

Supplementary Table 1 - part 1 - C18 3 min Isocratic method - IROA standard characterization

Compound Name	PARENT_CID	Neutral mass	Acid Rt	Organic Rt	Polarity
(2-AMINOETHYL)PHOSPHONATE	C03557	125.02418	1.21	1.19	POS
(R)-MALATE	C00711	134.02153	1.57	1.34	NEG
(R,R)-TARTARIC ACID	C00898	150.01644	1.40	1.45	NEG
(S)-LACTATE	C01432	90.03170	1.62	1.30	NEG
(S)-MALATE	C00711	134.02153	1.57	1.34	NEG
(S)-NICOTINE	C16150	162.11570	1.65	-	POS
(S,S)-TARTARIC ACID	C00898	150.01644	1.40	1.45	NEG
1,3-DIAMINOPROPANE	C00986	74.08440	1.09	1.07	POS
1-AMINOCYCLOPROPANE-1-CARBOXYLATE	C01234	101.04768	1.22	1.20	POS
1-HYDROXY-2-NAPHTHOATE	C03203	188.04735	1.61	1.27	NEG
1-METHYL-6,7-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINE	C09642	179.09464	1.79	1.35	POS
1-METHYLADENOSINE	C02494	281.11241	1.64	1.25	POS
2',4'-DIHYDROXYACETOPHENONE	C03663	152.04735	3.15	-	POS
2,4-DIHYDROXYPTERIDINE	C03212	164.03343	2.09	1.26	NEG
2,4-DIHYDROXYPYRIMIDINE-5-CARBOXYLIC ACID	C03030	156.01711	1.91	1.35	NEG
2,5-DIHYDROXYBENZOATE	C00628	154.02661	1.99	1.26	NEG
2,6-DIHYDROXYPYRIDINE	C03056	111.03202	1.99	-	POS
2-ACETAMIDO-2-DEOXY-BETA-D-GLUCOSYLAMINE	CA1416	220.10592	1.15	1.25	POS
2-AMINO-2-METHYLPROPANOATE	C03665	103.06333	1.23	1.22	POS
2-AMINOETHYL DIHYDROGEN PHOSPHATE	CA1062	141.01910	1.21	1.19	POS
2-AMINOPHENOL	C01987	109.05276	1.72	1.28	POS
2'-DEOXYADENOSINE	C00559	269.11241	2.96	-	POS
2'-DEOXYADENOSINE 5'-DIPHOSPHATE	C00206	411.03451	1.65	1.65	POS
2'-DEOXYADENOSINE 5'-TRIPHOSPHATE	C00131	491.00084	1.05	1.65	NEG
2'-DEOXYCYTIDINE 5'-DIPHOSPHATE	C00705	387.02327	1.49	1.60	NEG
2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE	C00239	307.05694	1.61	1.27	POS
2-DEOXY-D-GLUCOSE	C00586	164.06848	1.25	1.20	POS
2'-DEOXYGUANOSINE	C00330	285.10732	2.50	2.49	POS
2'-DEOXYGUANOSINE 5'-MONOPHOSPHATE	C00362	347.06309	1.64	1.26	POS
2'-DEOXYURIDINE 5'-MONO-PHOS-PHATE	C00365	308.04096	1.64	1.65	NEG
2-HYDROXYBUTYRIC ACID	C05984	104.04734	1.67	2.42	POS
2-HYDROXYPHENYLACETIC ACID	CA1444	152.04734	1.61	3.92	NEG
2-HYDROXYPYRIDINE	C02502	95.03711	2.27	-	POS
2-METHYLMALATE	C02226	130.02661	3.53	3.52	NEG
2-METHYLPROPANAL OXIME	C03219	87.06841	1.40	1.38	POS
2-OXOADIPATE	C00322	160.03718	2.48	2.47	NEG
2-QUINOLINECARBOXYLIC ACID	C06325	173.04768	-	1.27	NEG
3-(4-HYDROXYPHENYL)PYRUVATE	C01179	180.04226	-	1.29	NEG
3,4-DIHYDROXY-L-PHENYLALANINE	C00355	197.06881	1.64	1.25	POS
3,4-DIHYDROXYPHENYL GLYCOL	C05576	170.05791	1.91	1.27	NEG
3,4-DIHYDROXYPHENYLACETATE	C01161	168.04226	2.62	-	NEG
3',5'-CYCLIC AMP	C00575	329.05252	2.12	1.34	POS
3-AMINO-4-HYDROXYBENZOIC ACID	C12115	153.04259	1.64	1.30	POS
3-AMINO-5-HYDROXYBENZOIC ACID	C12107	153.04260	1.71	1.25	POS
3-AMINOISOBUTANOATE	C05145	103.06333	1.25	1.22	POS
3'-CMP	C05822	323.05186	1.64	1.26	POS
3-DEHYDROSHIKIMATE	C02637	172.03717	1.64	1.35	NEG
3-HYDROXY-3-METHYLGLUTARATE	C03761	162.05283	2.18	2.19	NEG
3-HYDROXYANTHRANILATE	C00632	153.04259	1.23	1.22	NEG
3-HYDROXYBENZOATE	C00587	138.03170	3.22	-	NEG
3-HYDROXYKYNURENINE	C02794	224.07971	1.93	1.26	POS
3-HYDROXYPHENYLACETATE	C05593	152.04735	3.23	-	POS
3-METHOXY-4-HYDROXYMANDELATE	C05584	198.05283	3.22	3.25	NEG
3-METHOXYTYRAMINE	C05587	167.09464	-	2.51	NEG
3-METHYLADENINE	C00913	149.07015	1.64	1.32	POS
3-METHYLHISTAMINE	C15526	125.09530	1.10	1.07	POS
3-NITRO-L-TYROSINE-change Rt	CA1195	226.05897	-	2.65	NEG
3-SULFINO-L-ALANINE	C00606	153.00958	1.26	1.32	POS
3-UREIDOPROPIONATE	C02642	132.05349	1.64	1.25	POS
4-ACETAMIDOBUTANOATE	C02946	145.07389	2.29	1.33	POS
4-AMINOBUTANOATE	C00334	103.06333	1.19	1.18	POS
4-GUANIDINOBUTANOATE	C01035	145.08513	1.64	1.26	POS
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID	C01717	189.04259	3.26	1.25	POS
4-HYDROXYBENZOATE	C00156	138.03170	1.54	1.27	NEG
4-HYDROXY-L-PHENYLGLYCINE	CA1445	167.05824	1.27	1.24	POS
4-HYDROXY-L-PROLINE	C01157	131.05824	1.23	1.20	POS
4-IMIDAZOLEACETIC ACID	C02835	126.04293	1.24	1.21	POS
4-METHYLCATECHOL	C06730	124.05243	3.20	-	POS
4-PYRIDOXATE	C00847	183.05316	2.49	1.26	POS
4-QUINOLINECARBOXYLIC ACID	C06414	173.04768	2.13	2.11	POS
5,6-DIHYDROURACIL	C00429	114.04293	1.64	1.25	POS
5-AMINOIMIDAZOLE-4-CARBOXAMIDE-1-BETA-D-RIBOFURANOSYL 5'-MONOPHOSPHAT	C04677	338.06275	1.63	1.26	POS

