

Table 7: *H. sapiens* Recon 1 metabolites. Alphabetized list of compartment-specific metabolites. Metabolite formula and charge were determined based on ionization state at pH 7.2 (see text for details).

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
10thf	10-Formyltetrahydrofolate	10-Formyl-THF	C20H21N7O7	-2	Cytosol
10thf	10-Formyltetrahydrofolate	10-Formyl-THF	C20H21N7O7	-2	Extracellular
10thf	10-Formyltetrahydrofolate	10-Formyl-THF	C20H21N7O7	-2	Lysosome
10thf	10-Formyltetrahydrofolate	10-Formyl-THF	C20H21N7O7	-2	Mitochondria
10thf5glu	10-formyltetrahydrofolate-[Glu](5)		C40H45N11O19	-6	Cytosol
10thf5glu	10-formyltetrahydrofolate-[Glu](5)		C40H45N11O19	-6	Extracellular
10thf5glu	10-formyltetrahydrofolate-[Glu](5)		C40H45N11O19	-6	Lysosome
10thf5glu	10-formyltetrahydrofolate-[Glu](5)		C40H45N11O19	-6	Mitochondria
10thf6glu	10-formyltetrahydrofolate-[Glu](6)		C45H51N12O22	-7	Cytosol
10thf6glu	10-formyltetrahydrofolate-[Glu](6)		C45H51N12O22	-7	Extracellular
10thf6glu	10-formyltetrahydrofolate-[Glu](6)		C45H51N12O22	-7	Lysosome
10thf6glu	10-formyltetrahydrofolate-[Glu](6)		C45H51N12O22	-7	Mitochondria
10thf7glu	10-formyltetrahydrofolate-[Glu](7)		C50H57N13O25	-8	Cytosol
10thf7glu	10-formyltetrahydrofolate-[Glu](7)		C50H57N13O25	-8	Extracellular
10thf7glu	10-formyltetrahydrofolate-[Glu](7)		C50H57N13O25	-8	Lysosome
10thf7glu	10-formyltetrahydrofolate-[Glu](7)		C50H57N13O25	-8	Mitochondria
11-cis-retfa	fatty acid 11-cis-retinol		C20H29OFULLR2CO	0	Cytosol
11-cis-retfa	fatty acid 11-cis-retinol		C20H29OFULLR2CO	0	Extracellular
11docrsl	11-Deoxycortisol	11-Deoxycortisol	C21H30O4	0	Cytosol
11docrsl	11-Deoxycortisol	11-Deoxycortisol	C21H30O4	0	Mitochondria
11docrsl	11-Deoxycortisol	11-Deoxycortisol	C21H30O4	0	Endoplasmic Reticulum
11docrstrn	11-Deoxycorticosterone	11-Deoxycorticosterone, 21-Hydroxy-4-pregnene-3,20-dione, Cortexone, DOC, Deoxycorticosterone	C21H30O3	0	Cytosol
11docrstrn	11-Deoxycorticosterone	11-Deoxycorticosterone, 21-Hydroxy-4-pregnene-3,20-dione, Cortexone, DOC, Deoxycorticosterone	C21H30O3	0	Mitochondria
11docrstrn	11-Deoxycorticosterone	11-Deoxycorticosterone, 21-Hydroxy-4-pregnene-3,20-dione, Cortexone, DOC, Deoxycorticosterone	C21H30O3	0	Endoplasmic Reticulum
12harachd	12 hydroxy arachidonic acid		C20H31O3	-1	Endoplasmic Reticulum
12HPET	12-Hydroperoxyeicosa-5,8,10,14-tetraenoate	(5Z,8Z,10E,14Z)-(12S)-12-Hydroperoxyeicosa-5,8,10,14-tetraenoic acid, 12-HPETE, 12-Hydroperoxyeicosatetraenoate, 12-Hydroperoxyeicosatetraenoic acid, 12-Hydroperoxyeicosatetraenoate, 12-Hydroperoxyeicosatetraenoic acid	C20H31O4	-1	Cytosol
12ppd-R	(R)-Propane-1,2-diol	(R)-1,2-Propanediol, (R)-Propylene glycol, D-1,2-propanediol	C3H8O2	0	Cytosol
12ppd-S	(S)-Propane-1,2-diol	(S)-1,2-Propanediol, (S)-Propylene glycol, L-1,2-propanediol	C3H8O2	0	Cytosol
12RHPET	12R-Hydroperoxyeicosatetraenoate	(5Z,8Z,10E,14Z)-(12R)-12-Hydroperoxyeicosa-5,8,10,14-tetraenoic acid, 12-HPETE, 12-Hydroperoxyeicosatetraenoic acid, 12-Hydroperoxyeicosatetraenoate, 12-Hydroperoxyeicosatetraenoic acid	C20H31O4	-1	Cytosol
13-cis-oretn	13-cis-oxo-retinoic acid		C20H27O3	-1	Cytosol
13-cis-oretn	13-cis-oxo-retinoic acid		C20H27O3	-1	Nucleus
13-cis-retn	13-cis-retinoate		C20H27O2	-1	Cytosol
13-cis-retn	13-cis-retinoate		C20H27O2	-1	Nucleus
13-cis-retn	13-cis-retinoate		C20H27O2	-1	Endoplasmic Reticulum
13-cis-retnglc	13-cis-retinoyl glucuronide		C26H35O8	-1	Cytosol
13-cis-retnglc	13-cis-retinoyl glucuronide		C26H35O8	-1	Extracellular
13-cis-retnglc	13-cis-retinoyl glucuronide		C26H35O8	-1	Endoplasmic Reticulum
13dampp	1,3-Diaminopropane	1,3-Propanediamine, Propane-1,3-diamine, Trimethylenediamine	C3H12N2	2	Cytosol
13dpg	3-Phospho-D-glyceroyl phosphate	(R)-2-Hydroxy-3-(phosphonoxy)-1-monoanhydride with phosphoric propanoic acid, 1,3-bis-phosphoglycerate, 3-Phospho-D-glyceroyl phosphate	C3H4O10P2	-4	Cytosol
15HPET	15-Hydroperoxyeicosatetraenoic acid	(5Z,8Z,11Z,13E)-(15S)-15-Hydroperoxyeicosa-5,8,11,13-tetraenoate, 15-HPETE, 15-Hydroperoxyeicosatetraenoate, 15-Hydroperoxyeicosatetraenoic acid, 15-Hydroperoxyeicosatetraenoate, 15-Hydroperoxyeicosatetraenoic acid	C20H31O4	-1	Cytosol
17ahprgnlone	17alpha-Hydroxypregnenolone	17alpha-Hydroxypregnenolone	C21H32O3	0	Cytosol
17ahprgnlone	17alpha-Hydroxypregnenolone	17alpha-Hydroxypregnenolone	C21H32O3	0	Endoplasmic Reticulum
17ahprgstrn	17alpha-Hydroxyprogesterone	17alpha-Hydroxy-4-pregnene-3,20-dione, 17alpha-Hydroxy-progesterone, 17alpha-Hydroxyprogesterone, Pregn-4-ene-3,20-dione-17-ol	C21H30O3	0	Cytosol
17ahprgstrn	17alpha-Hydroxyprogesterone	17alpha-Hydroxy-4-pregnene-3,20-dione, 17alpha-Hydroxy-progesterone, 17alpha-Hydroxyprogesterone, Pregn-4-ene-3,20-dione-17-ol	C21H30O3	0	Endoplasmic Reticulum
18harachd	18 hydroxy arachidonic acid		C20H31O3	-1	Endoplasmic Reticulum
1a2425thvid2	1-alpha,24R,25-Trihydroxyvitamin D2		C28H44O4	0	Mitochondria
1a2425thvid3	1-alpha,24R,25-Trihydroxyvitamin D3		C27H44O4	0	Mitochondria
1a25dhvid2	1-alpha,25-Dihydroxyvitamin D2		C28H44O3	0	Mitochondria
1a25dhvid3	1-alpha,25-Dihydroxyvitamin D3	Calcitriol, Rocaltrol (TN)	C27H44O3	0	Mitochondria
1glyc_hs	1 acyl phosphoglycerol	glycerol phosphate, glycerolipid, phoso glycerol, phosphate glycerol	C6H13O7PFULLRCO2	-1	Extracellular
1mncam	1-Methylnicotinamide		C7H9N2O	1	Cytosol
1mncam	1-Methylnicotinamide		C7H9N2O	1	Extracellular
1mpyr	1-Methylpyrrolinium	1-Methylpyrrolinium	C5H10N	1	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
1p2cbl	1-Pyrroline-2-carboxylate	1-Pyrroline-2-carboxylic acid	C5H6NO2	-1	Peroxisome
1p3h5c	L-1-Pyrroline-3-hydroxy-5-carboxylate	3-Hydroxy-L-1-pyrroline-5-carboxylate	C5H6NO3	-1	Mitochondria
1pipdn2c	delta1-Piperidine-2-carboxylate		C6H9NO2	0	Peroxisome
1pyr5c	1-Pyrroline-5-carboxylate	(S)-1-Pyrroline-5-carboxylate, 1-Pyrroline-5-carboxylic acid, L-1-Pyrroline-5-carboxylate	C5H6NO2	-1	Cytosol
1pyr5c	1-Pyrroline-5-carboxylate	(S)-1-Pyrroline-5-carboxylate, 1-Pyrroline-5-carboxylic acid, L-1-Pyrroline-5-carboxylate	C5H6NO2	-1	Mitochondria
20ahcsterol	20alpha-hydroxy cholesterol		C27H46O2	0	Mitochondria
23doguln	2,3-Dioxo-L-gulonate	2,3-diketo-gulonic acid, 2,3-diketogulonate, DKG, diketogulonate	C6H7O7	-1	Cytosol
23dpg	2,3-Diphospho-D-glycerate	2,3-Bisphospho-D-glycerate, 3-Phospho-D-glycerate, D-Greenwald ester, DPG	C3H3O10P2	-5	Cytosol
2425dhvitd2	24R,25-Dihydroxyvitamin D2		C28H44O3	0	Cytosol
2425dhvitd2	24R,25-Dihydroxyvitamin D2		C28H44O3	0	Extracellular
2425dhvitd2	24R,25-Dihydroxyvitamin D2		C28H44O3	0	Mitochondria
2425dhvitd3	24R,25-Dihydroxyvitamin D3		C27H44O3	0	Cytosol
2425dhvitd3	24R,25-Dihydroxyvitamin D3		C27H44O3	0	Extracellular
2425dhvitd3	24R,25-Dihydroxyvitamin D3		C27H44O3	0	Mitochondria
24nph	2,4 dihydroxy nitrophenol	2 hydroxy 4 nitrophenol, 2 hydroxy, 4 hydroxy nitrobenzene	C6H5NO4	0	Cytosol
24nph	2,4 dihydroxy nitrophenol	2 hydroxy 4 nitrophenol, 2 hydroxy, 4 hydroxy nitrobenzene	C6H5NO4	0	Extracellular
25aics	(S)-2-[5-Amino-1-(5-phospho-D-ribose)imidazole-4-carboxamido]succinate	1-(5'-Phosphoribosyl)-4-(N-succinocarboxamide)-5-aminimidazole, 1-(5'-Phosphoribosyl)-5-amino-4-(N-succinocarboxamide)-imidazole, 5'-Phosphoribosyl-4-(N-succinocarboxamide)-5-aminimidazole	C13H15N4O12P	-4	Cytosol
25hvitd2	25-Hydroxyvitamin D2		C28H44O2	0	Cytosol
25hvitd2	25-Hydroxyvitamin D2		C28H44O2	0	Extracellular
25hvitd2	25-Hydroxyvitamin D2		C28H44O2	0	Mitochondria
25hvitd3	25-Hydroxyvitamin D3	Calcidiol, Calcifediol anhydrous, Calcifediol, Calderol (TN)	C27H44O2	0	Cytosol
25hvitd3	25-Hydroxyvitamin D3	Calcidiol, Calcifediol anhydrous, Calcifediol, Calderol (TN)	C27H44O2	0	Extracellular
25hvitd3	25-Hydroxyvitamin D3	Calcidiol, Calcifediol anhydrous, Calcifediol, Calderol (TN)	C27H44O2	0	Mitochondria
2amac	2-Aminoacrylate	Dehydroalanine	C3H5NO2	0	Cytosol
2ameph	(2-Aminoethyl)phosphonate	2-Aminoethylphosphonate, Clatinate	C2H7NO3P	-1	Cytosol
2aobut	L-2-Amino-3-oxobutanoate	L-2-Amino-acetoacetate	C4H7NO3	0	Mitochondria
2c23dh56dhoxin	2-Carboxy-2,3-dihydro-5,6-dihydroxyindole	2-Carboxy-2,3-dihydro-5,6-dihydroxyindole, Leucodopachrome	C9H8NO4	-1	Cytosol
2coum	cis-2-Hydroxy cinnamate	2-Coumarinate	C9H7O3	-1	Cytosol
2dp6mep	2-Decaprenyl-6-methoxyphenol		C57H88O2	0	Mitochondria
2dp6mobq	2-Decaprenyl-6-methoxy-1,4-benzoquinone		C57H86O3	0	Mitochondria
2dp6mobq_me	2-Decaprenyl-3-methyl-6-methoxy-1,4-benzoquinone		C58H88O3	0	Mitochondria
2dpmbobq	2-Decaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone		C58H88O4	0	Mitochondria
2dr1p	2-Deoxy-D-ribose 1-phosphate	Deoxy-ribose 1-phosphate	C5H9O7P	-2	Cytosol
2dr5p	2-Deoxy-D-ribose 5-phosphate		C5H9O7P	-2	Cytosol
2hb	2-Hydroxybutyrate	2-Hydroxybutyric acid	C4H7O3	-1	Cytosol
2hb	2-Hydroxybutyrate	2-Hydroxybutyric acid	C4H7O3	-1	Extracellular
2hyoxplac	2-Hydroxyphenylacetate	2-Hydroxyphenylacetate	C8H7O3	-1	Cytosol
2kmb	2-keto-4-methylthiobutyrate	2-oxo-4-(methylthio)butyrate, 4-methylthio-2-oxobutanoate	C5H7O3S	-1	Cytosol
2maacoa	2-Methyl-3-acetoacetyl-CoA	2-Methylacetoacetyl-CoA	C26H38N7O18P3S	-4	Mitochondria
2mb2coa	trans-2-Methylbut-2-enoyl-CoA	(E)-2-Methylcrotonoyl-CoA, 2-Methylbut-2-enoyl-CoA, Tiglyl-CoA, methylcrotonoyl-CoA, methylcrotonyl-CoA, tigloyl-CoA	C26H38N7O17P3S	-4	Mitochondria
2mbcoa	2-Methylbutanoyl-CoA	2-Methylbutyryl-CoA	C26H40N7O17P3S	-4	Mitochondria
2mcaen	cis-2-Methylaconitate	(Z)-But-2-ene-1,2,3-tricarboxylate, cis-2-Methylaconitate	C7H5O6	-3	Cytosol
2mciit	2-Methylcitrate		C7H7O7	-3	Cytosol
2mciit	2-Methylcitrate		C7H7O7	-3	Extracellular
2mop	2-Methyl-3-oxopropanoate	(S)-methylmalonate semialdehyde, 3-Oxo-2-methylpropanoate, Methylmalonate semialdehyde	C4H5O3	-1	Mitochondria
2mp2coa	2-Methylprop-2-enoyl-CoA	Methacrylyl-CoA, Methylacrylyl-CoA	C25H36N7O17P3S	-4	Mitochondria
2obut	2-Oxobutanoate	2-Ketobutyric acid, 2-Oxobutanoic acid, 2-Oxobutyrate, 2-Oxobutyric acid, alpha-Ketobutyrate	C4H5O3	-1	Cytosol
2oxoadp	2-Oxoadipate	2-Oxoadipic acid	C6H6O5	-2	Cytosol
2oxoadp	2-Oxoadipate	2-Oxoadipic acid	C6H6O5	-2	Mitochondria
2pg	D-Glycerate 2-phosphate	2-Phospho-D-glycerate, 2-phosphoglyceric acid	C3H4O7P	-3	Cytosol
2pglyc	2-Phosphoglycolate	2-phosphoglycolic acid, Phosphoglycolic acid	C2H2O6P	-3	Cytosol
34dhcimm	3,4-Dihydroxy-trans-cinnamate	trans-Caffeate	C9H7O4	-1	Cytosol
34dhmald	3,4-Dihydroxymandelaldehyde		C8H8O4	0	Cytosol
34dhoxmand	3,4-Dihydroxymandelate		C8H7O5	-1	Cytosol
34dhoxpeg	3,4-Dihydroxyphenylethyleneglycol	3,4-Dihydroxyphenylethyleneglycol	C8H10O4	0	Cytosol
34dhoxpeg	3,4-Dihydroxyphenylethyleneglycol	3,4-Dihydroxyphenylethyleneglycol	C8H10O4	0	Extracellular
34dhpac	3,4-Dihydroxyphenylacetaldehyde	3,4-Dihydroxyphenylacetaldehyde, Protocatechuatealdehyde	C8H8O3	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
34dhpa	3,4-Dihydroxyphenylacetate	3,4-Dihydroxyphenyl acetate, 3,4-Dihydroxyphenyl acetic acid, 3,4-Dihydroxyphenylacetic acid, Homoprotocatechuate	C8H7O4	-1	Cytosol
34dhphe	3,4-Dihydroxy-L-phenylalanine	3-Hydroxy-L-tyrosine, Dihydroxy-L-phenylalanine, Hydroxy-L-tyrosine, L-Dopa, L-beta-(3,4-Dihydroxyphenyl)alanine, Levodopa	C9H11NO4	0	Cytosol
34dhphe	3,4-Dihydroxy-L-phenylalanine	3-Hydroxy-L-tyrosine, Dihydroxy-L-phenylalanine, Hydroxy-L-tyrosine, L-Dopa, L-beta-(3,4-Dihydroxyphenyl)alanine, Levodopa	C9H11NO4	0	Extracellular
34hpl	3-(4-Hydroxyphenyl)lactate	4-Hydroxyphenyllactate, p-Hydroxyphenyllactate	C9H9O4	-1	Mitochondria
34hpp	3-(4-Hydroxyphenyl)pyruvate	4-Hydroxyphenylpyruvate, p-Hydroxyphenylpyruvic acid	C9H7O4	-1	Cytosol
34hpp	3-(4-Hydroxyphenyl)pyruvate	4-Hydroxyphenylpyruvate, p-Hydroxyphenylpyruvic acid	C9H7O4	-1	Mitochondria
35cgmpp	3',5'-Cyclic GMP	Cyclic GMP, Guanosine 3',5'-cyclic monophosphate, Guanosine 3',5'-cyclic phosphate	C10H11NSO7P	-1	Cytosol
35cgmpp	3',5'-Cyclic GMP	Cyclic GMP, Guanosine 3',5'-cyclic monophosphate, Guanosine 3',5'-cyclic phosphate	C10H11NSO7P	-1	Extracellular
35cgmpp	3',5'-Cyclic GMP	Cyclic GMP, Guanosine 3',5'-cyclic monophosphate, Guanosine 3',5'-cyclic phosphate	C10H11NSO7P	-1	Golgi Apparatus
35cgmpp	3',5'-Cyclic GMP	Cyclic GMP, Guanosine 3',5'-cyclic monophosphate, Guanosine 3',5'-cyclic phosphate	C10H11NSO7P	-1	Nucleus
35dtyr	3,5-Diiodo-L-tyrosine	3,5-Diiodotyrosine, L-Diiodotyrosine	C9H9I2NO3	0	Cytosol
3aib	L-3-Amino-isobutanoate	(S)-3-Amino-isobutanoate, (S)-3-Amino-isobutyrate, L-3-Amino-isobutyrate, b-Aminoisobutyrate	C4H9NO2	0	Cytosol
3aib	L-3-Amino-isobutanoate	(S)-3-Amino-isobutanoate, (S)-3-Amino-isobutyrate, L-3-Amino-isobutyrate, b-Aminoisobutyrate	C4H9NO2	0	Extracellular
3aib	L-3-Amino-isobutanoate	(S)-3-Amino-isobutanoate, (S)-3-Amino-isobutyrate, L-3-Amino-isobutyrate, b-Aminoisobutyrate	C4H9NO2	0	Mitochondria
3aib-D	D-3-Amino-isobutanoate	D-3-Amino-isobutanoate	C4H9NO2	0	Cytosol
3aib-D	D-3-Amino-isobutanoate	D-3-Amino-isobutanoate	C4H9NO2	0	Extracellular
3aib-D	D-3-Amino-isobutanoate	D-3-Amino-isobutanoate	C4H9NO2	0	Mitochondria
3amp	3'-AMP	3'-Adenosine monophosphate, 3'-Adenylic acid, AMP 3'-phosphate, Adenosine 3'-phosphate, Adenosine-3'-monophosphate	C10H12NSO7P	-2	Lysosome
3dhguln	3-Dehydro-L-gulonate	3-keto-L-gulonate	C6H9O7	-1	Cytosol
3dpthb	3-Decaprenyl-4,5-dihydroxybenzoate		C57H85O4	-1	Mitochondria
3dpthb_me	3-Decaprenyl-4-hydroxy-5-methoxybenzoate		C58H87O4	-1	Mitochondria
3dpthb	3-Decaprenyl-4-hydroxybenzoate		C57H85O3	-1	Mitochondria
3dsphgn	3-Dehydrospinganine	3-Dehydro-D-sphinganine	C18H38NO2	1	Cytosol
3h26dm5coa	3-Hydroxy-2,6-dimethyl-5-methylene-heptanoyl-CoA		C31H48N7O18P3S	-4	Mitochondria
3h26dm5coa	3-Hydroxy-2,6-dimethyl-5-methylene-heptanoyl-CoA		C31H48N7O18P3S	-4	Peroxisome
3hanthr	3-Hydroxyanthranilate	3-Hydroxyanthranilic acid	C7H7NO3	0	Cytosol
3hbcoa	(S)-3-Hydroxybutanoyl-CoA	(S)-3-Hydroxybutyryl-CoA	C25H38N7O18P3S	-4	Mitochondria
3hbcoa	(S)-3-Hydroxybutanoyl-CoA	(S)-3-Hydroxybutyryl-CoA	C25H38N7O18P3S	-4	Peroxisome
3hbcoa-R	(R)-3-Hydroxybutanoyl-CoA	(3R)-3-Hydroxybutanoyl-CoA	C25H38N7O18P3S	-4	Mitochondria
3hibutcoa	(S)-3-Hydroxyisobutyryl-CoA		C25H38N7O18P3S	-4	Mitochondria
3hmbcoa	(S)-3-Hydroxy-2-methylbutyryl-CoA	(2S,3S)-3-Hydroxy-2-methylbutanoyl-CoA	C26H40N7O18P3S	-4	Mitochondria
3hmp	3-Hydroxy-2-methylpropanoate	(S)-3-hydroxyisobutyrate, 3-Hydroxyisobutyrate, 3-Hydroxyisobutyric acid	C4H7O3	-1	Mitochondria
3hpcoa	3-Hydroxypropionyl-CoA	3-Hydroxyisobutyryl coenzyme A, 3-Hydroxyisobutyryl-CoA, 3-Hydroxypropanoyl coenzyme A, 3-Hydroxypropanoyl-CoA, 3-Hydroxypropionyl coenzyme A	C24H36N7O18P3S	-4	Cytosol
3hpcoa	3-Hydroxypropionyl-CoA	3-Hydroxyisobutyryl coenzyme A, 3-Hydroxyisobutyryl-CoA, 3-Hydroxypropanoyl coenzyme A, 3-Hydroxypropanoyl-CoA, 3-Hydroxypropionyl coenzyme A	C24H36N7O18P3S	-4	Mitochondria
3hpcoa	3-Hydroxypropionyl-CoA	3-Hydroxyisobutyryl coenzyme A, 3-Hydroxyisobutyryl-CoA, 3-Hydroxypropanoyl coenzyme A, 3-Hydroxypropanoyl-CoA, 3-Hydroxypropionyl coenzyme A	C24H36N7O18P3S	-4	Peroxisome
3hpp	3-Hydroxypropanoate	3-Hydropropionic acid, 3-Hydroxyisobutyrate, 3-Hydroxyisobutyric acid, 3-Hydroxypropanoic acid, 3-Hydroxypropionate, 3-Hydroxypropionate, 3-Hydroxypropionic acid, Hydracrylic acid	C3H5O3	-1	Cytosol
3hlmelys	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine		C9H20N2O3	0	Cytosol
3hlmelys	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine		C9H20N2O3	0	Mitochondria
3hxyknam	3-Hydroxykynurenamine		C9H13N2O2	1	Cytosol
3ityr-L	3-Iodo-L-tyrosine	3-Iodo-L-tyrosine	C9H10INO3	0	Cytosol
3m4hpga	3-Methoxy-4-hydroxyphenylglycolaldehyde		C9H10O4	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
3mb2coa	3-Methylbut-2-enoyl-CoA	3-Methylcrotonoyl-CoA	C26H38N7O17P3S	-4	Mitochondria
3mgcoa	3-Methylglutaconyl-CoA	trans-3-Methylglutaconyl-CoA	C27H37N7O19P3S	-5	Mitochondria
3mlda	3-Methylimidazoleacetic acid	1-Methyl-4-imidazoleacetic acid, Tele-methylimidazoleacetic acid	C6H7N2O2	-1	Cytosol
3mlda	3-Methylimidazoleacetic acid	1-Methyl-4-imidazoleacetic acid, Tele-methylimidazoleacetic acid	C6H7N2O2	-1	Extracellular
3mldz	3-Methylimidazole acetaldehyde	1-Methylimidazole-4-acetaldehyde, Methylimidazoleacetaldehyde	C6H8N2O	0	Cytosol
3mob	3-Methyl-2-oxobutanoate	2-Keto-3-methylbutyric acid, 2-Ketovaline, 2-Oxo-methylbutanoate, 2-Oxoisopentanoate, 2-Oxoisovalerate, 3-Methyl-2-oxobutyric acid, alpha-Ketovaline	C5H7O3	-1	Cytosol
3mob	3-Methyl-2-oxobutanoate	2-Keto-3-methylbutyric acid, 2-Ketovaline, 2-Oxo-methylbutanoate, 2-Oxoisopentanoate, 2-Oxoisovalerate, 3-Methyl-2-oxobutyric acid, alpha-Ketovaline	C5H7O3	-1	Mitochondria
3mop	(S)-3-Methyl-2-oxopentanoate	(R)-2-oxo-3-methylpentanoate, (S)-2-oxo-3-methylpentanoate, 2-oxo-3-methylpentanoate, alpha-keto-beta-methylvalerate, alpha-oxo-beta-methylvalerate, ketoisoleucine	C6H9O3	-1	Cytosol
3mop	(S)-3-Methyl-2-oxopentanoate	(R)-2-oxo-3-methylpentanoate, (S)-2-oxo-3-methylpentanoate, 2-oxo-3-methylpentanoate, alpha-keto-beta-methylvalerate, alpha-oxo-beta-methylvalerate, ketoisoleucine	C6H9O3	-1	Mitochondria
3mox4hoxm	3-Methoxy-4-hydroxymandelate	Vanillylmandelic acid	C9H9O5	-1	Cytosol
3mox4hpac	3-Methoxy-4-hydroxyphenylacetaldehyde		C9H10O3	0	Cytosol
3moxtyr	3-Methoxytyramine		C9H14NO2	1	Cytosol
3odcoa	3-Oxodecanoyl-CoA		C31H48N7O18P3S	-4	Peroxisome
3oddcoa	3-Oxododecanoyl-CoA		C33H52N7O18P3S	-4	Peroxisome
3ohdcoa	3-Oxohexadecanoyl-CoA		C37H60N7O18P3S	-4	Peroxisome
3ohodcoa	3-Oxooctadecanoyl-CoA		C39H64N7O18P3S	-4	Peroxisome
3ohxcoa	3-Oxohexacosyl-CoA		C47H80N7O18P3S	-4	Peroxisome
3otdcoa	3-Oxotetradecanoyl-CoA		C35H56N7O18P3S	-4	Peroxisome
3padsel	3'-Phosphoadenylylselenate	3'-Phosphoadenosine-5'-phosphoselenate	C10H11N5O13P2Se	-4	Cytosol
3pg	3-Phospho-D-glycerate	3-Phosphoglycerate, 3-phosphoglyceric acid, D-Glycerate 3-phosphate	C3H4O7P	-3	Cytosol
3php	3-Phosphohydroxypyruvate	3-Phosphohydroxypyruvic acid, 3-Phosphonoxyypyruvate, 3-Phosphonoxyypyruvic acid	C3H2O7P	-3	Cytosol
3sala	3-Sulfino-L-alanine	3-Sulfinoalanine, 3-sulphino-L-alanine, L-Cysteine sulfonic acid, L-Cysteinesulfonic acid	C3H5NO4S	-2	Cytosol
3sala	3-Sulfino-L-alanine	3-Sulfinoalanine, 3-sulphino-L-alanine, L-Cysteine sulfonic acid, L-Cysteinesulfonic acid	C3H5NO4S	-2	Mitochondria
3snpyr	3-Sulfinyopyruvate	3-Sulfinyopyruvate, 3-Sulfinylpyruvate	C3H2O5S	-2	Cytosol
3snpyr	3-Sulfinyopyruvate	3-Sulfinyopyruvate, 3-Sulfinylpyruvate	C3H2O5S	-2	Mitochondria
3spxr	3-Sulfoxyruvate		C3H2O6S	-2	Cytosol
3spxr	3-Sulfoxyruvate		C3H2O6S	-2	Mitochondria
3uib	3-Ureidoisobutyrate		C5H9N2O3	-1	Cytosol
42A3HP24DB	4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate		C10H8NO5	-1	Cytosol
44mctr	4,4-dimethylcholesta-8,14,24-trienol	4,4'-dimethyl cholesta-8,14,24-triene-3-beta-ol, delta-8-14-24-dimethylsterol	C29H46O	0	Cytosol
44mctr	4,4-dimethylcholesta-8,14,24-trienol	4,4'-dimethyl cholesta-8,14,24-triene-3-beta-ol, delta-8-14-24-dimethylsterol	C29H46O	0	Endoplasmic Reticulum
44mzym	4,4-dimethylzymosterol	14-Desmethylanosterol, 4,4-dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol	C29H48O	0	Endoplasmic Reticulum
46dhoquin	4,6-Dihydroxyquinoline	Quinoline-4,6-diol	C9H7NO2	0	Cytosol
48dhoquin	4,8-Dihydroxyquinoline	Quinoline-4,8-diol	C9H7NO2	0	Cytosol
4aabtn	4-Acetamidobutanoate		C6H10NO3	-1	Cytosol
4aabtn	4-Acetamidobutanoate		C6H10NO3	-1	Mitochondria
4abut	4-Aminobutanoate	(4-Aminobutyl)guanidine, 4-Aminobutanoic acid, 4-Aminobutylate, 4-Aminobutyric acid, GABA, gamma-Aminobutyric acid	C4H9NO2	0	Cytosol
4abut	4-Aminobutanoate	(4-Aminobutyl)guanidine, 4-Aminobutanoic acid, 4-Aminobutylate, 4-Aminobutyric acid, GABA, gamma-Aminobutyric acid	C4H9NO2	0	Extracellular
4abut	4-Aminobutanoate	(4-Aminobutyl)guanidine, 4-Aminobutanoic acid, 4-Aminobutylate, 4-Aminobutyric acid, GABA, gamma-Aminobutyric acid	C4H9NO2	0	Lysosome
4abut	4-Aminobutanoate	(4-Aminobutyl)guanidine, 4-Aminobutanoic acid, 4-Aminobutylate, 4-Aminobutyric acid, GABA, gamma-Aminobutyric acid	C4H9NO2	0	Mitochondria
4abtn	4-Aminobutanol	4-Aminobutylaldehyde, 4-amino-Butylaldehyde, gamma-aminobutanol	C4H10NO	1	Cytosol
4aphdob	4-(2-Aminophenyl)-2,4-dioxobutanoate		C10H8NO4	-1	Cytosol
4fumacac	4-Fumarylacetoacetate	4-Fumarylacetoacetic acid, Fumarylacetoacetate	C8H6O6	-2	Cytosol
4h2ogl	4-Hydroxy-2-oxoglutarate	4-Hydroxy-2-oxoglutaric acid, D-4-Hydroxy-2-oxoglutarate	C5H4O6	-2	Cytosol
4h2ogl	4-Hydroxy-2-oxoglutarate	4-Hydroxy-2-oxoglutaric acid, D-4-Hydroxy-2-oxoglutarate	C5H4O6	-2	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
4hbz	4-Hydroxybenzoate	4-Hydroxybenzoic acid, Hydroxybenzenecarboxylic acid, Hydroxybenzoic acid	C7H5O3	-1	Mitochondria
4hbzcoa	4-hydroxybenoyl-CoA		C28H36N7O18P3S	-4	Mitochondria
4hdebrisoquine	4 hydroxy debrisoquine		C10H14N3O	1	Cytosol
4hdebrisoquine	4 hydroxy debrisoquine		C10H14N3O	1	Extracellular
4hglsa	L-4-Hydroxyglutamate semialdehyde		C5H9NO4	0	Mitochondria
4hoxpacd	4-Hydroxyphenylacetaldehyde	2-(4-Hydroxyphenyl)acetaldehyde	C8H8O2	0	Cytosol
4hphac	4-Hydroxyphenylacetate	4-Hydroxyphenylacetic acid	C8H7O3	-1	Cytosol
4hphac	4-Hydroxyphenylacetate	4-Hydroxyphenylacetic acid	C8H7O3	-1	Extracellular
4hpro-LT	trans-4-Hydroxy-L-proline		C5H9NO3	0	Mitochondria
4hpro-LT	trans-4-Hydroxy-L-proline		C5H9NO3	0	Endoplasmic Reticulum
4izp	4-Imidazolone-5-propanoate	4,5-Dihydro-4-oxo-5-imidazolepropanoate, 4-Imidazolone-5-propionic acid	C6H7N2O3	-1	Cytosol
4mlacac	4-Maleylacetate		C8H6O6	-2	Cytosol
4mop	4-Methyl-2-oxopentanoate	2-Oxoisocaproate, alpha-ketoisocaproate	C6H9O3	-1	Cytosol
4mop	4-Methyl-2-oxopentanoate	2-Oxoisocaproate, alpha-ketoisocaproate	C6H9O3	-1	Mitochondria
4mptnl	4-Methylpentanal	4-Methylpentanal	C6H12O	0	Mitochondria
4mtolbutamide	4 hydroxy tolbutamide	4 methyl hydroxy tolbutamide	C12H18N2O4S	0	Cytosol
4mtolbutamide	4 hydroxy tolbutamide	4 methyl hydroxy tolbutamide	C12H18N2O4S	0	Extracellular
4mzym_int1	4-Methylzymosterol intermediate 1		C29H46O3	0	Endoplasmic Reticulum
4mzym_int2	4-Methylzymosterol intermediate 2		C28H44O	0	Endoplasmic Reticulum
4nph	4-Nitrophenol	4-Hydroxynitrobenzene, Niphen, PNP, p-Nitrophenol	C6H5NO3	0	Cytosol
4nph	4-Nitrophenol	4-Hydroxynitrobenzene, Niphen, PNP, p-Nitrophenol	C6H5NO3	0	Extracellular
4nphsf	4-Nitrophenyl sulfate	IUPAC Name: 1-nitro-4-sulfooxy-benzene, Sulfuric acid mono(4-nitrophenyl) ester, p-Nitrophenol sulfate, p-Nitrophenyl sulfate	C6H4NO6S	-1	Cytosol
4nphsf	4-Nitrophenyl sulfate	IUPAC Name: 1-nitro-4-sulfooxy-benzene, Sulfuric acid mono(4-nitrophenyl) ester, p-Nitrophenol sulfate, p-Nitrophenyl sulfate	C6H4NO6S	-1	Extracellular
4ppan	D-4'-Phosphopantothenate	(R)-4'-Phosphopantothenate	C9H15NO8P	-3	Cytosol
4ppan	D-4'-Phosphopantothenate	(R)-4'-Phosphopantothenate	C9H15NO8P	-3	Mitochondria
4ppcys	N-((R)-4-Phosphopantothenoyl)-L-cysteine	(R)-4'-Phosphopantothenoyl-L-cysteine	C12H20N2O9PS	-3	Cytosol
4pyrdx	4-Pyridoxate	4-Pyridoxic acid	C8H9NO4	0	Cytosol
4pyrdx	4-Pyridoxate	4-Pyridoxic acid	C8H9NO4	0	Extracellular
4meabut	4-Trimethylammoniumbutanal		C7H16NO	1	Cytosol
4meabut	4-Trimethylammoniumbutanal		C7H16NO	1	Mitochondria
4meabutn	4-Trimethylammoniumbutanoate		C7H15NO2	0	Cytosol
56dhindlcrbxlt	5,6-Dihydroxyindole-2-carboxylate		C9H6NO4	-1	Cytosol
56dthm	5,6-Dihydrothymine	5,6-Dihydro-5-methyluracil, Dihydrothymine	C5H8N2O2	0	Cytosol
56dura	5,6-dihydrouracil	2, 3H)-Pyrimidinedione, 4(1H, 4-dihydroxy)pyrimidine, 5, 6-Dihydro-2, Dihydrouracil, Hydrouracil, dihydro-, dihydrouracil	C4H6N2O2	0	Cytosol
5a2opntn	5-Amino-2-oxopentanoate	2-Oxo-5-amino-pentanoate, 2-Oxo-5-aminopentanoate, alpha-Keto-delta-aminopentanoate	C5H9NO3	0	Peroxisome
5adtststerone	5alpha-Dihydrotestosterone	17beta-Hydroxy-5alpha-androstan-3-one, 17beta-Hydroxyandrost-3-one, 5alpha-Dihydrotestosterone, Androstanolone	C19H30O2	0	Cytosol
5adtststerone	5alpha-Dihydrotestosterone	17beta-Hydroxy-5alpha-androstan-3-one, 17beta-Hydroxyandrost-3-one, 5alpha-Dihydrotestosterone, Androstanolone	C19H30O2	0	Extracellular
5adtststerone	5alpha-Dihydrotestosterone	17beta-Hydroxy-5alpha-androstan-3-one, 17beta-Hydroxyandrost-3-one, 5alpha-Dihydrotestosterone, Androstanolone	C19H30O2	0	Endoplasmic Reticulum
5adtststeroneglc	5alpha-Dihydrotestosterone glucuronide		C25H38O8	0	Cytosol
5adtststeroneglc	5alpha-Dihydrotestosterone glucuronide		C25H38O8	0	Extracellular
5adtststeroneglc	5alpha-Dihydrotestosterone glucuronide		C25H38O8	0	Endoplasmic Reticulum
5adtststerones	5alpha-Dihydrotestosterone sulfate		C19H29O5S	-1	Cytosol
5adtststerones	5alpha-Dihydrotestosterone sulfate		C19H29O5S	-1	Extracellular
5aizc	5-amino-1-(5-phospho-D-ribose)imidazole-4-carboxylate	1-(5'-Phosphoribosyl)-4-carboxy-5-aminoimidazole, 1-(5'-Phosphoribosyl)-5-amino-4-carboxyimidazole, 1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxylate, 1-(5-Phospho-D-ribose)-5-amino-4-imidazolecarboxylate, 5'-Phosphoribosyl-carboxy-5-aminoimidazole, 5'-Phosphoribosyl-5-amino-4-imidazolecarboxylate	C9H11N3O9P	-3	Cytosol
5aop	5-Amino-4-oxopentanoate	5-Amino-4-oxovaleric acid, 5-Aminolevulinat	C5H9NO3	0	Cytosol
5aop	5-Amino-4-oxopentanoate	5-Amino-4-oxovaleric acid, 5-Aminolevulinat	C5H9NO3	0	Mitochondria
5dhf	pentaglutamyl folate (DHF)		C39H43N11O18	-6	Cytosol
5dhf	pentaglutamyl folate (DHF)		C39H43N11O18	-6	Extracellular
5dhf	pentaglutamyl folate (DHF)		C39H43N11O18	-6	Lysosome
5dhf	pentaglutamyl folate (DHF)		C39H43N11O18	-6	Mitochondria
5dpmev	(R)-5-Diphosphomevalonate		C6H10O10P2	-4	Peroxisome
5forthf	5-Formiminotetrahydrofolate		C20H22N8O6	-2	Cytosol
