

Table S2. Metabolites that were positively identified in tier 2 (HMDB)

NovaMT Library No.	External Identifier	Compounds
AFA00136000	C20279	(2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine
AAA00742000	C01142	(3S)-3,6-Diaminohexanoic acid - 2 tags
AAA00743000	C01186	(3S,5S)-3,5-Diaminohexanoic acid - 2 tags
AXA00705000	C06486	(6R)-6-(L-Erythro-1,2-Dihydroxypropyl)-5,6,7,8-tetrahydro-4a-hydroxypterin - 2 tags
AAA01484000	C03451	(R)-S-Lactoylglutathione
AXA00443000	C09642	(R)-Salsolinol - 2 tags
AAA00684000	C02356	(S)-2-Aminobutanoic acid/D-alpha-Aminobutyric acid
AAA01774000	C03741	(S)-4-Amino-5-oxopentanoic acid
AAA00744000	C03656	(S)-5-Amino-3-oxohexanoic acid
AAA00589000	C20249	(Z)-3-Peroxyaminoacrylic acid
ABA00497000	C14105	1,2-Dihydroxy-7-hydroxymethylnaphthalene - 2 tags
ABA00515000	C16196	1,2-Dihydroxynaphthalene-6-sulfonic acid
ABA00515000	C16196	1,2-Dihydroxynaphthalene-6-sulfonic acid - 2 tags
AAA00322000	C17018	1,4-Dihydroxy-6-naphthoic acid - 2 tags
AAA00644000	C01234	1-Aminocyclopropane-1-carboxylic acid
AXA00237000	C04545	1-Methylguanosine
AAA01623000	C03458	2,3,6-Trihydroxypyridine
AXA03843000	C16603	2,3-Dihydroxycarbamazepine
ABA00379000	C02923	2,3-Dihydroxytoluene - 2 tags
AXA00618000	C04441	2-(3-Carboxy-3-aminopropyl)-L-histidine - 2 tags
ABA00298000	C21248	2-Aminovalienone
AXA03073000	C02499	2-Biphenylol
AAA01231000	C17580	2-Deoxy-scylo-inosamine
APA00810000	C17756	2-Descarboxy-cyclo-dopa - 2 tags
AAA00919000	C00596	2-Hydroxy-2,4-pentadienoic acid
AAA00384000	C05298	2-Hydroxyestrone
AAA01479000	C03981	2-Hydroxyethylenedicarboxylic acid
ABA00147000	C02501	2-Hydroxymuconic acid
AXA00845000	C17883	2-Methoxy-4-vinylphenol
AXA01654000	C10675	3',4'-Dihydroxyacetophenone - 2 tags
AAA00905000	C05577	3,4-Dihydroxymandelaldehyde
AAA00906000	C05576	3,4-Dihydroxyphenylethyleneglycol - 2 tags
APA00413000	C06224	3,4-Dihydroxystyrene - 2 tags
AAA00286000	C01179	3-(4-Hydroxyphenyl)pyruvic acid
APA00895000	C12115	3-Amino-4-hydroxybenzoic acid - 2 tags
AFA00145000	C02512	3-Cyano-L-alanine
ABA00167000	C16472	3-Fluorocatechol - 2 tags
AAA00999000	C00632	3-Hydroxyanthranilic acid - 2 tags
ABA00397000	C03067	3-Hydroxybenzaldehyde
AAA01003000	C05636	3-Hydroxykynurenamine - 2 tags
AAA00907000	C05594	3-Methoxy-4-hydroxyphenylethyleneglycol
AAA00676000	C00606	3-Sulfinio-L-alanine
AAA01281000	C21258	4'-Oxonebramine - 2 tags
AAA01002000	C05637	4,8-Dihydroxyquinoline
AAA01726000	C20559	4-(beta-D-Ribofuranosyl)aniline 5'-phosphate
AAA00759000	C00555	4-Aminobutyraldehyde
ABA00125000	C04484	4-Carboxy-2-hydroxymuconate semialdehyde
APA00957000	C22137	4-Chloro-L-lysine
APA00957000	C22137	4-Chloro-L-lysine - 2 tags
AAA00770000	C02647	4-Guanidinobutanol
AAA00769000	C01035	4-Guanidinobutanoic acid - 2 tags
APA00045000	C21777	4-Hydroxy-L-tryptophan
AXA00645000	C17467	4-Hydroxybenzyl alcohol
AAA00862000	C05595	4-Hydroxyphenylacetylglutamic acid
AAA00854000	C06044	4-Hydroxyphenylethanol
APA00409000	C05627	4-Hydroxystyrene
AAA01649000	C15987	4-Methylaminobutyric acid
AXA03703000	C12739	5'-Deoxy-5-fluorouridine