5-AMINOLEVULINIC ACID	C00430	131.05824	1.22	1.19	POS
5-AMINOPENTANOATE	C00431	117.07898	1.31	1.24	POS
5'-DEOXYADENOSINE	C05198	251.10184	2.86	1.24	POS
5-HYDROXYINDOLEACETATE	C05635	191.05824	1.22	-	POS
5-HYDROXY-L-TRYPTOPHAN	C01017	220.08479	2.93	1.25	POS
5-HYDROXYMETHYLURACIL	C03088	142.03784	1.64	1.26	NEG
5-METHYLCYTOSINE HYDROCHLORIDE	C02376	125.05891	1.29	1.23	POS
5'-METHYLTHIOADENOSINE	C00170	297.08956	1.86	1.25	NEG
5-OXO-D-PROLINE	C01879	129.04259	1.74	1.26	NEG
5-OXO-L-PROLINE	C01879	129.04259	1.74	1.26	NEG
5-VALEROLACTONE	C02240	100.05243	3.33	-	POS
6-DEOXY-L-GALACTOSE	C00382	164.06848	1.55	1.57	NEG
6-HYDROXYDOPAMINE	CA1404	169.07390	1.64	1.24	POS
6-HYDROXYNICOTINATE	C01020	139.02694	2.50	2.55	POS
6-PHOSPHOGLUCONIC ACID	C00345	276.02464	1.50	1.60	NEG
ADENINE	C00147	135.05450	1.63	1.24	POS
ADENOSINE	C00212	267.09676	1.91	1.25	POS
ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE	C02353	267.09676	1.66	1.32	POS
ADENOSINE 3',5'-CYCLIC MONOPHOSPHATE	C00575	329.05252	2.12	1.34	POS
ADENOSINE 3',5'-DIPHOSPHATE	C00054	427.02942	2.20	-	POS
ADENOSINE 5'-DIPHOSPHATE	C00008	427.02942	1.50	1.58	POS
ADENOSINE 5'-DIPHOSPHORIBOSE	C00301	559.07168	1.63	1.86	NEG
ADENOSINE 5'-MONOPHOSPHATE	C00020	347.06309	1.64	1.27	POS
ADENOSINE-5'-DIPHOSPHOGLUCOSE	C00498	427.02942	1.63	-	NEG
AGMATINE SULFATE	C00179	130.12180	1.11	1.07	POS
ALLANTOIN	C01551	158.04399	1.28	1.26	NEG
ALPHA-AMINOADIPATE	C00956	161.06881	1.27	1.23	POS
ALPHA-D-GALACTOSE 1-PHOSPHATE	C00446	260.02971	1.27	1.29	NEG
ALPHA-D-GLUCOSE 1-PHOSPHATE	C00103	260.02972	1.27	1.29	POS
ALPHA-KETOGLUTARIC ACID	C00026	146.02153	1.93	1.89	NEG
ANILINE	C00292	93.05785	2.24	2.25	POS
ANILINE-2-SULFONIC ACID	C00292	173.01467	2.24	2.25	POS
ASCORBATE	C00072	176.03209	1.62	1.25	NEG
AZELAIC ACID	C08261	188.10486	-	1.26	NEG
BENZOATE	C00180	122.03678	1.99	1.32	NEG
BETA-ALANINE	C00099	89.04768	1.18	1.16	POS
BETAINE	C00719	117.07898	1.24	1.21	POS
BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE 2'-PHOSPHATE REDUCED	C00006	743.07545	1.64	1.64	POS
BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE PHOSPHATE	C00006	743.07545	1.64	1.64	POS
BIS(3-AMINOPROPYL)AMINE	C03375	131.14225	1.03	1.02	POS
BUTANAL	C01412	72.05752	2.65	-	POS
CADAVERINE	C01672	102.11570	1.08	1.07	POS
CARNOSINE	C00386	226.10659	1.10	1.10	POS
CHOLINE	C00114	104.10754	1.19	1.15	POS
CIS-4-HYDROXY-D-PROLINE	C01015	131.05824	1.21	1.19	POS
CITRAMALATE	C00815	148.11402	1.99	2.04	NEG
CITRATE	C00158	192.02701	1.74	1.80	NEG
CITRULLINE	C00327	175.09569	1.21	1.19	POS
CMP	C00055	323.05186	1.29	1.22	POS
CREATINE	C00300	131.06948	1.26	1.21	POS
CREATINE PHOSPHATE	C02305	211.03581	1.31	1.27	POS
CREATININE	C00791	113.05891	1.22	1.19	POS
CYS-GLY	C01419	178.04122	1.13	1.11	POS
CYSTEAMINE	C01678	77.02992	1.08	1.08	POS
CYTIDINE	C00475	243.08552	1.61	1.25	POS
CYTIDINE 2',3'-CYCLIC MONO-PHOS-PHATE	C02354	305.04129	1.34	1.23	POS
CYTIDINE 5'-DIPHOSPHATE	C00112	403.01819	1.47	1.54	NEG
CYTIDINE 5'-DIPHOSPHOCHOLINE	C00307	489.11459	1.23	1.20	POS
CYTOSINE	C00380	111.04326	1.61	1.24	POS
D-(-)-3-PHOSPHOGLYCERIC ACID	C00597	185.99294	1.30	2.00	POS
D-(+)-CELLOBIOSE	C00185	342.11622	1.21	-	POS
D-(+)-GALACTOSAMINE	C02262	179.07938	1.24	1.13	POS
D-(+)-GLUCOSAMINE	C00329	179.07938	1.16	1.13	POS
D-(+)-RAFFINOSE	C00492	594.22187	1.27	-	POS
D-ALANINE	C01401	89.04768	1.22	1.19	POS
DAMP	C00360	331.06817	1.64	1.26	POS
D-ASPARTATE	C16433	133.03751	1.22	1.20	POS
DEHYDROASCORBATE	C00425	174.01644	1.26	-	POS
DEHYDRO-L-(+)-ASCORBIC ACID DIMER	C00425	348.03288	1.26	-	POS
DEOXYCARNITINE	C05543	145.11028	1.24	1.21	POS
DEOXYCYTIDINE	C00881	227.09061	1.64	1.24	POS
DEOXYURIDINE	C00526	228.07462	2.13	1.27	NEG
D-FRUCTOSE	C01496	180.06339	1.23	-	NEG
D-FRUCTOSE 6-PHOSPHATE	C00085	260.02972	1.28	1.29	NEG
D-GALACTOSE	C01582	180.06339	1.23	-	NEG