5fthf	5-Formyltetrahydrofolate	Folic acid, L(-)-5-Formyl-5,6,7,8-tetrahydrofolic acid	C20H21N7O7	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
5thf	5-Formyltetrahydrofolate	Folinic acid, L(-)-5-Formyl-5,6,7,8-tetrahydrofolic acid	C20H21N7O7	-2	Extracellular
5g2oxpt	5-Guanidino-2-oxopentanoate	2-Oxo-5-guanidino-pentanoate, 2-Oxo-5-guanidinopentanoate, 5-Guanidino-2-oxo-pentanoate	C6H11N3O3	0	Peroxisome
5homeprazole	5 hydroxy omeprazole		C17H19N3O4S	0	Cytosol
5homeprazole	5 hydroxy omeprazole		C17H19N3O4S	0	Extracellular
5shoxindact	5-Hydroxyindoleacetaldehyde		C10H9NO2	0	Cytosol
5shoxindact	5-Hydroxyindoleacetaldehyde		C10H9NO2	0	Mitochondria
5shoxindoa	5-Hydroxyindoleacetate		C10H8NO3	-1	Cytosol
5shoxindoa	5-Hydroxyindoleacetate		C10H8NO3	-1	Mitochondria
5shoxnkyn	5-Hydroxy-N-formylkynurenine		C11H12N2O5	0	Cytosol
5HPET	5-Hydroperoxy-6-trans-8,11,14-cis-eicosatetraenoate	(6E,8Z,11Z,14Z)-(5S)-5-Hydroperoxyeicosa-6,8,11,14-tetraenoate, 5-HPETE, 5-Hydroperoxy-trans-8,11,14-cis-eicosatetraenoate	C20H31O4	-1	Cytosol
5htrp	5-Hydroxy-L-tryptophan	5-HTP	C11H12N2O3	0	Cytosol
5htrp	5-Hydroxy-L-tryptophan	5-HTP	C11H12N2O3	0	Extracellular
5hxkyn	5-Hydroxykynurenine		C10H12N2O4	0	Cytosol
5hxkynam	5-Hydroxykynurenamine		C9H13N2O2	1	Cytosol
5mdr1p	5-Methylthio-D-ribose 1-phosphate	5-Methylthio-D-ribose 1-phosphate, S5-Methyl-5-thio-D-ribose 1-phosphate	C6H11O7PS	-2	Cytosol
5mdru1p	5-Methylthio-5-deoxy-D-ribose 1-phosphate		C6H11O7PS	-2	Cytosol
5moxact	5-Methoxyindoleacetate		C11H10NO3	-1	Cytosol
5mta	5-Methylthioadenosine	5'-Deoxy-5'-(methylthio)adenosine, 5'-Methylthioadenosine, 5'-S-Methylthioadenosine, Methylthioadenosine	C11H15N5O3S	0	Cytosol
5mthf	5-Methyltetrahydrofolate	5-methyl-5,6,7,8-tetrahydrofolate, N5-methyl-5,6,7,8-tetrahydrofolate, N5-methyl-tetrahydrofolate	C20H24N7O6	-1	Cytosol
5mthf	5-Methyltetrahydrofolate	5-methyl-5,6,7,8-tetrahydrofolate, N5-methyl-5,6,7,8-tetrahydrofolate, N5-methyl-tetrahydrofolate	C20H24N7O6	-1	Extracellular
5oxpro	5-Oxoproline	5-Oxoproline, 5-Pyrrolidone-2-carboxylic acid, Pyroglutamate, Pyroglutamic acid	C5H6NO3	-1	Cytosol
5pnev	(R)-5-Phosphomevalonate	(R)-5-Phosphomevalonic acid, (R)-Mevalonic acid 5-phosphate	C6H10O7P	-3	Peroxisome
5thf	pentaglutamyl folate (THF)		C39H45N11O18	-6	Cytosol
5thf	pentaglutamyl folate (THF)		C39H45N11O18	-6	Extracellular
5thf	pentaglutamyl folate (THF)		C39H45N11O18	-6	Lysosome
5thf	pentaglutamyl folate (THF)		C39H45N11O18	-6	Mitochondria
6a2ohxnt	6-Amino-2-oxohexanoate	2-Oxo-6-aminocaproate	C6H11NO3	0	Peroxisome
6dhf	hexaglutamyl folate (DHF)		C44H49N12O21	-7	Cytosol
6dhf	hexaglutamyl folate (DHF)		C44H49N12O21	-7	Extracellular
6dhf	hexaglutamyl folate (DHF)		C44H49N12O21	-7	Lysosome
6dhf	hexaglutamyl folate (DHF)		C44H49N12O21	-7	Mitochondria
6hoxmelatn	6-Hydroxymelatonin		C13H16N2O3	0	Cytosol
6htststerone	6 beta hydroxy testosterone		C19H28O3	0	Cytosol
6htststerone	6 beta hydroxy testosterone		C19H28O3	0	Extracellular
6htststerone	6 beta hydroxy testosterone		C19H28O3	0	Endoplasmic Reticulum
6pgc	6-Phospho-D-gluconate	6-phosphogluconic acid, D-gluconate 6-phosphate	C6H10O10P	-3	Cytosol
6pgc	6-Phospho-D-gluconate	6-phosphogluconic acid, D-gluconate 6-phosphate	C6H10O10P	-3	Endoplasmic Reticulum
6pgl	6-phospho-D-glucono-1,5-lactone	D-Glucono-1,5-lactone 6-phosphate	C6H9O9P	-2	Cytosol
6pgl	6-phospho-D-glucono-1,5-lactone	D-Glucono-1,5-lactone 6-phosphate	C6H9O9P	-2	Endoplasmic Reticulum
6pthp	6-Pyruvoyl-5,6,7,8-tetrahydropterin	6-Pyruvoyl-tetrahydropterin, 6-Pyruvoyltetrahydropterin	C9H11NSO3	0	Cytosol
6pthp	6-Pyruvoyl-5,6,7,8-tetrahydropterin	6-Pyruvoyl-tetrahydropterin, 6-Pyruvoyltetrahydropterin	C9H11NSO3	0	Nucleus
6thf	hexaglutamyl folate (THF)		C44H51N12O21	-7	Cytosol
6thf	hexaglutamyl folate (THF)		C44H51N12O21	-7	Extracellular
6thf	hexaglutamyl folate (THF)		C44H51N12O21	-7	Lysosome
6thf	hexaglutamyl folate (THF)		C44H51N12O21	-7	Mitochondria
7dhcsterol	7-Dehydrocholesterol	7-dien-3beta-ol, Cholesta-5, Provitamin D3	C27H44O	0	Cytosol
7dhcsterol	7-Dehydrocholesterol	7-dien-3beta-ol, Cholesta-5, Provitamin D3	C27H44O	0	Endoplasmic Reticulum
7dhf	heptaglutamyl folate (DHF)		C49H55N13O24	-8	Cytosol
7dhf	heptaglutamyl folate (DHF)		C49H55N13O24	-8	Extracellular
7dhf	heptaglutamyl folate (DHF)		C49H55N13O24	-8	Lysosome
7dhf	heptaglutamyl folate (DHF)		C49H55N13O24	-8	Mitochondria
7dhf	heptaglutamyl folate (THF)		C49H57N13O24	-8	Cytosol
7dhf	heptaglutamyl folate (THF)		C49H57N13O24	-8	Extracellular
7dhf	heptaglutamyl folate (THF)		C49H57N13O24	-8	Lysosome
7dhf	heptaglutamyl folate (THF)		C49H57N13O24	-8	Mitochondria
9-cis-retfa	fatty acid 9-cis-retinol		C20H29OFULLR2CO	0	Cytosol
9-cis-retfa	fatty acid 9-cis-retinol		C20H29OFULLR2CO	0	Extracellular
aacoa	Acetoacetyl-CoA	3-acetoacetyl-CoA, 3-ketobutanoyl-CoA, 3-ketobutyryl-CoA, 3-oxobutanoyl-CoA, 3-oxobutyryl-CoA, Acetoacetyl coenzyme A	C25H36N7O18P3S	4	Cytosol
aacoa	Acetoacetyl-CoA	3-acetoacetyl-CoA, 3-ketobutanoyl-CoA, 3-ketobutyryl-CoA, 3-oxobutanoyl-CoA, 3-oxobutyryl-CoA, Acetoacetyl coenzyme A	C25H36N7O18P3S	4	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
aacoa	Acetoacetyl-CoA	3-acetoacetyl-CoA, 3-ketobutanoyl-CoA, 3-ketobutyryl-CoA, 3-oxobutanoyl-CoA, 3-oxobutyryl-CoA, Acetoacetyl coenzyme A	C25H36N7O18P3S	-4	Peroxisome
aact	Aminoacetone	1-Amino-2-propanone	C3H8NO	1	Cytosol
aact	Aminoacetone	1-Amino-2-propanone	C3H8NO	1	Mitochondria
abt	L-Arabinitol	L-Arabinol, L-Arabitol, L-Lyxitol	C5H12O5	0	Cytosol
abt	L-Arabinitol	L-Arabinol, L-Arabitol, L-Lyxitol	C5H12O5	0	Extracellular
ac	Acetate	Acetic acid, Ethanoic acid, Ethylic acid, Methanecarboxylic acid, Vinegar acid, vinegar	C2H3O2	-1	Cytosol
ac	Acetate	Acetic acid, Ethanoic acid, Ethylic acid, Methanecarboxylic acid, Vinegar acid, vinegar	C2H3O2	-1	Extracellular
ac	Acetate	Acetic acid, Ethanoic acid, Ethylic acid, Methanecarboxylic acid, Vinegar acid, vinegar	C2H3O2	-1	Golgi Apparatus
ac	Acetate	Acetic acid, Ethanoic acid, Ethylic acid, Methanecarboxylic acid, Vinegar acid, vinegar	C2H3O2	-1	Mitochondria
acac	Acetoacetate	3-Oxobutanoic acid, Acetoacetic acid, beta-Ketobutyric acid	C4H5O3	-1	Cytosol
acac	Acetoacetate	3-Oxobutanoic acid, Acetoacetic acid, beta-Ketobutyric acid	C4H5O3	-1	Extracellular
acac	Acetoacetate	3-Oxobutanoic acid, Acetoacetic acid, beta-Ketobutyric acid	C4H5O3	-1	Mitochondria
acac	Acetoacetate	3-Oxobutanoic acid, Acetoacetic acid, beta-Ketobutyric acid	C4H5O3	-1	Peroxisome
acACP	Acetyl-ACP		C13H23N2O8PRS	-1	Cytosol
acald	Acetaldehyde	Acetaldehyde, Acetic aldehyde, Aldehyde, Aldehyd C(2), Ethanal, Ethyl aldehyde, acetylaldehyde	C2H4O	0	Cytosol
acald	Acetaldehyde	Acetaldehyde, Acetic aldehyde, Aldehyde, Aldehyd C(2), Ethanal, Ethyl aldehyde, acetylaldehyde	C2H4O	0	Extracellular
acald	Acetaldehyde	Acetaldehyde, Acetic aldehyde, Aldehyde, Aldehyd C(2), Ethanal, Ethyl aldehyde, acetylaldehyde	C2H4O	0	Mitochondria
acald	Acetaldehyde	Acetaldehyde, Acetic aldehyde, Aldehyde, Aldehyd C(2), Ethanal, Ethyl aldehyde, acetylaldehyde	C2H4O	0	Endoplasmic Reticulum
acald	Acetaldehyde	Acetaldehyde, Acetic aldehyde, Aldehyde, Aldehyd C(2), Ethanal, Ethyl aldehyde, acetylaldehyde	C2H4O	0	Peroxisome
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Cytosol
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Golgi Apparatus
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Mitochondria
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Nucleus
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Endoplasmic Reticulum
accoa	Acetyl-CoA	Acetyl coenzyme A	C23H34N7O17P3S	-4	Peroxisome
acetol	Acetol	1-Hydroxy-2-propanone, 2-Ketopropyl alcohol, Acetone alcohol, Hydroxyacetone, Methylketol, Pyruvic alcohol, Pyruvinalcohol	C3H6O2	0	Cytosol
acetone	Acetone	2-Propanone, Dimethyl ketone	C3H6O	0	Cytosol
acetone	Acetone	2-Propanone, Dimethyl ketone	C3H6O	0	Extracellular
acetone	Acetone	2-Propanone, Dimethyl ketone	C3H6O	0	Mitochondria
acg5p	N-Acetyl-L-glutamyl 5-phosphate	N-Acetyl-L-glutamate 5-phosphate	C7H9NO8P	-3	Mitochondria
acg5sa	N-Acetyl-L-glutamyl 5-semialdehyde	2-Acetamido-5-oxopentanoate	C7H10NO4	-1	Mitochondria
acgagbside_hs	alpha GalNAc globoside (homo sapiens)	GalNAc alpha globoside	C52H92N3O27FULLRCO	0	Cytosol
acgagbside_hs	alpha GalNAc globoside (homo sapiens)	GalNAc alpha globoside	C52H92N3O27FULLRCO	0	Golgi Apparatus
acgagbside_hs	alpha GalNAc globoside (homo sapiens)	GalNAc alpha globoside	C52H92N3O27FULLRCO	0	Lysosome
acgal	N-Acetyl-D-galactosamine	2-Acetamido-2-deoxy-D-galactose, GalNAc, N-Acetyl-D-chondrosamine	C8H15NO6	0	Cytosol
acgal	N-Acetyl-D-galactosamine	2-Acetamido-2-deoxy-D-galactose, GalNAc, N-Acetyl-D-chondrosamine	C8H15NO6	0	Golgi Apparatus
acgal	N-Acetyl-D-galactosamine	2-Acetamido-2-deoxy-D-galactose, GalNAc, N-Acetyl-D-chondrosamine	C8H15NO6	0	Lysosome
acgal1p	N-Acetyl-D-galactosamine 1-phosphate		C8H14NO9P	-2	Cytosol
acgalfuc12gal14acglegalgusde_hs	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1		C58H102N3O31FULLRCO	0	Golgi Apparatus
acgalfucgalacgalfuc12gal14acglegalguside_hs	Type IIIA glycolipid	(Gal)3 (GalNAc)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	C78H135N4O45FULLRCO	0	Cytosol
acgalfucgalacgalfuc12gal14acglegalguside_hs	Type IIIA glycolipid	(Gal)3 (GalNAc)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	C78H135N4O45FULLRCO	0	Extracellular
acgalfucgalacgalfuc12gal14acglegalguside_hs	Type IIIA glycolipid	(Gal)3 (GalNAc)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	C78H135N4O45FULLRCO	0	Golgi Apparatus
acgalfucgalacgalfucgalcglgal14acglegalguside_hs	Type IIIAb	(Gal)4 (GalNAc)2 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	C92H158N5O55FULLRCO	0	Cytosol
acgalfucgalacgalfucgalcglgal14acglegalguside_hs	Type IIIAb	(Gal)4 (GalNAc)2 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	C92H158N5O55FULLRCO	0	Extracellular
acgalfucgalacgalfucgalcglgal14acglegalguside_hs	Type IIIAb	(Gal)4 (GalNAc)2 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	C92H158N5O55FULLRCO	0	Golgi Apparatus
acgalfucgalacgalfucgalcglgal14acglegalguside_hs	(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1		C72H125N4O41FULLRCO	0	Golgi Apparatus
acgalfucgalacgalfucgalcglgal14acglegalguside_hs	Type IA glycolipid	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C58H102N3O31FULLRCO	0	Golgi Apparatus
acgam	N-Acetyl-D-glucosamine	2-Acetamido-2-deoxy-D-glucose, GlcNAc, N-Acetylchitosamine	C8H15NO6	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
acgam	N-Acetyl-D-glucosamine	2-Acetamido-2-deoxy-D-glucose, GlcNAc, N-Acetylchitosamine	C8H15NO6	0	Extracellular
acgam	N-Acetyl-D-glucosamine	2-Acetamido-2-deoxy-D-glucose, GlcNAc, N-Acetylchitosamine	C8H15NO6	0	Lysosome
acgam1p	N-Acetyl-D-glucosamine 1-phosphate		C8H14NO9P	-2	Cytosol
acgam6p	N-Acetyl-D-glucosamine 6-phosphate		C8H14NO9P	-2	Cytosol
acgbgbside_hs	beta GalNAc globoside (homo sapiens)	IV3GalNAcb-Gb4Cer	C52H92N3O27FULLRCO	0	Cytosol
acgbgbside_hs	beta GalNAc globoside (homo sapiens)	IV3GalNAcb-Gb4Cer	C52H92N3O27FULLRCO	0	Golgi Apparatus
acgbgbside_hs	beta GalNAc globoside (homo sapiens)	IV3GalNAcb-Gb4Cer	C52H92N3O27FULLRCO	0	Lysosome
acglc13galacglgal14acglcgaluside_hs	nLc7Cer		C66H115N4O37FULLRCO	0	Golgi Apparatus
acglcgal14acglcgaluside_hs	nLc5Cer	(Gal)2 (Glc)1 (GlcNAc)2 (Cer)1	C52H92N3O27FULLRCO	0	Golgi Apparatus
acglcgalacglgal14acglcgaluside_hs	(Gal)3 (Glc)1 (GlcNAc)3 (Cer)1		C66H115N4O37FULLRCO	0	Golgi Apparatus
acglcgalgbside_hs	GlcNAc-Gal globoside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)1 (Cer)1	C58H102N3O32FULLRCO	0	Golgi Apparatus
acglcgaluside_hs	(Gal)1 (Glc)1 (GlcNAc)1 (Cer)1	Lc3Cer	C38H69N2O17FULLRCO	0	Golgi Apparatus
acglu	N-Acetyl-L-glutamate	N-Acetyl-L-glutamic acid	C7H9NO5	-2	Mitochondria
acgpail_hs	N-Acetyl-D-glucosaminylphosphatidylinositol		C17H29NO14PFULLRCO2FULLR2CO2	-1	Cytosol
ach	Acetylcholine	Acetylcholine, O-Acetylcholine	C7H16NO2	1	Cytosol
ach	Acetylcholine	Acetylcholine, O-Acetylcholine	C7H16NO2	1	Extracellular
ach	Acetylcholine	Acetylcholine, O-Acetylcholine	C7H16NO2	1	Nucleus
acmana	N-Acetyl-D-mannosamine	2-Acetamido-2-deoxy-D-mannose	C8H15NO6	0	Cytosol
acmanap	N-Acetyl-D-mannosamine 6-phosphate	N-Acetyl-D-mannosamine 6-phosphate, N-Acetylmannosamine 6-phosphate	C8H14NO9P	-2	Cytosol
acn13acngalgsbside_hs	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Disialosyl Gb5, Disialosylgalactosylgloboside, Disialosylglobopentaosylceramide, V3NeuAcIV6NeuAc-Gb5Cer;	C72H121N4O43FULLRCO	-2	Cytosol
acn13acngalgsbside_hs	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Disialosyl Gb5, Disialosylgalactosylgloboside, Disialosylglobopentaosylceramide, V3NeuAcIV6NeuAc-Gb5Cer;	C72H121N4O43FULLRCO	-2	Extracellular
acn13acngalgsbside_hs	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Disialosyl Gb5, Disialosylgalactosylgloboside, Disialosylglobopentaosylceramide, V3NeuAcIV6NeuAc-Gb5Cer;	C72H121N4O43FULLRCO	-2	Golgi Apparatus
acn23acngalgsbside_hs	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C72H121N4O43FULLRCO	-2	Cytosol
acn23acngalgsbside_hs	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C72H121N4O43FULLRCO	-2	Extracellular
acn23acngalgsbside_hs	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C72H121N4O43FULLRCO	-2	Golgi Apparatus
acnangal14acglcgalgalside_hs	3,8'-LD1	(Gal)2 (Glc)1 (GlcNAc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Cytosol
acnangal14acglcgalgalside_hs	3,8'-LD1	(Gal)2 (Glc)1 (GlcNAc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Extracellular
acnangal14acglcgalgalside_hs	3,8'-LD1	(Gal)2 (Glc)1 (GlcNAc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
acnangalgsbside_hs	disialyl galactosylgloboside (homo sapiens)	V3(NeuAc)2-Gb5Cer	C72H121N4O43FULLRCO	-2	Cytosol
acnangalgsbside_hs	disialyl galactosylgloboside (homo sapiens)	V3(NeuAc)2-Gb5Cer	C72H121N4O43FULLRCO	-2	Extracellular
acnangalgsbside_hs	disialyl galactosylgloboside (homo sapiens)	V3(NeuAc)2-Gb5Cer	C72H121N4O43FULLRCO	-2	Golgi Apparatus
acnam	N-Acetylneuraminate	5-Acetamido-3,5-dideoxy-D-glycero-D-galacto-2-nomulosonic acid, N-Acetylneuraminic acid, Neu5Ac	C11H18NO9	-1	Cytosol
acnam	N-Acetylneuraminate	5-Acetamido-3,5-dideoxy-D-glycero-D-galacto-2-nomulosonic acid, N-Acetylneuraminic acid, Neu5Ac	C11H18NO9	-1	Lysosome
acnam	N-Acetylneuraminate	5-Acetamido-3,5-dideoxy-D-glycero-D-galacto-2-nomulosonic acid, N-Acetylneuraminic acid, Neu5Ac	C11H18NO9	-1	Nucleus
acnamp	N-Acetylneuraminate 9-phosphate		C11H17NO12P	-3	Cytosol
acngal14acglcgalgalside_hs	Sialyl-3-paragloboside	(Gal)2 (Glc)1 (GlcNAc)1 (Neu5Ac)1 (Cer)1, 3'-LM1, IV3-a-Neu5Ac-nLc4Cer, Sialyl-3-paragloboside, snLc4Cer	C55H95N3O30FULLRCO	-1	Golgi Apparatus
acngalacglcgal14acglcgalgalside_hs	V13NeuAc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (Neu5Ac)1 (Cer)1	C69H118N4O40FULLRCO	-1	Cytosol
acngalacglcgal14acglcgalgalside_hs	V13NeuAc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (Neu5Ac)1 (Cer)1	C69H118N4O40FULLRCO	-1	Extracellular
acngalacglcgal14acglcgalgalside_hs	V13NeuAc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (Neu5Ac)1 (Cer)1	C69H118N4O40FULLRCO	-1	Golgi Apparatus
acngalacglcgalgalside_hs	(Gal)3 (Glc)1 (GlcNAc)1 (Cer)1		C55H95N3O30FULLRCO	-1	Golgi Apparatus
acngalgsbside_hs	sialyl galactosylgloboside (homo sapiens)	MSGG, Monosialyl-Gb5, Monosialylgalactosylgloboside, SSEA-4, V3NeuAc-Gb5Cer	C61H105N3O35FULLRCO	-1	Golgi Apparatus
acorn	N2-Acetyl-L-ornithine		C7H14N2O3	0	Cytosol
ACP	acyl carrier protein		C11H21N2O7PRS	-1	Cytosol
ACP	acyl carrier protein		C11H21N2O7PRS	-1	Mitochondria
acrn	O-Acetylcamitine		C9H17NO4	0	Cytosol
acrn	O-Acetylcamitine		C9H17NO4	0	Mitochondria
acrn	O-Acetylcamitine		C9H17NO4	0	Endoplasmic Reticulum
acrn	O-Acetylcamitine		C9H17NO4	0	Peroxisome
ade	Adenine	1H-Purin-6-amine, 6-Aminopurine, A, Ade, Adeninimine, Vitamin B4	C5H5N5	0	Cytosol
ade	Adenine	1H-Purin-6-amine, 6-Aminopurine, A, Ade, Adeninimine, Vitamin B4	C5H5N5	0	Extracellular
ade	Adenine	1H-Purin-6-amine, 6-Aminopurine, A, Ade, Adeninimine, Vitamin B4	C5H5N5	0	Lysosome
adhap_hs	acyl-dihydroxyacetone phosphate		C3H4O6PFULLRCO	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
adhap_hs	acyl-dihydroxyacetone phosphate		C3H4O6PFULLRSCO	-2	Peroxisome
adn	Adenosine	9-B-D-ribofuranosyl-9H-purin-6-amine, 9-beta-D-Ribofuranosyladenine, Adenine riboside, Adenocard, rA	C10H13NSO4	0	Cytosol
adn	Adenosine	9-B-D-ribofuranosyl-9H-purin-6-amine, 9-beta-D-Ribofuranosyladenine, Adenine riboside, Adenocard, rA	C10H13NSO4	0	Extracellular
adn	Adenosine	9-B-D-ribofuranosyl-9H-purin-6-amine, 9-beta-D-Ribofuranosyladenine, Adenine riboside, Adenocard, rA	C10H13NSO4	0	Lysosome
adn	Adenosine	9-B-D-ribofuranosyl-9H-purin-6-amine, 9-beta-D-Ribofuranosyladenine, Adenine riboside, Adenocard, rA	C10H13NSO4	0	Mitochondria
adocbl	Adenosylcobalamin	(5, (5'-Deoxy-5'-adenosyl)cobamide coenzyme, 5,5-Deoxy-5'-adenosyl vitamin B12, 5'-Deoxy-5'-adenosyl-5, 5'-Deoxy-5'-adenosylcobalamin, 6-Dimethylbenzimidazolylcobamide coenzyme, 6-Dimethylbenzimidazolyl-5-deoxyadenosylcobamide, 6-Dimethylbenzimidazolyl-Co-5'-deoxy-5'-adenosylcobamide, 6-dimethylbenzimidazolylcobamide coenzyme, 6-dimethylbenzimidazolylcobamide, Adenosylcobalamin, Calomide, Cobalamin coenzyme, Cobamamide, Coenzyme B12, DMBC coenzyme, Deoxyadenosylcobalamin, Dibencozide Funacomide, Vitamin B12 coenzyme, a-(5	C72H100CoN18O17P	0	Mitochondria
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Cytosol
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Extracellular
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Mitochondria
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Nucleus
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Endoplasmic Reticulum
adp	ADP	Adenosine 5'-diphosphate	C10H12NSO10P2	-3	Peroxisome
adpglc	ADPglucose	Adenosine diphosphoglucose	C16H23NSO15P2	-2	Cytosol
adpman	ADPmannose		C16H23NSO15P2	-2	Cytosol
adprbp	ADPribose 2'-phosphate		C15H20NSO17P3	-4	Cytosol
adprbp	ADPribose 2'-phosphate		C15H20NSO17P3	-4	Extracellular
adprib	ADPribose	ADP-D-ribose, ADP-ribose, adenine-diphosphate-ribose, adenosine diphosphate ribose	C15H21NSO14P2	-2	Cytosol
adprib	ADPribose	ADP-D-ribose, ADP-ribose, adenine-diphosphate-ribose, adenosine diphosphate ribose	C15H21NSO14P2	-2	Extracellular
adprib	ADPribose	ADP-D-ribose, ADP-ribose, adenine-diphosphate-ribose, adenosine diphosphate ribose	C15H21NSO14P2	-2	Mitochondria
adrn	adrenic acid	adrenic acid(22:4,n-6), docosa-7,10,13,16-tetraenoic acid	C22H35O2	-1	Cytosol
adrn	adrenic acid	adrenic acid(22:4,n-6), docosa-7,10,13,16-tetraenoic acid	C22H35O2	-1	Extracellular
adrn	adrenic acid	adrenic acid(22:4,n-6), docosa-7,10,13,16-tetraenoic acid	C22H35O2	-1	Peroxisome
adrncoa	adrenyl coenzyme A		C43H66N7O17P3S	-4	Cytosol
adrncoa	adrenyl coenzyme A		C43H66N7O17P3S	-4	Mitochondria
adrncoa	adrenyl coenzyme A		C43H66N7O17P3S	-4	Peroxisome
adrncrn	Adrenyl carnitine	adrenic acid carnitine	C29H49NO4	0	Cytosol
adrncrn	Adrenyl carnitine	adrenic acid carnitine	C29H49NO4	0	Mitochondria
adrl	Adrenaline	(R)-(-)-Adrenaline, (R)-(-)-Adrenaline, (R)-(-)-Epinephrine, (R)-(-)-Eprenamine, 2-benzenediol, [(1R)-1-Hydroxy-2-(methylamino)ethyl]-1, L-Adrenaline	C9H14NO3	1	Cytosol
adrl	Adrenaline	(R)-(-)-Adrenaline, (R)-(-)-Adrenaline, (R)-(-)-Epinephrine, (R)-(-)-Eprenamine, 2-benzenediol, [(1R)-1-Hydroxy-2-(methylamino)ethyl]-1, L-Adrenaline	C9H14NO3	1	Extracellular
adsel	Adenylselenate	Adenosine-5'-phosphoselenate	C10H12NSO10PSe	-2	Cytosol
aflatoxin	aflatoxin B1	2,3-Epoxyaflatoxin B1, Aflatoxin B1 2,3-epoxide, Aflatoxin B1 8,9-epoxide, Aflatoxin B1 8,9-oxide, Aflatoxin B1 epoxide, Aflatoxin B1-2,3-oxide [MeSH: aflatoxin B1-2,3-oxide]	C17H12O6	0	Cytosol
aflatoxin	aflatoxin B1	2,3-Epoxyaflatoxin B1, Aflatoxin B1 2,3-epoxide, Aflatoxin B1 8,9-epoxide, Aflatoxin B1 8,9-oxide, Aflatoxin B1 epoxide, Aflatoxin B1-2,3-oxide [MeSH: aflatoxin B1-2,3-oxide]	C17H12O6	0	Extracellular
agm	Agmatine	(4-Aminobutyl) guanidine	C5H16N4	2	Mitochondria
ahandrostan	3alpha-Hydroxy-5beta-androstan-17-one	3alpha-Hydroxy-5beta-androstan-17-one, 3alpha-Hydroxyetiocholan-17-one, Etiocholan-3alpha-ol-17-one	C19H30O2	0	Endoplasmic Reticulum
ahandrostanglc	Etiocholan-3alpha-ol-17-one 3-glucuronide		C25H38O8	0	Cytosol
ahandrostanglc	Etiocholan-3alpha-ol-17-one 3-glucuronide		C25H38O8	0	Extracellular
ahandrostanglc	Etiocholan-3alpha-ol-17-one 3-glucuronide		C25H38O8	0	Endoplasmic Reticulum
ahcys	S-Adenosyl-L-homocysteine	S-Adenosylhomocysteine	C14H20N6O5S	0	Cytosol
ahcys	S-Adenosyl-L-homocysteine	S-Adenosylhomocysteine	C14H20N6O5S	0	Mitochondria
ahcys	S-Adenosyl-L-homocysteine	S-Adenosylhomocysteine	C14H20N6O5S	0	Nucleus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ahcys	S-Adenosyl-L-homocysteine	S-Adenosylhomocysteine	C14H20N6O5S	0	Endoplasmic Reticulum
ahdt	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate, 6-(L-erythro-1,2-Dihydroxypropyl 3-triphosphate)-7-dihydropterin, 6-[(1S,2R)-1,2-Dihydroxy-3-triphosphoxypropyl]-7,8-dihydropterin, H2-neopterin triphosphate, dihydroneopterin triphosphate	C9H12N5O13P3	-4	Cytosol
ahdt	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine triphosphate, 6-(L-erythro-1,2-Dihydroxypropyl 3-triphosphate)-7-dihydropterin, 6-[(1S,2R)-1,2-Dihydroxy-3-triphosphoxypropyl]-7,8-dihydropterin, H2-neopterin triphosphate, dihydroneopterin triphosphate	C9H12N5O13P3	-4	Nucleus
aicar	5-Amino-1-(5-Phospho-D-ribose)imidazole-4-carboxamide	1-(5'-Phosphoribosyl)-5-amino-4-imidazolecarboxamide, 5'-Phospho-ribose-1,5-amino-4-imidazolecarboxamide, 5-Aminoimidazole-4-carboxamide ribotide, 5-Phosphoribosyl-4-carbamoyl-5-aminoimidazole, AICAR	C9H13N4O8P	-2	Cytosol
air	5-amino-1-(5-phospho-D-ribose)imidazole	1-(5'-Phosphoribosyl)-5-aminoimidazole, 1-(5-Phospho-D-ribose)-5-aminoimidazole, 5'-Phosphoribosyl-5-aminoimidazole, AIR, Aminoimidazole ribotide	C8H12N3O7P	-2	Cytosol
ak2g_hs	1-alkyl 2-acylglycerol		C5H10O2FULLRFULLR2CO2	0	Cytosol
ak2gchol_hs	1-alkyl 2-acylglycerol 3-phosphocholine		C10H20O5NPFULLRFULLR2CO	0	Cytosol
ak2gp_hs	1-alkyl 2-acylglycerol 3-phosphate		C5H9O6PFULLRFULLR2CO	-2	Cytosol
ak2gpe_hs	1-alkyl 2-acylglycerol 3-phosphoethanolamine		C7H16O5NPFULLRFULLR2CO	0	Cytosol
ak2lgchol_hs	1-alkyl 2-lysoglycerol 3-phosphocholine	1-Organyl-2-lyso-sn-glycero-3-phosphocholine, 1-Radyl-2-lyso-sn-glycero-3-phosphocholine	C10H21O5NPFULLR	0	Cytosol
ak2lgchol_hs	1-alkyl 2-lysoglycerol 3-phosphocholine	1-Organyl-2-lyso-sn-glycero-3-phosphocholine, 1-Radyl-2-lyso-sn-glycero-3-phosphocholine	C10H21O5NPFULLR	0	Extracellular
akdhap_hs	1-alkylidihydroxyacetone phosphate		C3H4O6PFULLRC2H4	-2	Cytosol
akdhap_hs	1-alkylidihydroxyacetone phosphate		C3H4O6PFULLRC2H4	-2	Peroxisome
akg	2-Oxoglutarate	2-Ketoglutaric acid, Oxoglutaric acid, alpha-Ketoglutarate, alpha-Ketoglutaric Acid	C5H4O5	-2	Cytosol
akg	2-Oxoglutarate	2-Ketoglutaric acid, Oxoglutaric acid, alpha-Ketoglutarate, alpha-Ketoglutaric Acid	C5H4O5	-2	Extracellular
akg	2-Oxoglutarate	2-Ketoglutaric acid, Oxoglutaric acid, alpha-Ketoglutarate, alpha-Ketoglutaric Acid	C5H4O5	-2	Mitochondria
akg	2-Oxoglutarate	2-Ketoglutaric acid, Oxoglutaric acid, alpha-Ketoglutarate, alpha-Ketoglutaric Acid	C5H4O5	-2	Endoplasmic Reticulum
akg	2-Oxoglutarate	2-Ketoglutaric acid, Oxoglutaric acid, alpha-Ketoglutarate, alpha-Ketoglutaric Acid	C5H4O5	-2	Peroxisome
akgp_hs	1-alkylglycerol 3-phosphate (homo sapiens)		C4H10O4PFULLR2CO2	-2	Cytosol
ala-B	beta-Alanine	3-Aminopropanoate, 3-aminopropionic acid	C3H7NO2	0	Cytosol
ala-B	beta-Alanine	3-Aminopropanoate, 3-aminopropionic acid	C3H7NO2	0	Extracellular
ala-B	beta-Alanine	3-Aminopropanoate, 3-aminopropionic acid	C3H7NO2	0	Mitochondria
ala-D	D-Alanine	D-2-Aminopropionic acid	C3H7NO2	0	Cytosol
ala-D	D-Alanine	D-2-Aminopropionic acid	C3H7NO2	0	Extracellular
ala-D	D-Alanine	D-2-Aminopropionic acid	C3H7NO2	0	Lysosome
ala-D	D-Alanine	D-2-Aminopropionic acid	C3H7NO2	0	Peroxisome
ala-L	L-Alanine	L-2-Aminopropionic acid, L-alpha-Alanine	C3H7NO2	0	Cytosol
ala-L	L-Alanine	L-2-Aminopropionic acid, L-alpha-Alanine	C3H7NO2	0	Extracellular
ala-L	L-Alanine	L-2-Aminopropionic acid, L-alpha-Alanine	C3H7NO2	0	Lysosome
ala-L	L-Alanine	L-2-Aminopropionic acid, L-alpha-Alanine	C3H7NO2	0	Mitochondria
ala-L	L-Alanine	L-2-Aminopropionic acid, L-alpha-Alanine	C3H7NO2	0	Peroxisome
aldstrn	Aldosterone	11beta,21-Dihydroxy-3,20-dioxo-4-pregnen-18-al, Aldosterone	C21H28O5	0	Cytosol
aldstrn	Aldosterone	11beta,21-Dihydroxy-3,20-dioxo-4-pregnen-18-al, Aldosterone	C21H28O5	0	Extracellular
aldstrn	Aldosterone	11beta,21-Dihydroxy-3,20-dioxo-4-pregnen-18-al, Aldosterone	C21H28O5	0	Mitochondria
alkylR1oh	hydroxy alkyl chain		C2H5OFULLR	0	Peroxisome
alpa_hs	lysophosphatidic acid (homo sapiens)		C3H6O5PFULLR2CO2	-2	Cytosol
alpa_hs	lysophosphatidic acid (homo sapiens)		C3H6O5PFULLR2CO2	-2	Mitochondria
alpm	S-aminomethylidihydropoamide		C9H21N2O5S2	1	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
alpro	S-Aminomethylidihydrolypoilprotein		CH6NS2X	1	Mitochondria
am6sa	2-Aminomuconate 6-semialdehyde	2-Aminomuconate semialdehyde	C6H7NO3	0	Cytosol
amet	S-Adenosyl-L-methionine	Acylcarnitine, S-Adenosylmethionine	C15H23N6O5S	1	Cytosol
amet	S-Adenosyl-L-methionine	Acylcarnitine, S-Adenosylmethionine	C15H23N6O5S	1	Mitochondria
