-01	0.98	FALSE
M226T890_pos	226.1227	890	3	8.64E-02	1.03	FALSE	8.35E-02	0.97	FALSE	1.33E-14	0.88	FALSE	5.65E-01	1.02	FALSE
M227T560_pos	227.1032	560	3	1.04E-01	1.10	FALSE	2.22E-01	1.08	FALSE	1.04E-07	1.34	FALSE	9.07E-01	0.99	FALSE
M227T757_pos	227.1278	757	3	5.27E-05	0.89	FALSE	2.99E-02	1.07	FALSE	1.37E-33	1.45	FALSE	1.67E-01	0.94	FALSE
M227T669_pos	227.1279	669	3	2.56E-01	1.04	FALSE	2.29E-01	1.04	FALSE	5.41E-30	1.45	FALSE	2.61E-02	0.94	FALSE
M227T383_pos	227.1392	383	3	3.96E-06	1.33	FALSE	2.69E-02	1.15	FALSE	2.92E-05	1.25	FALSE	8.37E-01	1.02	FALSE
M227T925_pos	227.1643	925	3	2.54E-02	0.92	FALSE	7.64E-01	1.01	FALSE	1.68E-02	1.08	FALSE	1.48E-06	1.40	FALSE
M227T882_pos	227.1643	882	3	1.45E-02	0.94	FALSE	1.13E-01	1.05	FALSE	4.11E-16	1.23	FALSE	9.93E-01	1.00	FALSE
M227T920_pos	227.2007	920	3	7.09E-02	0.93	FALSE	3.00E-02	1.10	FALSE	4.55E-01	0.97	FALSE	4.30E-03	1.28	FALSE
M227T981_pos	227.2007	981	3	2.51E-02	1.12	FALSE	4.26E-01	0.96	FALSE	7.12E-01	0.98	FALSE	6.16E-01	1.04	FALSE
M228T769_pos	228.1021	769	3	6.71E-03	0.79	FALSE	4.14E-01	1.07	FALSE	1.53E-05	1.39	FALSE	3.75E-01	0.93	FALSE
M228T550_pos	228.1233	550	3	2.88E-01	1.06	FALSE	5.95E-01	1.03	FALSE	1.13E-02	1.13	FALSE	2.52E-02	0.85	FALSE
M228T874_pos	228.1959	874	3	8.99E-02	1.04	FALSE	1.56E-01	1.03	FALSE	8.28E-09	0.90	FALSE	5.78E-03	0.89	FALSE
M230T473_pos	230.0958	473	3	5.25E-01	1.05	FALSE	7.72E-01	0.97	FALSE	3.30E-04	1.30	FALSE	2.97E-01	0.80	FALSE
M230T509_pos	230.0974	509	3	1.15E-03	0.68	FALSE	2.47E-01	0.86	FALSE	3.51E-02	1.24	FALSE	3.62E-01	0.78	FALSE
M230T442_pos	230.1132	442	3	2.72E-03	1.31	FALSE	4.03E-01	1.08	FALSE	4.87E-05	1.38	FALSE	2.37E-02	1.46	FALSE
M230T581_2_pos	230.1388	581	3	3.97E-06	1.24	FALSE	7.48E-01	1.02	FALSE	7.34E-03	1.11	FALSE	8.36E-01	0.97	FALSE
M230T868_pos	230.1753	868	3	7.48E-01	1.04	FALSE	9.64E-03	1.39	FALSE	3.60E-03	1.39	FALSE	7.89E-01	0.95	FALSE
M230T873_pos	230.2480	873	3	3.67E-01	1.03	FALSE	9.54E-02	0.94	FALSE	9.23E-01	1.00	FALSE	4.36E-01	1.07	FALSE
M231T359_pos	231.0806	359	3	4.72E-01	1.06	FALSE	3.92E-01	1.07	FALSE	5.08E-04	1.28	FALSE	6.40E-02	0.80	FALSE
M231T476_pos	231.1163	476	3	2.97E-01	0.90	FALSE	2.97E-02	0.81	FALSE	1.26E-04	1.39	FALSE	6.90E-02	0.69	FALSE
M231T1054_1_pos	231.2108	1054	3	4.85E-01	1.03	FALSE	1.77E-02	0.91	FALSE	9.77E-02	0.95	FALSE	6.09E-01	0.95	FALSE
M232T483_pos	232.1092	483	3	2.29E-02	1.21	FALSE	1.20E-01	1.15	FALSE	1.24E-07	1.50	FALSE	1.77E-01	1.18	FALSE
M232T666_pos	232.1181	666	3	1.17E-01	0.88	FALSE	2.40E-02	1.22	FALSE	5.89E-08	1.48	FALSE	5.12E-01	0.91	FALSE
M232T491_pos	232.1545	491	3	1.34E-01	0.70	FALSE	7.45E-01	1.08	FALSE	1.92E-01	1.31	FALSE	3.69E-03	0.85	FALSE
M233T378_pos	233.0956	378	3	8.82E-02	1.10	FALSE	8.69E-02	1.10	FALSE	2.17E-10	1.37	FALSE	4.67E-01	1.07	FALSE
M233T527_pos	233.1286	527	3	1.13E-02	1.13	FALSE	3.10E-01	1.05	FALSE	7.40E-17	1.48	FALSE	6.54E-01	0.97	FALSE
M233T1033_pos	233.2264	1033	3	4.49E-03	1.16	FALSE	4.80E-01	0.96	FALSE	7.28E-02	1.08	FALSE	5.41E-01	1.03	FALSE
M234T803_pos	234.0575	803	3	2.68E-12	1.24	FALSE	7.40E-01	1.01	FALSE	1.23E-20	0.77	FALSE	8.04E-01	1.01	FALSE
M234T461_pos	234.0795	461	3	2.08E-03	1.27	FALSE	4.36E-03	0.81	FALSE	7.17E-01	1.02	FALSE	2.16E-01	0.85	FALSE
M234T475_pos	234.1327	475	3	3.66E-02	1.13	FALSE	1.28E-01	1.09	FALSE	8.02E-01	1.01	FALSE	4.68E-01	1.09	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M235T373_pos	235.1106	373	3							HMDB0028778	Cysteinyl-Isoleucine	C9H18N2O3S	2.1
M235T706_pos	235.1694	706	3							HMDB0030016	Valerenic acid	C15H22O2	0.8
M235T940_pos	235.1693	940	3							HMDB0030016	Valerenic acid	C15H22O2	0.3
M235T974_pos	235.1693	974	3							HMDB0030016	Valerenic acid	C15H22O2	0.3
M235T1062_pos	235.1693	1062	3							HMDB0030016	Valerenic acid	C15H22O2	0.2
M235T1059_pos	235.2057	1059	3							HMDB0040179	2,6-Di-tert-butyl-4-ethylphenol	C16H26O	0.4
M235T1014_pos	235.2058	1014	3							HMDB0040179	2,6-Di-tert-butyl-4-ethylphenol	C16H26O	0.8
M235T1038_pos	235.2422	1038	3							HMDB0041082	(5Z,8Z)-1,5,8-Heptadecatriene	C17H30	0.6
M236T104_pos	236.0797	104	3							HMDB0304419	N,N-dihydroxy-L-tryptophan	C11H11N2O4	0.0
M236T697_pos	236.1283	697	3							HMDB0033610	Pandamarilactam 3x	C13H17NO3	0.6
M236T510_pos	236.1638	510	3							HMDB0060849	N,N-Didesmethyltramadol	C14H21NO2	2.8
M236T657_pos	236.1649	657	3							HMDB0060849	N,N-Didesmethyltramadol	C14H21NO2	1.5
M237T361_pos	237.0874	361	3							HMDB0001200	N2-Succinyl-L-ornithine	C11H12N2O4	1.7
M237T390_pos	237.1237	390	3							HMDB0015444	Hexobarbital	C12H16N2O3	1.3
M237T1014_pos	237.1480	1014	3							HMDB0034462	Heptyl 4-hydroxybenzoate	C14H20O3	2.2
M237T790_pos	237.1850	790	3						Terpenoids	HMDB0002352	Capsidiol	C15H24O2	0.6
M237T726_pos	237.1850	726	3							HMDB0002352	Capsidiol	C15H24O2	0.6
M237T1056_pos	237.2214	1056	3							HMDB0031851	rimethylbicyclo[2.2.1]hept-1-yl)cyc	C16H28O	0.6
M238T510_pos	238.0712	510	3							HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	0.8
M238T569_pos	238.0713	569	3							HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	1.1
M238T591_pos	238.1076	591	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.8
M238T670_pos	238.1076	670	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.8
M238T532_pos	238.1439	532	3							HMDB0259807	viloxazine	C13H19NO3	0.7
M238T461_pos	238.1445	461	3							HMDB0259807	viloxazine	C13H19NO3	3.2
M239T457_pos	239.0922	457	3							HMDB0002511	3,4,5-Trimethoxycinnamic acid	C12H14O5	3.2
M239T744_pos	239.0915	744	3							HMDB0002511	3,4,5-Trimethoxycinnamic acid	C12H14O5	0.5
M239T574_2_pos	239.1393	574	3							HMDB0014562	Secobarbital	C12H18N2O3	1.1
M239T1066_pos	239.1490	1066	3							HMDB0256256	Pentaethylene glycol	C10H22O6	0.4
M239T932_pos	239.1636	932	3							HMDB0038256	Geranyl acetoacetate	C14H22O3	2.3
M239T1041_pos	239.2007	1041	3							HMDB0029350	Geranyl 3-methylbutanoate	C15H26O2	0.5
M240T847_pos	240.0981	847	3							HMDB0245533	2-Acetylacteoside	C10H13N3O4	1.0
M240T432_pos	240.1343	432	3							HMDB0251741	Eldoral	C11H17N3O3	0.2
M241T468_pos	241.0709	468	3							HMDB0303951	oxy-2-succinylcyclohexa-2,4-diene	C11H12O6	1.0
M241T703_pos	241.1436	703	3							HMDB0014862	Imiquimod	C14H16N4	4.9
M241T564_pos	241.1546	564	3							HMDB0015407	Pirbuterol	C12H20N2O3	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M235T373_pos	235.1106	373	3	5.12E-01	0.95	FALSE	5.54E-01	0.95	FALSE	5.75E-07	1.43	FALSE	3.98E-01	0.86	FALSE
M235T706_pos	235.1694	706	3	2.78E-11	1.45	FALSE	7.07E-01	0.98	FALSE	1.30E-01	0.93	FALSE	2.98E-01	1.09	FALSE
M235T940_pos	235.1693	940	3	1.15E-01	0.95	FALSE	4.56E-01	0.97	FALSE	1.58E-02	1.07	FALSE	2.50E-01	0.87	FALSE
M235T974_pos	235.1693	974	3	9.87E-01	1.00	FALSE	9.50E-01	1.01	FALSE	1.90E-01	1.14	FALSE	8.23E-01	0.97	FALSE
M235T1062_pos	235.1693	1062	3	1.32E-01	1.06	FALSE	6.81E-01	1.02	FALSE	6.59E-01	0.98	FALSE	6.71E-01	1.04	FALSE
M235T1059_pos	235.2057	1059	3	6.49E-01	1.03	FALSE	3.27E-01	1.06	FALSE	6.29E-01	0.97	FALSE	4.47E-01	1.11	FALSE
M235T1014_pos	235.2058	1014	3	1.45E-05	1.27	FALSE	8.13E-03	0.86	FALSE	1.12E-02	1.13	FALSE	7.76E-04	1.48	FALSE
M235T1038_pos	235.2422	1038	3	5.81E-04	1.25	FALSE	2.74E-01	1.07	FALSE	2.39E-01	0.94	FALSE	3.91E-01	1.12	FALSE
M236T104_pos	236.0797	104	3	9.55E-01	1.01	FALSE	4.48E-01	0.92	FALSE	3.84E-02	1.23	FALSE	7.42E-01	0.92	FALSE
M236T697_pos	236.1283	697	3	2.63E-07	1.23	FALSE	6.28E-01	0.98	FALSE	6.69E-02	1.06	FALSE	4.27E-03	0.84	FALSE
M236T510_pos	236.1638	510	3	1.67E-02	1.12	FALSE	1.24E-01	1.08	FALSE	2.44E-12	1.35	FALSE	7.70E-01	0.98	FALSE
M236T657_pos	236.1649	657	3	1.62E-04	1.24	FALSE	3.09E-01	0.94	FALSE	1.35E-03	1.17	FALSE	4.87E-01	0.89	FALSE
M237T361_pos	237.0874	361	3	6.18E-01	1.03	FALSE	6.25E-01	0.98	FALSE	1.65E-07	1.27	FALSE	2.90E-01	0.92	FALSE
M237T390_pos	237.1237	390	3	8.70E-01	0.99	FALSE	6.07E-03	0.84	FALSE	2.72E-10	1.40	FALSE	1.59E-02	1.32	FALSE
M237T1014_pos	237.1480	1014	3	3.20E-01	0.98	FALSE	7.37E-01	1.01	FALSE	3.89E-01	1.01	FALSE	9.04E-01	0.99	FALSE
M237T790_pos	237.1850	790	3	5.75E-15	1.40	FALSE	5.64E-02	1.08	FALSE	3.69E-01	1.03	FALSE	6.98E-01	1.04	FALSE
M237T726_pos	237.1850	726	3	3.29E-14	1.43	FALSE	2.45E-01	1.06	FALSE	1.36E-01	0.95	FALSE	3.28E-01	1.12	FALSE
M237T1056_pos	237.2214	1056	3	8.88E-01	1.01	FALSE	6.67E-01	0.97	FALSE	5.31E-01	0.96	FALSE	7.74E-01	0.94	FALSE
M238T510_pos	238.0712	510	3	1.38E-02	0.89	FALSE	7.50E-01	1.02	FALSE	1.27E-17	1.49	FALSE	1.23E-01	0.88	FALSE
M238T569_pos	238.0713	569	3	3.28E-01	1.05	FALSE	4.78E-01	0.97	FALSE	2.00E-05	1.20	FALSE	4.68E-01	0.91	FALSE
M238T591_pos	238.1076	591	3	7.17E-04	1.22	FALSE	6.34E-02	1.12	FALSE	2.03E-07	1.31	FALSE	6.18E-01	0.95	FALSE
M238T670_pos	238.1076	670	3	3.22E-09	1.32	FALSE	1.45E-01	1.07	FALSE	7.10E-04	1.14	FALSE	9.58E-01	0.99	FALSE
M238T532_pos	238.1439	532	3	4.20E-03	1.26	FALSE	3.80E-01	1.08	FALSE	5.54E-05	1.34	FALSE	4.64E-01	1.08	FALSE
M238T461_pos	238.1445	461	3	7.70E-02	1.15	FALSE	1.02E-01	1.15	FALSE	1.07E-02	1.19	FALSE	4.05E-01	1.14	FALSE
M239T457_pos	239.0922	457	3	5.43E-01	1.06	FALSE	1.68E-02	1.26	FALSE	2.64E-03	1.27	FALSE	8.51E-02	1.24	FALSE
M239T744_pos	239.0915	744	3	1.11E-09	1.38	FALSE	4.87E-03	1.16	FALSE	7.85E-03	1.12	FALSE	7.00E-01	1.06	FALSE
M239T574_2_pos	239.1393	574	3	6.88E-01	1.02	FALSE	6.41E-01	0.98	FALSE	3.17E-12	1.31	FALSE	1.44E-01	0.89	FALSE
M239T1066_pos	239.1490	1066	3	6.98E-01	0.99	FALSE	7.55E-02	0.97	FALSE	9.23E-01	1.00	FALSE	9.31E-02	0.92	FALSE
M239T932_pos	239.1636	932	3	8.79E-02	1.08	FALSE	9.31E-01	1.00	FALSE	7.38E-07	1.22	FALSE	8.59E-02	0.81	FALSE
M239T1041_pos	239.2007	1041	3	3.63E-01	1.02	FALSE	8.00E-01	0.99	FALSE	2.42E-01	0.97	FALSE	6.81E-04	1.29	FALSE
M240T847_pos	240.0981	847	3	1.33E-02	1.26	FALSE	8.82E-04	0.74	FALSE	6.10E-01	0.96	FALSE	9.84E-01	1.00	FALSE
M240T432_pos	240.1343	432	3	5.55E-02	1.18	FALSE	4.48E-01	1.07	FALSE	1.66E-05	1.39	FALSE	4.74E-01	0.93	FALSE
M241T468_pos	241.0709	468	3	3.33E-05	1.42	FALSE	4.73E-01	0.94	FALSE	8.96E-01	1.01	FALSE	4.51E-01	1.10	FALSE
M241T703_pos	241.1436	703	3	1.13E-05	1.24	FALSE	5.46E-01	1.03	FALSE	6.00E-04	1.15	FALSE	4.22E-02	0.82	FALSE
M241T564_pos	241.1546	564	3	2.52E-01	0.92	FALSE	6.15E-01	0.96	FALSE	4.30E-04	1.27	FALSE	4.82E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M241T514_pos	241.1548	514	3							HMDB0015407	Pirbuterol	C12H20N2O3	0.5
M241T413_pos	241.1548	413	3							HMDB0015407	Pirbuterol	C12H20N2O3	0.5
M241T1016_pos	241.1799	1016	3							HMDB0032369	L-Menthyl acetoacetate	C14H24O3	0.4
M241T987_pos	241.2164	987	3							HMDB0029765	9-Pentadecenoic acid	C15H28O2	0.7
M241T1038_pos	241.2163	1038	3							HMDB0029765	9-Pentadecenoic acid	C15H28O2	0.5
M242T618_pos	242.0848	618	3							HMDB0040289	ylsulfinylmethyl)phenyl methylcarb	C11H15NO3S	1.0
M242T590_pos	242.1136	590	3							HMDB0002224	5-Methyldeoxycytidine	C10H15N3O4	0.5
M242T616_pos	242.1390	616	3							HMDB0242338	ethylpropyl]-4-propyl-6-oxa-2-aza	C12H19NO4	1.4
M243T968_2_pos	243.1958	968	3							HMDB0010730	3-Oxotetradecanoic acid	C14H26O3	1.4
M243T1077_pos	243.2320	1077	3							HMDB0000826	Pentadecanoic acid	C15H30O2	0.4
M244T360_pos	244.1292	360	3							HMDB0028805	Glutaminylproline	C10H17N3O4	0.2
M244T403_pos	244.1292	403	3							HMDB0028805	Glutaminylproline	C10H17N3O4	0.0
M244T742_pos	244.1545	742	3							HMDB0002366	Tiglylcarnitine	C12H21NO4	0.8
M245T756_pos	245.1384	756	3							HMDB0032472	Polyethylene, oxidized	C12H20O5	0.4
M245T1038_pos	245.2265	1038	3						Fatty acids	HMDB0260170	6,7,8,9,10,11,12,14,15,16,17-tetra	C18H28	0.5
M246T152_pos	246.1086	152	3							HMDB0028732	Asparaginylhydroxyproline	C9H15N3O5	0.7
M246T468_1_pos	246.1341	468	3							HMDB0241651	3-Oxobutanoylcarnitine	C11H19NO5	2.0
M247T1016_pos	247.2271	1016	3						Fatty acids	HMDB0034557	,8-Diethoxy-2,6-dimethyl-2-octan	C14H30O3	1.3
M247T1080_pos	247.2421	1080	3							HMDB0251572	Dodecylbenzene	C18H30	0.5
M248T512_pos	248.1490	512	3							HMDB0013127	3-Hydroxybutyrylcarnitine	C11H21NO5	1.1
M248T525_pos	248.1644	525	3							HMDB0014597	Meperidine	C15H21NO2	0.5
M248T883_pos	248.1857	883	3						Fatty acids				
M249T740_pos	249.1123	740	3							HMDB0029575	-hydroxy-4-methoxy-6-(2-phenyle	C14H16O4	0.7
M249T361_pos	249.1241	361	3							HMDB0004081	6-Hydroxymelatonin	C13H16N2O3	3.0
M249T409_pos	249.1237	409	3							HMDB0004081	6-Hydroxymelatonin	C13H16N2O3	1.2
M249T473_pos	249.1237	473	3							HMDB0004081	6-Hydroxymelatonin	C13H16N2O3	1.4
M249T913_pos	249.1482	913	3							HMDB0030757	(S)-Pterosin A	C15H20O3	1.1
M249T455_pos	249.1598	455	3							HMDB0015095	Pindolol	C14H20N2O2	0.4
M249T957_pos	249.1846	957	3							HMDB0032228	Dimethylbenzyl carbinyl hexanoate	C16H24O2	1.1
M249T891_pos	249.1852	891	3						Fatty acids	HMDB0032228	Dimethylbenzyl carbinyl hexanoate	C16H24O2	1.3
M250T577_pos	250.1803	577	3							HMDB0015004	Alprenolol	C15H23NO2	0.7
M250T676_pos	250.1802	676	3							HMDB0015004	Alprenolol	C15H23NO2	0.3
M251T868_2_pos	251.0796	868	3							HMDB0250519	Cppene	C8H15N2O5P	1.8
M251T674_pos	251.1033	674	3							HMDB0240342	N-Acetylkynurenine	C12H14N2O4	2.5
M251T860_pos	251.1256	860	3						Fatty acids	HMDB0250896	Dda-tetracycline	C10H14N6O2	2.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M241T514_pos	241.1548	514	3	3.32E-04	1.19	FALSE	1.68E-01	1.07	FALSE	4.69E-05	1.19	FALSE	1.45E-01	1.16	FALSE
M241T413_pos	241.1548	413	3	1.33E-05	1.38	FALSE	2.30E-02	1.18	FALSE	2.84E-04	1.26	FALSE	4.75E-01	1.12	FALSE
M241T1016_pos	241.1799	1016	3	2.62E-10	1.38	FALSE	5.86E-02	0.91	FALSE	2.25E-05	1.20	FALSE	5.50E-01	1.03	FALSE
M241T987_pos	241.2164	987	3	2.06E-01	1.07	FALSE	1.04E-01	1.09	FALSE	9.98E-01	1.00	FALSE	4.15E-01	1.11	FALSE
M241T1038_pos	241.2163	1038	3	4.98E-06	1.22	FALSE	8.05E-04	0.86	FALSE	3.50E-03	0.90	FALSE	5.65E-03	1.17	FALSE
M242T618_pos	242.0848	618	3	2.79E-01	1.06	FALSE	4.84E-01	1.04	FALSE	1.33E-04	1.19	FALSE	8.80E-01	1.02	FALSE
M242T590_pos	242.1136	590	3	7.75E-01	0.98	FALSE	4.16E-01	0.95	FALSE	4.42E-06	1.30	FALSE	4.48E-01	0.88	FALSE
M242T616_pos	242.1390	616	3	8.44E-03	1.23	FALSE	8.21E-02	1.16	FALSE	1.42E-05	1.36	FALSE	2.53E-02	1.36	FALSE
M243T968_2_pos	243.1958	968	3	7.87E-02	1.16	FALSE	7.67E-01	1.03	FALSE	1.12E-01	1.12	FALSE	6.07E-01	0.91	FALSE
M243T1077_pos	243.2320	1077	3	6.11E-02	1.26	FALSE	1.84E-01	0.86	FALSE	7.27E-01	1.04	FALSE	9.73E-01	0.99	FALSE
M244T360_pos	244.1292	360	3	4.65E-08	0.76	FALSE	2.64E-02	1.12	FALSE	1.04E-08	1.29	FALSE	2.80E-01	1.12	FALSE
M244T403_pos	244.1292	403	3	1.07E-03	1.18	FALSE	3.25E-03	1.17	FALSE	1.23E-10	1.35	FALSE	1.50E-02	1.10	FALSE
M244T742_pos	244.1545	742	3	3.07E-05	0.74	FALSE	3.33E-07	1.46	FALSE	2.74E-06	1.34	FALSE	1.72E-01	1.15	FALSE
M245T756_pos	245.1384	756	3	3.98E-07	0.87	FALSE	7.09E-08	1.16	FALSE	2.37E-29	1.37	FALSE	7.38E-02	0.93	FALSE
M245T1038_pos	245.2265	1038	3	9.28E-04	1.35	FALSE	1.36E-03	0.73	FALSE	3.24E-04	1.33	FALSE	7.63E-01	1.04	FALSE
M246T152_pos	246.1086	152	3	2.46E-02	1.21	FALSE	1.52E-01	0.89	FALSE	2.82E-07	1.50	FALSE	4.64E-02	0.78	FALSE
M246T468_1_pos	246.1341	468	3	1.28E-04	1.33	FALSE	3.90E-01	0.94	FALSE	1.04E-05	1.33	FALSE	8.07E-02	0.91	FALSE
M247T1016_pos	247.2271	1016	3	3.72E-01	0.97	FALSE	4.84E-01	1.03	FALSE	8.06E-01	1.01	FALSE	1.82E-01	1.18	FALSE
M247T1080_pos	247.2421	1080	3	2.75E-01	1.15	FALSE	6.89E-01	0.94	FALSE	2.37E-03	1.42	FALSE	9.33E-01	0.98	FALSE
M248T512_pos	248.1490	512	3	1.49E-02	1.27	FALSE	4.97E-01	0.93	FALSE	8.05E-02	1.16	FALSE	1.31E-01	0.86	FALSE
M248T525_pos	248.1644	525	3	1.94E-01	1.07	FALSE	8.34E-01	1.01	FALSE	6.43E-15	1.49	FALSE	4.73E-01	0.95	FALSE
M248T883_pos	248.1857	883	3	1.34E-02	0.94	FALSE	2.32E-01	1.03	FALSE	1.93E-02	1.06	FALSE	3.91E-01	1.10	FALSE
M249T740_pos	249.1123	740	3	4.06E-09	1.25	FALSE	4.26E-03	1.11	FALSE	1.62E-03	1.11	FALSE	1.48E-01	1.12	FALSE
M249T361_pos	249.1241	361	3	1.18E-04	1.27	FALSE	1.85E-01	0.92	FALSE	2.48E-01	1.06	FALSE	4.72E-01	1.03	FALSE
M249T409_pos	249.1237	409	3	3.36E-04	1.27	FALSE	2.00E-01	0.92	FALSE	2.12E-09	1.44	FALSE	2.65E-01	0.90	FALSE
M249T473_pos	249.1237	473	3	1.08E-02	1.26	FALSE	2.82E-01	0.90	FALSE	1.53E-02	1.21	FALSE	7.54E-01	0.96	FALSE
M249T913_pos	249.1482	913	3	2.37E-01	1.09	FALSE	1.77E-01	0.89	FALSE	8.31E-03	1.19	FALSE	4.12E-03	1.46	FALSE
M249T455_pos	249.1598	455	3	6.55E-06	1.39	FALSE	1.86E-01	1.10	FALSE	1.81E-06	1.35	FALSE	4.00E-02	0.86	FALSE
M249T957_pos	249.1846	957	3	4.91E-01	1.03	FALSE	1.13E-02	0.89	FALSE	4.29E-03	0.90	FALSE	2.82E-01	1.16	FALSE
M249T891_pos	249.1852	891	3	6.44E-01	0.98	FALSE	3.62E-02	1.08	FALSE	1.34E-16	1.33	FALSE	9.30E-01	0.99	FALSE
M250T577_pos	250.1803	577	3	7.36E-03	1.11	FALSE	2.89E-01	1.04	FALSE	3.17E-20	1.43	FALSE	4.65E-01	0.96	FALSE
M250T676_pos	250.1802	676	3	1.23E-02	1.23	FALSE	3.08E-01	0.91	FALSE	3.10E-03	1.24	FALSE	3.27E-01	0.82	FALSE
M251T868_2_pos	251.0796	868	3	2.77E-11	1.14	FALSE	7.22E-01	1.01	FALSE	5.74E-10	0.90	FALSE	6.71E-01	1.02	FALSE
M251T674_pos	251.1033	674	3	7.48E-01	1.02	FALSE	7.20E-01	1.02	FALSE	6.25E-10	1.38	FALSE	1.03E-02	0.88	FALSE
M251T860_pos	251.1256	860	3	2.32E-01	0.95	FALSE	5.83E-01	0.98	FALSE	2.79E-01	1.04	FALSE	4.16E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M251T496_pos	251.1393	496	3							HMDB0015443	Heptabarbital	C13H18N2O3	1.1
M251T445_pos	251.1392	445	3							HMDB0015443	Heptabarbital	C13H18N2O3	0.9
M251T397_pos	251.1393	397	3							HMDB0015443	Heptabarbital	C13H18N2O3	1.1
M251T839_pos	251.1643	839	3							HMDB0015371	Gemfibrozil	C15H22O3	0.6
M251T487_pos	251.1755	487	3							HMDB0015124	Rivastigmine	C14H22N2O2	0.4
M251T1008_pos	251.2003	1008	3							HMDB0035293	Norambreinolide	C16H26O2	1.0
M252T657_pos	252.1335	657	3							HMDB0246659	L-Leucine-p-nitroanilide	C12H17N3O3	2.9
M252T586_pos	252.1596	586	3							HMDB0245262	2-Nitrophenyl octyl ether	C14H21NO3	0.8
M252T1044_pos	252.2325	1044	3							HMDB0030275	Herculin	C16H29NO	1.4
M253T494_pos	253.0813	494	3							HMDB0004086	5-Hydroxy-N-formylkynurenine	C11H12N2O5	2.3
M253T571_1_pos	253.0937	571	3							HMDB0000071	Deoxyinosine	C10H12N4O4	2.2
M253T430_pos	253.1273	430	3							HMDB0040822	2,3-Butanediol glucoside	C10H20O7	3.6
M253T764_pos	253.1434	764	3							HMDB0033197	methyl-6-(1-oxobutyl)-1,3,5-cyclol	C14H20O4	0.1
M253T706_pos	253.1800	706	3							HMDB0030918	1-Hydroxyepiacorone	C15H24O3	0.9
M253T940_pos	253.1799	940	3						Terpenoids	HMDB0030918	1-Hydroxyepiacorone	C15H24O3	0.3
M253T783_pos	253.1800	783	3							HMDB0030918	1-Hydroxyepiacorone	C15H24O3	0.6
M253T1014_pos	253.2162	1014	3							HMDB0000477	7Z,10Z-Hexadecadienoic acid	C16H28O2	0.1
M254T418_pos	254.0663	418	3							HMDB0039506	N-Salicyloylaspartic acid	C11H11NO6	1.4
M254T402_pos	254.1028	402	3							HMDB0011716	N-Acetylvanilalanine	C12H15NO5	2.1
M254T761_pos	254.1757	761	3							HMDB0244460	,5-Trimethylcyclohexyl ester5-oxo	C14H23NO3	2.5
M254T879_pos	254.1754	879	3							HMDB0244460	,5-Trimethylcyclohexyl ester5-oxo	C14H23NO3	1.5
M254T1032_pos	254.2480	1032	3							HMDB0256086	Palmitoleamide	C16H31NO	0.5
M254T972_pos	254.2480	972	3							HMDB0256086	Palmitoleamide	C16H31NO	0.5
M255T371_pos	255.1345	371	3							HMDB0014356	Midodrine	C12H18N2O4	2.2
M255T878_pos	255.1591	878	3							HMDB0249518	C75 trans	C14H22O4	0.1
M255T798_pos	255.1592	798	3							HMDB0249518	C75 trans	C14H22O4	0.4
M255T791_pos	255.1956	791	3							HMDB0029604	Lubiminol	C15H26O3	0.6
M255T872_pos	255.1956	872	3							HMDB0029604	Lubiminol	C15H26O3	0.6
M257T414_pos	257.1140	414	3							HMDB0011648	D-Ribofuranosyl)-1,4-dihydronicot	C11H16N2O5	3.2
M257T827_pos	257.1747	827	3							HMDB0030993	ltetrahydro-2-oxo-3-furancarboxy	C14H24O4	0.0
M257T1007_pos	257.2113	1007	3						Fatty acids	HMDB0040904	Ipomeatetrahydrofuran	C15H28O3	0.8
M257T308_pos	257.2478	308	3							HMDB0000220	Palmitic acid	C16H32O2	1.3
M257T229_pos	257.2478	229	3							HMDB0000220	Palmitic acid	C16H32O2	1.2
M258T342_pos	258.1087	342	3							HMDB0000982	5-Methylcytidine	C10H15N3O5	1.1
M258T502_pos	258.1085	502	3							HMDB0000982	5-Methylcytidine	C10H15N3O5	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M251T496_pos	251.1393	496	3	1.50E-04	1.17	FALSE	8.31E-01	1.01	FALSE	1.63E-11	1.29	FALSE	5.64E-02	0.90	FALSE
M251T445_pos	251.1392	445	3	3.20E-02	1.11	FALSE	8.63E-01	0.99	FALSE	8.56E-12	1.37	FALSE	5.50E-01	0.95	FALSE
M251T397_pos	251.1393	397	3	6.82E-01	0.98	FALSE	2.70E-01	0.94	FALSE	1.09E-06	1.25	FALSE	3.14E-01	0.82	FALSE
M251T839_pos	251.1643	839	3	5.71E-01	1.02	FALSE	3.96E-01	1.03	FALSE	4.75E-02	1.06	FALSE	8.88E-01	1.02	FALSE
M251T487_pos	251.1755	487	3	3.04E-02	0.90	FALSE	3.51E-01	1.05	FALSE	3.10E-17	1.50	FALSE	2.61E-01	0.94	FALSE
M251T1008_pos	251.2003	1008	3	5.13E-01	1.04	FALSE	8.35E-01	1.01	FALSE	3.60E-01	1.05	FALSE	1.47E-01	1.15	FALSE
M252T657_pos	252.1335	657	3	5.82E-01	0.84	FALSE	6.32E-01	1.22	FALSE	8.12E-01	0.93	FALSE	4.30E-01	0.88	FALSE
M252T586_pos	252.1596	586	3	9.17E-02	1.10	FALSE	7.87E-02	1.11	FALSE	2.05E-08	1.32	FALSE	5.87E-02	1.35	FALSE
M252T1044_pos	252.2325	1044	3	8.69E-01	1.01	FALSE	5.50E-01	1.04	FALSE	2.75E-01	0.94	FALSE	6.53E-01	0.95	FALSE
M253T494_pos	253.0813	494	3	5.08E-02	0.76	FALSE	9.56E-01	1.01	FALSE	5.19E-01	0.93	FALSE	5.20E-01	0.90	FALSE
M253T571_1_pos	253.0937	571	3	6.41E-02	1.11	FALSE	4.89E-01	0.96	FALSE	4.00E-13	1.49	FALSE	1.20E-02	0.81	FALSE
M253T430_pos	253.1273	430	3	4.70E-05	1.26	FALSE	5.35E-01	1.04	FALSE	1.01E-03	1.17	FALSE	6.31E-01	1.06	FALSE
M253T764_pos	253.1434	764	3	1.77E-01	1.10	FALSE	1.51E-04	1.33	FALSE	9.55E-01	1.00	FALSE	6.76E-01	0.97	FALSE
M253T706_pos	253.1800	706	3	9.96E-03	1.29	FALSE	7.65E-01	0.97	FALSE	2.62E-02	1.21	FALSE	4.04E-01	0.92	FALSE
M253T940_pos	253.1799	940	3	1.99E-01	1.03	FALSE	9.30E-01	1.00	FALSE	3.56E-03	1.06	FALSE	1.20E-01	0.93	FALSE
M253T783_pos	253.1800	783	3	3.74E-09	1.28	FALSE	2.49E-03	1.14	FALSE	7.43E-04	1.13	FALSE	2.42E-01	0.89	FALSE
M253T1014_pos	253.2162	1014	3	8.80E-07	1.43	FALSE	4.01E-04	0.78	FALSE	1.35E-03	1.22	FALSE	9.45E-03	1.42	FALSE
M254T418_pos	254.0663	418	3	8.14E-04	0.70	FALSE	2.98E-01	0.89	FALSE	2.85E-01	1.10	FALSE	7.37E-01	0.92	FALSE
M254T402_pos	254.1028	402	3	7.78E-03	0.77	FALSE	4.61E-02	0.82	FALSE	1.14E-04	1.39	FALSE	5.52E-01	0.81	FALSE
M254T761_pos	254.1757	761	3	4.08E-12	1.30	FALSE	7.62E-02	1.07	FALSE	1.06E-01	1.05	FALSE	3.43E-04	0.78	FALSE
M254T879_pos	254.1754	879	3	4.42E-05	1.46	FALSE	1.21E-02	1.27	FALSE	1.48E-01	1.12	FALSE	1.60E-02	1.21	FALSE
M254T1032_pos	254.2480	1032	3	1.56E-01	0.92	FALSE	6.77E-01	1.03	FALSE	2.54E-01	0.94	FALSE	3.36E-01	1.16	FALSE
M254T972_pos	254.2480	972	3	2.60E-17	0.87	FALSE	1.51E-01	1.02	FALSE	3.36E-02	0.97	FALSE	5.02E-01	1.03	FALSE
M255T371_pos	255.1345	371	3	1.76E-02	0.86	FALSE	3.34E-01	1.07	FALSE	3.47E-10	1.45	FALSE	4.89E-01	1.11	FALSE
M255T878_pos	255.1591	878	3	1.19E-02	0.94	FALSE	3.72E-02	1.05	FALSE	2.27E-03	0.94	FALSE	5.90E-03	1.26	FALSE
M255T798_pos	255.1592	798	3	8.38E-01	0.99	FALSE	1.01E-01	1.07	FALSE	3.18E-02	1.07	FALSE	5.06E-02	0.79	FALSE
M255T791_pos	255.1956	791	3	6.84E-05	1.21	FALSE	3.20E-01	1.05	FALSE	1.36E-02	1.11	FALSE	2.78E-01	1.12	FALSE
M255T872_pos	255.1956	872	3	2.06E-01	1.11	FALSE	2.72E-01	1.09	FALSE	2.23E-01	1.09	FALSE	3.34E-01	1.22	FALSE
M257T414_pos	257.1140	414	3	1.52E-01	1.09	FALSE	5.63E-01	0.96	FALSE	1.71E-03	1.17	FALSE	4.96E-01	1.11	FALSE
M257T827_pos	257.1747	827	3	3.72E-02	0.93	FALSE	1.52E-01	0.95	FALSE	1.43E-01	1.05	FALSE	2.28E-01	0.89	FALSE
M257T1007_pos	257.2113	1007	3	2.76E-01	1.89	FALSE	5.31E-01	0.63	FALSE	1.23E-01	2.22	FALSE	8.68E-01	0.89	FALSE
M257T308_pos	257.2478	308	3	4.74E-01	0.96	FALSE	5.80E-01	1.04	FALSE	5.78E-01	0.97	FALSE	1.11E-01	1.30	FALSE
M257T229_pos	257.2478	229	3	5.13E-02	1.15	FALSE	7.45E-01	1.02	FALSE	9.15E-01	1.01	FALSE	6.25E-01	1.08	FALSE
M258T342_pos	258.1087	342	3	9.39E-01	0.99	FALSE	3.78E-01	0.92	FALSE	5.38E-06	1.44	FALSE	2.33E-01	0.77	FALSE
M258T502_pos	258.1085	502	3	9.46E-01	1.01	FALSE	3.15E-01	0.92	FALSE	2.07E-07	1.43	FALSE	2.63E-01	0.80	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M258T701_pos	258.1701	701	3							HMDB0013161	2-Hexenoylcarnitine	C13H23NO4	0.5
M259T534_pos	259.0753	534	3							HMDB0246637	ydroxy-3-phenoxyphenyl)propano	C10H14N2O4S	2.1
M259T367_pos	259.1292	367	3							HMDB0038614	gamma-L-Glutamyl-L-pipecolic acid	C11H18N2O5	1.4
M259T998_pos	259.1904	998	3							HMDB0000872	Tetradecanedioic acid	C14H26O4	0.2
M260T148_pos	260.1242	148	3							HMDB0028798	Glutaminylhydroxyproline	C10H17N3O5	0.4
M260T349_pos	260.1244	349	3							HMDB0028798	Glutaminylhydroxyproline	C10H17N3O5	1.1
M260T249_pos	260.1243	249	3							HMDB0028798	Glutaminylhydroxyproline	C10H17N3O5	0.9
M260T659_pos	260.1496	659	3							HMDB0241663	3-Oxopentanoylcarnitine	C12H21NO5	1.3
M261T82_pos	261.0308	82	3							HMDB0014672	Cyclophosphamide	C7H15Cl2N2O2P	5.0
M261T780_pos	261.1124	780	3							HMDB0030110	Celerin	C15H16O4	1.0
M261T1002_pos	261.2214	1002	3						Fatty acids	HMDB0245878	3-Gonal	C18H28O	0.4
M262T671_pos	262.1649	671	3							HMDB0061189	3-Hydroxyisovalerylcarnitine	C12H23NO5	0.2
M262T757_pos	262.1650	757	3							HMDB0061189	3-Hydroxyisovalerylcarnitine	C12H23NO5	0.5
M263T1034_pos	263.1992	1034	3							HMDB0032501	Santalyl acetate	C17H26O2	5.0
M265T957_pos	265.1793	957	3							HMDB0032090	Oxo-2,3-dinor-10,15-phytodienoic	C16H24O3	2.1
M265T878_pos	265.1800	878	3							HMDB0032090	Oxo-2,3-dinor-10,15-phytodienoic	C16H24O3	0.8
M265T601_pos	265.1913	601	3							HMDB0248344	Matrine 1beta-oxide	C15H24N2O2	0.9
M266T529_pos	266.1755	529	3							HMDB0015520	Oxprenolol	C15H23NO3	1.6
M266T642_pos	266.1753	642	3							HMDB0015520	Oxprenolol	C15H23NO3	0.7
M267T755_pos	267.1210	755	3							HMDB0246876	beta-Pregnane-3alpha,20alpha-dio	C10H14N6O3	3.7
M267T1032_pos	267.1722	1032	3							HMDB0303280	Potassium myristate	C14H27KO2	0.5
M267T1039_pos	267.2679	1039	3							HMDB0030965	9-Octadecenal	C18H34O	1.3
M269T608_pos	269.1496	608	3							HMDB0247322	(2-hydroxyethyl)amino-L-phenylala	C13H20N2O4	0.0
M269T992_pos	269.1772	992	3							HMDB0030347	N-(p-Hydroxyphenethyl)actinidine	C18H22NO	0.9
M269T690_pos	269.1750	690	3						Terpenoids	HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	0.9
M269T838_pos	269.1749	838	3						Terpenoids	HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	0.7
M269T1046_pos	269.2477	1046	3							HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	0.8
M269T993_pos	269.2480	993	3							HMDB0030997	Cyclohexaneundecanoic acid	C17H32O2	1.7
M270T630_pos	270.1338	630	3							HMDB0251804	Endralazine	C14H15N5O	4.0
M270T958_pos	270.2430	958	3						Fatty acids				
M271T501_1_pos	271.0815	501	3							HMDB0059806	Phenylglucuronide	C12H14O7	0.9
M271T442_pos	271.0816	442	3							HMDB0059806	Phenylglucuronide	C12H14O7	1.4
M271T919_pos	271.1891	919	3							HMDB0040459	Ethylene brassylate	C15H26O4	4.8
M271T704_pos	271.1906	704	3							HMDB0040459	Ethylene brassylate	C15H26O4	0.8
M271T902_pos	271.2270	902	3							HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M258T701_pos	258.1701	701	3	1.79E-04	1.32	FALSE	2.53E-01	1.09	FALSE	1.70E-01	1.09	FALSE	2.95E-03	0.82	FALSE
M259T534_pos	259.0753	534	3	3.32E-02	1.12	FALSE	9.05E-01	0.99	FALSE	3.88E-14	1.47	FALSE	1.94E-01	0.90	FALSE
M259T367_pos	259.1292	367	3	4.23E-01	1.06	FALSE	9.06E-01	1.01	FALSE	8.48E-01	0.99	FALSE	6.42E-01	1.12	FALSE
M259T998_pos	259.1904	998	3	9.08E-01	1.01	FALSE	8.38E-01	0.99	FALSE	2.03E-01	0.93	FALSE	3.97E-01	1.21	FALSE
M260T148_pos	260.1242	148	3	3.98E-04	0.75	FALSE	1.05E-01	0.87	FALSE	6.92E-03	1.21	FALSE	5.15E-02	0.63	FALSE
M260T349_pos	260.1244	349	3	5.36E-03	0.91	FALSE	7.01E-01	1.01	FALSE	5.48E-22	1.40	FALSE	4.31E-02	1.05	FALSE
M260T249_pos	260.1243	249	3	1.12E-02	1.12	FALSE	3.90E-02	1.10	FALSE	2.52E-18	1.45	FALSE	9.38E-01	1.00	FALSE
M260T659_pos	260.1496	659	3	1.34E-04	1.17	FALSE	6.25E-03	1.13	FALSE	2.32E-11	1.29	FALSE	1.83E-01	0.88	FALSE
M261T82_pos	261.0308	82	3	2.81E-01	0.91	FALSE	9.54E-01	1.00	FALSE	4.45E-01	1.06	FALSE	5.05E-04	0.83	FALSE
M261T780_pos	261.1124	780	3	2.90E-01	0.96	FALSE	1.65E-01	1.05	FALSE	7.71E-06	1.15	FALSE	1.24E-01	0.87	FALSE
M261T1002_pos	261.2214	1002	3	4.60E-02	1.12	FALSE	1.53E-02	0.86	FALSE	1.18E-02	1.13	FALSE	5.19E-01	0.93	FALSE
M262T671_pos	262.1649	671	3	5.10E-09	1.40	FALSE	4.41E-01	1.05	FALSE	2.96E-01	0.95	FALSE	6.00E-01	1.07	FALSE
M262T757_pos	262.1650	757	3	8.34E-01	0.99	FALSE	1.68E-07	1.16	FALSE	2.47E-20	1.28	FALSE	6.53E-02	0.89	FALSE
M263T1034_pos	263.1992	1034	3	1.68E-01	1.27	FALSE	9.14E-01	1.02	FALSE	2.71E-02	1.41	FALSE	8.46E-01	1.07	FALSE
M265T957_pos	265.1793	957	3	1.55E-01	0.94	FALSE	5.80E-01	0.97	FALSE	1.54E-03	0.88	FALSE	2.15E-01	1.18	FALSE
M265T878_pos	265.1800	878	3	1.67E-01	0.95	FALSE	3.42E-03	1.12	FALSE	5.15E-16	1.34	FALSE	1.98E-01	0.92	FALSE
M265T601_pos	265.1913	601	3	4.71E-01	0.94	FALSE	5.93E-04	1.39	FALSE	1.48E-06	1.48	FALSE	7.49E-01	0.95	FALSE
M266T529_pos	266.1755	529	3	4.60E-01	1.04	FALSE	1.43E-01	1.08	FALSE	2.57E-16	1.49	FALSE	5.01E-01	0.97	FALSE
M266T642_pos	266.1753	642	3	3.50E-02	1.09	FALSE	3.23E-03	1.13	FALSE	7.24E-19	1.42	FALSE	6.99E-01	1.01	FALSE
M267T755_pos	267.1210	755	3	3.12E-02	0.93	FALSE	1.33E-06	1.17	FALSE	2.31E-17	1.29	FALSE	9.55E-01	1.00	FALSE
M267T1032_pos	267.1722	1032	3	1.88E-02	0.83	FALSE	1.51E-01	0.89	FALSE	1.15E-01	1.12	FALSE	4.24E-01	0.81	FALSE
M267T1039_pos	267.2679	1039	3	1.16E-01	0.85	FALSE	5.71E-01	1.06	FALSE	5.50E-02	0.84	FALSE	6.84E-03	1.34	FALSE
M269T608_pos	269.1496	608	3	7.89E-02	1.10	FALSE	3.05E-01	0.95	FALSE	4.13E-06	1.24	FALSE	3.09E-02	0.83	FALSE
M269T992_pos	269.1772	992	3	7.17E-01	1.03	FALSE	2.51E-01	0.88	FALSE	6.95E-02	1.16	FALSE	4.95E-01	0.87	FALSE
M269T690_pos	269.1750	690	3	2.09E-08	1.32	FALSE	2.43E-01	0.94	FALSE	1.95E-04	1.17	FALSE	4.36E-01	0.96	FALSE
M269T838_pos	269.1749	838	3	1.63E-01	1.10	FALSE	7.57E-01	1.02	FALSE	2.39E-05	1.29	FALSE	1.38E-01	0.90	FALSE
M269T1046_pos	269.2477	1046	3	5.11E-01	1.05	FALSE	1.14E-01	0.88	FALSE	1.09E-04	1.29	FALSE	2.84E-01	0.76	FALSE
M269T993_pos	269.2480	993	3	5.06E-01	1.06	FALSE	7.23E-02	0.86	FALSE	1.20E-04	1.33	FALSE	9.01E-01	0.97	FALSE
M270T630_pos	270.1338	630	3	8.10E-02	1.11	FALSE	3.30E-01	1.06	FALSE	7.62E-06	1.27	FALSE	4.40E-02	0.80	FALSE
M270T958_pos	270.2430	958	3	2.03E-01	1.19	FALSE	4.43E-01	1.11	FALSE	7.18E-01	0.96	FALSE	3.99E-01	1.10	FALSE
M271T501_1_pos	271.0815	501	3	1.22E-02	1.20	FALSE	1.46E-01	1.11	FALSE	5.21E-08	1.43	FALSE	9.15E-01	0.99	FALSE
M271T442_pos	271.0816	442	3	1.71E-01	0.91	FALSE	7.47E-01	1.02	FALSE	1.11E-08	1.46	FALSE	4.96E-01	0.92	FALSE
M271T919_pos	271.1891	919	3	4.94E-01	1.02	FALSE	4.05E-01	1.02	FALSE	2.56E-04	0.92	FALSE	1.71E-08	-77.17	FALSE
M271T704_pos	271.1906	704	3	2.71E-08	1.33	FALSE	5.92E-01	1.03	FALSE	4.28E-01	1.03	FALSE	7.23E-01	0.98	FALSE
M271T902_pos	271.2270	902	3	9.37E-01	1.01	FALSE	6.88E-03	0.75	FALSE	1.71E-01	1.11	FALSE	1.76E-01	1.26	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M272T889_1_pos	272.1283	889	3							HMDB0014004	Norhydromorphone	C16H17NO3	0.8
M272T590_pos	272.1285	590	3							HMDB0014004	Norhydromorphone	C16H17NO3	1.3
M272T879_pos	272.1858	879	3							HMDB0241681	Hept-3-enoylcarnitine	C14H25NO4	0.7
M273T503_pos	273.1239	503	3							HMDB0035191	9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-t	C15H16N2O3	1.8
M273T889_pos	273.1318	889	3							HMDB0033663	Decarbamoylneosaxitoxin	C9H16N6O4	4.3
M273T1007_pos	273.1848	1007	3							HMDB0000151	Estradiol	C18H24O2	0.5
M273T568_pos	273.1921	568	3							HMDB0258266	methyl)amino)-1-oxohexyl)amino)p	C12H24N4O3	0.0
M273T1014_pos	273.2212	1014	3							HMDB0006046	5a-Androst-3-en-17-one	C19H28O	0.5