D-GLUCONATE	C00257	178.04774	1.23	1.22	POS
D-GLUCONO-1,5-LACTONE	C00198	178.04774	1.37	1.26	NEG
D-GLUCOSAMINE 6-PHOSPHATE	C00352	259.04571	1.20	1.17	POS
D-GLUCOSAMINE 6-SULFATE	CA1422	259.03619	1.21	1.19	NEG
D-GLUCOSE 6-PHOSPHATE	C00092	260.02972	1.26	1.28	NEG
D-GLUCOSE-6-PHOSPHATE	C00092	260.02972	1.26	1.28	NEG
D-GLUCURONIC ACID	C00191	194.04265	1.23	1.25	NEG
D-GLUCURONOLACTONE	C02670	176.03209	1.35	1.26	NEG
D-GLYCERIC ACID	C00258	106.02661	1.36	1.24	NEG
D-GULONIC ACID GAMA-LACTONE	C00800	178.04774	1.25	1.25	POS
DIETHANOLAMINE	C06772	105.07898	1.17	1.14	POS
DIETHYL 2-METHYL-3-OXOSUCCINATE	C04067	202.08413	-	1.26	NEG
DIHYDROXYACETONE PHOSPHATE	C00111	182.01439	1.20	1.28	NEG
DIHYDROXYMANDELIC ACID	C07470	184.03718	1.97	1.93	NEG
DIMETHYLBENZIMIDAZOLE	C03114	146.0844	-	1.27	NEG
DL-5-HYDROXYLYSINE	C01211	162.10044	1.10	1.10	NEG
D-LACTOSE	C00243	360.12678	1.13	1.12	NEG
DL-NORMETANEPHRINE	CA1379	183.08954	1.64	1.24	POS
D-MANNOSAMINE	C03570	179.07938	1.15	1.14	POS
D-MANNOSE 6-PHOSPHATE	C00275	260.02972	1.25	1.24	POS
DOPAMINE	C03758	153.07898	1.66	1.25	POS
D-ORNITHINE	C00515	132.08987	1.11	1.11	POS
D-PANTOTHENIC ACID	C00864	219.11067	-	2.63	POS
D-RIBOSE	C08353	150.05283	1.26	1.28	NEG
D-RIBOSE 5-PHOSPHATE	C00117	230.01916	1.27	1.29	NEG
D-RIBULOSE 1,5-BISPHOSPHATE	C01182	309.98548	2.19	1.51	NEG
D-SACCHARIC ACID	C00818	210.03757	1.28	1.28	NEG
D-TAGATOSE	C00795	180.06339	1.23	1.25	NEG
D-TRYPTOPHAN	C00806	204.08988	3.41	3.34	POS
D-XYLOSE	C01394	150.05283	1.26	1.25	NEG
EPINEPHRINE	C00788	183.08954	1.35	1.26	POS
ERYTHRITOL	C00503	122.05791	1.25	-	POS
ETHANOLAMINE PHOSPHATE	C00346	141.01910	1.21	1.19	POS
ETHYL 3-UREIDOPROPIONATE	CA1359	160.08479	1.43	1.54	POS
FORMYL-L-METHIONYL PEPTIDE	C03145	177.04597	1.18	1.25	NEG
FRUCTOSE 1,6-BIPHOSPHATE	C00354	339.99606	2.00	1.50	NEG
FUMARATE	C00122	116.01096	2.18	2.19	NEG
GALACTARATE	C01807	210.03757	1.28	1.29	NEG
GALACTITOL	C01697	182.07904	1.21	1.25	NEG
GLUCONIC ACID	CA1492	196.05830	1.26	1.25	NEG
GLUCOSAMINATE	C03752	195.07429	1.19	1.16	POS
GLUTARATE	C00489	132.04226	2.94	2.90	NEG
GLUTARIC ACID	C00489	132.04226	2.94	2.90	NEG
GLUTATHIONE	C00051	307.08381	1.64	1.24	POS
GLYCERALDEHYDE	C02154	90.03170	1.21	-	POS
GLYCERALDEHYDE 3-PHOSPHATE DIETHYL ACETAL	CA1402	169.99803	1.20	1.32	NEG
GLYCERATE	C00258	106.02661	1.36	1.24	NEG
GLYCEROL 2-PHOSPHATE	C02979	172.01367	1.30	1.30	NEG
GLYCINE	C00037	75.03203	1.18	1.17	POS
GUANIDINOACETATE	C00581	117.05383	1.20	1.19	POS
GUANINE	C00242	151.04941	2.23	-	POS
GUANOSINE	C00387	283.09167	2.22	1.25	POS
GUANOSINE 3',5'-CYCLIC MONOPHOSPHATE	C00942	345.04744	2.52	2.57	POS
GUANOSINE 5'-DIPHOSPHATE	C00035	443.02432	2.25	-	POS
GUANOSINE 5'-DIPHOSPHO-D-MANNOSE	C00096	605.07716	1.63	1.63	POS
GUANOSINE 5'-DIPHOSPHOGLUCOSE	C00394	443.02432	1.65	1.65	POS
GUANOSINE 5'-MONOPHOSPHATE	C00144	363.05800	1.64	1.63	POS
HEPTANOIC ACID	CA1393	130.09938	-	1.25	NEG
HEXANOATE	C01585	116.08373	-	1.25	NEG
HISTAMINE	C00388	111.07965	1.09	1.07	POS
HOMOCYSTEINE	C05330	135.03540	1.34	1.26	POS
HOMOCYSTINE	C01817	268.05515	1.31	1.24	POS
HOMOGENISATE	C00544	168.04226	2.50	3.25	NEG
HOMOSERINE	C00263	119.05824	1.19	1.19	POS
HYPOTAURINE	C00519	109.01975	1.22	1.19	POS
HYPOXANTHINE	C00262	136.03851	1.67	1.25	POS
INDOLE-3-ACETALDEHYDE	C00637	159.06841	-	1.34	NEG
INDOXYL SULFATE	C08481	133.05277	1.64	1.24	POS
INOSINE	C00294	268.08077	2.22	1.26	POS
INOSINE 5'-DIPHOSPHATE	C00104	428.01344	2.34	-	POS
INOSINE 5'-MONOPHOSPHATE	C00130	348.04710	1.64	1.69	NEG
INOSINE 5'-PHOSPHATE	C00130	348.04710	1.64	1.69	NEG
ISOCITRIC ACID	C00311	192.02701	1.61	1.34	NEG
ISOPENTENYL PYROPHOSPHATE	C00129	297.08547	1.15	-	POS
ITACONATE	C00490	130.02661	3.70	-	NEG

KYNURENINE	C01718	208.08479	3.32	1.31	POS
L-2,3-DIAMINOPROPIONIC ACID	C03401	104.05858	1.12	1.12	POS
L-ALANINE	C01401	89.04768	1.22	1.19	POS
L-ALLOTHREONINE	C05519	119.05824	1.21	1.18	POS
L-ANSERINE	C01262	303.11788	-	1.12	NEG
L-ARABITOL	CA1387	152.06848	-	1.25	NEG
L-ARGININE	C00062	174.11168	1.13	1.12	POS
L-ASPARAGINE	C16438	132.05349	1.20	1.18	POS
L-ASPARTATE	C16433	133.03751	1.22	1.20	POS
L-CARNITINE	C00318	161.10519	1.20	1.19	POS
L-CYSTATHIONINE	C00542	222.06743	1.16	1.16	POS
L-CYSTEIC ACID	C00506	187.01506	1.15	1.43	NEG
L-CYSTEINE	C00736	121.01975	1.25	1.25	POS
L-CYSTINE	C01420	240.02385	1.18	1.17	POS
LEUCINE	C16439	131.09463	1.99	1.26	POS
L-GLUTAMIC ACID	C00302	147.05316	1.21	1.20	POS
L-GLUTAMINE	C00303	146.06914	1.24	1.20	POS
L-HISTIDINE	C00135	155.06947	1.14	1.12	POS
L-HISTIDINOL	C00860	141.09021	1.10	1.07	POS
L-HOMOCYSTEINE THIOACTONE	CE1401	117.02483	1.30	1.24	POS
L-ISOLEUCINE	C16434	131.09463	1.40	1.24	POS
L-KYNURENINE	C01718	208.08479	3.32	1.31	POS
LL-2,6-DIAMINOHEPTANEDIOATE	C00666	190.09536	1.16	1.14	POS
L-LYSINE	C16440	146.10553	1.12	1.11	POS
L-METHIONINE	C01733	149.05105	1.61	1.26	NEG
L-METHIONINE SULFOXIMINE	C03510	180.05687	1.19	1.17	POS
L-NORVALINE	CA1395	117.07898	1.63	1.26	POS
L-ORNITHINE	C00077	132.08987	1.10	1.11	POS
L-PHENYLALANINE	C02057	165.07898	3.17	1.42	POS
L-PIPECOLIC ACID	C00408	129.07898	1.09	1.11	POS
L-PROLINE	C16435	115.06333	1.26	1.23	POS
L-RHAMNOSE	C00507	182.07904	1.25	1.20	NEG
L-SERINE	C00716	105.04259	1.19	1.17	POS
L-SORBOSE	C01452	180.06339	1.04	1.25	NEG
L-THREONINE	CA1381	119.05824	1.22	1.19	POS
L-TRYPTOPHAN	C00806	204.08988	3.41	3.34	POS
L-TRYPTOPHANAMIDE	C00977	203.10586	1.25	1.33	POS
L-TYROSINE	C01536	181.07389	1.92	1.26	POS
LUMICHROME	C01727	242.08038	1.11	-	POS
L-VALINE	C16436	117.07898	1.36	1.26	POS
MALEAMATE	C01596	115.02694	1.36	-	NEG
MALEIC ACID	C01384	116.01096	2.51	2.48	NEG
MALEIMIDE	C07272	97.01638	1.69	-	POS
MALTOSE	C00208	342.11622	1.24	1.26	NEG
MANDELIC ACID	CA1444	152.04734	1.61	3.92	NEG
MANNITOL	C00392	182.07904	1.24	1.25	POS
MANNOSE	C00159	180.06339	1.23	1.24	NEG
MELIBIOSE	C05402	342.11622	1.24	1.25	NEG
MERCAPTOPYRUVATE	C00957	119.98812	-	1.65	NEG
MESO-TARTARIC ACID	C00552	168.02701	1.64	-	NEG
MESOXALATE	C00830	117.99023	1.61	-	NEG
METHYL BETA-D-GALACTOSIDE	C03619	194.07904	2.09	1.33	NEG
METHYL INDOLE-3-ACETATE	CA1231	189.07898	3.01	-	POS
METHYLGUANIDINE	C02294	73.06400	1.22	1.19	POS
METHYLMALONATE	C02170	118.02661	2.43	2.37	NEG
MEVALOLACTONE	CA1383	130.06300	2.41	2.42	POS
MONO-METHYL GLUTARATE	CA1015	146.05791	-	2.05	NEG
MYO-INOSITOL	C00137	180.06339	1.22	1.25	NEG
N(PAI)-METHYL-L-HISTIDINE	C01152	169.08513	1.15	1.12	POS
N,N-DIMETHYL-1,4-PHENYLENEDIAMINE	C04203	136.10005	1.64	1.33	POS
N1-ACETYLSPERMINE	C02567	244.22631	1.09	1.03	POS
N-ACETYL-D-GALACTOSAMINE	C01074	221.08994	1.25	1.23	POS
N-ACETYL-DL-GLUTAMIC ACID	CA1454	189.06372	1.86	1.26	NEG
N-ACETYL-DL-METHIONINE	CA1210	191.06162	3.02	2.97	POS
N-ACETYL-DL-SERINE	CA1449	147.05316	1.56	1.27	NEG
N-ACETYL-D-MANNOSAMINE	C00645	221.08994	1.26	1.23	POS
N-ACETYLGLYCINE	CA1212	117.04259	1.64	1.26	NEG
N-ACETYL-L-ALANINE	CE1554	131.05824	1.99	1.37	NEG
N-ACETYL-L-ASPARTIC ACID	CA1200	175.04807	1.65	1.52	NEG
N-ACETYL-L-CYSTEINE	CE1310	162.02249	2.65	2.66	NEG
N-ACETYL-L-PHENYLALANINE	C03519	207.08954	1.32	-	POS
N-ACETYLNEURAMINATE	C00270	309.10598	1.30	1.31	POS
N-ACETYLPUTRESCINE	C02714	130.11061	1.27	1.23	POS
NAD	C00003	663.10912	1.64	1.24	POS
N-ALPHA-ACETYL-L-ASPARAGINE	CA1214	174.06406	1.44	1.26	NEG