NovaMT Library No.	External Identifier	Compounds
AXA00273000	C05198	5'-Deoxyadenosine
AAA00806000	C01110	5-Amino-2-oxopentanoic acid
APA00767000	C12455	5-Aminopentanal
AAA00740000	C00990	5-Aminopentanamide
AAA00768000	C03771	5-Guanidino-2-oxopentanoic acid
AAA00994000	C00643	5-Hydroxy-L-tryptophan
APA00422000	C12204	5-Hydroxyconiferaldehyde
APA00414000	C12205	5-Hydroxyconiferyl alcohol - 2 tags
AAA00608000	C16432	5-Hydroxyectoine
AAA01009000	C05634	5-Hydroxyindoleacetaldehyde
AAA01010000	C05635	5-Hydroxyindoleacetic acid
AAA01085000	C05844	5-L-Glutamyl-L-tyrosine
AAA01280000	C21256	6'-Oxolividamine
AAA00733000	C03239	6-Amino-2-oxohexanoic acid
AAA01015000	C05643	6-Hydroxymelatonin
AAA01671000	C01037	7,8-Diaminononanoic acid - 2 tags
AAA01707000	C16675	7-Aminomethyl-7-carbaguanine - 2 tags
AFA00195000	C17368	8-Dehydroxythienamycin
AXA00286000	C20155	8-Hydroxyguanine
AXA03712000	C07447	Acetylhydrazine
AAA00455000	C00147	Adenine
AAA00636000	C01888	Aminoacetone
AAA00593000	C20253	Aminoacrylic acid
AXA00049000	C04540	Aspartylglycosamine
AXA00795000	C03065	Beta-Guanidinopropionic acid
AXA00396000	C02486	Beta-Leucine
APA00426000	C12206	Caffeyl alcohol - 2 tags
APA00768000	C10850	Calystegin A3
AAA00778000	C18172	Carboxyspermidine
AAA00831000	C00386	Carnosine
APA00438000	C00590	Coniferyl alcohol
AAA00774000	C00791	Creatinine
AFA00001000	C01566	Cyanamide
AAA01745000	C04122	D-1-Aminopropan-2-ol O-phosphate
AAA00750000	C04020	D-Lysopine - 2 tags
AFA00011000	C06559	Deethylatrazine
AAA00573000	C00881	Deoxycytidine
AXA03600000	C14422	Diethylamine
APA00817000	C17755	Dopamine quinone
AAA00886000	C00822	Dopaquinone
AAA00418000	C00468	Estrone
AXA00427000	C06502	FAPy-adenine
AAA00784000	C10497	Feruloylputrescine - 2 tags
AAA01012000	C05647	Formyl-5-hydroxykynurenamine - 2 tags
ABA00560000	C01424	Gallic acid
AAA00668000	C00051	Glutathione
AXA00651000	C02037	Glycyl-glycine
AXA00216000	C01502	Guaiacol
AAA00476000	C00242	Guanine
AAA00513000	C06193	Guanosine 3'-phosphate
AXA02938000	C08306	Hexylamine
AAA00866000	C00530	Hydroquinone - 2 tags
AAA01079000	C00519	Hypotaurine
AYA00095000	C19911	Iminodiacetic acid
AXA01548000	C08295	Isoalliin
AAA00842000	C16673	Isoglutamine
AAA00743000	C01186	Isomer 1 of (3S,5S)-3,5-Diaminohexanoic acid - 2 tags
AXA00443000	C09642	Isomer 1 of (R)-Salsolinol - 2 tags
AAA00644000	C01234	Isomer 1 of 1-Aminocyclopropane-1-carboxylic acid
AXA03843000	C16603	Isomer 1 of 2,3-Dihydroxycarbamazepine
AAA00919000	C00596	Isomer 1 of 2-Hydroxy-2,4-pentadienoic acid
AXA00845000	C17883	Isomer 1 of 2-Methoxy-4-vinylphenol
APA00413000	C06224	Isomer 1 of 3,4-Dihydroxystyrene - 2 tags
AAA00286000	C01179	Isomer 1 of 3-(4-Hydroxyphenyl)pyruvic acid
AFA00145000	C02512	Isomer 1 of 3-Cyano-L-alanine
AAA01003000	C05636	Isomer 1 of 3-Hydroxykynurenamine - 2 tags

NovaMT Library No.	External Identifier	Compounds
AAA00907000	C05594	Isomer 1 of 3-Methoxy-4-hydroxyphenylethyleneglycol
AAA01726000	C20559	Isomer 1 of 4-(beta-D-Ribofuranosyl)aniline 5'-phosphate
AAA00759000	C00555	Isomer 1 of 4-Aminobutyraldehyde
APA00767000	C12455	Isomer 1 of 5-Aminopentanal
