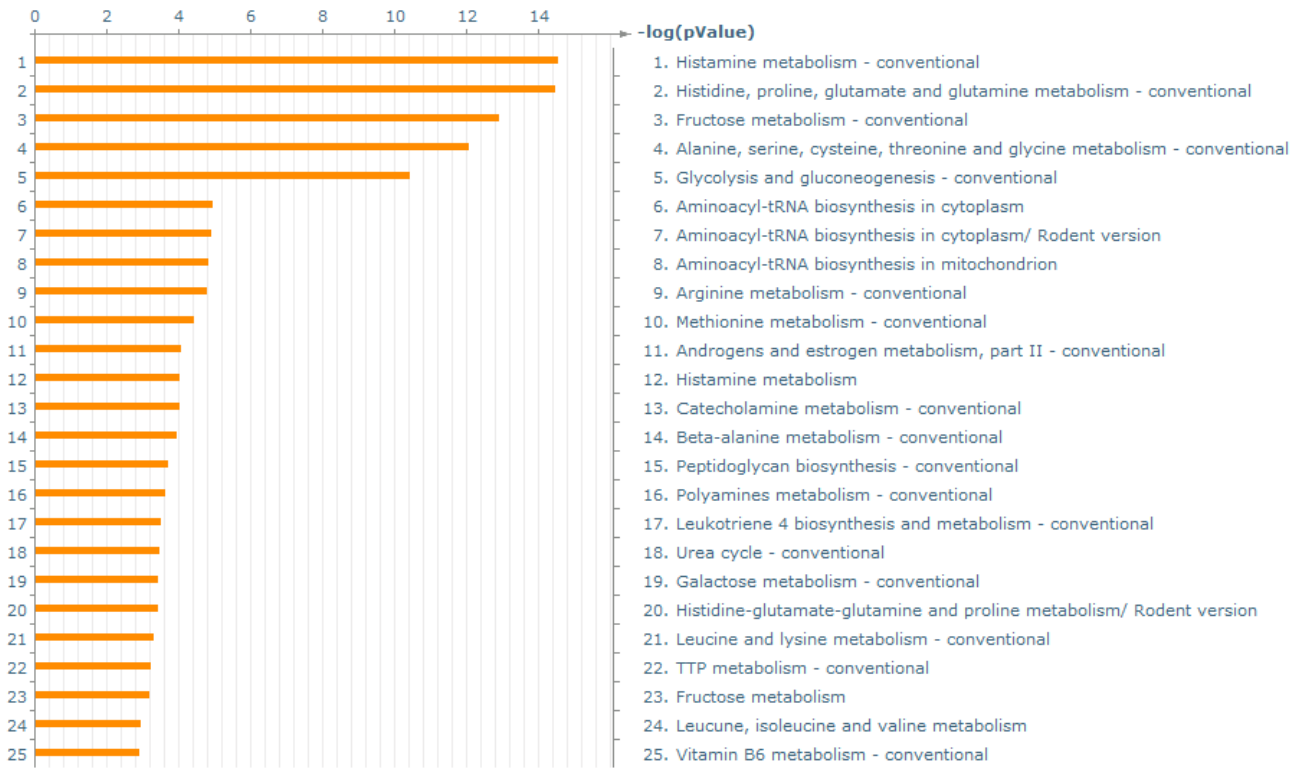

Figure S-1: Set of 25 canonical metabolic pathways relevant to the uploaded elemental formulae ranked according to their p-values (hypergeometric distribution).

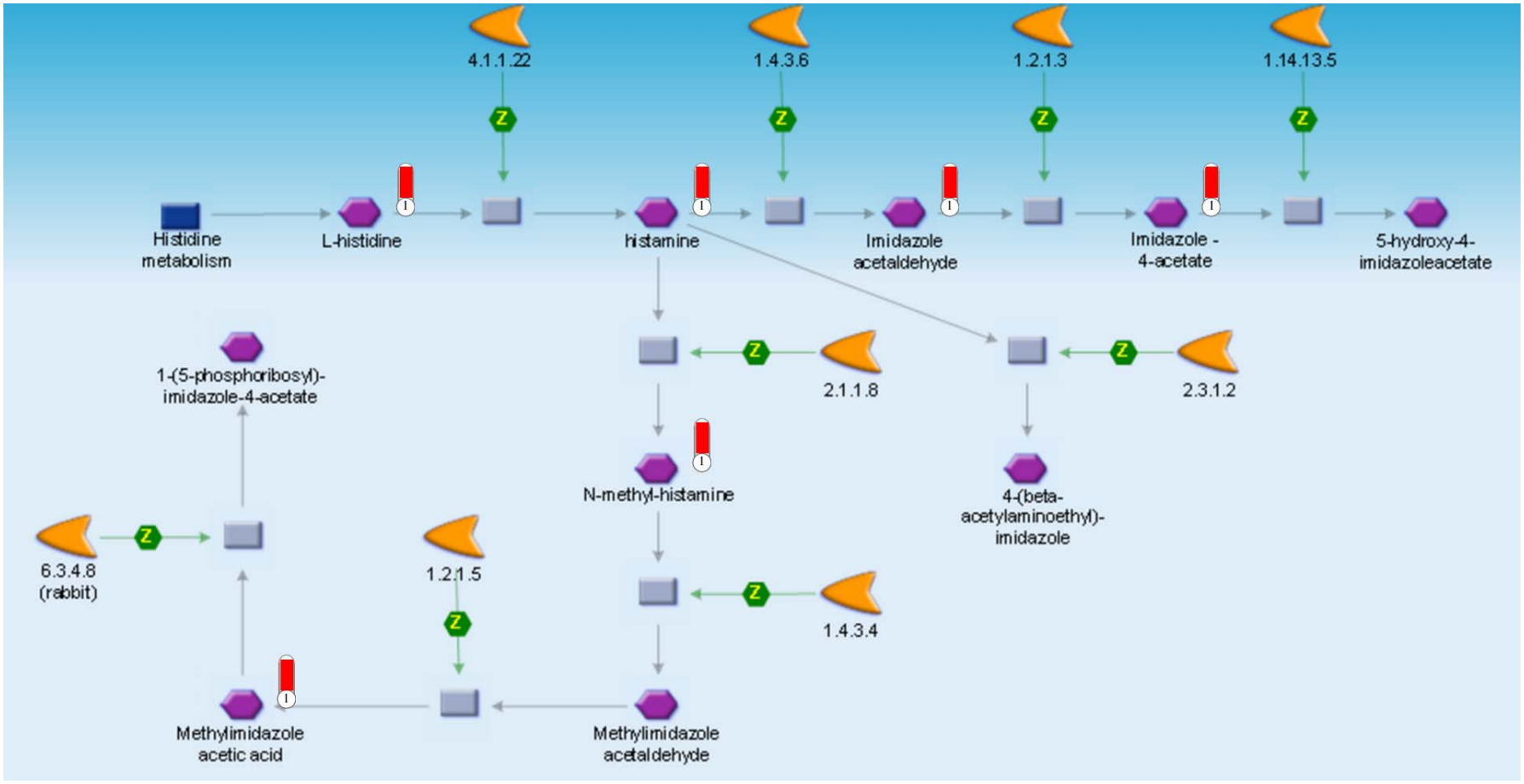

Figure S-2: Canonical pathway for histamine metabolism.