NALPHA-ACETYL-L-LYSINE	CA1219	188.11609	1.27	1.22	POS
N-AMIDINO-L-ASPARTATE	C03139	175.05931	1.24	1.21	POS
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	C03793	188.15248	1.12	1.12	POS
N-FORMYLGLYCINE	CA1268	103.02694	1.34	1.34	POS
NICOTINAMIDE	C00153	122.04801	1.64	1.26	POS
NICOTINAMIDE HYPOXANTHINE DINUCLEOTIDE	C04423	665.10040	1.64	1.30	POS
NICOTINAMIDE MONONUCLEOTIDE	C00455	334.05661	1.26	1.23	POS
NICOTINATE	C00253	123.03203	1.63	1.37	POS
NICOTINIC ACID ADENINE DINUCLEOTIDE PHOSPHATE	C13051	745.06677	1.64	1.69	POS
N-METHYL-D-ASPARTIC ACID	C12269	147.05316	1.24	1.22	POS
N-METHYL-L-GLUTAMATE	C01046	161.06881	1.24	1.22	POS
NORADRENALINE	C00547	169.07389	1.25	1.22	POS
NORLEUCINE	C01933	131.09463	2.10	1.27	POS
O-ACETYL-L-SERINE	C00979	147.05316	1.27	1.24	POS
OCTOPAMINE	C04227	153.07897	1.35	1.26	POS
O-PHOSPHO-DL-SERINE	CA1209	185.00893	1.26	1.36	NEG
O-PHOSPHO-L-SERINE	CA1388	185.00893	1.26	1.34	NEG
OPHTHALMIC ACID	CA1475	289.12739	1.64	1.26	POS
OROTATE	C00295	156.01711	1.14	-	POS
OROTIC ACID	C00295	174.02767	1.14	-	POS
OXALIC ACID	C00209	126.01644	1.07	-	POS
OXALOMALIC ACID	C01990	206.00627	1.27	-	NEG
PARAXANTHINE	C13747	180.06473	3.87	1.35	POS
PENTANOATE	C00803	102.06808	-	1.30	NEG
PHENETHYLAMINE	C05332	121.08915	-	1.27	NEG
PHENOL	C00146	94.04187	2.67	-	POS
PHENYLETHANOLAMINE	C02735	137.08406	2.66	-	POS
PHENYLPIRUVATE	C00166	164.04735	1.96	1.29	POS
PHOSPHO(ENOL)PYRUVIC ACID	C00074	167.98238	1.35	1.35	POS
PHOSPHOCHOLINE	C00588	183.06604	1.21	1.19	POS
PHOSPHOCREATINE	C02305	211.03581	1.31	1.27	POS
PHOSPHONOACETATE	C05682	139.98746	1.36	1.45	NEG
PICOLINIC ACID	C10164	123.03203	1.63	1.27	POS
PIPECOLATE	C00408	129.07898	1.09	1.11	POS
PROPANOATE	C00163	74.03678	3.00	1.37	POS
PROPIONATE	C00163	74.03678	3.00	1.37	POS
PTERIN	CA1303	163.04941	1.37	-	NEG
PURINE	C00465	120.04360	1.85	1.25	POS
PUTRESCINE	C00134	88.10005	1.06	1.07	POS
PYRIDINE-2,3-DICARBOXYLATE	C03722	167.02186	1.87	1.95	NEG
PYRIDOXAL	C00250	167.05824	1.63	1.33	POS
PYRIDOXAL 5'-PHOSPHATE	C00018	265.03514	1.64	1.51	POS
PYRIDOXAMINE	C00534	168.08988	1.11	1.11	POS
PYRIDOXINE	C00314	169.07389	1.64	1.26	POS
PYRUVATE	C00022	88.01605	1.98	1.64	NEG
QUINATE	C00296	192.06339	1.31	1.26	NEG
RIBITOL	C00474	152.06848	1.23	-	NEG
ROSMARINIC ACID	C10489	360.08452	-	1.25	NEG
S-(5'-ADENOSYL)-L-HOMOCYSTEINE	C00021	384.12159	1.65	1.24	POS
S-(5'-ADENOSYL)-L-METHIONINE	C00019	570.15665	1.15	-	POS
SALICYLAMIDE	CA1193	137.04768	0.51	-	POS
SARCOSINE	C00213	89.04768	1.18	-	POS
S-CARBOXYMETHYL-L-CYSTEINE	C03727	179.02523	1.31	1.26	POS
SELENOCYSTAMINE	CA1403	247.93309	1.09	1.09	POS
SELENOMETHIONINE	C05335	196.99550	1.78	1.26	POS
SEROTONIN	C00780	176.09496	3.01	2.66	POS
SHIKIMATE	C00493	174.05283	1.56	1.26	NEG
SN-GLYCERO-3-PHOSPHOCHOLINE	C00670	258.11011	-	1.20	NEG
SN-GLYCEROL 3-PHOSPHATE	C00093	370.22328	1.28	-	NEG
SPERMIDINE	C00315	145.15790	1.02	1.01	POS
SPERMINE	C00750	202.21575	1.01	1.00	POS
STACHYOSE	C01613	666.22186	1.24	1.20	POS
SUBERIC ACID	C08278	174.08921	-	1.28	NEG
SUCCINATE	C00042	118.02661	2.17	2.05	NEG
SUCROSE	C00089	342.11622	1.26	-	NEG
TAURINE	C00245	125.01467	1.21	1.20	POS
THEOPHYLLINE	C07130	180.06473	3.87	-	POS
THIAMINE	C00378	265.11231	1.20	1.14	POS
THIAMINE MONOPHOSPHATE	C01081	344.07081	1.18	1.15	POS
THIAMINE PYROPHOSPHATE	C00068	265.11176	-	1.65	NEG
THIOPURINE S-METHYLETHER	C03542	166.03132	1.63	-	POS
THIOUREA	C14415	76.00952	1.37	1.26	POS
THYMIDINE	C00214	242.09027	3.49	1.27	NEG
THYMIDINE 5'-MONOPHOSPHATE	C00364	322.05661	1.85	1.90	NEG
THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE	C00842	564.07576	1.66	1.65	POS

