Supporting Information

NMR/MS Translator for the Enhanced Simultaneous Analysis of Metabolomics Mixtures by NMR Spectroscopy and Mass Spectrometry: Application to Human Urine

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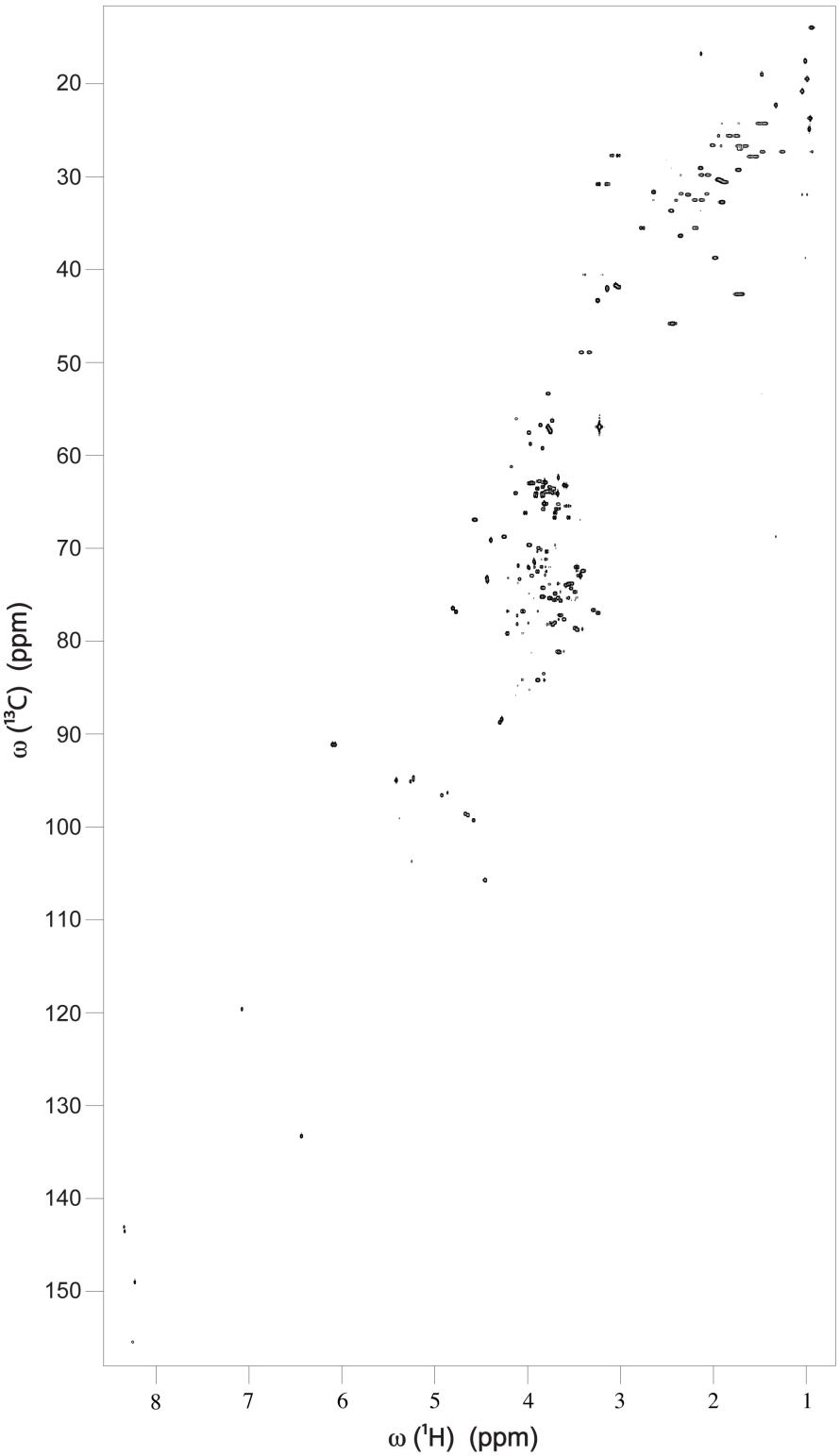

Figure S1. 2D ^{13}C-^{1}H HSQC spectrum of 26-compound model mixture. The spectrum was acquired at 600 MHz proton frequency at 298 K with 800 and 512 complex data points along the direct and indirect dimensions, respectively.

