

Supporting Information Table 1. Results of metabolite standards by three CE-MS, Cation, Anion and Nucleotide, methods.

Marked * anions were determined by nucleotide analysis conditions.

Cationic compound	m/z	Cationic compound	m/z	Anionic compound	m/z	Anionic compound	m/z
Urea	61	DL-β-Hydroxyphenethylamine	138	Acrylate	71	Phenaceturate	192
3-Aminopropionitrile	71	Urocanate	139	Glyoxylate	73	D-Glucuronate	193
Methylguanidine	74	6-Hydroxynicotinate	140	Propionate	73	O-Hydroxyhippurate	194
1,3-Diaminopropane	75	Tropine	142	Glycolate	75	Gluconate	195
L-Gly	76	4-Methyl-5-thiazoleethanol	144	Butyrate	87	Erythrose 4-phosphate	199
Isopropanolamine	76	Spermidine	146	Pyruvate	87	Sebacate	201
Thioacetate	77	γ-Guanidinobutyrate	146	Lactate	89	Indole-3-pyruvate	202
Cysteamine	78	Trientine	147	Thioglycolate	91	Xanthurenate	204
Pyridine	80	L-Lys	147	Chloroacetate	93	Ibuprofen	205
Pyrimidine	80	L-Gln	147	Methanesulfonate	95	Etidronate	205
3-Amino-1,2,4-triazole	85	Acetylcholine	147	Tiglate	99	DL-6,8-Thioctate amide	205
Piperidine	86	L-Albizziine	148	Isovalerate	101	DL-6,8-Thioctate ,reduced	205
Piperazine anhydrous	87	Isatin	148	2-Oxobutyrate	101	Benzylsuccinate	207
1,4-Butanediamine	89	L-Glu	148	Pentanoate	101	N-Benzyloxycarbonylglycine	208
L-β-Ala	90	O-Acetyl-L-serine	148	β-Hydroxypropyruvate	103	Mucin	209
L-Ala	90	D-Penicillamine	150	β-Hydroxybutyrate	103	2-Deoxyribose 5-phosphate	213
Sarcosine	90	L-Met	150	α-Hydroxybutyrate	103	4-Nitrophenyl phosphate	218
3-Amino-1,2,-propanediol	92	2,6-Dimethylaniline	150	2-Hydroxyisobutyrate	103	Pantothenate	218
2-Hydroxypyridine	96	3-Methyl adenine	150	Malonate	103	Ribose 5-phosphate	229
Aniline	94	Triethanolamine	151	Glycerate	105	Ribulose 5-phosphate	229
4-Hydroxymethyl imidazole	99	Guanine	152	Propionate	110	Pyridoxal 5-phosphate	246
1-Methyl-2-pyrrolidone	100	1-Adamantanamine	152	Maleamate	114	D-Glucosamine 6-phosphate	258
Succinimide	100	3,4-Dihydroxyphenethylamine	154	Hexanoate	115	Fructose 6-phosphate	259
α-Aminocyclopropane-1-carboxylat	102	L-His	156	Fumarate	115	Glucose 1-phosphate	259
Hexylamine	102	3-Indolyl acetonitrile	157	3-Methyl-2-oxobutanoate	115	Glucose 6-phosphate	259
Cadaverine(1,5-Diaminopentane)	103	Buforamin	158	Guanidoacetate	116	2,3-Diphosphoglycerate	265
α-Aminoisobutyrate	104	Allantoin	159	Methylmalonate	117	Gluconate 6-Phosphate	275
GABA	104	Ibotenate	159	Succinate	117	Argininosuccinate	289
N,N-Dimethylglycine	104	Indole-3-acetaldehyde	160	Benzoate	121	Nopaline	303
N-Methyl-DL-alanine	104	Tolazoline	161	Isonicotinate	122	N-Acetylneuramate	308
DL-2,3-Diaminopropionate	105	L-Carnitine	162	Nicotinate	122	Pyrrroloquinoline guinone	329
L-Ser	106	3-Indole ethanol	162	Diisopropyl phosphite	123	Fructose 1,6-diphosphate	339
Diethanolamine	106	Nicotine	163	L(+)-Tartarate	123	Ribose 1,5-diphosphate	389
Phenyl hydrazine	109	Pterin	164	2-Aminoethylphosphonate	124	7,8-Dihydrofolate	443
Hypotaurine	110	Phe	166	(S)-(+)-1-Aminoethylphosphonate	124	Adenylosuccinate	462
4-Aminophenol	110	Benzocaine	166	Citraconate	129	cTMP*	303
Cytosine	112	Phenylephrine	168	Itaconate	129	cCMP*	304
Uracil	113	Pyridoxal	168	Mesaconate	129	dCMP*	306
Creatinine	114	Mecamylamine	168	4-Methyl-2-oxovalerate	129	dUMP*	307
Dihydrouracil	115	Pyridoxine	170	Glutarate	131	TMP*	321