THYMINE	C00178	126.04293	2.25	2.31	POS
THYROTROPIN RELEASING HORMONE	C03958	362.17025	1.73	1.26	POS
TRANS-4-HYDROXYPROLINE	C01157	131.05824	1.23	1.20	POS
TRANS-ACONITATE	C02341	174.01644	1.40	2.58	NEG
TRIGONELLINE	C01004	137.04768	1.26	1.23	POS
TYRAMINE	C00483	137.08406	1.99	1.95	POS
URACIL	C00106	112.02728	1.64	1.25	POS
URATE	C00366	168.02834	1.64	1.26	NEG
URIDINE	C00299	244.06954	1.80	1.26	NEG
URIDINE 5'-DIPHOSPHATE	C00015	404.00220	1.65	-	POS
URIDINE 5'-DIPHOSPHOGALACTOSE	C00052	566.05503	1.37	1.42	POS
URIDINE 5'-DIPHOSPHOGLUCOSE	C00029	566.05503	1.32	1.37	POS
URIDINE 5'-DIPHOSPHOGLUCURONIC ACID	C00167	580.03430	-	2.61	NEG
URIDINE 5'-DIPHOSPHO-N-ACETYLGALACTOSAMINE	C00203	607.08154	1.38	1.41	POS
URIDINE 5'-DIPHOSPHO-N-ACETYLGLUCOSAMINE	C00043	607.08158	1.37	-	POS
URIDINE-5-MONOPHOSPHATE	C00105	324.03587	1.58	1.47	NEG
UROCANATE	C00785	138.04293	1.64	1.25	POS
XANTHINE	C00385	152.03343	1.81	1.25	NEG
XANTHOSINE	C01762	284.07569	2.84	1.26	NEG
XANTHOSINE 5'-MONOPHOSPHATE	C00655	364.04202	1.64	1.72	NEG
XANTHURENIC ACID	C02470	205.03751	1.35	-	POS
XYLITOL	C00379	152.06848	1.24	1.25	POS

Supplementary Table 1 - part 2 - HILIC 15 min method - IROA standard characterization

COMPOUND NAME	PARENT_CID	Neutral mass	Rt
(2-AMINOETHYL)PHOSPHONATE	C03557	125.02418	7.10
(R)-MALATE	C00711	134.02153	0.76
(R,R)-TARTARIC ACID	C00898	150.01644	1.15
(S)-LACTATE	C01432	90.03170	0.80
(S)-MALATE	C00711	134.02153	0.76
(S,S)-TARTARIC ACID	C00898	150.01644	1.15
1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE	LMGP01010380	565.37436	5.39
1,3-DIAMINOPROPANE	C00986	74.08440	7.48
10-HYDROXYDECANOATE	C02774	188.14125	0.70
1-AMINOCYCLOPROPANE-1-CARBOXYLATE	C01234	101.04768	4.97
1-HYDROXY-2-NAPHTHOATE	C03203	188.04735	0.76
1-METHYL-6,7-DIHYDROXY-1,2,3,4-TETRAHYDROISOQUINOLINE	C09642	179.09464	4.67
1-METHYLADENOSINE	C02494	281.11241	3.60
1-NAPHTHYLAMINE	C14790	143.07350	0.85
2,3-DIHYDROXYBENZOATE	C00196	154.02661	0.74
2',4'-DIHYDROXYACETOPHENONE	C03663	152.04735	0.74
2,4-DIHYDROXYPTERIDINE	C03212	164.03343	0.75
2,4-DIHYDROXYPYRIMIDINE-5-CARBOXYLIC ACID	C03030	156.01711	0.73
2,5-DIHYDROXYBENZOATE	C00628	154.02661	0.67
2-AMINO-2-METHYLPROPANOATE	C03665	103.06333	4.85
2-AMINOETHYL DIHYDROGEN PHOSPHATE	CA1062	141.01910	6.57
2-AMINOPHENOL	C01987	109.05276	2.84
2'-DEOXYADENOSINE 5'-DIPHOSPHATE	C00206	411.03451	7.73
2'-DEOXYCYTIDINE 5'-MONOPHOSPHATE	C00239	307.05694	6.30
2'-DEOXYGUANOSINE 5'-TRIPHOSPHATE	C00286	506.99575	11.78
2'-DEOXYURIDINE 5'-MONO-PHOS-PHATE	C00365	308.04096	4.98
2-HYDROXYBUTYRIC ACID	C05984	104.04734	0.77
2-HYDROXYPHENYLACETIC ACID	CA1444	152.04734	0.74
2-HYDROXYPYRIDINE	C02502	95.03711	1.08
2-METHYLGLUTARIC ACID	CA1107	146.05791	0.68
2-METHYLMALEATE	C02226	130.02661	0.68
2-METHYLPROPANAL OXIME	C03219	87.06841	0.75
2-METHYLPROPANOATE	C02632	88.05243	0.89
2-OXOADIPATE	C00322	160.03718	0.69
2-QUINOLINECARBOXYLIC ACID	C06325	173.04768	1.67
3-(2-HYDROXYPHENYL)PROPANOATE	C01198	166.06300	0.70
3-(4-HYDROXYPHENYL)LACTATE	C03672	182.05791	0.71
3-(4-HYDROXYPHENYL)PYRUVATE	C01179	180.04226	0.67
3,4-DIHYDROXYBENZOATE	C00230	154.02661	0.71
3,4-DIHYDROXY-L-PHENYLALANINE	C00355	197.06881	4.72
3,4-DIHYDROXYPHENYL GLYCOL	C05576	170.05791	0.73
3,4-DIHYDROXYPHENYLACETATE	C01161	168.04226	0.71
3',5'-CYCLIC AMP	C00575	329.05252	5.29
3,5-DIIODO-L-THYRONINE	C01060	524.89341	0.72
3,5-DIIODO-L-TYROSINE	C01060	468.88833	0.72
3ALPHA,12ALPHA-DIHYDROXY-5BETA-CHOLANATE	C04483	392.29266	0.70
3-AMINO-4-HYDROXYBENZOIC ACID	C12115	153.04259	0.81
3-AMINO-5-HYDROXYBENZOIC ACID	C12107	153.04260	0.74
3-AMINOISOBUTANOATE	C05145	103.06333	4.94
3'-CMP	C05822	323.05186	6.12
3-DEHYDROSHIKIMATE	C02637	172.03717	0.74
3-HYDROXY-3-METHYLGLUTARATE	C03761	162.05283	0.72
3-HYDROXYANTHRANILATE	C00632	153.04259	0.71
3-HYDROXYBENZALDEHYDE	C03067	122.03678	0.74
3-HYDROXYBENZOATE	C00587	138.03170	0.75
3-HYDROXYBENZYL ALCOHOL	C03351	124.05243	0.71
3-HYDROXYBUTANOIC ACID	C01089	104.04735	0.76
3-HYDROXYKYNURENINE	C02794	224.07971	4.55
3-HYDROXYPHENYLACETATE	C05593	152.04735	0.76