AAA00735000	C00431	Isomer 1 of 5-Aminopentanoic acid
AAA00608000	C16432	Isomer 1 of 5-Hydroxyectoine
AAA01010000	C05635	Isomer 1 of 5-Hydroxyindoleacetic acid
AAA00733000	C03239	Isomer 1 of 6-Amino-2-oxohexanoic acid
AAA00593000	C20253	Isomer 1 of Aminoacrylic acid
AAA00424000	C00062	Isomer 1 of Arginine
AXA00042000	C06313	Isomer 1 of Bipterin
APA00438000	C00590	Isomer 1 of Coniferyl alcohol
AAA00774000	C00791	Isomer 1 of Creatinine
AXA03600000	C14422	Isomer 1 of Diethylamine
AAA01327000	C00189	Isomer 1 of Ethanolamine
AAA01012000	C05647	Isomer 1 of Formyl-5-hydroxykynurenamine - 2 tags
AAA00832000	C00135	Isomer 1 of Histidine
AXA01548000	C08295	Isomer 1 of Isoalliin
APA00881000	C12212	Isomer 1 of Kanosamine
AXA00327000	C16511	Isomer 1 of L-Homocysteic acid
AAA00728000	C00408	Isomer 1 of L-Pipecolic acid
AFA00137000	C16138	Isomer 1 of L-Pyrrolysine
AAA00807000	C05939	Isomer 1 of Linatine
AAA00657000	C00073	Isomer 1 of Methionine
AXA00288000	C02728	Isomer 1 of N(6)-Methyllysine - 2 tags
AAA00976000	C02298	Isomer 1 of N-Acetylindoxyl
AAA00437000	C00437	Isomer 1 of N-Acetylornithine
AXA03615000	C11735	Isomer 1 of N-Ethylglycine
AAA00845000	C00439	Isomer 1 of N-Formimino-L-glutamic acid
ABA00216000	C04767	Isomer 1 of O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate - 2 tags
AAA01757000	C00931	Isomer 1 of Porphobilinogen
AAA01703000	C18239	Isomer 1 of Precursor Z
AAA00804000	C00148	Isomer 1 of Proline
AAA01599000	C00647	Isomer 1 of Pyridoxamine phosphate - 2 tags
AAA00658000	C00021	Isomer 1 of S-Adenosylhomocysteine (2 tags 2 charges)
AAA00763000	C00315	Isomer 1 of Spermidine - 2 tags
AFA00116000	C20916	Isomer 1 of Tabtoxin biosynthesis intermediate 6
AFA00118000	C20918	Isomer 1 of Tabtoxinine-beta-lactam
AAA00624000	C00188	Isomer 1 of Threonine
AAA00285000	C00082	Isomer 1 of Tyrosine (2 tags 2 charges)
AAA00743000	C01186	Isomer 2 of (3S,5S)-3,5-Diaminohexanoic acid - 2 tags
AAA00907000	C05594	Isomer 2 of 3-Methoxy-4-hydroxyphenylethyleneglycol
AAA00759000	C00555	Isomer 2 of 4-Aminobutyraldehyde
APA00767000	C12455	Isomer 2 of 5-Aminopentanal
AAA00735000	C00431	Isomer 2 of 5-Aminopentanoic acid
AAA00608000	C16432	Isomer 2 of 5-Hydroxyectoine
AAA01010000	C05635	Isomer 2 of 5-Hydroxyindoleacetic acid
AYA00010000	C07527	Isomer 2 of Benzocaine
AAA01327000	C00189	Isomer 2 of Ethanolamine
AXA00109000	C02155	Isomer 2 of Glycyl-Leucine
AAA00728000	C00408	Isomer 2 of L-Pipecolic acid
AAA00657000	C00073	Isomer 2 of Methionine
AXA00288000	C02728	Isomer 2 of N(6)-Methyllysine - 2 tags
AAA00845000	C00439	Isomer 2 of N-Formimino-L-glutamic acid
AAA00935000	C00079	Isomer 2 of Phenylalanine
AAA01757000	C00931	Isomer 2 of Porphobilinogen
AAA00658000	C00021	Isomer 2 of S-Adenosylhomocysteine (2 tags 2 charges)
AAA00622000	C00213	Isomer 2 of Sarcosine
AAA00624000	C00188	Isomer 2 of Threonine

NovaMT Library No.	External Identifier	Compounds
AAA00743000	C01186	Isomer 3 of (3S,5S)-3,5-Diaminohexanoic acid - 2 tags
APA00767000	C12455	Isomer 3 of 5-Aminopentanal
AAA00735000	C00431	Isomer 3 of 5-Aminopentanoic acid