amet	S-Adenosyl-L-methionine	Acylcarnitine, S-Adenosylmethionine	C15H23N6O5S	1	Nucleus
amet	S-Adenosyl-L-methionine	Acylcarnitine, S-Adenosylmethionine	C15H23N6O5S	1	Endoplasmic Reticulum
ametam	S-Adenosylmethioninamine	(5-Deoxy-5-adenosyl)(3-aminopropyl)methylsulfonium salt, S-Adenosyl-L-methioninamine	C14H24N6O3S	2	Cytosol
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Cytosol
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Extracellular
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Golgi Apparatus
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Lysosome
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Mitochondria
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Endoplasmic Reticulum
amp	AMP	5'-AMP, 5'-Adenosine monophosphate, 5'-Adenylic acid, Adenosine 5'-monophosphate, Adenosine 5'-phosphate, Adenylate, Adenylic acid	C10H12NSO7P	-2	Peroxisome
amuco	2-Aminomuconate	2-Aminomuconic acid, o-Aminomuconate	C6H6NO4	-1	Cytosol
andrstandn	androstanedione	5beta-Androstane-3,17-dione	C19H28O2	0	Endoplasmic Reticulum
andrstdn	Androstenedione	4-Androstene-3,17-dione, Androst-4-ene-3,17-dione	C19H26O2	0	Endoplasmic Reticulum
andrstm	Androsterone	3alpha-Hydroxy-5alpha-androstan-17-one	C19H30O2	0	Cytosol
andrstm	Androsterone	3alpha-Hydroxy-5alpha-androstan-17-one	C19H30O2	0	Extracellular
andrstm	Androsterone	3alpha-Hydroxy-5alpha-androstan-17-one	C19H30O2	0	Endoplasmic Reticulum
andrstmglc	androsterone glucuronide		C25H38O8	0	Cytosol
andrstmglc	androsterone glucuronide		C25H38O8	0	Extracellular
andrstmglc	androsterone glucuronide		C25H38O8	0	Endoplasmic Reticulum
anth	Anthraniolate	2-Aminobenzoate, Anthranilic acid, Vitamin L, Vitamin L1, o-Aminobenzoic acid	C7H6NO2	-1	Cytosol
antipyrene	antipyrene	Analgesine, Anodynine, Antipirin, Antipyrin, Apirelina, Parodyne, Phenazon [MeSH: pyrazon], Phenazone [MeSH: Antipyrine], Phenazonum, antipyrine [MeSH: Antipyrine]	C11H12N2O	0	Cytosol
antipyrene	antipyrene	Analgesine, Anodynine, Antipirin, Antipyrin, Apirelina, Parodyne, Phenazon [MeSH: pyrazon], Phenazone [MeSH: Antipyrine], Phenazonum, antipyrine [MeSH: Antipyrine]	C11H12N2O	0	Extracellular
ap4a	P1,P4-Bis(5'-adenosyl) tetraphosphate	AppppA	C20H24N10O19P4	-4	Cytosol
apnnox	alpha-Pinene-oxide	alpha-Pinene-oxide	C10H16O	0	Cytosol
apnnox	alpha-Pinene-oxide	alpha-Pinene-oxide	C10H16O	0	Extracellular
apoC	Apocboxylase (no lys residue)		XH	0	Cytosol
apoC	Apocboxylase (no lys residue)		XH	0	Mitochondria
apoC-Lys	Apocboxylase (Lys residue)		C6H13N2OX	0	Cytosol
apoC-Lys	Apocboxylase (Lys residue)		C6H13N2OX	0	Mitochondria
apoC-Lys_btn	Holocarboxylase (biotin covalent bound to Lys residue of apoC)		C16H27N4O3SX	0	Cytosol
apoC-Lys_btn	Holocarboxylase (biotin covalent bound to Lys residue of apoC)		C16H27N4O3SX	0	Mitochondria
appnn	(+)-alpha-Pinene	(+)-alpha-Pinene	C10H16	0	Cytosol
appnn	(+)-alpha-Pinene	(+)-alpha-Pinene	C10H16	0	Extracellular
aprgstm	20alpha-Hydroxyprogesterone	20(S)-Hydroxyprogesterone, 20alpha-Dihydroprogesterone, 20alpha-Hydroxy-4-pregnen-3-one, 20alpha-Hydroxypregn-4-en-3-one, 20alpha-Hydroxyprogesterone, Progesterol-20alpha	C21H32O2	0	Cytosol
aprgstm	20alpha-Hydroxyprogesterone	20(S)-Hydroxyprogesterone, 20alpha-Dihydroprogesterone, 20alpha-Hydroxy-4-pregnen-3-one, 20alpha-Hydroxypregn-4-en-3-one, 20alpha-Hydroxyprogesterone, Progesterol-20alpha	C21H32O2	0	Extracellular
aprut	N-Acetylputrescine		C6H15N2O	1	Cytosol
aps	Adenosine 5'-phosphosulfate	APS, Adenylylsulfate	C10H12NSO10PS	-2	Cytosol
aqcobal	Aquacob(III)alamin	Aquacobalamin	C62H93CoN13O15P	0	Cytosol
aqcobal	Aquacob(III)alamin	Aquacobalamin	C62H93CoN13O15P	0	Extracellular

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
arab-L	L-Arabinose		C5H10O5	0	Cytosol
arab-L	L-Arabinose		C5H10O5	0	Extracellular
arach	Arachidic acid	Arachidic acid, Eicosanoic acid, Icosanoic acid	C20H39O2	-1	Cytosol
arach	Arachidic acid	Arachidic acid, Eicosanoic acid, Icosanoic acid	C20H39O2	-1	Extracellular
arachcoa	arachidyl coenzyme A		C41H70N7O17P3S	-4	Cytosol
arachcoa	arachidyl coenzyme A		C41H70N7O17P3S	-4	Mitochondria
arachcoa	arachidyl coenzyme A		C41H70N7O17P3S	-4	Peroxisome
arachcrn	arachidyl carnitine	arachidic acid - carnitine	C27H53NO4	0	Cytosol
arachcrn	arachidyl carnitine	arachidic acid - carnitine	C27H53NO4	0	Mitochondria
arachd	arachidonic acid	(5Z,8Z,11Z,14Z)-Icosatetraenoic acid, Arachidonate, Arachidonic acid, cis-5,8,11,14-Eicosatetraenoic acid, eicosanoate 20:4	C20H31O2	-1	Cytosol
arachd	arachidonic acid	(5Z,8Z,11Z,14Z)-Icosatetraenoic acid, Arachidonate, Arachidonic acid, cis-5,8,11,14-Eicosatetraenoic acid, eicosanoate 20:4	C20H31O2	-1	Extracellular
arachd	arachidonic acid	(5Z,8Z,11Z,14Z)-Icosatetraenoic acid, Arachidonate, Arachidonic acid, cis-5,8,11,14-Eicosatetraenoic acid, eicosanoate 20:4	C20H31O2	-1	Endoplasmic Reticulum
arachdcoa	C20:4-CoA	Arachidonyl-CoA, arachidonate CoA, arachidonic acid Coenzyme A	C41H62N7O17P3S	-4	Cytosol
arachdcoa	C20:4-CoA	Arachidonyl-CoA, arachidonate CoA, arachidonic acid Coenzyme A	C41H62N7O17P3S	-4	Mitochondria
arachdcoa	C20:4-CoA	Arachidonyl-CoA, arachidonate CoA, arachidonic acid Coenzyme A	C41H62N7O17P3S	-4	Peroxisome
arachdcrn	C20:4 carnitine	Arachidonate carnitine	C27H45NO4	0	Cytosol
arachdcrn	C20:4 carnitine	Arachidonate carnitine	C27H45NO4	0	Mitochondria
arg-D	D-Arginine	D-2-Amino-5-guanidinovaleric acid	C6H15N4O2	1	Peroxisome
arg-L	L-Arginine	(S)-2-Amino-5-guanidinovaleric acid, Arg, Arginine	C6H15N4O2	1	Cytosol
arg-L	L-Arginine	(S)-2-Amino-5-guanidinovaleric acid, Arg, Arginine	C6H15N4O2	1	Extracellular
arg-L	L-Arginine	(S)-2-Amino-5-guanidinovaleric acid, Arg, Arginine	C6H15N4O2	1	Mitochondria
argsuc	N(omega)-(L-Arginino)succinate	L-Argininosuccinate, L-Argininosuccinic acid, L-Argininosuccinic acid, N-(L-Arginino)succinate	C10H17N4O6	-1	Cytosol
ascb-L	L-Ascorbate	Ascorbate, Ascorbic acid, L-Ascorbic acid, Vitamin C	C6H8O6	0	Cytosol
ascb-L	L-Ascorbate	Ascorbate, Ascorbic acid, L-Ascorbic acid, Vitamin C	C6H8O6	0	Extracellular
asn-L	L-Asparagine	2-Amino-3-carbamoylpropanoic acid, 2-Aminosuccinamic acid, Arg	C4H8N2O3	0	Cytosol
asn-L	L-Asparagine	2-Amino-3-carbamoylpropanoic acid, 2-Aminosuccinamic acid, Arg	C4H8N2O3	0	Extracellular
asn-L	L-Asparagine	2-Amino-3-carbamoylpropanoic acid, 2-Aminosuccinamic acid, Arg	C4H8N2O3	0	Mitochondria
Asn-X-Ser/Thr	protein-linked asparagine residue (N-glycosylation site)		XH	0	Lysosome
Asn-X-Ser/Thr	protein-linked asparagine residue (N-glycosylation site)		XH	0	Endoplasmic Reticulum
asp-D	D-Aspartate	D-2-Aminobutanedioic acid, D-Aspartic acid	C4H6NO4	-1	Cytosol
asp-D	D-Aspartate	D-2-Aminobutanedioic acid, D-Aspartic acid	C4H6NO4	-1	Extracellular
asp-D	D-Aspartate	D-2-Aminobutanedioic acid, D-Aspartic acid	C4H6NO4	-1	Peroxisome
asp-L	L-Aspartate	2-aminosuccinic acid, Asp, L-Aspartic acid	C4H6NO4	-1	Cytosol
asp-L	L-Aspartate	2-aminosuccinic acid, Asp, L-Aspartic acid	C4H6NO4	-1	Extracellular
asp-L	L-Aspartate	2-aminosuccinic acid, Asp, L-Aspartic acid	C4H6NO4	-1	Mitochondria
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Cytosol
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Extracellular
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Mitochondria
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Nucleus
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Endoplasmic Reticulum
atp	ATP	5'-adenylate triphosphate, Adenosine 5'-triphosphate	C10H12NSO13P3	-4	Peroxisome
avite1	alpha-Tocopherol	Aquasol E, Ephanyl, Eprolin, Esorb, Pheryl-E, Phytoergmine, Vita plus E, Vita plus Ealpha-Tocopherol, Viteolin, Waynecomycin	C29H50O2	0	Cytosol
avite1	alpha-Tocopherol	Aquasol E, Ephanyl, Eprolin, Esorb, Pheryl-E, Phytoergmine, Vita plus E, Vita plus Ealpha-Tocopherol, Viteolin, Waynecomycin	C29H50O2	0	Extracellular
avite2	alpha-Tocotrienol	1721-51-3, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-, CHEMID001721513, Tocotrienol, alpha, zeta 1-Tocopherol	C29H44O2	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
avite2	alpha-Tocotrienol	1721-51-3, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-, CHEMID001721513, Tocotrienol, alpha, zeta1-Tocopherol	C29H44O2	0	Extracellular
b2coa	Crotonoyl-CoA	2-Butenoyl-CoA, But-2-enoyl-CoA, Crotonyl-CoA, trans-But-2-enoyl-CoA	C25H36N7O17P3S	-4	Mitochondria
b2coa	Crotonoyl-CoA	2-Butenoyl-CoA, But-2-enoyl-CoA, Crotonyl-CoA, trans-But-2-enoyl-CoA	C25H36N7O17P3S	-4	Peroxisome
bampald	beta-Aminopropion aldehyde		C3H8NO	1	Cytosol
bampald	beta-Aminopropion aldehyde		C3H8NO	1	Mitochondria
bdg2hc	cis-beta-D-Glucosyl-2-hydroxycinnamate	beta-D-Glucosyl-2-coumarinate	C15H18O8	0	Cytosol
betald	Betaine aldehyde		C5H12NO	1	Cytosol
betald	Betaine aldehyde		C5H12NO	1	Mitochondria
bhb	(R)-3-Hydroxybutanoate	(R)-3-Hydroxybutanoic acid, (R)-3-Hydroxybutyric acid, 3-hydroxybutyrate	C4H7O3	-1	Cytosol
bhb	(R)-3-Hydroxybutanoate	(R)-3-Hydroxybutanoic acid, (R)-3-Hydroxybutyric acid, 3-hydroxybutyrate	C4H7O3	-1	Extracellular
bhb	(R)-3-Hydroxybutanoate	(R)-3-Hydroxybutanoic acid, (R)-3-Hydroxybutyric acid, 3-hydroxybutyrate	C4H7O3	-1	Mitochondria
bilgclcur	Bilirubin beta-digluconide	Bilirubin bis-gluconoside	C45H50N4O18	-2	Cytosol
bilgclcur	Bilirubin beta-digluconide	Bilirubin bis-gluconoside	C45H50N4O18	-2	Extracellular
bilgclcur	Bilirubin beta-digluconide	Bilirubin bis-gluconoside	C45H50N4O18	-2	Endoplasmic Reticulum
bilglcur	Bilirubin monogluconide	Bilirubin-gluconoside	C39H44N4O12	0	Cytosol
bilglcur	Bilirubin monogluconide	Bilirubin-gluconoside	C39H44N4O12	0	Extracellular
bilglcur	Bilirubin monogluconide	Bilirubin-gluconoside	C39H44N4O12	0	Endoplasmic Reticulum
bilirub	Bilirubin		C33H34N4O6	-2	Cytosol
bilirub	Bilirubin		C33H34N4O6	-2	Extracellular
bilirub	Bilirubin		C33H34N4O6	-2	Endoplasmic Reticulum
biliverd	Biliverdin		C33H32N4O6	-2	Cytosol
biocyt	Biocytin	N6-D-Biotinyl-L-lysine, epsilon-N-Biotinyl-L-lysine	C16H28N4O4S	0	Cytosol
biocyt	Biocytin	N6-D-Biotinyl-L-lysine, epsilon-N-Biotinyl-L-lysine	C16H28N4O4S	0	Extracellular
biocyt	Biocytin	N6-D-Biotinyl-L-lysine, epsilon-N-Biotinyl-L-lysine	C16H28N4O4S	0	Mitochondria
biocyt	Biocytin	N6-D-Biotinyl-L-lysine, epsilon-N-Biotinyl-L-lysine	C16H28N4O4S	0	Nucleus
btamp	Biotinyl-5'-AMP		C20H27N7O9PS	-1	Cytosol
btamp	Biotinyl-5'-AMP		C20H27N7O9PS	-1	Mitochondria
btcoa	Butanoyl-CoA	Butyryl-CoA	C25H38N7O17P3S	-4	Mitochondria
btn	Biotin	Coenzyme R, D-Biotin, Vitamin B7, Vitamin H	C10H15N2O3S	-1	Cytosol
btn	Biotin	Coenzyme R, D-Biotin, Vitamin B7, Vitamin H	C10H15N2O3S	-1	Extracellular
btn	Biotin	Coenzyme R, D-Biotin, Vitamin B7, Vitamin H	C10H15N2O3S	-1	Mitochondria
btn	Biotin	Coenzyme R, D-Biotin, Vitamin B7, Vitamin H	C10H15N2O3S	-1	Nucleus
but	Butyrate (n-C4:0)	Butanoate, Butanoic acid, Butyric acid	C4H7O2	-1	Cytosol
but	Butyrate (n-C4:0)	Butanoate, Butanoic acid, Butyric acid	C4H7O2	-1	Extracellular
but	Butyrate (n-C4:0)	Butanoate, Butanoic acid, Butyric acid	C4H7O2	-1	Mitochondria
bvite	beta-tocopherol	148-03-8, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)-, (2R)-rel-, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-, 3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-ol, CHEMID000148038, EINECS 205-708-5	C28H48O2	0	Cytosol
bvite	beta-tocopherol	148-03-8, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)-, (2R)-rel-, 2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-, 3,4-Dihydro-2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-ol, CHEMID000148038, EINECS 205-708-5	C28H48O2	0	Extracellular
bz	Benzoate	Benzenecarboxylic acid, Benzoic acid, Dracylic acid, Phenylformic acid	C7H5O2	-1	Cytosol
bz	Benzoate	Benzenecarboxylic acid, Benzoic acid, Dracylic acid, Phenylformic acid	C7H5O2	-1	Extracellular
bz	Benzoate	Benzenecarboxylic acid, Benzoic acid, Dracylic acid, Phenylformic acid	C7H5O2	-1	Endoplasmic Reticulum
c226coa	cervonyl coenzyme A	C226-CoA, Docosahexaenoic acid coenzyme a, cervonic acid coenzyme a, docosa-4,7,10,13,16,19-hexaenoic acid coenzyme a	C43H62N7O17P3S	-4	Cytosol
c226coa	cervonyl coenzyme A	C226-CoA, Docosahexaenoic acid coenzyme a, cervonic acid coenzyme a, docosa-4,7,10,13,16,19-hexaenoic acid coenzyme a	C43H62N7O17P3S	-4	Mitochondria
c226coa	cervonyl coenzyme A	C226-CoA, Docosahexaenoic acid coenzyme a, cervonic acid coenzyme a, docosa-4,7,10,13,16,19-hexaenoic acid coenzyme a	C43H62N7O17P3S	-4	Peroxisome
c226cm	cervonyl carnitine	cervonic acid carnitine	C29H45NO4	0	Cytosol
c226cm	cervonyl carnitine	cervonic acid carnitine	C29H45NO4	0	Mitochondria
c2m26dcoa	cis-2-Methyl-5-isopropylhexa-2,5-dienyl-CoA		C31H46N7O17P3S	-4	Mitochondria
c2m26dcoa	cis-2-Methyl-5-isopropylhexa-2,5-dienyl-CoA		C31H46N7O17P3S	-4	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ca2	Calcium	Ca ²⁺	Ca	2	Cytosol
ca2	Calcium	Ca ²⁺	Ca	2	Extracellular
cala	N-Carbamoyl-beta-alanine	3-Ureidopropionate, 3-Ureidopropionate, beta-Ureidopropionic acid	C4H7N2O3	-1	Cytosol
camp	cAMP	3',5'-Cyclic AMP, Adenosine 3[-5]-cyclic monophosphate, Cyclic adenylic acid	C10H11NSO6P	-1	Cytosol
camp	cAMP	3',5'-Cyclic AMP, Adenosine 3[-5]-cyclic monophosphate, Cyclic adenylic acid	C10H11NSO6P	-1	Extracellular
camp	cAMP	3',5'-Cyclic AMP, Adenosine 3[-5]-cyclic monophosphate, Cyclic adenylic acid	C10H11NSO6P	-1	Golgi Apparatus
carn	L-Carnosine	L-Carnosine, Nalpha-(beta-alanyl)-L-histidine	C9H14N4O3	0	Cytosol
caro	beta-Carotene		C40H56	0	Cytosol
caro	beta-Carotene		C40H56	0	Extracellular
carveol	(E)-carveol	(-)-trans-Carveol, (E)-carveol	C10H16O	0	Cytosol
carveol	(E)-carveol	(-)-trans-Carveol, (E)-carveol	C10H16O	0	Extracellular
chasp	N-Carbamoyl-L-aspartate		C5H6N2O5	-2	Cytosol
chl1	Cob(I)alamin	Chl, Vitamin B12s	C62H88CoN13O14P	-1	Mitochondria
chl2	Cob(II)alamin	Vitamin B12r	C62H92CoN13O14P	0	Cytosol
chl2	Cob(II)alamin	Vitamin B12r	C62H92CoN13O14P	0	Mitochondria
chp	Carbamoyl phosphate		CH2NO5P	-2	Cytosol
chp	Carbamoyl phosphate		CH2NO5P	-2	Mitochondria
chp	Carbamoyl phosphate		CH2NO5P	-2	Endoplasmic Reticulum
cca_d3	Calcitric acid (D3)	1alpha(OH)-23-carboxy-24,25,26,27-tetranor-D3	C22H33O4	-1	Cytosol
cca_d3	Calcitric acid (D3)	1alpha(OH)-23-carboxy-24,25,26,27-tetranor-D3	C22H33O4	-1	Extracellular
cca_d3	Calcitric acid (D3)	1alpha(OH)-23-carboxy-24,25,26,27-tetranor-D3	C22H33O4	-1	Mitochondria
cdp	CDP	Cytidine 5'-diphosphate, Cytidine diphosphate	C9H12N3O11P2	3	Cytosol
cdp	CDP	Cytidine 5'-diphosphate, Cytidine diphosphate	C9H12N3O11P2	-3	Mitochondria
cdp	CDP	Cytidine 5'-diphosphate, Cytidine diphosphate	C9H12N3O11P2	-3	Nucleus
cdpchol	CDPcholine	Cytidine 5'-diphosphocholine	C14H25N4O11P2	-1	Cytosol
edpdag_hs	CDP diacylglycerol (homo sapiens)	CDP-diacylglycerol	C12H17N3O11P2FULLRCO2FU LLR2CO2	-2	Cytosol
edpdag_hs	CDP diacylglycerol (homo sapiens)	CDP-diacylglycerol	C12H17N3O11P2FULLRCO2FU LLR2CO2	-2	Mitochondria
cdpea	CDPethanolamine		C11H19N4O11P2	-1	Cytosol
egly	Cys-Gly	L-Cysteinylglycine	C5H10N2O3S	0	Cytosol
egly	Cys-Gly	L-Cysteinylglycine	C5H10N2O3S	0	Extracellular
chito2pdol_L	N,N'-Diacylchitobiosyldiphosphodolichol, human liver homolog	Chitobiosyldiphosphodolichol	C1240H2028N20O170P20	-20	Cytosol
chito2pdol_U	N,N'-Diacylchitobiosyldiphosphodolichol, human uterine homolog	Chitobiosyldiphosphodolichol	C1185H1940N20O170P20	-20	Cytosol
chlstol	Cholesta-7,24-dien-3beta-ol	Cholesta-7,24-dien-3beta-ol	C27H44O	0	Endoplasmic Reticulum
chol	Choline	Bilineurine	C5H14NO	1	Cytosol
chol	Choline	Bilineurine	C5H14NO	1	Extracellular
chol	Choline	Bilineurine	C5H14NO	1	Golgi Apparatus
chol	Choline	Bilineurine	C5H14NO	1	Mitochondria
chol	Choline	Bilineurine	C5H14NO	1	Nucleus
chol	Choline	Bilineurine	C5H14NO	1	Endoplasmic Reticulum
cholate	Cholate	12alpha-Trihydroxy-5beta-cholanate, 12alpha-Trihydroxy-5beta-cholamic acid, 3alpha, 7alpha, Chololic acid, bile acid	C24H39O5	-1	Cytosol
cholate	Cholate	12alpha-Trihydroxy-5beta-cholanate, 12alpha-Trihydroxy-5beta-cholamic acid, 3alpha, 7alpha, Chololic acid, bile acid	C24H39O5	-1	Extracellular
cholcoa	Choloyl-CoA	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholant-24-one-CoA, Choloyl-CoA	C45H70N7O20P3S	-4	Peroxisome
cholcoads	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA	25(S)-3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholest-24-enoyl-CoA, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA	C48H74N7O20P3S	-4	Peroxisome
cholcoaone	3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholest-24-one-CoA, 3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA	C48H74N7O21P3S	-4	Peroxisome
cholcoar	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	25(R) 3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoyl-CoA, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	C48H76N7O20P3S	-4	Endoplasmic Reticulum
cholcoar	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	25(R) 3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoyl-CoA, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	C48H76N7O20P3S	-4	Peroxisome
cholcoas	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(S)	25(S)-3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoyl-coa	C48H76N7O20P3S	-4	Endoplasmic Reticulum
cholcoas	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(S)	25(S)-3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoyl-coa	C48H76N7O20P3S	-4	Peroxisome
cholp	Choline phosphate	O-Phosphocholine, Phosphocholine, Phosphorylcholine	C5H13NO4P	-1	Cytosol
cholp	Choline phosphate	O-Phosphocholine, Phosphocholine, Phosphorylcholine	C5H13NO4P	-1	Golgi Apparatus
cholp	Choline phosphate	O-Phosphocholine, Phosphocholine, Phosphorylcholine	C5H13NO4P	-1	Lysosome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Cytosol
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Extracellular
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Golgi Apparatus
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Lysosome
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Mitochondria
chsterol	Cholesterol	Cholest-5-en-3beta-ol	C27H46O	0	Endoplasmic Reticulum
chsterols	cholesterol sulfate		C27H45O4S	-1	Cytosol
chsterols	cholesterol sulfate		C27H45O4S	-1	Endoplasmic Reticulum
chtn	chitin	beta-1,4-poly-N-acetyl-D-glucosamine	C24H41N3O16	0	Cytosol
chtn	chitin	beta-1,4-poly-N-acetyl-D-glucosamine	C24H41N3O16	0	Extracellular
cit	Citrate	2, 2-Hydroxy-1, 2-Hydroxytricarballic acid, 3-propanetricarboxylic acid, Citric acid	C6H5O7	-3	Cytosol
cit	Citrate	2, 2-Hydroxy-1, 2-Hydroxytricarballic acid, 3-propanetricarboxylic acid, Citric acid	C6H5O7	-3	Extracellular
cit	Citrate	2, 2-Hydroxy-1, 2-Hydroxytricarballic acid, 3-propanetricarboxylic acid, Citric acid	C6H5O7	-3	Mitochondria
citmcoa-L	L-Citramalyl-CoA	(3S)-Citramalyl-CoA	C26H37N7O20P3S	-5	Mitochondria
citrl-L	L-Citrulline	2-Amino-5-ureidovaleric acid, Citrulline, N5-(aminocarbonyl)-L-Ornithine	C6H13N3O3	0	Cytosol
citrl-L	L-Citrulline	2-Amino-5-ureidovaleric acid, Citrulline, N5-(aminocarbonyl)-L-Ornithine	C6H13N3O3	0	Mitochondria
cl	Chloride	Cl-	Cl	-1	Cytosol
cl	Chloride	Cl-	Cl	-1	Extracellular
clpn_hs	cardiolipin (homo sapiens)		C9H1609P2FULLR2CO2FULLR2CO2	-2	Cytosol
clpnd	clupanodonic acid	docosa-7,10,13,16,19-pentaenoic acid, docosapentaenoic acid (n-3)	C22H33O2	-1	Cytosol
clpnd	clupanodonic acid	docosa-7,10,13,16,19-pentaenoic acid, docosapentaenoic acid (n-3)	C22H33O2	-1	Extracellular
clpndcoa	clupanodonyl CoA	clupanodonyl Coenzyme A, docosa-7,10,13,16,19-pentaenoyl coenzyme A	C43H64N7O17P3S	4	Cytosol
clpndcoa	clupanodonyl CoA	clupanodonyl Coenzyme A, docosa-7,10,13,16,19-pentaenoyl coenzyme A	C43H64N7O17P3S	4	Mitochondria
clpndcoa	clupanodonyl CoA	clupanodonyl Coenzyme A, docosa-7,10,13,16,19-pentaenoyl coenzyme A	C43H64N7O17P3S	4	Peroxisome
clpndcrn	clupanodonyl carnitine		C29H47NO4	0	Cytosol
clpndcrn	clupanodonyl carnitine		C29H47NO4	0	Mitochondria
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Cytosol
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Extracellular
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Golgi Apparatus
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Lysosome
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Mitochondria
cmp	CMP	3'-Cytidylic Acid, Cytidine-2'(3')-monophosphoric acid, Cytidine-2[(3)]-monophosphoric acid, Cytidine-5'-monophosphate, Cytidylic acid	C9H12N3O8P	-2	Nucleus
cmp2amep	CMP-2-aminoethylphosphonate	CMPciliatine	C11H19N4O10P2	-1	Cytosol
cmpacna	CMP-N-acetylneuraminate	CMP-Neu5Ac	C20H29N4O16P	-2	Cytosol
cmpacna	CMP-N-acetylneuraminate	CMP-Neu5Ac	C20H29N4O16P	-2	Golgi Apparatus
cmpacna	CMP-N-acetylneuraminate	CMP-Neu5Ac	C20H29N4O16P	-2	Nucleus
cmpntm2amep	CMP-N-trimethyl-2-aminoethylphosphonate	CMP-2-trimethylaminoethylphosphonate	C14H25N4O10P2	-1	Cytosol
cmusa	2-Amino-3-carboxymuconate semialdehyde		C7H6NO5	-1	Cytosol
co	Carbon monoxide		CO	0	Cytosol
co	Carbon monoxide		CO	0	Extracellular
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Cytosol
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Extracellular
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Golgi Apparatus
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Mitochondria
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Nucleus
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Endoplasmic Reticulum
co2	CO2	Carbon dioxide, Carbonic anhydride	CO2	0	Peroxisome
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Cytosol
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Golgi Apparatus
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Lysosome
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Mitochondria
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Nucleus
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Endoplasmic Reticulum
coa	Coenzyme A	CoA, CoA-SH, CoASH	C21H32N7O16P3S	-4	Peroxisome
coke	cocaine	beta-Cocain, 1-Cocain	C17H21NO4	0	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
core2	Core 2	beta-D-Galactosyl-1,3-(N-acetyl-beta-D-glucosaminy-1,6)-N-acetyl-D-galactosaminy-R	C22H37N2O15X	0	Golgi Apparatus
core3	Core 3	N-Acetyl-beta-D-glucosaminy-1,3-N-acetyl-D-galactosaminy-R	C16H27N2O10X	0	Golgi Apparatus
core4	Core 4	N-Acetyl-beta-D-glucosaminy-1,6-(N-acetyl-beta-glucosaminy-1,3)-N-acetyl-D-galactosaminy-R	C24H40N3O15X	0	Golgi Apparatus
core5	Core 5		C16H27N2O10X	0	Golgi Apparatus
core6	Core 6		C16H27N2O10X	0	Golgi Apparatus
core6	Core 6		C16H27N2O10X	0	Lysosome
core7	Core 7		C16H27N2O10X	0	Golgi Apparatus
core8	Core 8		C14H24NO10X	0	Golgi Apparatus
cortsn	Cortisone	11, 17alpha, 20-trione, 21-Dihydroxy-4-pregnene-3, Kendall's compound E, Reichstein's substance F	C21H28O5	0	Endoplasmic Reticulum
coucoa	p-coumaroyl-CoA	4-Coumaroyl-CoA, 4-Hydroxycinnamoyl-CoA	C30H38N7O18P3S1	-4	Mitochondria
coumarin	coumarin	1,2-Benzopyrone, 2-Propenoic acid, 3-(2-hydroxyphenyl)-, d-lactone, 2H-1-Benzopyran-2-one, 5,6-Benzo-2-pyrone, Benzo-a-pyrone, Coumarine, Coumarinic anhydride, Coumarin, Rattex, Tonka bean camphor, cis-o-Coumarinic acid lactone, o-Hydroxycinnamic acid lactone	C9H6O2	0	Cytosol
coumarin	coumarin	1,2-Benzopyrone, 2-Propenoic acid, 3-(2-hydroxyphenyl)-, d-lactone, 2H-1-Benzopyran-2-one, 5,6-Benzo-2-pyrone, Benzo-a-pyrone, Coumarine, Coumarinic anhydride, Coumarin, Rattex, Tonka bean camphor, cis-o-Coumarinic acid lactone, o-Hydroxycinnamic acid lactone	C9H6O2	0	Extracellular
cp3	Coproporphyrinogen III		C36H40N4O8	-4	Cytosol
creat	Creatine	Methylglycocyanine, alpha-Methylguanidino acetic acid	C4H9N3O2	0	Cytosol
creat	Creatine	Methylglycocyanine, alpha-Methylguanidino acetic acid	C4H9N3O2	0	Extracellular
creat	Creatine	Methylglycocyanine, alpha-Methylguanidino acetic acid	C4H9N3O2	0	Mitochondria
crm_hs	ceramide (homo sapiens)	Ceramide, N-Acylsphingosine	C18H36NO2FULLRCO	0	Cytosol
crm_hs	ceramide (homo sapiens)	Ceramide, N-Acylsphingosine	C18H36NO2FULLRCO	0	Golgi Apparatus
crm_hs	ceramide (homo sapiens)	Ceramide, N-Acylsphingosine	C18H36NO2FULLRCO	0	Lysosome
crm_hs	ceramide (homo sapiens)	Ceramide, N-Acylsphingosine	C18H36NO2FULLRCO	0	Endoplasmic Reticulum
crmp_hs	Ceramide 1-phosphate	Ceramide 1-phosphate, Ceramide phosphate	C18H35NO5PFULLRCO	-2	Cytosol
crmp_hs	Ceramide 1-phosphate	Ceramide 1-phosphate, Ceramide phosphate	C18H35NO5PFULLRCO	-2	Extracellular
cm	L-Carnitine	(S)-Carnitine, 3-Carboxy-2-hydroxy-N, L-gamma-Trimethyl-beta-hydroxybutyrobetaine, N-trimethyl-1-propanaminium, Vitamin BT	C7H15NO3	0	Cytosol
cm	L-Carnitine	(S)-Carnitine, 3-Carboxy-2-hydroxy-N, L-gamma-Trimethyl-beta-hydroxybutyrobetaine, N-trimethyl-1-propanaminium, Vitamin BT	C7H15NO3	0	Extracellular
cm	L-Carnitine	(S)-Carnitine, 3-Carboxy-2-hydroxy-N, L-gamma-Trimethyl-beta-hydroxybutyrobetaine, N-trimethyl-1-propanaminium, Vitamin BT	C7H15NO3	0	Mitochondria
cm	L-Carnitine	(S)-Carnitine, 3-Carboxy-2-hydroxy-N, L-gamma-Trimethyl-beta-hydroxybutyrobetaine, N-trimethyl-1-propanaminium, Vitamin BT	C7H15NO3	0	Endoplasmic Reticulum
cm	L-Carnitine	(S)-Carnitine, 3-Carboxy-2-hydroxy-N, L-gamma-Trimethyl-beta-hydroxybutyrobetaine, N-trimethyl-1-propanaminium, Vitamin BT	C7H15NO3	0	Peroxisome
crn	Creatinine	1-Methylglycocyanidine	C4H7N3O	0	Cytosol
crtsl	Cortisol	11beta, 17alpha, 20-dione, 21-Trihydroxy-4-pregnene-3, Hydrocortisone, Kendall's compound H, Reichstein's substance M	C21H30O5	0	Cytosol
crtsl	Cortisol	11beta, 17alpha, 20-dione, 21-Trihydroxy-4-pregnene-3, Hydrocortisone, Kendall's compound H, Reichstein's substance M	C21H30O5	0	Mitochondria