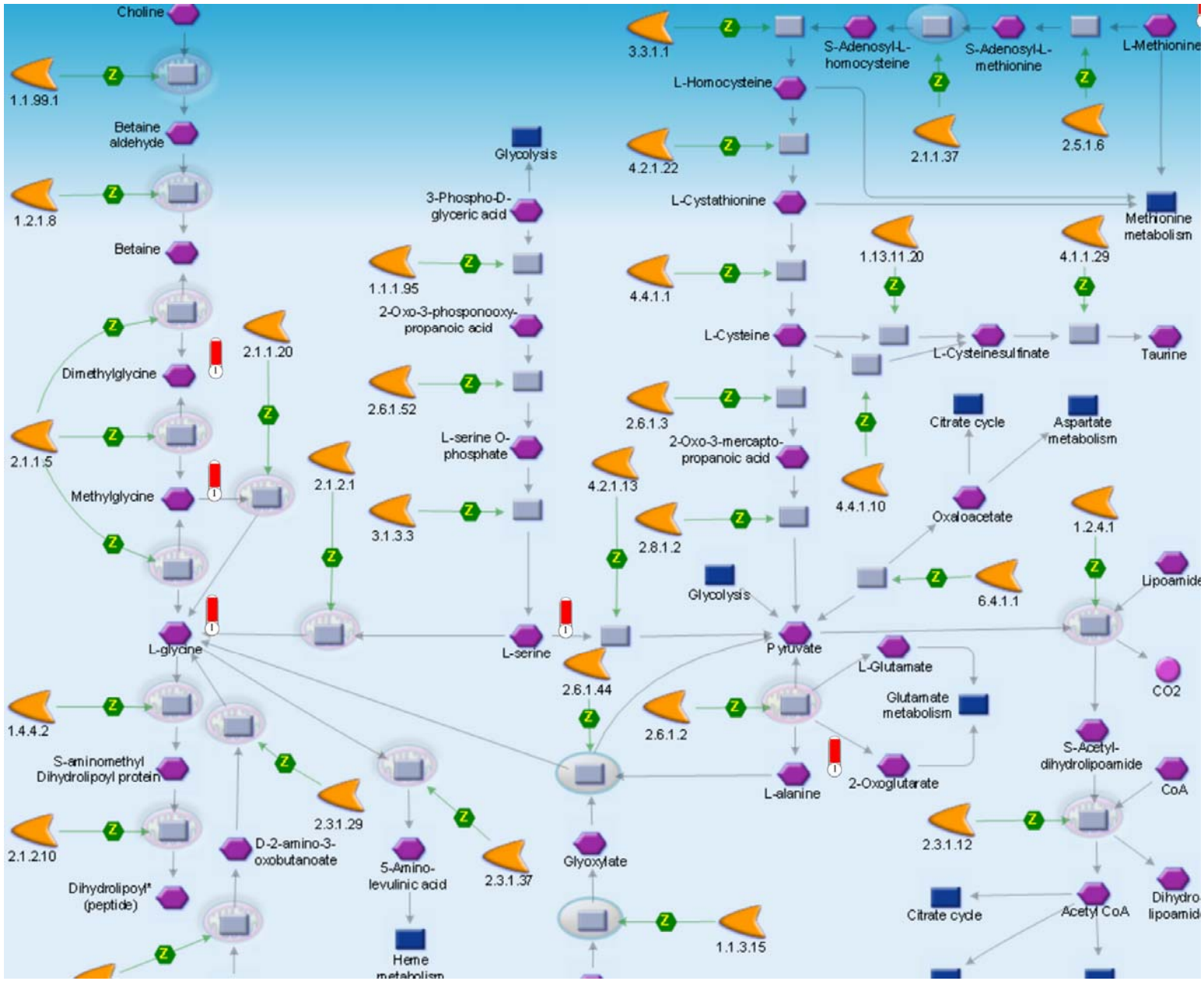

Figure S-3: Canonical pathway for alanine, serine, cysteine, threonine and glycine metabolism.

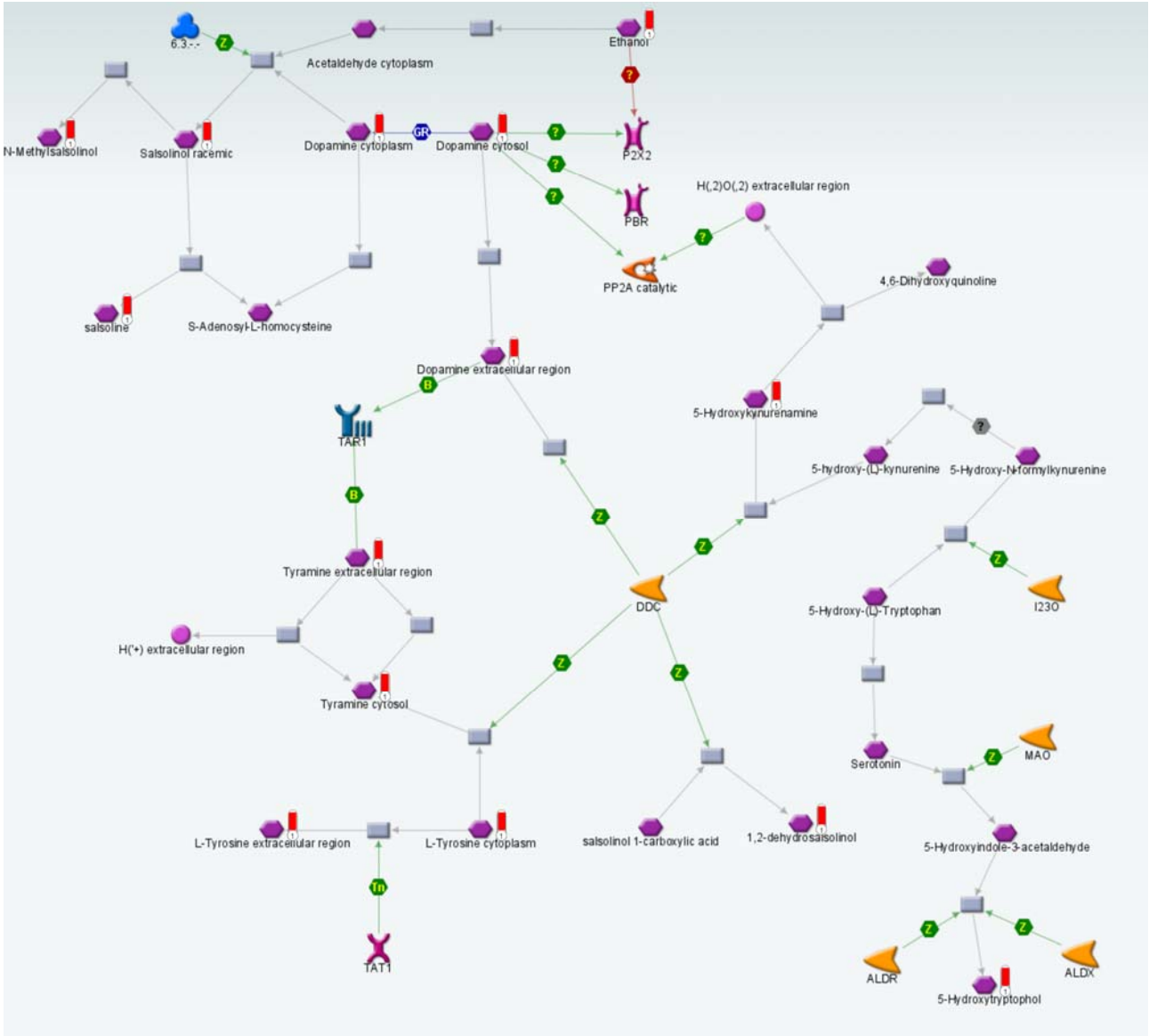

Figure S-4: Metabolic network built for tentatively identified aromatic amines in set of differentiating metabolites.

