

Table S3. Metabolites that were positively identified in tier 1 (CIL Library)

NovaMT Library No.	External Identifier	Compounds
AAA00641000	C00986	1,3-Diaminopropane (2 tags 2 charges)
AAA00758000	C00134	1,4-diaminobutane (2 tags 1 charge)
AAA00758000	C00134	1,4-diaminobutane (2 tags 2 charges)
AYA00001000	C01152	1-Methylhistidine
AXA00258000	C03665	2-Aminoisobutyric acid
AXA00106000	HMDB0003911_2	3-Aminoisobutanoic acid - H2O
	HMDB00000750	3-Hydroxymandelic acid
	HMDB0000750_2	3-Hydroxymandelic acid - COOH
AAA00829000	HMDB00000479	3-Methylhistidine
	HMDB0003464_2	4-Guanidinobutanoic acid - H2O
AAA00278000	C00156	4-Hydroxybenzoic acid
AAA00799000	C01157	4-Hydroxyproline
AAA00652000	C00170	5'-Methylthioadenosine
AXA00043000	C03088	5-Hydroxymethyluracil
AAA00453000	C00020	Adenosine monophosphate
AAA00596000	C00041	Alanine
AXA00982000	HMDB0028680	Alanyl-Alanine
AXA00985000	HMDB0028683	Alanyl-Aspartic Acid
AXA00988000	HMDB0028686	Alanyl-Glutamic acid
AXA00990000	HMDB0028689	Alanyl-Histidine
AXA00992000	HMDB0028691	Alanyl-Leucine
AXA00993000	HMDB0028692	Alanyl-Lysine (2 tags 2 charges)
AXA00994000	HMDB0028693	Alanyl-Methionine
AXA00995000	HMDB0028694	Alanyl-Phenylalanine
AXA00996000	HMDB0028695	Alanyl-Proline
AXA00998000	HMDB0028697	Alanyl-Threonine
AXA00791000	C00806	Alanyl-Tryptophan
AXA00999000	HMDB0028699	Alanyl-Tyrosine (2 tags 2 charges)
AXA01000000	HMDB0028700	Alanyl-Valine
AXA00058000	C21096	Alloisoleucine
AAA00727000	C00956	Aminoadipic acid
AAA00424000	C00062	Arginine
AXA01002000	HMDB0028702	Arginyl-Alanine
AXA01007000	HMDB0028707	Arginyl-Glutamine
AXA01012000	HMDB0028712	Arginyl-Isoleucine
AXA01019000	HMDB0028719	Arginyl-Threonine
AXA01026000	HMDB0028726	Asparaginyl-Asparagine
AXA01029000	HMDB0028729	Asparaginyl-Glutamine
AXA01034000	HMDB0028734	Asparaginyl-Isoleucine
AXA01035000	HMDB0028735	Asparaginyl-Leucine
AXA01037000	HMDB0028737	Asparaginyl-Methionine
AXA01038000	HMDB0028738	Asparaginyl-Phenylalanine
AXA01043000	HMDB0028743	Asparaginyl-Tyrosine (2 tags 2 charges)
AXA01044000	HMDB0028744	Asparaginyl-Valine
AXA04440000	C11045	Aspartame
AXA01047000	HMDB0028747	Aspartyl-Arginine
AXA01049000	HMDB0028749	Aspartyl-Aspartate
AXA01053000	HMDB0028753	Aspartyl-Glycine
AXA01055000	HMDB0028756	Aspartyl-Isoleucine
AXA01059000	HMDB0028761	Aspartyl-Proline
AYA00010000	C07527	Benzocaine
AAA00562000	C00099	Beta-Alanine
AXA00042000	C06313	Biopterin
AAA00736000	C01672	Cadaverine (2 tags 2 charges)
AAA00423000	C00327	Citrulline
AAA00616000	C00300	Creatine
AAA00620000	C02291	Cystathionine (2 tags 2 charges) - Isomer
AAA00674000	C00491	Cysteinyl-Alanine dimer (2 tags 2 charges)
		Cystine (2 tags 2 charges)
AAA00567000	C00055	Cytidine monophosphate - Isomer
AXA00324000	C01744	Desaminotyrosine
AFA00126000	C00666	Diaminopimelic acid (2 tags 2 charges)
AAA01327000	C00189	Ethanolamine
	HMDB0000112_2	Gamma-Aminobutyric acid - H2O
AXA00652000	C05282	Gamma-Glutamylglutamic acid