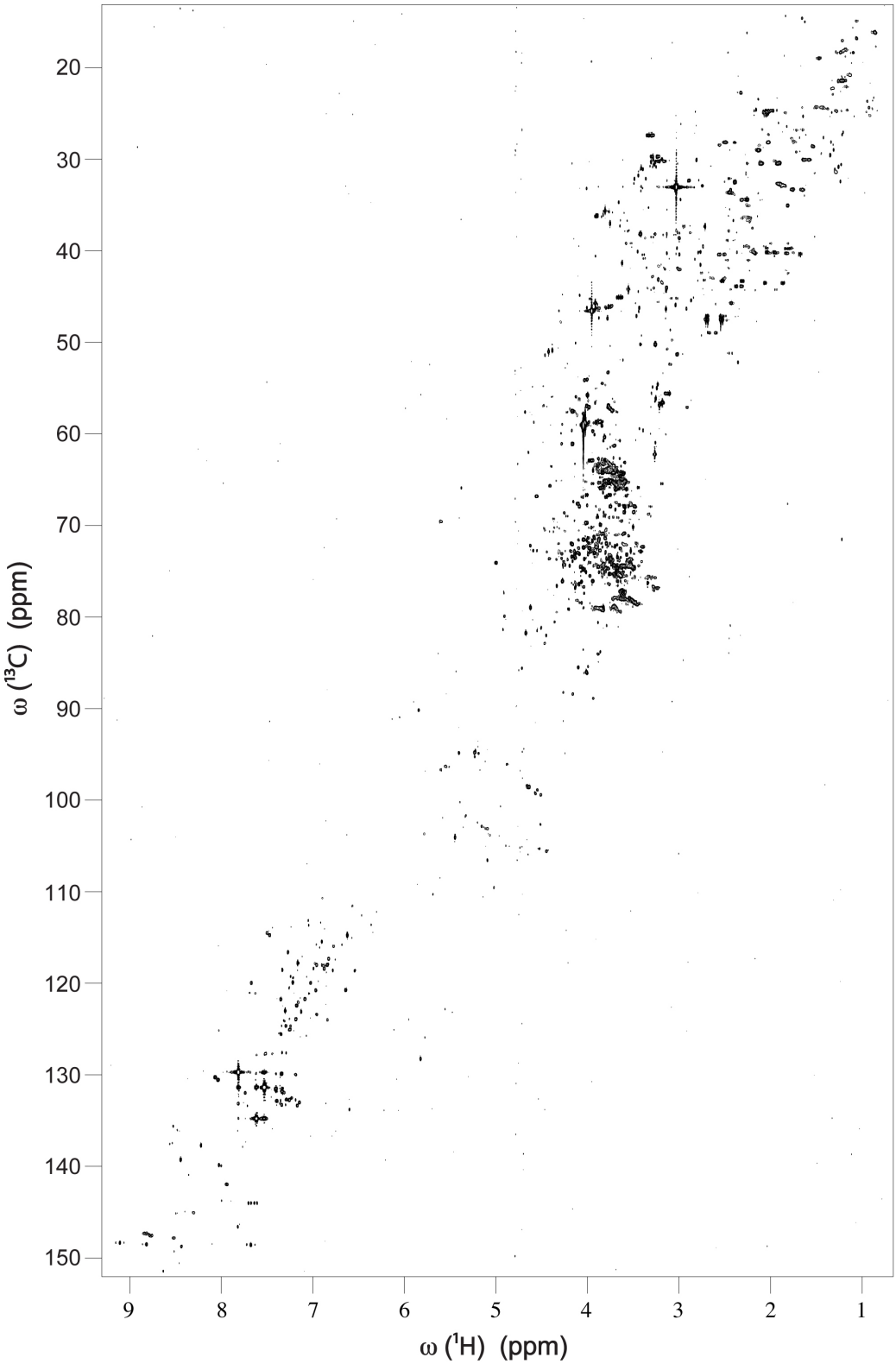

Figure S2. 2D ^{13}C-^{1}H HSQC spectrum of human urine collected from a pool of healthy individuals. The spectrum was acquired at 800 MHz proton frequency at 298 K with 1024 and 512 complex data points along the indirect and direct dimensions, respectively.