3-METHOXY-4-HYDROXYMANDELATE	C05584	198.05283	0.74
3-METHOXYTYRAMINE	C05587	167.09464	4.60
3-METHYGLUTARIC ACID	CA1192	146.05791	0.69
3-METHYL-2-OXINDOLE	CA1325	147.06841	0.71
3-METHYLADENINE	C00913	149.07015	5.17
3-METHYLHISTAMINE	C15526	125.09530	7.61
3-NITRO-L-TYROSINE	CA1195	226.05897	4.50
3-SULFINO-L-ALANINE	C00606	153.00958	4.99
3-UREIDOPROPIONATE	C02642	132.05349	0.77
4-ACETAMIDOBUTANOATE	C02946	145.07389	0.73
4-AMINOBENZOATE	C00568	137.04768	0.68
4-AMINOBUTANOATE	C00334	103.06333	4.96
4-COUMARATE	C00811	164.04735	0.70
4-GUANIDINOBUTANOATE	C01035	145.08513	4.73
4-HYDROXY-2-QUINOLINECARBOXYLIC ACID	C01717	189.04259	0.73
4-HYDROXYBENZALDEHYDE	C00633	122.03678	0.74
4-HYDROXYBENZOATE	C00156	138.03170	0.74
4-HYDROXY-L-PHENYLGLYCINE	CA1445	167.05824	4.64
4-HYDROXY-L-PROLINE	C01157	131.05824	5.37
4-HYDROXYPHENYLACETATE	C00642	152.04735	0.75
4-IMIDAZOLEACETIC ACID	C02835	126.04293	4.94
4-METHYL-2-OXO-PENTANOIC ACID	C00233	130.06299	0.69
4-PYRIDOXATE	C00847	183.05316	4.99
4-QUINOLINECARBOXYLIC ACID	C06414	173.04768	1.09
5,6-DIHYDROURACIL	C00429	114.04293	2.42
5-AMINOIMIDAZOLE-4-CARBOXAMIDE-1-BETA-D-RIBOFURANOSYL 5'-MONOPHOSPHATE	C04677	338.06275	6.23
5-AMINOPENTANOATE	C00431	117.07898	4.93
5'-DEOXYADENOSINE	C05198	251.10184	3.78
5-HYDROXYINDOLEACETATE	C05635	191.05824	0.73
5-HYDROXY-L-TRYPTOPHAN	C01017	220.08479	4.56
5-HYDROXYMETHYLURACIL	C03088	142.03784	0.76
5-METHYLCYTOSINE HYDROCHLORIDE	C02376	125.05891	5.00
5'-METHYLTHIOADENOSINE	C00170	297.08956	3.55
5-OXO-D-PROLINE	C01879	129.04259	0.75
5-OXO-L-PROLINE	C01879	129.04259	0.75
6-CARBOXYHEXANOATE	C02656	160.07356	0.70
6-DEOXY-L-GALACTOSE	C00382	164.06848	4.05
6-HYDROXYDOPAMINE	CA1404	169.07390	5.25
6-HYDROXYNICOTINATE	C01020	139.02694	0.75
ACETOACETATE	C00164	102.03169	0.79
ACETOIN	C00466	88.05243	0.89
ACETYL PHOSPHATE	C00227	139.98750	7.00
ADENINE	C00147	135.05450	4.70
ADENOSINE	C00212	267.09676	3.66
ADENOSINE 2',3'-CYCLIC MONOPHOSPHATE	C02353	267.09676	5.07
ADENOSINE 3',5'-CYCLIC MONOPHOSPHATE	C00575	329.05252	5.29
ADENOSINE 5'-DIPHOSPHORIBOSE	C00301	559.07168	9.06
ADENOSINE 5'-MONOPHOSPHATE	C00020	347.06309	6.14
ADENOSINE 5'-TRIPHOSPHATE	C00002	506.99575	11.82
ADIPIC ACID	CA1042	146.05791	0.71
AGMATINE SULFATE	C00179	130.12180	7.31
ALLANTOIN	C01551	158.04399	0.74
ALLOSE	C01487	180.06339	1.08
ALPHA-AMINOADIPATE	C00956	161.06881	4.89
ALPHA-D-GALACTOSE 1-PHOSPHATE	C00446	260.02971	6.05
ALPHA-D-GLUCOSE	C00293	180.06339	0.81
ALPHA-D-GLUCOSE 1-PHOSPHATE	C00103	260.02972	6.11
ALPHA-KETOGLUTARIC ACID	C00026	146.02153	0.76
ANILINE	C00292	93.05785	1.80
ANILINE-2-SULFONIC ACID	C00292-1	173.01467	0.70
ANTHRANILATE	C00108	137.04768	0.67



AZELAIC ACID	C08261	188.10486	0.70
BENZOATE	C00180	122.03678	0.70
BETA-ALANINE	C00099	89.04768	5.01
BETAINE	C00719	117.07898	5.81
BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE 2'-PHOSPHATE REDUCED	C00006	743.07545	10.32
BETA-NICOTINAMIDE ADENINE DINUCLEOTIDE PHOSPHATE	C00006	743.07545	10.32
BIOTIN	C00120	244.08817	0.76
BIS(2-ETHYLHEXYL)PHTHALATE	C03690	390.27701	0.71
BIS(3-AMINOPROPYL)AMINE	C03375	131.14225	8.66
BUTANOATE	C00246	88.05243	0.83
CADAVERINE	C01672	102.11570	7.38
CAFFEATE	C01481	180.04226	0.67
CAFFEINE	C07481	194.08038	0.98
CARNOSINE	C00386	226.10659	7.51
CATECHOL	C00090	110.03678	0.71
CHENODEOXYCHOLATE	C02528	392.29266	0.71
CHOLATE	C00695	408.28758	0.72
CHOLESTERYL ACETATE	CA1190	428.36543	0.69
CHOLINE	C00114	104.10754	5.74
CIS-4-HYDROXY-D-PROLINE	C01015	131.05824	5.20
CITRAMALATE	C00815	148.11402	1.12
CITRATE	C00158	192.02701	2.25
CITRULLINE	C00327	175.09569	5.91
CMP	C00055	323.05186	6.22
CORTISOL	C00735	362.20933	0.72
CORTISOL 21-ACETATE	C02821	404.21989	0.69
CREATINE	C00300	131.06948	4.98
CREATINE PHOSPHATE	C02305	211.03581	6.13
CREATININE	C00791	113.05891	5.01
CYS-GLY	C01419	178.04122	7.10
CYTIDINE	C00475	243.08552	5.02
CYTIDINE 2',3'-CYCLIC MONO-PHOS-PHATE	C02354	305.04129	5.63
CYTIDINE 5'-DIPHOSPHATE	C00112	403.01819	4.95
CYTIDINE 5'-DIPHOSPHOCHOLINE	C00307	489.11459	9.29
CYTOSINE	C00380	111.04326	5.02
D-(-)-3-PHOSPHOGLYCERIC ACID	C00597	185.99294	8.57
D-(-)-ARABINOSE	CA1283	150.05282	0.70
D-(+)-CELLOBIOSE	C00185	342.11622	4.05
D-(+)-GALACTOSAMINE	C02262	179.07938	5.53
D-(+)-GLUCOSAMINE	C00329	179.07938	5.50
D-ALANINE	C00133	89.04768	4.98
DAMP	C00360	331.06817	6.28
D-ASPARTATE	C16433	133.03751	4.86
DEHYDROASCORBATE	C00425	174.01644	0.75
DEHYDRO-L-(+)-ASCORBIC ACID DIMER	C00425	348.03288	0.75
DEOXYCARNITINE	C05543	145.11028	5.36
DEOXYCHOLATE	C04483	392.29266	0.70
DEOXYCYTIDINE	C00881	227.09061	5.01
DEOXYRIBOSE	C01801	134.05791	0.70
DEOXYURIDINE	C00526	228.07462	0.74
DETHIOBIOTIN	C01909	214.13174	0.74
D-FRUCTOSE	C01496	180.06339	0.80
D-FRUCTOSE 6-PHOSPHATE	C00085	260.02972	6.46
D-GALACTOSE	C01582	180.06339	1.13
D-GLUCONO-1,5-LACTONE	C00198	178.04774	0.75
D-GLUCOSAMINE 6-PHOSPHATE	C00352	259.04571	6.47
D-GLUCOSAMINE 6-SULFATE	CA1422	259.03619	0.78
D-GLUCOSE 6-PHOSPHATE	C00092	260.02972	6.76
D-GLUCURONIC ACID	C00191	194.04265	0.76
D-GLUCURONOLACTONE	C02670	176.03209	0.74
D-GLYCERIC ACID	C00258	106.02661	1.13