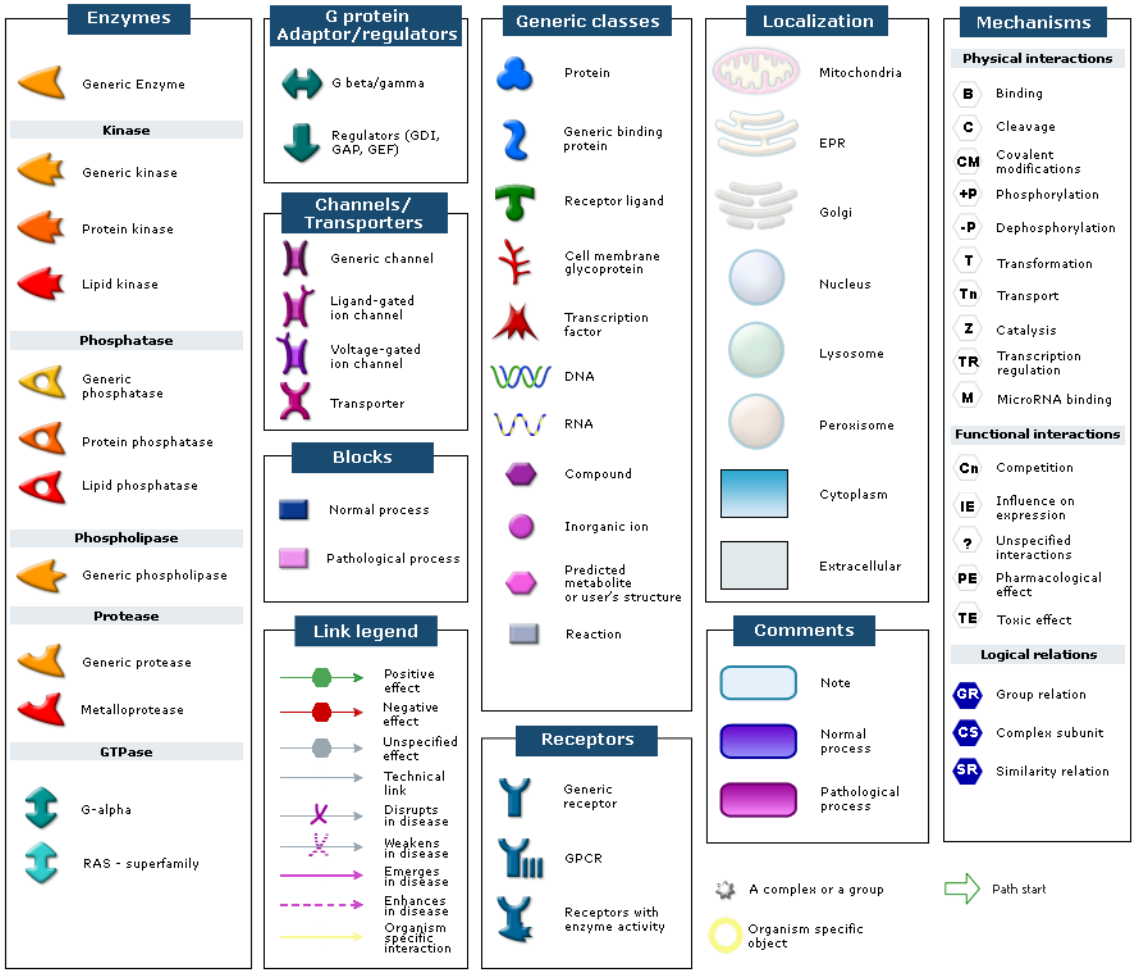

Figure S-5: Legend used in maps and pathways

a.

Classifier type	Feature selection method	Number of Features	SENS(%)	SPEC(%)	ACC(%)
fSVM	1:7:20,000 sub-sampling	2,858	100.0	93.8	96.7
fSVM_NL			100.0	93.8	96.7
fSVM	One-way ANOVA (p=0.05)	3,017	**100.0**	**100.0**	**100.0**
fSVM_NL			100.0	93.8	96.7
fSVM	One-way ANOVA (p=0.01)	1,320	92.9	93.8	93.3
fSVM_NL			92.9	100.0	96.7

b.

Classifier type	Feature selection method	Number of Features	SENS(%)	SPEC(%)	ACC(%)
fSVM	1:7:20,000 sub-sampling	2,858	**100.0**	**98.0**	**98.9**
fSVM_NL			**100.0**	**98.0**	**98.9**
fSVM	One-way ANOVA (p=0.05)	4,390	**100.0**	**98.0**	**98.9**
fSVM_NL			100.0	96.0	97.9
fSVM	One-way ANOVA (p=0.01)	2,084	**97.7**	**100.0**	**98.9**
fSVM_NL			97.7	98.0	97.9

c.

Classifier type	Feature selection method	Number of Features	SENS(%)	SPEC(%)	ACC(%)
SVM	No	20,000	100.0	93.8	96.7
SVM_NL			**100.0**	**100.0**	**100.0**
PLSDA (8LV)			**100.0**	**100.0**	**100.0**
SVM	RFE	12	92.9	93.8	93.3
SVM	L1SVM	6	92.9	93.8	93.3
SVM_NL	RFE	23	**100.0**	**100.0**	**100.0**
SVM_NL	SVMRW	25	100.0	93.8	96.7
SVM	1:7:20,000 sub-sampling	2,858	92.9	87.5	90.0
SVM_NL			92.9	93.8	93.3
PLSDA (8LV)			100.0	87.5	93.3
SVM	One-way ANOVA (p=0.05)	3,017	**100.0**	**100.0**	**100.0**
SVM_NL			100.0	87.5	93.3
PLSDA (8LV)			100.0	93.8	96.7
SVM	One-way ANOVA (p=0.01)	1,320	92.9	81.3	86.7
SVM_NL			100.0	81.3	90.0
PLSDA (8LV)			92.9	87.5	90.0

d.

Classifier type	Feature selection method	Number of Features	SENS(%)	SPEC(%)	ACC(%)
SVM	No	20,000	90.9	92	91.5
SVM_NL			**95.5**	**100**	**97.9**
PLSDA (8LV)			97.7	96	96.8
SVM	RFE	15[a]	97.7	94	95.7
SVM	L1SVM	14[a]	97.7	96	96.8
SVM_NL	RFE	18[a]	**100**	**96**	**97.9**
SVM_NL	SVMRW	35[a]	95.5	84	89.4
SVM	1:7:20,000 sub-sampling	2,858	95.5	92.0	93.6
SVM_NL			93.2	92.0	92.6
PLSDA (8LV)			93.2	90.0	91.5
SVM	One-way ANOVA (p=0.05)	4,390[a]	97.7	94.0	95.7
SVM_NL			95.5	94.0	94.7
PLSDA (8LV)			**97.7**	**98.0**	**97.9**
SVM	One-way ANOVA (p=0.01)	2,084[a]	**97.7**	**98.0**	**97.9**
SVM_NL			97.7	88.0	92.6
PLSDA (8LV)			93.2	92.0	92.6

[a]Average number of features selected over LOOCV.

Table S-1. Results from the multivariate classification of DART MS data. The best accuracies obtained are shown in bold. Simple subsampling or ANOVA feature selection in combination with fSVM classifiers were first applied only to the training dataset and then the test set predicted using the selected features subset: (a) 64-30-split validation, (b) LOOCV evaluation. SVM or PLSDA were first applied only to the training dataset and then the test set predicted using the selected features subset. (c) 64-30-split validation. (d) LOOCV.