Table S1. List of identified metabolites in the model mixture by the NMR/MS Translator and their *m/z* ratios in the MS^1 spectra (positive and negative mode). The list is used to reconstruct the MS^1 spectrum from the 2D ^{13}C-^1H HSQC spectrum in Figure 2. ACN and FA stand for acetonitrile and formic acid, respectively.

Metabolite	Feature	*m/z*[a]	ppm[b]	Metabolite	Feature	*m/z*[a]	ppm[b]
Lysine	$[M+H]^+$	147.1126	-4.78	Alanine	$[M+H]^+$	90.0548	-8.19
Isoleucine/ Leucine	$[M+H]^+$	132.1019	-4.06	Ribose	$[M+H]^+$	151.0626	12.63
Isoleucine/ Leucine	$[M+Na]^+$	154.0837	-4.47	Ribose	$[M+Na]^+$	173.0417	-5.18
Histidine	$[M+H]^+$	156.0765	-4.83	Ribose	$[M+FA-H]^-$	195.0511	3.18
Histidine	$[M+ACN+H]^+$	197.1008	-15.3	Lactose/Sucrose	$[M+H]^+$	343.1230	-3.17
Glutamine	$[M+H]^+$	147.0763	-4.84	Lactose/Sucrose	$[M+Na]^+$	365.1049	-2.91
Glutamine	$[M+Na]^+$	169.0578	-6.72	Lactose/Sucrose	$[M+H-H_2O]^+$	325.1127	-2.49
Glutamine	$[M-H]^-$	145.0617	2.67	Lactose/Sucrose	$[M-H]^-$	341.1090	1.88
Ornithine	$[M+H]^+$	133.0989	8.72	Lactose/Sucrose	$[M+Cl]^-$	377.0856	1.29
Ornithine	$[M+Na]^+$	155.0791	-3.50	Lactose/Sucrose	$[M+FA-H]^-$	387.1145	1.56
Ornithine	$[M+H-H_2O]^+$	115.0866	-4.69	Fructose/Glucose/Galactose	$[M+Na]^+$	203.0524	-3.78
Ornithine	$[M-H]^-$	131.0828	5.82	Fructose/Glucose/Galactose	$[M+H-2H_2O]^+$	145.0492	-5.88
Carnitine	$[M+H]^+$	162.1125	-3.33	Fructose/Glucose/Galactose	$[M+H-H_2O]^+$	163.0599	-4.64
Carnitine	$[M+Na]^+$	184.0942	-4.39	Fructose/Glucose/Galactose	$[M-H]^-$	179.0561	3.09
Shikimate	$[M+H-2H_2O]^+$	139.0389	-4.53	Fructose/Glucose/Galactose	$[M+Cl]^-$	215.0328	2.58
Shikimate	$[M-H]^-$	173.0454	2.58	Threonine	$[M+H]^+$	120.0654	-5.46
Arginine	$[M+H]^+$	175.1189	-3.32	Threonine	$[M+H-H_2O]^+$	102.0547	-7.42
Arginine	$[M+Na]^+$	197.1008	-3.10	Threonine	$[M-H]^-$	118.0512	7.01
Arginine	$[M+2H]^{2+}$	88.0632	-5.63	Proline	$[M+H]^+$	116.0705	-5.66
Arginine	$[M-H]^-$	173.1043	2.70	Proline	$[M+NH_4]^+$	133.0989	8.72
Glutamate	$[M+H]^+$	148.0602	-5.11	Proline	$[M+Na]^+$	138.0510	-15.46
Glutamate	$[M+H-H_2O]^+$	130.0497	-5.89	Methionine	$[M+H]^+$	150.0582	-4.20
Glutamate	$[M-H]^-$	146.0459	3.56	Methionine	$[M-H]^-$	148.0437	3.41
Glutamate	$[M-H_2O-H]^-$	128.0353	3.89	Serine	$[M+H]^+$	106.0497	-7.19
Inosine	$[M+H]^+$	269.0895	3.46	Serine	$[M+ACN+H]^+$	147.0763	-4.84
Inosine	$[M+Na]^+$	291.0696	-3.40	Serine	$[M+ACN+Na]^+$	169.0578	-6.72
Inosine	$[M-H]^-$	267.0736	2.60	Citrulline	$[M+H]^+$	176.1028	-3.99
Adenosine	$[M+H]^+$	268.1040	-2.23	Citrulline	$[M+Na]^+$	198.0849	-2.87
Adenosine	$[M+Cl]^-$	302.0665	2.83	Citrulline	$[M-H]^-$	174.0883	2.21
Adenosine	$[M+FA-H]^-$	312.0954	3.26	Valine	$[M+H]^+$	118.0861	-5.79
Cysteine	$[M+H]^+$	122.0268	-6.12				