crtsl	Cortisol	11beta, 17alpha, 20-dione, 21-Trihydroxy-4-pregnene-3, Hydrocortisone, Kendall's compound H, Reichstein's substance M	C21H30O5	0	Endoplasmic Reticulum
crtrsn	Corticosterone	11beta, 21-Dihydroxy-4-pregnene-3,20-dione, Kendall's compound B, Reichstein's substance H	C21H30O4	0	Cytosol
crtrsn	Corticosterone	11beta, 21-Dihydroxy-4-pregnene-3,20-dione, Kendall's compound B, Reichstein's substance H	C21H30O4	0	Mitochondria
crtrsn	Corticosterone	11beta, 21-Dihydroxy-4-pregnene-3,20-dione, Kendall's compound B, Reichstein's substance H	C21H30O4	0	Endoplasmic Reticulum
crvnc	cervonic acid, C22:6 n-3	DHE, Docosahexaenoic acid, docosa-4,7,10,13,16,19-hexaenoic acid	C22H31O2	-1	Cytosol
crvnc	cervonic acid, C22:6 n-3	DHE, Docosahexaenoic acid, docosa-4,7,10,13,16,19-hexaenoic acid	C22H31O2	-1	Extracellular

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
cs_hs_linkage	chondroitin sulfate/heparan sulfate linkage region (GlcA-(Gal)2-Xyl-L-Ser (protein))		C23H36O20X	-1	Golgi Apparatus
cs_a	chondroitin sulfate A (GalNAc4S-GlcA), free chain	(GalNAc4S-GlcA)2-Gal4S-Gal-Xyl	C45H67N2O46S3	5	Lysosome
cs_a,b,e_pre1	chondroitin sulfate A (GalNAc4S-GlcA), B (IdoA2S-GalNAc4S), and E (GalNAc4,6diS-GlcA), precursor 1	GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser (protein)	C31H47NO31S2X	-3	Golgi Apparatus
cs_a,b_pre2	chondroitin sulfate A (GalNAc4S-GlcA) and B (IdoA2S-GalNAc4S), precursor 2	GlcA-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C37H54NO37S2X	-4	Golgi Apparatus
cs_a,b_pre3	chondroitin sulfate A (GalNAc4S-GlcA) and B (IdoA2S-GalNAc4S), precursor 3	GalNAc-GlcA-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C45H67N2O42S2X	-4	Golgi Apparatus
cs_a_deg1	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 1	GalNAc-GlcA-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C45H68N2O43S2	-4	Lysosome
cs_a_deg2	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 2	GlcA-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C37H55NO38S2	-4	Lysosome
cs_a_deg3	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 3	GalNAc4S-GlcA-Gal4S-Gal-Xyl	C31H48NO32S2	-3	Lysosome
cs_a_deg4	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 4	GalNAc-GlcA-Gal4S-Gal-Xyl	C31H49NO29S	-2	Lysosome
cs_a_deg5	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 5	GlcA-Gal4S-Gal-Xyl	C23H36O24S	-2	Lysosome
cs_b	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), free chain	GalNAc4S-IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C45H66N2O49S4	-6	Lysosome
cs_b_deg1	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 1	GalNAc-IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C45H67N2O46S3	-5	Lysosome
cs_b_deg2	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 2	IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C37H54NO41S3	-5	Lysosome
cs_b_deg3	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 3	IdoA-GalNAc4S-GlcA-Gal4S-Gal-Xyl	C37H55NO38S2	-4	Lysosome
cs_b_pre4	chondroitin sulfate B (IdoA2S-GalNAc4S), precursor 4	GalNAc-IdoA-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C45H67N2O42S2X	4	Golgi Apparatus
cs_b_pre5	chondroitin sulfate B (IdoA2S-GalNAc4S), precursor 5		C45H66N2O45S3X	-5	Golgi Apparatus
cs_c	chondroitin sulfate C (GalNAc6S-GlcA), free chain	(GalNAc6S-GlcA)2-Gal6S-Gal-Xyl	C45H67N2O46S3	5	Lysosome
cs_c,d,e_pre1	chondroitin sulfate C (GalNAc6S-GlcA) and D (GlcNAc6S-GlcA2S), precursor 1	GalNAc6S-GlcA-Gal6S-Gal-Xyl-L-Ser (protein)	C31H47NO31S2X	-3	Golgi Apparatus
cs_c_deg1	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 1	GalNAc-GlcA-GalNAc6S-GlcA-Gal6S-Gal-Xyl	C45H68N2O43S2	-4	Lysosome
cs_c_deg2	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 2	GlcA-GalNAc6S-GlcA-Gal6S-Gal-Xyl	C37H55NO38S2	-4	Lysosome
cs_c_deg3	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 3	GalNAc6S-GlcA-Gal6S-Gal-Xyl	C31H48NO32S2	-3	Lysosome
cs_c_deg4	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 4	GalNAc-GlcA-Gal6S-Gal-Xyl	C31H49NO29S	-2	Lysosome
cs_c_deg5	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 5	GlcA-Gal6S-Gal-Xyl	C23H36O24S	-2	Lysosome
cs_c_pre2	chondroitin sulfate C (GalNAc6S-GlcA), precursor 2	GlcA-GalNAc6S-GlcA-Gal6S-Gal-Xyl-L-Ser (protein)	C37H54NO37S2X	4	Golgi Apparatus
cs_c_pre3	chondroitin sulfate C (GalNAc6S-GlcA), precursor 3	GalNAc-GlcA-GalNAc6S-GlcA-Gal6S-Gal-Xyl-L-Ser (protein)	C45H67N2O42S2X	4	Golgi Apparatus
cs_d	chondroitin sulfate D (GlcNAc6S-GlcA2S), free chain	(GalNAc6S-GlcA2S)2-Gal6S-Gal-Xyl	C45H65N2O52S5	-7	Lysosome
cs_d_deg1	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 1	GalNAc-GlcA2S-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl	C45H66N2O49S4	-6	Lysosome
cs_d_deg2	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 2	GlcA2S-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl	C37H53NO44S4	-6	Lysosome
cs_d_deg3	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 3	GlcA-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl	C37H54NO41S3	-5	Lysosome
cs_d_deg4	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 4	GalNAc6S-GlcA2S-Gal6S-Gal-Xyl	C31H47NO35S3	-4	Lysosome
cs_d_deg5	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 5	GalNAc-GlcA2S-Gal6S-Gal-Xyl	C31H48NO32S2	-3	Lysosome
cs_d_deg6	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 6	GlcA2S-Gal6S-Gal-Xyl	C23H35O27S2	-3	Lysosome
cs_d_pre2	chondroitin sulfate D (GlcNAc6S-GlcA2S) precursor 2	GalNAc6S-GlcA2S-Gal6S-Gal-Xyl-L-Ser (protein)	C31H46NO34S3X	-4	Golgi Apparatus
cs_d_pre3	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 3	GlcA-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl-L-Ser (protein)	C37H53NO40S3X	-5	Golgi Apparatus
cs_d_pre4	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 4	GalNAc-GlcA-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Golgi Apparatus
cs_d_pre5	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 5	GalNAc6S-GlcA-GalNAc6S-GlcA2S-Gal6S-Gal-Xyl-L-Ser (protein)	C45H65N2O48S4X	-6	Golgi Apparatus
cs_e	chondroitin sulfate E (GalNAc4,6diS-GlcA), free chain	(GalNAc4,6diS-GlcA)2-Gal4,6diS-Gal-Xyl	C45H64N2O55S6	-8	Lysosome
cs_e_deg1	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 1	GalNAc6S-GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl	C45H65N2O52S5	-7	Lysosome
cs_e_deg2	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 2	GalNAc-GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl	C45H66N2O49S4	-6	Lysosome
cs_e_deg3	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 3	GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl	C37H53NO44S4	-6	Lysosome
cs_e_deg4	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 4	GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl	C31H46NO38S4	-5	Lysosome
cs_e_deg5	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 5	GalNAc6S-GlcA-Gal4,6diS-Gal-Xyl	C31H47NO35S3	-4	Lysosome
cs_e_deg6	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 6	GalNAc-GlcA-Gal4,6diS-Gal-Xyl	C31H48NO32S2	-3	Lysosome
cs_e_deg7	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 7	GlcA-Gal4,6diS-Gal-Xyl	C23H35O27S2	-3	Lysosome
cs_e_pre2	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 2	GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C31H45NO37S4X	-5	Golgi Apparatus
cs_e_pre3	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 3	GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C37H52NO43S4X	-6	Golgi Apparatus
cs_e_pre4	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 4	GalNAc-GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H65N2O48S4X	-6	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
es_e_pre5a	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5a	GalNAc4S-GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H64N2O51S5X	-7	Golgi Apparatus
es_e_pre5b	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5b	GalNAc6S-GlcA-GalNAc4,6diS-GlcA-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H64N2O51S5X	-7	Golgi Apparatus
es_pre	chondroitin sulfate precursor (GalNAc-GlcA-(Gal)2-Xyl-L-Ser (protein))	GalNAc-GlcA-(Gal)2-Xyl-L-Ser (protein)	C31H49NO25X	-1	Golgi Apparatus
esn	Cytosine		C4H5N3O	0	Cytosol
esn	Cytosine		C4H5N3O	0	Extracellular
espg_a	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	(GalNAc4S-GlcA)2-Gal4S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Extracellular
espg_a	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	(GalNAc4S-GlcA)2-Gal4S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Golgi Apparatus
espg_a	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	(GalNAc4S-GlcA)2-Gal4S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Lysosome
espg_b	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S-proteoglycan)	GalNAc4S-IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C45H65N2O48S4X	-6	Extracellular
espg_b	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S-proteoglycan)	GalNAc4S-IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C45H65N2O48S4X	-6	Golgi Apparatus
espg_b	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S-proteoglycan)	GalNAc4S-IdoA2S-GalNAc4S-GlcA-Gal4S-Gal-Xyl-L-Ser	C45H65N2O48S4X	-6	Lysosome
espg_c	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	(GalNAc6S-GlcA)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Extracellular
espg_c	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	(GalNAc6S-GlcA)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Golgi Apparatus
espg_c	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	(GalNAc6S-GlcA)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H66N2O45S3X	-5	Lysosome
espg_d	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	(GalNAc6S-GlcA2S)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H64N2O51S5X	-7	Extracellular
espg_d	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	(GalNAc6S-GlcA2S)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H64N2O51S5X	-7	Golgi Apparatus
espg_d	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	(GalNAc6S-GlcA2S)2-Gal6S-Gal-Xyl-L-Ser (protein)	C45H64N2O51S5X	-7	Lysosome
espg_e	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	(GalNAc4,6diS-GlcA)2-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H63N2O54S6X	-8	Extracellular
espg_e	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	(GalNAc4,6diS-GlcA)2-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H63N2O54S6X	-8	Golgi Apparatus
espg_e	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	(GalNAc4,6diS-GlcA)2-Gal4,6diS-Gal-Xyl-L-Ser (protein)	C45H63N2O54S6X	-8	Lysosome
etp	CTP	Cytidine 5'-triphosphate, Cytidine triphosphate	C9H12N3O14P3	-4	Cytosol
etp	CTP	Cytidine 5'-triphosphate, Cytidine triphosphate	C9H12N3O14P3	-4	Mitochondria
etp	CTP	Cytidine 5'-triphosphate, Cytidine triphosphate	C9H12N3O14P3	-4	Nucleus
eyan	Hydrogen cyanide	CN-, Cyano	CHN	0	Cytosol
eyan	Hydrogen cyanide	CN-, Cyano	CHN	0	Extracellular
eyan	Hydrogen cyanide	CN-, Cyano	CHN	0	Mitochondria
eysam	Cysteamine		C2H8NS	1	Cytosol
eys-L	L-Cysteine	Cys, L-2-Amino-3-mercaptopropionic acid	C3H7NO2S	0	Cytosol
eys-L	L-Cysteine	Cys, L-2-Amino-3-mercaptopropionic acid	C3H7NO2S	0	Extracellular
eys-L	L-Cysteine	Cys, L-2-Amino-3-mercaptopropionic acid	C3H7NO2S	0	Mitochondria
cyst-L	L-Cystathionine		C7H14N2O4S	0	Cytosol
eytd	Cytidine	1-beta-ribofuranosyl-4-amino-1-beta-D-ribofuranosyl-2(1H)-pyrimidinone, cytosine riboside	C9H13N3O5	0	Cytosol
eytd	Cytidine	1-beta-ribofuranosyl-4-amino-1-beta-D-ribofuranosyl-2(1H)-pyrimidinone, cytosine riboside	C9H13N3O5	0	Extracellular
eytd	Cytidine	1-beta-ribofuranosyl-4-amino-1-beta-D-ribofuranosyl-2(1H)-pyrimidinone, cytosine riboside	C9H13N3O5	0	Lysosome
eytd	Cytidine	1-beta-ribofuranosyl-4-amino-1-beta-D-ribofuranosyl-2(1H)-pyrimidinone, cytosine riboside	C9H13N3O5	0	Mitochondria
eytd	Cytidine	1-beta-ribofuranosyl-4-amino-1-beta-D-ribofuranosyl-2(1H)-pyrimidinone, cytosine riboside	C9H13N3O5	0	Nucleus
dad-2	Deoxyadenosine	2'-Deoxyadenosine, dA	C10H13NSO3	0	Cytosol
dad-2	Deoxyadenosine	2'-Deoxyadenosine, dA	C10H13NSO3	0	Extracellular
dad-2	Deoxyadenosine	2'-Deoxyadenosine, dA	C10H13NSO3	0	Lysosome
dad-5	5'-Deoxyadenosine		C10H13NSO3	0	Extracellular
dadp	dADP	2'-Deoxyadenosine 5'-diphosphate	C10H12NSO9P2	-3	Cytosol
dadp	dADP	2'-Deoxyadenosine 5'-diphosphate	C10H12NSO9P2	-3	Mitochondria
dadp	dADP	2'-Deoxyadenosine 5'-diphosphate	C10H12NSO9P2	-3	Nucleus
dag_hs	diacylglycerol (homo sapiens)		C3H60FULLRCO2FULLR2CO2	0	Cytosol
dag_hs	diacylglycerol (homo sapiens)		C3H60FULLRCO2FULLR2CO2	0	Extracellular
dag_hs	diacylglycerol (homo sapiens)		C3H60FULLRCO2FULLR2CO2	0	Nucleus
dag_hs	diacylglycerol (homo sapiens)		C3H60FULLRCO2FULLR2CO2	0	Endoplasmic Reticulum
dak2gpe_hs	1-alkenyl 2-acylglycerol 3-phosphoethanolamine plasmalogen (homo sapiens)	plasmalogen	C7H14O5NPFULLRFULLR2CO	0	Cytosol
damp	dAMP	2'-Deoxyadenosine 5'-monophosphate, 2'-Deoxyadenosine 5'-phosphate, Deoxyadenosine monophosphate, Deoxyadenylic acid	C10H12NSO6P	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
damp	dAMP	2'-Deoxyadenosine 5'-monophosphate, 2'-Deoxyadenosine 5'-phosphate, Deoxyadenosine monophosphate, Deoxyadenylic acid	C10H12NSO6P	-2	Lysosome
datp	dATP	2'-Deoxyadenosine 5'-triphosphate, Deoxyadenosin 5'-triphosphate, Deoxyadenosine triphosphate	C10H12NSO12P3	-4	Cytosol
datp	dATP	2'-Deoxyadenosine 5'-triphosphate, Deoxyadenosin 5'-triphosphate, Deoxyadenosine triphosphate	C10H12NSO12P3	-4	Mitochondria
datp	dATP	2'-Deoxyadenosine 5'-triphosphate, Deoxyadenosin 5'-triphosphate, Deoxyadenosine triphosphate	C10H12NSO12P3	-4	Nucleus
dcacoa	Decanoyl-CoA (n-C10:0CoA)		C31H50N7O17P3S	-4	Cytosol
dcacoa	Decanoyl-CoA (n-C10:0CoA)		C31H50N7O17P3S	-4	Peroxisome
dcamp	N6-(1,2-Dicarboxyethyl)-AMP	Adenylosuccinate, Adenylosuccinic acid	C14H14NSO11P	-4	Cytosol
dcdp	dCDP	2'-Deoxycytidine 5'-diphosphate, 2'-Deoxycytidine diphosphate	C9H12N3O10P2	-3	Cytosol
dcdp	dCDP	2'-Deoxycytidine 5'-diphosphate, 2'-Deoxycytidine diphosphate	C9H12N3O10P2	-3	Mitochondria
dcdp	dCDP	2'-Deoxycytidine 5'-diphosphate, 2'-Deoxycytidine diphosphate	C9H12N3O10P2	-3	Nucleus
dcholcoa	chenodeoxycholyol coenzyme a	Chenodeoxycholyol-CoA, bile acid	C45H70N7O19P3S	-4	Peroxisome
dcmp	dCMP	2'-Deoxycytidine 5'-monophosphate, Deoxycytidine monophosphate, Deoxycydidylate, Deoxycydidylic acid	C9H12N3O7P	-2	Cytosol
dcmp	dCMP	2'-Deoxycytidine 5'-monophosphate, Deoxycytidine monophosphate, Deoxycydidylate, Deoxycydidylic acid	C9H12N3O7P	-2	Lysosome
dcmp	dCMP	2'-Deoxycytidine 5'-monophosphate, Deoxycytidine monophosphate, Deoxycydidylate, Deoxycydidylic acid	C9H12N3O7P	-2	Mitochondria
dcmp	dCMP	2'-Deoxycytidine 5'-monophosphate, Deoxycytidine monophosphate, Deoxycydidylate, Deoxycydidylic acid	C9H12N3O7P	-2	Nucleus
dcspn1	docosa-4,7,10,13,16-pentaenoic acid (n-6)	(All-Z)-4,7,10,13,16-docosapentaenoic acid, 4,7,10,13,16-Docosapentaenoic acid, (all-Z)-, 4,7,10,13,16-Docosapentaenoic acid, (all-Z)-, docosa-4,7,10,13,16-pentaenoic acid	C22H33O2	-1	Cytosol
dcspn1	docosa-4,7,10,13,16-pentaenoic acid (n-6)	(All-Z)-4,7,10,13,16-docosapentaenoic acid, 4,7,10,13,16-Docosapentaenoic acid, (all-Z)-, 4,7,10,13,16-Docosapentaenoic acid, (all-Z)-, docosa-4,7,10,13,16-pentaenoic acid	C22H33O2	-1	Extracellular
dcspn1coa	docosa-4,7,10,13,16-pentaenoyl coenzyme A		C43H64N7O17P3S	-4	Cytosol
dcspn1coa	docosa-4,7,10,13,16-pentaenoyl coenzyme A		C43H64N7O17P3S	-4	Mitochondria
dcspn1coa	docosa-4,7,10,13,16-pentaenoyl coenzyme A		C43H64N7O17P3S	-4	Peroxisome
dcspn1cm	docosa-4,7,10,13,16-pentaenoyl carnitine		C29H47NO4	0	Cytosol
dcspn1cm	docosa-4,7,10,13,16-pentaenoyl carnitine		C29H47NO4	0	Mitochondria
dctp	dCTP	2'-Deoxycytidine 5'-triphosphate, Deoxycytidine 5' triphosphate, Deoxycytidine triphosphate	C9H12N3O13P3	-4	Cytosol
dctp	dCTP	2'-Deoxycytidine 5'-triphosphate, Deoxycytidine 5' triphosphate, Deoxycytidine triphosphate	C9H12N3O13P3	-4	Mitochondria
dctp	dCTP	2'-Deoxycytidine 5'-triphosphate, Deoxycytidine 5' triphosphate, Deoxycytidine triphosphate	C9H12N3O13P3	-4	Nucleus
dcyt	Deoxycytidine	2'-Deoxycytidine, dC	C9H13N3O4	0	Cytosol
dcyt	Deoxycytidine	2'-Deoxycytidine, dC	C9H13N3O4	0	Extracellular
dcyt	Deoxycytidine	2'-Deoxycytidine, dC	C9H13N3O4	0	Lysosome
dcyt	Deoxycytidine	2'-Deoxycytidine, dC	C9H13N3O4	0	Mitochondria
dcyt	Deoxycytidine	2'-Deoxycytidine, dC	C9H13N3O4	0	Nucleus
dd2coa	trans-Dodec-2-enoyl-CoA	2-trans-Dodecenoyl-CoA	C33H52N7O17P3S	-4	Mitochondria
dd3coa	3-dodecenoyl CoA	3-cis-Dodecenoyl-CoA	C33H52N7O17P3S	-4	Mitochondria
ddca	Dodecanoate (n-C12:0)	Dodecanoic acid, Dodecylcarboxylate, Lauric acid	C12H23O2	-1	Cytosol
ddcaACP	Dodecanoyl-ACP (n-C12:0ACP)	Dodecanoyl-[acp], Dodecanoyl-[acyl-carrier protein], Fatty Acid C12 ACP, Lauroyl ACP	C23H43N2O8PRS	-1	Cytosol
ddcacoa	Dodecanoyl-CoA (n-C12:0CoA)	Lauroyl coenzyme A, Lauroyl-CoA	C33H54N7O17P3S	-4	Cytosol
ddcacoa	Dodecanoyl-CoA (n-C12:0CoA)	Lauroyl coenzyme A, Lauroyl-CoA	C33H54N7O17P3S	-4	Peroxisome
ddssterol	7-Dehydrodesmesterol	7-Dehydrodesmesterol	C27H42O	0	Endoplasmic Reticulum
debrisoquine	debrisoquine	2(1H)-Isoquinolinecarboximidamide, 3,4-dihydro-, 3,4-Dihydro-2(1H)-isoquinolinecarboximidine, 3,4-Dihydro-2(1H)-isoquinolinecarboximidamide, Debrisoquin [MeSH: Debrisoquin], Debrisoquine [MeSH: Debrisoquin], Isocaramidine	C10H14N3	1	Cytosol
debrisoquine	debrisoquine	2(1H)-Isoquinolinecarboximidamide, 3,4-dihydro-, 3,4-Dihydro-2(1H)-isoquinolinecarboximidine, 3,4-Dihydro-2(1H)-isoquinolinecarboximidamide, Debrisoquin [MeSH: Debrisoquin], Debrisoquine [MeSH: Debrisoquin], Isocaramidine	C10H14N3	1	Extracellular
decdp	all trans Decaprenyl diphosphate		C50H81O7P2	-3	Cytosol
decdp	all trans Decaprenyl diphosphate		C50H81O7P2	-3	Mitochondria
dedol_L	Dehydrodicolchol, human liver homolog		C1080H1748O10	0	Cytosol
dedol_U	Dehydrodicolchol, human uterine homolog		C1025H1660O10	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
dedoldp_L	Dehydrodicolchol diphosphate, human liver homolog	Dehydrodicolchyl diphosphate	C1080H1738O70P20	-30	Cytosol
dedoldp_U	Dehydrodicolchol diphosphate, human uterine homolog		C1025H1650O70P20	-30	Cytosol
dedolp_L	Dehydrodicolchol phosphate, human liver homolog		C1080H1738O40P10	-20	Cytosol
dedolp_U	Dehydrodicolchol phosphate, human uterine homolog		C1025H1650O40P10	-20	Cytosol
dem2emgacpail_prot_hs	deacylated-(phosphoethanolaminyldimannosyl)-(phosphoethanolaminyldimannosyl)-glucosaminyl-acylphosphatidylinositol	{[(Prot-PE-(Man)2],[PE])-Man-GlcN-PI	C37H70N3O34P3FULLR2CO2FU LLR2CO2X	0	Endoplasmic Reticulum
dgchol	Chenodeoxyglycocholate	Chenodeoxyglycocholate	C26H43NO5	0	Cytosol
dgchol	Chenodeoxyglycocholate	Chenodeoxyglycocholate	C26H43NO5	0	Extracellular
dgchol	Chenodeoxyglycocholate	Chenodeoxyglycocholate	C26H43NO5	0	Peroxisome
dgcholcoa	Chenodeoxyglycocholate-CoA	Chenodeoxyglycocholate-CoA	C45H70N7O19P3S	-4	Peroxisome
dgdp	dGDP	2'-Deoxyguanosine 5'-diphosphate	C10H12NSO10P2	-3	Cytosol
dgdp	dGDP	2'-Deoxyguanosine 5'-diphosphate	C10H12NSO10P2	-3	Mitochondria
dgdp	dGDP	2'-Deoxyguanosine 5'-diphosphate	C10H12NSO10P2	-3	Nucleus
dgmpp	dGMP	2'-Deoxyguanosine 5'-monophosphate, 2'-Deoxyguanosine 5'-phosphate, Deoxyguanosine monophosphate, Deoxyguanylic acid	C10H12NSO7P	-2	Cytosol
dgmpp	dGMP	2'-Deoxyguanosine 5'-monophosphate, 2'-Deoxyguanosine 5'-phosphate, Deoxyguanosine monophosphate, Deoxyguanylic acid	C10H12NSO7P	-2	Lysosome
dgmpp	dGMP	2'-Deoxyguanosine 5'-monophosphate, 2'-Deoxyguanosine 5'-phosphate, Deoxyguanosine monophosphate, Deoxyguanylic acid	C10H12NSO7P	-2	Mitochondria
dgpil_prot_hs	deacylated-glycophosphatidylinositol (GPI)-anchored protein	{[(Prot-PE-(Man),(PE)-Man],[PE])-Man-GlcN-PI	C39H76N4O37P4FULLR2CO2FU LLR2CO2X	0	Endoplasmic Reticulum
dgsn	Deoxyguanosine	2'-Deoxyguanosine, 2'-deoxyguanosine hemihydrate	C10H13NSO4	0	Cytosol
dgsn	Deoxyguanosine	2'-Deoxyguanosine, 2'-deoxyguanosine hemihydrate	C10H13NSO4	0	Extracellular
dgsn	Deoxyguanosine	2'-Deoxyguanosine, 2'-deoxyguanosine hemihydrate	C10H13NSO4	0	Lysosome
dgsn	Deoxyguanosine	2'-Deoxyguanosine, 2'-deoxyguanosine hemihydrate	C10H13NSO4	0	Mitochondria
dgtpp	dGTP	2'-Deoxyguanosine 5'-triphosphate, Deoxyguanosine 5'-triphosphate, Deoxyguanosine triphosphate	C10H12NSO13P3	-4	Cytosol
dgtpp	dGTP	2'-Deoxyguanosine 5'-triphosphate, Deoxyguanosine 5'-triphosphate, Deoxyguanosine triphosphate	C10H12NSO13P3	-4	Mitochondria
dgtpp	dGTP	2'-Deoxyguanosine 5'-triphosphate, Deoxyguanosine 5'-triphosphate, Deoxyguanosine triphosphate	C10H12NSO13P3	-4	Nucleus
dha	Dihydroxyacetone	1, 3-Dihydroxy-2-propanone, 3-Dihydroxyacetone, 3-Dihydroxypropan-2-one, Glycerone	C3H6O3	0	Cytosol
dhapp	Dihydroxyacetone phosphate	Glycerone phosphate	C3H5O6P	-2	Cytosol
dhapp	Dihydroxyacetone phosphate	Glycerone phosphate	C3H5O6P	-2	Peroxisome
dhbpt	6,7-Dihydrobiopterin	Dihydrobiopterin, Quinoid-dihydrobiopterin	C9H13NSO3	0	Cytosol
dhcholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate, 3alpha,7alpha-Dihydroxy-5beta-cholestanate	C27H45O4	-1	Mitochondria
dhcholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate, 3alpha,7alpha-Dihydroxy-5beta-cholestanate	C27H45O4	-1	Endoplasmic Reticulum
dhcholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate	3alpha,7alpha-Dihydroxy-5beta-cholestanate, 3alpha,7alpha-Dihydroxy-5beta-cholestanate	C27H45O4	-1	Peroxisome
dhcholestancoa	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	C48H76N7O19P3S	-4	Endoplasmic Reticulum
dhcholestancoa	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	C48H76N7O19P3S	-4	Peroxisome
dhcholoylcoa	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	C48H74N7O19P3S	-4	Endoplasmic Reticulum
dhcholoylcoa	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	C48H74N7O19P3S	-4	Peroxisome
dhcrrm_hs	dihydroceramide (homo sapiens)	N-Acylsphinganine	C18H38NO2FULLR2CO	0	Cytosol
dhdascb	Dehydroascorbate	DHA, Dehydroascorbic acid	C6H6O6	0	Cytosol
dhdascb	Dehydroascorbate	DHA, Dehydroascorbic acid	C6H6O6	0	Extracellular
dhea	Dehydroepiandrosterone	3beta-Hydroxyandrost-5-en-17-one, DHA, DHEA, Dehydroisoandrosterone	C19H28O2	0	Cytosol
dhea	Dehydroepiandrosterone	3beta-Hydroxyandrost-5-en-17-one, DHA, DHEA, Dehydroisoandrosterone	C19H28O2	0	Endoplasmic Reticulum
dheas	Dehydroepiandrosterone sulfate	3beta-Hydroxyandrost-5-en-17-one 3-sulfate, Dehydroepiandrosterone sulfate	C19H27O5S	-1	Cytosol
dheas	Dehydroepiandrosterone sulfate	3beta-Hydroxyandrost-5-en-17-one 3-sulfate, Dehydroepiandrosterone sulfate	C19H27O5S	-1	Extracellular
dheas	Dehydroepiandrosterone sulfate	3beta-Hydroxyandrost-5-en-17-one 3-sulfate, Dehydroepiandrosterone sulfate	C19H27O5S	-1	Endoplasmic Reticulum
dhf	7,8-Dihydrofolate	7,8-Dihydrofolic acid, Dihydrofolate, Dihydrofolic acid	C19H19N7O6	-2	Cytosol
dhf	7,8-Dihydrofolate	7,8-Dihydrofolic acid, Dihydrofolate, Dihydrofolic acid	C19H19N7O6	-2	Extracellular
dhf	7,8-Dihydrofolate	7,8-Dihydrofolic acid, Dihydrofolate, Dihydrofolic acid	C19H19N7O6	-2	Lysosome
dhf	7,8-Dihydrofolate	7,8-Dihydrofolic acid, Dihydrofolate, Dihydrofolic acid	C19H19N7O6	-2	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
dhlam	Dihydroliipoamide	Dihydrothioctamide	C8H17NO ₂	0	Mitochondria
dhlpro	Dihydroliipoalprotein		H ₂ S ₂ X	0	Mitochondria
dhocholoylcoa	3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane	3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane, 3alpha,7alpha-Dihydroxy-5beta-24-oxocholestanoyl-CoA, 5beta-Cholestane-3alpha,7alpha,12alpha,26-tetraol	C ₄₈ H ₇₄ N ₇ O ₂₀ P ₃ S	-4	Peroxisome
dhor-S	(S)-Dihydroorotate	(S)-4, 5-Dihydroorotate, Dihydro-L-orotic acid, L-Dihydroorotate, L-Dihydroorotic acid	C ₅ H ₅ N ₂ O ₄	-1	Cytosol
didp	dIDP	2'-Deoxyinosine 5'-diphosphate, 2'-Deoxyinosine-5-diphosphate	C ₁₀ H ₁₁ N ₄ O ₁₀ P ₂	-3	Cytosol
didp	dIDP	2'-Deoxyinosine 5'-diphosphate, 2'-Deoxyinosine-5-diphosphate	C ₁₀ H ₁₁ N ₄ O ₁₀ P ₂	-3	Mitochondria
didp	dIDP	2'-Deoxyinosine 5'-diphosphate, 2'-Deoxyinosine-5-diphosphate	C ₁₀ H ₁₁ N ₄ O ₁₀ P ₂	-3	Nucleus
digalsalside_hs	Digalactosylceramidesulfate	Digalactosylceramidesulfate	C ₃₀ H ₅₅ N ₁ O ₁₅ SFULLR _{CO}	-1	Cytosol
digalsalside_hs	Digalactosylceramidesulfate	Digalactosylceramidesulfate	C ₃₀ H ₅₅ N ₁ O ₁₅ SFULLR _{CO}	-1	Extracellular
digalsalside_hs	Digalactosylceramidesulfate	Digalactosylceramidesulfate	C ₃₀ H ₅₅ N ₁ O ₁₅ SFULLR _{CO}	-1	Golgi Apparatus
digalside_hs	Digalactosylceramide	Gal-Gal-Cer, Gal-alpha1->4Gal-beta1->1'Cer	C ₃₀ H ₅₆ N ₁ O ₁₂ FULLR _{CO}	0	Cytosol
digalside_hs	Digalactosylceramide	Gal-Gal-Cer, Gal-alpha1->4Gal-beta1->1'Cer	C ₃₀ H ₅₆ N ₁ O ₁₂ FULLR _{CO}	0	Golgi Apparatus
digalside_hs	Digalactosylceramide	Gal-Gal-Cer, Gal-alpha1->4Gal-beta1->1'Cer	C ₃₀ H ₅₆ N ₁ O ₁₂ FULLR _{CO}	0	Lysosome
dimp	dIMP	2'-Deoxyinosine 5'-phosphate	C ₁₀ H ₁₁ N ₄ O ₇ P	-2	Cytosol
din	Deoxyinosine	2'-deoxy-inosine	C ₁₀ H ₁₂ N ₄ O ₄	0	Cytosol
din	Deoxyinosine	2'-deoxy-inosine	C ₁₀ H ₁₂ N ₄ O ₄	0	Extracellular
diip	dITP	2'-Deoxyinosine 5'-triphosphate, 2'-Deoxyinosine-5-triphosphate	C ₁₀ H ₁₁ N ₄ O ₁₃ P ₃	-4	Cytosol
diip	dITP	2'-Deoxyinosine 5'-triphosphate, 2'-Deoxyinosine-5-triphosphate	C ₁₀ H ₁₁ N ₄ O ₁₃ P ₃	-4	Mitochondria
diip	dITP	2'-Deoxyinosine 5'-triphosphate, 2'-Deoxyinosine-5-triphosphate	C ₁₀ H ₁₁ N ₄ O ₁₃ P ₃	-4	Nucleus
dknpp	2,3-diketo-5-methylthio-1-phosphopentane	1-phospho-2,3-diketo-5-methylthiopentane	C ₆ H ₉ O ₆ P ₅	-2	Cytosol