AAA00604000	C00352	Glucosamine 6-phosphate

NovaMT Library No.	External Identifier	Compounds
AAA00438000	C00025 HMDB0000148_2	Glutamic Acid Glutamic Acid - H2O
AAA00432000	C00064	Glutamine
AXA01087000	HMDB0028790	Glutaminy-Alanine
AXA01092000	HMDB0028795	Glutaminy-Glutamine
AXA01096000	HMDB0028799	Glutaminy-Histidine
AXA01098000	HMDB0028801	Glutaminy-Leucine
AXA01100000	HMDB0028803	Glutaminy-Methionine
AXA01104000	HMDB0028807	Glutaminy-Threonine
AXA01107000	HMDB0028810	Glutaminy-Valine
AXA00399000	HMDB0003764	Glutamyl-Alanine
AXA01111000	HMDB0028815	Glutamyl-Aspartic acid
AXA01113000	HMDB0028817	Glutamyl-Glutamine
AXA01115000	HMDB0028819	Glutamyl-Glycine
AXA01117000	HMDB0028822	Glutamyl-Isoleucine
AXA01118000	HMDB0028823	Glutamyl-Leucine
AXA00416000	HMDB0028824	Glutamyl-Lysine (2 tags 2 charges)
AXA01420000		Glutamyl-Phenylalanine
AXA01121000	HMDB0028828	Glutamyl-Serine
AXA01109000	HMDB0028813	Glutamylarginine
AYA00014000		Gly-Norvaline
AAA00261000	C00037	Glycine
AXA01127000	HMDB0028835	Glycyl-Arginine
AXA01128000	HMDB0028836	Glycyl-Asparagine
AXA01133000	HMDB0028843	Glycyl-Histidine
AXA01134000	HMDB0028844	Glycyl-Isoleucine
AXA00109000	C02155	Glycyl-Leucine
AXA01135000	HMDB0028846	Glycyl-Lysine (2 tags 2 charges)
AXA01136000	HMDB0028847	Glycyl-Methionine
AXA01137000	HMDB0028848	Glycyl-Phenylalanine
AXA00095000	HMDB00000721	Glycyl-Proline
AXA01139000	HMDB0028851	Glycyl-Threonine
AXA01140000	HMDB0028852	Glycyl-Tryptophan
AXA01141000	HMDB0028853	Glycyl-Tyrosine (2 tags 2 charges)
AXA01142000	HMDB0028854	Glycyl-Valine
AXA00241000	C17349	Guanidine
AAA00485000	C00387	Guanosine
AAA00832000	C00135	Histidine
AXA01166000	HMDB0028881	Histidinyl-Aspartate
AXA01169000	HMDB0028884	Histidinyl-Glutamate
AXA01173000	HMDB0028888	Histidinyl-Isoleucine
AXA01174000	HMDB0028889	Histidinyl-Leucine
AXA01175000	HMDB0028890	Histidinyl-Lysine (2 tags 2 charges)
AXA01182000	HMDB0028897	Histidinyl-Tyrosine (2 tags 2 charges)
AXA00084000	C01924	Homoarginine
AAA00630000	C00263	Homoserine
AAA00897000	C05582	Homovanillic acid
AAA00459000	C00262	Hypoxanthine - Isomer
AAA00825000	C02835	Imidazoleacetic acid
AXA01186000	HMDB0028901	Isoleucyl-Arginine
AXA01187000	HMDB0028902	Isoleucyl-Asparagine
AXA01188000	HMDB0028903	Isoleucyl-Aspartate
AXA01191000	HMDB0028906	Isoleucyl-Glutamate
AXA01190000	HMDB0028905	Isoleucyl-Glutamine
AXA01196000	HMDB0028911	Isoleucyl-Leucine
AXA01197000	HMDB0028912	Isoleucyl-Lysine (2 tags 2 charges)
AXA01198000	HMDB0028913	Isoleucyl-Methionine
AXA01201000	HMDB0028917	Isoleucyl-Threonine
AXA01203000	HMDB0028919	Isoleucyl-Tyrosine (2 tags 2 charges)
AAA00453000	HMDB00003911_2 C00020	Isomer 1 of 3-Aminoisobutanoic acid - H2O
	HMDB0000112_2	Isomer 1 of Adenosine monophosphate
		Isomer 1 of Gamma-Aminobutyric acid - H2O
AAA00438000	C00025	Isomer 1 of Glutamic Acid
AXA01169000	HMDB0000148_2	Isomer 1 of Glutamic Acid - H2O
AXA01212000	HMDB0028928	Isomer 1 of Histidinyl-Glutamate