[a] Experimentally detected *m/z* ratio of an ion.

[b] *m/z* ratio difference (in units of ppm) between experimentally detected *m/z* ratio and theoretical *m/z* ratio of a given ion.

Table S2. List of all identified metabolites in human urine by 2D ^{13}C-^{1}H HSQC. The letter "M" behind several metabolite names (in parentheses) are used to denote that these metabolites were identified manually, whereas the rest of the metabolites were identified automatically by querying the COLMAR ^{13}C-^{1}H HSQC database.

Acetic acid	1,2-Propanediol
Acetylcarnitine	Quinolinic acid
Alanine	Quinic acid
1,6-Anhydro beta glucose	Saccharate
Arabitol	Serine
N-acetylneuraminic acid	Suberic acid
Allantoin	Sorbitol
Alpha-ketoglutaric acid	Succinic acid
3-Aminoisobutyric acid	Threitol
Ascorbate	Trigonelline
4-Acetamidobutyric acid	Trimethylamine-N-oxide
Allose	Tyrosine
2-Aminoadipic acid	Tartaric acid
Arabinose	Taurine
Arginine	Threonine
Asparagine	Uracil
Betaine	Valine
Carnitine	Xylitol
Creatinine	Xylose
Choline	Caffeine
Cystine	Sucrose
Citraconic acid	Lactose
N,N-Dimethylglycine	Ribose
Meso-erythritol	Galactitol
Ethanolamine	N-acetylputrescine
Fucose	3-Hydroxyisobutyric acid
Fructose	Dimethylamine
Glucuronate	Indoxyl sulfate
Glutamine	Alpha hydroxyisobutyric acid
Guanidineacetic acid	3-Hydroxyisovaleric acid
Glycerol	Methylguanidine
Glycine	1,3-Dimethyluric acid
Galactose	Dimethylsulfone
Gluconic acid	Indole-3-acetic acid
Glucose	Leucine
Homocitrulline	N-acetylaspartic acid
Hippuric acid	Adenosine
4-Hydroxy-3-methoxymandelic acid	Inosine
3-Hydroxy-3-methylglutaric acid	1-Methylhistidine (M)
4-Hydroxyphenylacetic acid	Glycolate (M)
Homovanillic acid	Citrate (M)
3-Hydroxyphenylacetic acid	Creatine (M)
Scyllo-inositol	Histidine (M)
Isethionic acid	Pantothenate (M)
Myo-inositol	Trans-aconitic acid (M)
Lactic acid	Threo-isocitric acid (M)
Lysine	Cis-aconitic acid (M)
Mannitol	Phenol (M)
Pimelic acid	Adipic acid (M)

Table S3. List of metabolites in human urine that have at least one consistent *m/z* ratio in the experimental urine MS^1 spectra (positive and negative ion mode) determined by the NMR/MS Translator. The list is used to reconstruct the MS^1 spectrum from the 2D ^{13}C-^1H HSQC in Figure 3. ACN and FA stand for acetonitrile and formic acid, respectively.

