

Abbreviations and Adducts Table

Figure.Row.Column	Abbreviated/Displayed Name	Longform, Other, or Isomer Name(s)	Adduct
S2.1.1.1	α -Ketoisocaproate [*]	-	M-H
S2.1.1.2	N-Acetyl-glucosamine	-	M-H+HCOONa
S2.1.1.3	1-O-16:0-LysoPC	1-O-Hexadecyl-lyso-sn-glycero-3-phosphocholine	M+FA-H
S2.1.1.4	4-Phosphoerythronate	-	M-H
S2.1.2.1	Piperidine	-	M+H
S2.1.2.2	β -Methylphenylpyruvate	(3S)-2-Oxo-3-phenylbutanoate	M-H+HCOONa
S2.1.2.3	5-MeO-6-Me-BI	5-Methoxy-6-methylbenzimidazole	M+H
S2.1.2.4	5-HTP	5-Hydroxy-L-tryptophan	M-H
S2.1.3.1	Glutamyl 5-phosphate	-	M-H
S2.1.3.2	Deglymidodrine	-	M+H
S2.1.3.3	N-Acetyl-L-leucine ^c	-	M+H
S2.1.3.4	2-Aminobutanoate	-	M+H-NH3
S2.1.4.1	α -Ketoarginine	5-Guanidino-2-oxopentanoate	M-H
S2.1.4.2	Mytatrienediol	-	M+H
S2.1.4.3	Homocysteine	-	M+2Na-H
S2.1.4.4	Ribose	-	M+H-2H2O
S2.1.5.1	Biliverdin ^l	-	M-H
S2.1.5.2	5-Methoxytryptamine	-	M+H
S2.1.5.3	Formate ^c	-	M-H+HCOONa
S2.1.5.4	Histidinal	-	M+H
S2.2.1.1	Levulinic acid ^c	-	M-H
S2.2.1.2	2-Oxo-6-acetamidocaproate	6-Acetamido-2-oxohexanoate	M+H
S2.2.1.3	N-Acetyl-L-alanine ^c	-	M+H-H2O
S2.2.1.4	2-OH-C24:0	2-Hydroxytetracosanoic acid	M+Cl
S2.2.2.1	Lovastatin acid	-	M+Hac-H
S2.2.2.2	10,16-DHPA	10,16-Dihydroxyhexadecanoic acid	M+H
S2.2.2.3	α -Ketoisocaproate ^c	-	M-H+HCOONa
S2.2.2.4	Pregnenolone sulfate	3 β -Hydroxypregn-5-en-20-one sulfate	M-H
S2.2.3.1	3-(Aminomethyl)indole	-	M+H-NH3
S2.2.3.2	L- α -Glycerophosphate	sn-Glycerol 1-phosphate	M+H
S2.2.3.3	3 β ,7 α -DiOH-5-cholestenolate	3 β ,7 α -Dihydroxy-5-cholestenolate	M-H
S2.2.3.4	Inosine-5'-carboxylate	-	M+H-H2O
S2.2.4.1	α -Keto-MTOB	4-Methylthio-2-oxobutanoic acid	M+Cl
S2.2.4.2	dTMP ^d	Thymidine 5'-monophosphate	M+FA-H
S2.2.4.3	Taurine	-	M+H
S2.2.4.4	Dexamethasone acetate	Dexamethasone acetate anhydrous	M-H
S2.2.5.1	5-HmdCDP	2'-Deoxy-5-hydroxymethylcytidine-5'-diphosphate	M-H+HCOONa
S2.2.5.2	2-Hydroxyphenylacetate	-	M+H
S2.2.5.3	Acetyllysine ^l	-	M-H
S2.2.5.4	α -Ketoisovalerate	-	M+2Na-H
S2.3.1.1	GSSG	Glutathione disulfide	M+FA-H
S2.3.1.2	Proline	-	M+H
S2.3.1.3	2-Hydroxyphytanate	-	M-H
S2.3.1.4	9,10-DHOME	-	M+Hac-H
S2.3.2.1	CHP-ThPP	3-Carboxy-1-hydroxypropylthiamine diphosphate	M+Cl
S2.3.2.2	Propionylcarnitine ^d	-	M+H+NH4
S2.3.2.3	Arachidonate	-	M-H
S2.3.2.4	15,16-Dihydrobiliverdin	-	M+H
S2.3.3.1	HMOA	4-Hydroxy-4-methyl-2-oxoadipate	M+Cl
S2.3.3.2	Histamine ^c	-	M+H
S2.3.3.3	5-Nitrosalicylate	-	M-H
S2.3.3.4	Uridine ^c	-	M-H+HCOONa
S2.3.4.1	Formaldehyde	-	M+Hac-H
S2.3.4.2	Acetoacetate	-	M-H
S2.3.4.3	D-(+)-Glucosamine ^d	-	M+H
S2.3.4.4	Arachidonoylcarnitine ^c	-	M+H
S2.3.5.1	Acetyl-serine	-	M-H
S2.3.5.2	4-Guanidinobutanal	-	M+H
S2.3.5.3	Valine	-	M-H+HCOONa
S2.3.5.4	Salicylamide ^c	-	M-H2O-H
S2.4.1.1	Trimethylsulfonium	-	M+Hac-H
S2.4.1.2	γ -Linolenic acid	(6Z,9Z,12Z)-Octadecatrienoic acid	M-H
S2.4.1.3	6-Hydroxyhexanoic acid	-	M-H
S2.4.1.4	DHAP	Glycerone phosphate	M+H
S2.4.2.1	Isoleucine	-	M-H+HCOONa
S2.4.2.2	Perindopril	-	M-H
S2.4.2.3	Normetanephine ^d	-	M+H-H2O
S2.4.2.4	Glutamate	-	M-H
S2.4.3.1	17 α -Estradiol ^c	-	2M-3H
S2.4.3.2	Nicotinate ^c	-	M+H
S2.4.3.3	Allantoin ^c	-	M+2Na-H
S2.4.3.4	Lauroylcarnitine ^c	-	M+H
S2.4.4.1	Pyridoxamine	-	M+Hac-H
S2.4.4.2	Indolylmethyl-cysteine	S-(Indolylmethylthiohydroxymoyl)-L-cysteine	M+H
S2.4.4.3	HMP	4-Amino-5-hydroxymethyl-2-methylpyrimidine	M+H

Footnote Table

Figure.Row.Column	Abbreviated/Displayed Name	Footnote
S2.1.5.1	Biliverdin ^l	^l Annotated isomers = Biliverdin-IX-5 and Biliverdin-IX- β (M-H adducts)
S2.2.4.2	dTMP ^d	^d Standard library isomers = 2'-Deoxyuridine 5'-monophosphate (M+Hac-H adduct)
S2.2.5.3	Acetyllysine ^l	^l Annotated isomer = 6-Acetamido-3-aminohexanoate (M-H adduct)
S2.3.2.2	Propionylcarnitine ^d	^d Standard library isomers = 5-Aminopentanoic acid (M+H adduct)
S2.3.4.3	D-(+)-Glucosamine ^d	^d Standard library isomers = D-Mannosamine (M+H adduct)
S2.4.2.3	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 S2.2.2.3.

^c Identity confirmed with authentic chemical standard.

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