M274T509_pos	274.1286	509	3							HMDB0013129	Glutaconylcarnitine	C12H19NO6	0.4
M274T901_pos	274.1441	901	3							HMDB0030187	(E,E)-Piperlonguminine	C16H19NO3	1.1
M274T591_pos	274.2013	591	3							HMDB0013238	Heptanoylcarnitine	C14H27NO4	0.1
M275T591_pos	275.1033	591	3							HMDB0035115	rahydro-1-methyl-beta-carboline-1	C14H14N2O4	2.3
M275T1033_1_pos	275.1146	1033	3							HMDB0246359	4-Aminophenylphosphorylcholine	C11H19N2O4P	3.3
M275T575_pos	275.1392	575	3							HMDB0034885	Imazamethabenz	C15H18N2O3	0.6
M275T1070_pos	275.1643	1070	3							HMDB0032697	-Furanoeudesm-4(15)-en-1-ol acet	C17H22O3	0.6
M275T827_pos	275.1852	827	3							HMDB0000394	3-Hydroxytetradecanedioic acid	C14H26O5	0.4
M275T914_pos	275.2008	914	3							HMDB0002725	Nandrolone	C18H26O2	0.8
M275T1008_pos	275.2219	1008	3						Fatty acids	HMDB0072858	MG(0:0/i-12:0/0:0)	C15H30O4	0.7
M276T495_pos	276.0871	495	3							HMDB0253996	lavendustin c	C14H13NO5	1.8
M276T174_pos	276.1554	174	3							HMDB0003869	epsilon-(gamma-Glutamyl)lysine	C11H21N3O5	0.1
M277T765_pos	277.1074	765	3							HMDB0030145	Ascochitine	C15H16O5	1.1
M277T655_pos	277.1184	655	3							HMDB0062178	N-lactoyl-Tryptophan	C14H16N2O4	0.5
M277T944_pos	277.2164	944	3							HMDB0002697	19-Norandrosterone	C18H28O2	0.8
M278T460_1_pos	278.1058	460	3							HMDB0254508	METAZACHLOR	C14H16ClN3O	1.2
M278T634_pos	278.2117	634	3							HMDB0005016	Venlafaxine	C17H27NO2	1.0
M278T1066_pos	278.2467	1066	3							HMDB0256035	4-(Dodecylamino)Phenol	C18H31NO	4.0
M278T971_pos	278.2481	971	3							HMDB0256035	4-(Dodecylamino)Phenol	C18H31NO	0.8
M279T341_pos	279.0650	341	3							HMDB0252357	Fluorescamine	C17H10O4	0.6
M279T444_pos	279.1365	444	3							HMDB0003426	Pantetheine	C11H22N2O4S	2.9
M279T637_pos	279.2073	637	3							HMDB0248370	Amydricaine	C16H26N2O2	2.2
M279T955_pos	279.2320	955	3							HMDB0001388	alpha-Linolenic acid	C18H30O2	0.6
M280T383_pos	280.1286	383	3							HMDB0028738	Asparaginyl-Phenylalanine	C13H17N3O4	2.2
M280T1076_pos	280.2636	1076	3						Fatty acids	HMDB0062656	Linoleamide	C18H33NO	0.2
M281T659_pos	281.0792	659	3							HMDB0031863	na-Glutamyl-S-methylcysteine sulf	C9H16N2O6S	3.4
M281T905_pos	281.1386	905	3							HMDB0035620	Artabsinolide A	C15H20O5	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M272T889_1_pos	272.1283	889	3	1.99E-01	7.90	FALSE	7.86E-01	1.45	FALSE	2.77E-01	3.67	FALSE	2.39E-01	-0.45	FALSE
M272T590_pos	272.1285	590	3	1.32E-03	1.30	FALSE	7.93E-01	0.98	FALSE	2.35E-02	1.17	FALSE	6.94E-01	1.10	FALSE
M272T879_pos	272.1858	879	3	1.65E-04	1.35	FALSE	1.67E-02	1.21	FALSE	8.75E-02	1.12	FALSE	8.45E-02	1.21	FALSE
M273T503_pos	273.1239	503	3	2.94E-05	1.19	FALSE	1.24E-01	1.07	FALSE	3.08E-13	1.32	FALSE	9.22E-01	1.01	FALSE
M273T889_pos	273.1318	889	3	2.11E-01	4.20	FALSE	7.77E-01	1.36	FALSE	2.81E-01	2.72	FALSE	2.40E-01	-0.33	FALSE
M273T1007_pos	273.1848	1007	3	3.34E-01	1.04	FALSE	3.55E-01	0.96	FALSE	3.37E-05	0.85	FALSE	3.27E-01	0.89	FALSE
M273T568_pos	273.1921	568	3	2.43E-04	1.24	FALSE	4.08E-01	1.05	FALSE	6.47E-08	1.32	FALSE	4.52E-01	1.08	FALSE
M273T1014_pos	273.2212	1014	3	3.69E-02	1.19	FALSE	1.37E-01	0.88	FALSE	7.79E-01	0.98	FALSE	8.01E-01	0.97	FALSE
M274T509_pos	274.1286	509	3	3.46E-01	1.05	FALSE	5.00E-01	0.96	FALSE	2.60E-13	1.45	FALSE	5.57E-01	0.98	FALSE
M274T901_pos	274.1441	901	3	8.57E-01	1.15	FALSE	2.44E-01	0.05	FALSE	4.62E-01	0.60	FALSE	2.37E-01	0.27	FALSE
M274T591_pos	274.2013	591	3	1.01E-01	0.93	FALSE	6.12E-01	0.98	FALSE	1.20E-16	1.41	FALSE	6.71E-01	1.02	FALSE
M275T591_pos	275.1033	591	3	1.59E-02	1.24	FALSE	4.06E-01	0.92	FALSE	2.82E-01	0.92	FALSE	5.01E-02	1.96	FALSE
M275T1033_1_pos	275.1146	1033	3	5.09E-02	1.09	FALSE	1.31E-01	0.93	FALSE	6.43E-01	0.98	FALSE	3.79E-01	1.09	FALSE
M275T575_pos	275.1392	575	3	3.37E-03	1.15	FALSE	4.55E-01	1.04	FALSE	4.48E-15	1.41	FALSE	5.00E-01	0.95	FALSE
M275T1070_pos	275.1643	1070	3	5.14E-01	1.04	FALSE	1.18E-01	0.90	FALSE	9.49E-01	1.00	FALSE	3.38E-01	1.19	FALSE
M275T827_pos	275.1852	827	3	4.37E-01	1.04	FALSE	2.92E-02	1.11	FALSE	3.23E-12	1.34	FALSE	1.24E-01	0.90	FALSE
M275T914_pos	275.2008	914	3	3.50E-04	1.24	FALSE	4.18E-02	0.87	FALSE	3.56E-03	1.17	FALSE	3.88E-01	0.94	FALSE
M275T1008_pos	275.2219	1008	3	2.44E-01	2.93	FALSE	9.27E-01	0.91	FALSE	1.61E-01	3.14	FALSE	7.89E-01	0.80	FALSE
M276T495_pos	276.0871	495	3	6.44E-03	0.70	FALSE	2.89E-02	1.34	FALSE	3.76E-04	1.50	FALSE	6.83E-02	1.15	FALSE
M276T174_pos	276.1554	174	3	4.64E-01	1.04	FALSE	2.08E-01	0.93	FALSE	1.88E-02	1.13	FALSE	7.92E-01	0.97	FALSE
M277T765_pos	277.1074	765	3	9.67E-06	1.23	FALSE	1.80E-02	1.12	FALSE	9.35E-02	1.07	FALSE	2.50E-01	1.12	FALSE
M277T655_pos	277.1184	655	3	8.53E-01	0.99	FALSE	5.27E-01	1.04	FALSE	1.56E-12	1.42	FALSE	1.42E-01	0.83	FALSE
M277T944_pos	277.2164	944	3	8.76E-06	1.32	FALSE	2.35E-02	0.87	FALSE	9.23E-07	1.31	FALSE	1.72E-02	0.80	FALSE
M278T460_1_pos	278.1058	460	3	5.50E-01	1.10	FALSE	8.00E-02	0.76	FALSE	6.23E-01	1.07	FALSE	8.00E-02	0.78	FALSE
M278T634_pos	278.2117	634	3	5.25E-02	1.12	FALSE	6.89E-01	1.02	FALSE	1.70E-06	1.28	FALSE	6.36E-01	0.97	FALSE
M278T1066_pos	278.2467	1066	3	6.36E-02	0.93	FALSE	3.60E-01	1.04	FALSE	3.46E-03	0.90	FALSE	7.59E-01	1.03	FALSE
M278T971_pos	278.2481	971	3	7.90E-01	1.01	FALSE	1.57E-01	1.05	FALSE	4.97E-02	0.94	FALSE	2.44E-01	1.06	FALSE
M279T341_pos	279.0650	341	3	9.68E-01	1.00	FALSE	3.66E-03	1.22	FALSE	1.45E-03	1.21	FALSE	9.55E-03	1.18	FALSE
M279T444_pos	279.1365	444	3	2.80E-02	0.68	FALSE	9.12E-01	0.98	FALSE	7.18E-02	0.76	FALSE	4.79E-01	1.90	FALSE
M279T637_pos	279.2073	637	3	3.35E-01	0.92	FALSE	9.81E-01	1.00	FALSE	1.25E-03	1.30	FALSE	5.09E-02	0.76	FALSE
M279T955_pos	279.2320	955	3	1.27E-01	1.14	FALSE	2.56E-01	0.90	FALSE	1.11E-01	1.12	FALSE	3.23E-01	0.80	FALSE
M280T383_pos	280.1286	383	3	3.60E-05	0.73	FALSE	1.91E-01	1.11	FALSE	3.85E-06	1.36	FALSE	4.73E-01	1.07	FALSE
M280T1076_pos	280.2636	1076	3	1.11E-01	0.95	FALSE	7.06E-03	1.10	FALSE	1.25E-01	0.96	FALSE	6.89E-01	1.04	FALSE
M281T659_pos	281.0792	659	3	1.22E-03	1.12	FALSE	7.23E-01	1.01	FALSE	4.52E-22	1.41	FALSE	2.99E-02	0.89	FALSE
M281T905_pos	281.1386	905	3	1.07E-02	1.06	FALSE	6.20E-02	0.96	FALSE	6.26E-10	0.88	FALSE	2.72E-02	1.30	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M281T922_pos	281.2112	922	3							HMDB0012535	12S-HHT	C17H28O3	0.4
M281T1020_pos	281.2478	1020	3						Fatty acids	HMDB0000673	Linoleic acid	C18H32O2	0.9
M282T832_pos	282.1124	832	3							HMDB0247920	Acetoxyacetylaminofluorene	C17H15NO3	0.1
M282T349_pos	282.1200	349	3							HMDB0003331	1-Methyladenosine	C11H15N5O4	1.2
M282T728_pos	282.1449	728	3							HMDB0254196	Lufironil	C13H19N3O4	0.1
M282T425_pos	282.1701	425	3							HMDB0244365	11-Maleimidoundecanoic acid	C15H23NO4	0.3
M282T493_pos	282.1702	493	3							HMDB0244365	11-Maleimidoundecanoic acid	C15H23NO4	0.6
M282T968_pos	282.2793	968	3							HMDB0247607	9-Octadecenamide	C18H35NO	0.5
M282T1041_pos	282.2792	1041	3						Fatty acids	HMDB0247607	9-Octadecenamide	C18H35NO	0.1
M283T1016_pos	283.2825	1016	3						Terpenoids				
M284T596_pos	284.1858	596	3							HMDB0060994	alpha-Hydroxymetoprolol	C15H25NO4	0.5
M285T1066_pos	285.1359	1066	3							HMDB0250372	Clovoxamine	C14H21ClN2O2	1.9
M285T694_pos	285.1488	694	3							HMDB0000372	16-Oxoestrone	C18H20O3	1.1
M285T682_pos	285.1803	682	3							HMDB0247560	ycarbonyl)piperidin-4-yl)azetidine-	C14H24N2O4	2.0
M285T1013_pos	285.1849	1013	3							HMDB0003422	Boldione	C19H24O2	0.1
M285T1038_pos	285.2788	1038	3							HMDB0000827	Stearic acid	C18H36O2	0.1
M285T229_pos	285.2792	229	3							HMDB0000827	Stearic acid	C18H36O2	1.2
M285T316_pos	285.2792	316	3							HMDB0000827	Stearic acid	C18H36O2	1.3
M285T66_pos	285.2792	66	3							HMDB0000827	Stearic acid	C18H36O2	1.3
M285T147_pos	285.2791	147	3							HMDB0000827	Stearic acid	C18H36O2	1.2
M286T578_pos	286.1110	578	3							HMDB0015166	Probenecid	C13H19NO4S	0.9
M286T779_pos	286.1437	779	3							HMDB0014440	Morphine	C17H19NO3	0.3
M286T613_pos	286.2014	613	3							HMDB0013324	2-Octenoylcarnitine	C15H27NO4	0.3
M287T86_pos	286.9588	86	3						Fatty acids				
M287T523_pos	287.0762	523	3							HMDB0029498	Dimethyl fukiic acid	C12H14O8	0.2
M287T581_pos	287.1388	581	3							HMDB0250542	Cromakalim	C16H18N2O3	0.6
M287T904_pos	287.2008	904	3							HMDB0000053	Androstenedione	C19H26O2	0.9
M287T1027_pos	287.2220	1027	3							HMDB0000672	Hexadecanedioic acid	C16H30O4	1.2
M288T984_pos	288.2536	984	3						Fatty acids	HMDB0032358	Lauroyl diethanolamide	C16H33NO3	1.0
M289T718_pos	289.1077	718	3							HMDB0029303	y-4-hydroxy)-phenyl-6,7-dihydroxy	C16H16O5	2.2
M289T475_pos	289.1191	475	3							HMDB0034881	-tetrahydro-1H-pyrido[3,4-b]indole	C15H16N2O4	2.8
M289T779_pos	289.1550	779	3							HMDB0034913	Imazamethabenz-methyl	C16H20N2O3	1.1
M290T770_pos	290.1397	770	3							HMDB0041836	Benzoyl ecgonine	C16H19NO4	3.3
M290T623_pos	290.1950	623	3							HMDB0241677	3-Hydroxyheptanoylcarnitine	C14H27NO5	4.3
M290T681_pos	290.1964	681	3							HMDB0241677	3-Hydroxyheptanoylcarnitine	C14H27NO5	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M281T922_pos	281.2112	922	3	2.34E-01	1.04	FALSE	1.51E-01	1.05	FALSE	2.09E-05	1.13	FALSE	9.25E-01	1.01	FALSE
M281T1020_pos	281.2478	1020	3	3.88E-01	0.91	FALSE	1.14E-01	0.84	FALSE	4.93E-03	1.30	FALSE	9.36E-01	0.99	FALSE
M282T832_pos	282.1124	832	3	6.77E-03	1.20	FALSE	9.20E-01	1.01	FALSE	2.24E-08	1.42	FALSE	5.04E-01	0.94	FALSE
M282T349_pos	282.1200	349	3	6.94E-07	0.79	FALSE	8.37E-01	0.99	FALSE	8.23E-20	1.50	FALSE	4.28E-01	1.08	FALSE
M282T728_pos	282.1449	728	3	5.78E-07	0.82	FALSE	9.70E-02	1.07	FALSE	6.05E-07	1.18	FALSE	4.96E-01	0.94	FALSE
M282T425_pos	282.1701	425	3	9.08E-03	1.18	FALSE	2.55E-01	0.93	FALSE	2.60E-10	1.43	FALSE	3.53E-01	0.95	FALSE
M282T493_pos	282.1702	493	3	3.57E-07	1.20	FALSE	5.09E-01	1.02	FALSE	5.08E-09	1.20	FALSE	2.27E-01	0.95	FALSE
M282T968_pos	282.2793	968	3	9.48E-01	1.00	FALSE	1.85E-01	0.92	FALSE	2.00E-01	0.94	FALSE	9.29E-01	1.02	FALSE
M282T1041_pos	282.2792	1041	3	3.03E-03	0.96	FALSE	1.10E-01	1.02	FALSE	6.41E-03	0.97	FALSE	8.91E-01	1.00	FALSE
M283T1016_pos	283.2825	1016	3	3.22E-01	0.99	FALSE	7.67E-01	1.00	FALSE	6.18E-01	1.00	FALSE	1.85E-01	0.96	FALSE
M284T596_pos	284.1858	596	3	8.26E-04	1.20	FALSE	5.76E-03	1.17	FALSE	1.55E-09	1.35	FALSE	7.02E-01	1.04	FALSE
M285T1066_pos	285.1359	1066	3	5.25E-01	1.05	FALSE	6.35E-04	0.77	FALSE	4.60E-03	0.83	FALSE	4.13E-01	1.12	FALSE
M285T694_pos	285.1488	694	3	1.11E-04	1.25	FALSE	1.93E-01	0.93	FALSE	1.17E-02	1.13	FALSE	6.63E-01	0.93	FALSE
M285T682_pos	285.1803	682	3	4.64E-01	1.09	FALSE	1.78E-01	0.86	FALSE	4.15E-04	1.43	FALSE	6.88E-01	0.95	FALSE
M285T1013_pos	285.1849	1013	3	7.25E-01	1.23	FALSE	3.52E-01	1.78	FALSE	2.08E-01	1.97	FALSE	8.77E-01	1.10	FALSE
M285T1038_pos	285.2788	1038	3	5.07E-01	0.86	FALSE	9.50E-01	0.98	FALSE	3.22E-01	0.82	FALSE	3.84E-04	1.41	FALSE
M285T229_pos	285.2792	229	3	4.59E-02	1.15	FALSE	6.25E-01	1.04	FALSE	8.46E-01	1.01	FALSE	5.52E-01	1.13	FALSE
M285T316_pos	285.2792	316	3	1.29E-01	1.11	FALSE	8.10E-01	1.02	FALSE	2.66E-01	1.07	FALSE	7.65E-01	1.06	FALSE
M285T66_pos	285.2792	66	3	1.66E-01	0.91	FALSE	9.25E-01	0.99	FALSE	6.02E-02	1.12	FALSE	9.74E-01	1.01	FALSE
M285T147_pos	285.2791	147	3	1.68E-01	1.09	FALSE	4.30E-01	0.95	FALSE	6.71E-01	1.02	FALSE	4.96E-01	0.87	FALSE
M286T578_pos	286.1110	578	3	9.78E-01	1.00	FALSE	3.21E-01	1.08	FALSE	1.36E-04	1.27	FALSE	8.23E-01	0.96	FALSE
M286T779_pos	286.1437	779	3	3.23E-01	0.95	FALSE	4.52E-05	1.24	FALSE	5.04E-09	1.31	FALSE	1.30E-01	0.88	FALSE
M286T613_pos	286.2014	613	3	1.00E-03	1.28	FALSE	5.08E-01	0.95	FALSE	2.35E-02	1.16	FALSE	4.05E-01	0.93	FALSE
M287T86_pos	286.9588	86	3	4.12E-02	1.10	FALSE	3.77E-02	1.11	FALSE	1.82E-04	1.17	FALSE	2.91E-01	0.81	FALSE
M287T523_pos	287.0762	523	3	1.30E-01	0.84	FALSE	6.64E-01	1.05	FALSE	2.03E-02	1.26	FALSE	7.97E-01	0.97	FALSE
M287T581_pos	287.1388	581	3	1.26E-02	0.78	FALSE	4.18E-01	0.93	FALSE	6.82E-02	1.17	FALSE	9.51E-01	1.01	FALSE
M287T904_pos	287.2008	904	3	2.87E-08	1.28	FALSE	3.27E-01	0.96	FALSE	1.28E-03	1.13	FALSE	7.03E-02	0.82	FALSE
M287T1027_pos	287.2220	1027	3	5.42E-04	0.86	FALSE	1.02E-03	1.16	FALSE	8.90E-03	0.91	FALSE	9.52E-01	0.99	FALSE
M288T984_pos	288.2536	984	3	3.61E-01	1.08	FALSE	2.10E-01	0.90	FALSE	3.27E-01	1.08	FALSE	4.76E-02	1.32	FALSE
M289T718_pos	289.1077	718	3	1.04E-03	1.27	FALSE	2.59E-01	0.92	FALSE	4.49E-02	1.14	FALSE	6.98E-01	1.05	FALSE
M289T475_pos	289.1191	475	3	2.02E-02	0.91	FALSE	2.83E-01	1.05	FALSE	7.04E-16	1.38	FALSE	4.17E-01	0.94	FALSE
M289T779_pos	289.1550	779	3	1.15E-02	1.12	FALSE	9.95E-03	0.89	FALSE	1.56E-01	1.06	FALSE	9.01E-01	1.02	FALSE
M290T770_pos	290.1397	770	3	6.61E-02	0.85	FALSE	4.26E-02	1.20	FALSE	7.36E-03	1.22	FALSE	7.74E-01	0.95	FALSE
M290T623_pos	290.1950	623	3	3.58E-01	0.65	FALSE	3.91E-01	1.62	FALSE	7.58E-01	0.88	FALSE	6.25E-01	0.88	FALSE
M290T681_pos	290.1964	681	3	1.09E-04	1.19	FALSE	2.10E-01	1.06	FALSE	8.36E-13	1.34	FALSE	2.80E-01	0.90	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M291T732_pos	291.1706	732	3							HMDB0015453	Procaterol	C16H22N2O3	0.8
M291T984_pos	291.1954	984	3							HMDB0031098	15Z)-4-Oxo-9,11,13,15-octadecate	C18H26O3	0.3
M291T972_pos	291.2320	972	3						Terpenoids	HMDB0000031	Androsterone	C19H30O2	0.5
M292T631_pos	292.1142	631	3							HMDB0252813	Glutamine-glutamate	C10H17N3O7	1.0
M292T680_pos	292.2273	680	3							HMDB0015447	Penbutolol	C18H29NO2	0.7
M293T710_pos	293.1496	710	3							HMDB0011687	Phenylbutyrylglutamine	C15H20N2O4	0.2
M293T539_pos	293.1500	539	3							HMDB0011687	Phenylbutyrylglutamine	C15H20N2O4	1.5
M293T380_pos	293.1499	380	3							HMDB0011687	Phenylbutyrylglutamine	C15H20N2O4	1.1
M293T913_pos	293.2112	913	3						Fatty acids	HMDB0030996	yltetrahydro-2-oxo-3-furancarboxy	C18H28O3	0.4
M295T429_pos	295.1300	429	3							HMDB0000594	gamma-Glutamylphenylalanine	C14H18N2O5	3.8
M295T797_pos	295.1541	797	3							HMDB0030555	Tocopheronic acid	C16H22O5	0.2
M295T912_pos	295.1905	912	3							HMDB0005783	Gingerol	C17H26O4	0.4
M295T949_pos	295.2269	949	3							HMDB0004668	13-OxoODE	C18H30O3	0.5
M295T1037_pos	295.2632	1037	3							HMDB0034381	Methyl linoleate	C19H34O2	0.1
M295T1068_pos	295.2996	1068	3							HMDB0035654	Phytal	C20H38O	0.1
M296T1062_pos	296.1842	1062	3							HMDB0014333	Esmolol	C16H25NO4	4.8
M297T613_pos	297.1131	613	3							HMDB0030772	Demethoxyegonol	C18H16O4	3.1
M297T1018_pos	297.2425	1018	3							HMDB0004667	13-HODE	C18H32O3	0.1
M299T748_pos	299.1282	748	3							HMDB0004808	7C-aglycone	C18H18O4	1.5
M299T1078_pos	299.1515	1078	3							HMDB0255576	Nialamide	C16H18N4O2	4.2
M299T969_pos	299.1621	969	3							HMDB0035233	Olomoucine	C15H18N6O	2.2
M299T908_pos	299.1852	908	3							HMDB0015643	Artemether	C16H26O5	0.5
M299T948_pos	299.1862	948	3							HMDB0014943	Minaprine	C17H22N4O	1.4
M299T986_pos	299.2584	986	3							HMDB0010736	3-Oxooctadecanoic acid	C18H34O3	1.1
M300T85_pos	299.9423	85	3							HMDB0249599	methylthio-1,2,5,6-tetrahydropht	C9H8Cl3NO2S	2.9
M301T555_pos	301.0855	555	3							HMDB0041849	Carboxytolbutamide	C12H16N2O5S	0.9
M301T762_pos	301.1551	762	3							HMDB0244456	-Amino-2,5-diethoxyphenyl)benza	C17H20N2O3	1.4
M301T986_pos	301.2163	986	3							HMDB0001852	all-trans-Retinoic acid	C20H28O2	0.2
M302T634_pos	302.1138	634	3							HMDB0259954	methyl-6-nitro-2H-1,4-benzoxazin-	C15H15N3O4	1.0
M302T1057_pos	302.2456	1057	3						Fatty acids				
M303T1067_pos	303.1465	1067	3							HMDB0028892	Histidylphenylalanine	C15H18N4O3	4.5
M303T917_pos	303.1704	917	3							HMDB0251775	Emivirine	C17H22N2O3	0.4
M304T897_pos	304.1745	897	3							HMDB0013328	Pimelylcarnitine	C14H25NO6	3.3
M305T947_pos	305.1861	947	3							HMDB0259093	Tilisolol	C17H24N2O3	0.4
M305T860_pos	305.1860	860	3							HMDB0259093	Tilisolol	C17H24N2O3	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M291T732_pos	291.1706	732	3	2.12E-02	1.27	FALSE	3.90E-04	0.71	FALSE	1.23E-01	0.87	FALSE	7.16E-01	1.08	FALSE
M291T984_pos	291.1954	984	3	1.23E-06	1.32	FALSE	6.88E-02	0.90	FALSE	1.19E-09	1.36	FALSE	5.44E-01	1.04	FALSE
M291T972_pos	291.2320	972	3	1.43E-06	1.47	FALSE	1.51E-02	0.83	FALSE	2.10E-07	1.44	FALSE	8.60E-01	1.02	FALSE
M292T631_pos	292.1142	631	3	1.00E-04	1.34	FALSE	3.29E-01	0.93	FALSE	3.10E-03	1.21	FALSE	8.69E-01	0.98	FALSE
M292T680_pos	292.2273	680	3	6.90E-03	1.22	FALSE	3.67E-01	1.07	FALSE	5.93E-04	1.25	FALSE	9.38E-01	0.99	FALSE
M293T710_pos	293.1496	710	3	8.88E-05	0.81	FALSE	5.41E-01	1.03	FALSE	5.96E-06	1.24	FALSE	5.74E-01	0.91	FALSE
M293T539_pos	293.1500	539	3	5.61E-02	2.21	FALSE	6.01E-01	0.82	FALSE	4.32E-01	1.31	FALSE	3.53E-01	0.37	FALSE
M293T380_pos	293.1499	380	3	2.62E-03	1.31	FALSE	3.16E-03	1.31	FALSE	1.12E-03	1.29	FALSE	3.91E-01	0.83	FALSE
M293T913_pos	293.2112	913	3	4.77E-01	0.97	FALSE	3.82E-01	0.96	FALSE	2.10E-06	1.21	FALSE	7.29E-01	0.97	FALSE
M295T429_pos	295.1300	429	3	1.94E-01	0.92	FALSE	6.16E-01	0.97	FALSE	2.23E-09	1.44	FALSE	1.85E-01	1.16	FALSE
M295T797_pos	295.1541	797	3	1.67E-02	1.14	FALSE	1.49E-01	1.09	FALSE	4.60E-02	1.10	FALSE	2.08E-01	0.83	FALSE
M295T912_pos	295.1905	912	3	4.98E-03	1.21	FALSE	5.24E-04	1.28	FALSE	1.28E-09	1.46	FALSE	3.31E-02	0.79	FALSE
M295T949_pos	295.2269	949	3	4.26E-01	1.05	FALSE	5.39E-02	0.88	FALSE	6.67E-02	1.10	FALSE	6.70E-01	0.91	FALSE
M295T1037_pos	295.2632	1037	3	2.97E-01	0.82	FALSE	2.50E-01	0.77	FALSE	4.70E-01	1.13	FALSE	5.22E-01	1.20	FALSE
M295T1068_pos	295.2996	1068	3	2.33E-01	1.09	FALSE	1.40E-04	1.33	FALSE	4.75E-01	1.04	FALSE	2.63E-01	0.82	FALSE
M296T1062_pos	296.1842	1062	3	1.46E-01	1.09	FALSE	3.48E-01	0.94	FALSE	5.16E-01	0.97	FALSE	6.93E-01	0.95	FALSE
M297T613_pos	297.1131	613	3	3.41E-05	1.24	FALSE	5.76E-01	1.03	FALSE	5.37E-10	1.33	FALSE	3.17E-02	1.21	FALSE
M297T1018_pos	297.2425	1018	3	9.55E-05	1.31	FALSE	2.03E-03	0.80	FALSE	9.27E-10	1.47	FALSE	3.05E-01	1.12	FALSE
M299T748_pos	299.1282	748	3	8.83E-02	0.95	FALSE	5.07E-01	0.98	FALSE	2.93E-17	1.30	FALSE	3.25E-03	0.81	FALSE
M299T1078_pos	299.1515	1078	3	3.62E-03	0.77	FALSE	5.46E-03	0.79	FALSE	3.21E-02	0.85	FALSE	2.28E-01	1.25	FALSE
M299T969_pos	299.1621	969	3	4.64E-03	0.84	FALSE	1.96E-02	1.16	FALSE	1.92E-10	0.71	FALSE	1.03E-01	1.12	FALSE
M299T908_pos	299.1852	908	3	7.97E-03	1.18	FALSE	1.03E-03	0.81	FALSE	6.17E-02	0.90	FALSE	5.04E-01	0.89	FALSE
M299T948_pos	299.1862	948	3	9.80E-05	0.81	FALSE	3.52E-05	1.26	FALSE	5.22E-01	0.97	FALSE	3.26E-01	1.10	FALSE
M299T986_pos	299.2584	986	3	2.85E-03	1.43	FALSE	7.44E-01	0.96	FALSE	4.59E-01	0.93	FALSE	1.94E-01	1.21	FALSE
M300T85_pos	299.9423	85	3	1.50E-01	1.09	FALSE	5.72E-01	1.03	FALSE	5.10E-03	1.15	FALSE	4.34E-04	0.68	FALSE
M301T555_pos	301.0855	555	3	1.22E-03	1.34	FALSE	1.20E-01	0.87	FALSE	4.70E-06	1.45	FALSE	3.56E-01	0.89	FALSE
M301T762_pos	301.1551	762	3	3.98E-01	1.06	FALSE	1.62E-07	0.71	FALSE	3.36E-05	1.27	FALSE	9.05E-02	0.79	FALSE
M301T986_pos	301.2163	986	3	8.72E-02	0.87	FALSE	2.94E-02	0.82	FALSE	4.47E-01	0.95	FALSE	2.53E-01	1.42	FALSE
M302T634_pos	302.1138	634	3	2.41E-01	1.12	FALSE	7.38E-01	1.03	FALSE	1.45E-04	1.38	FALSE	1.83E-01	1.11	FALSE
M302T1057_pos	302.2456	1057	3	8.12E-08	0.72	FALSE	4.76E-05	1.29	FALSE	9.65E-04	0.84	FALSE	7.03E-01	1.04	FALSE
M303T1067_pos	303.1465	1067	3	4.44E-01	0.95	FALSE	8.99E-05	0.76	FALSE	7.17E-04	0.81	FALSE	8.99E-01	0.98	FALSE
M303T917_pos	303.1704	917	3	3.89E-07	0.72	FALSE	6.26E-02	1.12	FALSE	3.35E-07	1.33	FALSE	6.28E-01	1.05	FALSE
M304T897_pos	304.1745	897	3	9.83E-07	0.81	FALSE	5.26E-01	0.97	FALSE	2.94E-03	1.12	FALSE	6.09E-02	1.25	FALSE
M305T947_pos	305.1861	947	3	4.37E-03	0.80	FALSE	5.57E-02	1.16	FALSE	8.27E-03	1.20	FALSE	4.61E-01	0.88	FALSE
M305T860_pos	305.1860	860	3	1.83E-04	0.80	FALSE	6.22E-01	1.03	FALSE	7.67E-01	1.02	FALSE	3.91E-02	1.31	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M305T949_pos	305.2118	949	3						Terpenoids	HMDB0000309	lpha,16beta-Dihydroxyandrosteno	C19H28O3	2.1
M306T973_pos	306.2436	973	3							HMDB0248273	Amafolone	C19H31NO2	2.6
M307T539_pos	307.1323	539	3							HMDB0062223	11c-Tetrahydro-6,11-dimethylbenz	C20H18O3	2.0
M307T775_pos	307.1653	775	3							HMDB0253499	Inproquone	C16H22N2O4	0.3
M307T930_pos	307.1906	930	3							HMDB0012799	4-Oxoretinal	C18H26O4	0.7
M308T923_pos	308.1260	923	3							HMDB0249634	Carbocysteine-lysine	C11H21N3O5S	4.8
M308T120_pos	308.1346	120	3							HMDB0059780	1,N2-propanodeoxyguanosine	C13H17N5O4	2.4
M308T1048_pos	308.2950	1048	3						Fatty acids				
M309T779_pos	309.1334	779	3							HMDB0037772	8-Acetylegelolide	C16H20O6	0.5
M309T923_pos	309.1295	923	3							HMDB0255498	Nebracetam	C12H16N6O4	3.6
M309T774_pos	309.2062	774	3							HMDB0029852	Methylgingerol	C18H28O4	0.4
M309T1035_pos	309.2404	1035	3							HMDB0256073	1,1,1-Trifluoroheptadecan-2-one	C17H31F3O	1.3
M310T518_pos	310.1652	518	3							HMDB0245639	zyl-9-(tetrahydro-2H-pyran-2-YL)a	C17H19N5O	3.2
M310T660_pos	310.2018	660	3							HMDB0015334	Nadolol	C17H27NO4	1.5
M310T899_pos	310.2018	899	3							HMDB0015334	Nadolol	C17H27NO4	1.7
M310T1049_pos	310.2745	1049	3						Fatty acids	HMDB0014942	Dicyclomine	C19H35NO2	1.4
M310T1052_pos	310.3106	1052	3							HMDB0032740	N-Hexadecanoylpyrrolidine	C20H39NO	0.6
M311T723_pos	311.1601	723	3							HMDB0250969	Delgocitini	C16H18N6O	4.3
M311T675_pos	311.2061	675	3							HMDB0303346	Magnesium octanoate	C16H30MgO4	2.0
M311T931_pos	311.2218	931	3							HMDB0013623	12(13)Ep-9-KODE	C18H30O4	0.4
M311T1013_pos	311.2373	1013	3							HMDB0014449	Desogestrel	C22H30O	1.1
M311T1058_pos	311.2564	1058	3						Fatty acids				
M312T383_pos	312.1450	383	3							HMDB0033939	Domoic acid	C15H21NO6	2.6
M312T399_pos	312.1807	399	3							HMDB0255678	Noberastine	C17H21N5O	3.7
M312T530_pos	312.2171	530	3							HMDB0013325	2-trans,4-cis-Decadienoylcarnitine	C17H29NO4	0.6
M312T928_pos	312.2536	928	3						Fatty acids				
M312T1050_pos	312.2905	1050	3						Fatty acids	HMDB0244503	13-Azaprostanoic acid	C19H37NO2	2.7
M313T890_pos	313.1999	890	3							HMDB0242731	Arteether	C17H28O5	3.2
M313T948_pos	313.2375	948	3							HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	0.5
M314T532_pos	314.2326	532	3							HMDB0013205	9-Decenoylcarnitine	C17H31NO4	0.1
M314T904_pos	314.2330	904	3							HMDB0013205	9-Decenoylcarnitine	C17H31NO4	1.3
M314T966_pos	314.2697	966	3							HMDB0013034	Palmitoylglycine	C18H35NO3	2.4
M315T973_pos	315.2532	973	3						Fatty acids	HMDB0000782	Octadecanedioic acid	C18H34O4	0.8
M316T476_pos	316.1554	476	3							HMDB0006921	(S)-3-Hydroxy-N-methylcoclaurine	C18H21NO4	3.5
M316T434_pos	316.2233	434	3							HMDB0094676	Val-Val-Val	C15H29N3O4	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M305T949_pos	305.2118	949	3	3.17E-03	0.78	FALSE	2.37E-01	0.91	FALSE	9.39E-01	0.99	FALSE	4.98E-01	0.85	FALSE
M306T973_pos	306.2436	973	3	2.50E-01	0.96	FALSE	3.36E-01	1.04	FALSE	2.42E-01	0.97	FALSE	2.26E-01	1.07	FALSE
M307T539_pos	307.1323	539	3	8.08E-01	0.99	FALSE	4.12E-01	1.04	FALSE	9.37E-13	1.40	FALSE	6.47E-03	0.92	FALSE
M307T775_pos	307.1653	775	3	3.80E-07	1.31	FALSE	2.35E-09	0.75	FALSE	5.14E-01	1.03	FALSE	2.34E-02	0.80	FALSE
M307T930_pos	307.1906	930	3	1.27E-07	1.35	FALSE	6.86E-01	1.02	FALSE	2.34E-01	1.06	FALSE	9.14E-01	0.99	FALSE
M308T923_pos	308.1260	923	3	5.54E-02	2.69	FALSE	2.34E-01	0.49	FALSE	9.75E-01	1.01	FALSE	1.21E-01	-0.26	FALSE
M308T120_pos	308.1346	120	3	3.87E-01	1.10	FALSE	8.61E-01	1.02	FALSE	2.64E-02	1.23	FALSE	7.96E-01	0.97	FALSE
M308T1048_pos	308.2950	1048	3	2.60E-04	0.92	FALSE	7.96E-03	1.06	FALSE	1.20E-01	0.97	FALSE	6.01E-01	0.98	FALSE
M309T779_pos	309.1334	779	3	6.60E-01	1.03	FALSE	9.69E-01	1.00	FALSE	1.17E-01	1.11	FALSE	2.68E-01	0.84	FALSE
M309T923_pos	309.1295	923	3	9.94E-02	1.79	FALSE	1.68E-01	0.56	FALSE	7.84E-01	1.09	FALSE	1.08E-01	-0.15	FALSE
M309T774_pos	309.2062	774	3	3.30E-02	1.10	FALSE	5.58E-01	1.03	FALSE	2.01E-02	0.91	FALSE	5.70E-01	0.92	FALSE
M309T1035_pos	309.2404	1035	3	7.90E-01	1.06	FALSE	1.44E-01	0.66	FALSE	1.35E-01	1.34	FALSE	5.33E-01	0.95	FALSE
M310T518_pos	310.1652	518	3	1.80E-01	1.92	FALSE	4.85E-01	1.47	FALSE	9.47E-01	1.03	FALSE	9.84E-01	1.02	FALSE
M310T660_pos	310.2018	660	3	2.94E-02	1.14	FALSE	1.98E-02	1.16	FALSE	9.09E-09	1.38	FALSE	7.56E-01	0.97	FALSE
M310T899_pos	310.2018	899	3	2.85E-01	1.11	FALSE	3.77E-04	1.42	FALSE	1.58E-03	1.30	FALSE	2.12E-01	1.19	FALSE
M310T1049_pos	310.2745	1049	3	8.03E-03	1.27	FALSE	4.87E-02	0.84	FALSE	1.78E-01	0.90	FALSE	2.27E-01	1.16	FALSE
M310T1052_pos	310.3106	1052	3	1.10E-01	1.10	FALSE	1.42E-01	1.10	FALSE	2.38E-03	1.17	FALSE	4.53E-01	0.87	FALSE
M311T723_pos	311.1601	723	3	3.38E-06	0.76	FALSE	1.18E-01	1.10	FALSE	3.31E-12	1.44	FALSE	5.34E-01	0.95	FALSE
M311T675_pos	311.2061	675	3	1.80E-08	1.21	FALSE	9.18E-01	1.00	FALSE	6.65E-02	0.95	FALSE	8.28E-01	0.98	FALSE
M311T931_pos	311.2218	931	3	9.27E-01	1.00	FALSE	1.59E-01	1.08	FALSE	7.64E-03	1.13	FALSE	6.54E-01	1.04	FALSE
M311T1013_pos	311.2373	1013	3	3.88E-01	0.93	FALSE	9.36E-01	1.01	FALSE	4.24E-01	1.06	FALSE	5.04E-01	0.78	FALSE
M311T1058_pos	311.2564	1058	3	2.30E-01	1.11	FALSE	2.85E-02	0.80	FALSE	1.50E-03	1.28	FALSE	9.71E-01	0.99	FALSE
M312T383_pos	312.1450	383	3	2.08E-01	1.18	FALSE	9.84E-01	1.00	FALSE	9.73E-03	1.34	FALSE	7.08E-01	1.16	FALSE
M312T399_pos	312.1807	399	3	3.13E-03	1.13	FALSE	5.97E-01	1.02	FALSE	5.48E-12	1.29	FALSE	5.17E-01	0.96	FALSE
M312T530_pos	312.2171	530	3	1.54E-02	1.22	FALSE	5.32E-02	1.17	FALSE	2.14E-04	1.31	FALSE	9.06E-01	0.98	FALSE
M312T928_pos	312.2536	928	3	2.34E-01	1.65	FALSE	1.08E-01	2.07	FALSE	3.18E-01	0.70	FALSE	2.08E-01	1.24	FALSE
M312T1050_pos	312.2905	1050	3	8.51E-01	0.98	FALSE	2.17E-01	0.85	FALSE	3.83E-01	0.91	FALSE	6.09E-01	1.11	FALSE
M313T890_pos	313.1999	890	3	3.17E-03	0.87	FALSE	1.60E-01	1.08	FALSE	7.65E-07	1.23	FALSE	2.39E-01	0.87	FALSE
M313T948_pos	313.2375	948	3	6.29E-09	1.49	FALSE	9.65E-02	0.89	FALSE	6.72E-04	1.22	FALSE	9.46E-01	1.01	FALSE
M314T532_pos	314.2326	532	3	7.55E-01	0.97	FALSE	6.23E-02	1.22	FALSE	2.32E-02	1.22	FALSE	3.25E-01	1.46	FALSE
M314T904_pos	314.2330	904	3	8.84E-04	1.22	FALSE	6.47E-03	1.18	FALSE	4.69E-02	1.11	FALSE	7.14E-02	1.13	FALSE
M314T966_pos	314.2697	966	3	1.10E-01	1.24	FALSE	4.08E-01	1.12	FALSE	2.17E-01	0.87	FALSE	8.51E-01	0.96	FALSE
M315T973_pos	315.2532	973	3	1.65E-07	1.36	FALSE	4.81E-05	0.78	FALSE	1.34E-01	1.08	FALSE	8.74E-01	0.98	FALSE
M316T476_pos	316.1554	476	3	2.51E-01	1.07	FALSE	3.91E-01	1.06	FALSE	1.53E-07	1.34	FALSE	4.03E-01	1.12	FALSE
M316T434_pos	316.2233	434	3	5.42E-03	1.12	FALSE	8.94E-01	1.01	FALSE	1.60E-22	1.50	FALSE	5.07E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M317T109_pos	317.0207	109	3							HMDB0256253	Pentaerythritol tetranitrate	C5H8N4O12	1.3
M317T1068_1_pos	317.1622	1068	3							HMDB0247071	6-Hydroxyazapropazone	C16H20N4O3	4.4
M317T551_pos	317.1597	551	3							HMDB0033643	Hydroxy-8-nor-2-fenchanone gluco	C15H24O7	0.8
M317T909_pos	317.1967	909	3							HMDB0029346	Neryl glucoside	C16H28O6	2.6
M318T657_pos	318.1377	657	3							HMDB0259283	Triticonazole	C17H20ClN3O	3.0
M318T879_pos	318.2276	879	3						Fatty acids	HMDB0061635	3-hydroxynonanoyl carnitine	C16H31NO5	0.3
M319T604_pos	319.1556	604	3							HMDB0031752	(S,E)-Zearalenone	C18H22O5	5.0
M319T926_pos	319.1906	926	3							HMDB0006709	Ubiquinone-2	C19H26O4	0.8
M319T907_pos	319.2269	907	3							HMDB0001337	Leukotriene A4	C20H30O3	0.6
M320T991_pos	320.2562	991	3						Fatty acids				
M320T1066_pos	320.2587	1066	3							HMDB0258886	Tetradecyl nicotinate	C20H33NO2	0.9
M321T656_pos	321.1448	656	3							HMDB0038970	Formylfusarochromanone	C16H20N2O5	0.9
M321T1033_2_pos	321.1577	1033	3							HMDB0254021	Lesopitron	C15H21ClN6	3.9
M321T898_pos	321.1681	898	3							HMDB0032698	ropanoyloxy)-9,10-epoxy-p-menth	C18H24O5	4.9
M325T870_pos	325.1135	870	3							HMDB0251271	Difructose anhydride III	C12H20O10	1.8
M325T621_pos	325.1860	621	3							HMDB0253911	rolinamide, 5-oxo-L-prolyl-L-norva	C15H24N4O4	3.1
M325T1044_pos	325.2351	1044	3						Fatty acids				
M326T381_pos	326.1497	381	3							HMDB0249843	7,8-dimethoxy-3-methyl-5H-2,3-b	C18H19N3O3	0.5
M326T493_pos	326.1616	493	3							HMDB0250222	ihydro-3-(4-methylphenyl)pyrido(3	C17H19N5O2	1.3
M326T976_pos	326.1753	976	3							HMDB0031997	Simulenoline	C20H23NO3	0.6
M327T779_pos	327.1440	779	3							HMDB0034755	Methoxybenzyl O-(2-sulfoglucosid	C16H22O7	0.5
M327T674_pos	327.1554	674	3							HMDB0255620	Nipradilol	C15H22N2O6	1.0
M327T1044_pos	327.1944	1044	3							HMDB0003039	Isoacitretin	C21H26O3	3.3
M327T1065_pos	327.2015	1065	3							HMDB0061835	Heptaethylene glycol	C14H30O8	0.4
M327T1045_pos	327.2527	1045	3							HMDB0031006	etoxy-2-hydroxy-16-heptadecen-4	C19H34O4	0.8
M328T660_pos	328.1905	660	3							HMDB0030355	(+)-O-Methylarmepavine	C20H25NO3	0.6
M328T974_pos	328.1913	974	3							HMDB0030355	(+)-O-Methylarmepavine	C20H25NO3	1.8
M329T1023_pos	329.1402	1023	3							HMDB0257012	PZXDYQVSAFZTBI-UHFFFAOYSA-N	C19H21ClN2O	4.1
M329T699_1_pos	329.1486	699	3							HMDB0029007	Phenylalanyltyrosine	C18H20N2O4	3.0
M329T1071_pos	329.1596	1071	3							HMDB0029777	Cymorcin monoglucoside	C16H24O7	0.4
M329T753_pos	329.1746	753	3							HMDB0029524	hydroxy-3-methoxyphenyl)-1-pher	C20H24O4	0.3
M330T806_pos	330.1341	806	3							HMDB0032805	N-trans-Feruloyloctopamine	C18H19NO5	1.5
M330T1033_pos	330.2646	1033	3							HMDB0006202	4,8 Dimethylnonanoyl carnitine	C18H35NO4	2.2
M330T760_pos	330.2641	760	3							HMDB0006202	4,8 Dimethylnonanoyl carnitine	C18H35NO4	0.5
M331T417_pos	331.1425	417	3							HMDB0242120	o)-2-nitroethenyl]amino]ethylsulfa	C13H22N4O4S	2.8

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M317T109_pos	317.0207	109	3	4.05E-01	1.07	FALSE	8.42E-02	1.15	FALSE	7.61E-02	1.13	FALSE	2.84E-01	0.81	FALSE
M317T1068_1_pos	317.1622	1068	3	5.66E-01	0.95	FALSE	1.29E-04	0.69	FALSE	7.34E-01	0.97	FALSE	9.85E-01	1.00	FALSE
M317T551_pos	317.1597	551	3	5.68E-02	0.89	FALSE	9.31E-01	1.01	FALSE	3.20E-03	1.17	FALSE	1.76E-02	1.20	FALSE
M317T909_pos	317.1967	909	3	8.97E-01	0.99	FALSE	5.35E-01	0.95	FALSE	1.05E-01	0.89	FALSE	3.77E-01	0.78	FALSE
M318T657_pos	318.1377	657	3	1.97E-02	0.83	FALSE	1.16E-01	1.15	FALSE	4.66E-04	1.29	FALSE	2.71E-01	0.80	FALSE
M318T879_pos	318.2276	879	3	6.64E-05	0.88	FALSE	8.55E-04	1.12	FALSE	7.26E-18	1.30	FALSE	9.75E-01	1.00	FALSE
M319T604_pos	319.1556	604	3	2.92E-03	1.35	FALSE	9.23E-01	1.01	FALSE	9.15E-03	1.26	FALSE	6.67E-01	1.09	FALSE
M319T926_pos	319.1906	926	3	6.20E-07	1.43	FALSE	5.31E-02	0.87	FALSE	7.75E-01	1.02	FALSE	3.89E-02	0.84	FALSE
M319T907_pos	319.2269	907	3	3.43E-06	1.30	FALSE	6.69E-01	0.98	FALSE	7.20E-03	1.14	FALSE	3.98E-01	0.91	FALSE
M320T991_pos	320.2562	991	3	1.09E-02	0.92	FALSE	5.36E-02	1.07	FALSE	1.46E-07	0.85	FALSE	9.14E-01	0.99	FALSE
M320T1066_pos	320.2587	1066	3	7.81E-01	1.07	FALSE	2.67E-01	1.33	FALSE	6.55E-01	0.91	FALSE	4.50E-01	1.24	FALSE
M321T656_pos	321.1448	656	3	5.39E-03	1.11	FALSE	3.72E-01	1.03	FALSE	3.01E-21	1.41	FALSE	4.86E-02	0.94	FALSE
M321T1033_2_pos	321.1577	1033	3	1.07E-01	2.08	FALSE	9.98E-01	1.00	FALSE	2.16E-01	1.61	FALSE	3.04E-01	1.93	FALSE
M321T898_pos	321.1681	898	3	1.15E-04	1.35	FALSE	2.92E-02	0.82	FALSE	2.06E-01	0.92	FALSE	5.45E-01	0.86	FALSE
M325T870_pos	325.1135	870	3	6.09E-03	-4.47	FALSE	1.63E-01	0.35	FALSE	3.61E-01	0.38	FALSE	5.05E-01	0.40	FALSE
M325T621_pos	325.1860	621	3	3.77E-01	0.79	FALSE	6.65E-01	1.13	FALSE	4.24E-01	1.21	FALSE	4.29E-01	0.84	FALSE
M325T1044_pos	325.2351	1044	3	7.91E-02	2.44	FALSE	9.96E-01	1.00	FALSE	3.24E-01	1.51	FALSE	7.92E-01	0.86	FALSE
M326T381_pos	326.1497	381	3	3.84E-12	1.47	FALSE	8.13E-01	0.99	FALSE	2.03E-01	1.06	FALSE	5.88E-01	0.96	FALSE
M326T493_pos	326.1616	493	3	5.59E-01	0.94	FALSE	1.33E-01	1.17	FALSE	2.03E-05	1.46	FALSE	2.48E-01	1.30	FALSE