The sensitivity (SENS), specificity (SPEC) and accuracy (ACC) were determined as follows: SENS = true positives (TP) / TP + false negatives (FN); SPEC = true negatives (TN) / TN + false positives (FP); ACC = (TP+TN) / (TP+FN+TN+FP). fSVM= functional support vector machine with linear kernel; fSVM_NL = functional support vector machine with nonlinear (NL) degree 2 polynomial kernel; SVM_NL = SVM with nonlinear degree 2 polynomial kernel; PLSDA (8LV) = partial least squares discriminant analysis with 8 latent variables; RFE = recursive feature elimination; L1SVM = L1-norm SVM; SVMRW = SVM following Weston's feature selection; PLSDA = partial least squares discriminant analysis.

Table S-2. Matching of spectral features in the *m/z* range 103~714 derived from the fSVM model with 1:7:20,000 sub-sampling to metabolomic database entries. All assignments should be treated as tentative until matches are verified by ultrahigh resolution MS, tandem MS experiments, NMR spectroscopy etc.

Feature Index in fSVM Model	Feature *m/z* in Model	Closest Peak Matched *(m/z)*	Ion Type	Experimental MW (Da)	Theoretical MW (Da)	Δm (mmu)	Estimated Elemental Formulae	Possible Match in Metabolome Databases	Source
1037	108.1764	108.0928	*Not Identified*						
1058	109.1530	109.0994	*Not Identified*						
1079	110.1295	110.0704	*Not Identified*						
1100	111.1061	111.056	*Not Identified*						
1121	112.0826	112.0896	$[M+H]^+$	111.0818	111.0796	-2.2	$C_5H_9N_3$	Histamine	MID68
1142	113.0592	113.1013	*Not Identified*						
1163	114.0357	114.0732	*Not Identified*						
1184	115.0123	115.0967	*Not Identified*						
1212	116.3143	116.0777	$[M+H]^+$	115.0699	115.0633	-6.6	$C_5H_9NO_2$	D-Proline	HMDB00162
1275	119.2440	119.0927	$[M+TMS+H]^+$	46.0454	46.0418	-3.6	C_2H_6O	Ethanol	HMDB00108
1359	123.1502	123.1186	*Not Identified*						
1380	124.1267	124.0865	*Not Identified*						

1401	125.1033	125.1333	*Not Identified*						
1422	126.0798	126.096	*Not Identified*						
1443	127.0564	127.1301	*Not Identified*						
1464	128.0329	128.0456	*Not Identified*						
1555	132.2646	132.1007	$[M+TMS+H]^+$	59.0534	59.0484	-5.0	CH_5N_3	Guanidine	HMDB01842
1576	133.2412	133.0813	$[M+TMS+H]^+$	60.0340	60.0324	-1.6	CH_4N_2O	Urea	HMDB00294
1702	139.1005	139.1499	*Not Identified*						
1723	140.0770	140.0754	*Not Identified*						
1744	141.0536	141.1415	*Not Identified*						
1765	142.0301	142.0894	*Not Identified*						
1814	144.3087	144.1093	$[M+TMS+H]^+$	71.0620	71.0609	-1.1	$C_3H_7N_2$	beta-Aminopropionitrile	MID7017
1856	146.2618	146.0839	$[M+TMS+H]^+$	73.0366	73.0528	16.2	C_3H_7NO	3-aminopropanal	HMDB01106
1877	147.2384	147.114	*Not Identified*						
1940	150.1680	150.1007	*Not Identified*						
1961	151.1446	151.1414	*Not Identified*						
1982	152.1211	152.0889	$[M+TMS+H]^+$	79.0416	79.0422	0.6	C_5H_5N	Pyridine	HMDB00926
2066	156.0273	156.0852	*Not Identified*						

2115	158.3059	158.1132	*Not Identified*						
2178	161.2356	161.1288	*Not Identified*						
2199	162.2121	162.0944	$[M+TMS+H]^+$	89.0470	89.0477	0.7	$C_3H_7NO_2$	L-Alanine	HMDB00161
2304	167.0949	167.0805	*Not Identified*						
2325	168.0714	168.094	*Not Identified*						
2367	170.0245	170.1123	*Not Identified*						
2416	172.3031	172.1059	$[M+TMS+H]^+$	99.0586	99.0684	9.8	C_5H_9NO	2-Piperidinone	HMDB11749
2458	174.2562	174.1174	*Not Identified*						
2479	175.2328	175.1408	*Not Identified*						
2500	176.2093	176.1053	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	103.0650	103.0633	-1.7	$C_4H_9NO_2$	L-a-aminobutyric acid	HMDB00452
2542	178.1624	178.0987	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	105.0514	105.0426	-8.8	$C_3H_7NO_3$	L-Serine	HMDB00187
2584	180.1155	180.1106	*Not Identified*						
2605	181.0921	181.1112	$[M+TMS+H]^+$	108.0638	108.0575	-6.3	C_7H_8O	p-Cresol	HMDB01858
2647	183.0452	183.0854	$[M+TMS+H]^+$	110.0380	110.0480	10.0	$C_5H_6N_2O$	Imidazole-4-acetaldehyde	HMDB03905
2668	184.0217	184.1321	$[M+TMS+H]^+$	111.0848	111.0796	-5.2	$C_5H_9N_3$	Histamine	HMDB00870
2696	185.3238	185.1208	*Not Identified*						
2717	186.3003	186.1425	*Not Identified*						

2738	187.2769	187.1185	$[M+TMS+H]^+$	114.0712	114.0681	-3.1	$C_6H_{10}O_2$	trans-Hex-2-enoic acid	HMDB10719
2759	188.2534	188.1084	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	115.0610	115.0633	2.3	$C_5H_9NO_2$	L-Proline	HMDB00162
2864	193.1362	193.1822	*Not Identified*						
2885	194.1127	194.1087	$[M+TMS+H]^+$	121.0614	121.0528	-8.6	C_7H_7NO	Benzamide	HMDB04461
2969	198.0189	198.127	$[M+TMS+H]^+$	125.0796	125.0953	15.7	$C_6H_{11}N_3$	1-Methylhistamine	HMDB00898
3018	200.2975	200.112	$[M+TMS+H]^+$	127.0646	127.0633	-1.3	$C_6H_9NO_2$	D-1-Piperideine-2-carboxylic acid	HMDB01084
3060	202.2506	202.0905	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	129.0432	129.0426	-0.6	$C_5H_7NO_3$	Pyroglutamic acid	HMDB00267
3102	204.2037	204.1398	$[M+TMS+H]^+$	131.0924	131.0946	2.2	$C_6H_{13}NO_2$	L-Isoleucine	HMDB00172
3186	208.1099	208.1152	$[M+TMS+H]^+$	135.0679	135.0684	0.5	C_8H_9NO	2-Phenylacetamide	HMDB10715
3207	209.0865	209.1359	$[M+TMS+H]^+$	136.0886	136.0749	-13.7	$C_6H_8N_4$	Tetrahydropteridine	HMDB01216
3228	210.0630	210.1228	$[M+TMS+H]^+$	137.0754	137.0841	8.7	$C_8H_{11}NO$	Tyramine	HMDB00306
3249	211.0396	211.1304	*Not Identified*						
3270	212.0161	212.1096	*Not Identified*						
3319	214.2947	214.1424	$[M+TMS+H]^+$	141.0950	141.0902	-4.8	$C_6H_{11}N_3O$	L-Histidinol	HMDB03431
3361	216.2478	216.1269	$[M+TMS+H]^+$	143.0796	143.0946	15.0	$C_7H_{13}NO_2$	Proline betaine	HMDB04827
3487	222.1071	222.1132	$[M+TMS+H]^+$	149.0658	149.0701	4.3	$C_6H_7N_5$	6-Methyladenine	HMDB02099
3550	225.0368	225.111	$[M+TMS+H]^+$	152.0636	152.0685	4.9	$C_5H_{12}O_5$	D-Arabitol	HMDB00568