Metabolite	**Feature**	***m/z***[a]	**ppm**[b]
Acetic acid	$[M+CH_3COO]^-$	119.0354	8.27
Acetylcarnitine	$[M+H]^+$	204.1230	-2.84
Acetylcarnitine	$[M+2Na-H]^+$	248.0933	23.58
Acetylcarnitine	$[M-H_2O-H]^-$	184.0979	2.80
Alanine	$[M+ACN+Na]^+$	153.0657	11.15
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M+Na]^+$	185.0398	-15.05
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M+H-H_2O]^+$	145.0467	-23.62
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M+K]^+$	201.0162	-1.58
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M-H]^-$	161.0463	8.27
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M-H_2O-H]^-$	143.0360	11.26
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M+Cl]^-$	197.0232	7.49
1,6-Anydro_beta_glucose/ 3_Hydroxy_3_methylglutaric_acid	$[M+CH_3COO]^-$	221.0659	-0.99
Arabitol/Xylitol	$[M-H]^-$	151.0615	5.55
Arabitol/Xylitol	$[M-H_2O-H]^-$	133.0509	6.50
Arabitol/Xylitol	$[M+Cl]^-$	187.0360	-6.86
Arabitol/Xylitol	$[M+FA-H]^-$	197.0686	12.48
Arabitol/Xylitol	$[M+F]^-$	171.0675	3.64
N-Acetylneuraminic acid	$[M-H]^-$	308.0988	1.92
Allantoin	$[M+F]^-$	177.0413	-6.09
Alpha-ketoglutaric acid	$[M-H]^-$	145.0142	3.77
Alpha-ketoglutaric acid	$[M+FA-H]^-$	191.0201	4.71
Alpha-ketoglutaric acid	$[M+CH_3COO]^-$	205.0356	3.67
Ascorbate	$[M+H-H_2O]^+$	159.0269	-15.40
Ascorbate	$[M-H]^-$	175.0250	4.20
4-Acetamidobutyric-acid	$[M+H]^+$	146.0813	-3.02
4-Acetamidobutyric-acid	$[M+Na]^+$	168.0632	-2.91
4-Acetamidobutyric-acid	$[M+H-2H_2O]^+$	110.0600	-5.45
4-Acetamidobutyric-acid	$[M+K]^+$	184.0368	-4.14
4-Acetamidobutyric-acid	$[M+2Na-H]^+$	190.0485	15.46
4-Acetamidobutyric-acid	$[M-H]^-$	144.0645	-11.15
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+H]^+$	181.0703	-5.01
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+Na]^+$	203.0510	-10.51
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+H-2H_2O]^+$	145.0467	-23.62
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+K]^+$	219.0258	-5.89
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+2Na-H]^+$	225.0333	-7.92
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M-H]^-$	179.0553	-1.50
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M-H_2O-H]^-$	161.0463	8.27
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+Cl]^-$	215.0333	4.85

Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+FA-H]^-$	225.0626	6.87
Allose/Fructose/Galactose/Glucose/scyllo-inositol/myo-inositol	$[M+F]^-$	199.0654	18.34
2-Aminoadipic_acid	$[M+Na-2H]^-$	182.0465	19.83
Arabinose/Xylose/Ribose	$[M+Na]^+$	173.0415	-6.44
Arabinose/Xylose/Ribose	$[M-H]^-$	149.0460	6.61
Arabinose/Xylose/Ribose	$[M-H_2O-H]^-$	131.0366	16.66
Arabinose/Xylose/Ribose	$[M+Cl]^-$	185.0221	2.49
Arabinose/Xylose/Ribose	$[M+FA-H]^-$	195.0519	7.46
Arabinose/Xylose/Ribose	$[M+CH_3COO]^-$	209.0634	-13.25
Arabinose/Xylose/Ribose	$[M+F]^-$	169.0516	2.28
Arginine	$[M+H]^+$	175.1196	0.82
Arginine	$[M+K-2H]^-$	211.0636	18.37
Asparagine	$[M+ACN+H]^+$	174.0904	14.74
Asparagine	$[M+Cl]^-$	167.0214	-5.46
Betaine/Valine	$[M+H]^+$	118.0855	-10.96
Betaine/Valine	$[M+Cl]^-$	152.0467	-7.67
Carnitine	$[M+H]^+$	162.1123	-4.40
Carnitine	$[M+H-H_2O]^+$	144.1013	-8.23
Creatinine	$[M+H]^+$	114.0661	-5.62
Creatinine	$[M+Na]^+$	136.0481	-4.63
Creatinine	$[M+K]^+$	152.0218	-5.18
Creatinine	$[M+2Na-H]^+$	158.0263	-27.15
Creatinine	$[M+Na-2H]^-$	134.0364	25.04
Creatinine	$[M+F]^-$	132.0572	-1.13
Cystine	$[M+F]^-$	259.0258	13.81
Citraconic_acid	$[M-H]^-$	129.0194	4.73
Citraconic_acid	$[M-H_2O-H]^-$	111.0089	5.92
Citraconic_acid	$[M+FA-H]^-$	175.0250	4.20
Citraconic_acid	$[M+CH_3COO]^-$	189.0401	0.89
meso_Erythritol/ Threitol	$[M+Na]^+$	145.0467	-7.04
meso_Erythritol/ Threitol	$[M+K]^+$	161.0214	-1.53
meso_Erythritol/ Threitol	$[M-H]^-$	121.0523	18.20
meso_Erythritol/ Threitol	$[M+Na-2H]^-$	143.0360	28.08
Fucose	$[M+Na]^+$	187.0571	-6.07
Fucose	$[M+K]^+$	203.0311	-5.10
Fucose	$[M-H]^-$	163.0622	9.21
Fucose	$[M-H_2O-H]^-$	145.0533	22.19
Fucose	$[M+Cl]^-$	199.0379	2.91
Fucose	$[M+K-2H]^-$	201.0210	22.07
Fucose	$[M+FA-H]^-$	209.0634	-13.25
Glucuronate	$[M+H-2H_2O]^+$	159.0269	-15.40
Glucuronate	$[M-H]^-$	193.0341	-3.76
Glucuronate	$[M-H_2O-H]^-$	175.0250	4.20
Glucuronate	$[M+K-2H]^-$	230.9974	28.87
Glutamine	$[M+Na]^+$	169.0600	6.43
Glutamine	$[M+H-H_2O]^+$	129.0653	-8.50
Glutamine	$[M+ACN+H]^+$	188.1037	1.07
Glutamine	$[M+Cl]^-$	181.0378	-0.98
Guanidineacetic_acid	$[M+H]^+$	118.0609	-6.57
Guanidineacetic_acid	$[M+ACN+Na]^+$	181.0703	0.90
Guanidineacetic_acid	$[M+F]^-$	136.0522	-0.54
Glycerol	$[M+CH_3COO]^-$	151.0615	5.55
Gluconic_acid	$[M-H]^-$	195.0519	7.46
Gluconic_acid	$[M-H_2O-H]^-$	177.0413	7.91
Gluconic_acid	$[M+Na-2H]^-$	217.0270	-24.79
Gluconic_acid	$[M+Cl]^-$	231.0287	6.49
Gluconic_acid	$[M+K-2H]^-$	233.0119	23.61