M326T976_pos	326.1753	976	3	7.38E-02	1.82	FALSE	1.78E-01	0.55	FALSE	8.88E-01	0.96	FALSE	4.84E-01	1.65	FALSE
M327T779_pos	327.1440	779	3	5.64E-01	1.04	FALSE	9.53E-01	1.00	FALSE	6.86E-02	1.12	FALSE	2.99E-01	0.87	FALSE
M327T674_pos	327.1554	674	3	7.73E-02	0.90	FALSE	3.73E-01	0.95	FALSE	9.42E-12	1.45	FALSE	3.88E-01	0.89	FALSE
M327T1044_pos	327.1944	1044	3	1.04E-03	1.26	FALSE	6.14E-02	0.87	FALSE	1.10E-03	1.22	FALSE	2.21E-04	1.42	FALSE
M327T1065_pos	327.2015	1065	3	2.00E-01	1.05	FALSE	5.55E-01	0.98	FALSE	2.47E-01	1.04	FALSE	2.92E-01	0.94	FALSE
M327T1045_pos	327.2527	1045	3	1.36E-01	2.05	FALSE	5.23E-01	1.34	FALSE	9.97E-01	1.00	FALSE	9.32E-01	0.96	FALSE
M328T660_pos	328.1905	660	3	3.78E-01	1.05	FALSE	7.65E-01	0.98	FALSE	6.68E-13	1.50	FALSE	1.92E-01	0.85	FALSE
M328T974_pos	328.1913	974	3	6.86E-01	1.24	FALSE	1.85E-01	0.29	FALSE	5.06E-01	0.73	FALSE	2.99E-01	32.27	FALSE
M329T1023_pos	329.1402	1023	3	6.26E-11	0.88	FALSE	7.23E-04	1.07	FALSE	7.91E-01	1.00	FALSE	1.06E-01	0.88	FALSE
M329T699_1_pos	329.1486	699	3	3.06E-01	1.17	FALSE	2.71E-02	0.73	FALSE	4.29E-01	1.11	FALSE	1.99E-01	0.77	FALSE
M329T1071_pos	329.1596	1071	3	4.65E-01	0.91	FALSE	7.46E-01	0.95	FALSE	5.78E-01	1.07	FALSE	6.24E-01	0.93	FALSE
M329T753_pos	329.1746	753	3	2.98E-01	1.04	FALSE	3.53E-03	1.12	FALSE	2.89E-12	1.28	FALSE	1.67E-01	0.91	FALSE
M330T806_pos	330.1341	806	3	2.68E-05	1.30	FALSE	7.08E-01	0.98	FALSE	7.21E-06	1.27	FALSE	7.95E-01	0.97	FALSE
M330T1033_pos	330.2646	1033	3	7.32E-01	1.05	FALSE	1.96E-01	1.20	FALSE	4.44E-01	0.91	FALSE	8.36E-02	1.73	FALSE
M330T760_pos	330.2641	760	3	2.56E-08	1.31	FALSE	1.66E-01	0.94	FALSE	1.24E-09	1.30	FALSE	1.99E-01	0.92	FALSE
M331T417_pos	331.1425	417	3	1.40E-05	1.30	FALSE	9.14E-01	1.01	FALSE	1.06E-03	1.19	FALSE	9.94E-02	0.91	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M331T983_pos	331.2633	983	3							HMDB0001976	Docosapentaenoic acid (22n-6)	C22H34O2	0.5
M332T998_pos	332.2221	998	3							HMDB0038596	dimethyl-1-oxocyclopenta[c]pyran-	C20H29NO3	0.3
M332T879_pos	332.2437	879	3							HMDB0061636	3-hydroxydecanoyl carnitine	C17H33NO5	1.8
M333T85_pos	332.9642	85	3						Amino acids and Peptides	HMDB0244457	-Amino-2,5-diethoxyphenyl)benza	C14H8N2S4	0.3
M333T858_pos	333.2066	858	3							HMDB0002358	Carnosic acid	C20H28O4	1.7
M333T886_pos	333.2637	886	3							HMDB0030935	9,10,13-Trihydroxystearic acid	C18H36O5	0.5
M334T791_pos	334.1652	791	3							HMDB0256290	Pentopril	C18H23NO5	0.9
M334T739_pos	334.2378	739	3							HMDB0249630	Carbetapentane	C20H31NO3	0.4
M335T463_pos	335.1110	463	3							HMDB0030651	Mukurozidiol	C17H18O7	4.5
M335T971_pos	335.2202	971	3							HMDB0001244	-Keto-13,14-dihydroprostaglandin	C20H30O4	4.5
M335T890_pos	335.2218	890	3							HMDB0001244	-Keto-13,14-dihydroprostaglandin	C20H30O4	0.4
M335T996_pos	335.2946	996	3						Fatty acids	HMDB0002823	Docosatrienoic acid	C22H38O2	0.6
M337T972_pos	337.2364	972	3						Terpenoids	HMDB0001085	Leukotriene B4	C20H32O4	2.7
M337T927_pos	337.2374	927	3							HMDB0001085	Leukotriene B4	C20H32O4	0.1
M338T1008_pos	338.2102	1008	3							HMDB0002835	Danazol	C22H27NO2	3.7
M338T1015_pos	338.2444	1015	3							HMDB0242033	N-Lauroyl Histidine	C18H31N3O3	1.8
M338T1043_pos	338.3419	1043	3							HMDB0244507	13-Docosenamide	C22H43NO	0.4
M339T830_pos	339.1809	830	3							HMDB0013032	mega-Carboxy-trinor-leukotriene E	C18H26O6	1.9
M340T742_pos	340.1759	742	3							HMDB0241127	5E,8Z)-Deca-3,5,8-trienedioylcarni	C17H25NO6	1.2
M340T997_pos	340.1913	997	3							HMDB0251701	Edivoxetine	C18H26FNO4	1.7
M340T710_pos	340.2093	710	3							HMDB0249447	Bursin	C14H25N7O3	0.4
M341T680_pos	341.1709	680	3							HMDB0257669	olidin-1-yl)-6-oxohexanoyl]pyrrolid	C16H24N2O6	0.4
M341T858_pos	341.1753	858	3							HMDB0030799	5-Deoxymyricanone	C21H24O4	1.6
M342T553_pos	342.1702	553	3							HMDB0014842	Naltrexone	C20H23NO4	0.6
M342T967_pos	342.2643	967	3							HMDB0013326	trans-2-Dodecenoylcarnitine	C19H35NO4	1.2
M342T1054_2_pos	342.2988	1054	3							HMDB0013308	Stearoylglycine	C20H39NO3	4.2
M342T964_pos	342.3369	964	3						Fatty acids				
M343T755_pos	343.1322	755	3							HMDB0060900	Clozapine N-oxide	C18H19ClN4O	0.6
M343T823_pos	343.1747	823	3							HMDB0032870	Jasmolone glucoside	C17H26O7	1.1
M344T714_2_pos	344.1502	714	3							HMDB0039755	trans-Feruloyl-4-O-methyldopami	C19H21NO5	2.8
M344T1045_pos	344.2798	1045	3							HMDB0240804	8-Methylundecanoylcarnitine	C19H37NO4	0.8
M345T690_pos	345.1341	690	3							HMDB0259305	True blue	C20H16N4O2	1.5
M345T676_pos	345.1808	676	3							HMDB0015118	Formoterol	C19H24N2O4	0.4
M346T1078_pos	346.2743	1078	3							HMDB0013649	Eicosapentaenoyl Ethanolamide	C22H35NO2	0.6
M347T752_pos	347.1855	752	3							HMDB0032819	Gibberellin A113	C20H26O5	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M331T983_pos	331.2633	983	3	6.49E-02	1.23	FALSE	5.37E-03	0.73	FALSE	7.36E-01	1.03	FALSE	1.10E-01	0.75	FALSE
M332T998_pos	332.2221	998	3	7.42E-01	1.26	FALSE	2.58E-01	0.19	FALSE	3.08E-01	0.52	FALSE	2.87E-01	24.28	FALSE
M332T879_pos	332.2437	879	3	5.64E-01	0.97	FALSE	1.57E-02	1.12	FALSE	7.95E-08	1.24	FALSE	8.01E-01	1.02	FALSE
M333T85_pos	332.9642	85	3	8.86E-02	1.08	FALSE	7.13E-01	0.98	FALSE	9.13E-01	1.00	FALSE	6.50E-02	0.87	FALSE
M333T858_pos	333.2066	858	3	3.96E-01	0.95	FALSE	4.16E-02	1.14	FALSE	6.18E-03	1.16	FALSE	7.39E-01	0.95	FALSE
M333T886_pos	333.2637	886	3	7.21E-01	1.05	FALSE	9.55E-02	0.76	FALSE	4.86E-01	0.92	FALSE	2.10E-01	0.78	FALSE
M334T791_pos	334.1652	791	3	3.03E-03	1.13	FALSE	6.11E-01	0.98	FALSE	5.99E-03	1.11	FALSE	6.56E-01	1.07	FALSE
M334T739_pos	334.2378	739	3	1.40E-01	1.11	FALSE	6.19E-01	1.04	FALSE	2.77E-07	1.39	FALSE	7.25E-01	1.03	FALSE
M335T463_pos	335.1110	463	3	1.88E-07	1.48	FALSE	6.91E-01	0.97	FALSE	5.81E-01	1.04	FALSE	1.13E-01	0.86	FALSE
M335T971_pos	335.2202	971	3	6.82E-04	1.18	FALSE	4.05E-07	0.77	FALSE	8.04E-01	1.01	FALSE	8.34E-01	0.98	FALSE
M335T890_pos	335.2218	890	3	5.11E-01	1.03	FALSE	3.12E-02	0.89	FALSE	1.48E-02	1.11	FALSE	8.08E-01	0.97	FALSE
M335T996_pos	335.2946	996	3	7.12E-01	1.04	FALSE	7.64E-01	1.04	FALSE	8.04E-01	1.02	FALSE	6.59E-01	1.11	FALSE
M337T972_pos	337.2364	972	3	4.37E-04	1.28	FALSE	6.22E-03	0.81	FALSE	3.62E-02	0.88	FALSE	8.25E-02	0.82	FALSE
M337T927_pos	337.2374	927	3	6.41E-01	0.97	FALSE	4.73E-01	0.95	FALSE	2.44E-03	1.17	FALSE	5.44E-01	1.13	FALSE
M338T1008_pos	338.2102	1008	3	6.27E-15	0.79	FALSE	2.04E-01	1.04	FALSE	8.95E-02	0.96	FALSE	5.40E-01	0.94	FALSE
M338T1015_pos	338.2444	1015	3	1.25E-14	0.79	FALSE	1.48E-01	1.04	FALSE	9.43E-01	1.00	FALSE	8.08E-01	0.98	FALSE
M338T1043_pos	338.3419	1043	3	6.47E-03	0.83	FALSE	3.77E-03	1.24	FALSE	4.23E-01	0.95	FALSE	2.28E-01	0.80	FALSE
M339T830_pos	339.1809	830	3	6.10E-02	1.27	FALSE	9.35E-02	0.78	FALSE	7.27E-02	1.22	FALSE	2.93E-01	1.89	FALSE
M340T742_pos	340.1759	742	3	4.18E-01	1.05	FALSE	2.75E-01	1.08	FALSE	6.35E-01	1.03	FALSE	4.25E-01	0.86	FALSE
M340T997_pos	340.1913	997	3	4.12E-01	1.32	FALSE	7.84E-02	0.43	FALSE	9.87E-01	1.00	FALSE	3.86E-01	11.75	FALSE
M340T710_pos	340.2093	710	3	4.80E-09	1.30	FALSE	8.38E-01	1.01	FALSE	4.93E-02	1.08	FALSE	7.08E-01	1.03	FALSE
M341T680_pos	341.1709	680	3	7.98E-06	1.35	FALSE	1.49E-02	0.85	FALSE	1.23E-07	1.37	FALSE	8.57E-01	0.98	FALSE
M341T858_pos	341.1753	858	3	2.64E-01	1.05	FALSE	2.94E-02	1.10	FALSE	3.23E-07	1.21	FALSE	1.49E-01	1.08	FALSE
M342T553_pos	342.1702	553	3	7.66E-09	0.70	FALSE	5.04E-01	0.96	FALSE	4.66E-08	1.34	FALSE	9.40E-01	0.99	FALSE
M342T967_pos	342.2643	967	3	6.79E-02	0.96	FALSE	6.61E-02	0.96	FALSE	1.93E-06	0.92	FALSE	9.18E-01	0.99	FALSE
M342T1054_2_pos	342.2988	1054	3	2.15E-03	1.46	FALSE	4.90E-02	0.77	FALSE	7.62E-01	0.97	FALSE	3.56E-01	1.17	FALSE
M342T964_pos	342.3369	964	3	4.65E-02	1.38	FALSE	3.98E-01	1.15	FALSE	9.56E-02	1.26	FALSE	5.55E-01	0.91	FALSE
M343T755_pos	343.1322	755	3	6.47E-01	1.06	FALSE	2.88E-01	0.88	FALSE	9.74E-03	1.32	FALSE	1.61E-01	0.73	FALSE
M343T823_pos	343.1747	823	3	7.64E-04	0.82	FALSE	1.60E-04	1.25	FALSE	7.53E-04	1.18	FALSE	3.64E-01	0.87	FALSE
M344T714_2_pos	344.1502	714	3	2.54E-01	0.93	FALSE	3.16E-01	1.07	FALSE	2.70E-08	1.39	FALSE	3.37E-02	0.89	FALSE
M344T1045_pos	344.2798	1045	3	1.03E-01	0.85	FALSE	1.81E-02	0.79	FALSE	2.54E-01	1.10	FALSE	4.77E-01	0.87	FALSE
M345T690_pos	345.1341	690	3	1.92E-03	1.22	FALSE	1.82E-03	1.23	FALSE	2.00E-01	1.07	FALSE	3.01E-01	1.19	FALSE
M345T676_pos	345.1808	676	3	8.17E-01	1.02	FALSE	2.06E-04	1.41	FALSE	1.50E-05	1.40	FALSE	2.59E-01	1.30	FALSE
M346T1078_pos	346.2743	1078	3	6.24E-02	1.33	FALSE	4.96E-02	0.75	FALSE	2.29E-01	0.85	FALSE	3.56E-01	1.27	FALSE
M347T752_pos	347.1855	752	3	1.40E-02	1.10	FALSE	2.33E-01	1.05	FALSE	2.82E-12	1.30	FALSE	4.54E-03	0.82	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M347T890_pos	347.1852	890	3							HMDB0032819	Gibberellin A113	C20H26O5	0.3
M347T820_pos	347.2429	820	3							HMDB0029885	Sorbitan laurate	C18H34O6	0.3
M349T914_pos	349.2000	914	3							HMDB0032010	Gibberellin A110	C20H28O5	2.8
M350T1041_pos	350.2666	1041	3						Fatty acids				
M351T1002_pos	351.0908	1002	3							HMDB0256368	sulfonyl)methyl]phenoxy}methyl)l	C18H14N4O2S	0.5
M351T910_pos	351.2532	910	3						Terpenoids	HMDB0000268	Tetrahydrocorticosterone	C21H34O4	0.6
M353T704_pos	353.1539	704	3							HMDB0244814	,4,5,5-tetramethylimidazoline-1-o	C25H20O2	0.9
M353T924_pos	353.2325	924	3							HMDB0001220	Prostaglandin E2	C20H32O5	0.7
M353T1072_pos	353.2679	1072	3						Fatty acids	HMDB0011539	MG(0:0/18:3(6Z,9Z,12Z)/0:0)	C21H36O4	2.1
M354T623_pos	354.2387	623	3							HMDB0253857	oxo-3-(2-(4-piperidinyl)ethyl)-1-pip	C18H31N3O4	0.1
M356T855_2_pos	356.1529	855	3							HMDB0014751	Amodiaquine	C20H22ClN3O	1.4
M356T1016_pos	356.2224	1016	3							HMDB0033449	Pipercide	C22H29NO3	1.0
M357T858_pos	357.2415	858	3							HMDB0039880	1-Formylneogrifolin	C23H32O3	2.5
M358T633_pos	358.2222	633	3							HMDB0241173	Undec-5-enedioylcarnitine	C18H31NO6	0.6
M358T885_pos	358.2227	885	3							HMDB0241173	Undec-5-enedioylcarnitine	C18H31NO6	0.7
M359T926_pos	359.1836	926	3							HMDB0005798	Malabaricone C	C21H26O5	4.8
M359T744_pos	359.1955	744	3							HMDB0253722	Itopride	C20H26N2O4	2.8
M362T106_pos	362.0851	106	3							HMDB0258407	SPARSOMYCIN	C13H19N3O5S2	3.2
M363T585_pos	363.1615	585	3							HMDB0257192	uorophenyl)-3-(1-cinnamyl-1H-pyr	C21H19FN4O	0.1
M365T752_pos	365.1961	752	3							HMDB0012550	12-Oxo-20-carboxy-leukotriene B4	C20H28O6	0.5
M366T958_pos	366.2627	958	3							HMDB0241394	Tetradeca-7,9,11-trienoylcarnitine	C21H35NO4	3.2
M367T853_pos	367.2696	853	3							HMDB0303247	Magnesium caprate	C20H38MgO4	0.8
M369T920_1_pos	369.1528	920	3							HMDB0039891	ydroxy-3-prenylbenzoic acid gluco	C18H24O8	4.4
M369T894_pos	369.2277	894	3							HMDB0001908	19-Hydroxy-PGE2	C20H32O6	1.4
M370T877_pos	370.2596	877	3							HMDB0241325	Hydroxytrideca-4,6-dienoylcarniti	C20H35NO5	2.2
M371T1064_pos	371.2277	1065	3							HMDB0094680	Octaethylene glycol	C16H34O9	0.4
M371T873_pos	371.2579	873	3							HMDB0000476	3-Oxo-4,6-choladienoic acid	C24H34O3	0.4
M371T969_pos	371.3673	969	3							HMDB0000941	Cholest-5-ene	C27H46	0.2
M372T1001_1_pos	372.2746	1001	3							HMDB0241348	3-Oxotridecanoylcarnitine	C20H37NO5	0.3
M373T956_pos	373.2736	956	3						Terpenoids	HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.3
M373T1007_pos	373.2737	1007	3						Terpenoids	HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.2
M373T1045_pos	373.2739	1045	3							HMDB0013627	Cervonoyl ethanolamide	C24H36O3	0.6
M373T1073_pos	373.2951	1073	3						Fatty acids	HMDB0092901	DG(8:0/10:0/0:0)	C21H40O5	0.7
M374T543_pos	374.1639	543	3							HMDB0250315	Clebopride	C20H24ClN3O2	2.4
M374T757_pos	374.2902	757	3							HMDB0061639	3-hydroxytridecanoyl carnitine	C20H39NO5	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M347T890_pos	347.1852	890	3	8.17E-01	1.01	FALSE	1.19E-01	1.09	FALSE	1.52E-03	1.17	FALSE	5.81E-01	0.89	FALSE
M347T820_pos	347.2429	820	3	2.38E-10	1.21	FALSE	5.69E-01	0.98	FALSE	2.84E-02	1.06	FALSE	4.55E-01	0.98	FALSE
M349T914_pos	349.2000	914	3	3.04E-02	0.90	FALSE	1.09E-01	1.09	FALSE	5.77E-02	1.09	FALSE	8.19E-01	1.02	FALSE
M350T1041_pos	350.2666	1041	3	6.28E-02	0.96	FALSE	5.26E-01	1.02	FALSE	4.33E-02	0.96	FALSE	1.93E-01	1.09	FALSE
M351T1002_pos	351.0908	1002	3	3.74E-01	0.95	FALSE	9.57E-01	1.00	FALSE	4.85E-01	1.04	FALSE	1.58E-01	1.26	FALSE
M351T910_pos	351.2532	910	3	1.14E-10	1.44	FALSE	2.10E-04	0.81	FALSE	1.54E-01	1.07	FALSE	3.10E-01	1.09	FALSE
M353T704_pos	353.1539	704	3	8.01E-01	0.99	FALSE	9.95E-01	1.00	FALSE	1.02E-06	1.25	FALSE	9.17E-01	0.99	FALSE
M353T924_pos	353.2325	924	3	6.10E-01	0.92	FALSE	9.74E-01	1.01	FALSE	7.38E-01	0.96	FALSE	1.36E-01	0.67	FALSE
M353T1072_pos	353.2679	1072	3	8.38E-01	1.12	FALSE	8.00E-02	0.19	FALSE	1.04E-01	2.24	FALSE	6.47E-01	0.92	FALSE
M354T623_pos	354.2387	623	3	1.80E-01	1.12	FALSE	1.45E-01	1.14	FALSE	1.89E-04	1.32	FALSE	5.01E-01	1.13	FALSE
M356T855_2_pos	356.1529	855	3	6.01E-01	1.03	FALSE	2.26E-03	1.23	FALSE	1.81E-04	1.24	FALSE	1.51E-02	1.07	FALSE
M356T1016_pos	356.2224	1016	3	4.60E-01	1.52	FALSE	8.11E-02	0.17	FALSE	4.04E-01	0.66	FALSE	3.92E-01	3.06	FALSE
M357T858_pos	357.2415	858	3	1.02E-02	1.14	FALSE	9.45E-01	1.00	FALSE	4.61E-01	0.97	FALSE	3.38E-01	1.05	FALSE
M358T633_pos	358.2222	633	3	2.85E-01	0.95	FALSE	2.22E-01	1.07	FALSE	3.79E-07	1.27	FALSE	2.52E-01	1.19	FALSE
M358T885_pos	358.2227	885	3	1.34E-01	0.90	FALSE	1.20E-01	1.13	FALSE	7.34E-09	1.48	FALSE	5.72E-01	1.08	FALSE
M359T926_pos	359.1836	926	3	5.46E-02	1.12	FALSE	4.31E-02	0.88	FALSE	1.60E-01	1.07	FALSE	5.21E-01	0.93	FALSE
M359T744_pos	359.1955	744	3	7.85E-03	0.81	FALSE	1.88E-02	1.22	FALSE	8.41E-06	1.38	FALSE	4.05E-01	1.13	FALSE
M362T106_pos	362.0851	106	3	1.94E-01	0.93	FALSE	3.42E-01	1.06	FALSE	3.10E-12	1.48	FALSE	6.29E-02	1.28	FALSE
M363T585_pos	363.1615	585	3	7.34E-02	0.89	FALSE	3.28E-01	1.07	FALSE	1.32E-05	1.28	FALSE	6.84E-01	0.95	FALSE
M365T752_pos	365.1961	752	3	3.05E-01	1.04	FALSE	1.93E-01	1.06	FALSE	6.19E-13	1.31	FALSE	5.29E-02	0.89	FALSE
M366T958_pos	366.2627	958	3	4.23E-01	0.94	FALSE	5.94E-01	0.95	FALSE	5.38E-01	0.96	FALSE	2.68E-02	1.28	FALSE
M367T853_pos	367.2696	853	3	7.00E-01	0.97	FALSE	2.30E-01	1.09	FALSE	1.65E-01	1.09	FALSE	6.84E-01	1.06	FALSE
M369T920_1_pos	369.1528	920	3	3.69E-02	0.91	FALSE	3.20E-01	0.96	FALSE	4.73E-05	0.86	FALSE	9.29E-01	0.99	FALSE
M369T894_pos	369.2277	894	3	1.28E-04	0.77	FALSE	7.38E-01	0.98	FALSE	4.62E-02	1.12	FALSE	7.03E-01	1.07	FALSE
M370T877_pos	370.2596	877	3	8.71E-05	1.17	FALSE	9.79E-01	1.00	FALSE	3.33E-02	1.08	FALSE	4.11E-01	0.93	FALSE
M371T1064_pos	371.2277	1065	3	8.52E-01	1.01	FALSE	2.01E-01	0.95	FALSE	3.67E-01	1.03	FALSE	4.16E-01	0.95	FALSE
M371T873_pos	371.2579	873	3	2.08E-03	1.20	FALSE	4.63E-01	0.96	FALSE	1.53E-02	1.13	FALSE	8.96E-01	0.98	FALSE
M371T969_pos	371.3673	969	3	4.79E-02	0.85	FALSE	9.64E-01	1.00	FALSE	3.93E-01	0.94	FALSE	3.50E-01	0.83	FALSE
M372T1001_1_pos	372.2746	1001	3	9.04E-02	0.84	FALSE	9.77E-01	1.00	FALSE	4.12E-02	0.84	FALSE	7.06E-01	1.12	FALSE
M373T956_pos	373.2736	956	3	4.21E-12	1.24	FALSE	4.61E-04	0.90	FALSE	2.73E-07	1.14	FALSE	4.49E-02	0.89	FALSE
M373T1007_pos	373.2737	1007	3	5.87E-04	1.15	FALSE	7.78E-01	0.99	FALSE	1.90E-15	1.37	FALSE	6.11E-02	0.91	FALSE
M373T1045_pos	373.2739	1045	3	6.29E-01	0.95	FALSE	6.09E-01	0.94	FALSE	2.84E-02	1.23	FALSE	6.72E-01	1.16	FALSE
M373T1073_pos	373.2951	1073	3	8.81E-02	2.13	FALSE	4.54E-01	1.39	FALSE	1.47E-01	1.73	FALSE	8.33E-01	0.90	FALSE
M374T543_pos	374.1639	543	3	3.94E-09	0.70	FALSE	5.73E-01	1.04	FALSE	2.05E-02	1.13	FALSE	6.10E-01	1.05	FALSE
M374T757_pos	374.2902	757	3	2.29E-02	1.11	FALSE	6.28E-01	0.98	FALSE	2.67E-06	1.22	FALSE	4.46E-02	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M376T797_pos	376.2378	797	3							HMDB0256570	Pipamperone	C21H30FN3O2	4.4
M377T938_pos	377.2310	938	3							HMDB0002294	Resolvin D2	C22H32O5	3.4
M380T649_pos	380.1820	649	3							HMDB0259448	nyl)-7,9-dihydro-9-(6-methoxy-3-p	C19H21N7O2	2.4
M381T627_pos	381.1764	627	3							HMDB0031954	ethyl-3-butenyl apiosyl-(1->6)-gluc	C16H28O10	2.3
M381T1071_pos	381.2768	1071	3							HMDB0244848	din-3-yl)-2,5-dimethyl-N,N-diprop	C22H32N6	1.7
M383T858_pos	383.2215	858	3							HMDB0029488	Farnesiferol A	C24H30O4	0.5
M383T923_pos	383.2939	923	3							HMDB0036368	(4,8,12-trimethyl-3,7,11-tridecatri	C26H38O2	1.5
M384T729_pos	384.2333	729	3							HMDB0259114	Trecadrine	C27H29NO	2.8
M385T1017_pos	385.3446	1017	3							HMDB0000032	7-Dehydrocholesterol	C27H44O	4.9
M386T1062_2_pos	386.3268	1062	3							HMDB0062517	Pentadecanoylcarnitine	C22H43NO4	0.9
M387T1062_pos	387.2538	1062	3							HMDB0000385	12a-Hydroxy-3-oxocholadienic acid	C24H34O4	2.1
M387T1060_pos	387.3615	1060	3							HMDB0000067	Cholesterol	C27H46O	1.7
M388T565_pos	388.1868	565	3							HMDB0256170	Pcera-1	C18H30NO6P	4.0
M389T1001_pos	389.1117	1001	3							HMDB0014546	Eszopiclone	C17H17ClN6O3	1.6
M389T873_pos	389.2687	873	3							HMDB0030366	Cavipetin C	C24H36O4	0.1
M391T896_pos	391.2099	896	3							HMDB0257369	utamyl-L-histidyl-3,3-dimethylprol	C18H26N6O4	2.6
M391T858_pos	391.2099	858	3							HMDB0257369	utamyl-L-histidyl-3,3-dimethylprol	C18H26N6O4	2.8
M391T916_pos	391.2844	916	3						Terpenoids	HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	0.2
M391T1032_pos	391.2844	1032	3							HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	0.4
M392T530_pos	392.1744	530	3							HMDB0254104	Linopirdine	C26H21N3O	3.4
M392T665_pos	392.2182	665	3							HMDB0258419	sphingosine phosphate	C18H34NO6P	3.8
M393T908_pos	393.1817	908	3							HMDB0013949	O-Desmethylcarvedilol	C23H24N2O4	2.1
M395T1033_pos	395.2551	1033	3							HMDB0011154	LysoPA(P-16:0/0:0)	C19H39O6P	1.5
M399T704_pos	399.1765	704	3							HMDB0249046	BENZOYLARGININE NITROANILIDE	C19H22N6O4	2.5
M400T1053_pos	400.2856	1053	3							HMDB0242007	N-Docosahexaenoyl Alanine	C25H37NO3	2.5
M401T1031_pos	401.3414	1031	3							HMDB0000501	7-Ketocholesterol	C27H44O2	0.0
M402T608_pos	402.2333	608	3							HMDB0248358	Amperozide	C23H29F2N3O	4.5
M402T825_pos	402.2389	825	3							HMDB0248039	ro-2-(4-amino-6-((4-phenyl-1-pipe	C23H27N7	2.9
M403T122_pos	403.0677	122	3							HMDB0034589	Shoyuflavone B	C19H14O10	4.4
M403T1071_pos	403.2329	1071	3							HMDB0034159	Acetyl tributyl citrate	C20H34O8	0.6
M403T1060_pos	403.3059	1060	3							HMDB0029887	Sorbitan palmitate	C22H42O6	1.3
M403T983_pos	403.3205	983	3							HMDB0029458	Oryzarol	C26H42O3	0.3
M404T721_pos	404.2333	721	3							HMDB0254511	metergoline	C25H29N3O2	0.0
M405T803_pos	405.2150	803	3							HMDB0015589	Flunarizine	C26H26F2N2	3.1
M405T1033_pos	405.2998	1033	3							HMDB0011555	G(0:0/22:5(4Z,7Z,10Z,13Z,16Z)/0:	C25H40O4	0.3

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M376T797_pos	376.2378	797	3	7.83E-01	1.01	FALSE	2.63E-01	1.04	FALSE	1.66E-01	1.04	FALSE	6.00E-01	1.07	FALSE
M377T938_pos	377.2310	938	3	4.41E-08	0.72	FALSE	1.97E-01	0.93	FALSE	4.67E-04	1.19	FALSE	4.36E-01	0.89	FALSE
M380T649_pos	380.1820	649	3	7.54E-01	0.90	FALSE	1.54E-01	0.59	FALSE	1.10E-01	0.62	FALSE	7.41E-01	1.13	FALSE
M381T627_pos	381.1764	627	3	2.96E-01	1.07	FALSE	3.77E-01	1.07	FALSE	1.49E-02	1.15	FALSE	4.33E-01	1.12	FALSE
M381T1071_pos	381.2768	1071	3	2.46E-01	1.14	FALSE	5.40E-02	0.79	FALSE	3.87E-01	1.09	FALSE	8.34E-01	0.93	FALSE
M383T858_pos	383.2215	858	3	2.35E-01	1.04	FALSE	2.72E-01	1.04	FALSE	6.41E-06	1.16	FALSE	2.57E-01	1.07	FALSE
M383T923_pos	383.2939	923	3	7.33E-02	1.28	FALSE	1.54E-01	1.23	FALSE	1.95E-03	0.69	FALSE	6.37E-01	1.14	FALSE
M384T729_pos	384.2333	729	3	4.06E-04	1.19	FALSE	4.77E-01	0.96	FALSE	1.33E-01	1.07	FALSE	6.01E-02	1.17	FALSE
M385T1017_pos	385.3446	1017	3	2.73E-01	1.17	FALSE	6.67E-01	0.94	FALSE	7.17E-02	1.25	FALSE	9.19E-01	1.04	FALSE
M386T1062_2_pos	386.3268	1062	3	8.96E-01	0.97	FALSE	2.02E-01	0.67	FALSE	7.00E-02	1.54	FALSE	4.77E-01	1.81	FALSE
M387T1062_pos	387.2538	1062	3	2.77E-01	1.07	FALSE	6.68E-01	0.97	FALSE	3.91E-01	1.05	FALSE	6.12E-01	0.95	FALSE
M387T1060_pos	387.3615	1060	3	3.36E-01	0.89	FALSE	1.38E-01	1.21	FALSE	1.53E-01	0.86	FALSE	4.24E-01	0.73	FALSE
M388T565_pos	388.1868	565	3	1.71E-01	0.92	FALSE	1.35E-03	0.83	FALSE	8.60E-01	0.99	FALSE	8.85E-03	1.39	FALSE
M389T1001_pos	389.1117	1001	3	7.47E-02	0.98	FALSE	8.90E-01	1.00	FALSE	2.02E-01	1.01	FALSE	9.79E-01	1.00	FALSE
M389T873_pos	389.2687	873	3	6.57E-04	1.17	FALSE	6.12E-01	0.98	FALSE	1.99E-01	1.05	FALSE	9.34E-01	0.99	FALSE
M391T896_pos	391.2099	896	3	2.40E-01	0.97	FALSE	2.66E-02	0.94	FALSE	1.38E-01	0.97	FALSE	9.15E-01	1.00	FALSE
M391T858_pos	391.2099	858	3	3.19E-01	0.98	FALSE	2.78E-01	1.03	FALSE	1.24E-01	1.03	FALSE	8.65E-01	0.99	FALSE
M391T916_pos	391.2844	916	3	2.20E-11	1.26	FALSE	2.82E-01	0.96	FALSE	6.95E-03	1.08	FALSE	8.64E-03	0.84	FALSE
M391T1032_pos	391.2844	1032	3	2.31E-04	1.17	FALSE	2.99E-01	1.05	FALSE	5.10E-10	1.27	FALSE	1.74E-01	0.88	FALSE
M392T530_pos	392.1744	530	3	1.35E-01	1.09	FALSE	9.83E-03	1.17	FALSE	1.44E-05	1.25	FALSE	9.95E-01	1.00	FALSE
M392T665_pos	392.2182	665	3	2.61E-01	0.89	FALSE	4.56E-01	1.08	FALSE	1.43E-05	1.47	FALSE	8.62E-01	1.02	FALSE
M393T908_pos	393.1817	908	3	2.90E-01	1.15	FALSE	3.70E-02	0.75	FALSE	2.84E-01	1.13	FALSE	4.40E-01	0.91	FALSE
M395T1033_pos	395.2551	1033	3	8.71E-01	0.96	FALSE	9.54E-01	1.02	FALSE	1.51E-01	1.40	FALSE	4.32E-01	1.13	FALSE
M399T704_pos	399.1765	704	3	1.31E-03	0.79	FALSE	9.87E-01	1.00	FALSE	2.62E-07	1.40	FALSE	4.56E-01	0.88	FALSE
M400T1053_pos	400.2856	1053	3	5.42E-02	1.09	FALSE	3.17E-01	0.96	FALSE	2.22E-09	0.79	FALSE	1.70E-01	1.15	FALSE
M401T1031_pos	401.3414	1031	3	5.36E-04	1.48	FALSE	1.07E-03	0.70	FALSE	8.90E-01	0.99	FALSE	1.39E-01	1.35	FALSE
M402T608_pos	402.2333	608	3	6.73E-01	0.98	FALSE	5.53E-01	1.03	FALSE	3.58E-02	1.09	FALSE	7.09E-01	0.97	FALSE
M402T825_pos	402.2389	825	3	1.70E-05	0.70	FALSE	3.68E-03	0.79	FALSE	2.81E-05	1.35	FALSE	9.44E-01	1.01	FALSE
M403T122_pos	403.0677	122	3	5.43E-02	0.85	FALSE	2.98E-01	1.10	FALSE	5.52E-04	1.30	FALSE	5.70E-01	0.90	FALSE
M403T1071_pos	403.2329	1071	3	3.45E-01	0.89	FALSE	5.80E-01	1.08	FALSE	9.18E-01	0.99	FALSE	7.06E-01	0.98	FALSE
M403T1060_pos	403.3059	1060	3	2.43E-01	-1.61	FALSE	2.91E-01	0.13	FALSE	3.21E-01	-0.52	FALSE	5.05E-02	0.51	FALSE
M403T983_pos	403.3205	983	3	4.98E-07	1.50	FALSE	5.42E-01	1.05	FALSE	1.42E-07	1.44	FALSE	9.66E-02	0.78	FALSE
M404T721_pos	404.2333	721	3	2.11E-03	1.22	FALSE	4.29E-01	0.95	FALSE	1.39E-01	1.09	FALSE	4.36E-01	0.94	FALSE
M405T803_pos	405.2150	803	3	3.41E-05	1.19	FALSE	6.52E-01	1.02	FALSE	1.74E-03	0.89	FALSE	9.79E-01	1.00	FALSE
M405T1033_pos	405.2998	1033	3	9.35E-02	1.12	FALSE	2.86E-01	1.08	FALSE	9.21E-06	1.30	FALSE	9.56E-01	1.01	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M407T932_pos	407.2795	932	3							HMDB0000391	7-Ketodeoxycholic acid	C24H38O5	0.7
M408T980_pos	408.3108	980	3						Terpenoids				
M409T614_pos	409.1803	614	3							HMDB0259951	-(2-((2-(2-ethoxyphenoxy)ethyl)am	C20H28N2O5S	2.8
M409T803_pos	409.2330	803	3							HMDB0062190	almitoyl-dihydroxyacetone-phosph	C19H37O7P	4.9
M410T1031_pos	410.2675	1031	3							HMDB0255789	1-yl-2,7,8,9,12,14,15,16-octahydro	C26H35NO3	3.6
M410T972_pos	410.3264	972	3						Terpenoids				
M413T745_pos	413.2073	745	3							HMDB0256185	9-ethoxy-8-methoxy-1,2,3,4,4a,10b	C23H28N2O5	0.6
M413T809_pos	413.2077	809	3							HMDB0256185	9-ethoxy-8-methoxy-1,2,3,4,4a,10b	C23H28N2O5	1.4
M413T1060_pos	413.2879	1060	3							HMDB0260484	G(20:3(8Z,11Z,14Z)-2OH(5,6)/0:0/0	C23H40O6	4.6
M413T993_pos	413.3052	993	3							HMDB0015567	Calcipotriol	C27H40O3	0.4
M414T828_pos	414.3218	828	3							HMDB0013333	3-Hydroxy-9-hexadecenoylcarnitine	C23H43NO5	0.9
M415T769_pos	415.2230	769	3							HMDB0247263	7-Hydroxymitragynine	C23H30N2O5	0.7
M415T737_2_pos	415.2626	737	3							HMDB0250057	)methyl]-17-prop-1-ynyl-2,6,7,8,12	C29H34O2	1.2
M415T1017_pos	415.3207	1017	3							HMDB0036941	Smilagenone	C27H42O3	0.0
M416T968_pos	416.2650	968	3							HMDB0241370	3-Hydroxytetradec-4-enedioylcarn	C21H37NO7	1.8
M417T625_pos	417.2110	625	3							HMDB0036340	l 7-epi-12-hydroxyjasmonate gluco	C20H32O9	2.1
M417T1000_pos	417.3363	1000	3							HMDB0000430	24,25-Dihydroxyvitamin D	C27H44O3	0.1
M420T1060_pos	420.3297	1060	3						Fatty acids				
M422T979_pos	422.3266	979	3							HMDB0006318	Gamma-linolenyl carnitine	C25H43NO4	0.3
M425T984_pos	425.2693	984	3							HMDB0249573	Camicinal	C25H33FN4O	4.3
M426T728_pos	426.2446	728	3							HMDB0249315	o)propyl)-1-((4-(((1,1-dimethyleth	C18H31N7O5	3.1
M426T896_pos	426.2855	896	3							HMDB0241487	8Z)-Hexadeca-6,8-dienedioylcarni	C23H39NO6	1.2
M427T789_2_pos	427.2310	789	3							HMDB0036011	Cinnzeylanine	C22H34O8	3.9
M427T1042_pos	427.3565	1042	3							HMDB0012167	4beta-methyl-5alpha-cholesta-8,2	C29H46O2	1.3
M429T893_pos	429.3000	893	3							HMDB0035506	Schidigeragenin B	C27H40O4	0.1
M429T948_pos	429.3003	948	3							HMDB0035506	Schidigeragenin B	C27H40O4	0.8
M431T1022_2_pos	431.1928	1022	3							HMDB0032622	Phenethyl rutinoside	C20H30O10	3.8
M431T1027_pos	431.2561	1027	3							HMDB0014660	Trandolapril	C24H34N2O5	4.7
M431T989_pos	431.2783	989	3							HMDB0040994	thyl-2E-pentenoyl)-2b,9a-dihydrox	C26H38O5	2.1
M431T918_pos	431.3156	918	3							HMDB0011590	(24:6(6Z,9Z,12Z,15Z,18Z,21Z)/0:0/	C27H42O4	0.1
M433T1019_pos	433.2943	1019	3							HMDB0014792	Latanoprost	C26H40O5	1.3
M433T1063_pos	433.3313	1063	3						Terpenoids	HMDB0006228	24-Hydroxycalcitriol	C27H44O4	0.2
M435T970_pos	435.3467	970	3							HMDB0000359	pha,7alpha-Dihydroxycoprostanic a	C27H46O4	0.4
M436T581_pos	436.2231	581	3							HMDB0033451	Cadabicine	C25H29N3O4	0.1
M436T937_pos	436.2235	937	3							HMDB0033451	Cadabicine	C25H29N3O4	1.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M407T932_pos	407.2795	932	3	3.12E-01	0.88	FALSE	2.98E-01	0.87	FALSE	6.46E-01	0.95	FALSE	7.93E-01	1.07	FALSE
M408T980_pos	408.3108	980	3	4.01E-01	0.96	FALSE	5.64E-01	1.03	FALSE	4.69E-01	0.97	FALSE	5.87E-01	0.91	FALSE
M409T614_pos	409.1803	614	3	1.49E-03	1.30	FALSE	3.31E-02	1.20	FALSE	1.46E-03	1.26	FALSE	8.58E-01	1.03	FALSE
M409T803_pos	409.2330	803	3	5.18E-05	0.74	FALSE	6.83E-05	1.35	FALSE	9.84E-07	1.37	FALSE	3.91E-01	0.93	FALSE
M410T1031_pos	410.2675	1031	3	2.22E-01	1.22	FALSE	1.77E-01	0.78	FALSE	3.23E-01	0.87	FALSE	5.65E-01	1.25	FALSE
M410T972_pos	410.3264	972	3	2.84E-17	1.36	FALSE	5.87E-13	0.79	FALSE	3.31E-12	0.81	FALSE	2.31E-01	1.08	FALSE
M413T745_pos	413.2073	745	3	1.27E-02	0.72	FALSE	4.66E-03	1.49	FALSE	1.56E-02	1.32	FALSE	1.48E-01	0.74	FALSE
M413T809_pos	413.2077	809	3	3.92E-03	1.44	FALSE	5.21E-03	0.71	FALSE	5.82E-02	0.81	FALSE	2.04E-01	0.88	FALSE
M413T1060_pos	413.2879	1060	3	9.16E-01	1.00	FALSE	8.86E-01	1.00	FALSE	3.70E-01	0.98	FALSE	7.44E-01	0.98	FALSE
M413T993_pos	413.3052	993	3	3.22E-02	0.75	FALSE	6.62E-01	1.06	FALSE	9.63E-01	1.01	FALSE	2.93E-01	0.68	FALSE
M414T828_pos	414.3218	828	3	1.87E-02	1.27	FALSE	5.07E-01	0.93	FALSE	3.20E-04	1.38	FALSE	2.83E-01	0.78	FALSE
M415T769_pos	415.2230	769	3	6.35E-02	0.75	FALSE	3.37E-02	1.43	FALSE	3.83E-02	1.32	FALSE	4.76E-01	1.19	FALSE
M415T737_2_pos	415.2626	737	3	1.40E-01	1.06	FALSE	5.91E-02	1.08	FALSE	3.62E-02	1.07	FALSE	1.12E-01	1.18	FALSE
M415T1017_pos	415.3207	1017	3	1.73E-01	1.14	FALSE	9.38E-02	0.84	FALSE	2.90E-01	0.92	FALSE	2.36E-01	1.34	FALSE
M416T968_pos	416.2650	968	3	8.66E-03	1.28	FALSE	3.92E-01	0.92	FALSE	3.41E-01	0.93	FALSE	9.89E-01	1.00	FALSE
M417T625_pos	417.2110	625	3	8.48E-01	0.97	FALSE	8.46E-01	0.96	FALSE	4.25E-01	1.13	FALSE	9.61E-01	1.03	FALSE
M417T1000_pos	417.3363	1000	3	4.41E-02	1.25	FALSE	6.55E-01	0.95	FALSE	2.13E-01	0.89	FALSE	3.19E-01	0.80	FALSE
M420T1060_pos	420.3297	1060	3	2.73E-01	-9.19	FALSE	3.11E-01	0.31	FALSE	2.87E-01	-0.03	FALSE	2.62E-01	0.76	FALSE
M422T979_pos	422.3266	979	3	4.31E-03	1.07	FALSE	5.49E-01	1.02	FALSE	4.79E-02	1.04	FALSE	4.10E-01	0.94	FALSE
M425T984_pos	425.2693	984	3	5.01E-05	1.27	FALSE	2.86E-01	0.94	FALSE	3.96E-08	1.34	FALSE	1.14E-01	0.88	FALSE
M426T728_pos	426.2446	728	3	7.93E-01	0.98	FALSE	3.60E-02	0.86	FALSE	3.12E-01	1.06	FALSE	1.05E-01	0.91	FALSE
M426T896_pos	426.2855	896	3	1.44E-01	1.07	FALSE	1.05E-02	1.14	FALSE	2.80E-15	1.45	FALSE	6.37E-01	1.05	FALSE
M427T789_2_pos	427.2310	789	3	9.94E-01	1.00	FALSE	1.85E-03	0.71	FALSE	8.86E-03	1.29	FALSE	3.92E-01	0.86	FALSE
M427T1042_pos	427.3565	1042	3	2.56E-01	1.14	FALSE	7.85E-01	0.97	FALSE	4.32E-01	1.08	FALSE	9.50E-01	0.99	FALSE
M429T893_pos	429.3000	893	3	1.43E-07	1.25	FALSE	2.80E-01	0.95	FALSE	5.15E-04	1.14	FALSE	2.56E-02	0.88	FALSE
M429T948_pos	429.3003	948	3	1.61E-09	1.49	FALSE	2.45E-01	0.92	FALSE	2.40E-04	1.23	FALSE	2.73E-01	0.83	FALSE
M431T1022_2_pos	431.1928	1022	3	3.17E-22	0.70	FALSE	7.57E-10	1.23	FALSE	2.05E-02	0.94	FALSE	3.21E-01	0.92	FALSE
M431T1027_pos	431.2561	1027	3	1.01E-02	1.17	FALSE	6.49E-03	0.84	FALSE	7.80E-01	0.99	FALSE	3.00E-01	1.29	FALSE
M431T989_pos	431.2783	989	3	1.38E-01	1.16	FALSE	7.85E-05	0.68	FALSE	2.27E-02	0.82	FALSE	9.45E-01	0.98	FALSE
M431T918_pos	431.3156	918	3	2.32E-08	1.38	FALSE	5.46E-01	0.97	FALSE	2.09E-03	1.16	FALSE	7.87E-01	0.95	FALSE
M433T1019_pos	433.2943	1019	3	5.18E-10	1.43	FALSE	2.14E-01	1.07	FALSE	5.31E-05	1.21	FALSE	3.72E-02	1.20	FALSE
M433T1063_pos	433.3313	1063	3	1.62E-01	1.21	FALSE	2.01E-01	0.84	FALSE	2.42E-01	0.87	FALSE	5.19E-01	1.12	FALSE
M435T970_pos	435.3467	970	3	3.91E-02	1.20	FALSE	8.62E-01	1.02	FALSE	6.09E-01	1.04	FALSE	4.68E-01	1.12	FALSE
M436T581_pos	436.2231	581	3	6.03E-01	0.92	FALSE	7.28E-01	0.95	FALSE	5.25E-01	1.09	FALSE	7.33E-01	0.92	FALSE
M436T937_pos	436.2235	937	3	8.58E-01	1.02	FALSE	4.08E-03	0.77	FALSE	2.34E-05	1.40	FALSE	3.96E-01	0.74	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M437T744_2_pos	437.2760	744	3							HMDB0032798	uranosyl-(1->2)-b-D-glucopyranosi	C21H40O9	3.3
M438T626_pos	438.2388	626	3							HMDB0033469	N1,N10-Dicoumaroylspermidine	C25H31N3O4	0.1
M438T837_pos	438.2391	837	3							HMDB0033469	N1,N10-Dicoumaroylspermidine	C25H31N3O4	0.9
M438T1066_pos	438.3790	1066	3						Fatty acids				
M441T777_pos	441.2025	777	3							HMDB0033468	Diferuloylputrescine	C24H28N2O6	1.2
M441T825_pos	441.2274	825	3							HMDB0244487	yl)-N-(5-(4-(dimethylamino)piperic	C22H29ClN8	0.6
M441T1066_pos	441.2979	1066	3							HMDB0243623	fluoro-27-nor-9,10-seco-5,7,10(19)	C26H39F3O2	1.0
M441T1067_pos	441.3729	1067	3							HMDB0001421	thyl-14a-formyl-5a-cholesta-8,24-d	C30H48O2	0.3
M442T826_pos	442.2316	826	3							HMDB0245941	3-N-(2-Fluoroethyl)spiperone	C25H29F2N3O2	3.4
M442T1058_pos	442.3877	1058	3							HMDB0240881	17-methyloctadecanoylcarnitine	C26H51NO4	3.0
M443T825_pos	443.2336	825	3							HMDB0257199	RHODAMINE 6G	C28H30N2O3	1.6
M443T1046_pos	443.2991	1046	3							HMDB0038242	Ascorbyl stearate	C24H42O7	2.8
M444T481_pos	444.1879	481	3							HMDB0250875	Dathf	C21H25N5O6	0.3
M444T810_pos	444.3109	810	3							HMDB0241987	N-Linoleoyl Tyrosine	C27H41NO4	0.1
M444T1048_2_pos	444.3089	1048	3							HMDB0241987	N-Linoleoyl Tyrosine	C27H41NO4	4.3
M446T681_pos	446.3265	681	3							HMDB0062337	N-Oleoyl tyrosine	C27H43NO4	0.1
M447T1058_pos	447.3470	1058	3							HMDB0012557	2-Oxo-20-trihydroxy-leukotriene B	C28H46O4	0.3
M447T992_pos	447.3470	992	3							HMDB0012557	2-Oxo-20-trihydroxy-leukotriene B	C28H46O4	0.4
M448T444_pos	448.2051	444	3							HMDB0252952	yl)-3-((4-methyl-6-(methylamino)-1	C21H24F3N7O	3.7
M449T712_pos	449.1449	712	3							HMDB0029481	Isosakuranin	C22H24O10	1.5
M449T965_pos	449.2898	965	3							HMDB0040993	4)-oplopen-3-one 2-(2-methylbut	C26H40O6	0.1
M449T996_pos	449.3264	996	3							HMDB0032783	Porrigenin A	C27H44O5	0.5