3620	228.2919	228.2617	*Not Identified*						
3641	229.2685	229.1891	*Not Identified*						
3662	230.2450	230.153	*Not Identified*						
3704	232.1981	232.1383	$[M+TMS+H]^+$	159.0910	159.0895	-1.5	$C_7H_{13}NO_3$	2-Methyl- butyrylglycine	HMDB00339
3767	235.1278	235.1697	*Not Identified*						
3830	238.0574	238.1238	$[M+TMS+H]^+$	165.0764	165.0651	-11.3	$C_6H_7N_5O$	7-Methylguanine	HMDB00897
3900	241.3126	241.1302	$[M+TMS+H]^+$	168.0828	168.0899	7.1	$C_8H_{12}N_2O_2$	Pyridoxamine	HMDB01431
3921	242.2891	242.1356	$[M+TMS+H]^+$	169.0882	169.0851	-3.1	$C_7H_{11}N_3O_2$	1-Methylhistidine	HMDB00001
3942	243.2657	243.2024	*Not Identified*						
3963	244.2422	244.1403	$[M+TMS+H]^+$	171.0929	171.0895	-3.4	$C_8H_{13}NO_3$	N-butanoyl-lhomoserine lactone	MID36732
4005	246.1953	246.1479	$[M+TMS+H]^+$	173.1006	173.1052	4.6	$C_8H_{15}NO_3$	Hexanoylglycine	HMDB00701
4047	248.1484	248.1361	$[M+TMS+H]^+$	175.0888	175.0957	6.9	$C_6H_{13}N_3O_3$	Citrulline	HMDB00904
4089	250.1015	250.1414	$[M+TMS+H]^+$	177.0940	177.0790	-15.0	$C_{10}H_{11}NO_2$	5-Hydroxytryptophol	HMDB01855
4131	252.0546	252.1394	$[M+TMS+H]^+$	179.0920	179.0946	2.6	$C_{10}H_{13}NO_2$	2(N)-Methyl-norsalsolinol	HMDB01189
4173	254.0077	254.1522	$[M+TMS+H]^+$	181.1048	181.0964	-8.4	$C_7H_{11}N_5O$	6-methyl-tetrahydropterin	HMDB02249
4243	257.2629	257.2311	$[M+TMS+H]^+$	184.1838	184.1827	-1.1	$C_{12}H_{24}O$	11-dodecen-1-ol	MID36478
4264	258.2394	258.2817	*Not Identified*						

4285	259.2160	259.1428	$[M+TMS+H]^+$	186.0954	186.1004	5.0	$C_8H_{14}N_2O_3$	Ala Pro	MID23860
4306	260.1925	260.1541	$[M+2TMS+H]^+$	115.0672	115.0633	-3.9	$C_5H_9NO_2$	Proline	MID29
4369	263.1222	263.2296	*Not Identified*						
4390	264.0987	264.196	*Not Identified*						
4432	266.0518	266.147	$[M+TMS+H]^+$	193.0997	193.1103	10.6	$C_{11}H_{15}NO_2$	(R)-N-Methylsalsolinol	HMDB03626
4496	268.0284	267.267	*Not Identified*						
4474	268.0049	268.1692	*Not Identified*						
4502	269.3070	269.1688	*Not Identified*						
4523	270.2835	270.1698	$[M+2TMS+H]^+$	125.0829	125.0953	12.4	$C_6H_{11}N_3$	1-Methylhistamine	HMDB00898
4544	271.2601	271.1195	$[M+2TMS+H]^+$	126.0326	126.0429	10.3	$C_5H_6N_2O_2$	Thymine	HMDB00262
4565	272.2366	272.1781	*Not Identified*						
4607	274.1897	274.13	$[M+2TMS+H]^+$	129.0431	129.0426	-0.5	$C_5H_7NO_3$	Pyroglutamic acid	MID3251
4691	278.0959	278.1682	*Not Identified*						
4712	279.0725	279.1551	$[M+2TMS+H]^+$	134.0682	134.0579	-10.3	$C_5H_{10}O_4$	Deoxyribose	HMDB03224
4733	280.0490	280.1564	$[M+2TMS+H]^+$	135.0695	135.0684	-1.1	C_8H_9NO	2-Phenylacetamide	HMDB10715
4754	281.0256	281.2894	*Not Identified*						
4775	282.0021	282.2802	*Not Identified*						

4803	283.3042	283.2658	*Not Identified*						
4824	284.2807	284.1606	$[M+2TMS+H]^+$	139.0737	139.0746	0.9	$C_6H_9N_3O$	Histidinal	HMDB12234
4845	285.2573	285.2806	*Not Identified*						
4908	288.1869	288.1624	$[M+TMS+H]^+$	215.1150	215.1157	0.7	$C_{10}H_{17}NO_4$	2-amino-8-oxo-9,10-epoxy-decanoic acid	MID35859
4992	292.0931	292.1655	$[M+3TMS+H]^+$	75.0391	75.0320	-7.1	$C_2H_5NO_2$	Glycine	HMDB00123
5013	293.0697	293.1588	$[M+2TMS+H]^+$	148.0719	148.0736	1.7	$C_6H_{12}O_4$	Mevalonic acid	HMDB00227
5034	294.0462	294.1537	$[M+2TMS+H]^+$	149.0668	149.0510	-15.8	$C_5H_{11}NO_2S$	L-Methionine	HMDB00696
5055	295.0228	295.1787	*Not Identified*						
5083	296.3248	297.2538	$[M+TMS+H]^+$	224.2065	224.2140	7.5	$C_{15}H_{28}O$	10-pentadecenal	MID36604
5125	298.2779	298.1833	$[M+2TMS+H]^+$	153.0964	153.0790	-17.4	$C_8H_{11}NO_2$	Dopamine	HMDB00073
5146	299.2545	299.2597	$[M+TMS+H]^+$	226.2124	226.1933	-19.1	$C_{14}H_{26}O_2$	5-Tetradecenoic acid	HMDB00499
5167	300.2310	300.1662	$[M+2TMS+H]^+$	155.0793	155.0695	-9.8	$C_6H_9N_3O_2$	L-Histidine	HMDB00177
5188	301.2076	301.1874	$[M+TMS+H]^+$	228.1401	228.1474	7.3	$C_{11}H_{20}N_2O_3$	L-isoleucyl-L-proline	HMDB11174
5209	302.1841	302.1712	$[M+2TMS+H]^+$	157.0843	157.0739	-10.4	$C_7H_{11}NO_3$	3-Methyl- crotonylglycine	HMDB00459
5230	303.1607	303.2969	*Not Identified*						
5251	304.1372	304.171	$[M+2TMS+H]^+$	159.0841	159.0895	5.4	$C_7H_{13}NO_3$	2-Methyl- butyrylglycine	HMDB00339
5293	306.0903	306.1762	$[M+3TMS+H]^+$	89.0498	89.0477	-2.1	$C_3H_7NO_2$	Beta-Alanine	HMDB00056

