

Abbreviations and Adducts Table

| Figure.Row.Column | Abbreviated/Displayed Name | Longform, Other, or Isomer Name(s) | Adduct |
|-------------------|---|--|------------|
| 2.1.1.1 | α -Ketoisocaproate ^a | - | M-H |
| 2.1.1.2 | N-Acetyl-glucosamine | - | M-H+HCOONa |
| 2.1.1.3 | 1-O-16:0-LysoPC | 1-O-Hexadecyl-lyso-sn-glycero-3-phosphocholine | M+FA-H |
| 2.1.1.4 | 4-Phosphoerythronate | - | M-H |
| 2.1.2.1 | Piperidine | - | M+H |
| 2.1.2.2 | β -Methylphenylpyruvate | (3S)-2-Oxo-3-phenylbutanoate | M-H+HCOONa |
| 2.1.2.3 | 5-MeO-6-Me-BI | 5-Methoxy-6-methylbenzimidazole | M+H |
| 2.1.2.4 | 5-HTP | 5-Hydroxy-L-tryptophan | M-H |
| 2.1.3.1 | Glutamyl 5-phosphate | - | M-H |
| 2.1.3.2 | Deglymidodrine | - | M+H |
| 2.1.3.3 | N-Acetyl-L-leucine ^c | - | M+H |
| 2.1.3.4 | 2-Aminobutanoate | - | M+H-NH3 |
| 2.1.4.1 | α -Ketoarginine | 5-Guanidino-2-oxopentanoate | M-H |
| 2.1.4.2 | Mytatrienediol | - | M+H |
| 2.1.4.3 | Homocysteine | - | M+2Na-H |
| 2.1.4.4 | Ribose | - | M+H-2H2O |
| 2.1.5.1 | Biliverdin ^l | - | M-H |
| 2.1.5.2 | 5-Methoxytryptamine | - | M+H |
| 2.1.5.3 | Formate ^c | - | M-H+HCOONa |
| 2.1.5.4 | Histidinal | - | M+H |
| 2.2.1.1 | Levulinic acid ^c | - | M-H |
| 2.2.1.2 | 2-Oxo-6-acetamidocaproate | 6-Acetamido-2-oxohexanoate | M+H |
| 2.2.1.3 | N-Acetyl-L-alanine ^c | - | M+H-H2O |
| 2.2.1.4 | 2-OH-C24:0 | 2-Hydroxytetracosanoic acid | M+Cl |
| 2.2.2.1 | Lovastatin acid | - | M+Hac-H |
| 2.2.2.2 | 10,16-DHPA | 10,16-Dihydroxyhexadecanoic acid | M+H |
| 2.2.2.3 | α -Ketoisocaproate ^c | - | M-H+HCOONa |
| 2.2.2.4 | Pregnenolone sulfate | 3 β -Hydroxypregn-5-en-20-one sulfate | M-H |
| 2.2.3.1 | 3-(Aminomethyl)indole | - | M+H-NH3 |
| 2.2.3.2 | L- α -Glycerophosphate | sn-Glycerol 1-phosphate | M+H |
| 2.2.3.3 | 3 β ,7 α -DiOH-5-cholestenoate | 3 β ,7 α -Dihydroxy-5-cholestenoate | M-H |
| 2.2.3.4 | Inosine-5'-carboxylate | - | M+H-H2O |
| 2.2.4.1 | α -Keto-MTOB | 4-Methylthio-2-oxobutanoic acid | M+Cl |
| 2.2.4.2 | dTMP ^d | Thymidine 5'-monophosphate | M+FA-H |
| 2.2.4.3 | Taurine | - | M+H |
| 2.2.4.4 | Dexamethasone acetate | Dexamethasone acetate anhydrous | M-H |
| 2.2.5.1 | 5-HmdCDP | 2'-Deoxy-5-hydroxymethylcytidine-5'-diphosphate | M-H+HCOONa |
| 2.2.5.2 | 2-Hydroxyphenylacetate | - | M+H |
| 2.2.5.3 | Acetyllysine ^l | - | M-H |
| 2.2.5.4 | α -Ketoisovalerate | - | M+2Na-H |
| 2.3.1.1 | GSSG | Glutathione disulfide | M+FA-H |
| 2.3.1.2 | Proline | - | M+H |
| 2.3.1.3 | 2-Hydroxyphytanate | - | M-H |
| 2.3.1.4 | 9,10-DHOME | - | M+Hac-H |
| 2.3.2.1 | CHP-ThPP | 3-Carboxy-1-hydroxypropylthiamine diphosphate | M+Cl |
| 2.3.2.2 | Propionylcarnitine ^d | - | M+H+NH4 |
| 2.3.2.3 | Arachidonate | - | M-H |
| 2.3.2.4 | 15,16-Dihydrobiliverdin | - | M+H |
| 2.3.3.1 | HMOA | 4-Hydroxy-4-methyl-2-oxoadipate | M+Cl |
| 2.3.3.2 | Histamine ^c | - | M+H |
| 2.3.3.3 | 5-Nitrosalicylate | - | M-H |
| 2.3.3.4 | Uridine ^c | - | M-H+HCOONa |
| 2.3.4.1 | Formaldehyde | - | M+Hac-H |
| 2.3.4.2 | Acetoacetate | - | M-H |
| 2.3.4.3 | D-(+)-Glucosamine ^d | - | M+H |
| 2.3.4.4 | Arachidonoylcarnitine ^c | - | M+H |
| 2.3.5.1 | Acetyl-serine | - | M-H |
| 2.3.5.2 | 4-Guanidinobutanal | - | M+H |
| 2.3.5.3 | Valine | - | M-H+HCOONa |
| 2.3.5.4 | Salicylamide ^c | - | M-H2O-H |
| 2.4.1.1 | Trimethylsulfonium | - | M+Hac-H |
| 2.4.1.2 | γ -Linolenic acid | (6Z,9Z,12Z)-Octadecatrienoic acid | M-H |
| 2.4.1.3 | 6-Hydroxyhexanoic acid | - | M-H |
| 2.4.1.4 | DHAP | Glycerone phosphate | M+H |
| 2.4.2.1 | Isoleucine | - | M-H+HCOONa |
| 2.4.2.2 | Perindopril | - | M-H |
| 2.4.2.3 | Normetanephine ^d | - | M+H-H2O |
| 2.4.2.4 | Glutamate | - | M-H |
| 2.4.3.1 | 17 α -Estradiol ^c | - | 2M-3H |
| 2.4.3.2 | Nicotinate ^c | - | M+H |
| 2.4.3.3 | Allantoin ^c | - | M+2Na-H |
| 2.4.3.4 | Lauroylcarnitine ^c | - | M+H |
| 2.4.4.1 | Pyridoxamine | - | M+Hac-H |
| 2.4.4.2 | Indolymethyl-cysteine | S-(Indolymethylthiohydroximoyl)-L-cysteine | M+H |
| 2.4.4.3 | HMP | 4-Amino-5-hydroxymethyl-2-methylpyrimidine | M+H |