M450T500_pos	450.2124	500	3							HMDB0039900	din 5-[E-feruloyl-(->3)-apiosyl-(1->	C23H31NO8	0.3
M450T759_pos	450.2387	759	3							HMDB0039857	Cadabicine methyl ether	C26H31N3O4	0.1
M450T751_pos	450.2749	751	3							HMDB0251669	oxy)-2-(4-(3-(pyrrolidin-1-yl)propox	C27H35N3O3	0.4
M451T759_pos	451.2422	759	3							HMDB0257146	Remogliflozin A	C23H34N2O7	3.7
M451T804_pos	451.3043	804	3							HMDB0303328	Sodium stearoyl 2-lactylate	C24H43NaO6	3.0
M452T895_pos	452.2547	895	3							HMDB0249799	Ceniserti	C24H30FN7O	4.8
M452T694_pos	452.2753	694	3							HMDB0011474	LysoPE(0:0/16:1(9Z))	C21H42NO7P	4.0
M455T1075_pos	455.2335	1075	3							HMDB0255908	Octimibate	C29H30N2O3	1.4
M459T742_pos	459.1993	742	3							HMDB0252405	Fluprostenol	C23H29F3O6	0.9
M459T1067_pos	459.3085	1067	3							HMDB0033728	Pubesenolide	C28H42O5	4.3
M460T1061_pos	460.2807	1061	3							HMDB0249489	yhexyl)-1-(2-cyclohexyl-2-hydroxye	C25H37N3O5	0.3
M461T857_1_pos	461.2299	857	3							HMDB0249311	ethoxy-4-pyrimidinyl)-1-piperazin	C25H28N6O3	0.7
M462T882_pos	462.2963	882	3							HMDB0244548	Z-Leu-Leu-Norvalinal	C25H39N3O5	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M437T744_2_pos	437.2760	744	3	9.01E-02	1.07	FALSE	2.17E-01	1.05	FALSE	2.76E-08	1.22	FALSE	8.48E-02	1.17	FALSE
M438T626_pos	438.2388	626	3	4.66E-01	0.96	FALSE	1.55E-01	1.09	FALSE	6.07E-12	1.46	FALSE	8.96E-02	1.33	FALSE
M438T837_pos	438.2391	837	3	4.60E-01	1.06	FALSE	1.27E-02	1.22	FALSE	8.77E-04	1.25	FALSE	2.47E-01	0.84	FALSE
M438T1066_pos	438.3790	1066	3	4.51E-02	0.97	FALSE	8.23E-01	1.00	FALSE	3.76E-03	0.96	FALSE	3.73E-01	1.04	FALSE
M441T777_pos	441.2025	777	3	3.14E-01	0.91	FALSE	9.16E-01	1.01	FALSE	7.29E-03	1.25	FALSE	7.79E-01	1.07	FALSE
M441T825_pos	441.2274	825	3	1.96E-01	1.07	FALSE	7.00E-02	1.11	FALSE	6.74E-10	1.33	FALSE	7.91E-01	1.03	FALSE
M441T1066_pos	441.2979	1066	3	6.86E-01	1.03	FALSE	1.16E-01	1.14	FALSE	8.53E-01	0.99	FALSE	4.38E-01	1.14	FALSE
M441T1067_pos	441.3729	1067	3	6.49E-01	1.14	FALSE	5.12E-01	1.21	FALSE	2.70E-01	1.32	FALSE	1.86E-01	2.16	FALSE
M442T826_pos	442.2316	826	3	8.16E-02	1.09	FALSE	1.93E-01	1.07	FALSE	7.00E-11	1.33	FALSE	9.93E-01	1.00	FALSE
M442T1058_pos	442.3877	1058	3	1.35E-01	0.74	FALSE	3.00E-01	1.22	FALSE	1.59E-01	0.78	FALSE	3.77E-01	0.61	FALSE
M443T825_pos	443.2336	825	3	5.01E-01	0.97	FALSE	3.79E-02	1.10	FALSE	1.04E-12	1.34	FALSE	6.61E-01	1.04	FALSE
M443T1046_pos	443.2991	1046	3	5.19E-01	0.96	FALSE	2.77E-01	0.94	FALSE	8.63E-01	1.01	FALSE	5.12E-01	0.89	FALSE
M444T481_pos	444.1879	481	3	5.41E-10	0.68	FALSE	9.84E-02	1.10	FALSE	1.86E-11	1.43	FALSE	5.08E-01	1.08	FALSE
M444T810_pos	444.3109	810	3	2.62E-05	1.41	FALSE	4.82E-01	1.06	FALSE	1.08E-06	1.42	FALSE	1.47E-01	1.25	FALSE
M444T1048_2_pos	444.3089	1048	3	1.66E-05	0.86	FALSE	4.35E-02	1.07	FALSE	2.29E-05	0.88	FALSE	1.54E-01	1.15	FALSE
M446T681_pos	446.3265	681	3	9.20E-08	1.32	FALSE	8.41E-03	0.87	FALSE	1.37E-04	1.18	FALSE	4.91E-01	1.07	FALSE
M447T1058_pos	447.3470	1058	3	6.66E-01	1.05	FALSE	6.77E-02	0.81	FALSE	9.78E-01	1.00	FALSE	8.61E-02	0.46	FALSE
M447T992_pos	447.3470	992	3	4.45E-05	0.78	FALSE	1.91E-01	1.08	FALSE	2.17E-01	0.94	FALSE	3.16E-01	1.07	FALSE
M448T444_pos	448.2051	444	3	2.85E-08	1.30	FALSE	2.59E-01	0.95	FALSE	6.82E-03	1.11	FALSE	2.22E-01	0.93	FALSE
M449T712_pos	449.1449	712	3	2.65E-01	1.50	FALSE	8.63E-01	0.93	FALSE	6.10E-02	1.84	FALSE	4.40E-01	2.30	FALSE
M449T965_pos	449.2898	965	3	1.70E-01	1.12	FALSE	7.06E-01	0.97	FALSE	2.81E-01	0.92	FALSE	5.13E-01	0.84	FALSE
M449T996_pos	449.3264	996	3	1.17E-05	1.18	FALSE	1.25E-01	0.94	FALSE	4.41E-08	1.20	FALSE	5.83E-01	1.03	FALSE
M450T500_pos	450.2124	500	3	3.78E-02	0.87	FALSE	1.10E-01	1.12	FALSE	4.51E-03	1.19	FALSE	7.53E-01	1.04	FALSE
M450T759_pos	450.2387	759	3	4.82E-01	1.07	FALSE	8.03E-02	0.84	FALSE	1.23E-02	1.24	FALSE	4.79E-02	1.41	FALSE
M450T751_pos	450.2749	751	3	9.22E-07	1.24	FALSE	4.04E-01	1.04	FALSE	4.84E-12	1.31	FALSE	9.45E-02	1.21	FALSE
M451T759_pos	451.2422	759	3	4.94E-02	0.86	FALSE	6.41E-01	1.04	FALSE	4.20E-05	1.33	FALSE	6.48E-01	1.07	FALSE
M451T804_pos	451.3043	804	3	4.54E-03	1.29	FALSE	2.99E-01	0.91	FALSE	1.21E-06	1.49	FALSE	2.59E-01	0.92	FALSE
M452T895_pos	452.2547	895	3	3.75E-01	1.20	FALSE	4.59E-01	1.16	FALSE	6.29E-01	1.09	FALSE	5.96E-01	0.89	FALSE
M452T694_pos	452.2753	694	3	1.05E-01	0.85	FALSE	2.17E-01	1.13	FALSE	1.37E-05	1.47	FALSE	9.47E-01	1.01	FALSE
M455T1075_pos	455.2335	1075	3	2.96E-01	1.04	FALSE	1.03E-01	1.06	FALSE	7.49E-02	0.95	FALSE	3.62E-02	1.29	FALSE
M459T742_pos	459.1993	742	3	1.20E-03	0.73	FALSE	1.16E-04	1.46	FALSE	7.03E-03	1.25	FALSE	9.99E-01	1.00	FALSE
M459T1067_pos	459.3085	1067	3	8.25E-01	0.99	FALSE	4.59E-01	0.96	FALSE	5.62E-04	1.18	FALSE	2.59E-01	0.89	FALSE
M460T1061_pos	460.2807	1061	3	5.22E-03	1.19	FALSE	9.41E-02	0.90	FALSE	3.67E-06	1.29	FALSE	4.73E-01	0.92	FALSE
M461T857_1_pos	461.2299	857	3	5.03E-01	1.04	FALSE	1.33E-03	1.23	FALSE	5.19E-08	1.33	FALSE	1.44E-01	1.22	FALSE
M462T882_pos	462.2963	882	3	2.90E-02	0.89	FALSE	7.15E-02	1.11	FALSE	4.91E-01	1.03	FALSE	5.37E-01	1.07	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M462T667_pos	462.3213	667	3							HMDB0241595	Z)-12-Hydroxyicosa-5,8,10,14,17-p	C27H43NO5	0.3
M464T726_pos	464.3372	726	3							HMDB0240765	3-Hydroxyarachidonoylcarnitine	C27H45NO5	0.3
M464T972_pos	464.3380	972	3							HMDB0240765	3-Hydroxyarachidonoylcarnitine	C27H45NO5	2.0
M465T938_pos	465.3213	938	3							HMDB0251684	Ecdysone	C27H44O6	0.6
M467T769_pos	467.2768	769	3							HMDB0247908	Acetildenafil	C25H34N6O3	0.5
M469T1033_pos	469.3292	1033	3							HMDB0241883	Z)-10-Nitrooctadeca-9,12-dienoylca	C25H44N2O6	4.2
M474T717_pos	474.2706	717	3							HMDB0015603	Ximelagatran	C24H35N5O5	1.0
M478T778_pos	478.3164	778	3							HMDB0241797	oxyoct-1-en-1-yl]-5-oxocyclopent-2	C27H43NO6	0.3
M479T985_pos	479.3368	985	3							HMDB0034086	Dolicholide	C28H46O6	0.1
M480T911_pos	480.3081	911	3							HMDB0011475	LysoPE(0:0/18:1(11Z))	C23H46NO7P	0.7
M480T979_pos	480.3332	979	3							HMDB0241589	)-12-Hydroperoxyicosa-5,8,10,14-	C27H45NO6	2.7
M481T645_pos	481.2621	645	3							HMDB0032839	Citronellyl beta-sophoroside	C22H40O11	4.6
M481T714_pos	481.2795	714	3							HMDB0255516	Neoandrographolide	C26H40O8	0.3
M482T943_pos	482.3239	943	3							HMDB0010381	LysoPC(15:0/0:0)	C23H48NO7P	0.5
M483T858_pos	483.2355	858	3							HMDB0029991	Dulciol C	C28H34O7	4.6
M484T838_pos	484.2440	838	3							HMDB0033470	Caffeoylferuloylspermidine	C26H33N3O6	0.4
M487T792_pos	487.2277	792	3							HMDB0248480	Antibiotic LL-AB 664	C18H30N8O8	3.6
M487T1046_pos	487.3261	1046	3							HMDB0030200	Hovenine A	C27H42N4O4	3.7
M487T973_pos	487.3419	973	3							HMDB0034526	Bassic acid	C30H46O5	0.3
M489T1051_pos	489.3194	1051	3							HMDB0249891	Antcin K	C29H44O6	3.4
M489T931_pos	489.3574	931	3							HMDB0034036	Pitheduloside I	C30H48O5	0.0
M489T1066_pos	489.3665	1066	3							HMDB0257531	a-1,7,13,19-tetraazatricyclo(11.11	C24H48N4O6	3.8
M491T647_pos	491.2864	647	3							HMDB0060118	y-13-O-D-glucuronoside-octadec-	C24H42O10	2.7
M492T1022_pos	492.2808	1022	3							HMDB0254083	Lidoflazine	C30H35F2N3O	2.6
M493T658_pos	493.2433	658	3							HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.2
M493T612_pos	493.2435	612	3							HMDB0060123	5,6-Epoxy-retinoyl-beta-D-glucuro	C26H36O9	0.5
M494T1048_pos	494.3323	1048	3							HMDB0257757	methyl-9-oxo-6-tricyclo[5.4.3.01,8	C28H47NO4S	4.9
M495T790_pos	495.2969	790	3							HMDB0034617	noxy-3,4-epoxy-14-hydroxy-12-cya	C27H42O8	3.4
M495T1060_2_pos	495.3434	1060	3							HMDB0062314	1-docosanoyl-glycero-3-phosphate	C25H51O7P	2.3
M495T1051_pos	495.3893	1051	3							HMDB0251574	taethylene glycol monododecyl et	C26H54O8	0.3
M496T821_pos	496.2422	821	3							HMDB0258291	Silodosin	C25H32F3N3O4	0.8
M497T1060_pos	497.3198	1060	3							HMDB0005772	Postin	C22H40N8O5	0.8
M500T818_pos	500.3219	818	3							HMDB0259406	xybutyl)-N-(2-methylpropyl)-N-((3	C27H41N5O4	2.5
M502T811_pos	502.2913	811	3							HMDB0011487	LysoPE(0:0/20:4(5Z,8Z,11Z,14Z))	C25H44NO7P	2.9
M503T776_pos	503.2617	776	3							HMDB0030362	Cavipetin B	C28H38O8	4.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M462T667_pos	462.3213	667	3	5.20E-06	1.28	FALSE	5.19E-01	0.96	FALSE	2.10E-15	1.49	FALSE	7.31E-01	0.98	FALSE
M464T726_pos	464.3372	726	3	1.62E-01	1.07	FALSE	1.43E-02	0.89	FALSE	4.96E-06	1.22	FALSE	4.79E-01	1.07	FALSE
M464T972_pos	464.3380	972	3	3.38E-02	1.20	FALSE	9.97E-02	0.86	FALSE	1.14E-01	1.13	FALSE	7.51E-01	0.93	FALSE
M465T938_pos	465.3213	938	3	6.58E-02	1.11	FALSE	5.08E-01	1.04	FALSE	4.38E-10	1.38	FALSE	3.16E-01	0.90	FALSE
M467T769_pos	467.2768	769	3	2.39E-02	1.21	FALSE	4.76E-02	1.20	FALSE	3.18E-02	1.17	FALSE	7.27E-01	1.08	FALSE
M469T1033_pos	469.3292	1033	3	2.36E-01	1.09	FALSE	4.00E-01	1.07	FALSE	8.93E-02	0.90	FALSE	7.35E-02	1.19	FALSE
M474T717_pos	474.2706	717	3	3.34E-03	0.79	FALSE	6.11E-04	1.32	FALSE	1.69E-05	1.36	FALSE	2.27E-01	1.16	FALSE
M478T778_pos	478.3164	778	3	8.75E-07	1.19	FALSE	2.68E-01	1.04	FALSE	2.08E-19	1.36	FALSE	2.33E-01	1.06	FALSE
M479T985_pos	479.3368	985	3	2.51E-06	1.30	FALSE	1.25E-01	0.92	FALSE	2.21E-08	1.32	FALSE	7.78E-02	0.78	FALSE
M480T911_pos	480.3081	911	3	3.25E-01	0.95	FALSE	6.37E-01	0.97	FALSE	4.09E-10	1.37	FALSE	6.84E-02	0.84	FALSE
M480T979_pos	480.3332	979	3	5.42E-01	1.02	FALSE	7.10E-01	0.99	FALSE	3.95E-03	1.07	FALSE	6.73E-01	0.94	FALSE
M481T645_pos	481.2621	645	3	2.43E-02	1.07	FALSE	8.45E-01	0.99	FALSE	6.20E-13	1.21	FALSE	1.16E-03	1.39	FALSE
M481T714_pos	481.2795	714	3	9.15E-07	1.25	FALSE	3.84E-02	1.10	FALSE	4.66E-06	1.20	FALSE	5.74E-02	1.20	FALSE
M482T943_pos	482.3239	943	3	9.07E-01	1.01	FALSE	3.61E-02	0.88	FALSE	2.73E-12	1.46	FALSE	1.09E-01	0.73	FALSE
M483T858_pos	483.2355	858	3	7.02E-02	1.05	FALSE	1.23E-03	1.10	FALSE	1.44E-02	0.94	FALSE	1.45E-01	1.09	FALSE
M484T838_pos	484.2440	838	3	1.48E-02	0.87	FALSE	1.43E-02	1.16	FALSE	4.79E-09	1.37	FALSE	3.06E-02	1.13	FALSE
M487T792_pos	487.2277	792	3	7.74E-01	1.03	FALSE	5.12E-02	0.83	FALSE	2.54E-05	1.43	FALSE	2.01E-01	0.89	FALSE
M487T1046_pos	487.3261	1046	3	8.92E-02	0.87	FALSE	8.89E-01	1.01	FALSE	2.65E-02	0.85	FALSE	8.11E-02	0.78	FALSE
M487T973_pos	487.3419	973	3	5.01E-02	1.23	FALSE	2.13E-01	0.86	FALSE	2.08E-01	1.12	FALSE	1.93E-01	1.36	FALSE
M489T1051_pos	489.3194	1051	3	2.45E-01	0.96	FALSE	3.16E-01	0.97	FALSE	2.31E-11	1.22	FALSE	5.11E-01	0.97	FALSE
M489T931_pos	489.3574	931	3	1.53E-19	1.47	FALSE	4.51E-03	0.89	FALSE	7.70E-08	1.20	FALSE	4.95E-02	1.14	FALSE
M489T1066_pos	489.3665	1066	3	2.01E-01	1.02	FALSE	8.29E-01	1.00	FALSE	8.34E-01	1.00	FALSE	9.18E-01	1.00	FALSE
M491T647_pos	491.2864	647	3	4.25E-02	0.86	FALSE	4.03E-03	0.81	FALSE	1.60E-02	1.17	FALSE	4.55E-01	0.89	FALSE
M492T1022_pos	492.2808	1022	3	3.60E-04	0.92	FALSE	1.37E-02	1.06	FALSE	5.51E-02	1.04	FALSE	9.69E-01	1.00	FALSE
M493T658_pos	493.2433	658	3	1.21E-01	1.11	FALSE	8.63E-04	1.26	FALSE	4.90E-09	1.44	FALSE	6.34E-03	1.36	FALSE
M493T612_pos	493.2435	612	3	1.79E-01	1.13	FALSE	3.36E-04	1.39	FALSE	5.83E-06	1.44	FALSE	6.49E-03	1.38	FALSE
M494T1048_pos	494.3323	1048	3	2.21E-01	1.46	FALSE	2.98E-01	0.68	FALSE	1.90E-01	1.42	FALSE	1.77E-01	1.17	FALSE
M495T790_pos	495.2969	790	3	7.61E-12	1.48	FALSE	7.94E-01	0.99	FALSE	1.09E-13	1.45	FALSE	4.78E-01	1.09	FALSE
M495T1060_2_pos	495.3434	1060	3	8.58E-01	1.01	FALSE	1.42E-01	0.89	FALSE	8.73E-01	1.01	FALSE	7.06E-01	0.91	FALSE
M495T1051_pos	495.3893	1051	3	7.75E-02	0.97	FALSE	8.28E-02	1.03	FALSE	2.53E-01	0.99	FALSE	1.68E-01	0.95	FALSE
M496T821_pos	496.2422	821	3	5.30E-15	0.72	FALSE	5.77E-07	1.22	FALSE	2.19E-09	1.23	FALSE	3.02E-02	1.11	FALSE
M497T1060_pos	497.3198	1060	3	2.16E-01	1.17	FALSE	2.79E-01	0.86	FALSE	5.00E-01	1.08	FALSE	6.56E-01	1.09	FALSE
M500T818_pos	500.3219	818	3	5.56E-02	0.93	FALSE	5.00E-03	1.11	FALSE	1.82E-02	1.08	FALSE	3.29E-01	1.14	FALSE
M502T811_pos	502.2913	811	3	1.49E-03	0.81	FALSE	1.46E-03	1.24	FALSE	5.62E-11	1.48	FALSE	2.47E-01	0.91	FALSE
M503T776_pos	503.2617	776	3	4.15E-01	0.98	FALSE	9.70E-04	1.11	FALSE	3.43E-08	1.16	FALSE	1.99E-01	1.10	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M503T984_2_pos	503.3368	984	3							HMDB0034551	Medicagenic acid	C30H46O6	0.2
M504T852_pos	504.2661	852	3							HMDB0247848	Lysyl-aspartyl-glutamyl-leucine	C21H37N5O9	0.5
M505T915_pos	505.3519	915	3							HMDB0034500	Protobassic acid	C30H48O6	1.0
M507T659_pos	507.2203	659	3							HMDB0038170	Isolimonic acid	C26H34O10	4.2
M508T686_pos	508.3635	686	3							HMDB0242380	Cholylvaline	C29H49NO6	0.5
M510T960_pos	510.3434	960	3							HMDB0242443	Cholylthreonine	C28H47NO7	1.6
M510T1053_pos	510.3552	1053	3							HMDB0011481	LysoPE(0:0/20:0)	C25H52NO7P	0.4
M511T780_pos	511.3033	780	3							HMDB0240602	LysoPG(18:1(9Z)/0:0)	C24H47O9P	0.4
M515T1074_pos	515.3561	1074	3							HMDB0247498	Butyryl trihexyl citrate	C28H50O8	3.4
M519T971_pos	519.3299	971	3							HMDB0034392	Perulactone	C30H46O7	3.3
M520T782_pos	520.3276	782	3							HMDB0241614	Z)-7,16,17-Trihydroxydocosa-4,8,1	C29H45NO7	1.5
M520T858_pos	520.3279	858	3							HMDB0241614	Z)-7,16,17-Trihydroxydocosa-4,8,1	C29H45NO7	1.9
M521T636_pos	521.2572	636	3							HMDB0029771	ydrovomifoliol 9-[apiosyl-(1->6)-glu	C24H40O12	3.9
M522T979_pos	522.3790	979	3						Terpenoids	HMDB0242373	Cholylisoleucine	C30H51NO6	0.1
M528T876_pos	528.3069	876	3							HMDB0011494	ysoPE(0:0/22:5(4Z,7Z,10Z,13Z,16Z	C27H46NO7P	3.0
M528T753_pos	528.2992	753	3							HMDB0251587	Doramapimod	C31H37N5O3	4.3
M539T1051_pos	539.4157	1051	3							HMDB0246126	taethyleneglycol monododecyl eth	C28H58O9	0.6
M553T1033_1_pos	552.5352	1033	3							HMDB0240678	Cer(d18:1/17:0)	C35H69NO3	0.4
M553T755_pos	553.3205	755	3							HMDB0004309	Triterpenoid	C30H48O7S	2.0
M565T653_pos	565.2835	653	3							HMDB0260018	methyl-21H,22H,23H,24H-porphy	C34H36N4O4	4.6
M567T847_pos	567.3046	847	3							HMDB0030461	Hordatine A	C28H38N8O5	1.4
M567T745_pos	567.3300	745	3							HMDB0041367	25-Cinnamoyl-vulgaroside	C34H46O7	2.9
M569T674_pos	569.3099	674	3							HMDB0244970	Enkephalinamide-Leu, Ala(2)-	C29H40N6O6	3.0
M571T908_pos	571.2781	908	3							HMDB0036360	Pipercyclobutanamide A	C34H38N2O6	3.8
M572T924_pos	572.2840	924	3							HMDB0005774	Endomorphin-2	C32H37N5O5	4.7
M583T1050_pos	583.4420	1050	3							HMDB0256665	Polidocanol	C30H62O10	0.7
M584T1078_pos	584.4734	1078	3						Fatty acids				
M587T667_pos	587.3275	667	3							HMDB0001278	Presqualene diphosphate	C30H52O7P2	2.4
M591T1019_1_pos	591.3180	1019	3							HMDB0004158	Urobilinogen	C33H42N4O6	0.4
M593T727_1_pos	593.3047	727	3							HMDB0253160	Hexobendine	C30H44N2O10	3.7
M593T940_pos	593.3338	940	3							HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.7
M595T736_pos	595.3501	736	3							HMDB0240259	Stercobilin	C33H46N4O6	1.8
M595T940_pos	595.3492	940	3							HMDB0240259	Stercobilin	C33H46N4O6	0.4
M597T1033_pos	597.3644	1033	3							HMDB0004157	Stercobilinogen	C33H48N4O6	0.5
M605T1071_pos	605.4232	1071	3							HMDB0256687	olyoxyethylene sorbitan monoolea	C32H60O10	4.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M503T984_2_pos	503.3368	984	3	3.58E-03	1.17	FALSE	4.37E-01	0.96	FALSE	2.76E-14	1.46	FALSE	1.59E-02	0.77	FALSE
M504T852_pos	504.2661	852	3	7.62E-02	1.12	FALSE	7.86E-06	0.75	FALSE	6.42E-03	1.16	FALSE	4.74E-01	0.88	FALSE
M505T915_pos	505.3519	915	3	2.82E-01	1.07	FALSE	1.54E-01	1.10	FALSE	8.40E-01	0.99	FALSE	2.15E-01	0.81	FALSE
M507T659_pos	507.2203	659	3	5.12E-03	1.09	FALSE	2.80E-01	1.04	FALSE	4.08E-22	1.36	FALSE	2.53E-01	0.93	FALSE
M508T686_pos	508.3635	686	3	1.80E-17	1.46	FALSE	2.40E-03	0.88	FALSE	1.94E-08	1.23	FALSE	8.33E-02	1.15	FALSE
M510T960_pos	510.3434	960	3	3.16E-01	0.96	FALSE	6.57E-04	1.16	FALSE	2.57E-03	1.11	FALSE	3.01E-01	1.13	FALSE
M510T1053_pos	510.3552	1053	3	9.44E-01	1.01	FALSE	7.97E-01	1.06	FALSE	1.86E-01	1.24	FALSE	7.72E-01	0.88	FALSE
M511T780_pos	511.3033	780	3	5.61E-02	1.14	FALSE	9.28E-01	1.01	FALSE	8.80E-03	1.17	FALSE	5.82E-01	1.05	FALSE
M515T1074_pos	515.3561	1074	3	5.09E-02	1.05	FALSE	8.21E-01	1.01	FALSE	3.08E-02	1.05	FALSE	3.91E-01	1.06	FALSE
M519T971_pos	519.3299	971	3	3.96E-01	1.04	FALSE	4.56E-01	0.97	FALSE	1.46E-01	1.06	FALSE	3.32E-01	0.95	FALSE
M520T782_pos	520.3276	782	3	3.59E-03	1.10	FALSE	2.68E-01	1.04	FALSE	3.27E-07	1.16	FALSE	7.85E-01	1.02	FALSE
M520T858_pos	520.3279	858	3	2.30E-01	1.06	FALSE	1.81E-02	1.12	FALSE	6.34E-15	1.40	FALSE	5.24E-02	1.19	FALSE
M521T636_pos	521.2572	636	3	4.60E-02	0.89	FALSE	7.04E-01	0.98	FALSE	5.87E-03	1.15	FALSE	5.94E-01	0.93	FALSE
M522T979_pos	522.3790	979	3	8.80E-01	1.00	FALSE	2.21E-01	1.04	FALSE	7.58E-05	1.12	FALSE	6.89E-01	1.04	FALSE
M528T876_pos	528.3069	876	3	1.47E-04	0.82	FALSE	2.85E-02	1.12	FALSE	1.95E-10	1.35	FALSE	9.82E-01	1.00	FALSE
M528T753_pos	528.2992	753	3	5.81E-03	0.79	FALSE	8.15E-01	0.98	FALSE	3.00E-07	1.50	FALSE	1.55E-01	0.79	FALSE
M539T1051_pos	539.4157	1051	3	9.17E-01	1.00	FALSE	7.63E-01	1.00	FALSE	7.19E-01	1.00	FALSE	3.22E-01	0.97	FALSE
M553T1033_1_pos	552.5352	1033	3	6.61E-02	0.78	FALSE	7.18E-01	0.95	FALSE	9.45E-01	1.01	FALSE	6.56E-01	1.11	FALSE
M553T755_pos	553.3205	755	3	5.18E-01	0.97	FALSE	2.59E-01	0.94	FALSE	5.63E-01	1.02	FALSE	8.05E-01	1.04	FALSE
M565T653_pos	565.2835	653	3	6.25E-01	1.03	FALSE	6.24E-01	1.03	FALSE	9.33E-03	1.15	FALSE	8.46E-01	0.98	FALSE
M567T847_pos	567.3046	847	3	4.52E-03	0.83	FALSE	4.69E-05	1.31	FALSE	3.82E-01	0.95	FALSE	9.70E-01	1.01	FALSE
M567T745_pos	567.3300	745	3	8.66E-01	0.99	FALSE	5.70E-01	1.05	FALSE	1.90E-03	1.23	FALSE	8.00E-01	0.96	FALSE
M569T674_pos	569.3099	674	3	8.30E-05	1.31	FALSE	2.10E-02	0.85	FALSE	2.49E-04	1.25	FALSE	8.68E-01	0.97	FALSE
M571T908_pos	571.2781	908	3	2.14E-01	7.58	FALSE	9.58E-01	1.06	FALSE	1.00E-01	16.61	FALSE	2.33E-01	-0.45	FALSE
M572T924_pos	572.2840	924	3	2.07E-01	6.14	FALSE	9.80E-01	0.97	FALSE	1.26E-01	7.39	FALSE	2.21E-01	-0.46	FALSE
M583T1050_pos	583.4420	1050	3	7.04E-02	0.97	FALSE	8.37E-01	1.00	FALSE	8.54E-01	1.00	FALSE	7.41E-01	0.99	FALSE
M584T1078_pos	584.4734	1078	3	2.24E-01	1.01	FALSE	8.26E-01	1.00	FALSE	7.31E-01	1.00	FALSE	7.48E-01	1.01	FALSE
M587T667_pos	587.3275	667	3	5.67E-01	0.97	FALSE	9.59E-01	1.00	FALSE	1.68E-02	1.13	FALSE	5.23E-01	0.93	FALSE
M591T1019_1_pos	591.3180	1019	3	2.78E-02	1.23	FALSE	8.40E-01	1.02	FALSE	6.08E-01	1.04	FALSE	4.59E-01	0.88	FALSE
M593T727_1_pos	593.3047	727	3	5.22E-01	1.23	FALSE	8.85E-01	1.06	FALSE	2.07E-01	0.70	FALSE	6.45E-02	0.86	FALSE
M593T940_pos	593.3338	940	3	1.03E-01	0.89	FALSE	2.99E-01	0.92	FALSE	6.70E-01	0.97	FALSE	2.85E-01	0.77	FALSE
M595T736_pos	595.3501	736	3	4.81E-03	1.21	FALSE	3.89E-04	0.79	FALSE	4.62E-04	1.23	FALSE	9.32E-01	1.01	FALSE
M595T940_pos	595.3492	940	3	5.81E-05	0.70	FALSE	1.03E-02	1.27	FALSE	3.48E-01	1.07	FALSE	2.36E-01	1.39	FALSE
M597T1033_pos	597.3644	1033	3	2.69E-02	0.77	FALSE	9.84E-03	1.37	FALSE	2.04E-01	1.14	FALSE	5.19E-02	1.30	FALSE
M605T1071_pos	605.4232	1071	3	6.10E-02	1.28	FALSE	4.56E-01	0.90	FALSE	4.08E-01	0.91	FALSE	5.67E-01	1.22	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M621T464_pos	621.2609	464	3						Carbohydrates				
M628T713_pos	628.3424	713	3							HMDB0249335	Boc-val-pro-arg-mca	C31H45N7O7	4.7
M628T1051_pos	628.4696	1051	3							HMDB0258449	Squalamine	C34H65N3O5S	3.5
M631T680_pos	631.3533	680	3							HMDB0014357	Remikiren	C33H50N4O6S	1.4
M642T759_pos	642.3840	759	3							HMDB0260055	2S)-2-[[(2R,6S)-2,6-dimethylpiperic	C34H51N5O7	3.3
M661T826_pos	661.3446	826	3							HMDB0002318	Capsianoside I	C32H52O14	2.5
M675T850_pos	675.3604	850	3						Amino acids and Peptides				
M818T1024_pos	817.5074	1024	3							HMDB0247884	yl-arginyl-prolyl-tyrosyl-isoleucyl-le	C38H64N12O8	3.8
M840T1062_pos	839.5708	1062	3							HMDB0061393	PC(DiMe(11,3)/DiMe(9,3))	C46H81NO10P	4.5
M91T714_neg	91.0553	714	3							HMDB0034168	Toluene	C7H8	0.3
M107T601_neg	107.0502	601	3							HMDB0001858	p-Cresol	C7H8O	0.0
M108T469_neg	108.0455	469	3							HMDB0001169	4-Aminophenol	C6H7NO	0.2
M131T526_neg	131.0715	526	3						Fatty acids	HMDB0000317	2-Hydroxy-3-methylpentanoic acid	C6H12O3	0.7
M135T714_neg	135.0452	714	3							HMDB0000209	Phenylacetic acid	C8H8O2	0.6
M136T513_neg	136.0769	513	3							HMDB0000306	Tyramine	C8H11NO	0.9
M137T745_neg	137.0245	745	3						Shikimates and Phenylpropanoids	HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.5
M137T607_neg	137.0245	607	3							HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.6
M138T402_neg	138.0562	402	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.9
M138T556_neg	138.0562	556	3							HMDB0012153	3,4-Dihydroxybenzylamine	C7H9NO2	0.7
M143T916_neg	143.1078	916	3						Fatty acids	HMDB0000482	Caprylic acid	C8H16O2	0.6
M144T433_neg	144.0667	433	3							HMDB0000730	Isobutyrylglycine	C6H11NO3	0.8
M146T627_neg	146.0612	627	3						Alkaloids	HMDB0005785	Indole-3-carbinol	C9H9NO	0.5
M149T784_neg	149.0609	784	3							HMDB0000764	Hydrocinnamic acid	C9H10O2	0.4
M152T469_neg	152.0354	469	3							HMDB0001476	3-Hydroxyanthranilic acid	C7H7NO3	0.6
M156T471_neg	156.0667	471	3							HMDB0000459	3-Methylcrotonylglycine	C7H11NO3	0.7
M162T569_neg	162.0561	569	3							HMDB0001424	4-(3-Pyridyl)-3-butenoic acid	C9H9NO2	0.5
M165T393_neg	165.0419	393	3							HMDB0001886	3-Methylxanthine	C6H6N4O2	0.5
M170T624_neg	170.0824	624	3							HMDB0247190	)-2-Oxotetrahydrofuran-3-Yl]butan	C8H13NO3	0.6
M171T761_neg	171.1027	761	3							HMDB0036188	Tetrahydrofurfuryl butyrate	C9H16O3	0.4
M173T455_neg	173.0820	455	3							HMDB0000893	Suberic acid	C8H14O4	0.5
M173T768_neg	173.1184	768	3						Fatty acids	HMDB0031513	\xc2\xb1)-3-Hydroxynonanoic acid	C9H18O3	0.3
M174T706_neg	174.0561	706	3						Alkaloids	HMDB0000197	Indoleacetic acid	C10H9NO2	0.5
M176T535_neg	176.0357	535	3						Alkaloids	HMDB0040612	4-Acetyl-2(3H)-benzoxazolone	C9H7NO3	1.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M621T464_pos	621.2609	464	3	8.90E-01	1.02	FALSE	6.26E-01	1.08	FALSE	8.02E-03	1.40	FALSE	8.69E-01	1.06	FALSE
M628T713_pos	628.3424	713	3	5.98E-01	1.03	FALSE	1.31E-09	0.68	FALSE	1.61E-06	1.28	FALSE	2.02E-02	1.34	FALSE
M628T1051_pos	628.4696	1051	3	1.69E-01	1.07	FALSE	3.09E-01	0.95	FALSE	5.05E-01	0.97	FALSE	5.42E-01	1.08	FALSE
M631T680_pos	631.3533	680	3	8.15E-01	0.99	FALSE	6.92E-01	0.97	FALSE	1.70E-01	1.08	FALSE	5.11E-01	0.92	FALSE
M642T759_pos	642.3840	759	3	1.34E-01	0.90	FALSE	6.13E-03	0.81	FALSE	4.08E-03	1.20	FALSE	1.65E-01	0.81	FALSE
M661T826_pos	661.3446	826	3	2.74E-08	0.70	FALSE	7.89E-02	1.12	FALSE	2.09E-06	1.30	FALSE	3.28E-01	1.16	FALSE
M675T850_pos	675.3604	850	3	6.58E-01	1.03	FALSE	6.87E-03	0.80	FALSE	1.10E-09	1.42	FALSE	6.08E-01	1.05	FALSE
M818T1024_pos	817.5074	1024	3	1.01E-12	1.14	FALSE	1.00E-02	0.95	FALSE	2.00E-06	0.93	FALSE	7.84E-01	1.01	FALSE
M840T1062_pos	839.5708	1062	3	2.45E-02	1.03	FALSE	2.77E-01	0.98	FALSE	8.57E-02	0.98	FALSE	1.27E-01	1.06	FALSE
M91T714_neg	91.0553	714	3	1.90E-10	1.29	FALSE	1.41E-02	1.10	FALSE	7.60E-06	1.17	FALSE	4.92E-01	1.06	FALSE
M107T601_neg	107.0502	601	3	9.61E-07	1.18	FALSE	4.49E-01	1.03	FALSE	1.50E-10	1.22	FALSE	4.05E-01	1.04	FALSE
M108T469_neg	108.0455	469	3	2.09E-05	1.17	FALSE	3.04E-01	1.04	FALSE	2.83E-23	1.45	FALSE	9.88E-01	1.00	FALSE
M131T526_neg	131.0715	526	3	6.64E-19	1.44	FALSE	2.29E-01	1.05	FALSE	1.74E-02	1.08	FALSE	7.10E-01	1.02	FALSE
M135T714_neg	135.0452	714	3	3.28E-15	1.46	FALSE	1.73E-02	1.12	FALSE	2.87E-04	1.15	FALSE	8.59E-01	1.02	FALSE
M136T513_neg	136.0769	513	3	4.68E-08	1.41	FALSE	2.48E-05	1.31	FALSE	3.25E-05	1.25	FALSE	6.10E-03	1.27	FALSE
M137T745_neg	137.0245	745	3	5.27E-02	1.53	FALSE	2.52E-01	0.75	FALSE	5.95E-01	0.90	FALSE	2.49E-01	1.50	FALSE
M137T607_neg	137.0245	607	3	5.55E-04	1.16	FALSE	2.29E-01	1.06	FALSE	4.16E-12	1.32	FALSE	9.08E-01	1.01	FALSE
M138T402_neg	138.0562	402	3	2.93E-03	1.10	FALSE	3.68E-01	1.03	FALSE	7.05E-19	1.33	FALSE	7.71E-01	1.01	FALSE
M138T556_neg	138.0562	556	3	1.56E-01	1.07	FALSE	2.44E-03	0.85	FALSE	5.26E-13	1.40	FALSE	4.48E-03	1.28	FALSE
M143T916_neg	143.1078	916	3	2.60E-01	1.53	FALSE	7.56E-01	0.89	FALSE	1.23E-01	1.67	FALSE	3.13E-01	0.46	FALSE
M144T433_neg	144.0667	433	3	1.02E-03	1.16	FALSE	9.92E-02	1.08	FALSE	4.94E-12	1.33	FALSE	6.40E-01	1.04	FALSE
M146T627_neg	146.0612	627	3	4.54E-03	1.16	FALSE	2.03E-01	1.07	FALSE	5.76E-12	1.41	FALSE	4.57E-02	1.16	FALSE
M149T784_neg	149.0609	784	3	2.16E-10	1.33	FALSE	4.33E-02	1.10	FALSE	8.73E-01	0.99	FALSE	4.05E-01	0.91	FALSE
M152T469_neg	152.0354	469	3	6.18E-09	1.26	FALSE	8.73E-02	1.07	FALSE	7.62E-21	1.43	FALSE	6.53E-01	1.03	FALSE
M156T471_neg	156.0667	471	3	6.03E-09	1.29	FALSE	2.89E-01	1.05	FALSE	6.61E-04	1.13	FALSE	9.83E-01	1.00	FALSE
M162T569_neg	162.0561	569	3	5.83E-01	0.97	FALSE	4.08E-01	0.95	FALSE	4.99E-08	1.31	FALSE	1.05E-01	1.20	FALSE
M165T393_neg	165.0419	393	3	1.78E-09	1.31	FALSE	5.35E-01	0.97	FALSE	1.34E-17	1.42	FALSE	6.00E-01	0.97	FALSE
M170T624_neg	170.0824	624	3	4.24E-01	1.04	FALSE	3.10E-04	0.82	FALSE	2.91E-04	1.16	FALSE	8.93E-01	0.99	FALSE
M171T761_neg	171.1027	761	3	7.27E-01	1.02	FALSE	2.99E-01	0.94	FALSE	3.08E-01	1.05	FALSE	2.72E-01	0.90	FALSE
M173T455_neg	173.0820	455	3	1.18E-15	1.38	FALSE	8.80E-01	1.01	FALSE	1.57E-10	1.24	FALSE	1.30E-01	0.88	FALSE
M173T768_neg	173.1184	768	3	5.77E-11	1.29	FALSE	2.06E-01	0.95	FALSE	6.84E-01	0.99	FALSE	6.82E-01	0.97	FALSE
M174T706_neg	174.0561	706	3	4.56E-01	1.11	FALSE	5.93E-01	1.08	FALSE	6.83E-02	1.24	FALSE	2.18E-01	0.84	FALSE
M176T535_neg	176.0357	535	3	7.33E-02	1.16	FALSE	6.43E-01	0.96	FALSE	8.40E-05	1.34	FALSE	6.65E-01	1.08	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M178T587_neg	178.0544	587	3							HMDB0252511	Fudosteine	C6H13NO3S	0.1
M182T402_neg	182.0459	402	3						Alkaloids	HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.3
M182T555_neg	182.0460	555	3							HMDB0000017	4-Pyridoxic acid	C8H9NO4	0.5
M184T487_neg	184.0616	487	3							HMDB0244794	bicyclo[3.1.0]hexane-2,6-dicarbox	C8H11NO4	0.3
M184T385_neg	184.0616	385	3							HMDB0244794	bicyclo[3.1.0]hexane-2,6-dicarbox	C8H11NO4	0.4
M184T181_neg	184.0728	181	3							HMDB0034912	hydro-1-methyl-4-oxo-1H-imidazo	C7H11N3O3	0.2
M186T600_neg	186.1136	600	3							HMDB0013010	N-Heptanoylglycine	C9H17NO3	0.4
M186T654_neg	186.1136	654	3							HMDB0013010	N-Heptanoylglycine	C9H17NO3	0.4
M188T758_neg	188.0717	758	3							HMDB0002302	Indole-3-propionic acid	C11H11NO2	0.2
M188T464_neg	188.0929	464	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.5
M188T418_neg	188.0929	418	3							HMDB0036604	N-Methylcalystegine B2	C8H15NO4	0.4
M190T627_neg	190.0510	627	3						Alkaloids	HMDB0000763	5-Hydroxyindoleacetic acid	C10H9NO3	0.0
M193T772_neg	193.0870	772	3							HMDB0031517	)-3-Hydroxy-5-phenylpentanoic ac	C11H14O3	0.1
M195T442_2_neg	195.0524	442	3						Alkaloids	HMDB0001857	1,3-Dimethyluric acid	C7H8N4O3	0.2
M198T514_neg	198.0773	514	3							HMDB0035177	ahydro-6-hydroxy-7-(hydroxymeth	C9H13NO4	0.4
M198T464_neg	198.0773	464	3							HMDB0035177	ahydro-6-hydroxy-7-(hydroxymeth	C9H13NO4	0.4
M200T683_neg	200.1293	683	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.3
M201T802_neg	201.1132	802	3						Fatty acids	HMDB0000792	Sebacic acid	C10H18O4	0.0
M203T648_neg	203.0925	648	3						Fatty acids	HMDB0303910	2-Hydroxyglutaric acid diethyl este	C9H16O5	0.1
M203T711_neg	203.1289	711	3							HMDB0033217	7-Methyl-3-methylene-1,2,6,7-oct	C10H20O4	0.2
M206T570_neg	206.0459	570	3						Alkaloids	HMDB0000978	-Aminophenyl)-2,4-dioxobutanoic	C10H9NO4	0.0
M207T877_neg	207.1027	877	3						Polyketides	HMDB0029867	Isoelemicin	C12H16O3	0.1
M208T383_neg	208.0616	383	3							HMDB0000735	Hydroxyphenylacetylglycine	C10H11NO4	0.3
M209T562_neg	209.0933	562	3							HMDB0015441	Aprobarbital	C10H14N2O3	0.4
M211T833_neg	211.1340	833	3							HMDB0029388	Cucurbic acid	C12H20O3	0.0
M215T853_neg	215.1289	853	3						Fatty acids	HMDB0000888	Undecanedioic acid	C11H20O4	0.1
M218T438_neg	218.1034	438	3						Fatty acids	HMDB0000210	Pantothenic acid	C9H17NO5	0.2
M222T394_neg	222.0884	394	3							HMDB0062375	trosamino)-1-(1-oxido-3-pyridinyl)-	C10H13N3O3	0.0
M222T609_2_neg	222.0772	609	3						Amino acids and Peptides	HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	0.1
M222T534_neg	222.0773	534	3						Amino acids and Peptides	HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	0.3
M223T895_neg	223.1340	895	3							HMDB0029670	Epoxyeremopetasinorol	C13H20O3	0.1
M224T637_neg	224.0928	637	3							HMDB0253254	Hydroxy Tyrosol -Acetate	C11H15NO4	0.0
M227T796_neg	227.1289	796	3							HMDB0000933	Traumatic acid	C12H20O4	0.0
M227T860_neg	227.1289	860	3						Fatty acids	HMDB0000933	Traumatic acid	C12H20O4	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M178T587_neg	178.0544	587	3	6.55E-01	0.97	FALSE	8.76E-01	1.01	FALSE	1.29E-01	1.09	FALSE	3.23E-02	0.83	FALSE
M182T402_neg	182.0459	402	3	3.86E-09	1.24	FALSE	1.75E-01	1.05	FALSE	4.57E-23	1.41	FALSE	8.14E-01	0.99	FALSE
M182T555_neg	182.0460	555	3	7.71E-02	1.11	FALSE	6.59E-02	0.90	FALSE	7.92E-13	1.48	FALSE	8.82E-02	1.21	FALSE
M184T487_neg	184.0616	487	3	5.93E-16	1.34	FALSE	2.37E-01	1.04	FALSE	2.06E-13	1.26	FALSE	7.97E-01	0.99	FALSE
M184T385_neg	184.0616	385	3	9.00E-19	1.35	FALSE	3.41E-01	1.03	FALSE	3.59E-05	1.12	FALSE	6.57E-01	0.98	FALSE
M184T181_neg	184.0728	181	3	1.10E-01	1.10	FALSE	4.32E-01	1.05	FALSE	3.96E-10	1.41	FALSE	5.40E-02	0.85	FALSE
M186T600_neg	186.1136	600	3	1.45E-18	1.49	FALSE	3.59E-01	1.04	FALSE	1.02E-01	1.06	FALSE	2.37E-01	0.97	FALSE
M186T654_neg	186.1136	654	3	8.25E-02	-2.25	FALSE	7.93E-01	1.45	FALSE	5.66E-02	-0.43	FALSE	2.09E-02	1.27	FALSE
M188T758_neg	188.0717	758	3	5.80E-02	1.11	FALSE	6.92E-01	0.98	FALSE	9.46E-05	1.21	FALSE	1.00E+00	1.00	FALSE
M188T464_neg	188.0929	464	3	2.03E-14	1.35	FALSE	4.70E-01	1.03	FALSE	3.78E-10	1.23	FALSE	1.65E-03	0.81	FALSE
M188T418_neg	188.0929	418	3	5.04E-03	0.86	FALSE	5.52E-01	0.97	FALSE	2.30E-06	1.25	FALSE	6.77E-01	1.03	FALSE
M190T627_neg	190.0510	627	3	1.14E-02	1.14	FALSE	2.63E-01	1.06	FALSE	2.26E-12	1.40	FALSE	6.79E-02	1.14	FALSE
M193T772_neg	193.0870	772	3	1.88E-06	1.23	FALSE	6.21E-01	1.02	FALSE	5.01E-03	1.11	FALSE	9.78E-01	1.00	FALSE
M195T442_2_neg	195.0524	442	3	1.94E-02	1.14	FALSE	1.12E-02	1.16	FALSE	1.16E-06	1.29	FALSE	5.17E-01	1.06	FALSE
M198T514_neg	198.0773	514	3	1.47E-09	1.47	FALSE	6.13E-05	1.29	FALSE	8.26E-05	1.23	FALSE	1.03E-02	1.25	FALSE
M198T464_neg	198.0773	464	3	3.05E-15	1.40	FALSE	8.09E-01	1.01	FALSE	2.39E-02	0.93	FALSE	6.56E-01	1.03	FALSE
M200T683_neg	200.1293	683	3	7.24E-16	1.46	FALSE	9.49E-01	1.00	FALSE	3.29E-01	1.04	FALSE	2.80E-02	0.89	FALSE
M201T802_neg	201.1132	802	3	8.55E-01	0.99	FALSE	7.69E-02	1.09	FALSE	1.05E-13	1.38	FALSE	4.19E-01	0.94	FALSE
M203T648_neg	203.0925	648	3	8.03E-08	0.74	FALSE	3.81E-01	1.05	FALSE	7.40E-10	1.36	FALSE	6.21E-01	1.03	FALSE
M203T711_neg	203.1289	711	3	1.40E-16	1.31	FALSE	2.36E-01	1.04	FALSE	2.90E-07	1.15	FALSE	2.43E-01	1.08	FALSE
M206T570_neg	206.0459	570	3	6.64E-01	0.98	FALSE	2.01E-01	0.93	FALSE	5.72E-08	1.33	FALSE	1.66E-01	1.17	FALSE
M207T877_neg	207.1027	877	3	6.79E-02	1.06	FALSE	9.37E-01	1.00	FALSE	2.35E-17	0.79	FALSE	5.54E-01	0.97	FALSE
M208T383_neg	208.0616	383	3	2.69E-02	0.70	FALSE	8.02E-01	1.04	FALSE	2.31E-01	1.18	FALSE	7.93E-01	0.99	FALSE
M209T562_neg	209.0933	562	3	1.20E-04	1.17	FALSE	6.09E-02	1.08	FALSE	1.06E-16	1.37	FALSE	1.94E-01	0.94	FALSE
M211T833_neg	211.1340	833	3	2.41E-08	1.37	FALSE	8.80E-01	1.01	FALSE	6.36E-01	1.02	FALSE	4.07E-01	1.09	FALSE
M215T853_neg	215.1289	853	3	7.33E-07	0.80	FALSE	4.55E-01	1.04	FALSE	1.79E-18	1.47	FALSE	4.76E-01	0.95	FALSE
M218T438_neg	218.1034	438	3	3.01E-05	1.17	FALSE	3.98E-02	1.08	FALSE	5.44E-22	1.44	FALSE	7.17E-01	0.99	FALSE