AXA01264000	HMDB0028982	Isomer 1 of Leucyl-Glutamate
AAA01331000	C00346	Isomer 1 of Methionyl-Serine
		Isomer 1 of O-Phosphoethanolamine

NovaMT Library No.	External Identifier	Compounds
AXA01276000	HMDB0028994	Isomer 1 of Phenylalanyl-Glutamate
AAA00624000	C00188	Isomer 1 of Threonine
AAA00548000	C00299	Isomer 1 of Uridine
AXA01399000	HMDB0029126	Isomer 1 of Valyl-Glutamate
AXA01400000	HMDB0029127	Isomer 1 of Valyl-Glycine
AAA00987000	C00328	Kynurenine
	HMDB0000684_2	Kynurenine - H2O
AAA00691000	C00123	Leucine
AXA01206000	HMDB0028922	Leucyl-Alanine
AXA01207000	HMDB0028923	Leucyl-Arginine
AXA01208000	HMDB0028924	Leucyl-Asparagine
AXA01209000	HMDB0028925	Leucyl-Aspartate
AXA01212000	HMDB0028928	Leucyl-Glutamate
AXA01211000	HMDB0028927	Leucyl-Glutamine
AXA01213000	HMDB0028929	Leucyl-Glycine
AYA00023000		Leucyl-Methionine sulfoxide
AXA00591000	HMDB0011175	Leucyl-Proline
AXA01221000	HMDB0028939	Leucyl-Threonine
AAA00739000	C00047	Lysine (2 tags 2 charges)
AXA01227000	HMDB0028945	Lysyl-Arginine (2 tags 2 charges)
AXA01228000	HMDB0028946	Lysyl-Asparagine (2 tags 2 charges)
AXA01229000	HMDB0028947	Lysyl-Aspartate (2 tags 2 charges)
AXA01232000	HMDB0028950	Lysyl-Glutamate (2 tags 2 charges)
AXA01231000	HMDB0028949	Lysyl-Glutamine (2 tags 2 charges)
AXA01233000	HMDB0028951	Lysyl-Glycine (2 tags 2 charges)
AXA01236000	HMDB0028954	Lysyl-Isoleucine (2 tags 2 charges)
AXA01241000	HMDB0028959	Lysyl-Proline (2 tags 2 charges)
AXA01243000	HMDB0028961	Lysyl-Threonine (2 tags 2 charges)
AXA01246000	HMDB0028964	Lysyl-Valine (2 tags 2 charges)
AAA00660000	C02989	Methionine Sulfoxide
AAA00660000	C02989	Methionine Sulfoxide - Isomer
AXA01248000	HMDB0028966	Methionyl-Alanine
AXA01255000	HMDB0028973	Methionyl-Glycine
AXA01258000	HMDB0028976	Methionyl-Isoleucine
AXA01260000	HMDB0028978	Methionyl-Lysine (2 tags 2 charges)
AXA01263000	HMDB0028981	Methionyl-Proline
AXA01264000	HMDB0028982	Methionyl-Serine
AXA01267000	HMDB0028985	Methionyl-Tyrosine (2 tags 2 charges)
AXA01268000	HMDB0028986	Methionyl-Valine
AXA00231000	C02294	Methylguanidine
AAA00739A01	HMDB0000446	N-Alpha-acetyllysine
AAA00738000	C02727	N6-Acetyl-Lysine
AAA01331000	C00346	O-Phosphoethanolamine
AAA00425000	C00077	Ornithine (2 tags 1 charge)
AAA00938000	C05852	Ortho-Hydroxyphenylacetic acid
AXA01270000	HMDB0028988	Phenylalanyl-Alanine
AXA01276000	HMDB0028994	Phenylalanyl-Glutamate
AXA01275000	HMDB0028993	Phenylalanyl-Glutamine
AYA00028000		Phenylalanyl-Leucine
AXA01280000	HMDB0029000	Phenylalanyl-Lysine (2 tags 2 charges)
AXA01282000	HMDB0029004	Phenylalanyl-Serine
AXA01283000	HMDB0029005	Phenylalanyl-Threonine
AXA01286000	HMDB0029008	Phenylalanyl-Valine
AAA00804000	C00148	Proline
AXA01288000	HMDB0029010	Prolyl-Alanine
AXA01289000	HMDB0029011	Prolyl-Arginine
AXA01290000	HMDB0029012	Prolyl-Asparagine
AXA01291000	HMDB0029013	Prolyl-Aspartate
AXA01294000	HMDB0029016	Prolyl-Glutamate