5335	308.0434	308.1673	$[M+2TMS+H]^+$	163.0804	163.0633	-17.1	$C_9H_9NO_2$	3-Methyldioxyindole	HMDB04186
5356	309.0200	309.1566	$[M+TMS+H]^+$	236.1092	236.1017	-7.5	$C_9H_{20}N_2OS_2$	S-aminomethyl-dihydrolipoamide	HMDB06239
5447	313.2517	313.2913	$[M+TMS+H]^+$	240.2440	240.2453	1.3	$C_{16}H_{32}O$	9-hexadecen-1-ol	MID36487
5489	315.2048	315.1044	$[M+2TMS+H]^+$	170.0175	169.9980	-19.5	$C_3H_7O_6P$	D-Glyceraldehyde 3-phosphate	HMDB01112
5552	318.1344	318.1817	$[M+2TMS+H]^+$	173.0948	173.1052	10.4	$C_8H_{15}NO_3$	Hexanoylglycine	HMDB00701
5594	320.0875	320.1781	$[M+2TMS+H]^+$	175.0912	175.0957	4.5	$C_6H_{13}N_3O_3$	Citrulline	HMDB00904
5657	323.0172	323.1745	*Not Identified*						
5685	324.3192	324.1645	$[M+TMS+H]^+$	251.1172	251.1018	-15.4	$C_{10}H_{13}N_5O_3$	Deoxyadenosine	HMDB00101
5706	325.2958	325.1855	$[M+2TMS+H]^+$	180.0986	180.0899	-8.7	$C_9H_{12}N_2O_2$	5-Hydroxy-kynurenamine	HMDB04076
5727	326.2723	326.1599	$[M+2TMS+H]^+$	181.0730	181.0739	0.9	$C_9H_{11}NO_3$	L-Tyrosine	HMDB00158
5748	327.2489	327.2764	$[M+TMS+H]^+$	254.2291	254.2246	-4.5	$C_{16}H_{30}O_2$	Hypogeic acid	HMDB02186
5790	329.2020	329.2859	$[M+TMS+H]^+$	256.2386	256.2402	1.6	$C_{16}H_{32}O_2$	Palmitic acid	HMDB00220
5832	331.1551	331.2722	$[M+2TMS+H]^+$	258.2249	258.2195	-5.4	$C_{15}H_{30}O_3$	2-hydroxy-pentadecanoic acid	MID35423
5853	332.1316	332.1598	$[M+TMS+H]^+$	259.1125	259.1168	4.3	$C_{10}H_{17}N_3O_5$	Ser Pro Gly	MID33557
5937	336.0378	336.235	*Not Identified*						
5986	338.3164	338.1905	*Not Identified*						
6112	344.1757	344.3206	*Not Identified*						

6049	341.2461	341.3034	*Not Identified*						
6133	345.1523	345.2206	$[M+TMS+H]^+$	272.1733	272.1776	4.3	$C_{18}H_{24}O_2$	Estradiol	HMDB00151
6154	346.1288	346.1878	$[M+TMS+H]^+$	273.1405	273.1325	-8.0	$C_{11}H_{19}N_3O_5$	Gly Pro Thr	MID22941
6175	347.1054	347.2285	$[M+2TMS+H]^+$	202.1416	202.1430	1.4	$C_8H_{18}N_4O_2$	Dimethyl-L-arginine	HMDB01539
6287	352.3136	352.2091	*Not Identified*						
6308	353.2902	353.2908	$[M+TMS+H]^+$	280.2435	280.2402	-3.3	$C_{18}H_{32}O_2$	Bovinic acid	HMDB03797
6350	355.2433	355.3029	$[M+TMS+H]^+$	282.2556	282.2559	0.3	$C_{18}H_{34}O_2$	Vaccenic acid	HMDB03231
6392	357.1964	357.3194	$[M+TMS+H]^+$	284.2720	284.2715	-0.5	$C_{18}H_{36}O_2$	Stearic acid	HMDB00827
6434	359.1495	359.3168	*Not Identified*						
6455	360.1260	360.3305	$[M+TMS+H]^+$	287.2832	287.2824	-0.8	$C_{17}H_{37}NO_2$	C17 Sphinganine	MID41558
6476	361.1026	361.3344	*Not Identified*						
6539	364.0322	364.1823	$[M+TMS+H]^+$	291.1350	291.1327	-2.3	$C_{13}H_{25}NO_2S_2$	S-(3-Methylbutanoyl)-dihydrolipoamide-E	HMDB06867
6588	366.3108	367.3389	*Not Identified*						
6651	369.2405	369.3507	$[M+TMS+H]^+$	296.3034	296.3079	4.5	$C_{20}H_{40}O$	11Z-eicosen-1-ol	MID36508
6693	371.1936	371.3576	*Not Identified*						
6756	374.1232	374.3349	$[M+TMS+H]^+$	301.2876	301.2981	10.5	$C_{18}H_{39}NO_2$	Sphinganine	HMDB00269
6798	376.0763	376.2339	$[M+2TMS+H]^+$	231.1470	231.1583	11.3	$C_{10}H_{21}N_3O_3$	Gamma-Aminobutyryl-lysine	HMDB01959

6840	378.0294	378.2119	$[M+3TMS+H]^+$	161.0855	161.0688	-16.7	$C_6H_{11}NO_4$	Aminoadipic acid	HMDB00510
6861	379.0060	379.1802	$[M+2TMS+H]^+$	234.0933	234.0852	-8.1	$C_8H_{14}N_2O_6$	L-beta-aspartyl-L-threonine	HMDB11169
6952	383.2377	383.3388	$[M+TMS+H]^+$	310.2915	310.2872	-4.3	$C_{20}H_{38}O_2$	14Z-eicosenoic acid	MID34768
6994	385.1908	385.3174	$[M+TMS+H]^+$	312.2700	312.2664	-3.6	$C_{19}H_{36}O_3$	10-oxo-nonadecanoic acid	MID35818
7036	387.1439	387.1435	*Not Identified*						
7057	388.1204	388.3615	*Not Identified*						
7099	390.0735	390.3692	*Not Identified*						
7120	391.0501	391.2645	$[M+TMS+H]^+$	318.2172	318.2195	2.3	$C_{20}H_{30}O_3$	5-HEPE	HMDB05081
7141	392.0266	392.229	$[M+3TMS+H]^+$	175.1026	175.0957	-6.9	$C_6H_{13}N_3O_3$	Argininic acid	HMDB03148
7190	394.3052	394.2083	$[M+3TMS+H]^+$	177.0819	177.0790	-2.9	$C_{10}H_{11}NO_2$	5-Hydroxytryptophol	HMDB01855
7232	396.2583	396.2009	$[M+3TMS+H]^+$	179.0745	179.0794	4.9	$C_6H_{13}NO_5$	Fructosamine	HMDB02030
7253	397.2349	397.2051	$[M+3TMS+H]^+$	180.0787	180.0634	-15.3	$C_6H_{12}O_6$	D-Glucose	HMDB00122
7295	399.1880	399.3415	$[M+TMS+H]^+$	326.2942	326.2821	-12.1	$C_{20}H_{38}O_3$	19-oxo-eicosanoic acid	MID35822
7316	400.1645	400.3961	*Not Identified*						
7337	401.1411	401.3334	$[M+TMS+H]^+$	328.2861	328.2977	11.6	$C_{20}H_{40}O_3$	2-hydroxy-eicosanoic acid	MID35451
7358	402.1176	402.368	Not Identified						
7379	403.0942	403.3303	$[M+TMS+H]^+$	330.2830	330.2770	-6.0	$C_{19}H_{38}O_4$	MG(0:0/16:0/0:0)	HMDB11533