D-GULONIC ACID GAMA-LACTONE	C00800	178.04774	0.75
DIETHANOLAMINE	C06772	105.07898	5.30
DIHYDROXYMANDELIC ACID	C07470	184.03718	0.72
DIMETHYLBENZIMIDAZOLE	C03114	146.08440	4.51
DL-5-HYDROXYLYSINE	C01211	162.10044	7.19
DL-NORMETANEPHRINE	CA1379	183.08954	4.70
D-MANNOSAMINE	C03570	179.07938	5.35
D-MANNOSE 6-PHOSPHATE	C00275	260.02972	5.87
DOPAMINE	C03758	153.07898	4.68
D-ORNITHINE	C00515	132.08987	7.18
D-PANTOTHENIC ACID	C00864	219.11067	0.75
D-PSICOSE	C06468	180.06339	1.40
D-RIBOSE	C08353	150.05283	0.70
D-RIBOSE 5-PHOSPHATE	C00117	230.01916	6.23
D-SACCHARIC ACID	C00818	210.03757	6.44
D-SORBITOL	C00749	180.06339	0.75
D-TRYPTOPHAN	C00806	204.08988	4.50
D-XYLOSE	C01394	150.05283	0.70
EPINEPHRINE	C00788	183.08954	4.88
ERYTHRITOL	C00503	122.05791	0.70
ETHANOLAMINE PHOSPHATE	C00346	141.01910	6.84
ETHYL 3-INDOLEACETATE	CA1213	203.09463	0.73
ETHYLMALONIC ACID	CA1366	132.04226	0.69
FERULATE	C01494	194.05791	0.70
FLAVIN ADENINE DINUCLEOTIDE	C00016	785.15714	8.78
FORMYL-L-METHIONYL PEPTIDE	C03145	177.04597	0.70
FRUCTOSE 1,6-BIPHOSPHATE	C00354	339.99606	3.35
FUMARATE	C00122	116.01096	0.71
GALACTARATE	C01807	210.03757	3.09
GALACTITOL	C01697	182.07904	2.92
GLUCONIC ACID	CA1492	196.05830	3.94
GLUCOSAMINATE	C03752	195.07429	5.73
GLUTARATE	C00489	132.04226	0.70
GLUTARIC ACID	C00489	132.04226	0.70
GLUTATHIONE	C00051	307.08381	5.02
GLYCERATE	C00258	106.02661	1.13
GLYCEROL 2-PHOSPHATE	C02979	172.01367	4.92
GLYCINE	C00037	75.03203	5.14
GLYCOCHOLATE	C01921	465.30904	0.72
GUANIDINOACETATE	C00581	117.05383	4.85
GUANOSINE	C00387	283.09167	3.22
GUANOSINE 3',5'-CYCLIC MONOPHOSPHATE	C00942	345.04744	0.73
GUANOSINE 5'-DIPHOSPHO-D-MANNOSE	C00096	605.07716	8.67
HEXANOATE	C01585	116.08373	0.70
HIPPURATE	C01586	179.05824	0.71
HISTAMINE	C00388	111.07965	7.37
HOMOCYSTINE	C01817	268.05515	6.53
HOMOGENISATE	C00544	168.04226	0.68
HOMOSERINE	C00263	119.05824	5.07
HOMOVANILLATE	C05582	182.05791	0.72
HYDROQUINONE	C00530	110.03678	0.67
HYPOTAURINE	C00519	109.01975	5.71
HYPOXANTHINE	C00262	136.03851	2.21
INDOLE-3-ACETALDEHYDE	C00637	159.06841	0.69
INDOLE-3-ACETAMIDE	C02693	174.07931	0.72
INDOLE-3-ACETATE	C00954	175.06333	0.73
INDOLE-3-ACETIC ACID	C00954	175.06333	0.73
INDOLE-3-ETHANOL	C00955	161.08406	0.72
INDOLE-3-PYRUVIC ACID	CA1282	203.05824	0.76
INDOXYL SULFATE	C08481	133.05277	0.48
INOSINE	C00294	268.08077	2.02

INOSINE 5'-MONOPHOSPHATE	C00130	348.04710	6.04
INOSINE 5'-PHOSPHATE	C00130	348.04710	6.04
ISOCITRIC ACID	C00311	192.02701	1.01
ITACONATE	C00490	130.02661	0.68
KYNURENINE	C01718	208.08479	4.60
L-2,3-DIAMINOPROPIONIC ACID	C03401	104.05858	6.87
L-2-PHOSPHOGLYCERIC ACID	CA1485	164.06848	0.70
L-ALANINE	C01401	89.04768	5.01
L-ALLOTHREONINE	C05519	119.05824	5.02
L-ARABITOL	CA1387	152.06848	0.81
L-ARGININE	C00062	174.11168	7.03
L-ASPARAGINE	C16438	132.05349	5.42
L-ASPARTATE	C16433	133.03751	4.86
LAUROYLCARNITINE	CA1406	343.27225	4.35
L-CARNITINE	C00318	161.10519	5.31
L-CYSTATHIONINE	C00542	222.06743	6.79
L-CYSTEINE	C00736	121.01975	4.83
L-CYSTINE	C01420	240.02385	6.77
LEUCINE	C16439	131.09463	4.61
L-GLUTAMIC ACID	C00302	147.05316	4.87
L-GLUTAMINE	C00303	146.06914	5.50
L-HISTIDINE	C00135	155.06947	7.06
L-HISTIDINOL	C00860	141.09021	7.31
L-HOMOCYSTEINE THIOLACTONE	CE1401	117.02483	4.80
LIPOAMIDE	C00248	205.05951	0.72
L-ISOLEUCINE	C16434	131.09463	4.61
L-KYNURENINE	C01718	208.08479	4.60
LL-2,6-DIAMINOHEPTANEDIOATE	C00666	190.09536	6.98
L-LYSINE	C16440	146.10553	7.23
L-METHIONINE	C01733	149.05105	4.72
L-METHIONINE SULFOXIMINE	C03510	180.05687	6.09
L-NORVALINE	CA1395	117.07898	4.71
L-ORNITHINE	C00077	132.08987	7.18
L-PHENYLALANINE	C02057	165.07898	4.57
L-PIPECOLIC ACID	C00408	129.07898	4.20
L-PROLINE	C16435	115.06333	5.21
L-SERINE	C00716	105.04259	5.10
L-SORBOSE	C01452	180.06339	0.80
L-THREONINE	CA1381	119.05824	5.03
L-TRYPTOPHAN	C00078	204.08988	4.51
L-TRYPTOPHANAMIDE	C00977	203.10586	4.70
L-TYROSINE	C01536	181.07389	4.66
L-VALINE	C16436	117.07898	4.81
MALEIC ACID	C01384	116.01096	0.66
MALONATE	C00383	104.01096	0.69
MALTOSE	C00208	342.11622	0.82
MANDELIC ACID	CA1444	152.04734	0.74
MANNITOL	C00392	182.07904	0.82
MANNOSE	C00159	180.06339	1.41
MELATONIN	C01598	232.12118	0.73
MELIBIOSE	C05402	342.11622	0.81
MERCAPTOPYRUVATE	C00957	119.98812	0.73
MESO-TARTARIC ACID	C00552	168.02701	0.75
METHYL BETA-D-GALACTOSIDE	C03619	194.07904	0.70
METHYL INDOLE-3-ACETATE	CA1231	189.07898	0.74
METHYL JASMONATE	C11512	224.14125	0.68
METHYLGUANIDINE	C02294	73.06400	4.93
METHYLMALONATE	C02170	118.02661	0.68
MEVALOLACTONE	CA1383	130.06300	0.72
MONO-ETHYL MALONATE	HMDB00576	132.04226	0.70
MONO-METHYL GLUTARATE	CA1015	146.05791	0.74