M222T394_neg	222.0884	394	3	1.73E-06	1.40	FALSE	5.30E-01	1.05	FALSE	2.27E-02	1.14	FALSE	9.85E-02	0.82	FALSE
M222T609_2_neg	222.0772	609	3	7.00E-07	1.27	FALSE	7.44E-01	1.02	FALSE	2.61E-04	1.16	FALSE	6.31E-01	1.09	FALSE
M222T534_neg	222.0773	534	3	5.07E-03	1.13	FALSE	2.18E-02	1.11	FALSE	6.31E-14	1.36	FALSE	3.46E-02	1.19	FALSE
M223T895_neg	223.1340	895	3	3.64E-03	1.12	FALSE	3.35E-02	0.91	FALSE	3.03E-09	0.80	FALSE	5.24E-01	1.06	FALSE
M224T637_neg	224.0928	637	3	2.72E-14	1.47	FALSE	1.67E-01	1.07	FALSE	3.08E-10	1.31	FALSE	5.20E-01	1.05	FALSE
M227T796_neg	227.1289	796	3	2.11E-05	1.18	FALSE	9.61E-01	1.00	FALSE	1.13E-02	1.09	FALSE	4.65E-02	1.13	FALSE
M227T860_neg	227.1289	860	3	1.27E-03	0.85	FALSE	2.08E-01	1.07	FALSE	8.56E-13	1.39	FALSE	1.72E-01	1.14	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M227T1066_neg	227.2017	1066	3							HMDB0000806	Myristic acid	C14H28O2	0.1
M229T700_neg	229.1081	700	3							HMDB0041448	Dicyclohexyl disulfide	C12H22S2	3.9
M229T892_neg	229.1445	892	3						Fatty acids	HMDB0000623	Dodecanedioic acid	C12H22O4	0.3
M229T684_neg	229.1444	684	3						Fatty acids	HMDB0000623	Dodecanedioic acid	C12H22O4	0.4
M230T569_neg	230.1033	569	3							HMDB0000726	Isovalerylglutamic acid	C10H17NO5	0.3
M231T883_neg	231.1500	883	3							HMDB0015693	Tymazoline	C14H20N2O	1.0
M231T770_neg	231.1602	770	3						Fatty acids				
M232T476_neg	232.1191	476	3							HMDB0013125	Hydroxypropionylcarnitine	C10H19NO5	0.3
M233T425_neg	233.1030	425	3							HMDB0260291	4-Carboxybutylperoxy)pentanoic a	C10H18O6	0.2
M236T515_neg	236.0565	515	3							HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	0.4
M236T670_neg	236.0929	670	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.1
M237T714_neg	237.1245	714	3							HMDB0014562	Secobarbital	C12H18N2O3	0.0
M238T760_neg	238.1085	760	3							HMDB0254628	Methyldopate	C12H17NO4	0.1
M241T718_neg	241.1234	718	3							HMDB0245327	Bisphenol B	C16H18O2	0.1
M241T920_neg	241.1445	920	3						Fatty acids	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	0.1
M241T1077_neg	241.2173	1077	3							HMDB0000826	Pentadecanoic acid	C15H30O2	0.0
M243T602_neg	243.0811	602	3							HMDB0248297	Amidephrine	C10H16N2O3S	1.0
M243T685_neg	243.0873	685	3							HMDB0031237	threo-Syringoylglycerol	C11H16O6	0.5
M243T613_neg	243.1238	613	3						Fatty acids	HMDB0032472	Polyethylene, oxidized	C12H20O5	0.0
M243T670_neg	243.1238	670	3						Fatty acids	HMDB0032472	Polyethylene, oxidized	C12H20O5	0.1
M243T925_neg	243.1602	925	3						Fatty acids	HMDB0002327	1,11-Undecanedicarboxylic acid	C13H24O4	0.1
M247T684_neg	247.1551	684	3						Fatty acids				
M251T877_neg	251.0925	877	3							HMDB0030668	,6-Trimethoxyphenyl)-1,3-butane	C13H16O5	0.1
M251T814_neg	251.1289	814	3							HMDB0033197	methyl-6-(1-oxobutyl)-1,3,5-cyclo	C14H20O4	0.0
M253T1075_neg	253.2173	1075	3							HMDB0002186	Hypogeic acid	C16H30O2	0.0
M254T397_neg	254.0702	397	3							HMDB0246171	o-3-phenylthieno[3,2-d]pyrimidin-	C11H14ClN3O2	0.2
M255T920_neg	255.1601	920	3						Fatty acids	HMDB0030993	ltetrahydro-2-oxo-3-furancarboxy	C14H24O4	0.1
M257T1034_neg	257.2122	1034	3							HMDB0031061	0-Hydroxymyristic acid methyl est	C15H30O3	0.0
M259T780_neg	259.0977	780	3							HMDB0030110	Celerin	C15H16O4	0.3
M261T681_neg	261.1609	681	3							HMDB0253250	Hydrogenated MDI	C15H22N2O2	0.1
M263T433_neg	263.1402	433	3							HMDB0015568	Vorinostat	C14H20N2O3	0.2
M268T629_neg	268.1191	629	3							HMDB0251804	Endralazine	C14H15N5O	4.9
M269T772_neg	269.0934	772	3							HMDB0060568	10,11-Dihydroxycarbamazepine	C15H14N2O3	0.7
M269T940_neg	269.1758	940	3						Fatty acids	HMDB0040459	Ethylene brassylate	C15H26O4	0.2
M269T783_neg	269.1758	783	3							HMDB0040459	Ethylene brassylate	C15H26O4	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M227T1066_neg	227.2017	1066	3	9.73E-01	1.00	FALSE	1.84E-02	0.71	FALSE	1.46E-03	0.68	FALSE	7.41E-01	0.90	FALSE
M229T700_neg	229.1081	700	3	7.79E-04	1.36	FALSE	4.54E-01	1.07	FALSE	9.52E-01	1.00	FALSE	2.23E-01	0.93	FALSE
M229T892_neg	229.1445	892	3	1.22E-04	0.86	FALSE	3.26E-02	1.09	FALSE	4.67E-22	1.44	FALSE	1.85E-01	1.12	FALSE
M229T684_neg	229.1444	684	3	3.31E-27	1.45	FALSE	1.22E-01	0.95	FALSE	5.32E-01	0.98	FALSE	3.40E-01	0.95	FALSE
M230T569_neg	230.1033	569	3	1.37E-02	0.86	FALSE	4.04E-01	0.95	FALSE	1.07E-11	1.47	FALSE	6.68E-01	0.97	FALSE
M231T883_neg	231.1500	883	3	2.65E-02	0.92	FALSE	1.13E-01	1.06	FALSE	1.07E-13	1.28	FALSE	1.10E-01	1.15	FALSE
M231T770_neg	231.1602	770	3	4.17E-07	1.25	FALSE	7.17E-01	0.98	FALSE	4.05E-01	0.97	FALSE	2.57E-01	1.09	FALSE
M232T476_neg	232.1191	476	3	6.43E-14	1.34	FALSE	1.72E-01	1.05	FALSE	4.41E-08	1.20	FALSE	1.62E-01	0.94	FALSE
M233T425_neg	233.1030	425	3	7.87E-01	0.99	FALSE	4.85E-01	1.04	FALSE	5.10E-18	1.49	FALSE	6.70E-01	1.02	FALSE
M236T515_neg	236.0565	515	3	1.09E-04	1.23	FALSE	6.82E-01	1.02	FALSE	4.15E-08	1.29	FALSE	3.17E-01	0.91	FALSE
M236T670_neg	236.0929	670	3	3.56E-06	1.21	FALSE	2.63E-01	1.05	FALSE	2.00E-02	1.09	FALSE	4.40E-01	1.14	FALSE
M237T714_neg	237.1245	714	3	7.06E-03	1.16	FALSE	1.15E-01	1.11	FALSE	2.55E-01	1.05	FALSE	2.32E-02	1.22	FALSE
M238T760_neg	238.1085	760	3	2.90E-03	1.21	FALSE	3.76E-01	1.06	FALSE	3.44E-08	1.38	FALSE	7.41E-01	0.96	FALSE
M241T718_neg	241.1234	718	3	2.93E-03	0.82	FALSE	8.45E-01	1.01	FALSE	6.54E-08	1.39	FALSE	1.49E-01	1.09	FALSE
M241T920_neg	241.1445	920	3	1.52E-04	1.08	FALSE	2.48E-01	0.98	FALSE	2.47E-07	0.91	FALSE	2.65E-01	0.95	FALSE
M241T1077_neg	241.2173	1077	3	1.02E-01	0.83	FALSE	1.75E-01	0.85	FALSE	1.27E-01	1.17	FALSE	2.68E-01	0.72	FALSE
M243T602_neg	243.0811	602	3	1.04E-01	1.06	FALSE	8.33E-02	1.07	FALSE	4.17E-19	1.39	FALSE	8.97E-05	1.32	FALSE
M243T685_neg	243.0873	685	3	2.58E-01	0.88	FALSE	3.08E-01	1.14	FALSE	4.83E-03	1.34	FALSE	6.78E-01	1.02	FALSE
M243T613_neg	243.1238	613	3	5.12E-15	1.36	FALSE	9.37E-02	1.06	FALSE	1.04E-03	1.11	FALSE	1.47E-01	1.17	FALSE
M243T670_neg	243.1238	670	3	6.99E-01	1.01	FALSE	1.40E-01	1.06	FALSE	1.95E-25	1.48	FALSE	3.48E-01	0.95	FALSE
M243T925_neg	243.1602	925	3	1.30E-04	0.88	FALSE	5.25E-02	1.07	FALSE	1.64E-21	1.37	FALSE	9.00E-02	1.13	FALSE
M247T684_neg	247.1551	684	3	4.71E-14	1.40	FALSE	8.68E-01	0.99	FALSE	1.49E-01	1.05	FALSE	3.58E-01	1.11	FALSE
M251T877_neg	251.0925	877	3	1.44E-03	1.09	FALSE	1.43E-01	0.96	FALSE	1.60E-17	0.80	FALSE	8.56E-01	1.01	FALSE
M251T814_neg	251.1289	814	3	1.04E-13	1.44	FALSE	2.70E-01	0.95	FALSE	8.70E-01	1.01	FALSE	3.30E-01	1.09	FALSE
M253T1075_neg	253.2173	1075	3	4.61E-02	0.86	FALSE	1.61E-03	0.77	FALSE	1.14E-02	1.19	FALSE	2.85E-01	1.23	FALSE
M254T397_neg	254.0702	397	3	4.75E-01	1.04	FALSE	4.98E-01	1.04	FALSE	2.29E-14	1.48	FALSE	3.78E-01	0.92	FALSE
M255T920_neg	255.1601	920	3	1.18E-01	0.93	FALSE	3.99E-01	1.04	FALSE	3.67E-16	1.43	FALSE	7.05E-01	1.03	FALSE
M257T1034_neg	257.2122	1034	3	8.13E-02	1.19	FALSE	1.28E-02	0.76	FALSE	5.66E-03	1.28	FALSE	8.38E-01	1.03	FALSE
M259T780_neg	259.0977	780	3	3.26E-01	1.03	FALSE	3.57E-01	1.03	FALSE	2.33E-08	1.18	FALSE	5.18E-03	0.86	FALSE
M261T681_neg	261.1609	681	3	5.20E-02	1.24	FALSE	3.73E-01	1.10	FALSE	1.39E-03	1.36	FALSE	1.60E-01	1.50	FALSE
M263T433_neg	263.1402	433	3	1.28E-05	1.30	FALSE	9.71E-01	1.00	FALSE	6.47E-11	1.43	FALSE	1.69E-01	0.89	FALSE
M268T629_neg	268.1191	629	3	5.17E-05	1.24	FALSE	2.07E-02	1.13	FALSE	1.59E-06	1.25	FALSE	1.87E-01	1.19	FALSE
M269T772_neg	269.0934	772	3	1.09E-01	1.08	FALSE	5.42E-01	1.03	FALSE	5.41E-12	1.34	FALSE	1.14E-01	0.88	FALSE
M269T940_neg	269.1758	940	3	3.54E-01	0.97	FALSE	1.62E-01	1.05	FALSE	6.07E-10	1.20	FALSE	6.62E-01	0.98	FALSE
M269T783_neg	269.1758	783	3	2.73E-10	1.38	FALSE	1.66E-03	1.17	FALSE	8.15E-02	1.08	FALSE	7.94E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M270T574_neg	270.0983	574	3							HMDB0246178	4-Aminophenylmannoside	C12H17NO6	0.1
M270T764_neg	270.1711	764	3							HMDB0241681	Hept-3-enoylcarnitine	C14H25NO4	0.1
M271T798_neg	271.1550	798	3						Fatty acids				
M271T791_neg	271.1915	791	3							HMDB0035918	7(14)-Bisabolene-2,3,10,11-tetrol	C15H28O4	0.1
M271T727_neg	271.1915	727	3							HMDB0035918	7(14)-Bisabolene-2,3,10,11-tetrol	C15H28O4	0.0
M275T968_neg	275.1653	968	3							HMDB0015586	Cyclandelate	C17H24O3	0.1
M279T681_neg	279.1715	681	3							HMDB0245010	2-Aminobenzylstatine	C15H24N2O3	0.2
M279T724_neg	279.1714	724	3							HMDB0245010	2-Aminobenzylstatine	C15H24N2O3	0.0
M281T627_neg	281.1395	627	3						Terpenoids	HMDB0033375	Octyl gallate	C15H22O5	0.1
M285T999_neg	285.2071	999	3						Fatty acids	HMDB0000672	Hexadecanedioic acid	C16H30O4	0.0
M287T667_neg	287.0927	667	3							HMDB0029303	y-4-hydroxy)-phenyl-6,7-dihydroxy	C16H16O5	0.6
M287T901_neg	287.2227	901	3							HMDB0037798	)-10,16-Dihydroxyhexadecanoic ac	C16H32O4	0.1
M289T1009_neg	289.1810	1009	3							HMDB0031098	15Z)-4-Oxo-9,11,13,15-octadecate	C18H26O3	0.1
M291T828_neg	291.1714	828	3						Alkaloids	HMDB0014662	Carteolol	C16H24N2O3	0.2
M293T916_neg	293.1761	916	3							HMDB0005783	Gingerol	C17H26O4	0.8
M297T793_neg	297.1343	793	3							HMDB0036159	Toxin T2 tetrol	C15H22O6	0.2
M297T900_neg	297.1707	900	3							HMDB0015643	Artemether	C16H26O5	0.1
M297T1038_neg	297.2435	1038	3							HMDB0010736	3-Oxooctadecanoic acid	C18H34O3	0.1
M299T1017_neg	299.2228	1017	3							HMDB0011531	MG(0:0/14:1(9Z)/0:0)	C17H32O4	0.1
M301T891_neg	301.2020	891	3						Fatty acids	HMDB0037830	xi-7-Hydroxyhexadecanedioic acid	C16H30O5	0.2
M303T830_neg	303.1714	830	3							HMDB0259093	Tilisolol	C17H24N2O3	0.1
M305T770_neg	305.1506	770	3							HMDB0253499	Inproquone	C16H22N2O4	0.2
M307T732_neg	307.1663	732	3							HMDB0060990	8-Hydroxycarteolol	C16H24N2O4	0.0
M309T1002_neg	309.2069	1002	3						Fatty acids	HMDB0013623	12(13)Ep-9-KODE	C18H30O4	0.6
M315T700_neg	315.1238	700	3							HMDB0250413	Combretastatin A4	C18H20O5	0.1
M315T551_neg	315.1452	551	3							HMDB0033643	Hydroxy-8-nor-2-fenchanone gluco	C15H24O7	1.0
M315T910_neg	315.1813	910	3							HMDB0029346	Neryl glucoside	C16H28O6	0.0
M321T382_neg	321.0494	382	3						Carbohydrates	HMDB0062560	Pyroglutamine	C10H15N2O8P	0.3
M321T904_neg	321.2072	904	3							HMDB0033615	(S)-[8]-Gingerol	C19H30O4	0.2
M321T946_neg	321.2073	946	3							HMDB0033615	(S)-[8]-Gingerol	C19H30O4	0.5
M326T897_neg	326.1974	897	3							HMDB0241110	5Z)-3-Hydroxydeca-4,6-dienoylcarn	C17H29NO5	0.3
M326T1033_neg	326.2702	1033	3						Fatty acids	HMDB0013246	Margaroylglycine	C19H37NO3	0.3
M331T403_neg	331.1147	403	3							HMDB0039002	Mytilin A	C13H20N2O8	0.1
M331T613_neg	331.1187	613	3						Terpenoids	HMDB0030664	3-Galloylcatechin	C18H20O6	0.1
M333T387_neg	333.1303	387	3							HMDB0012996	Lipoyllysine	C14H26N2O3S2	2.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M270T574_neg	270.0983	574	3	4.76E-02	0.85	FALSE	7.48E-01	0.97	FALSE	1.88E-07	1.46	FALSE	4.73E-01	1.12	FALSE
M270T764_neg	270.1711	764	3	7.76E-11	1.32	FALSE	5.12E-01	1.03	FALSE	7.83E-02	1.06	FALSE	2.96E-01	0.94	FALSE
M271T798_neg	271.1550	798	3	4.47E-01	1.04	FALSE	4.21E-01	1.04	FALSE	1.47E-10	1.34	FALSE	9.72E-01	1.00	FALSE
M271T791_neg	271.1915	791	3	1.95E-14	1.42	FALSE	2.08E-01	1.06	FALSE	9.48E-01	1.00	FALSE	5.35E-01	1.08	FALSE
M271T727_neg	271.1915	727	3	2.26E-08	1.28	FALSE	8.38E-01	1.01	FALSE	5.12E-01	0.98	FALSE	1.51E-01	1.19	FALSE
M275T968_neg	275.1653	968	3	2.17E-01	0.95	FALSE	8.76E-01	0.99	FALSE	1.74E-04	0.87	FALSE	8.48E-01	0.98	FALSE
M279T681_neg	279.1715	681	3	1.19E-03	1.32	FALSE	7.24E-02	1.17	FALSE	3.56E-01	1.07	FALSE	3.46E-01	0.82	FALSE
M279T724_neg	279.1714	724	3	4.06E-03	1.37	FALSE	3.30E-02	1.26	FALSE	1.74E-04	1.43	FALSE	2.47E-01	1.21	FALSE
M281T627_neg	281.1395	627	3	6.94E-09	1.28	FALSE	5.55E-01	0.97	FALSE	1.16E-07	1.22	FALSE	7.75E-01	1.02	FALSE
M285T999_neg	285.2071	999	3	6.73E-01	1.02	FALSE	7.10E-01	0.98	FALSE	4.52E-18	1.38	FALSE	1.51E-02	0.88	FALSE
M287T667_neg	287.0927	667	3	1.75E-06	1.21	FALSE	5.23E-02	1.08	FALSE	3.21E-18	1.39	FALSE	7.61E-02	1.13	FALSE
M287T901_neg	287.2227	901	3	9.38E-01	1.01	FALSE	1.15E-02	0.72	FALSE	2.63E-01	1.11	FALSE	9.12E-01	0.98	FALSE
M289T1009_neg	289.1810	1009	3	8.57E-01	1.02	FALSE	9.07E-01	0.98	FALSE	4.81E-02	1.26	FALSE	7.09E-02	0.60	FALSE
M291T828_neg	291.1714	828	3	1.93E-13	0.78	FALSE	4.88E-01	0.98	FALSE	9.73E-14	1.25	FALSE	2.14E-01	1.09	FALSE
M293T916_neg	293.1761	916	3	6.46E-08	0.67	FALSE	2.19E-02	1.18	FALSE	3.64E-08	1.43	FALSE	6.34E-02	0.67	FALSE
M297T793_neg	297.1343	793	3	2.72E-08	1.40	FALSE	1.13E-01	1.10	FALSE	9.66E-01	1.00	FALSE	2.03E-01	1.15	FALSE
M297T900_neg	297.1707	900	3	4.42E-02	0.91	FALSE	1.21E-02	0.88	FALSE	7.40E-12	1.33	FALSE	1.72E-01	0.85	FALSE
M297T1038_neg	297.2435	1038	3	8.05E-01	1.02	FALSE	9.46E-04	0.75	FALSE	1.47E-02	1.19	FALSE	6.07E-01	0.92	FALSE
M299T1017_neg	299.2228	1017	3	1.86E-08	1.26	FALSE	8.79E-01	0.99	FALSE	1.77E-19	1.42	FALSE	6.26E-01	1.02	FALSE
M301T891_neg	301.2020	891	3	8.45E-01	0.99	FALSE	7.88E-02	1.09	FALSE	2.74E-14	1.40	FALSE	1.63E-01	1.14	FALSE
M303T830_neg	303.1714	830	3	4.53E-12	0.69	FALSE	2.25E-04	1.21	FALSE	2.44E-07	1.26	FALSE	1.96E-01	1.11	FALSE
M305T770_neg	305.1506	770	3	8.07E-08	1.45	FALSE	1.39E-06	0.74	FALSE	1.50E-04	1.25	FALSE	3.27E-01	1.09	FALSE
M307T732_neg	307.1663	732	3	7.29E-01	1.05	FALSE	2.01E-02	0.73	FALSE	2.69E-01	0.87	FALSE	1.15E-01	1.32	FALSE
M309T1002_neg	309.2069	1002	3	5.12E-05	1.38	FALSE	1.30E-01	0.88	FALSE	5.28E-04	1.27	FALSE	6.47E-01	1.08	FALSE
M315T700_neg	315.1238	700	3	5.95E-11	1.27	FALSE	6.99E-02	1.07	FALSE	1.37E-12	1.25	FALSE	1.25E-01	1.10	FALSE
M315T551_neg	315.1452	551	3	7.42E-12	1.48	FALSE	8.61E-01	1.01	FALSE	3.85E-04	1.18	FALSE	7.04E-02	1.21	FALSE
M315T910_neg	315.1813	910	3	5.16E-05	0.91	FALSE	3.76E-02	1.05	FALSE	2.04E-15	1.20	FALSE	5.46E-02	0.85	FALSE
M321T382_neg	321.0494	382	3	5.92E-01	0.84	FALSE	3.34E-01	1.36	FALSE	1.58E-01	1.50	FALSE	9.29E-02	1.38	FALSE
M321T904_neg	321.2072	904	3	1.50E-16	1.33	FALSE	3.72E-01	0.97	FALSE	4.11E-02	0.95	FALSE	8.46E-01	0.99	FALSE
M321T946_neg	321.2073	946	3	6.52E-07	1.28	FALSE	1.35E-03	0.85	FALSE	4.45E-02	0.92	FALSE	7.79E-01	0.98	FALSE
M326T897_neg	326.1974	897	3	5.90E-01	1.05	FALSE	3.86E-03	1.35	FALSE	7.90E-05	1.42	FALSE	5.42E-02	1.29	FALSE
M326T1033_neg	326.2702	1033	3	6.33E-11	0.75	FALSE	6.11E-03	1.13	FALSE	4.04E-06	0.84	FALSE	9.92E-01	1.00	FALSE
M331T403_neg	331.1147	403	3	3.32E-02	1.12	FALSE	6.19E-01	1.03	FALSE	1.24E-10	1.38	FALSE	6.67E-01	0.94	FALSE
M331T613_neg	331.1187	613	3	2.41E-09	1.28	FALSE	8.68E-02	1.07	FALSE	2.00E-15	1.35	FALSE	5.48E-02	1.15	FALSE
M333T387_neg	333.1303	387	3	1.10E-01	1.11	FALSE	4.90E-01	1.05	FALSE	8.17E-05	1.26	FALSE	2.62E-01	0.84	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M333T947_neg	333.1708	947	3							HMDB0032699	-8-(2-methylbutanoyloxy)-9,10-ep	C19H26O5	0.1
M337T1017_neg	337.2385	1017	3						Fatty acids	HMDB0002265	14,15-DiHETrE	C20H34O4	0.1
M363T609_neg	363.1197	609	3						Alkaloids				
M381T753_neg	381.1922	753	3						Terpenoids	HMDB0012553	2-Oxo-20-trihydroxy-leukotriene B	C20H30O7	0.9
M387T960_neg	387.2542	960	3							HMDB0030366	Cavipetin C	C24H36O4	0.3
M389T980_neg	389.2698	980	3						Terpenoids	HMDB0000328	12-Ketodeoxycholic acid	C24H38O4	0.2
M391T686_neg	391.1404	686	3						Polyketides	HMDB0039564	Marmesin rhamnoside	C20H24O8	1.3
M391T883_neg	391.2492	883	3							HMDB0060730	20, 22-Dihydrodigoxigenin	C23H36O5	0.5
M395T616_neg	395.0074	616	3							HMDB0031554	Sucralose	C12H19Cl3O8	0.4
M397T950_neg	397.1691	950	3						Terpenoids				
M397T840_neg	397.2135	840	3							HMDB0041933	Mitragynine	C23H30N2O4	0.6
M399T878_neg	399.1117	878	3							HMDB0254796	(1-methyl-1h-indol-3-yl)-4-(1-meth	C22H16N4O4	4.7
M401T891_neg	401.1274	891	3							HMDB0257097	Rafabegron	C21H23ClN2O4	0.0
M403T877_neg	403.2703	877	3						Fatty acids				
M405T873_neg	405.2649	873	3							HMDB0000391	7-Ketodeoxycholic acid	C24H38O5	0.5
M407T916_neg	407.2804	916	3							HMDB0000312	pha,12beta-Trihydroxy-5beta-cho	C24H40O5	0.2
M407T813_neg	407.2805	813	3						Terpenoids	HMDB0000312	pha,12beta-Trihydroxy-5beta-cho	C24H40O5	0.5
M421T1007_neg	421.2961	1007	3						Terpenoids	HMDB0244296	7-Methyl-cholic acid	C25H42O5	0.5
M422T1048_neg	422.2679	1048	3						Fatty acids				
M433T960_neg	433.2597	960	3						Terpenoids	HMDB0033030	-Demethyl-10,29-dideoxy-11,12-di	C25H38O6	0.3
M435T978_neg	435.2753	978	3						Terpenoids	HMDB0061047	simvastatin hydroxy acid	C25H40O6	0.2
M453T916_neg	453.2859	916	3						Terpenoids	HMDB0296939	(2:0/20:3(8Z,11Z,14Z)-2OH(5,6)/0	C25H42O7	0.3
M453T813_neg	453.2862	813	3						Terpenoids	HMDB0296939	(2:0/20:3(8Z,11Z,14Z)-2OH(5,6)/0	C25H42O7	0.8
M457T825_neg	457.2234	825	3							HMDB0034760	Hydroxystrobilurin D	C26H34O7	0.6
M459T972_neg	459.2731	972	3							HMDB0030909	2,3-Secoporrigenin	C27H40O6	4.6
M465T781_neg	465.2860	781	3						Terpenoids				
M465T863_neg	465.2860	863	3						Polyketides				
M465T960_neg	465.2864	960	3						Terpenoids				
M472T821_neg	472.2455	821	3							HMDB0011480	LysoPE(0:0/18:4(6Z,9Z,12Z,15Z))	C23H40NO7P	3.1
M477T968_neg	477.2861	968	3						Terpenoids	HMDB0031896	Erinacine D	C27H42O7	0.6
M479T714_neg	479.2652	714	3							HMDB0255516	Neoandrographolide	C26H40O8	0.3
M479T777_neg	479.2653	777	3							HMDB0255516	Neoandrographolide	C26H40O8	0.5
M479T853_neg	479.2652	853	3							HMDB0255516	Neoandrographolide	C26H40O8	0.4
M482T837_neg	482.2300	837	3							HMDB0033470	Caffeoylferuloylspermidine	C26H33N3O6	0.7
M484T851_neg	484.2455	851	3							HMDB0248754	o)-2-((2-(dimethylamino)ethyl)(m	C27H31N7O2	2.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M333T947_neg	333.1708	947	3	3.82E-04	0.88	FALSE	6.06E-01	1.02	FALSE	1.30E-20	1.40	FALSE	1.53E-01	0.91	FALSE
M337T1017_neg	337.2385	1017	3	6.84E-02	1.21	FALSE	3.28E-01	1.11	FALSE	8.47E-03	1.27	FALSE	5.90E-01	1.07	FALSE
M363T609_neg	363.1197	609	3	1.18E-01	1.11	FALSE	1.80E-08	0.70	FALSE	1.79E-01	1.08	FALSE	1.34E-01	0.73	FALSE
M381T753_neg	381.1922	753	3	2.60E-03	1.18	FALSE	8.79E-01	1.01	FALSE	3.74E-06	1.26	FALSE	4.19E-01	0.92	FALSE
M387T960_neg	387.2542	960	3	7.93E-13	1.27	FALSE	2.01E-03	1.10	FALSE	1.82E-30	1.45	FALSE	4.65E-02	0.88	FALSE
M389T980_neg	389.2698	980	3	3.99E-04	1.08	FALSE	3.05E-01	1.02	FALSE	7.48E-11	1.14	FALSE	2.61E-02	0.86	FALSE
M391T686_neg	391.1404	686	3	7.78E-01	1.02	FALSE	2.90E-01	1.07	FALSE	1.41E-13	1.48	FALSE	4.76E-01	1.14	FALSE
M391T883_neg	391.2492	883	3	9.42E-08	1.18	FALSE	3.11E-01	1.03	FALSE	4.12E-02	1.05	FALSE	5.12E-01	0.96	FALSE
M395T616_neg	395.0074	616	3	9.74E-07	1.40	FALSE	7.57E-01	0.98	FALSE	4.19E-01	1.05	FALSE	4.74E-01	0.89	FALSE
M397T950_neg	397.1691	950	3	6.12E-01	0.95	FALSE	5.45E-01	0.94	FALSE	3.27E-02	1.21	FALSE	5.33E-02	0.66	FALSE
M397T840_neg	397.2135	840	3	8.95E-01	1.02	FALSE	2.27E-03	1.47	FALSE	6.82E-02	1.21	FALSE	7.47E-01	1.09	FALSE
M399T878_neg	399.1117	878	3	6.38E-04	0.85	FALSE	6.21E-02	1.10	FALSE	2.01E-13	1.39	FALSE	1.43E-01	0.85	FALSE
M401T891_neg	401.1274	891	3	5.53E-02	0.92	FALSE	9.34E-01	1.00	FALSE	2.39E-08	1.26	FALSE	5.43E-01	0.94	FALSE
M403T877_neg	403.2703	877	3	8.64E-05	1.27	FALSE	5.16E-01	0.96	FALSE	2.88E-01	0.95	FALSE	4.99E-01	0.93	FALSE
M405T873_neg	405.2649	873	3	2.20E-10	1.34	FALSE	6.61E-01	0.98	FALSE	2.78E-02	1.09	FALSE	8.86E-01	1.01	FALSE
M407T916_neg	407.2804	916	3	4.07E-15	1.35	FALSE	3.79E-01	0.97	FALSE	1.52E-01	1.04	FALSE	1.16E-02	0.89	FALSE
M407T813_neg	407.2805	813	3	4.21E-16	1.35	FALSE	4.47E-01	0.97	FALSE	5.12E-01	0.98	FALSE	1.43E-01	0.94	FALSE
M421T1007_neg	421.2961	1007	3	2.92E-05	1.23	FALSE	5.30E-01	0.97	FALSE	3.96E-11	1.34	FALSE	2.32E-01	0.91	FALSE
M422T1048_neg	422.2679	1048	3	1.55E-01	1.23	FALSE	6.39E-02	0.74	FALSE	2.71E-01	1.15	FALSE	5.34E-01	1.18	FALSE
M433T960_neg	433.2597	960	3	1.08E-12	1.25	FALSE	2.32E-03	1.10	FALSE	3.49E-30	1.43	FALSE	3.52E-02	0.87	FALSE
M435T978_neg	435.2753	978	3	4.18E-01	1.01	FALSE	2.11E-01	1.02	FALSE	2.33E-05	1.06	FALSE	3.40E-02	0.92	FALSE
M453T916_neg	453.2859	916	3	1.77E-11	1.32	FALSE	7.32E-01	0.99	FALSE	2.38E-01	1.04	FALSE	6.35E-02	0.92	FALSE
M453T813_neg	453.2862	813	3	1.25E-17	1.37	FALSE	1.26E-01	0.95	FALSE	7.41E-01	1.01	FALSE	1.26E-01	0.89	FALSE
M457T825_neg	457.2234	825	3	2.23E-02	1.13	FALSE	9.20E-02	1.10	FALSE	2.11E-06	1.25	FALSE	4.22E-01	1.09	FALSE
M459T972_neg	459.2731	972	3	7.70E-02	1.06	FALSE	2.48E-02	0.93	FALSE	4.42E-06	0.88	FALSE	6.74E-01	1.04	FALSE
M465T781_neg	465.2860	781	3	1.26E-09	1.39	FALSE	3.17E-02	1.12	FALSE	6.46E-01	0.98	FALSE	3.82E-01	1.14	FALSE
M465T863_neg	465.2860	863	3	1.31E-09	1.37	FALSE	5.21E-01	1.03	FALSE	8.13E-01	1.01	FALSE	1.60E-01	1.23	FALSE
M465T960_neg	465.2864	960	3	2.15E-01	0.83	FALSE	3.89E-01	1.15	FALSE	6.92E-01	0.95	FALSE	4.27E-01	0.88	FALSE
M472T821_neg	472.2455	821	3	1.16E-08	0.69	FALSE	1.03E-06	1.38	FALSE	4.70E-11	1.47	FALSE	1.24E-01	1.11	FALSE
M477T968_neg	477.2861	968	3	1.25E-05	1.24	FALSE	4.23E-01	1.04	FALSE	1.33E-09	1.31	FALSE	2.09E-01	0.94	FALSE
M479T714_neg	479.2652	714	3	3.83E-10	1.45	FALSE	1.88E-01	1.08	FALSE	2.46E-02	1.12	FALSE	6.97E-02	1.30	FALSE
M479T777_neg	479.2653	777	3	1.09E-01	0.92	FALSE	1.87E-02	1.15	FALSE	5.40E-13	1.45	FALSE	4.85E-01	1.08	FALSE
M479T853_neg	479.2652	853	3	1.43E-07	0.81	FALSE	4.29E-01	1.03	FALSE	2.17E-16	1.35	FALSE	9.79E-01	1.00	FALSE
M482T837_neg	482.2300	837	3	2.72E-01	0.94	FALSE	3.67E-06	1.33	FALSE	4.32E-07	1.31	FALSE	6.79E-01	1.03	FALSE
M484T851_neg	484.2455	851	3	3.51E-11	0.73	FALSE	5.51E-09	1.32	FALSE	7.75E-16	1.42	FALSE	3.79E-01	0.96	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M491T973_neg	491.2108	973	3							HMDB0254159	Loperamide oxide	C29H33ClN2O3	0.3
M491T961_neg	491.3378	961	3							HMDB0033907	Homodolicholide	C29H48O6	0.0
M501T984_neg	501.3223	984	3						Terpenoids	HMDB0034551	Medicagenic acid	C30H46O6	0.3
M503T825_neg	503.2288	825	3						Terpenoids	HMDB0039122	Crocin 4	C27H36O9	0.2
M505T718_neg	505.2116	718	3							HMDB0253269	Hydroxyglimepiride	C24H34N4O6S	2.1
M517T836_neg	517.3172	836	3						Terpenoids	HMDB0034392	Perulactone	C30H46O7	0.2
M531T595_neg	531.2383	595	3							HMDB0266521	2:0/20:4(6Z,8E,10E,14Z)-2OH(5S,1	C25H41O10P	3.6
M536T584_neg	536.1778	584	3							HMDB0034773	,4S)-1,8-Epoxy-p-menthan-3-ol glu	C25H31NO12	0.8
M559T858_neg	559.1643	858	3							HMDB0041489	4,5-Dihydropiperlonguminine	C24H32O15	4.6
M591T727_neg	591.3190	727	3							HMDB0001898	Mesobilirubinogen	C33H44N4O6	0.2
M616T1014_neg	616.4948	1014	3							HMDB0289957	Cer(d18:0/PGJ2)	C38H67NO5	0.3
M633T898_neg	633.3129	898	3						Fatty acids				
M675T855_neg	675.3749	855	3							HMDB0247977	Actein	C37H56O11	0.1
M691T1021_neg	690.5678	1021	3						Terpenoids				
M707T1013_neg	707.4891	1013	3							HMDB0116648	PG(a-13:0/i-18:0)	C37H73O10P	3.1
M780T978_neg	779.5467	978	3						Terpenoids				
M797T960_neg	797.4976	960	3							HMDB0264686	:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5	C43H75O11P	0.2
M802T1006_neg	801.5287	1006	3							HMDB0264646	PA(20:0/PGF2alpha)	C43H79O11P	0.0
M919T857_neg	919.4851	857	3							HMDB0276264	PI(16:2(9Z,12Z)/6 keto-PGF1alpha	C45H77O17P	2.7
M69T171_neg	68.9957	171	3							HMDB0252378	Trifluoromethane	CHF3	1.1
M80T584_neg	79.9573	584	3							HMDB0304277	bisulfite	HO3S	0.6
M85T526_neg	85.0659	526	3							HMDB0006478	Isovaleraldehyde	C5H10O	0.0
M87T526_neg	87.0816	526	3							HMDB0006007	Isopentanol	C5H12O	0.2
M93T565_neg	93.0346	565	3							HMDB0000228	Phenol	C6H6O	0.0
M93T607_neg	93.0346	607	3							HMDB0000228	Phenol	C6H6O	0.3
M99T1033_neg	98.9391	1033	3							HMDB0303252	Magnesium silicate	MgO3Si	3.4
M99T433_neg	99.0452	433	3							HMDB0000509	Senecioic acid	C5H8O2	0.1
M105T510_neg	105.0016	510	3							HMDB0254617	Methyl thioglycolate	C3H6O2S	0.3
M105T444_neg	105.0016	444	3							HMDB0254617	Methyl thioglycolate	C3H6O2S	0.2
M105T784_neg	105.0710	784	3							HMDB0059810	m-Xylene	C8H10	0.2
M109T485_neg	109.0295	485	3							HMDB0000957	Pyrocatechol	C6H6O2	0.2
M109T521_neg	109.0659	521	3							HMDB0029721	2,3,5-Trimethylfuran	C7H10O	0.2
M110T475_neg	110.0248	475	3							HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	0.2
M110T578_neg	110.0248	578	3							HMDB0004230	Pyrrole-2-carboxylic acid	C5H5NO2	0.3
M112T714_neg	112.0405	714	3							HMDB0001301	1-Pyrroline-5-carboxylic acid	C5H7NO2	0.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M491T973_neg	491.2108	973	3	7.16E-06	1.24	FALSE	1.44E-04	0.83	FALSE	6.54E-05	0.85	FALSE	3.77E-01	1.09	FALSE
M491T961_neg	491.3378	961	3	2.61E-08	1.25	FALSE	5.93E-04	0.87	FALSE	2.95E-02	1.07	FALSE	5.77E-01	1.04	FALSE
M501T984_neg	501.3223	984	3	7.25E-02	0.88	FALSE	4.75E-01	1.06	FALSE	4.15E-08	1.44	FALSE	8.04E-01	0.95	FALSE
M503T825_neg	503.2288	825	3	3.43E-02	1.12	FALSE	7.21E-02	1.11	FALSE	3.09E-07	1.28	FALSE	4.51E-01	1.08	FALSE
M505T718_neg	505.2116	718	3	3.84E-02	1.13	FALSE	6.81E-01	1.03	FALSE	3.79E-08	1.36	FALSE	6.34E-01	1.06	FALSE
M517T836_neg	517.3172	836	3	1.53E-01	0.92	FALSE	1.18E-01	1.10	FALSE	1.40E-10	1.42	FALSE	9.16E-01	1.02	FALSE
M531T595_neg	531.2383	595	3	1.25E-07	1.44	FALSE	7.46E-01	0.98	FALSE	4.80E-01	1.04	FALSE	1.20E-01	1.27	FALSE
M536T584_neg	536.1778	584	3	3.06E-03	1.31	FALSE	7.42E-01	0.97	FALSE	3.73E-04	1.33	FALSE	2.07E-01	0.62	FALSE
M559T858_neg	559.1643	858	3	1.00E-02	1.13	FALSE	9.78E-01	1.00	FALSE	8.83E-02	0.93	FALSE	4.46E-01	1.08	FALSE
M591T727_neg	591.3190	727	3	5.25E-06	1.27	FALSE	2.56E-06	1.29	FALSE	4.34E-04	1.17	FALSE	4.10E-03	0.73	FALSE
M616T1014_neg	616.4948	1014	3	1.69E-01	0.85	FALSE	6.08E-02	0.78	FALSE	6.38E-02	0.83	FALSE	8.89E-01	1.03	FALSE
M633T898_neg	633.3129	898	3	6.26E-06	1.35	FALSE	8.77E-01	0.99	FALSE	4.93E-01	1.04	FALSE	7.47E-02	0.76	FALSE
M675T855_neg	675.3749	855	3	7.17E-06	0.82	FALSE	6.36E-04	1.17	FALSE	1.80E-19	1.48	FALSE	5.31E-01	1.05	FALSE
M691T1021_neg	690.5678	1021	3	7.35E-09	0.73	FALSE	1.17E-02	1.15	FALSE	9.19E-03	0.89	FALSE	2.37E-01	1.11	FALSE
M707T1013_neg	707.4891	1013	3	3.50E-02	1.30	FALSE	1.51E-01	0.82	FALSE	8.01E-02	1.21	FALSE	8.19E-01	1.04	FALSE
M780T978_neg	779.5467	978	3	1.52E-07	1.18	FALSE	2.83E-01	1.03	FALSE	1.22E-12	1.22	FALSE	5.29E-02	0.87	FALSE
M797T960_neg	797.4976	960	3	1.43E-02	1.12	FALSE	1.70E-04	1.20	FALSE	4.57E-02	1.08	FALSE	1.04E-01	0.83	FALSE
M802T1006_neg	801.5287	1006	3	5.61E-03	0.90	FALSE	4.07E-01	1.03	FALSE	6.84E-01	1.01	FALSE	5.51E-01	0.95	FALSE
M919T857_neg	919.4851	857	3	1.89E-01	1.10	FALSE	2.64E-04	1.34	FALSE	1.54E-07	1.42	FALSE	1.38E-03	1.39	FALSE
M69T171_neg	68.9957	171	3	9.24E-02	1.17	FALSE	5.88E-01	1.06	FALSE	8.50E-02	1.15	FALSE	8.90E-01	1.03	FALSE
M80T584_neg	79.9573	584	3	1.41E-01	1.09	FALSE	8.31E-01	0.99	FALSE	9.90E-03	1.15	FALSE	7.54E-01	1.07	FALSE
M85T526_neg	85.0659	526	3	4.63E-18	1.38	FALSE	1.91E-01	1.05	FALSE	5.35E-05	1.13	FALSE	7.69E-01	1.01	FALSE
M87T526_neg	87.0816	526	3	1.38E-16	1.39	FALSE	5.24E-01	1.02	FALSE	6.66E-03	1.09	FALSE	5.04E-01	1.04	FALSE
M93T565_neg	93.0346	565	3	3.64E-01	0.93	FALSE	4.16E-01	1.08	FALSE	1.70E-07	1.48	FALSE	5.18E-01	0.95	FALSE
M93T607_neg	93.0346	607	3	4.39E-05	1.20	FALSE	1.70E-01	1.06	FALSE	1.15E-12	1.33	FALSE	8.04E-01	1.02	FALSE
M99T1033_neg	98.9391	1033	3	1.08E-02	0.91	FALSE	9.97E-01	1.00	FALSE	8.93E-01	1.00	FALSE	8.17E-01	0.98	FALSE
M99T433_neg	99.0452	433	3	1.47E-04	1.34	FALSE	2.02E-02	1.20	FALSE	3.48E-03	1.21	FALSE	4.68E-01	1.08	FALSE
M105T510_neg	105.0016	510	3	1.88E-09	1.34	FALSE	1.64E-03	1.17	FALSE	1.91E-08	1.27	FALSE	3.79E-01	0.92	FALSE
M105T444_neg	105.0016	444	3	6.41E-14	1.30	FALSE	2.77E-04	1.13	FALSE	7.77E-12	1.23	FALSE	5.11E-01	0.96	FALSE
M105T784_neg	105.0710	784	3	1.56E-09	1.34	FALSE	7.96E-02	1.09	FALSE	7.21E-01	0.99	FALSE	3.58E-01	0.88	FALSE
M109T485_neg	109.0295	485	3	7.37E-05	1.45	FALSE	9.15E-02	1.17	FALSE	1.09E-01	1.14	FALSE	7.76E-01	1.04	FALSE
M109T521_neg	109.0659	521	3	1.74E-10	1.41	FALSE	4.85E-01	0.96	FALSE	7.88E-07	1.26	FALSE	9.15E-02	0.86	FALSE
M110T475_neg	110.0248	475	3	5.30E-01	0.91	FALSE	1.25E-02	0.72	FALSE	4.56E-03	1.44	FALSE	3.15E-01	0.77	FALSE
M110T578_neg	110.0248	578	3	2.07E-01	0.82	FALSE	1.41E-02	0.70	FALSE	3.18E-02	1.35	FALSE	1.57E-01	0.67	FALSE
M112T714_neg	112.0405	714	3	1.53E-02	1.14	FALSE	3.64E-01	1.06	FALSE	9.00E-01	0.99	FALSE	1.36E-01	1.13	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M112T488_neg	112.0405	488	3							HMDB0001301	1-Pyrroline-5-carboxylic acid	C5H7NO2	0.5
M113T419_neg	113.0245	419	3							HMDB0031859	Norfuraneol	C5H6O3	0.6
M113T526_neg	113.0609	526	3							HMDB0000453	delta-Hexanolactone	C6H10O2	0.8
M114T412_neg	114.0925	412	3							HMDB0031651	N-(3-Methylbutyl)acetamide	C6H13NO	0.8
M114T465_neg	114.0925	465	3							HMDB0031651	N-(3-Methylbutyl)acetamide	C6H13NO	1.0
M115T533_neg	115.0224	533	3							HMDB0038556	Dihydro-2-methyl-3(2H)-thiophenc	C5H8OS	0.8
M115T847_neg	115.0401	847	3							HMDB0000019	alpha-Ketoisovaleric acid	C5H8O3	0.7
M116T573_neg	116.0506	573	3							HMDB0000738	Indole	C8H7N	0.6
M116T465_neg	116.0718	465	3							HMDB0000883	L-Valine	C5H11NO2	0.8
M118T499_neg	118.0332	499	3							HMDB0255064	N-Acetylcysteamine	C4H9NOS	0.1
M119T561_neg	118.9809	561	3							HMDB0001368	3-Mercaptopyruvic acid	C3H4O3S	0.7
M121T609_neg	121.0660	609	3							HMDB0029306	4-Ethylphenol	C8H10O	0.6
M121T662_neg	121.0660	662	3							HMDB0029306	4-Ethylphenol	C8H10O	0.7
M123T490_neg	123.0452	490	3							HMDB0000873	4-Methylcatechol	C7H8O2	0.7
M124T637_neg	124.0405	637	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.8
M124T770_neg	124.0405	770	3							HMDB0245816	3-Aminobenzene-1,2-diol	C6H7NO2	0.6
M126T695_neg	126.0561	695	3							HMDB0001084	1-Piperideine-2-carboxylic acid	C6H9NO2	0.7
M127T575_neg	127.0224	575	3							HMDB0041566	2-Methyl-5-(methylthio)furan	C6H8OS	0.9
M128T268_neg	128.0354	268	3							HMDB0000267	Pyroglutamic acid	C5H7NO3	0.7
M128T707_neg	128.0507	707	3							HMDB0011664	3-Methylene-indolenine	C9H7N	0.7
M128T626_neg	128.0507	627	3							HMDB0011664	3-Methylene-indolenine	C9H7N	1.0
M129T490_neg	129.0558	490	3							HMDB0000408	2-Methyl-3-ketovaleric acid	C6H10O3	1.0
M129T686_neg	129.0922	686	3							HMDB0000666	Heptanoic acid	C7H14O2	0.7
M129T747_neg	129.0922	747	3							HMDB0000666	Heptanoic acid	C7H14O2	0.5
M130T831_neg	130.0663	831	3							HMDB0000466	3-Methylindole	C9H9N	0.2
M130T706_neg	130.0663	706	3							HMDB0000466	3-Methylindole	C9H9N	0.6
M134T571_neg	134.0613	571	3							HMDB0001250	N-Acetylarylamine	C8H9NO	1.2
M135T216_neg	135.0122	216	3							HMDB0244530	etrahydrothiophene-3-ol 1,1-dioxic	C4H8O3S	0.7
M135T659_neg	135.0817	659	3							HMDB0029667	2,3,6-Trimethylphenol	C9H12O	0.8
M136T598_2_neg	136.0769	598	3							HMDB0000306	Tyramine	C8H11NO	0.8
M136T452_neg	136.0769	452	3							HMDB0000306	Tyramine	C8H11NO	0.9
M136T680_neg	136.0769	680	3							HMDB0000306	Tyramine	C8H11NO	0.8
M137T563_neg	137.0245	563	3							HMDB0000500	4-Hydroxybenzoic acid	C7H6O3	0.8
M137T575_neg	137.0358	575	3							HMDB0000301	Urocanic acid	C6H6N2O2	0.7
M137T536_neg	137.0610	536	3							HMDB0004284	Tyrosol	C8H10O2	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M112T488_neg	112.0405	488	3	5.43E-06	1.21	FALSE	4.07E-01	1.04	FALSE	2.64E-14	1.34	FALSE	2.16E-01	1.07	FALSE
M113T419_neg	113.0245	419	3	3.85E-03	1.25	FALSE	9.12E-01	0.99	FALSE	9.96E-03	0.84	FALSE	7.67E-01	1.07	FALSE
M113T526_neg	113.0609	526	3	2.42E-18	1.37	FALSE	2.84E-01	1.04	FALSE	6.76E-05	1.12	FALSE	6.47E-01	1.02	FALSE
M114T412_neg	114.0925	412	3	5.39E-01	1.04	FALSE	1.48E-01	1.11	FALSE	1.39E-09	1.49	FALSE	5.90E-01	1.06	FALSE
M114T465_neg	114.0925	465	3	1.33E-19	1.50	FALSE	4.88E-01	0.97	FALSE	4.20E-03	1.10	FALSE	2.51E-02	0.86	FALSE
M115T533_neg	115.0224	533	3	5.57E-09	1.43	FALSE	4.32E-01	1.05	FALSE	6.04E-04	1.19	FALSE	7.75E-01	0.97	FALSE