7400	404.0707	404.2066	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	259.1197	259.1168	-2.9	$C_{10}H_{17}N_3O_5$	Ser Pro Gly	MID22557
7442	406.0238	406.2184	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	261.1315	261.1325	1.0	$C_{10}H_{19}N_3O_5$	Ser Gly Val	MID23067
7491	408.3024	408.2776	*Not Identified*						
7533	410.2555	410.2265	$[M+TMS+H]^+$	337.1792	337.1750	-4.2	$C_{15}H_{23}N_5O_4$	Kyotorphin	HMDB05768
7596	413.1852	413.3419	$[M+TMS+H]^+$	340.2946	340.2977	3.1	$C_{21}H_{40}O_3$	2-oxo-heneicosanoic acid	MID35825
7659	416.1148	416.2254	$[M+2TMS+H]^+$	271.1385	271.1406	2.1	$C_{11}H_{19}N_4O_4$	2-(3-Carboxy-3-(methylammonio)propyl)-L-histidine	HMDB11654
7701	418.0679	418.3526	$[M+TMS+H]^+$	345.3053	345.3032	-2.1	$C_{23}H_{39}NO$	N-propyl arachidonoyl amine	MID36681
7722	419.0445	419.2884	$[M+3TMS+H]^+$	202.1620	202.1430	-19.0	$C_8H_{18}N_4O_2$	Dimethyl-L-arginine	HMDB01539
7792	422.2996	422.2203	$[M+2TMS+H]^+$	277.1334	277.1175	-15.9	$C_{12}H_{15}N_5O_3$	Queuine	HMDB01495
7813	423.2762	423.2556	$[M+TMS+H]^+$	350.2083	350.2093	1.0	$C_{20}H_{30}O_5$	8-iso-15-keto-PGE2	HMDB02341
7834	424.2527	424.2178	$[M+3TMS+H]^+$	207.0914	207.0752	-16.2	$C_8H_{17}NOS_2$	Dihydrolipoamide	HMDB00985
7855	425.2293	425.3162	$[M+TMS+H]^+$	352.2689	352.2614	-7.5	$C_{21}H_{36}O_4$	MG(0:0/18:3(6Z,9Z,12Z)/0:0)	HMDB11539
7918	428.1589	428.3949	$[M+TMS+H]^+$	355.3476	355.3450	-2.6	$C_{22}H_{45}NO_2$	N-(2-hydroxyethyl)icosanamide	MID3723
7939	429.1355	429.3694	$[M+TMS+H]^+$	356.3221	356.3290	6.9	$C_{22}H_{44}O_3$	2-hydroxy behenic	MID35454
7981	431.0886	431.3533	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	358.3060	358.3083	2.3	$C_{21}H_{42}O_4$	MG(18:0/0:0/0:0)	HMDB11131
8072	435.3203	435.3824	$[M+TMS+H]^+$	362.3351	362.3185	-16.6	$C_{24}H_{42}O_2$	5beta-Cholane-3alpha,24-diol	MID42895

8114	437.2734	437.3135	$[M+2TMS+H]^+$	292.2266	292.2402	13.6	$C_{19}H_{32}O_2$	3b,17b-Dihydroxyetiocholane	HMDB00369
8163	439.5520	439.2287	$[M+TMS+H]^+$	366.1814	366.1652	-16.2	$C_{15}H_{22}N_6O_5$	Pro His Asn	MID23382
8240	443.1327	443.2628	$[M+TMS+H]^+$	370.2155	370.2329	17.4	$C_{16}H_{30}N_6O_4$	Val Arg Pro	MID23376
8282	445.0858	445.2388	$[M+3TMS+H]^+$	228.1124	228.1110	-1.4	$C_{10}H_{16}N_2O_4$	Prolylhydroxyproline	HMDB06695
8324	447.0389	447.3446	$[M+2TMS+H]^+$	302.2577	302.2457	-12.0	$C_{17}H_{34}O_4$	MG(0:0/14:0/0:0)	HMDB11530
8345	448.0154	448.3935	*Not Identified*						
8394	450.2940	450.2371	$[M+3TMS+H]^+$	233.1107	233.0916	-19.1	$C_{10}H_{11}N_5O_2$	Dihydroxycoprostanoic acid	HMDB01974
8415	451.2706	451.2253	$[M+3TMS+H]^+$	234.0989	234.1004	1.5	$C_{12}H_{14}N_2O_3$	5-Methoxytryptophan	HMDB02339
8604	460.0595	460.4028	$[M+TMS+H]^+$	387.3555	387.3501	-5.4	$C_{26}H_{45}NO$	25-Azacholesterol	HMDB01028
8695	464.2912	464.2809	$[M+3TMS+H]^+$	247.1545	247.1532	-1.3	$C_{10}H_{21}N_3O_4$	Lys Thr	MID23652
8779	468.1974	468.2377	$[M+3TMS+H]^+$	251.1113	251.1018	-9.5	$C_{10}H_{13}N_5O_3$	Deoxyadenosine	HMDB00101
8842	471.1271	471.3956	$[M+TMS+H]^+$	398.3483	398.3548	6.5	$C_{28}H_{46}O$	4a-Methylzymosterol	HMDB01217
8884	473.0802	473.3847	$[M+TMS+H]^+$	400.3374	400.3341	-3.3	$C_{27}H_{44}O_2$	7-Ketocholesterol	HMDB00501
8926	475.0333	475.3655	$[M+2TMS+H]^+$	330.2786	330.2770	-1.6	$C_{19}H_{38}O_4$	MG(0:0/16:0/0:0)	HMDB11533
8996	478.2884	478.2522	$[M+3TMS+H]^+$	261.1258	261.1325	6.7	$C_{10}H_{19}N_3O_5$	Ser Gly Val	MID23067
9080	482.1946	482.26	$[M+2TMS+H]^+$	337.1731	337.1750	1.9	$C_{15}H_{23}N_5O_4$	Kyotorphin	HMDB05768
9143	485.1243	485.3228	*Not Identified*						

9185	487.0774	487.2499	$[M+TMS+H]^+$	414.2026	414.2049	2.3	$C_{17}H_{30}N_6O_4S_1$	Lys Met His	MID23058
9248	490.0070	490.2768	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	345.1899	345.1900	0.1	$C_{15}H_{27}N_3O_6$	Val Glu Val	MID22736
9297	492.2856	492.2743	$[M+3TMS+H]^+$	275.1479	275.1481	0.2	$C_{11}H_{21}N_3O_5$	Epsilon-(gamma-Glutamyl)-lysine	HMDB03869
9339	494.2387	494.2575	$[M+3TMS+H]^+$	277.1311	277.1175	-13.6	$C_{12}H_{15}N_5O_3$	Queuine	HMDB01495
9381	496.1918	496.2643	$[M+2TMS+H]^+$	351.1774	351.1794	2.0	$C_{17}H_{25}N_3O_5$	Val Tyr Ala	MID22964
9465	500.0980	500.4358	$[M+2TMS+H]^+$	355.3489	355.3450	-3.9	$C_{22}H_{45}NO_2$	N-(2-hydroxyethyl) icosanamide	MID3723
9507	502.0511	502.4386	*Not Identified*						
9528	503.0277	503.39	$[M+TMS+H]^+$	430.3426	430.3447	2.1	$C_{28}H_{46}O_3$	1α-hydroxy-25-methoxyvitamin D3	MID42264
9619	507.2594	507.5022	*Not Identified*						
9640	508.2359	508.2806	$[M+3TMS+H]^+$	291.1542	291.1430	-11.2	$C_{11}H_{21}N_3O_6$	Ala Thr Thr	MID22878
9682	510.1890	510.2765	$[M+2TMS+H]^+$	365.1896	365.1951	5.5	$C_{18}H_{27}N_3O_5$	Ser Phe Ile	MID22773
9808	516.0483	516.45	*Not Identified*						
9829	517.0249	518.2985	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	301.1721	301.1638	-8.3	$C_{13}H_{23}N_3O_5$	Pro Ser Val	MID23420
9850	518.0014	518.4984	*Not Identified*						
9899	520.2800	520.5065	*Not Identified*						
9941	522.2331	522.2826	$[M+TMS+H]^+$	449.2352	449.2387	3.5	$C_{20}H_{31}N_7O_5$	Gln Arg Phe	MID22049