Homocitrulline	$[M+Na]^+$	212.1015	1.88
Hippuric_acid	$[M+H]^+$	180.0653	-4.17
Hippuric_acid	$[M+Na]^+$	202.0473	-3.74
Hippuric_acid	$[M+K]^+$	218.0206	-6.07
Hippuric_acid	$[M+2Na-H]^+$	224.0292	-3.60
Hippuric_acid	$[M-H]^-$	178.0515	6.17
Hippuric_acid	$[M+Cl]^-$	214.0280	4.11
Hippuric_acid	$[M+FA-H]^-$	224.0596	16.31
Hippuric_acid	$[M+CH_3COO]^-$	238.0771	23.43
4_Hydroxy_3_methoxymandelic_acid	$[M+Na]^+$	221.0407	-8.47
4_Hydroxy_3_methoxymandelic_acid	$[M+ACN+Na]^+$	262.0681	-3.85
4_Hydroxy_3_methoxymandelic_acid	$[M+Li]^+$	205.0671	-8.53
4_Hydroxy_3_methoxymandelic_acid	$[M+F]^-$	217.0480	-14.99
4_Hydroxyphenylacetic_acid/ 3_Hydroxyphenylacetic_acid	$[M-H]^-$	151.0402	4.62
4_Hydroxyphenylacetic_acid/ 3_Hydroxyphenylacetic_acid	$[M+CH_3COO]^-$	211.0636	14.03
4_Hydroxyphenylacetic_acid/ 3_Hydroxyphenylacetic_acid	$[M+F]^-$	171.0406	-29.88
Homovanillic_acid	$[M+Na]^+$	205.0487	5.04
Homovanillic_acid	$[M+Cl]^-$	217.0270	1.30
Isethionic_acid	$[M-H]^-$	124.9914	4.43
Lactic_acid	$[M+Na-2H]^-$	111.0089	27.59
Lactic_acid	$[M+FA-H]^-$	135.0303	7.34
Lactic_acid	$[M+CH_3COO]^-$	149.0460	6.61
Lysine	$[M+K-2H]^-$	183.0507	-15.52
Pimelic_acid	$[M+2Na-H]^+$	205.0487	16.77
Pimelic_acid	$[M-H]^-$	159.0676	11.50
Pimelic_acid	$[M+K-2H]^-$	197.0232	7.79
Pimelic_acid	$[M+FA-H]^-$	205.0724	5.95
1,2_Propanediol	$[M+ACN+H]^+$	118.0855	-10.96
1,2_Propanediol	$[M+FA-H]^-$	121.0523	18.20
1,2_Propanediol	$[M+CH_3COO]^-$	135.0649	-6.53
Quinolinic_acid	$[M-H]^-$	166.0156	9.58
Quinic_acid	$[M-H]^-$	191.0566	5.51
Quinic_acid	$[M-H_2O-H]^-$	173.0492	24.30
Quinic_acid	$[M+Cl]^-$	227.0340	7.64
Quinic_acid	$[M+F]^-$	211.0636	8.62
Saccharate	$[M-H_2O-H]^-$	191.0201	4.71
Saccharate	$[M+Cl]^-$	245.0126	25.26
Saccharate	$[M+K-2H]^-$	246.9927	28.73
Serine	$[M+ACN+Na]^+$	169.0600	6.43
Suberic_acid	$[M-H]^-$	173.0823	5.26
Suberic_acid	$[M+Cl]^-$	209.0634	25.34
Succinic_acid	$[M+CH_3COO]^-$	177.0413	7.91
Trigonelline	$[M+H]^+$	138.0546	-6.56
Trigonelline	$[M+Na]^+$	160.0364	-6.65
Trigonelline	$[M+K]^+$	176.0110	-1.96
Trigonelline	$[M+FA-H]^-$	182.0465	6.62
Trigonelline	$[M+CH_3COO]^-$	196.0599	-5.63
Tyrosine	$[M+H]^+$	182.0800	-9.66
Tartaric_acid	$[M-H]^-$	149.0097	7.25
Taurine	$[M+NH_4]^+$	143.0531	28.26
Taurine	$[M-H]^-$	124.0079	8.84
Threonine	$[M+K]^+$	158.0263	27.74
Uracil	$[M+CH_3COO]^-$	171.0406	0.32
Caffeine	$[M-H_2O-H]^-$	175.0621	0.87
Caffeine	$[M+K-2H]^-$	231.0287	0.97
Caffeine	$[M+F]^-$	213.0785	-1.08