AYA00026000		Prolyl-Isoleucine
AYA00027000		Prolyl-Leucine
AXA01297000	HMDB0029022	Prolyl-Lysine (2 tags 2 charges)
AXA00595000	HMDB0011179	Prolyl-Phenylalanine
AXA01299000	HMDB0029026	Prolyl-Serine
AXA01300000	HMDB0029027	Prolyl-Threonine
AXA01302000	HMDB0029029	Prolyl-Tyrosine (2 tags 2 charges)
AXA01303000	HMDB0029030	Prolyl-Valine
AAA01047000	C00230	Protocatechuic acid (2 tags 2 charges)
ABA00075000	C00090	Pyrocatechol (2 tags 2 charges)

NovaMT Library No.	External Identifier	Compounds
AAA00658000	C00021	S-Adenosylhomocysteine (2 tags 2 charges)
AAA00622000	C00213	Sarcosine
AXA01319000	HMDB0029046	Seriny-Phenylalanine
AAA01008000	C00780	Serotonin (2 tags 2 charges)
AXA01305000	HMDB0029032	Seryl-Alanine
AXA01306000	HMDB0029033	Seryl-Arginine
AXA01307000	HMDB0029034	Seryl-Asparagine
AXA01308000	HMDB0029035	Seryl-Aspartic acid
AXA01314000	HMDB0029041	Seryl-Histidine
AXA01318000	HMDB0029045	Seryl-Methionine
AXA01321000	HMDB0029048	Seryl-Serine
AXA01322000	HMDB0029049	Seryl-Threonine
AXA01323000	HMDB0029050	Seryl-Tryptophan
AXA01325000	HMDB0029052	Seryl-Valine
AXA00390000	HMDB00003334	Symmetric dimethylarginine
AAA00624000	C00188	Threonine
AXA01333000	HMDB0029060	Threoninyl-Glutamate
AXA01334000	HMDB0029061	Threoninyl-Glycine
AXA01336000	HMDB0029063	Threoninyl-Histidine
AXA01337000	HMDB0029064	Threoninyl-Isoleucine
AXA01338000	HMDB0029065	Threoninyl-Leucine
AXA01339000	HMDB0029066	Threoninyl-Lysine (2 tags 2 charges)
AXA01340000	HMDB0029067	Threoninyl-Methionine
AXA01341000	HMDB0029068	Threoninyl-Phenylalanine
AXA01344000	HMDB0029071	Threoninyl-Threonine
AXA01346000	HMDB0029073	Threoninyl-Tyrosine (2 tags 2 charges)
AAA00556000	C00178	Thymine
AAA00640000	C00078	Tryptophan
AXA01361000	HMDB0029088	Tryptophyl-Lysine (2 tags 2 charges)
AXA01368000	HMDB0029095	Tryptophyl-Tyrosine
AAA00285000	C00082	Tyrosine (2 tags 2 charges)
AXA01371000	HMDB0029098	Tyrosyl-Alanine (2 tags 2 charges)
AXA01373000	HMDB0029100	Tyrosyl-Asparagine (2 tags 2 charges)
AXA01381000	HMDB0029108	Tyrosyl-Isoleucine (2 tags 2 charges)
AXA01385000	HMDB0029112	Tyrosyl-Phenylalanine (2 tags 2 charges)
AXA01388000	HMDB0029115	Tyrosyl-Threonine (2 tags 2 charges)
AXA01391000	HMDB0029118	Tyrosyl-Valine (2 tags 2 charges)
AAA00549000	C00106	Uracil
AAA00548000	C00299	Uridine
	HMDB0000296_2	Uridine - H2O
AAA00840000	C00785	Urocanic acid
AAA00705000	C00183	Valine
AXA01393000	HMDB0029120	Valyl-Alanine
AXA01396000	HMDB0029123	Valyl-Aspartate
AXA01399000	HMDB0029126	Valyl-Glutamate
AXA01400000	HMDB0029127	Valyl-Glycine
AXA01404000	HMDB0029131	Valyl-Leucine
AXA01405000	HMDB0029132	Valyl-Lysine (2 tags 2 charges)
AXA01406000	HMDB0029133	Valyl-Methionine
AXA01407000	HMDB0029134	Valyl-Phenylalanine
AXA01413000	HMDB0029140	Valyl-Valine
ABA00533000	C06672	Vanillic acid
AAA00466000	C00385	Xanthine
AAA01000000	C02470	Xanthurenic acid
AAA01692000	C00568	p-Aminobenzoic acid
AXA00596000	HMDB0011180	prolyl-proline