dnlcg	dihomo-gamma-linolenic acid (n-6)	(Z,Z,Z)-8,11,14-Eicosatrienoate, (Z,Z,Z)-8,11,14-Icosatrienoate, 8,11,14-Eicosatrienoate, 8,11,14-Icosatrienoate, Dihomo-gamma-linolenic acid, icos 6,9,12-trienoic acid	C ₂₀ H ₃₃ O ₂	-1	Cytosol
dnlcg	dihomo-gamma-linolenic acid (n-6)	(Z,Z,Z)-8,11,14-Eicosatrienoate, (Z,Z,Z)-8,11,14-Icosatrienoate, 8,11,14-Eicosatrienoate, 8,11,14-Icosatrienoate, Dihomo-gamma-linolenic acid, icos 6,9,12-trienoic acid	C ₂₀ H ₃₃ O ₂	-1	Extracellular
dnlcgoa	dihomo-gamma-linolenyl coenzyme A		C ₄₁ H ₆₄ N ₇ O ₁₇ P ₃ S	-4	Cytosol
dnlcgoa	dihomo-gamma-linolenyl coenzyme A		C ₄₁ H ₆₄ N ₇ O ₁₇ P ₃ S	-4	Mitochondria
dnlcgcrn	dihomo-gamma-linolenyl carnitine		C ₂₇ H ₄₇ N ₃ O ₄	0	Cytosol
dnlcgcrn	dihomo-gamma-linolenyl carnitine		C ₂₇ H ₄₇ N ₃ O ₄	0	Mitochondria
dmanipyrine	demethylated antipyrine		C ₁₀ H ₁₀ N ₂ O	0	Cytosol
dmanipyrine	demethylated antipyrine		C ₁₀ H ₁₀ N ₂ O	0	Extracellular
dmgly	N,N-Dimethylglycine	Dimethylglycine	C ₄ H ₉ N ₂ O	0	Cytosol
dmgly	N,N-Dimethylglycine	Dimethylglycine	C ₄ H ₉ N ₂ O	0	Mitochondria
dnhptcoa	2,6 dimethylheptanoyl-CoA	dimethyl heptanoyl coenzyme A	C ₃₀ H ₅₂ N ₇ O ₁₇ P ₃ S	-4	Cytosol
dnhptcoa	2,6 dimethylheptanoyl-CoA	dimethyl heptanoyl coenzyme A	C ₃₀ H ₅₂ N ₇ O ₁₇ P ₃ S	-4	Mitochondria
dnhptcrn	2,6 dimethylheptanoyl carnitine	dimethyl heptanoyl carnitine	C ₁₆ H ₃₅ N ₃ O ₄	0	Cytosol
dnhptcrn	2,6 dimethylheptanoyl carnitine	dimethyl heptanoyl carnitine	C ₁₆ H ₃₅ N ₃ O ₄	0	Extracellular
dnhptcrn	2,6 dimethylheptanoyl carnitine	dimethyl heptanoyl carnitine	C ₁₆ H ₃₅ N ₃ O ₄	0	Mitochondria
dnnoncoa	4,8 dimethylnonanoyl-CoA	4,8 dimethylnonanoyl coenzyme a	C ₃₂ H ₅₄ N ₇ O ₁₇ P ₃ S	-4	Cytosol
dnnoncoa	4,8 dimethylnonanoyl-CoA	4,8 dimethylnonanoyl coenzyme a	C ₃₂ H ₅₄ N ₇ O ₁₇ P ₃ S	-4	Mitochondria
dnnoncoa	4,8 dimethylnonanoyl-CoA	4,8 dimethylnonanoyl coenzyme a	C ₃₂ H ₅₄ N ₇ O ₁₇ P ₃ S	-4	Peroxisome
dnnoncrn	4,8 dimethylnonanoyl carnitine		C ₁₈ H ₃₇ N ₃ O ₄	0	Mitochondria
dnnoncrn	4,8 dimethylnonanoyl carnitine		C ₁₈ H ₃₇ N ₃ O ₄	0	Peroxisome
dmpp	Dimethylallyl diphosphate	2-Isopentenyl diphosphate, Prenyl diphosphate, delta2-Isopentenyl diphosphate, dimethylallyl pyrophosphate	C ₅ H ₉ O ₇ P ₂	-3	Cytosol
dmpp	Dimethylallyl diphosphate	2-Isopentenyl diphosphate, Prenyl diphosphate, delta2-Isopentenyl diphosphate, dimethylallyl pyrophosphate	C ₅ H ₉ O ₇ P ₂	-3	Peroxisome
dna	DNA		C ₁₀ H ₁₇ O ₈ P ₂	0	Nucleus
dna5mtc	DNA 5-methylcytosine		C ₁₁ H ₁₉ O ₈ P ₂	0	Nucleus
dnad	Deamino-NAD+	Deamido-NAD+	C ₂₁ H ₂₄ N ₆ O ₁₅ P ₂	-2	Cytosol
dnad	Deamino-NAD+	Deamido-NAD+	C ₂₁ H ₂₄ N ₆ O ₁₅ P ₂	-2	Mitochondria
dnad	Deamino-NAD+	Deamido-NAD+	C ₂₁ H ₂₄ N ₆ O ₁₅ P ₂	-2	Nucleus
doldp_L	Dolichol diphosphate, human liver homolog		C ₁₀₈ O ₁₈₁ H ₁₇₅₈ O ₇₀ P ₂₀	-30	Endoplasmic Reticulum
doldp_U	Dolichol diphosphate, human uterine homolog		C ₁₀₂ S ₅ H ₁₆₇₀₀ O ₇₀ P ₂₀	-30	Endoplasmic Reticulum
dolgclp_L	Dolichyl beta-D-glucosyl phosphate, human liver homolog		C ₁₁₄₀ H ₁₈₆₈ O ₉₀ P ₁₀	-10	Cytosol
dolgclp_L	Dolichyl beta-D-glucosyl phosphate, human liver homolog		C ₁₁₄₀ H ₁₈₆₈ O ₉₀ P ₁₀	-10	Endoplasmic Reticulum
dolgclp_U	Dolichyl beta-D-glucosyl phosphate, human uterine homolog		C ₁₀₈ S ₅ H ₁₇₈₀₀ O ₉₀ P ₁₀	-10	Cytosol
dolgclp_U	Dolichyl beta-D-glucosyl phosphate, human uterine homolog		C ₁₀₈ S ₅ H ₁₇₈₀₀ O ₉₀ P ₁₀	-10	Endoplasmic Reticulum
doichol_L	Dolichol, human liver homolog		C ₁₀₈ O ₁₈ H ₁₇₆₈ O ₁₀	0	Cytosol
doichol_L	Dolichol, human liver homolog		C ₁₀₈ O ₁₈ H ₁₇₆₈ O ₁₀	0	Endoplasmic Reticulum
doichol_U	Dolichol, human uterine homolog		C ₁₀₂ S ₅ H ₁₆₈₀₀ O ₁₀	0	Cytosol
doichol_U	Dolichol, human uterine homolog		C ₁₀₂ S ₅ H ₁₆₈₀₀ O ₁₀	0	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
dolmanp_L	Dolichyl phosphate D-mannose, human liver homolog	Dolichyl D-mannosyl phosphate	C1140H1868O90P10	-10	Cytosol
dolmanp_L	Dolichyl phosphate D-mannose, human liver homolog	Dolichyl D-mannosyl phosphate	C1140H1868O90P10	-10	Endoplasmic Reticulum
dolmanp_U	Dolichyl phosphate D-mannose, human uterine homolog	Dolichyl D-mannosyl phosphate	C1085H1780O90P10	-10	Cytosol
dolmanp_U	Dolichyl phosphate D-mannose, human uterine homolog	Dolichyl D-mannosyl phosphate	C1085H1780O90P10	-10	Endoplasmic Reticulum
dolp_L	Dolichol phosphate, human liver homolog	Dolichyl phosphate	C1080H1758O40P10	-20	Cytosol
dolp_L	Dolichol phosphate, human liver homolog	Dolichyl phosphate	C1080H1758O40P10	-20	Endoplasmic Reticulum
dolp_U	Dolichol phosphate, human uterine homolog	Dolichyl phosphate	C1025H1670O40P10	-20	Cytosol
dolp_U	Dolichol phosphate, human uterine homolog	Dolichyl phosphate	C1025H1670O40P10	-20	Endoplasmic Reticulum
dopa	Dopamine	2-(3,4-Dihydroxyphenyl)ethylamine, 3,4-Dihydroxyphenethylamine, 4-(2-Aminoethyl)-1,2-benzenediol, 4-(2-Aminoethyl)benzene-1,2-diol	C8H12NO2	1	Cytosol
dopa	Dopamine	2-(3,4-Dihydroxyphenyl)ethylamine, 3,4-Dihydroxyphenethylamine, 4-(2-Aminoethyl)-1,2-benzenediol, 4-(2-Aminoethyl)benzene-1,2-diol	C8H12NO2	1	Extracellular
dopaqn	Dopaquinone		C9H9NO4	0	Cytosol
dopasf	Dopamine 3-O-sulfate		C8H11NO5S	0	Cytosol
dopasf	Dopamine 3-O-sulfate		C8H11NO5S	0	Extracellular
dpcoa	Dephospho-CoA		C21H33N7O13P2S	-2	Cytosol
dpcoa	Dephospho-CoA		C21H33N7O13P2S	-2	Lysosome
drnb	Deoxyribose	2-Deoxy-D-ribose, 2-Deoxy-beta-D-erythro-pentose, Thymine	C5H10O4	0	Cytosol
drnb	Deoxyribose	2-Deoxy-D-ribose, 2-Deoxy-beta-D-erythro-pentose, Thymine	C5H10O4	0	Extracellular
dsmsterol	Desmosterol	24-Dehydrocholesterol, Cholesta-5,24-dien-3beta-ol, Desmosterol	C27H44O	0	Endoplasmic Reticulum
dst_antigen	disialyl-T antigen		C36H56N3O26X	-2	Golgi Apparatus
dtup	dTDP	Thymidine 5'-diphosphate	C10H13N2O11P2	-3	Cytosol
dtup	dTDP	Thymidine 5'-diphosphate	C10H13N2O11P2	-3	Mitochondria
dtup	dTDP	Thymidine 5'-diphosphate	C10H13N2O11P2	-3	Nucleus
dtup4d6dg	dTDP-4-dehydro-6-deoxy-D-glucose	dTDP-4-oxo-6-deoxy-D-glucose	C16H22N2O15P2	-2	Cytosol
dtup4d6dm	dTDP-4-dehydro-6-deoxy-L-mannose	dTDP-4-oxo-6-deoxy-L-mannose, dTDP-4-oxo-L-rhamnose	C16H22N2O15P2	-2	Cytosol
dtupglu	dTDPglucose	dTDP-D-glucose	C16H24N2O16P2	-2	Cytosol
dtuprnm	dTDP-L-rhamnose	dTDP-6-deoxy-L-mannose, dTDP-L-rhamnose	C16H24N2O15P2	-2	Cytosol
dtmp	dTMP	5-Thymidylic acid, Deoxythymidine 5'-phosphate, Deoxythymidylic acid, Thymidine 5'-phosphate, Thymidine monophosphate, Thymidylate, Thymidylic acid	C10H13N2O8P	-2	Cytosol
dtmp	dTMP	5-Thymidylic acid, Deoxythymidine 5'-phosphate, Deoxythymidylic acid, Thymidine 5'-phosphate, Thymidine monophosphate, Thymidylate, Thymidylic acid	C10H13N2O8P	-2	Lysosome
dtmp	dTMP	5-Thymidylic acid, Deoxythymidine 5'-phosphate, Deoxythymidylic acid, Thymidine 5'-phosphate, Thymidine monophosphate, Thymidylate, Thymidylic acid	C10H13N2O8P	-2	Mitochondria
dtu	Dithiothreitol	1, 3-butanediol, 4-Dimercapto-2, 4-Dithiothreitol, DTT, threo-1	C4H10O2S2	0	Cytosol
dtuOX	Oxidized dithiothreitol		C4H8O2S2	0	Cytosol
dtup	dTTP	TTP, Thymidine 5'-triphosphate, Thymidine triphosphate	C10H13N2O14P3	-4	Cytosol
dtup	dTTP	TTP, Thymidine 5'-triphosphate, Thymidine triphosphate	C10H13N2O14P3	-4	Mitochondria
dtup	dTTP	TTP, Thymidine 5'-triphosphate, Thymidine triphosphate	C10H13N2O14P3	-4	Nucleus
duap	dUDP	2'-Deoxyuridine 5'-diphosphate	C9H11N2O11P2	-3	Cytosol
duap	dUDP	2'-Deoxyuridine 5'-diphosphate	C9H11N2O11P2	-3	Mitochondria
duap	dUDP	2'-Deoxyuridine 5'-diphosphate	C9H11N2O11P2	-3	Nucleus
dump	dUMP	2'-Deoxyuridine 5'-phosphate, Deoxyuridine 5'-phosphate, Deoxyuridine monophosphate, Deoxyuridylic acid	C9H11N2O8P	-2	Cytosol
dump	dUMP	2'-Deoxyuridine 5'-phosphate, Deoxyuridine 5'-phosphate, Deoxyuridine monophosphate, Deoxyuridylic acid	C9H11N2O8P	-2	Mitochondria
dump	dUMP	2'-Deoxyuridine 5'-phosphate, Deoxyuridine 5'-phosphate, Deoxyuridine monophosphate, Deoxyuridylic acid	C9H11N2O8P	-2	Nucleus
duri	Deoxyuridine	2'-Deoxyuridine, 2-Deoxyuridine	C9H12N2O5	0	Cytosol
duri	Deoxyuridine	2'-Deoxyuridine, 2-Deoxyuridine	C9H12N2O5	0	Extracellular
duri	Deoxyuridine	2'-Deoxyuridine, 2-Deoxyuridine	C9H12N2O5	0	Mitochondria
duri	Deoxyuridine	2'-Deoxyuridine, 2-Deoxyuridine	C9H12N2O5	0	Nucleus
dtup	dUTP	2'-Deoxyuridine 5'-triphosphate	C9H11N2O14P3	-4	Cytosol
dtup	dUTP	2'-Deoxyuridine 5'-triphosphate	C9H11N2O14P3	-4	Mitochondria
dtup	dUTP	2'-Deoxyuridine 5'-triphosphate	C9H11N2O14P3	-4	Nucleus
dxtrn	phosphorylase-limit dextrin (glycogenin-1,6[4[1,4-Glc], 4[1,4-Glc]])		C48H81O41X	0	Cytosol
e4hglu	L-erythro-4-Hydroxyglutamate		C5H8NO5	-1	Cytosol
e4hglu	L-erythro-4-Hydroxyglutamate		C5H8NO5	-1	Mitochondria
e4p	D-Erythrose 4-phosphate	4-phospho D-erythrose	C4H7O7P	-2	Cytosol
eaflatoxin	8,9 epoxy aflatoxin B1		C17H12O7	0	Cytosol
eaflatoxin	8,9 epoxy aflatoxin B1		C17H12O7	0	Extracellular

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
eandrstrm	epiandrosterone	16alpha-Hydroxydehydroepiandrosterone, 5-Androstene-3beta,16alpha-diol-17-one	C19H28O3	0	Endoplasmic Reticulum
ebastine	ebastine	4-Diphenylmethoxy-1-(3-(4-tert-butylbenzoyl)propyl)piperidine, Ebastel, Ebastina, Ebastine, Ebastinum, Kestine, ebastine	C32H39NO2	0	Cytosol
ebastine	ebastine	4-Diphenylmethoxy-1-(3-(4-tert-butylbenzoyl)propyl)piperidine, Ebastel, Ebastina, Ebastine, Ebastinum, Kestine, ebastine	C32H39NO2	0	Extracellular
ebastine	ebastine	4-Diphenylmethoxy-1-(3-(4-tert-butylbenzoyl)propyl)piperidine, Ebastel, Ebastina, Ebastine, Ebastinum, Kestine, ebastine	C32H39NO2	0	Endoplasmic Reticulum
ebastineoh	hydroxylated ebastine		C32H39NO3	0	Cytosol
ebastineoh	hydroxylated ebastine		C32H39NO3	0	Extracellular
ebastineoh	hydroxylated ebastine		C32H39NO3	0	Endoplasmic Reticulum
ecgon	ecgonine		C9H14NO3	-1	Endoplasmic Reticulum
egme	ecgonine methyl ester		C10H17NO3	0	Endoplasmic Reticulum
eicostet	eicosatetraenoic acid	8,11,14,17-Eicosatetraenoic acid	C20H31O2	-1	Cytosol
eicostet	eicosatetraenoic acid	8,11,14,17-Eicosatetraenoic acid	C20H31O2	-1	Extracellular
eicostetcoa	eicosatetraenyl coenzyme A	8,11,14,17-Eicosatetraenoic acid coenzyme a	C41H62N7O17P3S	-4	Cytosol
eicostetcoa	eicosatetraenyl coenzyme A	8,11,14,17-Eicosatetraenoic acid coenzyme a	C41H62N7O17P3S	-4	Mitochondria
eicostetcrn	Eicosatetraenyl carnitine		C27H45NO4	0	Cytosol
eicostetcrn	Eicosatetraenyl carnitine		C27H45NO4	0	Mitochondria
elaid	elaidic acid	(E)-9-Octadecenoic acid, (E)-Oleic acid, 9-Octadecenoic acid, (E)-, 9-trans-Octadecenoic acid D9-trans-Octadecenoic acid, Elaidinsäure, acide elaidique, elaidic acid, trans-9-Octadecenoic acid, trans-D9-Octadecenoic acid, trans-Elaidic acid, trans-Oleic acid	C18H33O2	-1	Cytosol
elaid	elaidic acid	(E)-9-Octadecenoic acid, (E)-Oleic acid, 9-Octadecenoic acid, (E)-, 9-trans-Octadecenoic acid D9-trans-Octadecenoic acid, Elaidinsäure, acide elaidique, elaidic acid, trans-9-Octadecenoic acid, trans-D9-Octadecenoic acid, trans-Elaidic acid, trans-Oleic acid	C18H33O2	-1	Extracellular
elaidcm	Elaidic carnitine	elaidic acid carnitine	C25H47NO4	0	Cytosol
elaidcm	Elaidic carnitine	elaidic acid carnitine	C25H47NO4	0	Mitochondria
em2emgacpail_hs	(phosphoethanolaminyldimannosyl)(phosphoethanolaminyldimannosyl)-glucosaminyl-acylphosphatidylinositol (H7)	[PE-(Man)2],[PE]-Man-GlcN-acylPI	C53H100N3O35P3FULLR2CO2FULR2CO2	0	Endoplasmic Reticulum
em2emgacpail_prot_hs	(phosphoethanolaminyldimannosyl)(phosphoethanolaminyldimannosyl)-glucosaminyl-acylphosphatidylinositol	[[PE-(Man)2],[PE]-Man-GlcN-acylPI-prot	C53H100N3O35P3FULLR2CO2FULR2CO2X	0	Endoplasmic Reticulum
em3gacpail_hs	phosphoethanolaminyldimannosyl-acylphosphatidylinositol (H6)	PE-(Man)3-GlcN-acylPI	C51H94N3O32P2FULLR2CO2FULR2CO2	0	Endoplasmic Reticulum
emem2gacpail_hs	(phosphoethanolaminyldimannosyl)(phosphoethanolaminyldimannosyl)-glucosaminyl-acylphosphatidylinositol (H7)	[PE-Man],[PE]-[Man]2-GlcN-acylPI	C53H100N3O35P3FULLR2CO2FULR2CO2	0	Endoplasmic Reticulum
emgacpail_hs	phosphoethanolaminyldimannosyl-acylphosphatidylinositol (H5)	PE-Man-GlcN-acylPI	C39H74N2O22P2FULLR2CO2FULR2CO2	0	Endoplasmic Reticulum
eryth	L-Erythrulose	L-glycero-Tetrolose	C4H8O4	0	Cytosol
estradiol	Estradiol	Estradiol-17beta, beta-Estradiol	C18H24O2	0	Cytosol
estradiol	Estradiol	Estradiol-17beta, beta-Estradiol	C18H24O2	0	Endoplasmic Reticulum
estradiolglc	estradiol glucuronide	Estradiol-17beta 3-glucuronide	C24H32O8	0	Cytosol
estradiolglc	estradiol glucuronide	Estradiol-17beta 3-glucuronide	C24H32O8	0	Extracellular
estradiolglc	estradiol glucuronide	Estradiol-17beta 3-glucuronide	C24H32O8	0	Endoplasmic Reticulum
estriol	estriol	1,3,5(10)-Estratriene-3,16-alpha,17beta-triol, Estriol	C18H24O3	0	Cytosol
estriol	estriol	1,3,5(10)-Estratriene-3,16-alpha,17beta-triol, Estriol	C18H24O3	0	Endoplasmic Reticulum
estriolglc	16-Glucuronide-estriol	16-Glucuronide, 16-Glucuronide-estriol, 16alpha,17beta-Estriol 16-(beta-D-glucuronide)	C24H32O9	0	Cytosol
estriolglc	16-Glucuronide-estriol	16-Glucuronide, 16-Glucuronide-estriol, 16alpha,17beta-Estriol 16-(beta-D-glucuronide)	C24H32O9	0	Extracellular
estriolglc	16-Glucuronide-estriol	16-Glucuronide, 16-Glucuronide-estriol, 16alpha,17beta-Estriol 16-(beta-D-glucuronide)	C24H32O9	0	Endoplasmic Reticulum
estrone	Estrone	3, 3-Hydroxy-1, 5(10)-estratrien-17-one	C18H22O2	0	Cytosol
estrone	Estrone	3, 3-Hydroxy-1, 5(10)-estratrien-17-one	C18H22O2	0	Endoplasmic Reticulum
estronegl	estrone glucuronide		C24H30O8	0	Cytosol
estronegl	estrone glucuronide		C24H30O8	0	Extracellular
estronegl	estrone glucuronide		C24H30O8	0	Endoplasmic Reticulum
estrones	Estrone 3-sulfate	Estrone 3-sulfate	C18H21O5S	-1	Cytosol
estrones	Estrone 3-sulfate	Estrone 3-sulfate	C18H21O5S	-1	Extracellular
estrones	Estrone 3-sulfate	Estrone 3-sulfate	C18H21O5S	-1	Endoplasmic Reticulum
etfox	Electron transfer flavoprotein oxidized		R	0	Mitochondria
etfrd	Electron transfer flavoprotein reduced		RH2	0	Mitochondria
etfa	Ethanolamine	Aminoethanol, Hydroxyethylamine	C2H8NO	1	Cytosol
ethamp	Ethanolamine phosphate	O-Phosphoethanolamine, O-Phosphorylethanolamine, Phosphoethanolamine	C2H7NO4P	-1	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ethamp	Ethanolamine phosphate	O-Phosphoethanolamine, O-Phosphorylethanolamine, Phosphoethanolamine	C2H7NO4P	-1	Endoplasmic Reticulum
etoh	Ethanol	Ethyl alcohol, Methylcarbinol	C2H6O	0	Cytosol
etoh	Ethanol	Ethyl alcohol, Methylcarbinol	C2H6O	0	Extracellular
etoh	Ethanol	Ethyl alcohol, Methylcarbinol	C2H6O	0	Peroxisome
f1a	F1alpha		C22H37N2O15X	0	Golgi Apparatus
f1a	F1alpha		C22H37N2O15X	0	Lysosome
f1p	D-Fructose 1-phosphate	Fructofuranose 1-phosphate, Fructose 1-phosphate	C6H11O9P	-2	Cytosol
f26bp	D-Fructose 2,6-bisphosphate		C6H10O12P2	-4	Cytosol
f5hoxkyn	Formyl-5-hydroxykynurenamine		C10H13N2O3	1	Cytosol
f6p	D-Fructose 6-phosphate	D-Fructose 6-phosphoric acid, Neuberg ester, beta-D-Fructose 6-phosphate	C6H11O9P	-2	Cytosol
fad	Flavin adenine dinucleotide oxidized	FAD, Flavin adenine dinucleotide, Riboflavine 5'-adenosine diphosphate	C27H31N9O15P2	-2	Cytosol
fad	Flavin adenine dinucleotide oxidized	FAD, Flavin adenine dinucleotide, Riboflavine 5'-adenosine diphosphate	C27H31N9O15P2	-2	Mitochondria
fad	Flavin adenine dinucleotide oxidized	FAD, Flavin adenine dinucleotide, Riboflavine 5'-adenosine diphosphate	C27H31N9O15P2	-2	Endoplasmic Reticulum
fad	Flavin adenine dinucleotide oxidized	FAD, Flavin adenine dinucleotide, Riboflavine 5'-adenosine diphosphate	C27H31N9O15P2	-2	Peroxisome
fadh2	Flavin adenine dinucleotide reduced	flavin adenine dinucleotide (reduced form)	C27H33N9O15P2	-2	Cytosol
fadh2	Flavin adenine dinucleotide reduced	flavin adenine dinucleotide (reduced form)	C27H33N9O15P2	-2	Mitochondria
fadh2	Flavin adenine dinucleotide reduced	flavin adenine dinucleotide (reduced form)	C27H33N9O15P2	-2	Endoplasmic Reticulum
fadh2	Flavin adenine dinucleotide reduced	flavin adenine dinucleotide (reduced form)	C27H33N9O15P2	-2	Peroxisome
fald	Formaldehyde	Formalin, Methanal, Methylene oxide, Oxomethane, Oxomethylene	CH2O	0	Cytosol
fald	Formaldehyde	Formalin, Methanal, Methylene oxide, Oxomethane, Oxomethylene	CH2O	0	Lysosome
fald	Formaldehyde	Formalin, Methanal, Methylene oxide, Oxomethane, Oxomethylene	CH2O	0	Mitochondria
fald	Formaldehyde	Formalin, Methanal, Methylene oxide, Oxomethane, Oxomethylene	CH2O	0	Peroxisome
fdp	D-Fructose 1,6-bisphosphate	beta-D-fructofuranose-1,6-diphosphate, fbp, fructose diphosphate, fructose-1,6-bisphosphate	C6H10O12P2	-4	Cytosol
fe2	Fe2+	Fe(II), Iron, Iron dication, Reduced Iron	Fe	2	Cytosol
fe2	Fe2+	Fe(II), Iron, Iron dication, Reduced Iron	Fe	2	Extracellular
fe2	Fe2+	Fe(II), Iron, Iron dication, Reduced Iron	Fe	2	Mitochondria
fe3	Fe3+	Fe(III), Iron trication	Fe	3	Extracellular
fgam	N2-Formyl-N1-(5-phospho-D-ribose)glycinamide	5'-Phosphoribosyl-N-formylglycinamide, N-FormylGAR, N-Formylglycinamide ribonucleotide	C8H13N2O9P	-2	Cytosol
fcycC	Ferricytochrome c		C42H54FeN8O6S2	3	Mitochondria
fmn	FMN	Flavin mononucleotide, Riboflavin-5-phosphate	C17H19N4O9P	-2	Cytosol
fn2m2masn	N4-[N-Acetyl-beta-D-glucosaminy]-(1,2)-alpha-D-mannosyl-(1,3)-[N-acetyl-beta-D-glucosaminy]-(1,2)-alpha-D-mannosyl-(1,6)-beta-D-mannosyl-(1,4)-N-acetyl-beta-D-glucosaminy]-(1,4)-[alpha-L-fucosyl-(1,6)]-N-acetyl-beta-D-glucosaminy]asparagine		C56H93N4O39X	0	Golgi Apparatus
fna5moxam	Formyl-N-acetyl-5-methoxykynurenamine		C13H16N2O4	0	Cytosol
foctC	Ferrocyclochrome C		C42H54FeN8O6S2	2	Mitochondria
fol	Folate	Folic acid, Pteroylglutamic acid	C19H18N7O6	-1	Cytosol
fol	Folate	Folic acid, Pteroylglutamic acid	C19H18N7O6	-1	Extracellular
for	Formate	Formic acid, Hydrogencarboxylic acid, Methanoic acid, aminic acid	CH1O2	-1	Cytosol
for	Formate	Formic acid, Hydrogencarboxylic acid, Methanoic acid, aminic acid	CH1O2	-1	Extracellular
for	Formate	Formic acid, Hydrogencarboxylic acid, Methanoic acid, aminic acid	CH1O2	-1	Mitochondria
for	Formate	Formic acid, Hydrogencarboxylic acid, Methanoic acid, aminic acid	CH1O2	-1	Nucleus
for	Formate	Formic acid, Hydrogencarboxylic acid, Methanoic acid, aminic acid	CH1O2	-1	Endoplasmic Reticulum
forglu	N-Formimidoyl-L-glutamate	N-Formimino-L-glutamate	C6H8N2O4	-2	Cytosol
formcoa	Formyl-CoA		C22H36N7O17P3S	0	Cytosol
formcoa	Formyl-CoA		C22H36N7O17P3S	0	Peroxisome
fpram	2-(Formamido)-N1-(5-phospho-D-ribose)acetamidine	1-(5'-Phosphoribosyl)-N-formylglycinamide, 2-(Formamido)-N1-(5'-phosphoribosyl)acetamidine, Phosphoribosyl-N-formylglycinamide, 5'-Phosphoribosylformylglycinamide	C8H15N3O8P	-1	Cytosol
fpica	5-Formamido-1-(5-phospho-D-ribose)imidazole-4-carboxamide	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide, 5'-Phosphoribosyl-5-formamido-4-imidazolecarboxamide, 5-Formamid-1-(5-phosphoribosyl)imidazole-4-carboxamide	C10H13N4O9P	-2	Cytosol
frdp	Farnesyl diphosphate	2-trans,6-trans-Farnesyl diphosphate, FPP, Farnesyl pyrophosphate, trans,trans-Farnesyl diphosphate	C15H25O7P2	-3	Cytosol
frdp	Farnesyl diphosphate	2-trans,6-trans-Farnesyl diphosphate, FPP, Farnesyl pyrophosphate, trans,trans-Farnesyl diphosphate	C15H25O7P2	-3	Endoplasmic Reticulum
frdp	Farnesyl diphosphate	2-trans,6-trans-Farnesyl diphosphate, FPP, Farnesyl pyrophosphate, trans,trans-Farnesyl diphosphate	C15H25O7P2	-3	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
fru	D-Fructose	D-Arabino-hexulose, Fruit sugar, Levulose	C6H12O6	0	Cytosol
fru	D-Fructose	D-Arabino-hexulose, Fruit sugar, Levulose	C6H12O6	0	Extracellular
fuc12gal14aclegalguside_hs	Type IIIH glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, IV2-a-Fuc-nLc4Cer, IV2Fuc-nLc4Cer	C50H89N2O26FULLRCO	0	Golgi Apparatus
fuc132galacleggal14aclegalguside_hs	V3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1, Lex	C64H112N3O36FULLRCO	0	Golgi Apparatus
fuc13galacleggal14aclegalguside_hs	III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C64H112N3O36FULLRCO	0	Cytosol
fuc13galacleggal14aclegalguside_hs	III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C64H112N3O36FULLRCO	0	Extracellular
fuc13galacleggal14aclegalguside_hs	III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C64H112N3O36FULLRCO	0	Golgi Apparatus
fuc14galaclegalguside_hs	Lea glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, Fuc-Lc4Cer, III4-a-Fuc-Lc4Cer	C50H89N2O26FULLRCO	0	Cytosol
fuc14galaclegalguside_hs	Lea glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, Fuc-Lc4Cer, III4-a-Fuc-Lc4Cer	C50H89N2O26FULLRCO	0	Extracellular
fuc14galaclegalguside_hs	Lea glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, Fuc-Lc4Cer, III4-a-Fuc-Lc4Cer	C50H89N2O26FULLRCO	0	Golgi Apparatus
fuc1p-L	L-Fucose 1-phosphate	6-Deoxy-L-galactose 1-phosphate, L-Fucose 1-phosphate	C6H11O8P	-2	Cytosol
fucacgalfucgalaclegalguside_hs	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	ALeb	C64H112N3O35FULLRCO	0	Cytosol
fucacgalfucgalaclegalguside_hs	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	ALeb	C64H112N3O35FULLRCO	0	Extracellular
fucacgalfucgalaclegalguside_hs	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	ALeb	C64H112N3O35FULLRCO	0	Golgi Apparatus
fucacngal14aclegalguside_hs	IV3-a-NeuAc, III3-a-Fuc-nLc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, IV3-a-NeuAc, III3-a-Fuc-nLc4Cer, IV3NeuAc, III3Fuc-nLc4Cer	C61H105N3O34FULLRCO	-1	Cytosol
fucacngal14aclegalguside_hs	IV3-a-NeuAc, III3-a-Fuc-nLc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, IV3-a-NeuAc, III3-a-Fuc-nLc4Cer, IV3NeuAc, III3Fuc-nLc4Cer	C61H105N3O34FULLRCO	-1	Extracellular
fucacngal14aclegalguside_hs	IV3-a-NeuAc, III3-a-Fuc-nLc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, IV3-a-NeuAc, III3-a-Fuc-nLc4Cer, IV3NeuAc, III3Fuc-nLc4Cer	C61H105N3O34FULLRCO	-1	Golgi Apparatus
fucacngalaclegalguside_hs	IV3-a-Neu5Ac, III4-a-Fuc-Lc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, Fuc-3-isoLM1	C61H105N3O34FULLRCO	-1	Cytosol
fucacngalaclegalguside_hs	IV3-a-Neu5Ac, III4-a-Fuc-Lc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, Fuc-3-isoLM1	C61H105N3O34FULLRCO	-1	Extracellular
fucacngalaclegalguside_hs	IV3-a-Neu5Ac, III4-a-Fuc-Lc4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Neu5Ac)1 (Cer)1, Fuc-3-isoLM1	C61H105N3O34FULLRCO	-1	Golgi Apparatus
fucfuc12gal14aclegalguside_hs	Ley glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, III3, IV2Fuc-nLc4Cer, IV2-a-Fuc, III3-a-Fuc-nLc4Cer	C56H99N2O30FULLRCO	0	Cytosol
fucfuc12gal14aclegalguside_hs	Ley glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, III3, IV2Fuc-nLc4Cer, IV2-a-Fuc, III3-a-Fuc-nLc4Cer	C56H99N2O30FULLRCO	0	Extracellular
fucfuc12gal14aclegalguside_hs	Ley glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, III3, IV2Fuc-nLc4Cer, IV2-a-Fuc, III3-a-Fuc-nLc4Cer	C56H99N2O30FULLRCO	0	Golgi Apparatus
fucfuc132galacleggal14aclegalguside_hs	V3Fuc, III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1, dimeric Lex	C70H122N3O40FULLRCO	0	Cytosol
fucfuc132galacleggal14aclegalguside_hs	V3Fuc, III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1, dimeric Lex	C70H122N3O40FULLRCO	0	Extracellular
fucfuc132galacleggal14aclegalguside_hs	V3Fuc, III3Fuc-nLc6Cer	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1, dimeric Lex	C70H122N3O40FULLRCO	0	Golgi Apparatus
fucfucfucgalacleg13galaclegal14aclegalguside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	trimeric Lex	C90H155N4O54FULLRCO	0	Cytosol
fucfucfucgalacleg13galaclegal14aclegalguside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	trimeric Lex	C90H155N4O54FULLRCO	0	Extracellular
fucfucfucgalacleg13galaclegal14aclegalguside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	trimeric Lex	C90H155N4O54FULLRCO	0	Golgi Apparatus
fucfucfucgalacleggal14aclegalguside_hs	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1		C76H132N3O44FULLRCO	0	Cytosol
fucfucfucgalacleggal14aclegalguside_hs	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1		C76H132N3O44FULLRCO	0	Extracellular
fucfucfucgalacleggal14aclegalguside_hs	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1		C76H132N3O44FULLRCO	0	Golgi Apparatus
fucfucgalacleg13galaclegal14aclegalguside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	dimeric Lex	C84H145N4O50FULLRCO	0	Golgi Apparatus
fucfucgalacleggal14aclegalguside_hs	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1		C70H122N3O40FULLRCO	0	Golgi Apparatus
fucfucgalacleggalacleggal14aclegalguside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1		C84H145N4O50FULLRCO	0	Golgi Apparatus
fucfucgalaclegalguside_hs	Leb glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, IV2-a-Fuc, III4-a-Fuc-Lc4Cer, IV2Fuc, III4Fuc-Lc4Cer	C56H99N2O30FULLRCO	0	Cytosol
fucfucgalaclegalguside_hs	Leb glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, IV2-a-Fuc, III4-a-Fuc-Lc4Cer, IV2Fuc, III4Fuc-Lc4Cer	C56H99N2O30FULLRCO	0	Extracellular
fucfucgalaclegalguside_hs	Leb glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1, IV2-a-Fuc, III4-a-Fuc-Lc4Cer, IV2Fuc, III4Fuc-Lc4Cer	C56H99N2O30FULLRCO	0	Golgi Apparatus
fuegal14aclegalguside_hs	Lacto-N-fucopentaosyl III ceramide	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, III3-a-Fuc-nLc4Cer, III3Fuc-nLc4Cer, LNF III cer., Lacto-N-fucopentaosyl III ceramide., SSEA-1	C50H89N2O26FULLRCO	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
fucgal14acglegalgluside_hs	Lacto-N-fucopentaosyl III ceramide	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, III3-a-Fuc-nLc4Cer, III3Fuc-nLc4Cer, LNF III cer., Lacto-N-fucopentaosyl III ceramide, SSEA-1	C50H89N2O26FULLRCO	0	Extracellular