AAA00657000	C00073	Isomer 3 of Methionine
AXA00288000	C02728	Isomer 3 of N(6)-Methyllysine - 2 tags
AAA00845000	C00439	Isomer 3 of N-Formimino-L-glutamic acid
AXA00288000	C02728	Isomer 4 of N(6)-Methyllysine - 2 tags
AFA00121000	C20919	Isotabtoxin
AXA00092000	C03975	Isoxanthopterin
APA00881000	C12212	Kanosamine
APA00963000	C03401	L-2,3-Diaminopropanoic acid
AXA01509000	C02926	L-3-Aminodihydro-2(3H)-furanone
AAA00670000	C00506	L-Cysteic acid
AAA00621000	C00097	L-Cysteine/D-Cysteine
AAA00818000	C01100	L-Histidinol phosphate
AXA00327000	C16511	L-Homocysteic acid
AAA00739000	C00047	L-Lysine/D-Lysine
AAA00901000	C05588	L-Metanephrine - 2 tags
AXA00239000	C01933	L-Norleucine
AAA00728000	C00408	L-Pipecolic acid
AFA00137000	C16138	L-Pyrrolysine
AAA01328000	C03872	L-Serine-phosphoethanolamine - 2 tags
AAA01746000	C12147	L-Threonine O-3-phosphate
APA00960000	C22140	L-gamma-Glutamyl-(3R)-L-beta-ethynylserine
AAA00807000	C05939	Linatine
APA00602000	C04900	Luteolin 7-O-[beta-D-glucuronosyl-(1->2)-beta-D-glucuronide]-4'-O-beta-D-glucuronide - 2 tags
AXA00659000	C07194	Methyldopa - 2 tags
AXA02555000	C14452	Morpholine
AXA00288000	C02728	N(6)-Methyllysine - 2 tags
AAA00610000	C06442	N(gamma)-Acetyldiaminobutyric acid
AAA00422000	C03406	N-(L-Arginino)succinic acid
AAA00976000	C02298	N-Acetylxindoxyl
AAA00437000	C00437	N-Acetylmethionine
AAA00765000	C02714	N-Acetylputrescine
AXA03615000	C11735	N-Ethylglycine
AAA00845000	C00439	N-Formimino-L-glutamic acid
AFA00155000	C20313	N-Hydroxy-L-valine
AYA00009000	C12269	N-Methyl aspartic acid
AAA00794000	C03415	N2-Succinyl-L-ornithine
AXA00322000	C01029	N8-Acetylspermidine - 2 tags
ABA00216000	C04767	O-(1->4)-alpha-L-Dihydrostreptosyl-streptidine 6-phosphate - 2 tags
AAA00686000	C21016	Ophthalmic acid
AXA01777000	C03002	Paucine - 2 tags
ABA00557000	C02183	Phloroglucinol
APA00639000	C05901	Piceatannol
AAA01757000	C00931	Porphobilinogen
AAA01703000	C18239	Precursor Z
AAA01568000	C00018	Pyridoxal phosphate
AAA01598000	C00534	Pyridoxamine - 2 tags
AAA01599000	C00647	Pyridoxamine phosphate - 2 tags
AAA01709000	C02587	Pyrimidodiazepine - 2 tags
APA00638000	C03582	Resveratrol
AFA00218000	C14180	S-(Hydroxymethyl)glutathione
AAA00658000	C00021	S-Adenosyl-L-homocysteine
AAA00667000	C05526	S-Glutathionyl-L-cysteine - 2 tags
AAA00763000	C00315	Spermidine - 2 tags
AFA00116000	C20916	Tabtoxin biosynthesis intermediate 6
AFA00118000	C20918	Tabtoxinine-beta-lactam
AFA00120000	C20920	Tabtoxinine-delta-lactam
AAA00263000	C00245	Taurine
AXA04525000	C09908	Thymol
AAA01072000	C05340	beta-Alanyl-L-arginine - 2 tags
APA00806000	C17751	cyclo-Dopa 5-O-glucoside
AFA00143000	C05715	gamma-Amino-gamma-cyanobutanoic acid

NovaMT Library No.	External Identifier	Compounds
AFA00144000	C05711	gamma-Glutamyl-beta-cyanoalanine
AAA00761000	C15700	gamma-Glutamyl-gamma-aminobutyraldehyde
AAA00760000	C15699	gamma-L-Glutamylputrescine
AAA00861000	C05596	p-Hydroxyphenylacetyl glycine
AXA00433000	C04548	p-Synephrine - 2 tags
AAA01324000	C01233	sn-Glycero-3-phosphoethanolamine
AAA00921000	C12623	trans-2,3-Dihydroxycinnamic acid