1-Methylhydantoin	115	1-Methyl-4-phenyl-1,2,3,6-tetrahydropyrid	174	3-Ureido propionate	131	CMP*	322
L-Pro	116	L-Arg	175	Malate	133	UMP*	323
L-Val	118	N-Ethyl-L-Glutamine	175	p-Toluate	135	cAMP*	328
L-Norvaline	118	N-Acetyl-L-ornithine	175	m-Toluate	135	dAMP*	330
Guanidinoacetate	118	Gramine	175	p-Hydroxybenzoate	137	dIMP*	331
Benzimidazole	119	L-Citrulline	176	m-Hydroxybenzoate	137	cGMP*	344
L-Homoserine	120	Fusarate	180	Salicylate	137	AMP*	346
L-Thr	120	o-Phenanthroline	181	Acetyl phosphate	139	dGMP*	346
α-Methyl-DL-serine	120	L-Tyr	182	Ethanolamine phosphate	140	IMP*	347
Benzamide	121	Carbachol	183	Valproate	143	GMP*	362
Purine	121	Quisqualate	190	Caprylate	143	Xanthosine 5-monophosphate*	363
L-Cys	122	Castanospermine	190	Valproate	143	dCDP*	386
N,N-Dimethylaniline	122	2,6-Diaminoheptanedioate	191	2-Oxoglutarate	145	TDP*	401
Benzamide	122	Caffeine	195	threo-b-Methyl-aspartate	146	CDP*	402
β-Phenylethylamine	122	L-β-(3,4-dihydroxyphenyl)alanine(DOPA)	198	trans-Cinnamate	147	UDP*	403
Taurine	126	Thiabenbazole	202	2-Carboxybenzaldehyde	149	dADP*	410
1-Methylhistamine	126	Spermine	203	p-Hydroxyphenylacetate	151	ADP*	426
5-Methyl cytosine	126	L-Trp	205	L-Cysteine sulfinate	152	Adenosine 3',5'-diphosphate*	426
Imidazole-4-acetate	127	Minoxidil	210	2,5-Dihydroxybenzoate	153	dGDP*	426
Isoguvacine(RBI)	128	Zakcutabine	212	Protocatechuate	153	Adenosine-5'-phosphatesulfate*	426
Octylamine	130	Pherazopyridine	214	Dihydroorotate	157	IDP*	427
Oxoproline	130	Baclofen	214	Acetylcysteine	162	GDP*	442
Cyanurate	130	Harmaline	215	p-Coumarate	163	Flavin mononucleotide*	455
1-Amino-1-cyclopentane-carboxyla	130	N-Acetyl-D(+)-glucosamine	222	o-Coumarate	163	dCTP*	466
1,1-Dimethyl biguanide	130	Cystathionine	223	β-Phenylpyruvate	163	dUTP*	467
N-Acetylputrescine	131	Carnosine	227	3,4-Dihydroxyphenylacetate	167	TTP*	481
Creatine	132	Porphobilinogen	227	Phosphoenol pyruvate	167	CTP*	482
L-Ile	132	2'-Deoxyuridine	229	L-Cysteate	168	UTP*	483
L-Leu	132	L-Homocarnosine	241	Glyphosate	168	dATP*	490
L-Hydroxyproline	132	Thymidine	243	Dihydroxyacetone phosphate	169	dITP*	491
δ-Aminolevulinat	132	Cytidine	244	Glycerol 3-phosphate	171	ATP	506
ε-Amino-n-caproate	132	Uridine	245	2-Quinolincarboxylate	172	dGTP*	506
L-Norleucine	132	Octopine	247	cis-Aconitate	173	ITP*	507
β-Guanidinopropionate	132	Adenosine	268	Phenyl phosphate	173	GTP*	522
L-Ornithine	133	Inosine	269	(-)-Shikimate	173	UDP-glucose*	565
L-Asn	133	Eserine	276	Ascorbate	175	UDP-glucuronate*	579
D-Omithine	133	Guanosine	284	Carbamoylaspartate	175	GDP-mannose*	604
4-Aminoindole	133	Nopaline	305	S-Carboxymethyl-L-cysteine	178	UDP-N-acetylglucosamine*	606
5-Aminoindole	133	Glutathione	308	Glucose	179	CMP-N-acetylneuramate*	614
Gly-Gly	133	Neamine	323	p-hydroxyphenylpyruvate	179	NAD*	662
L-Asp	134	S-Adenosyl-L-homocystein	385	Dihydrocafeate	181	NADH*	664
Adenine	136	Leu-Leu-Tyr	408	O-Phospho-L-serine	184	NADP*	742
2-Aminoimidazole	134	Leupeptin	427	3-Phosphoglycerate	185	NADPH*	744
DL-Homocysteine	136	Piperacillin	518	2-Phosphoglycerate	185	CoA*	766
Hypoxanthine	137			Azelaate	187	FAD*	784
Pralidoxime	137			N-Acetyl-L-glutamate	188	Acetyl CoA*	808
Tyramine	138			N-Acetyl-L-methionine	190	n-Proryl CoA*	822
Anthranilate	138			Citrate	191	Malonyl CoA*	852
p-Aminobenzoate	138			iso-Citrate	191	Succinyl CoA*	866