Footnote Table

| Figure.Row.Column | Abbreviated/Displayed Name | Footnote |
|-------------------|---------------------------------|---|
| 2.1.5.1 | Biliverdin ^l | ^l Annotated isomers = Biliverdin-IX-5 and Biliverdin-IX- β (M-H adducts) |
| 2.2.4.2 | dTMP ^d | ^d Standard library isomers = 2'-Deoxyuridine 5'-monophosphate (M+Hac-H adduct) |
| 2.2.5.3 | Acetyllysine ^l | ^l Annotated isomer = 6-Acetamido-3-aminohexanoate (M-H adduct) |
| 2.3.2.2 | Propionylcarnitine ^d | ^d Standard library isomers = 5-Aminopentanoic acid (M+H adduct) |
| 2.3.4.3 | D-(+)-Glucosamine ^d | ^d Standard library isomers = D-Mannosamine (M+H adduct) |
| 2.4.2.3 | Normetanephine ^d | ^d Standard library isomers = 1,3-Dihydro-(2H)-indol-2-one ^c (M+CH4O+H adduct) |

* M-H adduct presented but also identified with authentic standard as M-H+HCOONa adduct; see Figure.Row.Column 2.2.2.3.

^c Identity confirmed with authentic chemical standard.

^l Isomer annotated or isomer present in library of authentic chemical standards. See Footnote Table for details.