fucgal14acglegalgluside_hs	Lacto-N-fucopentaosyl III ceramide	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, III3-a-Fuc-nLc4Cer, III3Fuc-nLc4Cer, LNF III cer., Lacto-N-fucopentaosyl III ceramide, SSEA-1	C50H89N2O26FULLRCO	0	Golgi Apparatus
fucgalacalfuc12gal14acglegalgluside_hs	Type IIIH glycolipid	(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	C70H122N3O40FULLRCO	0	Golgi Apparatus
fucgalacalfucgalaclegal14acglegalgluside_hs	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1		C84H145N4O50FULLRCO	0	Golgi Apparatus
fucgalac1e13galaclegal14acglegalgluside_hs	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)1 (Cer)1	Lex	C78H135N4O46FULLRCO	0	Golgi Apparatus
fucgalaclegal14acglegalgluside_hs	VI2Fuc-nLc6	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C64H112N3O36FULLRCO	0	Golgi Apparatus
fucgalaclegalgluside_hs	Type III glycolipid	(Gal)2 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1, IV2-a-Fuc-Lc4Cer, IV2Fuc-Lc4Cer	C50H89N2O26FULLRCO	0	Golgi Apparatus
fucalfucgalaclegalgluside_hs	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1		C62H109N2O35FULLRCO	0	Cytosol
fucalfucgalaclegalgluside_hs	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1		C62H109N2O35FULLRCO	0	Extracellular
fucalfucgalaclegalgluside_hs	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1		C62H109N2O35FULLRCO	0	Golgi Apparatus
fucalghside_hs	fucosyl galactosylglucoside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (LFuc)1 (Cer)1, Fuc-Gal globoside, Globo-H	C56H99N2O31FULLRCO	0	Cytosol
fucalghside_hs	fucosyl galactosylglucoside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (LFuc)1 (Cer)1, Fuc-Gal globoside, Globo-H	C56H99N2O31FULLRCO	0	Extracellular
fucalghside_hs	fucosyl galactosylglucoside (homo sapiens)	(Gal)3 (GalNAc)1 (Glc)1 (LFuc)1 (Cer)1, Fuc-Gal globoside, Globo-H	C56H99N2O31FULLRCO	0	Golgi Apparatus
fuc-L	L-Fucose	6-Deoxy-L-galactose	C6H12O5	0	Cytosol
fuc-L	L-Fucose	6-Deoxy-L-galactose	C6H12O5	0	Extracellular
fuc-L	L-Fucose	6-Deoxy-L-galactose	C6H12O5	0	Lysosome
fum	Fumarate	Fumaric acid, Trans-butenedioic acid, allomaleic acid, boletic acid	C4H2O4	-2	Cytosol
fum	Fumarate	Fumaric acid, Trans-butenedioic acid, allomaleic acid, boletic acid	C4H2O4	-2	Mitochondria
g1m6masnB1	glucosyl-(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C64H107N2O50X	0	Golgi Apparatus
g1m6masnB1	glucosyl-(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C64H107N2O50X	0	Endoplasmic Reticulum
g1m7masnB	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)		C70H117N2O55X	0	Golgi Apparatus
g1m7masnB	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)		C70H117N2O55X	0	Endoplasmic Reticulum
g1m7masnC	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform C (protein)		C70H117N2O55X	0	Golgi Apparatus
g1m7masnC	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform C (protein)		C70H117N2O55X	0	Endoplasmic Reticulum
g1m8masn	(alpha-D-Glucosyl)-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C76H127N2O60X	0	Golgi Apparatus
g1m8masn	(alpha-D-Glucosyl)-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C76H127N2O60X	0	Endoplasmic Reticulum
g1m8mpdol_L	alpha-D-Glucosyl-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1840H3028N200670P20	-20	Endoplasmic Reticulum
g1m8mpdol_U	alpha-D-Glucosyl-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1785H2940N200670P20	-20	Endoplasmic Reticulum
g1p	D-Glucose 1-phosphate	Cori ester, Glucose 1-phosphate, alpha-D-Glucose phosphate	C6H11O9P	-2	Cytosol
g2m8masn	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C82H137N2O65X	0	Golgi Apparatus
g2m8masn	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C82H137N2O65X	0	Endoplasmic Reticulum
g2m8mpdol_L	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1900H3128N200720P20	-20	Endoplasmic Reticulum
g2m8mpdol_U	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1845H3040N200720P20	-20	Endoplasmic Reticulum
g3m8masn	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C88H147N2O70X	0	Golgi Apparatus
g3m8masn	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)		C88H147N2O70X	0	Endoplasmic Reticulum
g3m8mpdol_L	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1960H3228N200770P20	-20	Endoplasmic Reticulum
g3m8mpdol_U	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1905H3140N200770P20	-20	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
g3p	Glyceraldehyde 3-phosphate	(2R)-2-Hydroxy-3-(phosphonoxy)-propanal, D-glyceraldehyde 3-phosphate	C3H5O6P	-2	Cytosol
g3pc	sn-Glycerol-3-phosphocholine	Glycerophosphocholine	C8H20NO6P	0	Cytosol
g6p	D-Glucose 6-phosphate	Glucose 6-phosphate, Robinson ester, alpha-D-Glucose 6-phosphate	C6H11O9P	-2	Cytosol
g6p	D-Glucose 6-phosphate	Glucose 6-phosphate, Robinson ester, alpha-D-Glucose 6-phosphate	C6H11O9P	-2	Endoplasmic Reticulum
gal_hs	GA1 (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Cer)1	C44H79N2O22FULLRCO	0	Golgi Apparatus
ga2_hs	GA2 (homo sapiens)	(Gal)1 (GalNAc)1 (Glc)1 (Cer)1	C38H69N2O17FULLRCO	0	Golgi Apparatus
gacpai_hs	glucosaminyl-acylphosphatidylinositol	GlcN-acylPI	C31H58NO14PFULLR2CO2	0	Cytosol
gacpai_hs	glucosaminyl-acylphosphatidylinositol	GlcN-acylPI	C31H58NO14PFULLR2CO2	0	Endoplasmic Reticulum
gal	D-Galactose	Galactose, alpha-Galactose(D)	C6H12O6	0	Cytosol
gal	D-Galactose	Galactose, alpha-Galactose(D)	C6H12O6	0	Extracellular
gal	D-Galactose	Galactose, alpha-Galactose(D)	C6H12O6	0	Lysosome
gal14aclegalgalside_hs	Lactoneotetraosylceramide	(Gal)2 (Glc)1 (GlcNAc)1 (Cer)1, LA1-, Lacto-N-neotetraosylceramide, Lactoneotetraosylceramide, Neolactotetraosylceramide-, Paragloboside-, nLc6Cer	C44H79N2O22FULLRCO	0	Golgi Apparatus
gal1p	alpha-D-Galactose 1-phosphate	D-Galactose 1-phosphate, alpha-D-Galactose 1-phosphate	C6H11O9P	-2	Cytosol
galacgalfuc12gal14aclegalgalside_hs		(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C64H112N3O36FULLRCO	0	Golgi Apparatus
galacgalfucgalaclegall14aclegalgalside_hs		(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C78H135N4O46FULLRCO	0	Golgi Apparatus
galacglc13galaclegall14aclegalgalside_hs	nLc8Cer	(Gal)4 (Glc)1 (GlcNAc)3 (Cer)1	C72H125N4O42FULLRCO	0	Golgi Apparatus
galacleggal14aclegalgalside_hs	i-antigen	(Gal)3 (Glc)1 (GlcNAc)2 (Cer)1, nLc6Cer;	C58H102N3O32FULLRCO	0	Golgi Apparatus
galacleggalacleggal14aclegalgalside_hs	i-antigen	(Gal)4 (Glc)1 (GlcNAc)3 (Cer)1, LacNAc-Lc6Cer, Lactosioctaosylceramide, iso-nLc8Cer;	C72H125N4O42FULLRCO	0	Golgi Apparatus
galacleggalgbside_hs	Gal-GlcNAc-Gal globoside (homo sapiens)	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)1 (Cer)1	C64H112N3O37FULLRCO	0	Cytosol
galacleggalgbside_hs	Gal-GlcNAc-Gal globoside (homo sapiens)	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)1 (Cer)1	C64H112N3O37FULLRCO	0	Extracellular
galacleggalgbside_hs	Gal-GlcNAc-Gal globoside (homo sapiens)	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)1 (Cer)1	C64H112N3O37FULLRCO	0	Golgi Apparatus
galacleggalgbside_hs	Le4Cer	(Gal)2 (Glc)1 (GlcNAc)1 (Cer)1	C44H79N2O22FULLRCO	0	Golgi Apparatus
galfuc12gal14aclegalgalside_hs		(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C56H99N2O31FULLRCO	0	Cytosol
galfuc12gal14aclegalgalside_hs		(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C56H99N2O31FULLRCO	0	Extracellular
galfuc12gal14aclegalgalside_hs		(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C56H99N2O31FULLRCO	0	Golgi Apparatus
galfucgalacleggal14aclegalgalside_hs		(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C70H122N3O41FULLRCO	0	Cytosol
galfucgalacleggal14aclegalgalside_hs		(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C70H122N3O41FULLRCO	0	Extracellular
galfucgalacleggal14aclegalgalside_hs		(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	C70H122N3O41FULLRCO	0	Golgi Apparatus
galfucgalacleggalgalside_hs	Type IB glycolipid	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	C56H99N2O31FULLRCO	0	Golgi Apparatus
galgalfucgalacleggalacleggal14aclegalgalside_hs		(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	C96H165N4O60FULLRCO	0	Cytosol
galgalfucgalacleggalacleggal14aclegalgalside_hs		(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	C96H165N4O60FULLRCO	0	Extracellular
galgalfucgalacleggalacleggal14aclegalgalside_hs		(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	C96H165N4O60FULLRCO	0	Golgi Apparatus
galgalgaltherm_hs	Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->4)-Glc(beta 1->4)-Cer, Gal-Gal-Gal-Gal-Glu-Cer	C54H96N3O32FULLRCO	0	Cytosol
galgalgaltherm_hs	Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->4)-Glc(beta 1->4)-Cer, Gal-Gal-Gal-Gal-Glu-Cer	C54H96N3O32FULLRCO	0	Extracellular
galgalgaltherm_hs	Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->4)-Glc(beta 1->4)-Cer, Gal-Gal-Gal-Gal-Glu-Cer	C54H96N3O32FULLRCO	0	Golgi Apparatus
galgaltherm_hs	Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Gal(alpha 1->3)-Gal(alpha 1->3)-Gal(alpha 1->4)-Glc(beta 1->4)-Cer, Gal-Gal-Gal-G-Glu-Cer	C48H86N2O27FULLRCO	0	Golgi Apparatus
galgbside_hs	galactosylgloboside (homo sapiens)	Gal-GalNAc-Gal-Gal-Glc-Cer, Gb5Cer, SSEA-3, galactose globoside	C50H89N2O27FULLRCO	0	Golgi Apparatus
galgalside_hs	galactosyl glucosyl ceramide	(Gal)1 (Glc)1 (Cer)1, Cer-Glc-Gal, Gal-Glc-Cer	C30H56NO12FULLRCO	0	Cytosol
galgalside_hs	galactosyl glucosyl ceramide	(Gal)1 (Glc)1 (Cer)1, Cer-Glc-Gal, Gal-Glc-Cer	C30H56NO12FULLRCO	0	Golgi Apparatus
galgalside_hs	galactosyl glucosyl ceramide	(Gal)1 (Glc)1 (Cer)1, Cer-Glc-Gal, Gal-Glc-Cer	C30H56NO12FULLRCO	0	Lysosome
galside_hs	galactocerebroside (homo sapiens)	1-beta-D-galactoceramide, Cer-Gal	C24H46NO7FULLRCO	0	Cytosol
galside_hs	galactocerebroside (homo sapiens)	1-beta-D-galactoceramide, Cer-Gal	C24H46NO7FULLRCO	0	Golgi Apparatus
galside_hs	galactocerebroside (homo sapiens)	1-beta-D-galactoceramide, Cer-Gal	C24H46NO7FULLRCO	0	Lysosome
galt	Galactitol	Dulcitol, Dulcose	C6H14O6	0	Cytosol
galtherm_hs	Gal-Gal-Gal-Glc-Cer (homo sapiens)	Gal(alpha 1->3)-Gal(alpha 1->4)-Gal(beta 1->4)-Glc(beta 1->4)-Cer, Gal-Gal-Gal-Glu-Cer	C42H76NO22FULLRCO	0	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
gam	D-Glucosamine	2-Amino-2-deoxy-D-glucose, Chitosamine, GlcN	C6H14NO5	1	Cytosol
gam	D-Glucosamine	2-Amino-2-deoxy-D-glucose, Chitosamine, GlcN	C6H14NO5	1	Extracellular
gam6p	D-Glucosamine 6-phosphate	D-Glucosamine phosphate	C6H13NO8P	-1	Cytosol
gar	N1-(5-Phospho-D-ribose1)glycinamide	5'-Phosphoribosylglycinamide, GAR, Glycinamide ribonucleotide	C7H14N2O8P	-1	Cytosol
gbside_hs	globoside (homo sapiens)	GalNac-Gal-Gal-Glc-Cer, Gb4Cer, P-antigen	C44H79N2O22FULLRCO	0	Cytosol
gbside_hs	globoside (homo sapiens)	GalNac-Gal-Gal-Glc-Cer, Gb4Cer, P-antigen	C44H79N2O22FULLRCO	0	Extracellular
gbside_hs	globoside (homo sapiens)	GalNac-Gal-Gal-Glc-Cer, Gb4Cer, P-antigen	C44H79N2O22FULLRCO	0	Golgi Apparatus
gbside_hs	globoside (homo sapiens)	GalNac-Gal-Gal-Glc-Cer, Gb4Cer, P-antigen	C44H79N2O22FULLRCO	0	Lysosome
gcald	Glycolaldehyde	Hydroxyacetaldehyde	C2H4O2	0	Cytosol
gcald	Glycolaldehyde	Hydroxyacetaldehyde	C2H4O2	0	Mitochondria
gchola	glycocholate	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(carboxymethyl)-amide, Glycocholate, Glycocholic acid, bile acid	C26H43NO6	0	Cytosol
gchola	glycocholate	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(carboxymethyl)-amide, Glycocholate, Glycocholic acid, bile acid	C26H43NO6	0	Extracellular
gchola	glycocholate	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(carboxymethyl)-amide, Glycocholate, Glycocholic acid, bile acid	C26H43NO6	0	Peroxisome
gd1a_hs	GD1a (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
gd1alpha_hs	GD1a (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
gd1b_hs	GD1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
gd1b2_hs	GD1beta (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Cytosol
gd1b2_hs	GD1beta (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Extracellular
gd1b2_hs	GD1beta (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
gd1c_hs	GD1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Cytosol
gd1c_hs	GD1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Extracellular
gd1c_hs	GD1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C66H111N4O38FULLRCO	-2	Golgi Apparatus
gd2_hs	GD2 (homo sapiens)	(Gal)1 (GalNAc)1 (Glc)1 (Neu5Ac)2 (Cer)1	C60H101N4O33FULLRCO	-2	Golgi Apparatus
gd3_hs	GD3 (homo sapiens)	(Gal)1 (Glc)1 (Neu5Ac)2 (Cer)1, CD60a	C52H88N3O28FULLRCO	-2	Cytosol
gd3_hs	GD3 (homo sapiens)	(Gal)1 (Glc)1 (Neu5Ac)2 (Cer)1, CD60a	C52H88N3O28FULLRCO	-2	Golgi Apparatus
gdchola	glycochenodeoxycholate	Glycochenodeoxycholate, bile acid, bile salt	C26H43NO5	0	Cytosol
gdchola	glycochenodeoxycholate	Glycochenodeoxycholate, bile acid, bile salt	C26H43NO5	0	Extracellular
gdchola	glycochenodeoxycholate	Glycochenodeoxycholate, bile acid, bile salt	C26H43NO5	0	Peroxisome
gdp	GDP	Guanosine 5'-diphosphate, Guanosine diphosphate	C10H12N5O11P2	-3	Cytosol
gdp	GDP	Guanosine 5'-diphosphate, Guanosine diphosphate	C10H12N5O11P2	-3	Extracellular
gdp	GDP	Guanosine 5'-diphosphate, Guanosine diphosphate	C10H12N5O11P2	-3	Golgi Apparatus
gdp	GDP	Guanosine 5'-diphosphate, Guanosine diphosphate	C10H12N5O11P2	-3	Mitochondria
gdp	GDP	Guanosine 5'-diphosphate, Guanosine diphosphate	C10H12N5O11P2	-3	Nucleus
gdpddman	GDP-4-dehydro-6-deoxy-D-mannose	GDP-4-dehydro-6-deoxy-D-mannose, GDP-4-dehydro-6-deoxy-D-talose, GDP-4-dehydro-D-rhamnose, GDP-4-oxo-6-deoxy-D-mannose	C16H21N5O15P2	-2	Cytosol
gdpfuc	GDP-L-fucose		C16H23N5O15P2	-2	Cytosol
gdpfuc	GDP-L-fucose		C16H23N5O15P2	-2	Golgi Apparatus
gdpmann	GDP-D-mannose		C16H23N5O16P2	-2	Cytosol
ggdp	Geranylgeranyl diphosphate	GGPP, Geranylgeranyl pyrophosphate, all-trans-Geranylgeranyl diphosphate, all-trans-Geranylgeranyl pyrophosphate	C20H33O7P2	-3	Cytosol
ggn	primed glycogenin (glycogenin-8[1,4-Glc])		C48H81O41X	0	Cytosol
glac	D-glucurono-6,3-lactone		C6H8O6	0	Cytosol
glac	D-glucurono-6,3-lactone		C6H8O6	0	Mitochondria
glac	D-glucurono-6,3-lactone		C6H8O6	0	Endoplasmic Reticulum
gk1man	glucose-1,3-mannose oligosaccharide		C12H22O11	0	Golgi Apparatus
gk2man	(2)glucose-1,3-mannose oligosaccharide		C18H32O16	0	Golgi Apparatus
gk3man	glucose-1,2-(2)glucose-1,3-mannose oligosaccharide		C24H42O21	0	Golgi Apparatus
gk-D	D-Glucose	Dextrose, Glucose, Grape sugar, alpha-D-Glucose, beta-D-Glucose	C6H12O6	0	Cytosol
gk-D	D-Glucose	Dextrose, Glucose, Grape sugar, alpha-D-Glucose, beta-D-Glucose	C6H12O6	0	Extracellular
gk-D	D-Glucose	Dextrose, Glucose, Grape sugar, alpha-D-Glucose, beta-D-Glucose	C6H12O6	0	Golgi Apparatus
gk-D	D-Glucose	Dextrose, Glucose, Grape sugar, alpha-D-Glucose, beta-D-Glucose	C6H12O6	0	Lysosome
gk-D	D-Glucose	Dextrose, Glucose, Grape sugar, alpha-D-Glucose, beta-D-Glucose	C6H12O6	0	Endoplasmic Reticulum
gkr	D-Glucarate	D-Gluconic acid, D-Glucosaccharic acid, D-Saccharic acid, L-Gularic acid	C6H8O8	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
glcr	D-Glucarate	D-Glucaric acid, D-Glucosaccharic acid, D-Saccharic acid, L-Gularic acid	C6H8O8	-2	Mitochondria
glcur	D-Glucuronate	GlcA, Glucuronate, Glucuronic acid	C6H9O7	-1	Cytosol
glcur	D-Glucuronate	GlcA, Glucuronate, Glucuronic acid	C6H9O7	-1	Lysosome
glcur	D-Glucuronate	GlcA, Glucuronate, Glucuronic acid	C6H9O7	-1	Endoplasmic Reticulum
glcur1p	D-Glucuronate 1-phosphate	GlcA-1P	C6H8O10P	-3	Cytosol
gln-L	L-Glutamine	Gln, L-2-Aminoglutaramic acid	C5H10N2O3	0	Cytosol
gln-L	L-Glutamine	Gln, L-2-Aminoglutaramic acid	C5H10N2O3	0	Extracellular
gln-L	L-Glutamine	Gln, L-2-Aminoglutaramic acid	C5H10N2O3	0	Mitochondria
glu5p	L-Glutamate 5-phosphate	L-Glutamyl 5-phosphate	C5H8NO7P	-2	Mitochondria
glu5sa	L-Glutamate 5-semialdehyde	L-Glutamate gamma-semialdehyde	C5H9NO3	0	Cytosol
glu5sa	L-Glutamate 5-semialdehyde	L-Glutamate gamma-semialdehyde	C5H9NO3	0	Mitochondria
gluala	5-L-Glutamyl-L-alanine		C8H13N2O5	-1	Extracellular
glucys	gamma-L-Glutamyl-L-cysteine	5-L-Glutamyl-L-cysteine, L-gamma-Glutamylcysteine	C8H13N2O5S	-1	Cytosol
glu-L	L-Glutamate	Glu, L-Glutamic acid, L-Glutaminic acid	C5H8NO4	-1	Cytosol
glu-L	L-Glutamate	Glu, L-Glutamic acid, L-Glutaminic acid	C5H8NO4	-1	Extracellular
glu-L	L-Glutamate	Glu, L-Glutamic acid, L-Glutaminic acid	C5H8NO4	-1	Lysosome
glu-L	L-Glutamate	Glu, L-Glutamic acid, L-Glutaminic acid	C5H8NO4	-1	Mitochondria
glu-L	L-Glutamate	Glu, L-Glutamic acid, L-Glutaminic acid	C5H8NO4	-1	Endoplasmic Reticulum
gluside_hs	glucocerebroside (homo sapiens)	1-beta-D-glucoceramide, Cer-Glu, glucosyl ceramide	C24H46NO7FULLRCO	0	Cytosol
gluside_hs	glucocerebroside (homo sapiens)	1-beta-D-glucoceramide, Cer-Glu, glucosyl ceramide	C24H46NO7FULLRCO	0	Golgi Apparatus
gluside_hs	glucocerebroside (homo sapiens)	1-beta-D-glucoceramide, Cer-Glu, glucosyl ceramide	C24H46NO7FULLRCO	0	Lysosome
gluside_hs	glucocerebroside (homo sapiens)	1-beta-D-glucoceramide, Cer-Glu, glucosyl ceramide	C24H46NO7FULLRCO	0	Endoplasmic Reticulum
glutcoa	Glutaryl-CoA		C26H37N7O19P3S	-5	Mitochondria
glx	Glyoxylate	Acetic acid, Glyoxalate, Glyoxylic acid	C2H1O3	-1	Cytosol
glx	Glyoxylate	Acetic acid, Glyoxalate, Glyoxylic acid	C2H1O3	-1	Mitochondria
glx	Glyoxylate	Acetic acid, Glyoxalate, Glyoxylic acid	C2H1O3	-1	Peroxisome
gly	Glycine	Aminoacetic acid, Gly	C2H5NO2	0	Cytosol
gly	Glycine	Aminoacetic acid, Gly	C2H5NO2	0	Extracellular
gly	Glycine	Aminoacetic acid, Gly	C2H5NO2	0	Lysosome
gly	Glycine	Aminoacetic acid, Gly	C2H5NO2	0	Mitochondria
gly	Glycine	Aminoacetic acid, Gly	C2H5NO2	0	Peroxisome
glyald	D-Glyceraldehyde	(R)-glyceraldehyde	C3H6O3	0	Cytosol
glyb	Glycine betaine	Betaine, Trimethylaminoacetate	C5H11NO2	0	Cytosol
glyb	Glycine betaine	Betaine, Trimethylaminoacetate	C5H11NO2	0	Extracellular
glyb	Glycine betaine	Betaine, Trimethylaminoacetate	C5H11NO2	0	Mitochondria
glyc	Glycerol	1,2,3-trihydroxypropane, 3-propanetriol, Glycerin	C3H8O3	0	Cytosol
glyc	Glycerol	1,2,3-trihydroxypropane, 3-propanetriol, Glycerin	C3H8O3	0	Extracellular
glyc	Glycerol	1,2,3-trihydroxypropane, 3-propanetriol, Glycerin	C3H8O3	0	Mitochondria
glyc3p	Glycerol 3-phosphate	Glycerophosphoric acid, Phosphatidyl glycerol, sn-Glycerol 3-phosphate, sn-Gro-1-P	C3H7O6P	-2	Cytosol
glyc3p	Glycerol 3-phosphate	Glycerophosphoric acid, Phosphatidyl glycerol, sn-Glycerol 3-phosphate, sn-Gro-1-P	C3H7O6P	-2	Mitochondria
glyclt	Glycolate	Glycolic acid, Hydroxyacetic acid	C2H3O3	-1	Cytosol
glyclt	Glycolate	Glycolic acid, Hydroxyacetic acid	C2H3O3	-1	Mitochondria
glyclt	Glycolate	Glycolic acid, Hydroxyacetic acid	C2H3O3	-1	Peroxisome
glyc-R	(R)-Glycerate	D-Glycerate, Glycerate, Glyceric acid	C3H5O4	-1	Cytosol
glyc-S	(S)-Glycerate	L-glycerate	C3H5O4	-1	Cytosol
glyc-S	(S)-Glycerate	L-glycerate	C3H5O4	-1	Extracellular
glygn1	glycogen, structure 1 (glycogenin-1[1,4-Glc])		C66H111O56X	0	Cytosol
glygn2	glycogen, structure 2 (glycogenin-1,6-[7[1,4-Glc], 4[1,4-Glc]])		C66H111O56X	0	Cytosol
glygn2	glycogen, structure 2 (glycogenin-1,6-[7[1,4-Glc], 4[1,4-Glc]])		C66H111O56X	0	Extracellular
glygn3	glycogen, structure 3 (glycogenin-7[1,4-Glc])		C42H71O36X	0	Cytosol
glygn4	glycogen, structure 4 (glycogenin-1,6-[2[1,4-Glc], 1[4-Glc]])		C18H31O16X	0	Extracellular
glygn5	glycogen, structure 5 (glycogenin-2[1,4-Glc])		C12H21O11X	0	Extracellular
gm1_hs	ganglioside GM1 (homo sapiens)	Cer-Glc-Gal-NeuAc-GlaNAc-Gal	C55H95N3O30FULLRCO	-1	Golgi Apparatus
gm1a_hs	GM1alpha (homo sapiens)	III6NeuAc-Gg4Cer	C55H95N3O30FULLRCO	-1	Golgi Apparatus
gm1b_hs	GM1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)1 (Cer)1	C55H95N3O30FULLRCO	-1	Golgi Apparatus
gm2_hs	ganglioside GM2 (homo sapiens)	Cer-Glc-Gal-NeuAc-GalNAc	C49H85N3O25FULLRCO	-1	Golgi Apparatus
gm2a_hs	GM2alpha (homo sapiens)	(Gal)1 (GalNAc)1 (Glc)1 (Neu5Ac)1 (Cer)1	C49H85N3O25FULLRCO	-1	Golgi Apparatus
gm3_hs	ganglioside GM3 (homo sapiens)	Cer-Glc-Gal-NeuAc	C41H72N2O20FULLRCO	-1	Golgi Apparatus
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Cytosol
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Extracellular
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Golgi Apparatus
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Lysosome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Mitochondria
gmp	GMP	Guanosine 5'-monophosphate, Guanosine 5'-phosphate, Guanosine monophosphate, Guanylic acid	C10H12N5O8P	-2	Nucleus
gncore1	GlcNAc-alpha-1,4-Core 1		C22H37N2O15X	0	Golgi Apparatus
gncore2	GlcNAc-alpha-1,4-Core 2		C30H50N3O20X	0	Golgi Apparatus
gp1c_hs	GP1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Cytosol
gp1c_hs	GP1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Extracellular
gp1c_hs	GP1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Golgi Apparatus
gp1calpha_hs	GP1c alpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Cytosol
gp1calpha_hs	GP1c alpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Extracellular
gp1calpha_hs	GP1c alpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)5 (Cer)1	C99H159N7O62FULLRCO	-5	Golgi Apparatus
gpail_hs	D-glucosaminylphosphatidylinositol		C15H28NO13PFULLR2CO2FULLR2CO2	0	Cytosol
gpi_hs	glycophosphatidylinositol (GPI) anchor precursor (3-(phosphoethanolaminylo-mannosyl)-glucosaminyl-acylphosphatidylinositol) (H8)	{[PE-Man-].[PE-Man].[PE]}-Man-GlcN-acylPI	C55H106N4O38P4FULLR2CO2FULLR2CO2	0	Endoplasmic Reticulum
gpi_prot_hs	glycophosphatidylinositol (GPI)-anchored protein	{[(Prot-PE-Man),(PE-Man).[PE]]}-Man-GlcN-acylPI	C55H106N4O38P4FULLR2CO2FULLR2CO2X	0	Endoplasmic Reticulum
gpi_sig	glycophosphatidylinositol (GPI) signal sequence (C-terminal peptide)		Y	0	Endoplasmic Reticulum
gq1b_hs	GQ1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Cytosol
gq1b_hs	GQ1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Extracellular
gq1b_hs	GQ1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Golgi Apparatus
gq1balpha_hs	GQ1balpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Cytosol
gq1balpha_hs	GQ1balpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Extracellular
gq1balpha_hs	GQ1balpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Golgi Apparatus
gq1c_hs	GQ1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)4 (Cer)1	C88H143N6O54FULLRCO	-4	Golgi Apparatus
grdp	Geranyl diphosphate	GPP	C10H17O7P2	-3	Cytosol
grdp	Geranyl diphosphate	GPP	C10H17O7P2	-3	Peroxisome
gsn	Guanosine	Guanine riboside, rG	C10H13N5O5	0	Cytosol
gsn	Guanosine	Guanine riboside, rG	C10H13N5O5	0	Extracellular
gsn	Guanosine	Guanine riboside, rG	C10H13N5O5	0	Lysosome
gsn	Guanosine	Guanine riboside, rG	C10H13N5O5	0	Mitochondria
gt1a_hs	GT1a (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Cytosol
gt1a_hs	GT1a (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Extracellular
gt1a_hs	GT1a (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Golgi Apparatus
gt1alpha_hs	GT1alpha (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Golgi Apparatus
gt1b_hs	GT1b (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Golgi Apparatus
gt1c_hs	GT1c (homo sapiens)	(Gal)2 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C77H127N5O46FULLRCO	-3	Golgi Apparatus
gt2_hs	GT2 (homo sapiens)	(Gal)1 (GalNAc)1 (Glc)1 (Neu5Ac)3 (Cer)1	C71H117N5O41FULLRCO	-3	Golgi Apparatus
gt3_hs	GT3 (homo sapiens)	(Gal)1 (Glc)1 (Neu5Ac)3 (Cer)1	C63H104N4O36FULLRCO	-3	Cytosol
gt3_hs	GT3 (homo sapiens)	(Gal)1 (Glc)1 (Neu5Ac)3 (Cer)1	C63H104N4O36FULLRCO	-3	Golgi Apparatus
gthox	Oxidized glutathione	Glutathione disulfide, L-Glutathione oxidized	C20H30N6O12S2	-2	Cytosol
gthox	Oxidized glutathione	Glutathione disulfide, L-Glutathione oxidized	C20H30N6O12S2	-2	Extracellular
gthox	Oxidized glutathione	Glutathione disulfide, L-Glutathione oxidized	C20H30N6O12S2	-2	Mitochondria
gthrd	Reduced glutathione	5-L-Glutamyl-L-cysteinylglycine, Glutathione, N-(gamma-L-Glutamyl-L-cysteinyl)glycine, gamma-L-Glutamyl-L-cysteinyl-glycine	C10H16N3O6S	-1	Cytosol
gthrd	Reduced glutathione	5-L-Glutamyl-L-cysteinylglycine, Glutathione, N-(gamma-L-Glutamyl-L-cysteinyl)glycine, gamma-L-Glutamyl-L-cysteinyl-glycine	C10H16N3O6S	-1	Extracellular
gthrd	Reduced glutathione	5-L-Glutamyl-L-cysteinylglycine, Glutathione, N-(gamma-L-Glutamyl-L-cysteinyl)glycine, gamma-L-Glutamyl-L-cysteinyl-glycine	C10H16N3O6S	-1	Mitochondria
gthrd	Reduced glutathione	5-L-Glutamyl-L-cysteinylglycine, Glutathione, N-(gamma-L-Glutamyl-L-cysteinyl)glycine, gamma-L-Glutamyl-L-cysteinyl-glycine	C10H16N3O6S	-1	Endoplasmic Reticulum
gtp	GTP	Guanosine 5'-triphosphate	C10H12N5O14P3	-4	Cytosol
gtp	GTP	Guanosine 5'-triphosphate	C10H12N5O14P3	-4	Extracellular
gtp	GTP	Guanosine 5'-triphosphate	C10H12N5O14P3	-4	Mitochondria
gtp	GTP	Guanosine 5'-triphosphate	C10H12N5O14P3	-4	Nucleus
gua	Guanine	2-Amino-6-hydroxypurine, 2-Aminohypoxanthine, G	C5H5N5O	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
gua	Guanine	2-Amino-6-hydroxypurine, 2-Aminohypoxanthine, G	C5H5N5O	0	Extracellular
gudac	Guanidinoacetate	Glycocyamine, Guanidinoacetic acid, Guanidoacetate, N-Amidinoglycine	C3H7N3O2	0	Cytosol
gullac	L-Gulono-1,4-lactone	L-Gulonic acid gamma-lactone, L-Gulono-gamma-lactone, L-Gulonolactone, gamma-Gulonolactone	C6H10O6	0	Cytosol
gullac	L-Gulono-1,4-lactone	L-Gulonic acid gamma-lactone, L-Gulono-gamma-lactone, L-Gulonolactone, gamma-Gulonolactone	C6H10O6	0	Endoplasmic Reticulum
guln	L-Gulonate	Gulonate, Gulonic acid, L-Gulonic acid	C6H11O7	-1	Cytosol