10025	526.1393	526.2566	$[M+3TMS+H]^+$	309.1302	309.1325	2.3	$C_{14}H_{19}N_3O_5$	Tyr Gly Ala	MID23104
10109	530.0455	530.4306	$[M+TMS+H]^+$	457.3833	457.3920	8.7	$C_{30}H_{51}NO_2$	3'-O-Aminopropyl-25-hydroxyvitamin D3	MID42610
10130	531.0221	531.2916	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	458.2442	458.2338	-10.4	$C_{23}H_{38}O_7S$	3-Sulfodeoxycholic acid	HMDB02504
10158	532.3241	532.3106	$[M+TMS+H]^+$	459.2632	459.2554	-7.8	$C_{17}H_{33}N_9O_6$	Arg Arg Glu	MID23106
10200	534.2772	534.5247	*Not Identified*						
10326	540.1365	540.2642	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	323.1378	323.1481	10.3	$C_{15}H_{21}N_3O_5$	Tyr Ala Ala	MID22475
10501	548.2744	548.2722	$[M+TMS+H]^+$	475.2248	475.2179	-6.9	$C_{21}H_{29}N_7O_6$	Trp Asp Arg	MID22780
10543	550.2275	550.2827	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	333.1563	333.1536	-2.7	$C_{13}H_{23}N_3O_7$	Asp Val Thr	MID23209
10732	559.0165	559.2889	$[M+2TMS+H]^+$	414.2020	414.2049	2.9	$C_{17}H_{30}N_6O_4S_1$	Lys Met His	MID23058
10886	566.1778	566.2841	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	349.1577	349.1485	-9.2	$C_{13}H_{23}N_3O_8$	Glu Thr Thr	MID21841
10928	568.1309	568.293	$[M+TMS+H]^+$	495.2456	495.2482	2.6	$C_{26}H_{33}N_5O_5$	Trp Lys Tyr	MID21781
11103	576.2688	576.4439	$[M+TMS+H]^+$	503.3965	503.4008	4.3	$C_{28}H_{57}NO_4S$	2-hexacosanamido-ethanesulfonic acid	MID3740
11145	578.2219	578.543	*Not Identified*						
11229	582.1281	582.3106	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	365.1842	365.1951	10.9	$C_{18}H_{27}N_3O_5$	Ser Phe Ile	MID22773
11313	586.0343	586.3148	$[M+TMS+H]^+$	513.2674	513.2760	8.6	$C_{26}H_{43}NO_7S$	Sulfolithocholylglycine	HMDB02639
11446	592.2191	592.5467	*Not Identified*						

11572	598.0784	598.295	$[M+3TMS+H]^+$	381.1686	381.1536	-15.0	$C_{17}H_{23}N_3O_7$	Phe Ser Glu	MID23135
11663	602.3101	602.3189	$[M+TMS+H]^+$, $[M+2TMS+H]^+$	529.2716	529.2709	-0.7	$C_{26}H_{43}NO_8S$	N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfooxy)cholan-24-yl]-Glycine	HMDB02409
11684	603.2867	603.3334	$[M+2TMS+H]^+$	458.2465	458.2390	-7.5	$C_{21}H_{30}N_8O_4$	Arg Phe His	MID21269
11705	604.2632	604.3471	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	387.2207	387.2230	2.3	$C_{17}H_{33}N_9O_6$	Arg Arg Glu	MID23106
11831	610.1225	610.3368	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	393.2104	393.2264	16.0	$C_{20}H_{31}N_3O_5$	Ile Val Tyr	MID23584
11873	612.0756	612.2989	$[M+3TMS+H]^+$	395.1725	395.1693	-3.2	$C_{18}H_{25}N_3O_7$	Thr Glu Phe	MID23502
12027	619.237	619.3249	$[M+TMS+H]^+$	546.2776	546.2703	-7.3	$C_{28}H_{34}N_8O_4$	Arg Trp Trp	MID19915
12048	620.2135	620.3034	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	403.1815	403.1770	-4.5	$C_{14}H_{25}N_7O_7$	Asn Arg Asp	MID22139
12216	628.0259	628.3128	$[M+TMS+H]^+$	555.2693	555.2654	-3.9	$C_{28}H_{37}N_5O_7$	Leucine Enkephalin	MID24069
12265	630.3045	630.3436	*Not Identified*						
12307	632.2576	632.371	$[M+3TMS+H]^+$	415.2446	415.2543	9.7	$C_{17}H_{33}N_7O_5$	Ile Arg Gln	MID22784
12391	636.1638	636.3449	$[M+3TMS+H]^+$	419.2185	419.2169	-1.6	$C_{20}H_{29}N_5O_5$	Trp Ser Lys	MID22695
12433	638.1169	638.3212	$[M+3TMS+H]^+$	421.1961	421.1948	-1.3	$C_{19}H_{27}N_5O_6$	Gln Phe Gln	MID22749
12475	640.07	640.328	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	423.2016	423.2006	-1.0	$C_{20}H_{29}N_3O_7$	Tyr Ile Glu	MID22318

12650	648.2079	648.3302	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	431.2038	431.2128	9.0	$C_{16}H_{29}N_7O_7$	Gln Glu Arg	MID21914
12692	650.161	650.3447	$[M+3TMS+H]^+$	433.2183	433.2220	3.7	$C_{15}H_{31}N_9O_4S_1$	Arg Cys Arg	MID21431
12776	654.0672	654.3428	$[M+3TMS+H]^+$	437.2164	437.2274	11.0	$C_{20}H_{31}N_5O_6$	Tyr Lys Gln	MID22135
12909	660.252	660.3563	$[M+2TMS+H]^+$	515.2694	515.2917	22.3	$C_{26}H_{45}NO_7S$	Taurocholic Acid	MID34542
12993	664.1582	664.4789	*Not Identified*						
13119	670.0175	670.3398	*Not Identified*						
13210	674.2492	674.3549	$[M+2TMS+H]^+$	529.2680	529.2709	2.9	$C_{26}H_{43}NO_8S$	N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfooxy)cholan-24-yl]-Glycine	MID6670
13469	686.2933	686.3726	$[M+3TMS+H]^+$	469.2462	469.2438	-2.4	$C_{23}H_{31}N_7O_4$	Lys His Trp	MID22014
13511	688.2464	688.352						Not Identified	
13574	691.1761	691.3389	$[M+2TMS+H]^+$, $[M+3TMS+H]^+$	474.2125	474.2339	21.4	$C_{21}H_{30}N_8O_5$	His Tyr Arg	MID22969
13749	699.314	699.3891	$[M+3TMS+H]^+$	482.2627	482.2516	-11.1	$C_{25}H_{38}O_9$	11-beta-hydroxy-androsterone-3-glucuronide	HMDB10351
13770	700.2905	700.323	*Not Identified*						
13812	702.2436	702.3626	*Not Identified*						
14071	714.2877	714.3688	$[M+3TMS+H]^+$	497.2424	497.2499	7.5	$C_{23}H_{31}N_9O_4$	Arg His Trp	MID20604