M115T847_neg	115.0401	847	3	5.35E-07	1.39	FALSE	9.62E-01	1.00	FALSE	8.49E-01	1.01	FALSE	1.14E-01	0.82	FALSE
M116T573_neg	116.0506	573	3	4.36E-01	1.06	FALSE	2.89E-01	0.92	FALSE	6.13E-01	1.04	FALSE	6.06E-02	1.40	FALSE
M116T465_neg	116.0718	465	3	1.38E-05	1.19	FALSE	7.60E-01	0.99	FALSE	5.68E-04	1.13	FALSE	1.21E-02	0.83	FALSE
M118T499_neg	118.0332	499	3	1.92E-06	1.21	FALSE	5.19E-07	1.22	FALSE	7.16E-09	1.22	FALSE	2.59E-01	1.07	FALSE
M119T561_neg	118.9809	561	3	2.16E-03	0.78	FALSE	8.01E-02	1.17	FALSE	2.65E-04	1.29	FALSE	1.95E-01	0.83	FALSE
M121T609_neg	121.0660	609	3	8.21E-06	1.34	FALSE	3.93E-01	0.94	FALSE	1.57E-03	1.19	FALSE	1.17E-01	1.31	FALSE
M121T662_neg	121.0660	662	3	7.54E-05	1.40	FALSE	6.76E-01	0.96	FALSE	2.98E-02	1.17	FALSE	6.42E-01	1.10	FALSE
M123T490_neg	123.0452	490	3	8.50E-08	1.28	FALSE	8.42E-01	1.01	FALSE	7.33E-11	1.30	FALSE	6.04E-01	1.04	FALSE
M124T637_neg	124.0405	637	3	1.05E-14	1.40	FALSE	3.82E-01	1.04	FALSE	5.89E-11	1.28	FALSE	4.86E-01	1.05	FALSE
M124T770_neg	124.0405	770	3	8.75E-02	1.09	FALSE	1.13E-01	1.08	FALSE	1.99E-16	1.46	FALSE	5.93E-01	0.95	FALSE
M126T695_neg	126.0561	695	3	3.99E-03	1.20	FALSE	2.99E-01	1.07	FALSE	1.41E-04	1.24	FALSE	1.99E-01	0.85	FALSE
M127T575_neg	127.0224	575	3	6.48E-01	0.97	FALSE	9.16E-01	0.99	FALSE	2.47E-04	1.21	FALSE	1.66E-01	0.85	FALSE
M128T268_neg	128.0354	268	3	6.93E-03	0.78	FALSE	8.21E-01	1.02	FALSE	2.64E-03	1.28	FALSE	3.12E-01	1.52	FALSE
M128T707_neg	128.0507	707	3	5.78E-01	1.07	FALSE	7.72E-01	1.04	FALSE	4.38E-02	1.25	FALSE	6.05E-01	0.93	FALSE
M128T626_neg	128.0507	627	3	3.60E-01	1.05	FALSE	1.93E-01	1.07	FALSE	9.85E-15	1.47	FALSE	9.58E-02	1.14	FALSE
M129T490_neg	129.0558	490	3	5.81E-11	1.27	FALSE	4.81E-02	1.07	FALSE	2.05E-03	1.10	FALSE	1.44E-02	1.17	FALSE
M129T686_neg	129.0922	686	3	7.39E-01	0.97	FALSE	2.17E-01	1.15	FALSE	3.58E-02	1.22	FALSE	1.43E-01	1.13	FALSE
M129T747_neg	129.0922	747	3	2.44E-08	0.74	FALSE	2.87E-01	1.06	FALSE	7.95E-11	1.37	FALSE	2.72E-02	0.71	FALSE
M130T831_neg	130.0663	831	3	7.91E-03	1.19	FALSE	2.47E-02	1.16	FALSE	4.79E-03	1.17	FALSE	5.85E-01	1.07	FALSE
M130T706_neg	130.0663	706	3	5.41E-01	1.08	FALSE	6.01E-01	1.07	FALSE	3.92E-02	1.26	FALSE	1.75E-01	0.84	FALSE
M134T571_neg	134.0613	571	3	1.00E+00	1.00	FALSE	2.86E-01	0.93	FALSE	6.27E-07	1.33	FALSE	6.78E-01	0.95	FALSE
M135T216_neg	135.0122	216	3	1.60E-03	1.31	FALSE	3.67E-02	0.84	FALSE	4.84E-04	1.30	FALSE	5.08E-01	1.07	FALSE
M135T659_neg	135.0817	659	3	2.09E-10	1.25	FALSE	9.01E-01	1.00	FALSE	3.60E-11	1.23	FALSE	4.78E-01	0.96	FALSE
M136T598_2_neg	136.0769	598	3	2.68E-03	1.27	FALSE	7.79E-02	0.86	FALSE	1.91E-01	1.09	FALSE	3.14E-02	1.16	FALSE
M136T452_neg	136.0769	452	3	1.13E-05	1.21	FALSE	4.12E-01	1.04	FALSE	7.29E-20	1.47	FALSE	5.29E-02	0.90	FALSE
M136T680_neg	136.0769	680	3	2.40E-02	1.17	FALSE	8.51E-02	1.14	FALSE	1.90E-03	1.21	FALSE	8.39E-01	1.05	FALSE
M137T563_neg	137.0245	563	3	6.70E-01	0.96	FALSE	4.40E-01	1.07	FALSE	2.72E-07	1.49	FALSE	2.90E-01	0.93	FALSE
M137T575_neg	137.0358	575	3	2.31E-02	0.81	FALSE	4.47E-01	0.93	FALSE	1.41E-05	1.44	FALSE	2.27E-01	0.87	FALSE
M137T536_neg	137.0610	536	3	2.72E-01	1.16	FALSE	2.50E-01	0.84	FALSE	1.35E-01	1.19	FALSE	8.98E-01	0.98	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M137T621_neg	137.0609	621	3							HMDB0004284	Tyrosol	C8H10O2	0.8
M138T254_neg	138.0198	254	3							HMDB0001232	4-Nitrophenol	C6H5NO3	0.7
M139T148_neg	139.0071	148	3							HMDB0245842	3-Chlorophenylhydrazone	C6H5ClN2	1.9
M139T802_neg	139.1129	802	3							HMDB0030957	(3Z,6Z)-3,6-Nonadien-1-ol	C9H16O	0.7
M140T385_neg	140.0718	385	3							HMDB0014731	Ethosuximide	C7H11NO2	1.0
M140T181_neg	140.0830	181	3							HMDB0003431	L-Histidinol	C6H11N3O	0.5
M141T488_neg	141.0558	488	3							HMDB0033551	yl-3-hydroxy-4-methyl-2(5H)-fura	C7H10O3	0.9
M141T406_neg	141.0671	406	3							HMDB0240650	Ectoine	C6H10N2O2	1.0
M141T724_neg	141.0922	724	3							HMDB0000392	2-Octenoic acid	C8H14O2	0.8
M142T479_neg	142.0333	479	3							HMDB0246712	-(1-Hydroxyethyl)-4-methylthiazol	C6H9NOS	0.8
M142T231_neg	142.0623	231	3							HMDB0250642	Cyclocreatine	C5H9N3O2	0.7
M143T415_neg	143.0351	415	3							HMDB0000393	3-Hexenedioic acid	C6H8O4	0.7
M143T537_neg	143.0715	537	3							HMDB0001988	4-Hydroxycyclohexylcarboxylic acid	C7H12O3	0.7
M143T753_neg	143.1079	753	3							HMDB0000482	Caprylic acid	C8H16O2	0.7
M144T571_neg	144.0456	571	3							HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.6
M144T627_neg	144.0456	627	3							HMDB0029737	Indole-3-carboxaldehyde	C9H7NO	0.7
M145T382_neg	145.0508	382	3						Fatty acids	HMDB0000422	2-Methylglutaric acid	C6H10O4	0.8
M145T631_neg	145.0871	631	3							HMDB0002207	3-Hydroxyisoheptanoic acid	C7H14O3	0.8
M147T375_neg	147.0664	375	3							HMDB0000227	Mevalonic acid	C6H12O4	0.9
M149T772_neg	149.0973	772	3							HMDB0001878	Thymol	C10H14O	0.5
M150T576_neg	150.0562	576	3							HMDB0001859	Acetaminophen	C8H9NO2	0.9
M150T468_neg	150.0926	468	3							HMDB0001387	N-Methylphenylethanolamine	C9H13NO	0.8
M151T535_neg	151.0766	535	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	1.1
M151T737_neg	151.0766	737	3							HMDB0032132	2-Isopropyl-1,4-benzenediol	C9H12O2	0.8
M153T622_neg	153.0194	622	3						Shikimates and Phenylpropanoids	HMDB0000152	Gentisic acid	C7H6O4	0.6
M154T513_neg	154.0875	513	3							HMDB0030353	Arecoline	C8H13NO2	1.0
M155T433_neg	155.0464	433	3							HMDB0000544	5-Hydroxymethyl-4-methyluracil	C6H8N2O3	0.9
M155T779_neg	155.1079	779	3							HMDB0004362	4-Hydroxynonenal	C9H16O2	0.7
M156T513_neg	156.0667	513	3							HMDB0000459	3-Methylcrotonylglycine	C7H11NO3	0.8
M157T927_neg	157.0871	927	3							HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	0.8
M157T693_neg	157.0871	693	3							HMDB0000451	cis-4-Hydroxycyclohexylacetic acid	C8H14O3	0.6
M159T453_neg	159.0664	453	3							HMDB0000555	3-Methyladipic acid	C7H12O4	0.7
M159T508_neg	159.0928	508	3							HMDB0000303	Tryptamine	C10H12N2	0.2
M160T686_neg	160.0405	686	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M137T621_neg	137.0609	621	3	3.06E-06	1.41	FALSE	3.51E-01	1.07	FALSE	7.09E-01	1.02	FALSE	9.56E-01	0.99	FALSE
M138T254_neg	138.0198	254	3	5.64E-02	0.84	FALSE	4.12E-01	1.08	FALSE	4.01E-04	1.34	FALSE	6.93E-01	1.06	FALSE
M139T148_neg	139.0071	148	3	1.55E-01	1.20	FALSE	7.66E-01	0.96	FALSE	8.84E-03	1.34	FALSE	5.47E-01	1.15	FALSE
M139T802_neg	139.1129	802	3	8.40E-01	0.99	FALSE	2.16E-01	1.05	FALSE	1.33E-12	1.30	FALSE	5.40E-01	0.94	FALSE
M140T385_neg	140.0718	385	3	3.90E-17	1.37	FALSE	1.02E-01	1.06	FALSE	1.70E-02	1.07	FALSE	3.13E-02	0.91	FALSE
M140T181_neg	140.0830	181	3	4.53E-02	1.13	FALSE	7.46E-01	0.98	FALSE	2.46E-12	1.49	FALSE	1.38E-02	0.83	FALSE
M141T488_neg	141.0558	488	3	2.94E-04	1.19	FALSE	1.44E-01	1.07	FALSE	4.36E-07	1.23	FALSE	7.05E-01	1.04	FALSE
M141T406_neg	141.0671	406	3	6.68E-01	0.97	FALSE	4.43E-01	1.06	FALSE	6.17E-04	1.24	FALSE	1.33E-01	0.75	FALSE
M141T724_neg	141.0922	724	3	5.67E-07	0.75	FALSE	8.32E-01	1.01	FALSE	4.49E-11	1.41	FALSE	8.70E-01	0.97	FALSE
M142T479_neg	142.0333	479	3	2.90E-01	1.04	FALSE	9.26E-01	1.00	FALSE	9.06E-26	1.48	FALSE	1.75E-01	0.96	FALSE
M142T231_neg	142.0623	231	3	1.15E-03	1.43	FALSE	8.90E-01	1.02	FALSE	1.13E-04	1.45	FALSE	9.55E-01	0.99	FALSE
M143T415_neg	143.0351	415	3	6.97E-01	0.98	FALSE	3.00E-01	1.06	FALSE	1.41E-04	1.20	FALSE	1.58E-01	1.23	FALSE
M143T537_neg	143.0715	537	3	2.61E-18	1.36	FALSE	9.15E-01	1.00	FALSE	1.36E-02	1.07	FALSE	9.45E-01	1.00	FALSE
M143T753_neg	143.1079	753	3	1.45E-03	0.85	FALSE	1.59E-01	1.08	FALSE	5.32E-16	1.48	FALSE	8.38E-02	0.88	FALSE
M144T571_neg	144.0456	571	3	1.08E-01	1.12	FALSE	9.40E-01	1.01	FALSE	1.60E-06	1.35	FALSE	3.24E-01	1.19	FALSE
M144T627_neg	144.0456	627	3	5.21E-02	1.10	FALSE	3.36E-01	1.05	FALSE	1.41E-10	1.33	FALSE	3.26E-02	1.16	FALSE
M145T382_neg	145.0508	382	3	3.89E-01	1.06	FALSE	3.39E-04	1.29	FALSE	3.61E-07	1.36	FALSE	2.25E-01	1.15	FALSE
M145T631_neg	145.0871	631	3	3.04E-15	1.42	FALSE	8.10E-01	1.01	FALSE	8.81E-01	0.99	FALSE	4.42E-01	1.05	FALSE
M147T375_neg	147.0664	375	3	2.07E-08	1.26	FALSE	9.68E-02	1.07	FALSE	2.66E-16	1.37	FALSE	5.28E-02	1.16	FALSE
M149T772_neg	149.0973	772	3	5.08E-06	1.26	FALSE	3.28E-01	1.05	FALSE	2.27E-02	1.10	FALSE	7.41E-01	1.05	FALSE
M150T576_neg	150.0562	576	3	2.75E-05	1.44	FALSE	2.27E-02	0.81	FALSE	4.28E-05	0.73	FALSE	8.47E-01	0.97	FALSE
M150T468_neg	150.0926	468	3	1.33E-02	1.16	FALSE	2.41E-01	1.08	FALSE	4.84E-09	1.37	FALSE	3.47E-01	0.92	FALSE
M151T535_neg	151.0766	535	3	9.89E-05	1.35	FALSE	9.65E-01	1.00	FALSE	1.24E-03	1.24	FALSE	8.03E-01	1.02	FALSE
M151T737_neg	151.0766	737	3	4.08E-02	0.86	FALSE	3.35E-01	1.07	FALSE	5.47E-08	1.42	FALSE	2.92E-01	0.91	FALSE
M153T622_neg	153.0194	622	3	7.73E-02	1.21	FALSE	1.50E-01	0.85	FALSE	2.52E-03	1.33	FALSE	5.65E-01	0.91	FALSE
M154T513_neg	154.0875	513	3	4.73E-05	1.31	FALSE	5.26E-05	1.32	FALSE	8.03E-11	1.48	FALSE	6.97E-02	1.19	FALSE
M155T433_neg	155.0464	433	3	5.17E-01	1.05	FALSE	8.96E-01	0.99	FALSE	5.70E-05	1.29	FALSE	5.96E-01	0.95	FALSE
M155T779_neg	155.1079	779	3	1.30E-01	0.93	FALSE	5.57E-01	1.03	FALSE	6.85E-06	1.20	FALSE	9.35E-02	0.85	FALSE
M156T513_neg	156.0667	513	3	4.73E-02	1.10	FALSE	1.30E-01	1.08	FALSE	4.02E-07	1.24	FALSE	9.61E-01	1.00	FALSE
M157T927_neg	157.0871	927	3	6.21E-03	1.40	FALSE	2.36E-01	0.85	FALSE	6.95E-03	0.75	FALSE	1.02E-01	0.80	FALSE
M157T693_neg	157.0871	693	3	1.33E-02	0.91	FALSE	1.12E-01	1.06	FALSE	1.16E-01	0.95	FALSE	1.04E-01	0.88	FALSE
M159T453_neg	159.0664	453	3	7.31E-02	1.21	FALSE	3.61E-02	0.78	FALSE	1.17E-01	0.87	FALSE	1.84E-01	0.88	FALSE
M159T508_neg	159.0928	508	3	1.95E-03	0.75	FALSE	2.64E-01	1.11	FALSE	1.60E-04	0.74	FALSE	4.21E-01	1.11	FALSE
M160T686_neg	160.0405	686	3	4.49E-01	0.94	FALSE	3.62E-01	0.92	FALSE	1.30E-06	1.43	FALSE	1.07E-01	0.57	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M160T543_neg	160.0406	543	3							HMDB0002285	2-Indolecarboxylic acid	C9H7NO2	1.0
M161T555_neg	161.0278	555	3							HMDB0012134	Dihydroxy-3-keto-5-methylthiopen	C6H10O3S	0.4
M161T466_neg	161.0456	466	3							HMDB0000321	2-Hydroxyadipic acid	C6H10O5	0.5
M161T440_neg	161.0820	440	3						Fatty acids	HMDB0059918	2-(1-Ethoxyethoxy)propanoic acid	C7H14O4	0.7
M163T719_neg	163.0766	719	3							HMDB0000329	2-Phenylbutyric acid	C10H12O2	0.7
M164T760_neg	164.1082	760	3							HMDB0001943	Pseudoephedrine	C10H15NO	0.4
M164T552_neg	164.1082	552	3							HMDB0001943	Pseudoephedrine	C10H15NO	0.6
M165T1001_neg	165.0409	1001	3							HMDB0034394	S-Propyl 1-propanesulfinothioate	C6H14OS2	2.5
M165T385_neg	165.0666	385	3							HMDB0247540	3,4-Dihydroxyphenylacetamidine	C8H10N2O2	2.1
M167T921_neg	167.0714	921	3							HMDB0029680	2,6-Dimethoxy-4-methylphenol	C9H12O3	0.4
M167T882_neg	167.1442	882	3							HMDB0031128	10-Undecenal	C11H20O	0.6
M168T506_neg	168.0667	506	3							HMDB0000216	Norepinephrine	C8H11NO3	0.7
M168T662_neg	168.0667	662	3							HMDB0000216	Norepinephrine	C8H11NO3	0.5
M169T485_neg	169.0983	485	3							HMDB0015333	Levetiracetam	C8H14N2O2	0.4
M170T711_neg	170.0824	711	3							HMDB0247190	)-2-Oxotetrahydrofuran-3-Yl]butan	C8H13NO3	1.0
M171T541_neg	171.0664	541	3							HMDB0000341	2-Octenedioic acid	C8H12O4	0.7
M171T487_neg	171.0776	487	3							HMDB0000721	Glycylproline	C7H12N2O3	0.6
M171T555_neg	171.0927	555	3							HMDB0012488	1,2,3,4-Tetrahydro-beta-carboline	C11H12N2	0.7
M172T627_neg	172.0405	627	3							HMDB0000842	Quinaldic acid	C10H7NO2	0.5
M172T361_neg	172.0616	361	3							HMDB0006488	-Acetyl-L-glutamate 5-semialdehyd	C7H11NO4	0.6
M172T290_neg	172.0616	290	3						Amino acids and Peptides	HMDB0006488	-Acetyl-L-glutamate 5-semialdehyd	C7H11NO4	0.5
M172T583_neg	172.0981	583	3							HMDB0000701	Hexanoylglycine	C8H15NO3	0.8
M172T370_neg	172.1092	370	3							HMDB0059607	otonoyl-CoA:carbon-dioxide ligase	C7H15N3O2	0.6
M173T426_neg	173.0456	426	3							HMDB0003070	Shikimic acid	C7H10O5	0.5
M173T729_neg	173.0820	729	3							HMDB0000893	Suberic acid	C8H14O4	0.4
M174T831_neg	174.0561	831	3							HMDB0000197	Indoleacetic acid	C10H9NO2	0.3
M175T773_neg	175.0765	773	3							HMDB0029699	Cinnamyl acetate	C11H12O2	0.3
M175T502_neg	175.0977	502	3							HMDB0250311	Cladinose	C8H16O4	0.6
M178T727_neg	178.0543	727	3							HMDB0029442	(R)C(R)S-S-Propylcysteine sulfoxide	C6H13NO3S	0.5
M179T539_neg	179.0572	539	3							HMDB0001860	Paraxanthine	C7H8N4O2	1.4
M179T917_neg	179.0715	917	3							HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	0.5
M179T783_neg	179.0714	783	3							HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	0.4
M179T670_neg	179.0715	670	3							HMDB0011751	3-Methoxybenzenepropanoic acid	C10H12O3	0.9
M179T659_neg	179.1078	659	3							HMDB0030007	tramethyl-1,6-dioxaspiro[4.4]nona	C11H16O2	0.5
M181T669_neg	181.1235	669	3							HMDB0030006	Tetramethyl-1,6-dioxaspiro[4.4]no	C11H18O2	0.6

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M160T543_neg	160.0406	543	3	2.75E-04	1.38	FALSE	2.19E-02	0.81	FALSE	7.81E-02	1.14	FALSE	4.97E-01	0.90	FALSE
M161T555_neg	161.0278	555	3	4.04E-04	1.20	FALSE	1.34E-03	1.19	FALSE	8.99E-13	1.40	FALSE	9.51E-01	1.00	FALSE
M161T466_neg	161.0456	466	3	2.30E-08	0.69	FALSE	2.09E-01	1.09	FALSE	3.55E-06	1.30	FALSE	2.66E-01	0.79	FALSE
M161T440_neg	161.0820	440	3	8.03E-19	1.47	FALSE	6.78E-01	1.02	FALSE	5.84E-02	1.07	FALSE	3.76E-01	0.93	FALSE
M163T719_neg	163.0766	719	3	1.18E-01	1.38	FALSE	3.62E-01	0.81	FALSE	4.07E-01	0.86	FALSE	2.74E-01	0.76	FALSE
M164T760_neg	164.1082	760	3	2.04E-01	1.08	FALSE	2.52E-01	1.07	FALSE	5.59E-07	1.31	FALSE	7.35E-01	0.96	FALSE
M164T552_neg	164.1082	552	3	2.97E-02	1.13	FALSE	1.25E-01	1.10	FALSE	4.14E-09	1.36	FALSE	8.21E-01	0.97	FALSE
M165T1001_neg	165.0409	1001	3	5.33E-06	0.83	FALSE	6.06E-03	1.12	FALSE	3.53E-03	0.90	FALSE	4.68E-01	1.07	FALSE
M165T385_neg	165.0666	385	3	6.42E-01	1.03	FALSE	1.50E-01	1.09	FALSE	2.27E-14	1.49	FALSE	1.05E-01	0.87	FALSE
M167T921_neg	167.0714	921	3	3.66E-02	1.05	FALSE	6.67E-02	0.96	FALSE	4.61E-12	0.87	FALSE	9.68E-01	1.00	FALSE
M167T882_neg	167.1442	882	3	9.57E-02	0.92	FALSE	8.20E-01	1.01	FALSE	1.19E-01	1.07	FALSE	9.16E-01	1.01	FALSE
M168T506_neg	168.0667	506	3	4.40E-03	0.73	FALSE	8.01E-01	1.03	FALSE	6.79E-03	1.30	FALSE	2.17E-01	1.12	FALSE
M168T662_neg	168.0667	662	3	7.03E-01	1.02	FALSE	2.82E-06	0.74	FALSE	3.08E-06	1.30	FALSE	8.03E-03	1.38	FALSE
M169T485_neg	169.0983	485	3	2.92E-02	0.88	FALSE	6.62E-01	1.03	FALSE	1.51E-11	1.46	FALSE	6.79E-01	1.05	FALSE
M170T711_neg	170.0824	711	3	7.58E-03	0.79	FALSE	5.76E-01	0.95	FALSE	6.22E-06	1.44	FALSE	1.17E-01	0.75	FALSE
M171T541_neg	171.0664	541	3	5.58E-09	1.29	FALSE	7.48E-01	0.99	FALSE	6.74E-01	0.99	FALSE	4.05E-01	1.11	FALSE
M171T487_neg	171.0776	487	3	1.60E-09	0.67	FALSE	7.87E-01	0.98	FALSE	7.31E-12	1.50	FALSE	9.12E-01	1.01	FALSE
M171T555_neg	171.0927	555	3	1.69E-04	1.36	FALSE	8.61E-02	1.15	FALSE	1.97E-01	1.09	FALSE	2.79E-01	0.91	FALSE
M172T627_neg	172.0405	627	3	1.23E-01	1.08	FALSE	1.06E-01	1.09	FALSE	4.41E-12	1.40	FALSE	1.20E-02	1.20	FALSE
M172T361_neg	172.0616	361	3	1.41E-01	1.10	FALSE	1.36E-01	1.11	FALSE	3.60E-10	1.46	FALSE	4.70E-01	0.94	FALSE
M172T290_neg	172.0616	290	3	5.42E-02	1.16	FALSE	3.03E-01	1.09	FALSE	2.93E-05	1.33	FALSE	8.51E-01	0.97	FALSE
M172T583_neg	172.0981	583	3	2.04E-01	-6.43	FALSE	1.26E-01	-3.22	FALSE	1.95E-01	-0.10	FALSE	9.59E-01	0.99	FALSE
M172T370_neg	172.1092	370	3	6.51E-01	0.93	FALSE	9.05E-01	0.98	FALSE	4.17E-01	0.90	FALSE	6.28E-02	0.66	FALSE
M173T426_neg	173.0456	426	3	3.14E-01	0.97	FALSE	6.65E-01	1.01	FALSE	4.53E-12	1.18	FALSE	6.45E-01	0.97	FALSE
M173T729_neg	173.0820	729	3	5.48E-01	1.04	FALSE	2.17E-03	1.23	FALSE	9.73E-10	1.43	FALSE	8.08E-01	1.03	FALSE
M174T831_neg	174.0561	831	3	2.05E-03	1.30	FALSE	2.17E-01	1.11	FALSE	3.26E-07	1.47	FALSE	6.88E-01	0.93	FALSE
M175T773_neg	175.0765	773	3	7.93E-01	1.01	FALSE	2.68E-01	1.07	FALSE	5.27E-04	1.19	FALSE	9.20E-01	1.01	FALSE
M175T502_neg	175.0977	502	3	4.67E-16	1.32	FALSE	4.56E-01	1.02	FALSE	1.37E-05	1.13	FALSE	4.76E-01	1.04	FALSE
M178T727_neg	178.0543	727	3	1.06E-02	1.37	FALSE	3.54E-01	1.13	FALSE	3.45E-02	1.25	FALSE	5.66E-01	0.81	FALSE
M179T539_neg	179.0572	539	3	1.32E-03	1.15	FALSE	3.57E-01	1.04	FALSE	3.58E-04	1.15	FALSE	3.33E-01	1.09	FALSE
M179T917_neg	179.0715	917	3	6.35E-05	1.47	FALSE	3.70E-01	0.91	FALSE	1.78E-01	1.12	FALSE	4.62E-01	0.87	FALSE
M179T783_neg	179.0714	783	3	3.06E-01	1.14	FALSE	8.40E-02	0.78	FALSE	4.91E-01	1.08	FALSE	7.47E-01	1.05	FALSE
M179T670_neg	179.0715	670	3	1.70E-02	1.26	FALSE	8.93E-01	0.99	FALSE	3.95E-01	1.07	FALSE	8.09E-01	0.96	FALSE
M179T659_neg	179.1078	659	3	7.49E-05	1.22	FALSE	5.65E-01	1.03	FALSE	6.01E-12	1.37	FALSE	8.80E-01	1.02	FALSE
M181T669_neg	181.1235	669	3	7.41E-02	1.11	FALSE	4.72E-01	1.04	FALSE	9.55E-03	1.14	FALSE	5.63E-01	0.91	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M182T655_neg	182.0825	655	3							HMDB0000068	Epinephrine	C9H13NO3	1.1
M182T566_neg	182.0824	566	3							HMDB0000068	Epinephrine	C9H13NO3	0.5
M183T803_neg	183.0816	803	3							HMDB0249075	Benzyl phenyl ether	C13H12O	0.5
M183T592_neg	183.1025	592	3							HMDB0036117	(-)-3-Thujene	C10H16O3	0.7
M183T807_neg	183.1027	807	3						Fatty acids	HMDB0036117	(-)-3-Thujene	C10H16O3	0.3
M183T859_neg	183.1391	859	3							HMDB0031062	(Z)-3-Methyl-3-decenoic acid	C11H20O2	0.4
M184T658_neg	184.0616	658	3							HMDB0244794	obicyclo[3.1.0]hexane-2,6-dicarbox	C8H11NO4	0.4
M185T709_neg	185.0820	709	3							HMDB0030988	propyl)tetrahydro-2-oxo-3-furanca	C9H14O4	0.2
M185T655_neg	185.0820	655	3							HMDB0030988	propyl)tetrahydro-2-oxo-3-furanca	C9H14O4	0.3
M185T608_neg	185.0820	608	3							HMDB0030988	propyl)tetrahydro-2-oxo-3-furanca	C9H14O4	0.2
M185T573_neg	185.1085	573	3							HMDB0029836	,3,4-Tetrahydro-2-methyl-b-carbol	C12H14N2	0.2
M185T1011_neg	185.1547	1011	3							HMDB0000947	Undecanoic acid	C11H22O2	0.2
M187T418_neg	187.0071	418	3							HMDB0240655	o-Cresol sulfate	C7H8O4S	0.5
M187T469_neg	187.0613	469	3							HMDB0059767	Tetrahydro-2,5-furan-diacetic acid	C8H12O5	0.4
M187T529_neg	187.0977	529	3							HMDB0000784	Azelaic acid	C9H16O4	0.5
M187T179_neg	187.1088	179	3							HMDB0000206	N6-Acetyl-L-lysine	C8H16N2O3	0.2
M188T571_neg	188.0355	571	3						Alkaloids	HMDB0000715	Kynurenic acid	C10H7NO3	0.8
M188T411_neg	188.0565	411	3							HMDB0000590	Glutarylglycine	C7H11NO5	0.5
M189T545_neg	189.1133	545	3						Fatty acids				
M190T499_neg	190.0547	499	3							HMDB0247004	L-Cysteine, N-acetyl-, ethyl ester	C7H13NO3S	1.7
M191T439_neg	191.0562	439	3						Fatty acids	HMDB0003072	Quinic acid	C7H12O6	0.3
M191T583_neg	191.0750	583	3							HMDB0246980	2-yl 2-hydroxy-4-methylsulfanylbu	C8H16O3S	1.1
M192T361_neg	192.0667	361	3							HMDB0000821	Phenylacetylglycine	C10H11NO3	0.2
M194T559_neg	194.0459	559	3							HMDB0000840	Salicyluric acid	C9H9NO4	0.1
M194T682_neg	194.0824	682	3							HMDB0014903	Metyrosine	C10H13NO3	0.4
M194T379_neg	194.1188	379	3							HMDB0060953	2-hydroxymexiletine	C11H17NO2	0.5
M195T596_neg	195.0664	596	3							HMDB0000434	Homoveratric acid	C10H12O4	0.6
M196T619_neg	196.0980	619	3							HMDB0004063	Metanephrine	C10H15NO3	0.4
M197T547_neg	197.0649	547	3							HMDB0036134	(2-Furanylmethyl)thio]-2-pentano	C10H14O2S	3.8
M197T370_neg	197.0680	370	3							HMDB0004400	Acetylamino-6-amino-3-methylura	C7H10N4O3	0.1
M197T212_neg	197.0680	212	3							HMDB0004400	Acetylamino-6-amino-3-methylura	C7H10N4O3	0.0
M197T741_neg	197.0819	741	3							HMDB0004998	Guaifenesin	C10H14O4	0.1
M197T689_neg	197.0932	689	3							HMDB0014606	Metharbital	C9H14N2O3	0.1
M197T743_neg	197.0971	743	3							HMDB0032078	Dibenzyl ether	C14H14O	0.2
M199T491_neg	199.0724	491	3							HMDB0247200	-Hydroxyethoxy)methyl-5-methylu	C8H12N2O4	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M182T655_neg	182.0825	655	3	2.98E-01	0.92	FALSE	1.98E-01	1.11	FALSE	5.13E-01	1.04	FALSE	6.41E-02	1.34	FALSE
M182T566_neg	182.0824	566	3	4.56E-02	1.09	FALSE	7.56E-01	0.99	FALSE	1.74E-06	1.21	FALSE	9.50E-01	0.99	FALSE
M183T803_neg	183.0816	803	3	1.04E-19	1.32	FALSE	4.49E-01	0.98	FALSE	8.86E-27	0.74	FALSE	1.44E-01	0.94	FALSE
M183T592_neg	183.1025	592	3	1.59E-08	1.39	FALSE	1.88E-01	0.93	FALSE	4.14E-01	1.04	FALSE	4.11E-01	0.88	FALSE
M183T807_neg	183.1027	807	3	3.18E-01	0.96	FALSE	9.38E-01	1.00	FALSE	8.72E-11	1.26	FALSE	5.53E-01	1.03	FALSE
M183T859_neg	183.1391	859	3	1.78E-03	0.90	FALSE	6.43E-01	1.02	FALSE	2.68E-12	1.23	FALSE	1.05E-01	0.89	FALSE
M184T658_neg	184.0616	658	3	3.04E-06	1.33	FALSE	8.83E-04	0.82	FALSE	5.83E-12	1.46	FALSE	8.55E-02	1.21	FALSE
M185T709_neg	185.0820	709	3	6.01E-01	0.98	FALSE	1.92E-02	1.11	FALSE	8.77E-07	1.20	FALSE	2.52E-01	1.06	FALSE
M185T655_neg	185.0820	655	3	2.87E-11	1.17	FALSE	4.41E-01	1.02	FALSE	3.57E-03	0.94	FALSE	8.36E-01	1.01	FALSE
M185T608_neg	185.0820	608	3	2.06E-03	1.13	FALSE	5.61E-03	1.12	FALSE	8.03E-03	1.09	FALSE	3.29E-01	1.08	FALSE
M185T573_neg	185.1085	573	3	4.60E-01	1.05	FALSE	9.24E-01	0.99	FALSE	1.60E-01	1.08	FALSE	3.44E-02	1.45	FALSE
M185T1011_neg	185.1547	1011	3	1.57E-01	1.16	FALSE	4.22E-03	0.73	FALSE	2.51E-01	0.90	FALSE	8.45E-01	0.94	FALSE
M187T418_neg	187.0071	418	3	3.01E-02	-2.58	FALSE	8.31E-02	0.18	FALSE	6.00E-02	-0.26	FALSE	8.55E-01	0.94	FALSE
M187T469_neg	187.0613	469	3	3.34E-04	1.15	FALSE	5.29E-01	1.03	FALSE	3.84E-03	1.11	FALSE	5.47E-01	1.05	FALSE
M187T529_neg	187.0977	529	3	1.10E-02	0.77	FALSE	6.12E-01	0.95	FALSE	3.39E-02	0.83	FALSE	3.13E-01	1.25	FALSE
M187T179_neg	187.1088	179	3	8.78E-01	0.99	FALSE	3.92E-02	0.89	FALSE	8.15E-01	1.01	FALSE	4.44E-01	1.13	FALSE
M188T571_neg	188.0355	571	3	9.20E-02	1.15	FALSE	4.99E-02	1.19	FALSE	1.86E-04	1.33	FALSE	5.21E-01	1.13	FALSE
M188T411_neg	188.0565	411	3	3.39E-05	0.77	FALSE	4.65E-01	1.05	FALSE	1.61E-06	1.30	FALSE	6.29E-01	1.03	FALSE
M189T545_neg	189.1133	545	3	1.42E-07	1.46	FALSE	9.67E-01	1.00	FALSE	1.48E-01	1.09	FALSE	1.67E-01	1.08	FALSE
M190T499_neg	190.0547	499	3	2.51E-08	1.30	FALSE	1.14E-03	1.17	FALSE	9.03E-02	1.07	FALSE	3.48E-02	1.18	FALSE
M191T439_neg	191.0562	439	3	2.03E-01	0.66	FALSE	7.37E-01	1.14	FALSE	2.36E-01	1.40	FALSE	5.09E-01	0.78	FALSE
M191T583_neg	191.0750	583	3	6.22E-02	1.21	FALSE	5.61E-01	0.94	FALSE	3.23E-03	1.30	FALSE	1.91E-01	1.19	FALSE
M192T361_neg	192.0667	361	3	5.99E-01	0.95	FALSE	8.65E-01	1.02	FALSE	3.25E-05	1.49	FALSE	4.74E-01	1.25	FALSE
M194T559_neg	194.0459	559	3	1.24E-06	1.41	FALSE	5.09E-01	1.05	FALSE	2.29E-07	1.38	FALSE	1.25E-01	0.76	FALSE
M194T682_neg	194.0824	682	3	1.13E-01	1.11	FALSE	4.99E-02	1.14	FALSE	5.22E-06	1.31	FALSE	9.09E-01	1.01	FALSE
M194T379_neg	194.1188	379	3	6.79E-03	1.18	FALSE	7.28E-01	0.98	FALSE	2.76E-06	1.30	FALSE	1.16E-01	0.81	FALSE
M195T596_neg	195.0664	596	3	4.77E-04	1.23	FALSE	2.01E-01	0.92	FALSE	2.26E-11	1.44	FALSE	3.32E-03	1.38	FALSE
M196T619_neg	196.0980	619	3	3.00E-03	1.15	FALSE	8.51E-01	1.01	FALSE	7.16E-07	1.24	FALSE	3.53E-01	1.08	FALSE
M197T547_neg	197.0649	547	3	1.96E-04	1.25	FALSE	2.92E-01	1.07	FALSE	7.59E-11	1.43	FALSE	7.22E-01	1.03	FALSE
M197T370_neg	197.0680	370	3	5.03E-06	1.46	FALSE	9.93E-01	1.00	FALSE	7.54E-01	1.02	FALSE	7.13E-01	0.91	FALSE
M197T212_neg	197.0680	212	3	2.05E-02	1.23	FALSE	3.29E-01	0.92	FALSE	8.57E-01	1.01	FALSE	7.05E-01	1.08	FALSE
M197T741_neg	197.0819	741	3	2.76E-04	0.82	FALSE	2.58E-02	1.13	FALSE	4.66E-12	1.42	FALSE	7.73E-01	1.05	FALSE
M197T689_neg	197.0932	689	3	7.05E-01	1.02	FALSE	2.08E-01	1.06	FALSE	1.41E-16	1.43	FALSE	5.29E-01	0.96	FALSE
M197T743_neg	197.0971	743	3	6.77E-02	1.30	FALSE	9.30E-01	1.01	FALSE	2.67E-01	0.87	FALSE	4.47E-01	0.72	FALSE
M199T491_neg	199.0724	491	3	6.48E-07	1.36	FALSE	2.03E-01	1.08	FALSE	6.31E-08	1.34	FALSE	4.73E-01	0.89	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M199T374_neg	199.0615	374	3							HMDB0033091	(1-Formyl-1-propenyl)pentanedioi	C9H12O5	1.3
M199T677_neg	199.0976	677	3							HMDB0000603	cis-4-Decenedioic acid	C10H16O4	0.3
M199T730_neg	199.0976	730	3							HMDB0000603	cis-4-Decenedioic acid	C10H16O4	0.2
M199T775_neg	199.0976	775	3							HMDB0000603	cis-4-Decenedioic acid	C10H16O4	0.1
M199T669_neg	199.1340	669	3							HMDB0032662	(S)-9-Hydroxy-10-undecenoic acid	C11H20O3	0.3
M200T727_neg	200.1293	727	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.4
M200T805_neg	200.1293	805	3							HMDB0000832	Capryloylglycine	C10H19NO3	0.2
M201T434_neg	201.0769	434	3							HMDB0032306	Diethyl oxalpropionate	C9H14O5	0.4
M201T653_neg	201.1133	653	3							HMDB0000792	Sebacic acid	C10H18O4	0.3
M201T591_neg	201.1133	591	3							HMDB0000792	Sebacic acid	C10H18O4	0.4
M201T192_neg	201.1245	192	3							HMDB0028900	Isoleucyl-Alanine	C9H18N2O3	0.3
M202T725_neg	202.0542	725	3							HMDB0240543	N-Acetyl-S-allylcysteine	C8H13NO3S	0.6
M203T511_neg	203.0562	511	3							HMDB0041031	5-(hydroxymethyl)-2-methoxy-2-c	C8H12O6	0.2
M203T696_neg	203.0827	696	3							HMDB0000929	L-Tryptophan	C11H12N2O2	0.7
M203T665_neg	203.1289	665	3							HMDB0033217	7-Methyl-3-methylene-1,2,6,7-oct	C10H20O4	0.3
M204T484_neg	204.1242	484	3							HMDB0004231	Panthenol	C9H19NO4	0.4
M204T163_neg	204.1242	163	3							HMDB0004231	Panthenol	C9H19NO4	0.1
M206T401_neg	206.0569	401	3							HMDB0060664	Isoniazid pyruvate	C9H9N3O3	1.1
M206T369_neg	206.0823	369	3							HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	0.1
M206T624_neg	206.0823	624	3							HMDB0000512	N-Acetyl-L-phenylalanine	C11H13NO3	0.2
M207T475_neg	207.0873	475	3							HMDB0029968	Ethyl beta-D-glucopyranoside	C8H16O6	0.7
M207T573_neg	207.0887	573	3							HMDB0245925	3-Methyl-1-propylxanthine	C9H12N4O2	0.1
M207T487_neg	207.1140	487	3							HMDB0015217	Pilocarpine	C11H16N2O2	0.6
M207T905_neg	207.1391	905	3							HMDB0029668	Eremopetasinorol	C13H20O2	0.1
M208T649_neg	208.0616	649	3							HMDB0000735	Hydroxyphenylacetylglycine	C10H11NO4	0.2
M208T758_neg	208.0980	758	3							HMDB0254817	thoxy-3,4-methylenedioxyamphet	C11H15NO3	0.3
M209T656_neg	209.0820	656	3							HMDB0013070	Sinapyl alcohol	C11H14O4	0.3
M209T541_neg	209.0821	541	3							HMDB0013070	Sinapyl alcohol	C11H14O4	0.6
M209T904_neg	209.0949	904	3							HMDB0303275	Potassium caprate	C10H19KO2	0.4
M209T744_neg	209.1184	744	3							HMDB0032797	Jasmonic acid	C12H18O3	0.2
M210T782_neg	210.0774	782	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	1.2
M210T597_neg	210.0773	597	3							HMDB0001434	3-Methoxytyrosine	C10H13NO4	0.5
M210T723_neg	210.1136	723	3							HMDB0014861	Methoxamine	C11H17NO3	0.3
M211T642_neg	211.0815	642	3							HMDB0033750	D-Glycero-D-galacto-heptitol	C7H16O7	4.1
M211T893_neg	211.1340	893	3						Fatty acids	HMDB0029388	Cucurbic acid	C12H20O3	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M199T374_neg	199.0615	374	3	5.96E-02	1.14	FALSE	5.56E-01	1.04	FALSE	3.49E-07	1.38	FALSE	1.22E-01	0.89	FALSE
M199T677_neg	199.0976	677	3	2.62E-04	1.19	FALSE	3.09E-01	1.05	FALSE	4.44E-01	1.03	FALSE	7.12E-01	1.06	FALSE
M199T730_neg	199.0976	730	3	5.96E-11	0.77	FALSE	6.04E-02	1.08	FALSE	3.01E-16	1.35	FALSE	2.17E-01	1.09	FALSE
M199T775_neg	199.0976	775	3	3.55E-02	0.91	FALSE	4.60E-01	0.97	FALSE	7.55E-09	1.27	FALSE	1.29E-01	0.86	FALSE
M199T669_neg	199.1340	669	3	9.06E-02	1.19	FALSE	2.86E-01	0.89	FALSE	5.16E-01	0.94	FALSE	9.35E-02	1.49	FALSE
M200T727_neg	200.1293	727	3	2.24E-01	2.71	FALSE	1.85E-01	2.89	FALSE	1.07E-01	0.30	FALSE	6.75E-01	0.97	FALSE
M200T805_neg	200.1293	805	3	4.10E-09	1.48	FALSE	4.26E-04	1.26	FALSE	4.12E-04	1.22	FALSE	5.26E-01	0.89	FALSE
M201T434_neg	201.0769	434	3	1.98E-01	0.92	FALSE	6.80E-01	0.97	FALSE	8.39E-03	1.17	FALSE	3.39E-01	0.91	FALSE
M201T653_neg	201.1133	653	3	6.42E-05	1.32	FALSE	5.55E-01	0.96	FALSE	2.35E-01	0.93	FALSE	3.51E-01	1.14	FALSE
M201T591_neg	201.1133	591	3	1.14E-08	1.33	FALSE	4.61E-02	1.10	FALSE	9.35E-04	1.15	FALSE	3.07E-01	1.16	FALSE
M201T192_neg	201.1245	192	3	6.94E-04	1.29	FALSE	4.47E-03	1.26	FALSE	2.57E-08	1.47	FALSE	1.57E-01	1.31	FALSE
M202T725_neg	202.0542	725	3	1.43E-03	1.30	FALSE	6.70E-01	1.04	FALSE	2.17E-01	1.09	FALSE	7.81E-01	0.96	FALSE
M203T511_neg	203.0562	511	3	2.09E-01	1.19	FALSE	9.87E-01	1.00	FALSE	6.02E-01	1.06	FALSE	9.24E-01	1.03	FALSE
M203T696_neg	203.0827	696	3	4.33E-05	1.48	FALSE	5.26E-01	1.06	FALSE	2.45E-02	1.20	FALSE	4.55E-01	0.90	FALSE
M203T665_neg	203.1289	665	3	9.50E-05	1.29	FALSE	6.22E-01	1.03	FALSE	3.63E-01	0.95	FALSE	1.47E-01	1.20	FALSE
M204T484_neg	204.1242	484	3	7.41E-01	0.96	FALSE	9.87E-01	1.00	FALSE	5.95E-02	1.25	FALSE	7.66E-02	0.42	FALSE
M204T163_neg	204.1242	163	3	2.53E-06	1.41	FALSE	4.55E-01	1.06	FALSE	1.91E-02	1.16	FALSE	4.84E-01	1.10	FALSE
M206T401_neg	206.0569	401	3	7.17E-02	0.87	FALSE	8.34E-01	1.02	FALSE	4.09E-05	1.34	FALSE	1.87E-02	1.27	FALSE
M206T369_neg	206.0823	369	3	6.38E-12	1.31	FALSE	8.86E-03	1.10	FALSE	1.52E-10	1.24	FALSE	9.40E-02	1.12	FALSE
M206T624_neg	206.0823	624	3	6.86E-15	1.45	FALSE	8.06E-03	1.13	FALSE	3.33E-02	1.09	FALSE	1.30E-01	1.16	FALSE
M207T475_neg	207.0873	475	3	2.91E-08	1.19	FALSE	2.58E-01	0.96	FALSE	1.85E-05	1.12	FALSE	7.79E-01	1.02	FALSE
M207T573_neg	207.0887	573	3	5.14E-01	1.05	FALSE	8.80E-01	1.01	FALSE	2.78E-05	1.34	FALSE	2.65E-02	0.72	FALSE
M207T487_neg	207.1140	487	3	7.20E-07	1.45	FALSE	5.09E-01	1.05	FALSE	1.65E-01	1.09	FALSE	3.73E-01	1.14	FALSE
M207T905_neg	207.1391	905	3	6.96E-05	1.10	FALSE	7.14E-01	0.99	FALSE	6.82E-18	0.82	FALSE	6.26E-01	0.98	FALSE
M208T649_neg	208.0616	649	3	1.19E-08	1.29	FALSE	2.38E-03	0.87	FALSE	6.24E-08	1.23	FALSE	2.05E-01	1.11	FALSE
M208T758_neg	208.0980	758	3	2.08E-02	0.92	FALSE	3.99E-02	1.08	FALSE	1.15E-03	1.11	FALSE	9.96E-01	1.00	FALSE
M209T656_neg	209.0820	656	3	7.27E-04	1.41	FALSE	8.37E-01	0.98	FALSE	1.86E-01	1.12	FALSE	8.63E-01	0.98	FALSE
M209T541_neg	209.0821	541	3	1.21E-13	1.48	FALSE	3.61E-01	1.05	FALSE	1.09E-07	1.27	FALSE	1.60E-01	1.13	FALSE
M209T904_neg	209.0949	904	3	2.44E-01	1.04	FALSE	9.23E-01	1.00	FALSE	2.38E-01	0.97	FALSE	4.96E-01	1.08	FALSE
M209T744_neg	209.1184	744	3	2.66E-03	1.19	FALSE	8.39E-01	1.01	FALSE	3.16E-01	1.05	FALSE	2.54E-01	1.13	FALSE
M210T782_neg	210.0774	782	3	3.63E-01	0.93	FALSE	2.03E-01	1.11	FALSE	3.41E-01	1.07	FALSE	5.50E-01	0.94	FALSE
M210T597_neg	210.0773	597	3	2.97E-03	1.20	FALSE	7.82E-01	1.02	FALSE	1.63E-11	1.47	FALSE	4.38E-01	1.11	FALSE
M210T723_neg	210.1136	723	3	7.64E-01	0.98	FALSE	8.55E-08	1.41	FALSE	3.24E-03	1.17	FALSE	1.63E-01	0.84	FALSE
M211T642_neg	211.0815	642	3	5.83E-01	0.92	FALSE	8.40E-01	0.97	FALSE	8.25E-02	0.78	FALSE	2.38E-01	1.64	FALSE
M211T893_neg	211.1340	893	3	4.03E-07	0.70	FALSE	1.35E-02	0.84	FALSE	1.83E-09	0.68	FALSE	1.65E-01	1.11	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M212T410_neg	212.0756	410	3							HMDB0032418	4-Methyl-5-thiazolyl)ethyl butano	C10H15NO2S	2.5
M213T471_neg	213.0349	471	3							HMDB0246327	4-Acetamidobenzenesulfonamide	C8H10N2O3S	4.4
M213T721_neg	213.0924	721	3							HMDB0012111	-(1R,2R)-1,2-Diphenylethane-1,2-d	C14H14O2	1.3
M213T550_neg	213.1134	550	3							HMDB0030984	ltetrahydro-2-oxo-3-furancarboxy	C11H18O4	0.6
M213T811_neg	213.1133	811	3							HMDB0030984	ltetrahydro-2-oxo-3-furancarboxy	C11H18O4	0.1
M213T1047_neg	213.1860	1047	3							HMDB0000910	Tridecanoic acid	C13H26O2	0.2
M214T675_neg	214.1086	675	3							HMDB0013124	Propenoylcarnitine	C10H17NO4	0.4
M214T563_neg	214.1086	563	3							HMDB0013124	Propenoylcarnitine	C10H17NO4	0.3
M214T515_neg	214.1086	515	3							HMDB0013124	Propenoylcarnitine	C10H17NO4	0.4
M215T361_neg	215.1402	361	3						Amino acids and Peptides	HMDB0029140	Valylvaline	C10H20N2O3	0.5
M215T531_neg	215.1402	531	3							HMDB0029140	Valylvaline	C10H20N2O3	0.4
M216T354_neg	216.0699	354	3							HMDB0015328	Captopril	C9H15NO3S	0.5
M216T557_neg	216.0701	557	3							HMDB0247169	Mercapto-2-methyl-1-oxopropyl)-L	C9H15NO3S	0.6