MYO-INOSITOL	C00137	180.06339	0.81
N(PAI)-METHYL-L-HISTIDINE	C01152	169.08513	7.51
N,N-DIMETHYL-1,4-PHENYLENEDIAMINE	C04203	136.10005	4.76
N1-ACETYLSPERMINE	C02567	244.22631	8.84
N6-(DELTA2-ISOPENTENYL)-ADENINE	C04083	203.11710	4.05
N-ACETYL-D-GALACTOSAMINE	C01074	221.08994	0.81
N-ACETYL-DL-GLUTAMIC ACID	CA1454	189.06372	0.75
N-ACETYL-DL-METHIONINE	CA1210	191.06162	0.72
N-ACETYL-DL-SERINE	CA1449	147.05316	0.75
N-ACETYL-D-TRYPTOPHAN	C03137	246.10044	0.71
N-ACETYLGLYCINE	CA1212	117.04259	0.74
N-ACETYL-L-ALANINE	CE1554	131.05824	0.71
N-ACETYL-L-ASPARTIC ACID	CA1200	175.04807	0.73
N-ACETYL-L-CYSTEINE	CE1310	162.02249	0.70
N-ACETYL-L-LEUCINE	C02710	173.10519	0.71
N-ACETYL-L-PHENYLALANINE	C03519	207.08954	0.71
N-ACETYLNEURAMINATE	C00270	309.10598	3.28
N-ACETYLPUTRESCINE	C02714	130.11061	5.77
N-ACETYLSEROTONIN	C00978	218.10553	0.74
NAD	C00003	663.10912	8.54
N-ALPHA-ACETYL-L-ASPARAGINE	CA1214	174.06406	0.76
NALPHA-ACETYL-L-LYSINE	CA1219	188.11609	5.34
N-AMIDINO-L-ASPARTATE	C03139	175.05931	4.64
NEPSILON,NEPSILON,NEPSILON-TRIMETHYLLYSINE	C03793	188.15248	8.36
N-FORMYLGLYCINE	CA1268	103.02694	0.74
NICOTINAMIDE	C00153	122.04801	1.87
NICOTINAMIDE MONONUCLEOTIDE	C00455	334.05661	6.59
NICOTINATE	C00253	123.03203	1.08
N-METHYL-D-ASPARTIC ACID	C12269	147.05316	4.78
N-METHYL-L-GLUTAMATE	C01046	161.06881	4.91
NORADRENALINE	C00547	169.07389	4.87
NORLEUCINE	C01933	131.09463	4.59
O-ACETYL-L-CARNITINE	C02571	203.11576	5.11
O-ACETYL-L-SERINE	C00979	147.05316	4.92
OCTOPAMINE	C04227	153.07897	4.64
OMEGA-HYDROXYDODECANOIC ACID	C08317	216.17255	0.69
O-PHOSPHO-DL-SERINE	CA1209	185.00893	7.77
O-PHOSPHO-L-SERINE	CA1388	185.00893	7.99
OPHTHALMIC ACID	CA1475	289.12739	5.21
OXALOMALIC ACID	C01990	206.00627	5.44
PALATINOSE	C01742	342.11621	3.49
PARAXANTHINE	C13747	180.06473	1.04
PHENYLACETIC ACID	C07086	136.05243	0.74
PHENYLETHANOLAMINE	C02735	137.08406	4.57
PHENYLPYRUVATE	C00166	164.04735	0.71
PHOSPHOCHOLINE	C00588	183.06604	7.88
PHOSPHOCREATINE	C02305	211.03581	6.13
PHOSPHONOACETATE	C05682	139.98746	7.08
PIPECOLATE	C00408	129.07898	4.20
PTERIN	CA1303	163.04941	2.02
PURINE	C00465	120.04360	1.96
PUTRESCINE	C00134	88.10005	7.42
PYRIDOXAL	C00250	167.05824	4.56
PYRIDOXAMINE	C00534	168.08988	7.03
PYRIDOXINE	C00314	169.07389	5.07
PYRUVATE	C00022	88.01605	0.67
QUINATE	C00296	192.06339	4.56
REICHSTEIN'S SUBSTANCE S	C05488	346.21441	0.70
RESORCINOL MONOACETATE	C12064	152.04735	0.75
RIBITOL	C00474	152.06848	0.82
RIBOFLAVIN	C00255	376.13829	0.78

ROSMARINIC ACID	C10489	360.08452	0.66
S-(5'-ADENOSYL)-L-HOMOCYSTEINE	C00021	384.12159	6.35
SALICYLAMIDE	CA1193	137.04768	0.72
SALICYLATE	C00805	138.03170	0.71
SARCOSINE	C00213	89.04768	5.21
S-CARBOXYMETHYL-L-CYSTEINE	C03727	179.02523	4.71
SELENOCYSTAMINE	CA1403	247.93309	7.22
SELENOMETHIONINE	C05335	196.99550	4.66
SEROTONIN	C00780	176.09496	4.56
S-HEXYL-GLUTATHIONE	C02886	391.17771	4.57
SHIKIMATE	C00493	174.05283	0.76
SPERMIDINE	C00315	145.15790	8.73
SPERMINE	C00750	202.21575	11.62
SPHINGANINE	C00836	301.29808	4.27
SUBERIC ACID	C08278	174.08921	0.71
SUCCINATE	C00042	118.02661	0.71
SUCROSE	C00089	342.11622	0.82
TAURINE	C00245	125.01467	3.69
TAUROLITHOCHOLATE	C02592	483.30185	0.70
THEOBROMINE	C07480	180.06473	1.04
THEOPHYLLINE	C07130	180.06473	0.77
THIAMINE	C00378	265.11231	7.61
THIAMINE MONOPHOSPHATE	C01081	344.07081	8.66
THIAMINE PYROPHOSPHATE	C00068	265.11176	7.04
THIOPURINE S-METHYLETHER	C03542	166.03132	0.90
THYMIDINE	C00214	242.09027	0.76
THYMIDINE 5'-MONOPHOSPHATE	C00364	322.05661	4.13
THYMIDINE-5'-DIPHOSPHO-ALPHA-D-GLUCOSE	C00842	564.07576	8.05
THYMINE	C00178	126.04293	0.73
THYROTROPIN RELEASING HORMONE	C03958	362.17025	6.58
TRANS-4-HYDROXYPROLINE	C01157	131.05824	5.37
TRANS-ACONITATE	C02341	174.01644	0.68
TRANS-CYCLOHEXANE-1,2-DIOL	C03739	116.08373	0.66
TRIGONELLINE	C01004	137.04768	5.69
TRYPTAMINE	C00398	160.10005	4.48
TYRAMINE	C00483	137.08406	4.56
URACIL	C00106	112.02728	0.75
URATE	C00366	168.02834	0.77
URIDINE	C00299	244.06954	0.74
URIDINE 5'-DIPHOSPHOGALACTOSE	C00052	566.05503	8.31
URIDINE 5'-DIPHOSPHOGLUCOSE	C00029	566.05503	8.29
URIDINE 5'-DIPHOSPHO-N-ACETYLGALACTOSAMINE	C00203	607.08154	8.17
URIDINE 5'-DIPHOSPHO-N-ACETYLGLUCOSAMINE	C00043	607.08158	8.17
URIDINE-5-MONOPHOSPHATE	C00105	324.03587	4.98
UROCANATE	C00785	138.04293	4.42
VITAMIN D2	C05441	396.33922	0.68
XANTHINE	C00385	152.03343	1.08
XANTHOSINE	C01762	284.07569	0.79
XANTHOSINE 5'-MONOPHOSPHATE	C00655	364.04202	5.94
XANTHURENIC ACID	C02470	205.03751	3.78
XYLITOL	C00379	152.06848	0.81