guln	L-Gulonate	Gulonate, Gulonic acid, L-Gulonic acid	C6H11O7	-1	Endoplasmic Reticulum
h	H+	Hydrogen Ion, Proton	H	1	Cytosol
h	H+	Hydrogen Ion, Proton	H	1	Extracellular
h	H+	Hydrogen Ion, Proton	H	1	Golgi Apparatus
h	H+	Hydrogen Ion, Proton	H	1	Lysosome
h	H+	Hydrogen Ion, Proton	H	1	Mitochondria
h	H+	Hydrogen Ion, Proton	H	1	Nucleus
h	H+	Hydrogen Ion, Proton	H	1	Endoplasmic Reticulum
h	H+	Hydrogen Ion, Proton	H	1	Peroxisome
h2co3	carbonic acid		H2CO3	0	Cytosol
h2co3	carbonic acid		H2CO3	0	Mitochondria
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Cytosol
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Extracellular
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Golgi Apparatus
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Lysosome
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Mitochondria
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Nucleus
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Endoplasmic Reticulum
h2o	H2O	Dihydrogen oxide, Water	H2O	0	Peroxisome
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Cytosol
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Extracellular
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Lysosome
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Mitochondria
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Nucleus
h2o2	Hydrogen peroxide	H2O2, hydrogen dioxide, peroxide	H2O2	0	Peroxisome
ha	hyaluronan	Hyaluronate, Hyaluronic acid	C28H40N2O22	-2	Extracellular
ha	hyaluronan	Hyaluronate, Hyaluronic acid	C28H40N2O22	-2	Lysosome
ha_deg1	hyaluronan degradation product 1		C22H33N2O16	-1	Lysosome
ha_pre1	hyaluronan biosynthesis, precursor 1		C14H20N011	-1	Extracellular
ha_pre1	hyaluronan biosynthesis, precursor 1		C14H20N011	-1	Lysosome
hco3	Bicarbonate	Acid carbonate, HCO3-, Hydrogencarbonate	CHO3	-1	Cytosol
hco3	Bicarbonate	Acid carbonate, HCO3-, Hydrogencarbonate	CHO3	-1	Extracellular
hco3	Bicarbonate	Acid carbonate, HCO3-, Hydrogencarbonate	CHO3	-1	Mitochondria
hcoumarin	hydroxy coumarin	7 hydroxy coumarin	C9H6O3	0	Cytosol
hcoumarin	hydroxy coumarin	7 hydroxy coumarin	C9H6O3	0	Extracellular
hcys-L	L-Homocysteine	L-2-Amino-4-mercaptobutyric acid, L-Homocysteine	C4H9NO2S	0	Cytosol
hdca	Hexadecanoate (n-C16:0)	Cetylic acid, Hexadecanoic acid, Hexadecylic acid, Palmitic acid, palmitate	C16H31O2	-1	Cytosol
hdca	Hexadecanoate (n-C16:0)	Cetylic acid, Hexadecanoic acid, Hexadecylic acid, Palmitic acid, palmitate	C16H31O2	-1	Extracellular
hdca	Hexadecanoate (n-C16:0)	Cetylic acid, Hexadecanoic acid, Hexadecylic acid, Palmitic acid, palmitate	C16H31O2	-1	Endoplasmic Reticulum
hdca	Hexadecanoate (n-C16:0)	Cetylic acid, Hexadecanoic acid, Hexadecylic acid, Palmitic acid, palmitate	C16H31O2	-1	Peroxisome
hdcea	Hexadecenoate (n-C16:1)	(9Z)-Hexadecenoic acid, Palmitoleic acid, cis-9-Hexadecenoic acid, hexadecenoic acid	C16H29O2	-1	Cytosol
hdcea	Hexadecenoate (n-C16:1)	(9Z)-Hexadecenoic acid, Palmitoleic acid, cis-9-Hexadecenoic acid, hexadecenoic acid	C16H29O2	-1	Extracellular
hdcecm	Hexadecenyl carnitine		C23H43NO4	0	Cytosol
hdcecm	Hexadecenyl carnitine		C23H43NO4	0	Mitochondria
hdcoa	Hexadecenoyl-CoA (n-C16:1CoA)	(2E)-Hexadecenoyl-CoA, palmitoleic coenzyme A, trans-2-Hexadecenoyl-CoA, trans-Hexadec-2-enoyl-CoA	C37H60N7O17P3S	-4	Cytosol
hdcoa	Hexadecenoyl-CoA (n-C16:1CoA)	(2E)-Hexadecenoyl-CoA, palmitoleic coenzyme A, trans-2-Hexadecenoyl-CoA, trans-Hexadec-2-enoyl-CoA	C37H60N7O17P3S	-4	Mitochondria
hdd2coa	trans-Hexadec-2-enoyl-CoA		C37H60N7O17P3S	-4	Cytosol
hdd2coa	trans-Hexadec-2-enoyl-CoA		C37H60N7O17P3S	-4	Mitochondria
hdd2coa	trans-Hexadec-2-enoyl-CoA		C37H60N7O17P3S	-4	Peroxisome
hdd2cm	trans-Hexadec-2-enoyl carnitine		C23H43NO4	0	Cytosol
hdd2cm	trans-Hexadec-2-enoyl carnitine		C23H43NO4	0	Mitochondria
hdeACP	cis-hexadec-9-enoyl-[acyl-carrier protein] (n-C16:1)	Hexadecenoyl-ACP (n-C16:1ACP), cis-palmitol-9-oyl-[acyl-carrier protein] (n-C16:1)	C27H49N2O8PRS	-1	Cytosol
hestratriol	4,17 dihydroxy estradiol	4 hydroxy 17 beta estradiol	C18H24O3	0	Cytosol
hestratriol	4,17 dihydroxy estradiol	4 hydroxy 17 beta estradiol	C18H24O3	0	Extracellular
hestratriol	4,17 dihydroxy estradiol	4 hydroxy 17 beta estradiol	C18H24O3	0	Endoplasmic Reticulum
hexc	hexacosanoate (n-C26:0)	cerotic acid, hexacosanoic acid	C26H51O2	-1	Cytosol
hexc	hexacosanoate (n-C26:0)	cerotic acid, hexacosanoic acid	C26H51O2	-1	Extracellular
hexccoa	Hexacosanoyl-CoA (n-C26:0CoA)	cerotic acid coenzyme a, cerotyl-CoA	C47H82N7O17P3S	-4	Cytosol
hexccoa	Hexacosanoyl-CoA (n-C26:0CoA)	cerotic acid coenzyme a, cerotyl-CoA	C47H82N7O17P3S	-4	Mitochondria
hexccoa	Hexacosanoyl-CoA (n-C26:0CoA)	cerotic acid coenzyme a, cerotyl-CoA	C47H82N7O17P3S	-4	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
hexccm	hexacosanoyl carnitine		C33H65NO4	0	Cytosol
hexccm	hexacosanoyl carnitine		C33H65NO4	0	Mitochondria
hgntis	Homogentisate	2,5-Dihydroxyphenylacetate, 2,5-Dihydroxyphenylacetic acid, Homogentisic acid	C8H7O4	-1	Cytosol
his-L	L-Histidine	(S)-alpha-Amino-1H-imidazole-4-propionic acid, Glyoxaline-5-alanine, His	C6H9N3O2	0	Cytosol
his-L	L-Histidine	(S)-alpha-Amino-1H-imidazole-4-propionic acid, Glyoxaline-5-alanine, His	C6H9N3O2	0	Extracellular
hista	Histamine		C5H10N3	1	Cytosol
hista	Histamine		C5H10N3	1	Extracellular
hLkynr	3-Hydroxy-L-kyurenine		C10H12N2O4	0	Cytosol
hmbil	Hydroxymethylbilane		C40H38N4O17	-8	Cytosol
hmgcoa	Hydroxymethylglutaryl-CoA	(S)-3-Hydroxy-3-methylglutaryl-CoA, 3-Hydroxy-3-methylglutaryl-CoA, HMG-CoA, Hydroxymethylglutaroyl coenzyme A	C27H39N7O20P3S	-5	Cytosol
hmgcoa	Hydroxymethylglutaryl-CoA	(S)-3-Hydroxy-3-methylglutaryl-CoA, 3-Hydroxy-3-methylglutaryl-CoA, HMG-CoA, Hydroxymethylglutaroyl coenzyme A	C27H39N7O20P3S	-5	Mitochondria
hmgcoa	Hydroxymethylglutaryl-CoA	(S)-3-Hydroxy-3-methylglutaryl-CoA, 3-Hydroxy-3-methylglutaryl-CoA, HMG-CoA, Hydroxymethylglutaroyl coenzyme A	C27H39N7O20P3S	-5	Endoplasmic Reticulum
hmgcoa	Hydroxymethylglutaryl-CoA	(S)-3-Hydroxy-3-methylglutaryl-CoA, 3-Hydroxy-3-methylglutaryl-CoA, HMG-CoA, Hydroxymethylglutaroyl coenzyme A	C27H39N7O20P3S	-5	Peroxisome
hnifedipine	hydroxy nifedipine		C17H18N2O7	0	Cytosol
hom-L	L-Homoserine	2-Amino-4-hydroxybutyric acid	C4H9NO3	0	Cytosol
hom-L	L-Homoserine	2-Amino-4-hydroxybutyric acid	C4H9NO3	0	Extracellular
homoval	Homovanillic acid		C9H9O4	-1	Cytosol
hpdca	heptadecanoate	Heptadecanoic acid, Margeric acid, n-Heptadecanoic Acid,	C17H33O2	-1	Cytosol
hpdca	heptadecanoate	Heptadecanoic acid, Margeric acid, n-Heptadecanoic Acid,	C17H33O2	-1	Extracellular
hpdcacoa	heptadecanoyl coa	Heptadecanoic acid coa, Margeric acid coa, n-Heptadecanoic Acid coenzyme a	C38H64N7O17P3S	-4	Cytosol
hpdcacoa	heptadecanoyl coa	Heptadecanoic acid coa, Margeric acid coa, n-Heptadecanoic Acid coenzyme a	C38H64N7O17P3S	-4	Mitochondria
hpdcaern	heptadecanoyl carnitine	heptadecanoate carnitine, heptadecanoyl acid carnitine	C24H47NO4	0	Cytosol
hpdcaern	heptadecanoyl carnitine	heptadecanoate carnitine, heptadecanoyl acid carnitine	C24H47NO4	0	Mitochondria
hpyr	Hydroxypyruvate	3-Hydroxypyruvate, 3-Hydroxypyruvic acid, Hydroxypyruvic acid	C3H3O4	-1	Cytosol
hpyr	Hydroxypyruvate	3-Hydroxypyruvate, 3-Hydroxypyruvic acid, Hydroxypyruvic acid	C3H3O4	-1	Mitochondria
hpyr	Hydroxypyruvate	3-Hydroxypyruvate, 3-Hydroxypyruvic acid, Hydroxypyruvic acid	C3H3O4	-1	Peroxisome
hretn	4 hydroxy retinoic acid		C20H27O3	-1	Cytosol
hretn	4 hydroxy retinoic acid		C20H27O3	-1	Nucleus
hs	heparan sulfate, free chain		C79H114N5O102S12	-13	Lysosome
hs_deg1	heparan sulfate, degradation product 1		C79H115N5O99S11	-12	Lysosome
hs_deg10	heparan sulfate, degradation product 10		C55H80N3O70S8	-9	Lysosome
hs_deg11	heparan sulfate, degradation product 11		C55H81N3O67S7	-8	Lysosome
hs_deg12	heparan sulfate, degradation product 12		C55H82N3O64S6	-7	Lysosome
hs_deg13	heparan sulfate, degradation product 13		C55H83N3O61S5	-6	Lysosome
hs_deg14	heparan sulfate, degradation product 14		C57H84N3O62S5	-7	Lysosome
hs_deg15	heparan sulfate, degradation product 15		C49H71N2O57S5	-7	Lysosome
hs_deg16	heparan sulfate, degradation product 16		C49H72N2O54S4	-6	Lysosome
hs_deg17	heparan sulfate, degradation product 17		C43H65N2O48S4	-5	Lysosome
hs_deg18	heparan sulfate, degradation product 18		C43H66N2O45S3	-4	Lysosome
hs_deg19	heparan sulfate, degradation product 19		C43H67N2O42S2	-3	Lysosome
hs_deg2	heparan sulfate, degradation product 2		C79H116N5O96S10	-11	Lysosome
hs_deg20	heparan sulfate, degradation product 20		C45H68N2O43S2	-4	Lysosome
hs_deg21	heparan sulfate, degradation product 21		C37H55N3O38S2	-4	Lysosome
hs_deg22	heparan sulfate, degradation product 22		C37H56N3O35S	-3	Lysosome
hs_deg23	heparan sulfate, degradation product 23		C31H49N2O29S	-2	Lysosome
hs_deg24	heparan sulfate, degradation product 24		C31H50N2O26	-1	Lysosome
hs_deg25	heparan sulfate, degradation product 25		C23H37O21	-1	Lysosome
hs_deg3	heparan sulfate, degradation product 3		C81H117N5O97S10	-12	Lysosome
hs_deg4	heparan sulfate, degradation product 4		C73H104N4O92S10	-12	Lysosome
hs_deg5	heparan sulfate, degradation product 5		C67H97N4O86S10	-11	Lysosome
hs_deg6	heparan sulfate, degradation product 6		C67H98N4O83S9	-10	Lysosome
hs_deg7	heparan sulfate, degradation product 7		C67H99N4O80S8	-9	Lysosome
hs_deg8	heparan sulfate, degradation product 8		C69H100N4O81S8	-10	Lysosome
hs_deg9	heparan sulfate, degradation product 9		C61H87N3O76S8	-10	Lysosome
hs_pre1	heparan sulfate, precursor 1	GlcNAc-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C31H49NO25X	-1	Golgi Apparatus
hs_pre10	heparan sulfate, precursor 10	(GlcN2S-GlcA)4-GlcNAc-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C79H121N5O77S4X	-5	Golgi Apparatus
hs_pre11	heparan sulfate, precursor 11	(GlcN2S-IdoA-GlcN2S-GlcA)2-GlcNAc-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C79H121N5O77S4X	-5	Golgi Apparatus
hs_pre12	heparan sulfate, precursor 12	GlcN2S-IdoA-GlcN2S-GlcA2S-GlcN2S-IdoA2S-GlcN2S-GlcA-GlcNAc-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C79H119N5O83S6X	-7	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
hs_pre13	heparan sulfate, precursor 13	GlcN2S-IdoA-GlcN2,6diS-GlcA2S-GlcN2,6diS-IdoA2S-GlcN2,6diS-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C79H116N5O92S9X	-10	Golgi Apparatus
hs_pre14	heparan sulfate, precursor 14		C79H115N5O95S10X	-11	Golgi Apparatus
hs_pre15	heparan sulfate, precursor 15		C79H114N5O98S11X	-12	Golgi Apparatus
hs_pre2	heparan sulfate, precursor 2	GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C37H56N031X	-2	Golgi Apparatus
hs_pre3	heparan sulfate, precursor 3	GlcNac-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C45H69N2036X	-2	Golgi Apparatus
hs_pre4	heparan sulfate, precursor 4	GlcA-GlcNac-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C51H76N2042X	-3	Golgi Apparatus
hs_pre5	heparan sulfate, precursor 5	(GlcNac-GlcA)2-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C59H89N3047X	-3	Golgi Apparatus
hs_pre6	heparan sulfate, precursor 6	GlcA-(GlcNac-GlcA)2-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C65H96N3053X	-4	Golgi Apparatus
hs_pre7	heparan sulfate, precursor 7	(GlcNac-GlcA)3-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C73H109N4058X	-4	Golgi Apparatus
hs_pre8	heparan sulfate, precursor 8	GlcA-(GlcNac-GlcA)3-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C79H116N4064X	-5	Golgi Apparatus
hs_pre9	heparan sulfate, precursor 9	(GlcNac-GlcA)4-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein)	C87H129N5069X	-5	Golgi Apparatus
hspg	heparan sulfate proteoglycan	GlcN2S-IdoA-GlcN2,6diS-GlcA2S-GlcN2,3,6triS-IdoA2S-GlcN2,6diS-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein), Heparan sulfate, Heparin monosulfate, Heparin sulfate, Heparitin sulfate;	C79H113N5O101S12X	-13	Extracellular
hspg	heparan sulfate proteoglycan	GlcN2S-IdoA-GlcN2,6diS-GlcA2S-GlcN2,3,6triS-IdoA2S-GlcN2,6diS-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein), Heparan sulfate, Heparin monosulfate, Heparin sulfate, Heparitin sulfate;	C79H113N5O101S12X	-13	Golgi Apparatus
hspg	heparan sulfate proteoglycan	GlcN2S-IdoA-GlcN2,6diS-GlcA2S-GlcN2,3,6triS-IdoA2S-GlcN2,6diS-GlcA-GlcNac-GlcA-Gal-Gal-Xyl-L-Ser (protein), Heparan sulfate, Heparin monosulfate, Heparin sulfate, Heparitin sulfate;	C79H113N5O101S12X	-13	Lysosome
htaxol	hydroxylated taxol	6 alpha hydroxy paclitaxel, 6 alpha hydroxy taxol	C47H31NO15	0	Cytosol
htaxol	hydroxylated taxol	6 alpha hydroxy paclitaxel, 6 alpha hydroxy taxol	C47H31NO15	0	Extracellular
hxan	Hypoxanthine	1,7-Dihydro-6H-purin-6-one, 6-Hydroxypurine, Purine-6-ol	C5H4N4O	0	Cytosol
hxan	Hypoxanthine	1,7-Dihydro-6H-purin-6-one, 6-Hydroxypurine, Purine-6-ol	C5H4N4O	0	Extracellular
hxan	Hypoxanthine	1,7-Dihydro-6H-purin-6-one, 6-Hydroxypurine, Purine-6-ol	C5H4N4O	0	Lysosome
hxan	Hypoxanthine	1,7-Dihydro-6H-purin-6-one, 6-Hydroxypurine, Purine-6-ol	C5H4N4O	0	Peroxisome
hxdcal	Hexadecanal	16-Hexadecanal, Palmitaldehyde	C16H32O	0	Endoplasmic Reticulum
hypaur	Hypotaurine	2-Aminoethanesulfonic acid	C2H6NO2S	-1	Cytosol
i	Iodide	I-	I	-1	Cytosol
i	Iodide	I-	I	-1	Extracellular
ibcoa	Isobutyryl-CoA	2-Methylpropanoyl-CoA, 2-Methylpropionyl-CoA	C25H38N7O17P3S	-4	Mitochondria
icit	Isocitrate	1-Hydroxypropane-1, 1-Hydroxytricarballic acid, 2, 3-tricarboxylic acid, Isocitric acid	C6H5O7	-3	Cytosol
icit	Isocitrate	1-Hydroxypropane-1, 1-Hydroxytricarballic acid, 2, 3-tricarboxylic acid, Isocitric acid	C6H5O7	-3	Mitochondria
icit	Isocitrate	1-Hydroxypropane-1, 1-Hydroxytricarballic acid, 2, 3-tricarboxylic acid, Isocitric acid	C6H5O7	-3	Peroxisome
id3acald	Indole-3-acetaldehyde	2-(Indol-3-yl)acetaldehyde, Indoleacetaldehyde	C10H9NO	0	Cytosol
id3acald	Indole-3-acetaldehyde	2-(Indol-3-yl)acetaldehyde, Indoleacetaldehyde	C10H9NO	0	Mitochondria
idour	L-Iduronate	D-Ido-hexuronic acid, IdoA, L-Iduronic acid	C6H9O7	-1	Cytosol
idour	L-Iduronate	D-Ido-hexuronic acid, IdoA, L-Iduronic acid	C6H9O7	-1	Lysosome
idp	IDP	5'-inosinate diphosphate, Inosine 5'-diphosphate, Inosine diphosphate	C10H11N4O11P2	-3	Cytosol
idp	IDP	5'-inosinate diphosphate, Inosine 5'-diphosphate, Inosine diphosphate	C10H11N4O11P2	-3	Extracellular
idp	IDP	5'-inosinate diphosphate, Inosine 5'-diphosphate, Inosine diphosphate	C10H11N4O11P2	-3	Mitochondria
idp	IDP	5'-inosinate diphosphate, Inosine 5'-diphosphate, Inosine diphosphate	C10H11N4O11P2	-3	Nucleus
ile-L	L-Isoleucine	2-Amino-3-methylvaleric acid, Ile	C6H13NO2	0	Cytosol
ile-L	L-Isoleucine	2-Amino-3-methylvaleric acid, Ile	C6H13NO2	0	Extracellular
ile-L	L-Isoleucine	2-Amino-3-methylvaleric acid, Ile	C6H13NO2	0	Mitochondria
im4ac	Imidazole-4-acetate	4-Imidazoleacetate, Imidazoleacetic acid	C5H5N2O2	-1	Cytosol
im4ac	Imidazole-4-acetate	4-Imidazoleacetate, Imidazoleacetic acid	C5H5N2O2	-1	Mitochondria
im4act	Imidazole-4-acetaldehyde	Imidazole acetaldehyde	C5H6N2O	0	Cytosol
im4act	Imidazole-4-acetaldehyde	Imidazole acetaldehyde	C5H6N2O	0	Mitochondria
imp	IMP	5'-Inosinate, 5'-Inosine monophosphate, 5'-Inosinic acid, Inosine 5'-monophosphate, Inosine 5'-phosphate, Inosine monophosphate, Inosinic acid	C10H11N4O8P	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
imp	IMP	5'-Inosinate, 5'-Inosine monophosphate, 5'-Inosinic acid, Inosine 5'-monophosphate, Inosine 5'-phosphate, Inosine monophosphate, Inosinic acid	C10H11N4O8P	-2	Extracellular
imp	IMP	5'-Inosinate, 5'-Inosine monophosphate, 5'-Inosinic acid, Inosine 5'-monophosphate, Inosine 5'-phosphate, Inosine monophosphate, Inosinic acid	C10H11N4O8P	-2	Mitochondria
ind3ac	Indole-3-acetate	3-indoleacetate, Indole-3-acetic acid, Indoleacetate, Indoleacetic acid	C10H8NO2	-1	Cytosol
ind3ac	Indole-3-acetate	3-indoleacetate, Indole-3-acetic acid, Indoleacetate, Indoleacetic acid	C10H8NO2	-1	Mitochondria
inost	myo-Inositol	1D-myo-Inositol, 1L-myo-Inositol, Bios I, Cyclohexitol, D-myo-Inositol, Dambosose, Inositol, myo-Inositol, Meat sugar, meso-Inositol	C6H12O6	0	Cytosol
inost	myo-Inositol	1D-myo-Inositol, 1L-myo-Inositol, Bios I, Cyclohexitol, D-myo-Inositol, Dambosose, Inositol, myo-Inositol, Meat sugar, meso-Inositol	C6H12O6	0	Extracellular
ins	Inosine	Hypoxanthine ribonucleoside	C10H12N4O5	0	Cytosol
ins	Inosine	Hypoxanthine ribonucleoside	C10H12N4O5	0	Extracellular
ins	Inosine	Hypoxanthine ribonucleoside	C10H12N4O5	0	Lysosome
ins	Inosine	Hypoxanthine ribonucleoside	C10H12N4O5	0	Mitochondria
iodine	Iodine	I2	I2	0	Cytosol
ipdp	Isopentenyl diphosphate	Isopentenyl pyrophosphate, Isoprenyl pyrophosphate, delta3-Isopentenyl diphosphate, delta3-methyl-3-butenyl diphosphate	C5H9O7P2	-3	Cytosol
ipdp	Isopentenyl diphosphate	Isopentenyl pyrophosphate, Isoprenyl pyrophosphate, delta3-Isopentenyl diphosphate, delta3-methyl-3-butenyl diphosphate	C5H9O7P2	-3	Peroxisome
itaccoa	Itaconyl-CoA		C26H35N7O19P3S	-5	Mitochondria
itacon	Itaconate	Itaconic acid, Methylene succinic acid	C5H4O4	-2	Mitochondria
itp	ITP	Inosine 5'-triphosphate, Inosine triphosphate, Inosine triphosphosphate	C10H11N4O14P3	-4	Cytosol
itp	ITP	Inosine 5'-triphosphate, Inosine triphosphate, Inosine triphosphosphate	C10H11N4O14P3	-4	Mitochondria
itp	ITP	Inosine 5'-triphosphate, Inosine triphosphate, Inosine triphosphosphate	C10H11N4O14P3	-4	Nucleus
ivcoa	Isovaleryl-CoA	3-Methylbutanoyl-CoA	C26H40N7O17P3S	-4	Mitochondria
k	potassium	K+, Potassium	K	1	Cytosol
k	potassium	K+, Potassium	K	1	Extracellular
k	potassium	K+, Potassium	K	1	Golgi Apparatus
kdn	2-keto-3-deoxy-D-glycero-D-galactonic acid	3-deoxy-D-glycero-D-galacto-nonulsonic acid, a-D-KDN, deaminouramic acid	C9H15O9	-1	Cytosol
kdn	2-keto-3-deoxy-D-glycero-D-galactonic acid 9-phosphate		C9H14O12P	-3	Cytosol
ksi	keratan sulfate 1		C247H393N17O213S12X	-13	Extracellular
ksi	keratan sulfate 1		C247H393N17O213S12X	-13	Golgi Apparatus
ksi	keratan sulfate 1		C247H393N17O213S12X	-13	Lysosome
ksi_deg1	keratan sulfate 1, degradation product 1		C241H383N17O209S12X	-13	Extracellular
ksi_deg1	keratan sulfate 1, degradation product 1		C241H383N17O209S12X	-13	Lysosome
ksi_deg10	keratan sulfate 1, degradation product 10		C188H302N13O163S9	-9	Lysosome
ksi_deg11	keratan sulfate 1, degradation product 11		C180H289N12O158S9	9	Lysosome
ksi_deg12	keratan sulfate 1, degradation product 12		C174H279N12O153S9	-9	Lysosome
ksi_deg13	keratan sulfate 1, degradation product 13		C174H280N12O150S8	-8	Lysosome
ksi_deg14	keratan sulfate 1, degradation product 14		C166H267N11O145S8	-8	Lysosome
ksi_deg15	keratan sulfate 1, degradation product 15		C160H257N11O140S8	-8	Lysosome
ksi_deg16	keratan sulfate 1, degradation product 16		C160H258N11O137S7	-7	Lysosome
ksi_deg17	keratan sulfate 1, degradation product 17		C152H245N10O132S7	-7	Lysosome
ksi_deg18	keratan sulfate 1, degradation product 18		C146H235N10O127S7	-7	Lysosome
ksi_deg19	keratan sulfate 1, degradation product 19		C146H236N10O124S6	-6	Lysosome
ksi_deg2	keratan sulfate 1, degradation product 2		C241H384N17O210S12	-13	Lysosome
ksi_deg20	keratan sulfate 1, degradation product 20		C138H223N9O119S6	-6	Lysosome
ksi_deg21	keratan sulfate 1, degradation product 21		C132H213N9O114S6	-6	Lysosome
ksi_deg22	keratan sulfate 1, degradation product 22		C132H214N9O111S5	-5	Lysosome
ksi_deg23	keratan sulfate 1, degradation product 23		C124H201N8O106S5	-5	Lysosome
ksi_deg24	keratan sulfate 1, degradation product 24		C118H191N8O101S5	-5	Lysosome
ksi_deg25	keratan sulfate 1, degradation product 25		C118H192N8O98S4	-4	Lysosome
ksi_deg26	keratan sulfate 1, degradation product 26		C110H179N7O93S4	-4	Lysosome
ksi_deg27	keratan sulfate 1, degradation product 27		C104H169N7O88S4	-4	Lysosome
ksi_deg28	keratan sulfate 1, degradation product 28		C104H170N7O85S3	-3	Lysosome
ksi_deg29	keratan sulfate 1, degradation product 29		C96H157N6O80S3	-3	Lysosome
ksi_deg3	keratan sulfate 1, degradation product 3		C233H371N16O205S12	-13	Lysosome
ksi_deg30	keratan sulfate 1, degradation product 30		C90H147N6O75S3	-3	Lysosome
ksi_deg31	keratan sulfate 1, degradation product 31		C90H148N6O72S2	-2	Lysosome
ksi_deg32	keratan sulfate 1, degradation product 32		C82H135N5O67S2	-2	Lysosome
ksi_deg33	keratan sulfate 1, degradation product 33		C76H125N5O62S2	-2	Lysosome
ksi_deg34	keratan sulfate 1, degradation product 34		C76H126N5O59S1	-1	Lysosome
ksi_deg35	keratan sulfate 1, degradation product 35		C68H113N4O54S1	-1	Lysosome
ksi_deg36	keratan sulfate 1, degradation product 36		C62H103N4O49S1	-1	Lysosome
ksi_deg37	keratan sulfate 1, degradation product 37		C62H104N4O46	0	Lysosome
ksi_deg38	keratan sulfate 1, degradation product 38		C54H91N3O41	0	Lysosome
ksi_deg39	keratan sulfate 1, degradation product 39		C48H81N3O36	0	Lysosome
ksi_deg4	keratan sulfate 1, degradation product 4		C222H355N15O197S12	-12	Lysosome
ksi_deg40	keratan sulfate 1, degradation product 40		C40H68N2O31	0	Lysosome
ksi_deg41	keratan sulfate 1, degradation product 41		C34H58N2O26	0	Lysosome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
kxi_deg5	keratan sulfate I, degradation product 5		C22H356N15O194S11	-11	Lysosome
kxi_deg6	keratan sulfate I, degradation product 6		C210H336N15O184S11	-11	Lysosome
kxi_deg7	keratan sulfate I, degradation product 7		C210H337N15O181S10	-10	Lysosome
kxi_deg8	keratan sulfate I, degradation product 8		C194H311N13O171S10	-10	Lysosome
kxi_deg9	keratan sulfate I, degradation product 9		C188H301N13O166S10	-10	Lysosome
kxi_pre1	keratan sulfate I biosynthesis, precursor 1		C79H129N5O57X	-1	Golgi Apparatus
kxi_pre10	keratan sulfate I biosynthesis, precursor 10		C129H209N9O98S2X	-3	Golgi Apparatus
kxi_pre11	keratan sulfate I biosynthesis, precursor 11		C129H208N9O101S3X	-4	Golgi Apparatus
kxi_pre12	keratan sulfate I biosynthesis, precursor 12		C135H218N9O106S3X	-4	Golgi Apparatus
kxi_pre13	keratan sulfate I biosynthesis, precursor 13		C143H231N10O111S3X	-4	Golgi Apparatus
kxi_pre14	keratan sulfate I biosynthesis, precursor 14		C143H230N10O114S4X	-5	Golgi Apparatus
kxi_pre15	keratan sulfate I biosynthesis, precursor 15		C149H240N10O119S4X	-5	Golgi Apparatus
kxi_pre16	keratan sulfate I biosynthesis, precursor 16		C157H253N11O124S4X	-5	Golgi Apparatus
kxi_pre17	keratan sulfate I biosynthesis, precursor 17		C157H252N11O127S5X	-6	Golgi Apparatus
kxi_pre18	keratan sulfate I biosynthesis, precursor 18		C163H262N11O132S5X	-6	Golgi Apparatus
kxi_pre19	keratan sulfate I biosynthesis, precursor 19		C171H275N12O137S5X	-6	Golgi Apparatus
kxi_pre2	keratan sulfate I biosynthesis, precursor 2		C87H142N6O62X	-1	Golgi Apparatus
kxi_pre20	keratan sulfate I biosynthesis, precursor 20		C171H274N12O140S6X	-7	Golgi Apparatus
kxi_pre21	keratan sulfate I biosynthesis, precursor 21		C177H284N12O145S6X	-7	Golgi Apparatus
kxi_pre22	keratan sulfate I biosynthesis, precursor 22		C185H297N13O150S6X	-7	Golgi Apparatus
kxi_pre23	keratan sulfate I biosynthesis, precursor 23		C185H296N13O153S7X	-8	Golgi Apparatus
kxi_pre24	keratan sulfate I biosynthesis, precursor 24		C191H306N13O158S7X	-8	Golgi Apparatus
kxi_pre25	keratan sulfate I biosynthesis, precursor 25		C199H319N14O163S7X	-8	Golgi Apparatus
kxi_pre26	keratan sulfate I biosynthesis, precursor 26		C199H318N14O166S8X	-9	Golgi Apparatus
kxi_pre27	keratan sulfate I biosynthesis, precursor 27		C205H328N14O171S8X	-9	Golgi Apparatus
kxi_pre28	keratan sulfate I biosynthesis, precursor 28		C213H341N15O176S8X	-9	Golgi Apparatus
kxi_pre29	keratan sulfate I biosynthesis, precursor 29		C213H340N15O179S9X	-10	Golgi Apparatus
kxi_pre3	keratan sulfate I biosynthesis, precursor 3		C93H152N6O67X	-1	Golgi Apparatus
kxi_pre30	keratan sulfate I biosynthesis, precursor 30		C219H350N15O184S9X	-10	Golgi Apparatus
kxi_pre31	keratan sulfate I biosynthesis, precursor 31		C227H363N16O189S9X	-10	Golgi Apparatus
kxi_pre32	keratan sulfate I biosynthesis, precursor 32		C227H362N16O192S10X	-11	Golgi Apparatus
kxi_pre33	keratan sulfate I biosynthesis, precursor 33		C233H372N16O197S10X	-11	Golgi Apparatus
kxi_pre34	keratan sulfate I biosynthesis, precursor 34		C241H385N17O202S10X	-11	Golgi Apparatus
kxi_pre35	keratan sulfate I biosynthesis, precursor 35		C241H384N17O205S11X	-12	Golgi Apparatus
kxi_pre36	keratan sulfate I biosynthesis, precursor 36		C247H394N17O210S11X	-12	Golgi Apparatus
kxi_pre4	keratan sulfate I biosynthesis, precursor 4		C101H165N7O72X	-1	Golgi Apparatus
kxi_pre5	keratan sulfate I biosynthesis, precursor 5		C101H164N7O75SX	-2	Golgi Apparatus
kxi_pre6	keratan sulfate I biosynthesis, precursor 6		C107H174N7O80SX	-2	Golgi Apparatus
kxi_pre7	keratan sulfate I biosynthesis, precursor 7		C115H187N8O85S2X	-2	Golgi Apparatus
kxi_pre8	keratan sulfate I biosynthesis, precursor 8		C115H186N8O88S2X	-3	Golgi Apparatus
kxi_pre9	keratan sulfate I biosynthesis, precursor 9		C121H196N8O93S2X	-3	Golgi Apparatus
kxii_core2	keratan sulfate II (core 2-linked)		C81H129N6O67S3X	-4	Extracellular
kxii_core2	keratan sulfate II (core 2-linked)		C81H129N6O67S3X	-4	Golgi Apparatus
kxii_core2	keratan sulfate II (core 2-linked)		C81H129N6O67S3X	-4	Lysosome
kxii_core2_deg1	keratan sulfate II (core 2-linked), degradation product 1		C70H113N5O59S3X	-3	Lysosome
kxii_core2_deg2	keratan sulfate II (core 2-linked), degradation product 2		C70H114N5O56S2X	-2	Lysosome
kxii_core2_deg3	keratan sulfate II (core 2-linked), degradation product 3		C58H94N5O46S2X	-2	Lysosome