M216T659_neg	216.1243	659	3							HMDB0240784	O-Propanoyl-D-carnitine	C10H19NO4	0.6
M217T384_neg	217.1085	384	3							HMDB0000350	3-Hydroxysebacic acid	C10H18O5	1.5
M217T699_neg	217.1446	699	3							HMDB0254850	2,3-Dihydroxypropyl octanoate	C11H22O4	0.1
M219T475_neg	219.0875	475	3							HMDB0242729	2-O-Isopropylidene-D-glucofurano	C9H16O6	0.2
M220T667_neg	220.0979	667	3							HMDB0014798	Metaxalone	C12H15NO3	0.0
M220T467_neg	220.1344	467	3							HMDB0030305	Dioscorine	C13H19NO2	0.3
M221T539_neg	221.1030	539	3							HMDB0032705	Isopropyl beta-D-glucoside	C9H18O6	0.2
M221T865_neg	221.1183	865	3							HMDB0032121	Annuionone B	C13H18O3	0.1
M221T390_neg	221.1297	390	3							HMDB0060678	-Hydroxymonoethylglycinexylidid	C12H18N2O2	0.7
M222T459_neg	222.0773	459	3							HMDB0000866	N-Acetyl-L-tyrosine	C11H13NO4	0.3
M223T772_neg	223.0975	772	3							HMDB0030680	Diplosporin	C12H16O4	0.3
M223T644_neg	223.1088	644	3							HMDB0014386	Butalbital	C11H16N2O3	0.3
M223T491_neg	223.1089	491	3							HMDB0014386	Butalbital	C11H16N2O3	0.2
M223T449_neg	223.1090	449	3							HMDB0014386	Butalbital	C11H16N2O3	1.0
M224T737_neg	224.0120	737	3						Alkaloids				
M224T660_neg	224.0566	660	3							HMDB0037264	-4,7-dimethoxy-2H-1,4-benzoxazin	C10H11NO5	0.6
M224T505_neg	224.1042	505	3							HMDB0041953	Nnal-N-oxide	C10H15N3O3	0.4
M225T736_neg	225.0144	736	3							HMDB0243907	1-Iodoheptane	C7H15I	0.6
M225T697_neg	225.0409	697	3							HMDB0012199	Chorismate	C10H10O6	2.1
M225T834_neg	225.1132	834	3							HMDB0040705	Allixin	C12H18O4	0.1
M226T504_neg	226.0180	504	3							HMDB0304937	6-Hydroxyindoxyl sulfate	C9H9NO4S	0.3
M226T674_neg	226.0830	674	3							HMDB0000014	Deoxycytidine	C9H13N3O4	1.5

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M212T410_neg	212.0756	410	3	1.93E-03	0.73	FALSE	2.05E-01	1.14	FALSE	1.69E-05	1.46	FALSE	3.88E-01	1.21	FALSE
M213T471_neg	213.0349	471	3	9.01E-05	1.44	FALSE	7.00E-01	1.04	FALSE	1.83E-03	1.28	FALSE	2.41E-01	0.66	FALSE
M213T721_neg	213.0924	721	3	1.81E-03	0.82	FALSE	7.20E-01	1.02	FALSE	7.44E-07	1.31	FALSE	3.42E-02	1.25	FALSE
M213T550_neg	213.1134	550	3	1.98E-03	1.23	FALSE	2.44E-01	0.92	FALSE	2.14E-02	1.14	FALSE	6.03E-02	0.76	FALSE
M213T811_neg	213.1133	811	3	3.78E-04	1.47	FALSE	7.61E-01	0.97	FALSE	7.89E-01	1.02	FALSE	7.86E-01	0.94	FALSE
M213T1047_neg	213.1860	1047	3	9.20E-02	0.85	FALSE	9.75E-01	1.00	FALSE	7.57E-01	1.03	FALSE	8.78E-01	0.96	FALSE
M214T675_neg	214.1086	675	3	2.01E-01	1.34	FALSE	1.62E-01	0.73	FALSE	5.59E-01	0.89	FALSE	7.50E-01	1.05	FALSE
M214T563_neg	214.1086	563	3	2.78E-06	1.27	FALSE	8.28E-01	0.99	FALSE	2.66E-03	1.14	FALSE	5.51E-01	0.92	FALSE
M214T515_neg	214.1086	515	3	1.13E-21	1.39	FALSE	6.24E-01	1.02	FALSE	1.59E-03	1.09	FALSE	5.00E-01	0.97	FALSE
M215T361_neg	215.1402	361	3	1.80E-13	1.42	FALSE	1.80E-03	1.16	FALSE	6.80E-16	1.41	FALSE	8.48E-01	1.01	FALSE
M215T531_neg	215.1402	531	3	9.33E-02	0.90	FALSE	8.38E-01	1.01	FALSE	7.84E-02	1.10	FALSE	3.99E-01	1.15	FALSE
M216T354_neg	216.0699	354	3	3.95E-03	1.34	FALSE	6.06E-01	0.95	FALSE	7.76E-01	1.02	FALSE	2.32E-01	1.14	FALSE
M216T557_neg	216.0701	557	3	9.19E-01	0.99	FALSE	3.99E-01	0.92	FALSE	1.41E-04	1.39	FALSE	1.25E-01	0.65	FALSE
M216T659_neg	216.1243	659	3	2.43E-08	1.19	FALSE	5.82E-01	0.98	FALSE	8.33E-08	0.87	FALSE	7.80E-01	1.02	FALSE
M217T384_neg	217.1085	384	3	1.76E-02	0.87	FALSE	5.44E-01	0.96	FALSE	9.81E-06	1.27	FALSE	6.93E-02	0.74	FALSE
M217T699_neg	217.1446	699	3	2.21E-01	0.93	FALSE	9.24E-01	1.01	FALSE	6.71E-03	1.14	FALSE	1.42E-01	0.78	FALSE
M219T475_neg	219.0875	475	3	1.62E-01	1.17	FALSE	2.20E-01	1.15	FALSE	6.74E-02	0.84	FALSE	1.12E-01	0.35	FALSE
M220T667_neg	220.0979	667	3	1.72E-01	0.92	FALSE	2.30E-10	1.47	FALSE	1.95E-09	1.38	FALSE	2.31E-01	1.09	FALSE
M220T467_neg	220.1344	467	3	1.43E-04	1.35	FALSE	7.02E-01	0.97	FALSE	1.69E-01	1.10	FALSE	4.71E-01	0.95	FALSE
M221T539_neg	221.1030	539	3	9.28E-01	1.01	FALSE	7.21E-01	1.02	FALSE	5.59E-08	1.38	FALSE	5.47E-01	0.86	FALSE
M221T865_neg	221.1183	865	3	3.23E-14	1.18	FALSE	7.63E-02	0.96	FALSE	3.79E-06	0.92	FALSE	4.63E-01	0.96	FALSE
M221T390_neg	221.1297	390	3	4.97E-03	1.18	FALSE	5.38E-01	1.04	FALSE	4.43E-09	1.37	FALSE	7.27E-01	0.96	FALSE
M222T459_neg	222.0773	459	3	2.59E-02	0.88	FALSE	7.94E-01	0.98	FALSE	2.39E-07	1.30	FALSE	1.06E-03	0.67	FALSE
M223T772_neg	223.0975	772	3	9.37E-02	1.11	FALSE	2.36E-02	1.16	FALSE	2.02E-01	1.07	FALSE	6.62E-01	1.05	FALSE
M223T644_neg	223.1088	644	3	2.40E-01	1.05	FALSE	6.12E-06	1.21	FALSE	4.98E-17	1.40	FALSE	6.84E-01	1.02	FALSE
M223T491_neg	223.1089	491	3	8.36E-22	1.41	FALSE	2.08E-01	1.04	FALSE	4.90E-04	1.10	FALSE	6.36E-01	0.98	FALSE
M223T449_neg	223.1090	449	3	2.22E-05	1.19	FALSE	2.81E-01	1.05	FALSE	4.92E-11	1.28	FALSE	3.51E-01	1.04	FALSE
M224T737_neg	224.0120	737	3	8.72E-01	1.03	FALSE	5.52E-02	1.41	FALSE	6.15E-01	1.08	FALSE	3.55E-01	1.20	FALSE
M224T660_neg	224.0566	660	3	2.79E-01	1.10	FALSE	1.45E-01	1.14	FALSE	7.15E-01	1.03	FALSE	3.91E-01	1.16	FALSE
M224T505_neg	224.1042	505	3	2.97E-01	1.08	FALSE	6.98E-01	1.03	FALSE	2.06E-02	1.15	FALSE	2.62E-02	1.38	FALSE
M225T736_neg	225.0144	736	3	3.90E-02	1.44	FALSE	6.64E-02	1.39	FALSE	7.09E-02	0.76	FALSE	9.06E-01	1.03	FALSE
M225T697_neg	225.0409	697	3	3.60E-01	0.93	FALSE	5.43E-01	0.95	FALSE	7.75E-04	1.25	FALSE	3.15E-01	0.84	FALSE
M225T834_neg	225.1132	834	3	6.54E-03	0.87	FALSE	1.60E-01	1.08	FALSE	3.65E-15	1.49	FALSE	1.20E-01	0.76	FALSE
M226T504_neg	226.0180	504	3	3.02E-03	1.26	FALSE	2.66E-02	1.19	FALSE	9.28E-07	1.40	FALSE	1.15E-01	1.11	FALSE
M226T674_neg	226.0830	674	3	7.73E-01	1.02	FALSE	6.39E-02	1.13	FALSE	7.51E-02	1.10	FALSE	6.30E-01	1.09	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M227T803_neg	227.0714	803	3							HMDB0015497	Oxybenzone	C14H12O3	0.2
M227T933_neg	227.1653	933	3							HMDB0035881	11-Hydroxy-9-tridecenoic acid	C13H24O3	0.0
M228T371_neg	228.0990	371	3							HMDB0028739	Asparaginyl-Proline	C9H15N3O4	0.1
M228T408_neg	228.1243	408	3							HMDB0013126	Butenylcarnitine	C11H19NO4	0.6
M229T454_1_neg	229.0826	454	3							HMDB0002335	Aspartyl-L-proline	C9H14N2O5	1.6
M229T454_2_neg	229.1195	454	3							HMDB0028876	Hydroxyprolyl-Valine	C10H18N2O4	0.6
M229T667_neg	229.1352	667	3							HMDB0015614	Ibudilast	C14H18N2O	2.2
M229T1011_neg	229.1809	1011	3							HMDB0036133	-(1-methylethyl)cyclohexyl]oxy]-1	C13H26O3	0.1
M230T615_neg	230.0855	615	3							HMDB0257407	-(2-methyl-3-(methylthio)-1-oxop	C10H17NO3S	0.6
M230T493_neg	230.1399	493	3							HMDB0002013	Butyrylcarnitine	C11H21NO4	0.7
M230T727_neg	230.1405	727	3							HMDB0247129	thoxy-2-(piperazin-1-yl)quinazolin	C12H17N5	2.9
M231T500_neg	231.1351	500	3							HMDB0013075	Spermic acid 2	C10H20N2O4	0.1
M232T803_neg	232.0439	803	3							HMDB0038592	Brassicanal B	C12H11NO2S	0.4
M233T973_neg	233.1547	973	3							HMDB0030016	Valerenic acid	C15H22O2	0.1
M234T530_neg	234.0810	530	3							HMDB0249714	Cbhcy	C9H17NO4S	2.0
M234T696_neg	234.1136	696	3							HMDB0033610	Pandamarilactam 3x	C13H17NO3	0.1
M235T519_neg	235.0721	519	3							HMDB0001200	N2-Succinyl-L-ornithine	C11H12N2O4	1.3
M235T879_neg	235.0977	879	3							HMDB0037683	Ethyl vanillin isobutyrate	C13H16O4	0.4
M235T448_neg	235.1453	448	3							HMDB0014859	Procaine	C13H20N2O2	0.4
M236T570_neg	236.0567	570	3							HMDB0034251	N-Benzoylaspartic acid	C11H11NO5	0.9
M236T581_neg	236.0929	581	3							HMDB0013067	Salsoline-1-carboxylate	C12H15NO4	0.1
M237T764_neg	237.1133	764	3							HMDB0033191	methyl-6-(1-oxopropyl)-1,3,5-cyclo	C13H18O4	0.3
M237T563_neg	237.1246	563	3							HMDB0014562	Secobarbital	C12H18N2O3	0.4
M237T393_neg	237.1342	393	3							HMDB0256256	Pentaethylene glycol	C10H22O6	0.7
M237T840_neg	237.1496	840	3							HMDB0038256	Geranyl acetoacetate	C14H22O3	0.1
M239T755_neg	239.0596	755	3							HMDB0033071	ppyl 1-(propylsulfinyl)propyl disulfi	C9H20OS3	3.2
M239T1031_neg	239.0596	1031	3							HMDB0033071	ppyl 1-(propylsulfinyl)propyl disulfi	C9H20OS3	3.1
M239T914_neg	239.0597	914	3							HMDB0033071	ppyl 1-(propylsulfinyl)propyl disulfi	C9H20OS3	2.6
M239T772_neg	239.0925	772	3							HMDB0030254	,4,5-Trimethoxyphenyl)propanoic	C12H16O5	0.1
M239T1062_neg	239.2017	1062	3							HMDB0029765	9-Pentadecenoic acid	C15H28O2	0.2
M240T363_neg	240.0879	363	3							HMDB0014567	Methocarbamol	C11H15NO5	0.7
M240T691_neg	240.0878	691	3							HMDB0014567	Methocarbamol	C11H15NO5	0.3
M241T782_neg	241.0508	782	3							HMDB0032040	Benzoyl peroxide	C14H10O4	0.8
M241T851_neg	241.0507	851	3							HMDB0032040	Benzoyl peroxide	C14H10O4	0.4
M241T743_neg	241.0870	743	3							HMDB0002209	Equol	C15H14O3	0.0

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M227T803_neg	227.0714	803	3	9.73E-03	1.23	FALSE	4.31E-01	0.94	FALSE	1.16E-02	0.84	FALSE	8.30E-01	0.93	FALSE
M227T933_neg	227.1653	933	3	1.87E-05	1.22	FALSE	8.78E-03	0.88	FALSE	6.53E-03	0.90	FALSE	4.21E-01	1.07	FALSE
M228T371_neg	228.0990	371	3	2.61E-01	1.08	FALSE	1.48E-01	1.10	FALSE	3.66E-05	1.27	FALSE	6.12E-01	0.95	FALSE
M228T408_neg	228.1243	408	3	5.25E-01	1.04	FALSE	2.26E-01	1.09	FALSE	3.76E-07	1.36	FALSE	8.04E-01	0.96	FALSE
M229T454_1_neg	229.0826	454	3	5.03E-01	0.95	FALSE	1.69E-01	1.11	FALSE	1.36E-07	1.40	FALSE	8.29E-01	1.02	FALSE
M229T454_2_neg	229.1195	454	3	4.12E-05	1.22	FALSE	5.48E-01	1.03	FALSE	8.82E-01	1.01	FALSE	9.81E-01	1.00	FALSE
M229T667_neg	229.1352	667	3	7.42E-02	1.23	FALSE	5.19E-01	0.93	FALSE	1.98E-01	0.88	FALSE	5.28E-01	1.21	FALSE
M229T1011_neg	229.1809	1011	3	2.03E-01	1.29	FALSE	5.84E-02	0.68	FALSE	8.91E-01	0.98	FALSE	9.13E-01	1.07	FALSE
M230T615_neg	230.0855	615	3	4.50E-01	1.06	FALSE	3.55E-02	1.20	FALSE	1.82E-05	1.38	FALSE	4.15E-01	0.84	FALSE
M230T493_neg	230.1399	493	3	7.64E-04	0.76	FALSE	4.23E-01	1.07	FALSE	4.11E-06	1.38	FALSE	8.04E-01	1.04	FALSE
M230T727_neg	230.1405	727	3	1.14E-02	0.84	FALSE	5.98E-01	0.96	FALSE	2.40E-06	0.75	FALSE	7.29E-01	1.04	FALSE
M231T500_neg	231.1351	500	3	2.36E-02	0.84	FALSE	7.86E-01	0.98	FALSE	1.09E-01	1.11	FALSE	7.97E-01	1.04	FALSE
M232T803_neg	232.0439	803	3	1.07E-09	1.27	FALSE	7.04E-01	0.99	FALSE	1.69E-21	0.70	FALSE	4.48E-01	0.95	FALSE
M233T973_neg	233.1547	973	3	1.64E-06	0.80	FALSE	9.40E-03	1.13	FALSE	1.93E-07	0.81	FALSE	4.86E-01	0.96	FALSE
M234T530_neg	234.0810	530	3	6.91E-01	0.97	FALSE	3.84E-01	0.93	FALSE	9.46E-05	1.31	FALSE	7.37E-01	0.97	FALSE
M234T696_neg	234.1136	696	3	3.85E-02	1.20	FALSE	4.78E-01	1.07	FALSE	3.87E-02	1.17	FALSE	3.77E-02	0.70	FALSE
M235T519_neg	235.0721	519	3	2.08E-04	1.21	FALSE	9.53E-01	1.00	FALSE	2.84E-09	1.31	FALSE	3.48E-01	0.93	FALSE
M235T879_neg	235.0977	879	3	6.34E-01	0.98	FALSE	3.77E-01	1.04	FALSE	3.29E-03	0.89	FALSE	6.59E-01	1.06	FALSE
M235T448_neg	235.1453	448	3	8.64E-02	0.86	FALSE	4.95E-01	0.94	FALSE	5.17E-03	1.24	FALSE	4.21E-01	1.19	FALSE
M236T570_neg	236.0567	570	3	1.25E-06	1.28	FALSE	7.14E-01	1.02	FALSE	1.87E-08	1.29	FALSE	2.66E-01	1.11	FALSE
M236T581_neg	236.0929	581	3	1.44E-01	1.11	FALSE	1.96E-02	1.19	FALSE	9.65E-07	1.36	FALSE	5.00E-02	1.26	FALSE
M237T764_neg	237.1133	764	3	9.11E-07	1.21	FALSE	2.80E-01	1.04	FALSE	6.76E-06	1.16	FALSE	3.15E-01	1.11	FALSE
M237T563_neg	237.1246	563	3	1.51E-14	1.50	FALSE	6.62E-01	0.98	FALSE	8.06E-01	1.01	FALSE	3.24E-01	0.93	FALSE
M237T393_neg	237.1342	393	3	2.36E-02	0.69	FALSE	6.16E-01	0.92	FALSE	9.86E-01	1.00	FALSE	1.92E-01	0.67	FALSE
M237T840_neg	237.1496	840	3	4.38E-02	1.08	FALSE	4.96E-02	0.92	FALSE	2.74E-01	0.96	FALSE	2.07E-01	0.89	FALSE
M239T755_neg	239.0596	755	3	2.75E-02	1.19	FALSE	2.66E-01	1.09	FALSE	8.88E-01	1.01	FALSE	3.93E-02	1.40	FALSE
M239T1031_neg	239.0596	1031	3	1.26E-06	0.70	FALSE	5.32E-02	1.16	FALSE	1.21E-01	0.91	FALSE	9.00E-01	1.03	FALSE
M239T914_neg	239.0597	914	3	2.71E-01	1.08	FALSE	4.51E-01	1.06	FALSE	7.14E-01	0.98	FALSE	1.98E-01	1.38	FALSE
M239T772_neg	239.0925	772	3	2.89E-06	1.21	FALSE	8.26E-01	1.01	FALSE	3.83E-04	1.13	FALSE	8.43E-01	1.03	FALSE
M239T1062_neg	239.2017	1062	3	4.55E-02	0.77	FALSE	4.36E-01	0.90	FALSE	9.24E-02	1.21	FALSE	1.89E-01	1.37	FALSE
M240T363_neg	240.0879	363	3	8.72E-02	0.94	FALSE	6.76E-01	1.02	FALSE	5.92E-18	1.33	FALSE	1.79E-02	1.15	FALSE
M240T691_neg	240.0878	691	3	1.95E-03	0.79	FALSE	8.75E-01	1.01	FALSE	3.03E-07	1.41	FALSE	6.83E-02	1.26	FALSE
M241T782_neg	241.0508	782	3	1.34E-02	1.17	FALSE	5.35E-01	0.96	FALSE	4.57E-01	1.04	FALSE	8.01E-01	1.05	FALSE
M241T851_neg	241.0507	851	3	5.01E-04	1.22	FALSE	9.65E-02	0.91	FALSE	4.07E-14	0.67	FALSE	3.26E-01	0.91	FALSE
M241T743_neg	241.0870	743	3	1.16E-04	0.76	FALSE	4.08E-01	1.06	FALSE	5.93E-05	1.29	FALSE	1.98E-01	1.10	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M241T726_neg	241.1445	726	3						Fatty acids	HMDB0030987	2-Carboxy-4-dodecanolide	C13H22O4	0.0
M243T732_neg	243.1238	732	3							HMDB0032472	Polyethylene, oxidized	C12H20O5	0.1
M243T404_neg	243.1461	404	3							HMDB0252056	Ethyl N2-acetyl-L-argininate	C10H20N4O3	0.5
M244T785_neg	244.1561	785	3							HMDB0000378	2-Methylbutyroylcarnitine	C12H23NO4	2.7
M245T908_neg	245.1394	908	3						Fatty acids	HMDB0000413	3-Hydroxydodecanedioic acid	C12H22O5	0.1
M246T468_neg	246.0983	468	3							HMDB0002095	Malonylcarnitine	C10H17NO6	0.0
M246T523_neg	246.0989	523	3							HMDB0002095	Malonylcarnitine	C10H17NO6	2.3
M246T514_neg	246.1348	514	3							HMDB0013127	3-Hydroxybutyrylcarnitine	C11H21NO5	0.3
M247T362_neg	247.1091	362	3							HMDB0004081	6-Hydroxymelatonin	C13H16N2O3	1.1
M247T517_neg	247.1187	517	3							HMDB0031876	Prenyl glucoside	C11H20O6	0.0
M248T177_neg	248.0401	177	3							HMDB0258136	nino-3-carboxypropanoyl]oxybuta	C8H11NO8	4.3
M248T691_neg	248.0928	691	3						Amino acids and Peptides				
M248T620_neg	248.0929	620	3						Amino acids and Peptides				
M249T845_neg	249.0322	845	3							HMDB0251449	Diphenyl phosphate	C12H11O4P	0.0
M249T950_neg	249.1132	950	3							HMDB0002012	Ubiquinone-1	C14H18O4	0.1
M249T393_neg	249.1341	393	3							HMDB0034750	Isopentyl beta-D-glucoside	C11H22O6	1.0
M251T757_neg	251.1029	757	3							HMDB0013940	N-Desmethylpromazine	C12H16N2O4	3.3
M251T565_neg	251.0961	565	3							HMDB0247351	yl-3-(pyridine-4-carbonylamino)thi	C11H16N4OS	4.6
M251T456_neg	251.0965	456	3							HMDB0247351	yl-3-(pyridine-4-carbonylamino)thi	C11H16N4OS	2.7
M251T519_neg	251.1131	519	3							HMDB0040822	2,3-Butanediol glucoside	C10H20O7	1.9
M252T674_neg	252.0337	674	3							HMDB0250934	Deferitrin	C11H11NO4S	0.2
M252T880_neg	252.1606	880	3							HMDB0244460	,5-Trimethylcyclohexyl ester5-oxo	C14H23NO3	0.2
M253T722_neg	253.0752	722	3							HMDB0255529	Neosalacinol	C9H18O6S	0.2
M253T917_neg	253.1080	917	3							HMDB0032796	3-dihydroxy-3-methylbutyl)-4-hydr	C13H18O5	0.4
M253T836_neg	253.1082	836	3							HMDB0032796	3-dihydroxy-3-methylbutyl)-4-hydr	C13H18O5	0.2
M253T718_neg	253.1447	718	3							HMDB0249518	C75 trans	C14H22O4	0.5
M255T499_neg	255.0985	499	3							HMDB0011648	D-Ribofuranosyl)-1,4-dihydronicot	C11H16N2O5	0.4
M255T719_neg	255.1238	719	3							HMDB0031772	oxy-1-(2,4,5-trimethoxyphenyl)-2-p	C13H20O5	0.0
M256T680_neg	256.0647	680	3							HMDB0040288	lsulfonylmethyl)phenyl methylcarl	C11H15NO4S	0.7
M256T503_neg	256.0650	503	3							HMDB0244399	butyl-1-(2-sulfophenyl)methanimir	C11H15NO4S	0.4
M256T706_neg	256.1554	706	3							HMDB0013161	2-Hexenoylcarnitine	C13H23NO4	0.0
M256T987_neg	256.1924	987	3							HMDB0013272	N-Lauroylglycine	C14H27NO3	2.1
M257T537_neg	257.0609	537	3						Amino acids and Peptides	HMDB0246637	ydroxy-3-phenoxyphenyl)propano	C10H14N2O4S	3.1
M259T497_neg	259.0738	497	3							HMDB0245532	2-Acetylacteoside	C10H13FN2O5	0.9

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M241T726_neg	241.1445	726	3	1.88E-04	1.22	FALSE	9.85E-02	0.91	FALSE	9.96E-01	1.00	FALSE	6.96E-01	0.90	FALSE
M243T732_neg	243.1238	732	3	1.72E-01	1.21	FALSE	2.20E-01	0.84	FALSE	4.70E-01	1.09	FALSE	9.14E-02	0.54	FALSE
M243T404_neg	243.1461	404	3	5.26E-13	1.46	FALSE	7.66E-01	0.98	FALSE	2.37E-09	1.31	FALSE	1.33E-01	1.16	FALSE
M244T785_neg	244.1561	785	3	1.90E-01	1.07	FALSE	8.82E-01	1.01	FALSE	1.68E-10	0.73	FALSE	2.38E-01	0.84	FALSE
M245T908_neg	245.1394	908	3	5.07E-02	0.28	FALSE	6.47E-01	0.75	FALSE	8.93E-02	2.51	FALSE	6.69E-10	-23.69	FALSE
M246T468_neg	246.0983	468	3	6.12E-02	0.76	FALSE	7.75E-01	1.04	FALSE	6.91E-01	0.95	FALSE	8.18E-01	1.04	FALSE
M246T523_neg	246.0989	523	3	7.69E-03	0.84	FALSE	1.47E-03	1.25	FALSE	2.85E-10	1.47	FALSE	4.10E-02	0.76	FALSE
M246T514_neg	246.1348	514	3	9.50E-02	0.92	FALSE	5.11E-02	0.90	FALSE	3.92E-03	1.14	FALSE	7.66E-02	0.77	FALSE
M247T362_neg	247.1091	362	3	3.03E-04	1.24	FALSE	8.22E-01	1.01	FALSE	3.52E-07	1.31	FALSE	6.32E-01	1.05	FALSE
M247T517_neg	247.1187	517	3	1.93E-13	1.46	FALSE	7.80E-01	1.01	FALSE	3.30E-14	1.41	FALSE	4.66E-02	1.12	FALSE
M248T177_neg	248.0401	177	3	1.54E-04	0.68	FALSE	3.63E-01	0.90	FALSE	1.38E-01	1.14	FALSE	4.71E-01	1.19	FALSE
M248T691_neg	248.0928	691	3	6.78E-01	1.03	FALSE	5.60E-01	0.96	FALSE	1.37E-04	1.29	FALSE	3.26E-01	0.83	FALSE
M248T620_neg	248.0929	620	3	1.72E-03	1.23	FALSE	8.14E-01	1.02	FALSE	1.17E-06	1.33	FALSE	3.01E-01	0.86	FALSE
M249T845_neg	249.0322	845	3	4.46E-01	0.96	FALSE	2.69E-02	0.89	FALSE	1.19E-03	0.86	FALSE	7.06E-01	0.92	FALSE
M249T950_neg	249.1132	950	3	4.67E-02	0.93	FALSE	5.18E-01	0.98	FALSE	1.52E-01	0.96	FALSE	7.23E-02	1.09	FALSE
M249T393_neg	249.1341	393	3	1.38E-01	1.13	FALSE	4.04E-01	0.93	FALSE	7.48E-02	1.14	FALSE	4.32E-01	0.88	FALSE
M251T757_neg	251.1029	757	3	1.30E-03	1.33	FALSE	6.66E-02	1.18	FALSE	1.49E-02	1.21	FALSE	8.07E-01	1.09	FALSE
M251T565_neg	251.0961	565	3	1.12E-09	1.44	FALSE	3.27E-02	1.13	FALSE	1.50E-05	1.24	FALSE	1.40E-01	1.15	FALSE
M251T456_neg	251.0965	456	3	2.86E-01	1.07	FALSE	2.87E-02	1.15	FALSE	1.02E-04	1.24	FALSE	2.08E-01	0.92	FALSE
M251T519_neg	251.1131	519	3	2.05E-08	1.29	FALSE	7.62E-01	0.99	FALSE	8.88E-01	0.99	FALSE	4.12E-01	1.05	FALSE
M252T674_neg	252.0337	674	3	2.07E-01	0.95	FALSE	9.22E-01	1.00	FALSE	2.37E-18	1.46	FALSE	1.80E-01	1.17	FALSE
M252T880_neg	252.1606	880	3	5.06E-04	1.44	FALSE	9.44E-03	1.32	FALSE	1.16E-01	1.15	FALSE	1.35E-01	1.24	FALSE
M253T722_neg	253.0752	722	3	1.96E-01	1.12	FALSE	8.70E-01	1.01	FALSE	5.15E-04	1.30	FALSE	2.91E-01	1.20	FALSE
M253T917_neg	253.1080	917	3	9.01E-01	0.99	FALSE	2.96E-02	0.87	FALSE	3.78E-01	1.05	FALSE	8.94E-01	1.01	FALSE
M253T836_neg	253.1082	836	3	1.09E-08	0.75	FALSE	2.93E-04	1.19	FALSE	1.27E-06	1.23	FALSE	3.16E-01	1.08	FALSE
M253T718_neg	253.1447	718	3	1.73E-11	1.36	FALSE	3.54E-01	0.96	FALSE	4.35E-10	0.78	FALSE	1.97E-01	0.85	FALSE
M255T499_neg	255.0985	499	3	4.75E-01	1.05	FALSE	7.21E-01	1.02	FALSE	5.40E-07	1.33	FALSE	3.60E-02	1.20	FALSE
M255T719_neg	255.1238	719	3	4.38E-01	1.10	FALSE	5.94E-01	0.93	FALSE	5.04E-01	1.07	FALSE	3.23E-01	0.86	FALSE
M256T680_neg	256.0647	680	3	4.13E-02	0.91	FALSE	7.21E-04	1.18	FALSE	3.53E-07	1.24	FALSE	6.52E-01	0.95	FALSE
M256T503_neg	256.0650	503	3	3.51E-01	1.09	FALSE	5.38E-01	0.94	FALSE	4.98E-04	1.32	FALSE	3.61E-01	0.76	FALSE
M256T706_neg	256.1554	706	3	2.55E-09	1.33	FALSE	4.94E-01	0.97	FALSE	1.28E-01	1.06	FALSE	6.08E-02	0.84	FALSE
M256T987_neg	256.1924	987	3	5.31E-02	1.70	FALSE	9.42E-01	1.02	FALSE	2.34E-01	1.32	FALSE	6.77E-01	1.20	FALSE
M257T537_neg	257.0609	537	3	1.81E-01	1.08	FALSE	7.58E-01	1.02	FALSE	1.38E-12	1.44	FALSE	3.19E-01	0.89	FALSE
M259T497_neg	259.0738	497	3	6.95E-02	0.80	FALSE	8.79E-01	1.02	FALSE	9.26E-01	0.99	FALSE	7.18E-01	0.92	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M259T629_neg	259.0978	629	3							HMDB0030110	Celerin	C15H16O4	1.0
M259T712_neg	259.0985	712	3							HMDB0030110	Celerin	C15H16O4	3.4
M259T678_neg	259.1454	678	3							HMDB0033481	Baptifoline	C15H20N2O2	0.6
M259T830_neg	259.1817	830	3							HMDB0014413	Ropinirole	C16H24N2O	0.4
M260T485_neg	260.1141	485	3							HMDB0033865	Lotaustralin	C11H19NO6	0.6
M260T654_neg	260.1505	654	3							HMDB0061189	3-Hydroxyisovalerylcarnitine	C12H23NO5	0.5
M261T689_neg	261.1032	689	3							HMDB0247598	9-Hydroxyellipticine	C17H14N2O	0.6
M261T467_neg	261.1455	467	3							HMDB0241810	-Amino-3-hydroxybutanoylcarnitin	C11H22N2O5	0.5
M262T665_neg	262.1113	665	3							HMDB0249267	Didesethyl Chloroquine	C14H18ClN3	1.3
M262T723_neg	262.1446	723	3							HMDB0032305	n-4-yl)benzo[d][1,3]dioxole-5-carb	C15H21NO3	0.8
M262T680_neg	262.1449	680	3							HMDB0032305	n-4-yl)benzo[d][1,3]dioxole-5-carb	C15H21NO3	0.0
M263T754_neg	263.0925	754	3							HMDB0036544	Heliantriol A1	C14H16O5	0.0
M263T861_neg	263.1289	861	3							HMDB0001931	gamma-CEHC	C15H20O4	0.1
M263T903_neg	263.1288	903	3							HMDB0001931	gamma-CEHC	C15H20O4	0.3
M264T765_neg	264.1243	765	3							HMDB0243530	diol, 2-(p-methoxybenzyl)-, 3-aceta	C14H19NO4	0.5
M265T384_neg	265.0841	384	3							HMDB0255007	N-(4-Aminobenzoyl)-L-glutamic aci	C12H14N2O5	4.1
M265T741_neg	265.1081	741	3							HMDB0040891	bis(4-hydroxyphenyl)-1,4,6-heptat	C14H18O5	0.1
M265T670_neg	265.1063	670	3							HMDB0246876	beta-Pregnane-3alpha,20alpha-dio	C10H14N6O3	3.0
M265T666_neg	265.1193	666	3							HMDB0029005	Phenylalanylthreonine	C13H18N2O4	0.4
M266T502_neg	266.1510	502	3							HMDB0249665	Carbuterol	C13H21N3O3	0.1
M267T622_neg	267.0874	622	3							HMDB0245694	-O-Benzylidene-alpha-D-glucopyra	C13H16O6	0.0
M267T922_neg	267.1601	922	3							HMDB0036150	4,11,13,15-Tetrahydroridentin B	C15H24O4	0.3
M269T632_neg	269.0607	632	3							HMDB0240217	3-(Cystein-S-yl)acetaminophen	C11H14N2O4S	1.9
M269T640_neg	269.1031	640	3							HMDB0243491	-(Hydroxymethyl)-6-phenylmethox	C13H18O6	0.0
M269T431_neg	269.1252	431	3							HMDB0254886	Morinidazole	C11H18N4O4	1.4
M269T727_neg	269.1758	727	3							HMDB0040459	Ethylene brassylate	C15H26O4	0.1
M269T1001_neg	269.2122	1001	3							HMDB0010733	3-Oxohexadecanoic acid	C16H30O3	0.0
M270T467_neg	270.0475	467	3							HMDB0259510	Methyl-D-glucamine dithiocarbam	C8H17NO5S2	0.2
M271T714_neg	271.0979	714	3							HMDB0004810	5C-aglycone	C16H16O4	1.0
M272T874_neg	272.1870	874	3							HMDB0013238	Heptanoylcarnitine	C14H27NO4	1.0
M273T84_neg	272.9589	84	3							HMDB0012285	Ribose-1-arsenate	C5H11AsO8	3.1
M273T763_1_neg	273.0769	763	3							HMDB0003306	Phloretin	C15H14O5	0.3
M273T562_neg	273.1246	562	3							HMDB0034885	Imazamethabenz	C15H18N2O3	0.7
M273T763_2_neg	273.1707	763	3						Fatty acids	HMDB0000394	3-Hydroxytetradecanedioic acid	C14H26O5	0.0
M273T826_neg	273.1707	826	3						Fatty acids	HMDB0000394	3-Hydroxytetradecanedioic acid	C14H26O5	0.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M259T629_neg	259.0978	629	3	2.11E-02	1.22	FALSE	6.91E-01	1.04	FALSE	1.35E-06	1.47	FALSE	6.10E-01	1.11	FALSE
M259T712_neg	259.0985	712	3	7.15E-01	1.02	FALSE	6.79E-01	0.98	FALSE	2.29E-10	1.37	FALSE	1.35E-02	0.82	FALSE
M259T678_neg	259.1454	678	3	2.99E-04	1.18	FALSE	1.09E-01	1.08	FALSE	3.29E-15	1.40	FALSE	3.78E-01	0.96	FALSE
M259T830_neg	259.1817	830	3	1.88E-13	0.69	FALSE	1.61E-03	1.16	FALSE	3.66E-10	1.30	FALSE	1.35E-02	1.30	FALSE
M260T485_neg	260.1141	485	3	7.59E-06	0.77	FALSE	2.18E-01	1.07	FALSE	2.80E-13	1.48	FALSE	5.62E-01	0.96	FALSE
M260T654_neg	260.1505	654	3	9.98E-02	1.11	FALSE	1.77E-01	1.10	FALSE	4.08E-03	1.18	FALSE	7.35E-01	0.96	FALSE
M261T689_neg	261.1032	689	3	1.29E-01	1.10	FALSE	5.26E-01	1.04	FALSE	1.53E-10	1.46	FALSE	6.19E-01	1.07	FALSE
M261T467_neg	261.1455	467	3	5.67E-05	1.32	FALSE	2.40E-01	0.92	FALSE	7.06E-02	0.90	FALSE	7.72E-01	1.02	FALSE
M262T665_neg	262.1113	665	3	5.43E-06	1.45	FALSE	6.63E-01	1.04	FALSE	2.46E-03	1.24	FALSE	5.90E-01	1.08	FALSE
M262T723_neg	262.1446	723	3	2.72E-02	1.20	FALSE	1.10E-02	1.25	FALSE	2.21E-03	1.25	FALSE	2.11E-01	1.26	FALSE
M262T680_neg	262.1449	680	3	8.86E-02	1.16	FALSE	4.16E-03	1.31	FALSE	3.61E-02	1.17	FALSE	1.33E-01	1.40	FALSE
M263T754_neg	263.0925	754	3	6.54E-06	1.50	FALSE	8.84E-01	1.01	FALSE	6.48E-02	1.15	FALSE	5.68E-01	1.09	FALSE
M263T861_neg	263.1289	861	3	3.05E-01	1.06	FALSE	9.83E-01	1.00	FALSE	1.41E-01	1.08	FALSE	6.04E-02	1.21	FALSE
M263T903_neg	263.1288	903	3	1.17E-05	0.85	FALSE	5.77E-02	1.08	FALSE	8.69E-22	1.42	FALSE	9.57E-01	1.00	FALSE
M264T765_neg	264.1243	765	3	1.68E-07	1.32	FALSE	5.14E-01	1.04	FALSE	4.60E-01	1.03	FALSE	6.49E-01	1.09	FALSE
M265T384_neg	265.0841	384	3	1.45E-01	1.28	FALSE	9.72E-01	0.99	FALSE	2.80E-01	0.85	FALSE	3.18E-01	1.09	FALSE
M265T741_neg	265.1081	741	3	7.09E-08	1.41	FALSE	2.77E-01	1.07	FALSE	9.39E-01	1.00	FALSE	6.80E-02	1.25	FALSE
M265T670_neg	265.1063	670	3	2.44E-03	1.20	FALSE	4.97E-02	1.13	FALSE	4.51E-02	0.90	FALSE	4.97E-02	1.43	FALSE
M265T666_neg	265.1193	666	3	2.16E-14	1.34	FALSE	9.44E-02	1.06	FALSE	4.70E-06	1.16	FALSE	2.90E-01	1.05	FALSE
M266T502_neg	266.1510	502	3	1.15E-04	1.28	FALSE	6.41E-01	1.03	FALSE	8.15E-01	1.01	FALSE	7.50E-02	0.83	FALSE
M267T622_neg	267.0874	622	3	6.44E-04	1.41	FALSE	4.31E-01	1.09	FALSE	8.09E-01	0.98	FALSE	7.15E-01	0.92	FALSE
M267T922_neg	267.1601	922	3	4.43E-02	0.93	FALSE	9.69E-01	1.00	FALSE	6.40E-07	1.17	FALSE	1.02E-01	0.88	FALSE
M269T632_neg	269.0607	632	3	1.05E-01	1.10	FALSE	6.91E-01	1.02	FALSE	8.63E-05	1.22	FALSE	5.98E-01	1.04	FALSE
M269T640_neg	269.1031	640	3	9.80E-01	1.00	FALSE	8.73E-01	1.01	FALSE	2.43E-06	1.38	FALSE	9.15E-02	0.60	FALSE
M269T431_neg	269.1252	431	3	1.60E-07	1.41	FALSE	4.63E-01	1.05	FALSE	1.45E-02	1.14	FALSE	1.89E-01	1.21	FALSE
M269T727_neg	269.1758	727	3	3.19E-06	1.22	FALSE	8.94E-01	1.01	FALSE	4.40E-01	0.97	FALSE	1.09E-01	1.23	FALSE
M269T1001_neg	269.2122	1001	3	5.06E-02	1.13	FALSE	2.32E-03	0.82	FALSE	5.82E-02	1.11	FALSE	4.37E-01	0.88	FALSE
M270T467_neg	270.0475	467	3	8.76E-01	0.99	FALSE	8.95E-02	1.13	FALSE	9.74E-09	1.34	FALSE	1.91E-03	1.36	FALSE
M271T714_neg	271.0979	714	3	3.83E-03	1.17	FALSE	8.07E-01	1.01	FALSE	4.56E-06	1.24	FALSE	7.60E-01	0.97	FALSE
M272T874_neg	272.1870	874	3	4.47E-02	1.05	FALSE	1.89E-02	0.94	FALSE	9.70E-02	1.04	FALSE	1.60E-01	0.90	FALSE
M273T84_neg	272.9589	84	3	3.37E-01	1.03	FALSE	4.46E-02	1.07	FALSE	8.44E-12	1.23	FALSE	7.01E-05	0.69	FALSE
M273T763_1_neg	273.0769	763	3	1.96E-04	1.20	FALSE	5.82E-02	0.91	FALSE	1.15E-14	1.42	FALSE	6.54E-01	0.95	FALSE
M273T562_neg	273.1246	562	3	1.39E-10	1.33	FALSE	4.89E-01	1.03	FALSE	4.22E-17	1.41	FALSE	9.36E-01	1.00	FALSE
M273T763_2_neg	273.1707	763	3	1.52E-11	1.32	FALSE	1.88E-01	1.06	FALSE	2.75E-01	1.04	FALSE	1.90E-01	0.92	FALSE
M273T826_neg	273.1707	826	3	3.53E-01	0.96	FALSE	1.77E-01	1.07	FALSE	3.11E-06	1.21	FALSE	9.15E-01	0.99	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M274T608_neg	274.1660	608	3							HMDB0013131	3-Hydroxyhexanoylcarnitine	C13H25NO5	0.0
M275T656_neg	275.1039	656	3						Amino acids and Peptides	HMDB0062178	N-lactoyl-Tryptophan	C14H16N2O4	0.6
M275T821_neg	275.1136	821	3						Fatty acids	HMDB0034263	Triethyl citrate	C12H20O7	0.1
M276T1014_neg	276.1607	1014	3							HMDB0036325	Dinorcapsaicin	C16H23NO3	0.7
M277T1030_neg	277.1445	1030	3							HMDB0001518	alpha-CEHC	C16H22O4	0.0
M277T679_neg	277.1559	679	3							HMDB0013243	Leucylphenylalanine	C15H22N2O3	0.4
M278T627_neg	278.1035	627	3							HMDB0032807	Niazirin	C14H17NO5	0.5
M278T512_neg	278.1395	512	3							HMDB0031802	(\xc2\xb1)-Metalaxyl	C15H21NO4	0.9
M278T688_neg	278.1398	688	3							HMDB0031802	(\xc2\xb1)-Metalaxyl	C15H21NO4	0.0
M280T729_neg	280.1300	729	3							HMDB0254196	Lufironil	C13H19N3O4	1.1
M281T575_neg	281.0936	575	3							HMDB0245789	rmethyl)-5,5-diphenylimidazolidine	C16H14N2O3	1.5
M282T898_neg	282.1170	898	3							HMDB0257152	reparixin	C14H21NO3S	0.2
M283T678_neg	283.1551	678	3							HMDB0060593	Alpha-dihydroartemisinin	C15H24O5	0.2
M284T369_neg	284.1252	369	3							HMDB0002171	Glycylprolylhydroxyproline	C12H19N3O5	0.1
M285T698_neg	285.1708	698	3							HMDB0240222	Thonzylamine	C16H22N4O	4.5
M285T838_neg	285.1708	838	3						Fatty acids	HMDB0240222	Thonzylamine	C16H22N4O	4.7
M285T890_neg	285.2071	890	3							HMDB0000672	Hexadecanedioic acid	C16H30O4	0.0
M285T1065_neg	285.2435	1065	3							HMDB0031042	Avocadene	C17H34O3	0.1
M287T753_neg	287.0229	753	3							HMDB0029191	5-Hydroxysebacate	C11H12O7S	0.9
M287T956_neg	287.1656	956	3							HMDB0000153	Estriol	C18H24O3	1.0
M287T704_neg	287.1864	704	3							HMDB0031885	6-Hydroxypentadecanedioic acid	C15H28O5	0.0
M288T747_neg	288.1243	747	3							HMDB0041836	Benzoyl ecgonine	C16H19NO4	0.5
M289T484_neg	289.0722	484	3							HMDB0001871	Epicatechin	C15H14O6	1.4
M289T662_neg	289.0753	662	3							HMDB0250129	Chloroxuron	C15H15ClN2O2	1.2
M290T496_neg	290.1610	496	3							HMDB0241031	5-dihydroxy-3-methylpentanoylca	C13H25NO6	0.4
M291T537_neg	291.1351	537	3							HMDB0011687	Phenylbutyrylglutamine	C15H20N2O4	0.1
M293T755_neg	293.1032	755	3							HMDB0039825	Cyclocalopin F	C15H18O6	0.3
M293T603_neg	293.1240	603	3							HMDB0031693	thyl (S)-3-hydroxybutyrate glucosid	C12H22O8	0.5
M297T694_neg	297.0653	694	3							HMDB0242752	6-Methylthioinosine	C11H14N4O4S	3.4
M297T676_neg	297.0920	676	3							HMDB0256886	anyl)-6-ethyl-7-oxo-1-azabicyclo[3.	C13H18N2O4S	1.8
M298T670_neg	298.0874	670	3							HMDB0015536	Imipenem	C12H17N3O4S	2.2
M298T997_neg	298.2389	997	3							HMDB0013300	Pentadecanoylglycine	C17H33NO3	0.5
M299T728_neg	299.0926	728	3							HMDB0030875	Phomarin	C17H16O5	0.3
M299T680_neg	299.1284	680	3							HMDB0030755	Myrigalone E	C18H20O4	1.6
M299T729_neg	299.1288	729	3							HMDB0030755	Myrigalone E	C18H20O4	0.4

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M274T608_neg	274.1660	608	3	4.47E-06	1.23	FALSE	6.70E-01	0.98	FALSE	3.12E-08	1.24	FALSE	2.47E-01	0.92	FALSE
M275T656_neg	275.1039	656	3	7.77E-06	0.78	FALSE	6.11E-01	1.03	FALSE	3.97E-09	1.35	FALSE	6.18E-01	0.95	FALSE
M275T821_neg	275.1136	821	3	3.87E-03	0.70	FALSE	9.22E-02	0.82	FALSE	7.85E-01	1.03	FALSE	5.92E-01	0.87	FALSE
M276T1014_neg	276.1607	1014	3	6.95E-01	1.02	FALSE	6.17E-01	0.97	FALSE	1.92E-01	0.93	FALSE	4.05E-01	0.89	FALSE
M277T1030_neg	277.1445	1030	3	3.91E-01	0.94	FALSE	4.62E-01	0.95	FALSE	4.08E-01	0.95	FALSE	1.82E-01	1.27	FALSE
M277T679_neg	277.1559	679	3	1.87E-11	0.70	FALSE	3.80E-01	1.05	FALSE	6.38E-12	1.38	FALSE	5.88E-01	0.97	FALSE
M278T627_neg	278.1035	627	3	4.50E-08	1.36	FALSE	7.53E-01	1.02	FALSE	3.04E-09	1.34	FALSE	1.19E-01	0.89	FALSE
M278T512_neg	278.1395	512	3	1.65E-01	1.11	FALSE	2.92E-01	1.08	FALSE	1.15E-03	1.23	FALSE	9.82E-03	0.70	FALSE
M278T688_neg	278.1398	688	3	1.56E-10	1.29	FALSE	2.47E-01	1.05	FALSE	2.05E-03	1.11	FALSE	6.35E-01	0.98	FALSE
M280T729_neg	280.1300	729	3	9.41E-04	0.87	FALSE	8.78E-01	1.01	FALSE	1.36E-10	1.28	FALSE	8.84E-01	0.98	FALSE
M281T575_neg	281.0936	575	3	9.55E-03	0.73	FALSE	9.71E-01	1.00	FALSE	3.15E-02	1.25	FALSE	1.28E-01	0.78	FALSE
M282T898_neg	282.1170	898	3	2.78E-01	0.89	FALSE	5.31E-02	1.28	FALSE	2.31E-01	1.12	FALSE	3.51E-01	0.85	FALSE
M283T678_neg	283.1551	678	3	3.29E-08	1.47	FALSE	8.20E-03	0.83	FALSE	7.88E-01	0.98	FALSE	9.94E-01	1.00	FALSE
M284T369_neg	284.1252	369	3	8.07E-01	1.01	FALSE	9.62E-01	1.00	FALSE	2.71E-09	1.36	FALSE	2.96E-01	0.86	FALSE
M285T698_neg	285.1708	698	3	6.26E-08	1.35	FALSE	5.17E-01	0.97	FALSE	8.04E-01	0.99	FALSE	9.15E-01	0.99	FALSE
M285T838_neg	285.1708	838	3	8.05E-01	1.01	FALSE	1.23E-01	1.08	FALSE	1.71E-06	1.21	FALSE	7.78E-01	0.97	FALSE
M285T890_neg	285.2071	890	3	9.80E-02	1.10	FALSE	6.46E-01	0.97	FALSE	4.77E-01	1.04	FALSE	9.54E-01	1.01	FALSE
M285T1065_neg	285.2435	1065	3	4.05E-01	0.90	FALSE	4.18E-03	0.70	FALSE	7.45E-01	0.96	FALSE	9.90E-01	1.00	FALSE
M287T753_neg	287.0229	753	3	4.96E-03	1.18	FALSE	8.08E-01	1.01	FALSE	2.88E-06	1.28	FALSE	6.20E-01	0.93	FALSE
M287T956_neg	287.1656	956	3	7.73E-04	1.38	FALSE	6.00E-01	0.95	FALSE	2.19E-02	1.21	FALSE	3.59E-02	1.34	FALSE
M287T704_neg	287.1864	704	3	5.40E-11	1.36	FALSE	4.39E-01	1.04	FALSE	1.08E-01	1.06	FALSE	8.94E-01	0.99	FALSE
M288T747_neg	288.1243	747	3	4.98E-05	1.17	FALSE	6.87E-01	1.02	FALSE	6.03E-09	1.23	FALSE	2.82E-02	0.85	FALSE