Sucrose/Lactose	$[M+Na]^+$	365.1044	-4.47
Sucrose/Lactose	$[M+K]^+$	381.0792	-1.99
Sucrose/Lactose	$[M+Na-2H]^-$	363.0805	-27.09
Sucrose/Lactose	$[M+Cl]^-$	377.0852	0.38
Sucrose/Lactose	$[M-2H]^{2-}$	170.0480	-13.16
Galactitol/ Mannitol/Sorbitol	$[M+Na]^+$	205.0671	-8.43
Galactitol/ Mannitol/Sorbitol	$[M+K]^+$	221.0407	-9.16
Galactitol/ Mannitol/Sorbitol	$[M-H_2O-H]^-$	163.0622	9.21
Galactitol/ Mannitol/Sorbitol	$[M+Cl]^-$	217.0480	0.37
Galactitol/ Mannitol/Sorbitol	$[M+F]^-$	201.0763	-5.79
3_Hydroxyisobutyric_acid/ Alpha_hydroxyisobutyric_acid	$[M+ACN+H]^+$	146.0813	-3.02
3_Hydroxyisobutyric_acid/ Alpha_hydroxyisobutyric_acid	$[M+ACN+Na]^+$	168.0632	-2.91
3_Hydroxyisobutyric_acid/ Alpha_hydroxyisobutyric_acid	$[M+FA-H]^-$	149.0460	6.61
3_Hydroxyisobutyric_acid Alpha_hydroxyisobutyric_acid	$[M+CH_3COO]^-$	163.0622	9.21
Indoxyl_Sulfate	$[M-H]^-$	212.0027	4.60
3_Hydroxyisovaleric_acid	$[M+ACN+Na]^+$	182.0800	3.55
3_Hydroxyisovaleric_acid	$[M+FA-H]^-$	163.0622	9.21
3_Hydroxyisovaleric_acid	$[M+CH_3COO]^-$	177.0793	16.81
1,3_Dimethyluric_acid	$[M-H]^-$	195.0519	0.61
1,3_Dimethyluric_acid	$[M-H_2O-H]^-$	177.0413	0.37
1,3_Dimethyluric_acid	$[M+Cl]^-$	231.0287	0.71
1,3_Dimethyluric_acid	$[M+K-2H]^-$	233.0119	17.87
Dimethyl_sulfone	$[M+ACN+Na]^+$	158.0263	7.37
Dimethyl_sulfone	$[M+CH_3COO]^-$	153.0214	-5.01
Indole_3_acetic_acid	$[M+H]^+$	176.0684	-15.81
Indole_3_acetic_acid	$[M+Li]^+$	182.0800	3.44
Leucine	$[M+2Na-H]^+$	176.0684	11.51
N_acetyl_L_aspartic_acid	$[M+K]^+$	214.0092	-11.87
N_acetyl_L_aspartic_acid	$[M-H]^-$	174.0422	11.17
N_acetyl_L_aspartic_acid	$[M+F]^-$	194.0454	-5.32
Adenosine	$[M+ACN+H]^+$	309.1226	-27.54
Inosine	$[M+K-2H]^-$	305.0348	19.49
1_Methyl_L_Histidine	$[M+H]^+$	170.0922	-4.51
1_Methyl_L_Histidine	$[M+Na]^+$	192.0730	-9.95
1_Methyl_L_Histidine	$[M+K]^+$	208.0479	-4.26
1_Methyl_L_Histidine	$[M+Li]^+$	176.1035	13.34
1_Methyl_L_Histidine	$[M+CH_3OH+H]^+$	202.1180	-5.96
Glycolate	$[M+CH_3COO]^-$	135.0303	7.34
Citrate/ Threo_isocitric_acid	$[M+Na]^+$	215.0156	-5.43
Citrate/ Threo_isocitric_acid	$[M+2Na-H]^+$	236.9980	-2.96
Citrate/ Threo_isocitric_acid	$[M-H]^-$	191.0201	4.71
Citrate/ Threo_isocitric_acid	$[M-H_2O-H]^-$	173.0094	4.28
Citrate/ Threo_isocitric_acid	$[M+Na-2H]^-$	213.0057	21.41
Citrate/ Threo_isocitric_acid	$[M+Cl]^-$	226.9963	1.88
Creatine	$[M+H]^+$	132.0758	-11.36
Creatine	$[M+H-H_2O]^+$	114.0661	-5.62
Creatine	$[M+Na-2H]^-$	152.0467	20.18
Histidine	$[M+H]^+$	156.0768	-3.37
Histidine	$[M+Na]^+$	178.0575	-9.65
Histidine	$[M+K]^+$	194.0325	-3.40
Histidine	$[M+CH_3OH+H]^+$	188.1037	1.07
Histidine	$[M-H]^-$	154.0627	6.53
Histidine	$[M-H_2O-H]^-$	136.0522	7.86
Histidine	$[M+Na-2H]^-$	176.0471	19.67
Histidine	$[M+Cl]^-$	190.0385	0.79
Pantothenate	$[M-H]^-$	218.1037	4.02

Pantothenate	$[M+K-2H]^-$	256.0593	2.34
Pantothenate	$[M+FA-H]^-$	264.1076	-2.70
Trans-/Cis-aconitic_acid	$[M+K]^+$	212.9783	-8.47
Trans-/Cis-aconitic_acid	$[M-H]^-$	173.0094	4.28
Adipic acid	$[M+2Na-H]^+$	191.0263	-17.28
Adipic acid	$[M-H]^-$	145.0533	22.19
Adipic acid	$[M+FA-H]^-$	191.0566	5.51
Adipic acid	$[M+CH_3COO]^-$	205.0724	5.95

[a] Experimentally detected *m/z* ratio of an ion.

[b] *m/z* ratio difference (in units of ppm) between experimentally detected *m/z* ratio and theoretical *m/z* ratio of a given ion.