M289T484_neg	289.0722	484	3	1.30E-01	1.14	FALSE	6.66E-01	1.04	FALSE	3.06E-01	0.93	FALSE	7.69E-02	0.59	FALSE
M289T662_neg	289.0753	662	3	3.06E-08	1.33	FALSE	5.39E-01	1.03	FALSE	4.68E-05	1.19	FALSE	6.93E-01	0.95	FALSE
M290T496_neg	290.1610	496	3	1.51E-01	1.08	FALSE	9.12E-01	0.99	FALSE	5.17E-13	1.42	FALSE	3.17E-01	0.93	FALSE
M291T537_neg	291.1351	537	3	4.13E-01	1.31	FALSE	8.42E-01	1.07	FALSE	7.24E-02	1.69	FALSE	3.65E-01	0.42	FALSE
M293T755_neg	293.1032	755	3	7.60E-01	0.97	FALSE	3.35E-01	1.11	FALSE	4.46E-01	0.94	FALSE	2.12E-01	1.55	FALSE
M293T603_neg	293.1240	603	3	2.01E-01	1.75	FALSE	5.17E-01	1.38	FALSE	1.19E-01	1.81	FALSE	1.13E-01	2.73	FALSE
M297T694_neg	297.0653	694	3	9.98E-04	0.81	FALSE	3.00E-01	1.07	FALSE	7.24E-01	0.98	FALSE	3.00E-01	1.20	FALSE
M297T676_neg	297.0920	676	3	1.74E-01	0.92	FALSE	4.01E-02	1.15	FALSE	1.32E-06	1.32	FALSE	4.83E-01	0.92	FALSE
M298T670_neg	298.0874	670	3	9.82E-02	1.16	FALSE	2.23E-01	1.12	FALSE	8.72E-02	1.14	FALSE	4.33E-01	1.12	FALSE
M298T997_neg	298.2389	997	3	4.10E-03	0.85	FALSE	2.30E-02	1.15	FALSE	1.02E-06	0.78	FALSE	8.58E-01	1.04	FALSE
M299T728_neg	299.0926	728	3	6.76E-01	0.97	FALSE	2.39E-01	0.92	FALSE	9.06E-03	1.16	FALSE	6.60E-01	0.93	FALSE
M299T680_neg	299.1284	680	3	5.89E-10	1.34	FALSE	1.98E-01	0.94	FALSE	1.93E-01	1.05	FALSE	9.55E-01	1.01	FALSE
M299T729_neg	299.1288	729	3	1.17E-01	0.84	FALSE	3.88E-01	0.90	FALSE	3.27E-01	1.10	FALSE	7.88E-01	1.07	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M299T827_neg	299.1290	827	3							HMDB0030755	Myrigalone E	C18H20O4	0.3
M300T616_neg	300.1243	616	3						Alkaloids	HMDB0015323	Oxymorphone	C17H19NO4	0.5
M301T803_neg	301.0385	803	3							HMDB0060031	Vanilloylglycine	C12H14O7S	1.0
M301T693_neg	301.1445	693	3						Shikimates and Phenylpropanoids	HMDB0000530	6-Ketoestriol	C18H22O4	0.3
M301T917_neg	301.1559	917	3							HMDB0251775	Emivirine	C17H22N2O3	0.6
M301T558_neg	301.1659	558	3							HMDB0031094	Glycerol tributanoate	C15H26O6	0.6
M301T706_neg	301.1657	706	3						Fatty acids	HMDB0031094	Glycerol tributanoate	C15H26O6	0.2
M302T693_neg	302.1476	693	3							HMDB0028708	Arginylglutamic acid	C11H21N5O5	2.0
M303T601_neg	303.0877	601	3							HMDB0029175	3-Sn-phosphatidylethanolamine	C16H16O6	1.0
M303T1044_neg	303.1966	1044	3							HMDB0000309	lpha,16beta-Dihydroxyandrosteno	C19H28O3	0.0
M303T891_neg	303.2078	891	3							HMDB0246631	xamide, 1-butyl-N-(4-hydroxy-2,6-	C18H28N2O2	0.1
M305T865_neg	305.0820	865	3							HMDB0032848	dihydroxy-4-(4-hydroxyphenyl)-1H	C19H14O4	0.3
M305T688_neg	305.0936	688	3							HMDB0245142	xy-1-naphthaldehyde salicyloylhy	C18H14N2O3	1.3
M305T700_neg	305.1508	700	3							HMDB0253499	Inproquone	C16H22N2O4	0.3
M305T932_neg	305.1758	932	3							HMDB0012799	4-Oxoretinal	C18H26O4	0.0
M306T724_neg	306.1349	724	3							HMDB0038582	oxy-4-methoxy-1-oxobutyl)-2,2-di	C16H21NO5	0.5
M307T837_neg	307.1661	837	3							HMDB0060990	8-Hydroxycarteolol	C16H24N2O4	0.9
M308T898_neg	308.1870	898	3							HMDB0015334	Nadolol	C17H27NO4	0.9
M311T1017_1_neg	311.1687	1017	3							HMDB0032549	N-Undecylbenzenesulfonic acid	C17H28O3S	0.1
M311T959_neg	311.2228	959	3						Fatty acids	HMDB0003871	13-L-Hydroperoxylinoleic acid	C18H32O4	0.0
M312T904_neg	312.2186	904	3							HMDB0013205	9-Decenoylcarnitine	C17H31NO4	1.8
M313T781_neg	313.1657	781	3							HMDB0029848	(-)-trans-Carveol glucoside	C16H26O6	0.0
M313T973_neg	313.2384	973	3						Fatty acids	HMDB0000782	Octadecanedioic acid	C18H34O4	0.0
M315T748_neg	315.1241	748	3							HMDB0038323	Verimol B	C18H20O5	0.9
M317T604_neg	317.1394	604	3							HMDB0031752	(S,E)-Zearalenone	C18H22O5	0.2
M317T773_neg	317.1507	773	3							HMDB0255714	Noopept	C17H22N2O4	0.1
M319T820_neg	319.1915	820	3							HMDB0012798	4-Oxoretinal	C19H28O4	0.2
M319T866_neg	319.2025	866	3							HMDB0253572	Iprovalicar	C18H28N2O3	0.6
M320T710_neg	320.1504	710	3							HMDB0252656	GD2 Ganglioside	C18H19N5O	3.9
M321T1075_neg	321.2056	1075	3							HMDB0033615	(S)-[8]-Gingerol	C19H30O4	4.9
M325T779_neg	325.1293	779	3							HMDB0034755	Methoxybenzyl O-(2-sulfoglucosid	C16H22O7	0.0
M325T674_neg	325.1405	674	3							HMDB0255620	Nipradilol	C15H22N2O6	0.0
M327T785_neg	327.0877	785	3							HMDB0029677	Zapotinin	C18H16O6	1.0
M327T913_neg	327.2177	913	3							HMDB0035919	Corchorifatty acid F	C18H32O5	0.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M299T827_neg	299.1290	827	3	5.39E-01	1.04	FALSE	6.52E-01	0.97	FALSE	4.50E-08	1.37	FALSE	2.17E-01	0.88	FALSE
M300T616_neg	300.1243	616	3	1.74E-04	1.49	FALSE	4.46E-01	0.92	FALSE	4.89E-01	0.94	FALSE	1.49E-01	0.72	FALSE
M301T803_neg	301.0385	803	3	2.50E-01	0.95	FALSE	1.48E-01	1.06	FALSE	4.64E-06	1.19	FALSE	3.51E-02	0.82	FALSE
M301T693_neg	301.1445	693	3	2.30E-05	1.46	FALSE	5.13E-01	0.94	FALSE	3.53E-01	1.07	FALSE	2.84E-01	0.78	FALSE
M301T917_neg	301.1559	917	3	2.50E-05	0.77	FALSE	6.55E-01	0.97	FALSE	1.39E-03	1.18	FALSE	4.23E-01	1.06	FALSE
M301T558_neg	301.1659	558	3	2.82E-14	1.40	FALSE	6.96E-01	0.98	FALSE	9.57E-02	1.06	FALSE	1.96E-01	1.10	FALSE
M301T706_neg	301.1657	706	3	6.58E-01	0.93	FALSE	7.17E-02	0.69	FALSE	4.21E-01	1.13	FALSE	7.27E-01	0.95	FALSE
M302T693_neg	302.1476	693	3	1.31E-04	1.35	FALSE	4.37E-01	0.94	FALSE	6.44E-02	1.13	FALSE	8.35E-02	0.72	FALSE
M303T601_neg	303.0877	601	3	4.08E-07	1.40	FALSE	2.69E-01	1.08	FALSE	2.01E-05	1.27	FALSE	4.83E-01	1.07	FALSE
M303T1044_neg	303.1966	1044	3	2.29E-05	1.34	FALSE	1.67E-03	0.80	FALSE	3.12E-02	1.13	FALSE	2.43E-02	1.28	FALSE
M303T891_neg	303.2078	891	3	1.70E-01	0.94	FALSE	1.47E-01	1.07	FALSE	1.11E-12	1.35	FALSE	7.34E-02	1.17	FALSE
M305T865_neg	305.0820	865	3	7.56E-01	0.99	FALSE	9.95E-01	1.00	FALSE	1.69E-05	0.86	FALSE	9.52E-01	1.01	FALSE
M305T688_neg	305.0936	688	3	1.66E-03	1.41	FALSE	6.88E-01	0.95	FALSE	4.03E-01	1.08	FALSE	7.83E-01	1.08	FALSE
M305T700_neg	305.1508	700	3	8.69E-06	1.32	FALSE	8.16E-05	0.79	FALSE	7.72E-01	1.02	FALSE	7.92E-02	0.93	FALSE
M305T932_neg	305.1758	932	3	2.59E-03	1.23	FALSE	4.79E-02	0.87	FALSE	9.69E-01	1.00	FALSE	3.71E-02	0.75	FALSE
M306T724_neg	306.1349	724	3	1.65E-03	1.33	FALSE	7.32E-03	1.28	FALSE	1.88E-02	1.20	FALSE	6.95E-02	1.28	FALSE
M307T837_neg	307.1661	837	3	4.39E-01	1.07	FALSE	4.04E-01	1.08	FALSE	1.74E-01	1.11	FALSE	7.46E-01	0.93	FALSE
M308T898_neg	308.1870	898	3	3.36E-01	1.10	FALSE	2.05E-03	1.37	FALSE	5.14E-05	1.42	FALSE	9.32E-02	1.30	FALSE
M311T1017_1_neg	311.1687	1017	3	9.66E-01	0.99	FALSE	1.12E-01	1.56	FALSE	4.97E-01	1.17	FALSE	5.87E-01	0.91	FALSE
M311T959_neg	311.2228	959	3	1.24E-01	1.15	FALSE	4.79E-01	0.93	FALSE	4.03E-02	1.18	FALSE	9.27E-01	1.01	FALSE
M312T904_neg	312.2186	904	3	2.27E-03	1.21	FALSE	8.85E-01	1.01	FALSE	2.92E-05	1.26	FALSE	5.71E-01	1.07	FALSE
M313T781_neg	313.1657	781	3	2.48E-02	0.88	FALSE	4.68E-01	1.04	FALSE	2.36E-11	1.43	FALSE	2.95E-01	1.18	FALSE
M313T973_neg	313.2384	973	3	5.77E-06	1.37	FALSE	4.11E-04	0.76	FALSE	9.00E-01	1.01	FALSE	7.65E-01	1.03	FALSE
M315T748_neg	315.1241	748	3	2.38E-01	1.04	FALSE	8.06E-02	0.94	FALSE	1.88E-10	1.23	FALSE	7.49E-01	1.02	FALSE
M317T604_neg	317.1394	604	3	3.01E-07	1.45	FALSE	4.97E-01	0.95	FALSE	7.00E-01	1.02	FALSE	2.42E-01	0.89	FALSE
M317T773_neg	317.1507	773	3	3.85E-01	1.07	FALSE	6.67E-02	0.87	FALSE	4.84E-08	1.45	FALSE	7.97E-01	1.02	FALSE
M319T820_neg	319.1915	820	3	1.88E-01	1.08	FALSE	4.42E-05	0.80	FALSE	5.00E-01	1.03	FALSE	1.85E-01	1.12	FALSE
M319T866_neg	319.2025	866	3	4.98E-01	0.96	FALSE	3.98E-02	1.14	FALSE	5.87E-01	0.97	FALSE	5.16E-02	1.34	FALSE
M320T710_neg	320.1504	710	3	8.53E-05	0.74	FALSE	4.36E-02	1.17	FALSE	5.62E-04	1.26	FALSE	8.66E-02	0.67	FALSE
M321T1075_neg	321.2056	1075	3	1.51E-01	0.82	FALSE	8.30E-01	1.03	FALSE	7.79E-01	1.03	FALSE	8.21E-01	1.09	FALSE
M325T779_neg	325.1293	779	3	2.67E-01	1.09	FALSE	6.85E-01	0.97	FALSE	2.06E-02	1.18	FALSE	2.65E-01	0.85	FALSE
M325T674_neg	325.1405	674	3	3.20E-02	0.88	FALSE	7.65E-01	1.02	FALSE	7.46E-12	1.47	FALSE	2.99E-01	0.89	FALSE
M327T785_neg	327.0877	785	3	1.92E-03	0.83	FALSE	7.30E-02	1.12	FALSE	5.34E-11	1.44	FALSE	6.63E-01	1.05	FALSE
M327T913_neg	327.2177	913	3	9.61E-01	1.00	FALSE	9.60E-01	1.00	FALSE	2.22E-03	1.14	FALSE	1.32E-01	0.84	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M327T1062_neg	327.2905	1062	3							HMDB0032477	Polyoxyethylene 40 monostearate	C20H40O3	0.1
M328T702_neg	328.1052	702	3							HMDB0010329	Dopamine glucuronide	C14H19NO8	4.2
M328T806_neg	328.1192	806	3							HMDB0032805	N-trans-Feruloyloctopamine	C18H19NO5	0.4
M329T1010_neg	329.1758	1010	3							HMDB0002121	Carnosol	C20H26O4	0.1
M329T915_neg	329.2333	915	3							HMDB0004708	9,12,13-TriHOME	C18H34O5	0.3
M331T745_neg	331.1191	745	3							HMDB0030664	3-Galloylcatechin	C18H20O6	1.1
M331T706_neg	331.1219	706	3							HMDB0244252	ppropyl-6-fluoro-1,4-dihydro-4-oxo	C16H17FN4O3	2.2
M331T797_neg	331.1559	797	3							HMDB0030787	(R)-Marmin	C19H24O5	2.5
M331T953_neg	331.1915	953	3							HMDB0002358	Carnosic acid	C20H28O4	0.0
M332T791_neg	332.1506	791	3							HMDB0256290	Pentopril	C18H23NO5	0.9
M333T786_neg	333.1087	786	3							HMDB0034937	Capparilloside A	C16H18N2O6	1.5
M333T781_neg	333.1452	781	3							HMDB0037499	1-Ethenylhexyl butanoate	C17H22N2O5	1.2
M333T822_neg	333.1712	822	3							HMDB0032699	-8-(2-methylbutanoyloxy)-9,10-ep	C19H26O5	1.4
M333T909_neg	333.2072	909	3							HMDB0001244	-Keto-13,14-dihydroprostaglandin	C20H30O4	0.3
M337T381_neg	337.1407	381	3							HMDB0001272	Nicotine glucuronide	C16H22N2O6	0.5
M338T774_neg	338.1613	774	3							HMDB0241127	5E,8Z)-Deca-3,5,8-trienedioylcarni	C17H25NO6	1.0
M340T763_neg	340.1771	763	3							HMDB0240793	4-Dimethylideneoctanedioylcarniti	C17H27NO6	1.6
M341T143_neg	341.1089	143	3						Carbohydrates	HMDB0000048	Melibiose	C12H22O11	0.0
M341T956_neg	341.2698	956	3							HMDB0242141	Eicosanedioic acid	C20H38O4	0.1
M342T680_neg	342.1018	680	3							HMDB0031942	Niazinin	C15H21NO6S	0.4
M342T991_neg	342.2651	991	3							HMDB0240804	8-Methylundecanoylcarnitine	C19H37NO4	0.4
M344T769_neg	344.1504	769	3							HMDB0242457	-yl)-2-methoxyphenyl)amino)pyrin	C19H23NO5	0.2
M345T680_neg	345.1347	680	3						Terpenoids	HMDB0003559	Gibberellin A3	C19H22O6	1.0
M347T713_neg	347.1001	713	3							HMDB0001557	Riboflavin reduced	C15H16N4O6	1.1
M347T599_neg	347.1499	599	3							HMDB0034988	Gibberellin A60	C19H24O6	0.2
M347T693_neg	347.1502	693	3						Shikimates and Phenylpropanoids	HMDB0034988	Gibberellin A60	C19H24O6	0.4
M347T823_neg	347.1969	823	3							HMDB0015695	Roxatidine acetate	C19H28N2O4	2.0
M348T898_neg	348.1798	898	3							HMDB0247746	Abeado	C15H23N7O3	2.4
M350T589_neg	350.1626	589	3							HMDB0014808	Pirenzepine	C19H21N5O2	1.0
M352T595_1_neg	352.1306	595	3							HMDB0248684	nyl)-1,2,4-oxadiazol-3-yl)phenoxy)	C19H19N3O4	0.9
M353T555_neg	353.0880	555	3						Shikimates and Phenylpropanoids	HMDB0002336	Biflorin	C16H18O9	0.6
M353T940_neg	353.2333	940	3							HMDB0001139	Prostaglandin F2a	C20H34O5	0.0
M354T855_neg	354.1382	855	3							HMDB0014751	Amodiaquine	C20H22ClN3O	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M327T1062_neg	327.2905	1062	3	2.91E-03	1.42	FALSE	4.32E-01	0.91	FALSE	3.22E-01	1.11	FALSE	6.04E-01	1.10	FALSE
M328T702_neg	328.1052	702	3	9.10E-01	1.01	FALSE	5.04E-01	0.93	FALSE	2.46E-05	1.47	FALSE	1.67E-01	0.80	FALSE
M328T806_neg	328.1192	806	3	6.99E-07	1.39	FALSE	9.72E-01	1.00	FALSE	5.95E-07	1.34	FALSE	7.22E-01	0.95	FALSE
M329T1010_neg	329.1758	1010	3	9.55E-01	0.95	FALSE	1.57E-01	0.07	FALSE	2.95E-01	2.18	FALSE	8.38E-01	1.21	FALSE
M329T915_neg	329.2333	915	3	3.22E-03	1.22	FALSE	2.79E-01	0.92	FALSE	6.39E-02	1.11	FALSE	5.77E-01	1.09	FALSE
M331T745_neg	331.1191	745	3	3.74E-04	1.26	FALSE	3.21E-01	1.07	FALSE	9.60E-04	1.20	FALSE	5.97E-01	1.09	FALSE
M331T706_neg	331.1219	706	3	1.75E-01	0.89	FALSE	6.59E-01	0.96	FALSE	7.70E-03	1.23	FALSE	5.38E-01	1.14	FALSE
M331T797_neg	331.1559	797	3	7.84E-02	1.13	FALSE	4.12E-01	1.06	FALSE	1.95E-01	1.08	FALSE	2.70E-01	1.15	FALSE
M331T953_neg	331.1915	953	3	3.81E-01	1.06	FALSE	9.11E-02	0.89	FALSE	6.50E-03	1.17	FALSE	1.06E-02	0.74	FALSE
M332T791_neg	332.1506	791	3	9.95E-11	1.37	FALSE	8.14E-01	1.01	FALSE	2.39E-01	0.95	FALSE	6.11E-01	1.08	FALSE
M333T786_neg	333.1087	786	3	3.75E-02	1.21	FALSE	1.68E-01	0.86	FALSE	5.54E-03	0.80	FALSE	1.32E-01	1.57	FALSE
M333T781_neg	333.1452	781	3	1.53E-03	1.24	FALSE	2.53E-08	0.67	FALSE	3.73E-01	0.95	FALSE	1.02E-01	0.70	FALSE
M333T822_neg	333.1712	822	3	1.55E-12	1.47	FALSE	2.28E-02	0.89	FALSE	9.30E-02	0.93	FALSE	6.38E-01	0.95	FALSE
M333T909_neg	333.2072	909	3	3.73E-08	1.25	FALSE	1.67E-01	0.95	FALSE	9.55E-01	1.00	FALSE	3.37E-01	1.05	FALSE
M337T381_neg	337.1407	381	3	1.22E-03	1.41	FALSE	9.56E-02	1.20	FALSE	3.50E-01	1.09	FALSE	6.42E-01	0.89	FALSE
M338T774_neg	338.1613	774	3	1.09E-04	1.49	FALSE	6.83E-01	0.95	FALSE	9.71E-01	1.00	FALSE	6.87E-01	0.95	FALSE
M340T763_neg	340.1771	763	3	9.24E-01	0.99	FALSE	2.96E-03	0.76	FALSE	5.01E-04	1.29	FALSE	5.82E-01	0.96	FALSE
M341T143_neg	341.1089	143	3	7.24E-01	0.93	FALSE	7.88E-01	0.95	FALSE	1.45E-01	1.28	FALSE	8.95E-01	0.91	FALSE
M341T956_neg	341.2698	956	3	7.44E-04	1.41	FALSE	2.82E-01	1.12	FALSE	2.10E-01	0.90	FALSE	5.56E-02	1.42	FALSE
M342T680_neg	342.1018	680	3	4.28E-01	0.93	FALSE	3.92E-01	1.09	FALSE	1.82E-06	1.50	FALSE	1.91E-01	0.74	FALSE
M342T991_neg	342.2651	991	3	3.72E-03	0.88	FALSE	5.01E-03	1.14	FALSE	1.29E-04	0.86	FALSE	4.03E-01	0.92	FALSE
M344T769_neg	344.1504	769	3	6.57E-01	0.98	FALSE	1.71E-08	1.27	FALSE	7.32E-12	1.29	FALSE	8.28E-01	0.99	FALSE
M345T680_neg	345.1347	680	3	2.37E-08	1.33	FALSE	8.15E-01	0.99	FALSE	2.88E-03	1.14	FALSE	3.73E-01	1.07	FALSE
M347T713_neg	347.1001	713	3	3.27E-02	1.23	FALSE	5.16E-01	1.07	FALSE	2.36E-03	1.30	FALSE	5.58E-01	0.88	FALSE
M347T599_neg	347.1499	599	3	1.96E-06	1.41	FALSE	8.70E-02	1.13	FALSE	2.31E-01	1.08	FALSE	2.34E-01	1.14	FALSE
M347T693_neg	347.1502	693	3	4.96E-06	1.45	FALSE	5.77E-01	0.95	FALSE	4.15E-01	1.06	FALSE	7.12E-01	0.91	FALSE
M347T823_neg	347.1969	823	3	2.95E-01	0.95	FALSE	6.98E-01	1.02	FALSE	6.94E-01	1.02	FALSE	6.66E-02	1.15	FALSE
M348T898_neg	348.1798	898	3	1.22E-01	0.90	FALSE	4.00E-01	1.06	FALSE	5.86E-02	0.89	FALSE	3.39E-02	1.30	FALSE
M350T589_neg	350.1626	589	3	2.82E-01	1.13	FALSE	9.32E-01	1.01	FALSE	4.60E-01	0.93	FALSE	5.10E-01	1.06	FALSE
M352T595_1_neg	352.1306	595	3	1.52E-01	1.07	FALSE	3.45E-03	1.16	FALSE	8.52E-18	1.50	FALSE	5.87E-01	1.07	FALSE
M353T555_neg	353.0880	555	3	1.42E-01	-36.81	FALSE	1.26E-01	-12.23	FALSE	6.09E-02	-12.22	FALSE	6.11E-01	1.37	FALSE
M353T940_neg	353.2333	940	3	9.23E-02	1.08	FALSE	5.41E-01	1.03	FALSE	2.87E-04	1.15	FALSE	4.08E-01	0.91	FALSE
M354T855_neg	354.1382	855	3	1.24E-01	0.85	FALSE	4.34E-01	1.10	FALSE	1.78E-02	1.25	FALSE	2.99E-01	0.79	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M355T920_neg	355.0854	920	3							HMDB0253981	Laquinimod	C19H17ClN2O3	0.1
M359T707_neg	359.0778	707	3						Shikimates and Phenylpropanoids	HMDB0003572	Rosmarinic acid	C18H16O8	1.6
M359T756_neg	359.1249	756	3							HMDB0006045	Dityrosine	C18H20N2O6	0.1
M359T740_neg	359.1504	740	3							HMDB0037235	Quassinol	C20H24O6	1.1
M363T577_neg	363.1451	577	3							HMDB0033420	Gibberellin A55	C19H24O7	0.6
M363T968_neg	363.2178	968	3							HMDB0000903	Tetrahydrocortisone	C21H32O5	0.2
M367T692_neg	367.2126	692	3							HMDB0001908	19-Hydroxy-PGE2	C20H32O6	0.0
M367T858_neg	367.2127	858	3							HMDB0001908	19-Hydroxy-PGE2	C20H32O6	0.2
M370T880_neg	370.0963	880	3							HMDB0259149	Triaminophenyl phosphate	C18H18N3O4P	0.2
M371T957_neg	371.1898	957	3							HMDB0247995	Androstane-3,17-diol 17-sulfate	C19H32O5S	0.2
M372T828_neg	372.1488	828	3							HMDB0250315	Clebopride	C20H24ClN3O2	0.9
M372T776_neg	372.1817	776	3							HMDB0039503	N-Jasmonoyltyrosine	C21H27NO5	0.2
M377T744_neg	377.1251	744	3							HMDB0029304	3,4-DHPEA-EA	C19H22O8	2.4
M377T933_neg	377.2334	933	3							HMDB0035508	Annoglabasin F	C22H34O5	0.2
M385T764_neg	385.1692	764	3							HMDB0255928	Olamufloxacin	C20H23FN4O3	2.7
M385T848_neg	385.1692	848	3							HMDB0255928	Olamufloxacin	C20H23FN4O3	2.7
M387T144_neg	387.1145	144	3						Carbohydrates				
M390T780_neg	390.1675	780	3							HMDB0257086	rboxy-3-carboxanilidopropyl)alany	C19H25N3O6	1.1
M391T783_neg	391.1401	783	3							HMDB0039564	Marmesin rhamnoside	C20H24O8	0.7
M399T1008_neg	399.1292	1008	3							HMDB0015561	Zuclopenthixol	C22H25ClN2OS	2.9
M399T846_neg	399.1594	846	3							HMDB0041278	hydroxy-2-methylbutanoyloxy)-7(1	C20H29ClO6	3.5
M399T701_neg	399.2219	701	3							HMDB0240579	na-Pregnan-3beta,20beta-diol 3-su	C21H36O5S	2.1
M403T832_neg	403.2251	832	3							HMDB0014905	Benzquinamide	C22H32N2O5	3.2
M405T933_neg	405.2648	933	3							HMDB0000391	7-Ketodeoxycholic acid	C24H38O5	0.4
M407T865_neg	407.2804	865	3						Terpenoids	HMDB0000312	pha,12beta-Trihydroxy-5beta-cho	C24H40O5	0.3
M418T725_neg	418.2139	725	3							HMDB0248012	Adimolol	C25H29N3O3	0.7
M421T863_neg	421.2598	863	3							HMDB0254177	Lovastatin acid	C24H38O6	0.6
M424T898_neg	424.1282	898	3							HMDB0250235	nylphenyl)-6-oxo-1,4-dihydropyrro	C25H19N3O4	4.9
M424T896_neg	424.2715	896	3							HMDB0241487	8Z)-Hexadeca-6,8-dienedioylcarni	C23H39NO6	2.4
M426T683_neg	426.1705	683	3							HMDB0259648	yl)-4-fluoro-1H-indol-1-yl)-6-(hydro	C24H26FNO5	4.0
M429T393_neg	429.1616	393	3						Carbohydrates				
M429T989_neg	429.2646	989	3							HMDB0040994	thyl-2E-pentenoyl)-2b,9a-dihydrox	C26H38O5	0.2
M434T937_neg	434.2087	937	3							HMDB0033451	Cadabicine	C25H29N3O4	0.5
M439T777_neg	439.1879	777	3							HMDB0033468	Diferuloylputrescine	C24H28N2O6	1.1

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M355T920_neg	355.0854	920	3	3.06E-02	0.84	FALSE	8.55E-01	1.02	FALSE	6.58E-07	1.43	FALSE	4.68E-01	1.08	FALSE
M359T707_neg	359.0778	707	3	2.91E-02	-5.55	FALSE	6.52E-02	-142.90	FALSE	6.48E-02	-34.19	FALSE	3.83E-01	0.28	FALSE
M359T756_neg	359.1249	756	3	9.24E-02	0.91	FALSE	5.49E-02	0.89	FALSE	4.16E-10	1.39	FALSE	2.70E-02	1.28	FALSE
M359T740_neg	359.1504	740	3	6.64E-01	0.98	FALSE	2.98E-01	0.95	FALSE	9.75E-02	1.08	FALSE	7.76E-01	1.04	FALSE
M363T577_neg	363.1451	577	3	4.89E-04	1.34	FALSE	5.85E-01	1.05	FALSE	1.70E-03	0.80	FALSE	7.25E-01	1.08	FALSE
M363T968_neg	363.2178	968	3	2.77E-08	1.32	FALSE	9.21E-04	0.84	FALSE	3.63E-04	1.16	FALSE	4.38E-01	0.96	FALSE
M367T692_neg	367.2126	692	3	1.12E-08	1.35	FALSE	3.46E-01	0.95	FALSE	4.16E-04	1.17	FALSE	9.97E-02	0.85	FALSE
M367T858_neg	367.2127	858	3	9.05E-02	1.06	FALSE	7.00E-01	0.99	FALSE	1.99E-04	1.12	FALSE	1.65E-01	0.93	FALSE
M370T880_neg	370.0963	880	3	1.04E-02	1.28	FALSE	6.87E-01	1.04	FALSE	4.05E-01	0.93	FALSE	1.60E-01	1.33	FALSE
M371T957_neg	371.1898	957	3	9.41E-02	1.15	FALSE	8.57E-01	0.98	FALSE	4.15E-01	1.06	FALSE	8.05E-01	1.04	FALSE
M372T828_neg	372.1488	828	3	5.94E-02	0.80	FALSE	5.87E-01	0.93	FALSE	4.09E-02	1.24	FALSE	2.49E-01	0.70	FALSE
M372T776_neg	372.1817	776	3	7.81E-01	0.98	FALSE	4.57E-01	0.95	FALSE	6.82E-06	1.27	FALSE	1.35E-03	0.73	FALSE
M377T744_neg	377.1251	744	3	2.80E-02	0.80	FALSE	8.28E-02	1.21	FALSE	2.19E-03	1.32	FALSE	3.17E-01	1.18	FALSE
M377T933_neg	377.2334	933	3	1.53E-01	1.09	FALSE	2.83E-01	1.07	FALSE	1.44E-06	1.29	FALSE	7.60E-01	0.96	FALSE
M385T764_neg	385.1692	764	3	2.23E-06	1.30	FALSE	6.74E-01	0.98	FALSE	4.48E-04	1.18	FALSE	8.93E-01	0.98	FALSE
M385T848_neg	385.1692	848	3	1.54E-01	1.09	FALSE	5.59E-01	0.96	FALSE	3.00E-02	1.12	FALSE	1.97E-01	0.78	FALSE
M387T144_neg	387.1145	144	3	1.69E-01	1.41	FALSE	2.30E-01	0.71	FALSE	4.04E-01	1.20	FALSE	9.78E-01	1.02	FALSE
M390T780_neg	390.1675	780	3	1.82E-02	0.71	FALSE	7.90E-01	1.04	FALSE	4.00E-01	1.11	FALSE	6.72E-01	0.89	FALSE
M391T783_neg	391.1401	783	3	2.07E-01	1.10	FALSE	7.63E-01	1.02	FALSE	1.16E-04	1.30	FALSE	1.99E-01	0.80	FALSE
M399T1008_neg	399.1292	1008	3	1.02E-01	10.56	FALSE	4.75E-01	0.52	FALSE	5.05E-01	0.55	FALSE	8.65E-01	0.89	FALSE
M399T846_neg	399.1594	846	3	7.83E-05	0.73	FALSE	3.23E-01	1.08	FALSE	2.19E-02	1.17	FALSE	8.35E-01	1.05	FALSE
M399T701_neg	399.2219	701	3	4.75E-06	1.38	FALSE	4.01E-01	1.06	FALSE	2.96E-02	1.14	FALSE	2.81E-01	1.17	FALSE
M403T832_neg	403.2251	832	3	7.20E-01	0.98	FALSE	3.41E-05	1.33	FALSE	1.86E-01	0.93	FALSE	5.12E-01	1.11	FALSE
M405T933_neg	405.2648	933	3	7.90E-02	0.86	FALSE	5.74E-01	0.95	FALSE	5.16E-01	0.95	FALSE	4.03E-01	0.90	FALSE
M407T865_neg	407.2804	865	3	7.44E-11	1.44	FALSE	1.65E-02	0.87	FALSE	1.17E-01	0.93	FALSE	1.29E-01	0.90	FALSE
M418T725_neg	418.2139	725	3	3.31E-05	1.44	FALSE	1.11E-02	0.81	FALSE	2.29E-01	0.91	FALSE	1.11E-02	0.71	FALSE
M421T863_neg	421.2598	863	3	7.57E-01	1.01	FALSE	2.60E-01	1.04	FALSE	2.58E-14	1.26	FALSE	3.48E-01	0.95	FALSE
M424T898_neg	424.1282	898	3	1.96E-01	0.89	FALSE	9.03E-01	1.01	FALSE	4.70E-03	1.24	FALSE	3.05E-01	1.26	FALSE
M424T896_neg	424.2715	896	3	6.68E-02	1.08	FALSE	1.52E-01	1.06	FALSE	5.05E-14	1.32	FALSE	2.71E-01	1.09	FALSE
M426T683_neg	426.1705	683	3	1.71E-02	0.87	FALSE	1.14E-02	1.18	FALSE	4.02E-06	1.28	FALSE	9.41E-01	1.01	FALSE
M429T393_neg	429.1616	393	3	2.04E-02	1.28	FALSE	6.72E-01	0.96	FALSE	6.96E-01	0.96	FALSE	5.75E-01	0.88	FALSE
M429T989_neg	429.2646	989	3	5.36E-01	1.03	FALSE	8.32E-01	1.01	FALSE	1.76E-16	1.43	FALSE	1.32E-04	0.76	FALSE
M434T937_neg	434.2087	937	3	1.75E-01	1.13	FALSE	3.62E-03	0.76	FALSE	1.34E-06	1.49	FALSE	2.11E-01	0.73	FALSE
M439T777_neg	439.1879	777	3	8.75E-01	0.98	FALSE	8.69E-01	1.02	FALSE	1.77E-01	1.18	FALSE	9.36E-01	1.03	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M440T1039_neg	440.1872	1039	3							HMDB0248840	Bacmecillinam	C20H31N3O6S	2.6
M445T947_neg	445.2962	947	3							HMDB0030913	Cepagenin	C27H42O5	0.5
M446T934_neg	446.2920	934	3						Terpenoids				
M447T993_neg	447.3117	993	3							HMDB0032783	Porrigenin A	C27H44O5	0.3
M448T909_neg	448.3070	909	3						Terpenoids	HMDB0000631	Deoxycholic acid glycine conjugate	C26H43NO5	0.4
M449T950_neg	449.3273	950	3							HMDB0000601	Coprocholic acid	C27H46O5	0.2
M451T867_neg	451.2702	867	3						Terpenoids	HMDB0296927	0/20:4(6Z,8E,10E,14Z)-2OH(5S,12F	C25H40O7	0.3
M451T924_neg	451.2703	924	3						Terpenoids	HMDB0296927	0/20:4(6Z,8E,10E,14Z)-2OH(5S,12F	C25H40O7	0.4
M453T606_neg	453.2278	606	3							HMDB0303362	alpha-Guttiferin	C27H34O6	1.1
M457T1007_neg	457.2573	1007	3						Terpenoids	HMDB0037611	Lucidenic acid A	C27H38O6	4.9
M459T1027_neg	459.2730	1027	3						Terpenoids	HMDB0030909	2,3-Secoporrigenin	C27H40O6	4.8
M460T1028_neg	460.2765	1028	3							HMDB0259789	Verdamicin	C20H39N5O7	2.5
M463T937_neg	463.3067	937	3						Terpenoids	HMDB0251684	Ecdysone	C27H44O6	0.4
M463T893_neg	463.3067	893	3							HMDB0251684	Ecdysone	C27H44O6	0.4
M464T945_neg	464.3024	945	3						Terpenoids	HMDB0000138	Glycocholic acid	C26H43NO6	1.4
M465T1068_neg	465.1533	1068	3							HMDB0015438	Spirapril	C22H30N2O5S2	2.0
M467T1018_neg	467.3377	1018	3							HMDB0258186	Scymnol	C27H48O6	0.3
M477T749_neg	477.2496	749	3						Terpenoids				
M479T964_neg	479.3015	964	3						Terpenoids	HMDB0030180	Crustecdysone	C27H44O7	0.2
M483T983_neg	483.3325	983	3							HMDB0242008	N-Docosahexaenoyl Arginine	C28H44N4O3	3.2
M487T809_neg	487.2362	809	3							HMDB0002421	7-Sulfocholic acid	C24H40O8S	1.8
M489T690_neg	489.2137	690	3							HMDB0034434	Austalide F	C26H34O9	1.5
M490T1007_neg	490.1978	1007	3							HMDB0248875	Barnidipine	C27H29N3O6	1.1
M491T1025_neg	491.2108	1025	3							HMDB0254159	Loperamide oxide	C29H33ClN2O3	0.2
M491T677_neg	491.2150	677	3							HMDB0247776	ropanoyl]amino]-3-methylbutanoy	C23H32N4O8	0.6
M491T947_neg	491.3016	947	3						Terpenoids	HMDB0302988	24(28)-Dehydromakisterone	C28H44O7	0.3
M493T793_neg	493.2445	793	3							HMDB0033655	7-(3-methylpentanoate) 11-(3-hyd	C26H38O9	0.4
M493T994_neg	493.3172	994	3						Terpenoids				
M501T777_neg	501.2471	777	3							HMDB0030362	Cavipetin B	C28H38O8	4.5
M503T814_neg	503.3379	814	3							HMDB0034500	Protobassic acid	C30H48O6	0.2
M505T659_neg	505.2078	659	3							HMDB0038170	Isolimonic acid	C26H34O10	0.2
M505T1025_neg	505.2782	1025	3							HMDB0033198	0R,22R)-5,6,14,20,27-Pentahydro	C28H42O8	5.0
M507T687_neg	507.2233	687	3							HMDB0033164	Acetyl-T2 Toxin	C26H36O10	0.5
M521T676_neg	521.1304	676	3						Shikimates and Phenylpropanoids	HMDB0033705	Salviaflaside	C24H26O13	0.7

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M440T1039_neg	440.1872	1039	3	1.26E-04	1.35	FALSE	1.17E-03	0.75	FALSE	7.04E-02	0.89	FALSE	3.09E-02	1.32	FALSE
M445T947_neg	445.2962	947	3	1.61E-08	1.46	FALSE	2.16E-01	1.09	FALSE	2.00E-08	1.39	FALSE	1.87E-01	0.82	FALSE
M446T934_neg	446.2920	934	3	9.65E-02	1.96	FALSE	6.94E-02	0.33	FALSE	7.82E-01	0.91	FALSE	6.91E-01	1.26	FALSE
M447T993_neg	447.3117	993	3	9.45E-06	1.18	FALSE	1.09E-01	0.94	FALSE	1.42E-01	1.05	FALSE	6.77E-02	0.86	FALSE
M448T909_neg	448.3070	909	3	3.89E-01	1.66	FALSE	1.71E-01	0.24	FALSE	2.68E-01	0.56	FALSE	5.89E-01	1.43	FALSE
M449T950_neg	449.3273	950	3	9.15E-09	1.29	FALSE	2.49E-03	0.87	FALSE	3.97E-04	1.14	FALSE	5.07E-01	1.05	FALSE
M451T867_neg	451.2702	867	3	3.51E-01	1.05	FALSE	3.47E-02	1.13	FALSE	1.74E-04	1.19	FALSE	9.23E-01	0.99	FALSE
M451T924_neg	451.2703	924	3	9.52E-01	0.99	FALSE	7.90E-01	1.03	FALSE	5.63E-01	1.05	FALSE	3.52E-01	0.79	FALSE
M453T606_neg	453.2278	606	3	3.59E-04	1.48	FALSE	8.51E-01	1.02	FALSE	2.11E-04	1.43	FALSE	2.53E-01	0.84	FALSE
M457T1007_neg	457.2573	1007	3	4.18E-12	0.76	FALSE	5.76E-03	1.11	FALSE	2.86E-04	0.89	FALSE	2.12E-02	0.78	FALSE
M459T1027_neg	459.2730	1027	3	7.80E-06	0.80	FALSE	1.01E-03	1.18	FALSE	2.59E-04	0.86	FALSE	8.36E-01	0.98	FALSE
M460T1028_neg	460.2765	1028	3	8.76E-06	0.75	FALSE	2.37E-04	1.28	FALSE	3.53E-06	0.77	FALSE	1.67E-01	1.21	FALSE
M463T937_neg	463.3067	937	3	3.25E-02	1.10	FALSE	2.49E-01	0.95	FALSE	5.54E-09	1.26	FALSE	5.46E-01	0.94	FALSE
M463T893_neg	463.3067	893	3	2.65E-08	1.34	FALSE	5.31E-01	1.03	FALSE	8.88E-02	1.08	FALSE	3.96E-01	1.10	FALSE
M464T945_neg	464.3024	945	3	1.35E-01	2.31	FALSE	6.29E-02	0.20	FALSE	1.45E-01	0.50	FALSE	6.94E-01	1.46	FALSE
M465T1068_neg	465.1533	1068	3	9.98E-01	1.00	FALSE	6.77E-01	0.86	FALSE	7.32E-01	0.92	FALSE	1.37E-01	3.06	FALSE
M467T1018_neg	467.3377	1018	3	4.69E-01	0.77	FALSE	1.25E-01	0.57	FALSE	4.42E-01	1.27	FALSE	8.31E-01	0.95	FALSE
M477T749_neg	477.2496	749	3	6.19E-03	1.19	FALSE	9.79E-01	1.00	FALSE	9.79E-02	1.09	FALSE	5.29E-01	0.94	FALSE
M479T964_neg	479.3015	964	3	1.43E-04	1.16	FALSE	7.69E-01	1.01	FALSE	4.59E-08	1.21	FALSE	6.58E-01	0.96	FALSE
M483T983_neg	483.3325	983	3	6.03E-01	0.90	FALSE	5.93E-01	0.89	FALSE	7.11E-01	1.07	FALSE	4.54E-01	1.17	FALSE
M487T809_neg	487.2362	809	3	3.13E-01	0.93	FALSE	3.27E-01	1.08	FALSE	1.78E-05	1.31	FALSE	5.15E-01	0.88	FALSE
M489T690_neg	489.2137	690	3	9.47E-01	1.01	FALSE	3.30E-01	0.86	FALSE	5.67E-01	1.09	FALSE	2.77E-01	0.81	FALSE
M490T1007_neg	490.1978	1007	3	1.17E-03	0.87	FALSE	5.61E-01	0.97	FALSE	7.93E-04	1.14	FALSE	9.36E-01	1.01	FALSE
M491T1025_neg	491.2108	1025	3	1.38E-08	1.24	FALSE	1.72E-02	0.91	FALSE	1.84E-03	0.90	FALSE	5.36E-01	1.06	FALSE
M491T677_neg	491.2150	677	3	1.96E-01	1.11	FALSE	7.73E-01	0.98	FALSE	8.46E-04	1.28	FALSE	9.44E-01	1.01	FALSE
M491T947_neg	491.3016	947	3	2.74E-02	1.10	FALSE	3.00E-01	1.05	FALSE	4.80E-14	1.37	FALSE	6.48E-03	0.81	FALSE
M493T793_neg	493.2445	793	3	1.46E-01	0.92	FALSE	7.61E-02	1.11	FALSE	5.33E-12	1.42	FALSE	1.31E-01	1.23	FALSE
M493T994_neg	493.3172	994	3	1.28E-03	1.20	FALSE	7.31E-01	0.98	FALSE	9.57E-05	1.22	FALSE	1.14E-01	0.88	FALSE
M501T777_neg	501.2471	777	3	4.90E-01	1.05	FALSE	2.26E-01	1.09	FALSE	9.89E-04	0.83	FALSE	6.55E-02	1.26	FALSE
M503T814_neg	503.3379	814	3	2.11E-10	1.34	FALSE	9.42E-02	0.92	FALSE	8.48E-03	1.11	FALSE	1.12E-01	0.83	FALSE
M505T659_neg	505.2078	659	3	3.70E-01	0.89	FALSE	1.04E-01	1.25	FALSE	1.19E-01	1.19	FALSE	2.00E-01	1.54	FALSE
M505T1025_neg	505.2782	1025	3	3.63E-02	1.15	FALSE	2.76E-04	0.78	FALSE	4.14E-01	0.95	FALSE	8.81E-01	0.98	FALSE
M507T687_neg	507.2233	687	3	2.00E-02	1.25	FALSE	2.41E-02	1.25	FALSE	1.89E-04	1.37	FALSE	5.25E-02	1.59	FALSE
M521T676_neg	521.1304	676	3	3.02E-02	-10.15	FALSE	1.86E-01	6.36	FALSE	2.17E-02	-16.77	FALSE	3.17E-01	0.19	FALSE

XCMS			Confi-dence level	In-house library match			HMDB MS2 match		CANOPUS	HMDB MS1 match			
Feature ID	m/z	rt, sec		name	mz	rt, sec	MF	Structure	NPC Pathway	HMDB ID	Structure	MF	MS1 ppm error
M525T777_neg	525.2707	777	3						Terpenoids	HMDB0253387	Iganidipine	C28H38N4O6	2.2
M529T589_neg	529.2230	589	3							HMDB0266517	PA(2:0/PGJ2)	C25H39O10P	4.1
M537T1047_neg	537.3259	1047	3						Fatty acids				
M549T147_neg	549.1674	147	3						Carbohydrates				
M573T858_neg	573.2317	858	3							HMDB0259107	Toosendanin	C30H38O11	4.3
M581T817_neg	581.2060	817	3							HMDB0304418	Mg-protoporphyrin	C34H30MgN4O4	0.8
M585T388_neg	585.2152	388	3						Carbohydrates				
M595T892_neg	595.3500	892	3							HMDB0004157	Stercobilinogen	C33H48N4O6	0.2
M603T673_neg	603.3286	673	3							HMDB0258791	Telinavir	C33H44N6O5	2.3
M611T777_neg	611.2166	777	3							HMDB0031148	Protochlorophyllide	C35H32MgN4O5	2.6
M611T852_neg	611.2165	852	3							HMDB0031148	Protochlorophyllide	C35H32MgN4O5	2.4
M613T818_neg	613.2324	818	3						Fatty acids	HMDB0304019	agnesium-protoporphyrin IX 13-mo	C35H34MgN4O5	2.8
M639T766_neg	639.1933	766	3						Shikimates and Phenylpropanoids	HMDB0256632	Plantamajoside	C29H36O16	0.4
M723T535_neg	723.2932	535	3						Carbohydrates				
M782T977_neg	781.5600	977	3						Terpenoids				
M800T957_neg	799.5118	957	3							HMDB0264640	PA(20:0/PGE2)	C43H77O11P	1.6
M851T80_neg	851.3495	80	3							HMDB0006901	Heme A	C49H56FeN4O6	2.2

XCMS			Confi-dence level	Sample preparation Beads/DLE			Methanol storage No/Yes			Lyophilization No/Yes			Lysing Matrix E/D		
Feature ID	m/z	rt, sec		p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance	p adj	fold change	significance
M525T777_neg	525.2707	777	3	1.48E-01	0.93	FALSE	1.95E-02	1.14	FALSE	1.12E-12	1.43	FALSE	3.22E-01	1.11	FALSE
M529T589_neg	529.2230	589	3	6.29E-01	0.95	FALSE	3.21E-01	0.91	FALSE	2.68E-02	1.21	FALSE	3.79E-01	1.15	FALSE
M537T1047_neg	537.3259	1047	3	6.26E-03	1.41	FALSE	4.22E-01	0.91	FALSE	2.21E-02	0.78	FALSE	4.99E-01	1.14	FALSE
M549T147_neg	549.1674	147	3	4.64E-01	0.85	FALSE	7.59E-01	1.08	FALSE	3.66E-01	1.19	FALSE	6.48E-01	1.26	FALSE
M573T858_neg	573.2317	858	3	7.26E-01	0.98	FALSE	1.21E-01	1.08	FALSE	8.11E-02	1.08	FALSE	9.07E-01	1.02	FALSE
M581T817_neg	581.2060	817	3	7.46E-02	1.16	FALSE	1.26E-01	0.87	FALSE	4.14E-01	0.94	FALSE	6.83E-01	1.10	FALSE
M585T388_neg	585.2152	388	3	7.59E-01	0.85	FALSE	1.31E-06	-7.24	FALSE	2.86E-06	-17.49	FALSE	1.88E-01	3.31	FALSE
M595T892_neg	595.3500	892	3	2.28E-02	0.88	FALSE	8.24E-02	1.11	FALSE	9.48E-05	1.22	FALSE	3.50E-01	1.11	FALSE
M603T673_neg	603.3286	673	3	1.52E-03	1.48	FALSE	7.80E-03	0.73	FALSE	2.46E-03	1.39	FALSE	6.47E-02	0.46	FALSE
M611T777_neg	611.2166	777	3	3.48E-01	0.92	FALSE	4.27E-01	0.93	FALSE	2.22E-01	1.10	FALSE	7.35E-01	1.06	FALSE
M611T852_neg	611.2165	852	3	2.95E-03	0.81	FALSE	1.44E-01	0.90	FALSE	6.67E-02	1.12	FALSE	6.33E-01	0.93	FALSE
M613T818_neg	613.2324	818	3	5.92E-01	0.96	FALSE	3.40E-01	0.93	FALSE	3.41E-01	1.06	FALSE	7.64E-01	1.07	FALSE
M639T766_neg	639.1933	766	3	5.08E-01	1.73	FALSE	5.89E-01	1.78	FALSE	1.11E-01	3.56	FALSE	1.65E-01	2.59	FALSE
M723T535_neg	723.2932	535	3	2.67E-03	1.45	FALSE	6.19E-01	1.07	FALSE	3.16E-03	0.73	FALSE	2.18E-01	0.80	FALSE
M782T977_neg	781.5600	977	3	2.11E-08	1.28	FALSE	2.10E-04	0.85	FALSE	4.82E-02	1.07	FALSE	4.42E-01	1.07	FALSE
M800T957_neg	799.5118	957	3	9.48E-01	1.00	FALSE	9.74E-01	1.00	FALSE	5.33E-04	0.85	FALSE	6.97E-03	0.67	FALSE
M851T80_neg	851.3495	80	3	2.30E-01	0.88	FALSE	4.99E-01	1.07	FALSE	6.54E-04	1.39	FALSE	6.40E-01	0.89	FALSE