kxii_core2_deg4	keratan sulfate II (core 2-linked), degradation product 4		C58H95N5O43SX	-1	Lysosome
kxii_core2_deg5	keratan sulfate II (core 2-linked), degradation product 5		C50H82N4O38SX	-1	Lysosome
kxii_core2_deg6	keratan sulfate II (core 2-linked), degradation product 6		C44H72N4O33SX	-1	Lysosome
kxii_core2_deg7	keratan sulfate II (core 2-linked), degradation product 7		C44H73N4O30X	0	Lysosome
kxii_core2_deg8	keratan sulfate II (core 2-linked), degradation product 8		C36H60N3O25X	0	Lysosome
kxii_core2_deg9	keratan sulfate II (core 2-linked), degradation product 9		C30H50N3O20X	0	Lysosome
kxii_core2_pre1	keratan sulfate II biosynthesis, precursor 1		C33H53N3O23X	-1	Golgi Apparatus
kxii_core2_pre10	keratan sulfate II biosynthesis, precursor 10		C81H130N6O64S2X	-3	Golgi Apparatus
kxii_core2_pre2	keratan sulfate II biosynthesis, precursor 2		C39H63N3O28X	-1	Golgi Apparatus
kxii_core2_pre3	keratan sulfate II biosynthesis, precursor 3		C47H76N4O33X	-1	Golgi Apparatus
kxii_core2_pre4	keratan sulfate II biosynthesis, precursor 4		C53H86N4O38X	-1	Golgi Apparatus
kxii_core2_pre5	keratan sulfate II biosynthesis, precursor 5		C61H99N5O43X	-1	Golgi Apparatus
kxii_core2_pre6	keratan sulfate II biosynthesis, precursor 6		C61H98N5O46SX	-2	Golgi Apparatus
kxii_core2_pre7	keratan sulfate II biosynthesis, precursor 7		C67H108N5O51SX	-2	Golgi Apparatus
kxii_core2_pre8	keratan sulfate II biosynthesis, precursor 8		C75H121N6O56SX	-2	Golgi Apparatus
kxii_core2_pre9	keratan sulfate II biosynthesis, precursor 9		C75H120N6O59S2X	-3	Golgi Apparatus
kxii_core4	keratan sulfate II (core 4-linked)		C89H142N7O72S3X	-4	Extracellular
kxii_core4	keratan sulfate II (core 4-linked)		C89H142N7O72S3X	-4	Golgi Apparatus
kxii_core4	keratan sulfate II (core 4-linked)		C89H142N7O72S3X	-4	Lysosome
kxii_core4_deg1	keratan sulfate II (core 4-linked), degradation product 1		C78H126N6O64S3X	-3	Lysosome
kxii_core4_deg2	keratan sulfate II (core 4-linked), degradation product 2		C78H127N6O61S2X	-2	Lysosome
kxii_core4_deg3	keratan sulfate II (core 4-linked), degradation product 3		C66H107N6O51S2X	-2	Lysosome
kxii_core4_deg4	keratan sulfate II (core 4-linked), degradation product 4		C66H108N6O48SX	-1	Lysosome
kxii_core4_pre1	keratan sulfate II biosynthesis, precursor 1		C36H60N3O25X	0	Golgi Apparatus
kxii_core4_pre10	keratan sulfate II biosynthesis, precursor 10		C89H143N7O69S2X	-3	Golgi Apparatus
kxii_core4_pre2	keratan sulfate II biosynthesis, precursor 2		C47H76N4O33X	-1	Golgi Apparatus
kxii_core4_pre3	keratan sulfate II biosynthesis, precursor 3		C55H89N5O38X	-1	Golgi Apparatus
kxii_core4_pre4	keratan sulfate II biosynthesis, precursor 4		C61H99N5O43X	-1	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ksii_core4_pre5	keratan sulfate II biosynthesis, precursor 5		C69H112N6O48X	-1	Golgi Apparatus
ksii_core4_pre6	keratan sulfate II biosynthesis, precursor 6		C69H111N6O51SX	-2	Golgi Apparatus
ksii_core4_pre7	keratan sulfate II biosynthesis, precursor 7		C75H121N6O56SX	-2	Golgi Apparatus
ksii_core4_pre8	keratan sulfate II biosynthesis, precursor 8		C83H134N7O61SX	-2	Golgi Apparatus
ksii_core4_pre9	keratan sulfate II biosynthesis, precursor 9		C83H133N7O64S2X	-3	Golgi Apparatus
kynate	4-Hydroxy-2-quinolinecarboxylic acid	4-Hydroxy-2-quinolinecarboxylic acid, Kynurenate, Kynurenic acid	C10H6NO3	-1	Cytosol
L2aadp	L-2-Aminoadipate	L-2-Aminoadipic acid, L-alpha-Aminoadipate, L-alpha-Aminoadipic acid	C6H10NO4	-1	Cytosol
L2aadp	L-2-Aminoadipate	L-2-Aminoadipic acid, L-alpha-Aminoadipate, L-alpha-Aminoadipic acid	C6H10NO4	-1	Mitochondria
L2aadp6sa	L-2-Aminoadipate 6-semialdehyde		C6H11NO3	0	Cytosol
L2aadp6sa	L-2-Aminoadipate 6-semialdehyde		C6H11NO3	0	Mitochondria
l2fn2m2masn	[[galactosyl-(1,4)-N-Acetyl-glucosaminyl-(1,2)-mannosyl-(1,3)-]1-[N-acetyl-glucosaminyl-(1,2)-mannosyl-(1,6)-]mannosyl-(1,4)-N-acetyl-glucosaminyl-(1,4)-[fucosyl-(1,6)-N-acetyl-glucosaminyl] asparagine		C68H113N4O49X	0	Golgi Apparatus
l2n2m2mn	de-Fuc, reducing GlcNAc removed, de-Sia form of PA6 (w/peptide linkage)		C54H91N3O41	0	Cytosol
l2n2m2mn	de-Fuc, reducing GlcNAc removed, de-Sia form of PA6 (w/peptide linkage)		C54H91N3O41	0	Lysosome
l2xser	(Gal)2-Xyl-L-Ser (protein)		C17H29O14X	0	Golgi Apparatus
lac-D	D-Lactate	(R)-Lactate, D-2-Hydroxypropanoic acid, D-2-Hydroxypropionic acid, D-Lactic acid	C3H5O3	-1	Cytosol
lac-D	D-Lactate	(R)-Lactate, D-2-Hydroxypropanoic acid, D-2-Hydroxypropionic acid, D-Lactic acid	C3H5O3	-1	Extracellular
lac-D	D-Lactate	(R)-Lactate, D-2-Hydroxypropanoic acid, D-2-Hydroxypropionic acid, D-Lactic acid	C3H5O3	-1	Mitochondria
lac-L	L-Lactate	(S)-Lactate, Hydroxypropionic acid, L-Lactic acid	C3H5O3	-1	Cytosol
lac-L	L-Lactate	(S)-Lactate, Hydroxypropionic acid, L-Lactic acid	C3H5O3	-1	Extracellular
lac-L	L-Lactate	(S)-Lactate, Hydroxypropionic acid, L-Lactic acid	C3H5O3	-1	Mitochondria
lald-D	D-Lactaldehyde	(R)-Lactaldehyde, D-2-Hydroxypropionaldehyde	C3H6O2	0	Cytosol
lald-D	D-Lactaldehyde	(R)-Lactaldehyde, D-2-Hydroxypropionaldehyde	C3H6O2	0	Mitochondria
lald-L	L-Lactaldehyde	(S)-Lactaldehyde, L-2-Hydroxypropionaldehyde	C3H6O2	0	Cytosol
lald-L	L-Lactaldehyde	(S)-Lactaldehyde, L-2-Hydroxypropionaldehyde	C3H6O2	0	Mitochondria
lanost	Lanosterol		C30H50O	0	Cytosol
lanost	Lanosterol		C30H50O	0	Endoplasmic Reticulum
lcts	Lactose	1-beta-D-Galactopyranosyl-4-alpha-D-glucopyranose, Milk sugar, lactobiose	C12H22O11	0	Cytosol
lcts	Lactose	1-beta-D-Galactopyranosyl-4-alpha-D-glucopyranose, Milk sugar, lactobiose	C12H22O11	0	Extracellular
lcts	Lactose	1-beta-D-Galactopyranosyl-4-alpha-D-glucopyranose, Milk sugar, lactobiose	C12H22O11	0	Golgi Apparatus
lcts	Lactose	1-beta-D-Galactopyranosyl-4-alpha-D-glucopyranose, Milk sugar, lactobiose	C12H22O11	0	Lysosome
Lcyst	L-Cysteate	2-Amino-3-sulfopropionic acid, 3-Sulfolanine, L-Cysteic acid	C3H6NO5S	-1	Cytosol
Lcyst	L-Cysteate	2-Amino-3-sulfopropionic acid, 3-Sulfolanine, L-Cysteic acid	C3H6NO5S	-1	Mitochondria
Lcystin	L-Cystine	L-Dicysteine, L-alpha-Diamino-beta-dithiolic acid	C6H12N2O4S2	0	Cytosol
Lcystin	L-Cystine	L-Dicysteine, L-alpha-Diamino-beta-dithiolic acid	C6H12N2O4S2	0	Extracellular
L-dpchrn	L-Dopachrome	2-L-Carboxy-2,3-dihydroindole-5,6-quinone	C9H6NO4	-1	Cytosol
leuktrA4	Leukotriene A4	(7E,9E,11Z,14Z)-(5S,6S)-5,6-Epoxyeicosa-7,9,11,14-tetraenoate, (7E,9E,11Z,14Z)-(5S,6S)-5,6-Epoxyeicosa-7,9,11,14-tetr, LTA4, Leukotriene A4	C20H29O3	-1	Cytosol
leuktrA4	Leukotriene A4	(7E,9E,11Z,14Z)-(5S,6S)-5,6-Epoxyeicosa-7,9,11,14-tetraenoate, (7E,9E,11Z,14Z)-(5S,6S)-5,6-Epoxyeicosa-7,9,11,14-tetr, LTA4, Leukotriene A4	C20H29O3	-1	Endoplasmic Reticulum
leuktrB4	Leukotriene B4	(6Z,8E,10E,14Z)-(5S,12R)-5,12-Dihydroxyeicosa-6,8,10,14-tetraenoate, (6Z,8E,10E,14Z)-(5S,12R)-5,12-Dihydroxyeicosa-6,8,10,14-tetraenoate, Leukotriene B4	C20H31O4	-1	Cytosol
leuktrB4	Leukotriene B4	(6Z,8E,10E,14Z)-(5S,12R)-5,12-Dihydroxyeicosa-6,8,10,14-tetraenoate, (6Z,8E,10E,14Z)-(5S,12R)-5,12-Dihydroxyeicosa-6,8,10,14-tetraenoate, Leukotriene B4	C20H31O4	-1	Endoplasmic Reticulum
leuktrB4wcooh	w-carboxy leukotriene B4	20 carboxy leukotriene B4, omega carboxy leukotriene B4, omega carboxylated leukotriene B4	C20H28O6	-2	Endoplasmic Reticulum
leuktrB4woh	w-hydroxyl leukotriene B4	20 hydroxy leukotriene B4, omega hydroxy leukotriene B4, omega-hydroxylated leukotriene B4	C20H31O5	-1	Endoplasmic Reticulum
leuktrC4	Leukotriene C4		C30H45N3O9S	-2	Cytosol
leuktrC4	Leukotriene C4		C30H45N3O9S	-2	Extracellular

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
leuktrC4	Leukotriene C4		C30H45N3O9S	-2	Endoplasmic Reticulum
leuktrD4	Leukotriene D4	LTD4, Leukotriene D4	C25H39N2O6S	-1	Cytosol
leuktrD4	Leukotriene D4	LTD4, Leukotriene D4	C25H39N2O6S	-1	Endoplasmic Reticulum
leuktrE4	leukotriene E4	5S-hydroxy,6R-(S-cysteinyl),7E,9E,11Z,14Z- eicosatetraenoic acid, C05952, LMFA03020002, LTE4, leukotriene E4	C23H36NO5S	-1	Cytosol
leuktrF4	leukotriene F4	C06462, LTF4, Leukotriene F4	C28H42N2O8S	-2	Cytosol
leu-L	L-Leucine	2-amino-4-methylvaleric acid, Leu	C6H13NO2	0	Cytosol
leu-L	L-Leucine	2-amino-4-methylvaleric acid, Leu	C6H13NO2	0	Extracellular
leu-L	L-Leucine	2-amino-4-methylvaleric acid, Leu	C6H13NO2	0	Mitochondria
Lfmkynr	L-Formylkynurenine	N-Formyl-L-kynurenine	C11H12N2O4	0	Cytosol
lgnc	lignoceric acid	Lignoceric acid, Tetracosanoic acid	C24H47O2	-1	Cytosol
lgnc	lignoceric acid	Lignoceric acid, Tetracosanoic acid	C24H47O2	-1	Extracellular
lgnccoa	lignoceryl coenzyme A		C45H78N7O17P3S	-4	Cytosol
lgnccoa	lignoceryl coenzyme A		C45H78N7O17P3S	-4	Mitochondria
lgnccoa	lignoceryl coenzyme A		C45H78N7O17P3S	-4	Peroxisome
lgncrm	lignoceryl carnitine		C31H61NO4	0	Cytosol
lgncrm	lignoceryl carnitine		C31H61NO4	0	Mitochondria
lgt-S	(R)-S-Lactoylglutathione		C13H20N3O8S	-1	Cytosol
lgt-S	(R)-S-Lactoylglutathione		C13H20N3O8S	-1	Mitochondria
limnen	Limonene	Limonene	C10H16	0	Cytosol
limnen	Limonene	Limonene	C10H16	0	Extracellular
lipoate	Lipoate	Lipoic acid, Thioctic acid, alpha-Lipoic acid	C8H14O2S2	0	Cytosol
lipoate	Lipoate	Lipoic acid, Thioctic acid, alpha-Lipoic acid	C8H14O2S2	0	Extracellular
Lkynr	L-Kynurenine	3-Anthraniloyl-L-alanine	C10H12N2O3	0	Cytosol
lnelc	linoalaidic acid (all trans C18:2)	9-cis,11-trans-Octadecadienoate, C18:2, Linoalaidic acid	C18H31O2	-1	Cytosol
lnelc	linoalaidic acid (all trans C18:2)	9-cis,11-trans-Octadecadienoate, C18:2, Linoalaidic acid	C18H31O2	-1	Extracellular
lnelcACP	linoalaidic acid ACP (all trans)		C29H51N2O8PRS	-1	Cytosol
lnelcco	linoalaidyl coenzyme A		C39H62N7O17P3S	-4	Cytosol
lnelcco	linoalaidyl coenzyme A		C39H62N7O17P3S	-4	Mitochondria
lnelccrm	Linoalaidyl carnitine		C25H45NO4	0	Cytosol
lnelccrm	Linoalaidyl carnitine		C25H45NO4	0	Mitochondria
lnlc	linoleic acid (all cis C18:2) n-6	9,12-Octadecadienoic acid, 9-cis,12-cis- Octadecadienoate, 9-cis,12-cis-Octadecadienoic acid, Linoleate, Linoleic acid	C18H31O2	-1	Cytosol
lnlc	linoleic acid (all cis C18:2) n-6	9,12-Octadecadienoic acid, 9-cis,12-cis- Octadecadienoate, 9-cis,12-cis-Octadecadienoic acid, Linoleate, Linoleic acid	C18H31O2	-1	Extracellular
lnlcACP	linoleic acid ACP (all cis)		C29H51N2O8PRS	-1	Cytosol
lnlcco	linoleic coenzyme A	linoleic acid coenzyme A, linoleic coenzyme A	C39H62N7O17P3S	-4	Cytosol
lnlcco	linoleic coenzyme A	linoleic acid coenzyme A, linoleic coenzyme A	C39H62N7O17P3S	-4	Mitochondria
lnlccrm	Linoleyl carnitine	linoleic acid carnitine	C25H45NO4	0	Cytosol
lnlccrm	Linoleyl carnitine	linoleic acid carnitine	C25H45NO4	0	Mitochondria
lnlnca	alpha-Linolenic acid, C18:3, n-3	(9Z,12Z,15Z)-Octadecatrienoic acid, 9,12,15- Octadecatrienoic acid, Linolenate, alpha-Linolenic acid	C18H29O2	-1	Cytosol
lnlnca	alpha-Linolenic acid, C18:3, n-3	(9Z,12Z,15Z)-Octadecatrienoic acid, 9,12,15- Octadecatrienoic acid, Linolenate, alpha-Linolenic acid	C18H29O2	-1	Extracellular
lnlnccoa	alpha-Linolenoyl-CoA	alpha-Linolenoyl-CoA	C39H60N7O17P3S	-4	Cytosol
lnlnccoa	alpha-Linolenoyl-CoA	alpha-Linolenoyl-CoA	C39H60N7O17P3S	-4	Mitochondria
lnlnccrm	alpha-linolenyl carnitine		C25H43NO4	0	Cytosol
lnlnccrm	alpha-linolenyl carnitine		C25H43NO4	0	Mitochondria
lnlncg	gamma-linolenic acid	6,9,12-Octadecatrienoic acid, gamma-linolenic acid	C18H29O2	-1	Cytosol
lnlncg	gamma-linolenic acid	6,9,12-Octadecatrienoic acid, gamma-linolenic acid	C18H29O2	-1	Extracellular
lnlncco	gamma-linolenoyl-CoA	gamma-Linolenoyl-CoA	C39H60N7O17P3S	-4	Cytosol
lnlncco	gamma-linolenoyl-CoA	gamma-Linolenoyl-CoA	C39H60N7O17P3S	-4	Mitochondria
lnlncco	gamma-linolenoyl-CoA	gamma-Linolenoyl-CoA	C39H60N7O17P3S	-4	Peroxisome
lnlnccrm	gamma-linolenyl carnitine		C25H43NO4	0	Cytosol
lnlnccrm	gamma-linolenyl carnitine		C25H43NO4	0	Mitochondria
lpam	Lipoamide	Thioctic Acid Amide	C8H15NO2S	0	Mitochondria
lpchol_hs	lysophosphatidylcholine (homo sapiens)	1-Acyl-sn-glycero-3-phosphocholine, 1-Acyl-sn- glycerol-3-phosphocholine, 2-Lysolecithin, 2- Lysophosphatidylcholine, alpha- Acylglycerophosphocholine, lysolecithin	C8H19NO5PFULLR2CO2	0	Cytosol
lpchol_hs	lysophosphatidylcholine (homo sapiens)	1-Acyl-sn-glycero-3-phosphocholine, 1-Acyl-sn- glycerol-3-phosphocholine, 2-Lysolecithin, 2- Lysophosphatidylcholine, alpha- Acylglycerophosphocholine, lysolecithin	C8H19NO5PFULLR2CO2	0	Extracellular
Lpipecol	L-Pipecolate	2-Piperidinecarboxylic acid, Pipecolic acid, Pipicolinic acid	C6H11NO2	0	Peroxisome
lpro	Lipoylprotein		S2X	0	Mitochondria
lthstrl	5alpha-Cholest-7-en-3beta-ol	5alpha-Cholest-7-en-3beta-ol, Lathosterol	C27H46O	0	Endoplasmic Reticulum
lum3	Lumisterol 3		C27H44O	0	Cytosol
lxsr	Gal-Xyl-L-Ser (protein)		C11H19O9X	0	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
lys-L	L-Lysine	2,6-diaminohexanoic acid, Lys, Lysine acid	C6H15N2O2	1	Cytosol
lys-L	L-Lysine	2,6-diaminohexanoic acid, Lys, Lysine acid	C6H15N2O2	1	Extracellular
lys-L	L-Lysine	2,6-diaminohexanoic acid, Lys, Lysine acid	C6H15N2O2	1	Mitochondria
lys-L	L-Lysine	2,6-diaminohexanoic acid, Lys, Lysine acid	C6H15N2O2	1	Nucleus
lys-L	L-Lysine	2,6-diaminohexanoic acid, Lys, Lysine acid	C6H15N2O2	1	Peroxisome
lyxt	L-lyxonate	L-Lyxonic acid	C5H9O6	-1	Cytosol
m(em)3gacpail_hs	mannosyl-3-(phosphoethanolaminy)-glucosaminyl-acylphosphatidylinositol (M4A)	[[[Man-1],[PE-]Man-],(PE-]Man-1],[PE-]Man-GlcN-acylPI	C61H116N4O43P4FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
m(em)3gacpail_prot_hs	mannosyl-3-(phosphoethanolaminy)-glucosaminyl-acylphosphatidylinositol-Protein (M4A)		C61H116N4O43P4FULLR2CO2F ULLR2CO2X	0	Endoplasmic Reticulum
m1mpdol_L	alpha-D-mannosyl-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1360H2228N200270P20	-20	Cytosol
m1mpdol_U	alpha-D-mannosyl-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1305H2140N200270P20	-20	Cytosol
m2emgacpail_hs	(dimannosyl1,(phosphoethanolaminy)-mannosyl-glucosaminyl-acylphosphatidylinositol (H6)	[(Man)2-1],[PE-]Man-GlcN-acylPI	C51H94N2O32P2FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
m2gacpail_hs	dimannosyl-1-glucosaminyl-acylphosphatidylinositol (H3)	(Man)2-GlcN-acylPI	C43H78N2O44P4FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
m2mn	(alpha-D-mannosyl)2-beta-D-mannosyl-N-acetylglucosamine		C26H45NO21	0	Cytosol
m2mn	(alpha-D-mannosyl)2-beta-D-mannosyl-N-acetylglucosamine		C26H45NO21	0	Lysosome
m2mpdol_L	(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1420H2328N200320P20	-20	Cytosol
m2mpdol_U	(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1365H2240N200320P20	-20	Cytosol
m3emgacpail_hs	(trimannosyl1,(phosphoethanolaminy)-mannosyl-glucosaminyl-acylphosphatidylinositol (M4C)	[(Man)3-1],[PE-]Man-GlcN-acylPI	C57H104N2O37P2FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
m3gacpail_hs	trimannosyl-1-glucosaminyl-acylphosphatidylinositol (H4)	(Man)3-GlcN-acylPI	C49H88N2O39P4FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
m3mpdol_L	(alpha-D-mannosyl)3-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1480H2428N200370P20	-20	Cytosol
m3mpdol_U	(alpha-D-mannosyl)3-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1425H2340N200370P20	-20	Cytosol
m4masn	(alpha-D-mannosyl)4-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C46H77N2O35X	0	Golgi Apparatus
m4mpdol_L	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1540H2528N200420P20	-20	Cytosol
m4mpdol_L	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1540H2528N200420P20	-20	Endoplasmic Reticulum
m4mpdol_U	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1485H2440N200420P20	-20	Cytosol
m4mpdol_U	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1485H2440N200420P20	-20	Endoplasmic Reticulum
m5masnB1	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C52H87N2O40X	0	Golgi Apparatus
m5masnB2	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C52H87N2O40X	0	Golgi Apparatus
m5masnC	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C52H87N2O40X	0	Golgi Apparatus
m5mpdol_L	(alpha-D-Mannosyl)5-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1600H2628N200470P20	-20	Endoplasmic Reticulum
m5mpdol_U	(alpha-D-Mannosyl)5-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1545H2540N200470P20	-20	Endoplasmic Reticulum
m6masnA	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C58H97N2O45X	0	Golgi Apparatus
m6masnB1	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C58H97N2O45X	0	Golgi Apparatus
m6masnB2	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C58H97N2O45X	0	Golgi Apparatus
m6masnC	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C58H97N2O45X	0	Golgi Apparatus
m6mpdol_L	(alpha-D-Mannosyl)6-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1660H2728N200520P20	-20	Endoplasmic Reticulum
m6mpdol_U	(alpha-D-Mannosyl)6-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1605H2640N200520P20	-20	Endoplasmic Reticulum
m7masnA	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-asparagine, isoform A (protein)		C64H107N2O50X	0	Golgi Apparatus
m7masnB	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-asparagine, isoform B (protein)		C64H107N2O50X	0	Golgi Apparatus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
m7masnB	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-asparagine, isoform B (protein)		C64H107N2O50X	0	Endoplasmic Reticulum
m7masnC	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-asparagine, isoform C (protein)		C64H107N2O50X	0	Golgi Apparatus
m7mpdol_L	(alpha-D-Mannosyl)7-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1720H2828N20O570P20	-20	Endoplasmic Reticulum
m7mpdol_U	(alpha-D-Mannosyl)7-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1665H2740N20O570P20	-20	Endoplasmic Reticulum
m8masn	(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C70H117N2O55X	0	Golgi Apparatus
m8masn	(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-asparagine (protein)		C70H117N2O55X	0	Endoplasmic Reticulum
m8mpdol_L	(alpha-D-Mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog		C1780H2928N20O620P20	-20	Endoplasmic Reticulum
m8mpdol_U	(alpha-D-Mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog		C1725H2840N20O620P20	-20	Endoplasmic Reticulum
mag_hs	monoacylglycerol 2 (homo sapiens)		C3H7O2FULLR2CO2	0	Cytosol
mag_hs	monoacylglycerol 2 (homo sapiens)		C3H7O2FULLR2CO2	0	Extracellular
malACP	Malonyl-[acyl-carrier protein]		C14H22N2O10PRS	-2	Cytosol
malACP	Malonyl-[acyl-carrier protein]		C14H22N2O10PRS	-2	Mitochondria
malcoa	Malonyl-CoA	Malonyl coenzyme A	C24H33N7O19P3S	5	Cytosol
malcoa	Malonyl-CoA	Malonyl coenzyme A	C24H33N7O19P3S	-5	Mitochondria
malcoa	Malonyl-CoA	Malonyl coenzyme A	C24H33N7O19P3S	-5	Peroxisome
mal-L	L-Malate	(S)-Malate, L-2-Hydroxybutanedioic acid, L-Aspartic acid, L-Malic acid, Malate	C4H4O5	-2	Cytosol
mal-L	L-Malate	(S)-Malate, L-2-Hydroxybutanedioic acid, L-Aspartic acid, L-Malic acid, Malate	C4H4O5	-2	Mitochondria
malt	Maltose	1-alpha-D-Glucopyranosyl-4-alpha-D-glucopyranose, Malt sugar	C12H22O11	0	Cytosol
malt	Maltose	1-alpha-D-Glucopyranosyl-4-alpha-D-glucopyranose, Malt sugar	C12H22O11	0	Extracellular
malt	Maltose	1-alpha-D-Glucopyranosyl-4-alpha-D-glucopyranose, Malt sugar	C12H22O11	0	Lysosome
maltr	Maltotriose	Amylotriose, Maltotriose	C18H32O16	0	Cytosol
maltr	Maltotriose	Amylotriose, Maltotriose	C18H32O16	0	Extracellular
maltr	Maltotriose	Amylotriose, Maltotriose	C18H32O16	0	Lysosome
man	D-Mannose	Carubiose, Mannose, Seminose	C6H12O6	0	Cytosol
man	D-Mannose	Carubiose, Mannose, Seminose	C6H12O6	0	Extracellular
man	D-Mannose	Carubiose, Mannose, Seminose	C6H12O6	0	Golgi Apparatus
man	D-Mannose	Carubiose, Mannose, Seminose	C6H12O6	0	Lysosome
man	D-Mannose	Carubiose, Mannose, Seminose	C6H12O6	0	Endoplasmic Reticulum
man1p	D-Mannose 1-phosphate	alpha-D-Mannose 1-phosphate	C6H11O9P	-2	Cytosol
man6p	D-Mannose 6-phosphate		C6H11O9P	-2	Cytosol
melanin	Melanin		C9H6NO4	-1	Cytosol
melatn	Melatonin	Melatonin, N-Acetyl-5-methoxytryptamine	C13H16N2O2	0	Cytosol
mem2emgacpail_hs	([[[(mannosyl),(phosphoethanolaminy)]-dimannosyl],[phosphoethanolaminy]]-mannosyl-glucosaminyl-acylphosphatidylinositol (M4B)	[[[Man-],[PE-](Man)2-],[PE-]Man-GlcN-acylPI	C59H110N3O40P3FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
mem2emgacpail_prot_hs	([[[(mannosyl),(phosphoethanolaminy)]-dimannosyl],[phosphoethanolaminy]]-mannosyl-glucosaminyl-acylphosphatidylinositol-Protein (M4B)		C59H110N3O40P3FULLR2CO2F ULLR2CO2X	0	Endoplasmic Reticulum
memgacpail_hs	(mannosyl),(phosphoethanolaminy)-mannosyl-glucosylaminyl-acylphosphatidylinositol (B)	[[Man-],[PE-]Man-GlcN-acylPI	C45H84N2O27P2FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum
meoh	Methanol	Methyl alcohol	CH4O1	0	Cytosol
meoh	Methanol	Methyl alcohol	CH4O1	0	Extracellular
meoh	Methanol	Methyl alcohol	CH4O1	0	Lysosome
meoh	Methanol	Methyl alcohol	CH4O1	0	Endoplasmic Reticulum
mepi	Metanephrine	L-Metanephrine	C10H16NO3	1	Cytosol
mepi	Metanephrine	L-Metanephrine	C10H16NO3	-1	Extracellular
mercplac	3-Mercaptolactate		C3H5O3S	-1	Cytosol
mercplaccys	3-mercaptolactate-cysteine disulfide		C6H10O5S2N	-1	Cytosol
mercplaccys	3-mercaptolactate-cysteine disulfide		C6H10O5S2N	-1	Extracellular
mercppyr	Mercaptopyruvate	3-Mercaptopyruvate	C3H3O3S	-1	Cytosol
mercppyr	Mercaptopyruvate	3-Mercaptopyruvate	C3H3O3S	-1	Mitochondria
mescoa	Mesaconyl-CoA		C26H35N7O19P3S	-5	Mitochondria
mescon	Mesaconate	2-Methylfumarate, Mesaconic acid, Methylfumaric acid	C5H4O4	-2	Mitochondria
methf	5,10-Methylenetetrahydrofolate	(6R)-5,10-methylenetetrahydrofolate, 5,10-methylenetetrahydrofolate, N5,N10-methenyl-5,6,7,8-tetrahydrofolate, N5,N10-methenyl-tetrahydrofolate	C20H20N7O6	-1	Cytosol
methf	5,10-Methylenetetrahydrofolate	(6R)-5,10-methylenetetrahydrofolate, 5,10-methylenetetrahydrofolate, N5,N10-methenyl-5,6,7,8-tetrahydrofolate, N5,N10-methenyl-tetrahydrofolate	C20H20N7O6	-1	Mitochondria
met-L	L-Methionine	L-2-Amino-4-methylthiobutyric acid, Met	C5H11NO2S	0	Cytosol
met-L	L-Methionine	L-2-Amino-4-methylthiobutyric acid, Met	C5H11NO2S	0	Extracellular
mev-R	(R)-Mevalonate	3,5-Dihydroxy-3-methylvaleric acid, Mevalonic acid	C6H11O4	-1	Endoplasmic Reticulum
mev-R	(R)-Mevalonate	3,5-Dihydroxy-3-methylvaleric acid, Mevalonic acid	C6H11O4	-1	Peroxisome
mgacpail_hs	mannosyl-glucosaminyl-acylphosphatidylinositol (H2)	Man-GlcN-acylPI	C37H68NO19FULLR2CO2F ULLR2CO2	0	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
mhista	N-Methylhistamine	1-Methyl-4-(2-aminoethyl)imidazole, Methylhistamine	C6H12N3	1	Cytosol
mi13456p	1D-myo-Inositol 1,3,4,5,6-pentakisphosphate	D-myo-Inositol 1,3,4,5,6-pentakisphosphate, Inositol 1,3,4,5,6-pentakisphosphate	C6H7O21P5	-10	Cytosol
mi13456p	1D-myo-Inositol 1,3,4,5,6-pentakisphosphate	D-myo-Inositol 1,3,4,5,6-pentakisphosphate, Inositol 1,3,4,5,6-pentakisphosphate	C6H7O21P5	-10	Nucleus
mi1345p	1D-myo-Inositol 1,3,4,5-tetrakisphosphate	D-myo-Inositol 1,3,4,5-tetrakisphosphate, Inositol 1,3,4,5-tetrakisphosphate	C6H8O18P4	-8	Cytosol
mi1345p	1D-myo-Inositol 1,3,4,5-tetrakisphosphate	D-myo-Inositol 1,3,4,5-tetrakisphosphate, Inositol 1,3,4,5-tetrakisphosphate	C6H8O18P4	-8	Nucleus
mi1346p	1D-myo-Inositol 1,3,4,6-tetrakisphosphate	D-myo-Inositol 1,3,4,6-tetrakisphosphate, Inositol 1,3,4,6-tetrakisphosphate	C6H8O18P4	-8	Cytosol
mi1346p	1D-myo-Inositol 1,3,4,6-tetrakisphosphate	D-myo-Inositol 1,3,4,6-tetrakisphosphate, Inositol 1,3,4,6-tetrakisphosphate	C6H8O18P4	-8	Nucleus
mi134p	1D-myo-Inositol 1,3,4-trisphosphate	Inositol 1,3,4-trisphosphate	C6H9O15P3	-6	Cytosol
mi13p	1D-myo-Inositol 1,3-bisphosphate	D-myo-Inositol 1,3-bisphosphate, Inositol 1,3-bisphosphate, myo-Inositol 1,3-bisphosphate	C6H10O12P2	-4	Cytosol
mi1456p	1D-myo-Inositol 1,4,5,6-tetrakisphosphate		C6H8O18P4	-8	Nucleus
mi145p	1D-myo-Inositol 1,4,5-trisphosphate	IP3, Inositol 1,4,5-trisphosphate	C6H9O15P3	-6	Cytosol
mi145p	1D-myo-Inositol 1,4,5-trisphosphate	IP3, Inositol 1,4,5-trisphosphate	C6H9O15P3	-6	Nucleus
mi14p	1D-myo-Inositol 1,4-bisphosphate	1D-myo-Inositol 1,4-bisphosphate, Inositol 1, myo-Inositol 1	C6H10O12P2	-4	Cytosol
mi14p	1D-myo-Inositol 1,4-bisphosphate	1D-myo-Inositol 1,4-bisphosphate, Inositol 1, myo-Inositol 1	C6H10O12P2	-4	Nucleus
mi1p-D	1D-myo-Inositol 1-phosphate	1D-myo-Inositol 1-monophosphate, 1L-myo-Inositol 1-phosphate, D-myo-Inositol 1-phosphate, Inositol 1-phosphate, L-myo-Inositol 1-phosphate, myo-Inositol 1-phosphate	C6H11O9P	-2	Cytosol
mi1p-D	1D-myo-Inositol 1-phosphate	1D-myo-Inositol 1-monophosphate, 1L-myo-Inositol 1-phosphate, D-myo-Inositol 1-phosphate, Inositol 1-phosphate, L-myo-Inositol 1-phosphate, myo-Inositol 1-phosphate	C6H11O9P	-2	Nucleus
mi3456p	1D-myo-Inositol 3,4,5,6-tetrakisphosphate	D-myo-Inositol 3,4,5,6-tetrakisphosphate, Inositol 3,4,5,6-tetrakisphosphate	C6H8O18P4	-8	Cytosol
mi34p	1D-myo-Inositol 3,4-bisphosphate	D-myo-Inositol 3,4-bisphosphate, Inositol 3,4-bisphosphate	C6H10O12P2	-4	Cytosol
mi3p-D	1D-myo-Inositol 3-phosphate	1D-myo-Inositol 3-monophosphate, D-myo-Inositol 3-monophosphate, D-myo-Inositol 3-phosphate, Inositol 3-monophosphate, Inositol 3-phosphate, myo-Inositol 3-monophosphate, myo-Inositol 3-phosphate	C6H11O9P	-2	Cytosol
mi4p-D	1D-myo-Inositol 4-phosphate	1D-myo-Inositol 4-monophosphate, D-myo-Inositol 4-phosphate, Inositol 4-phosphate	C6H11O9P	-2	Cytosol
micit	methylisocitrate	(2S,3R)-3-Hydroxybutane-1,2,3-tricarboxylate, Methylisocitrate, Methylisocitric acid	C7H7O7	-3	Cytosol
minohp	myo-Inositol hexakisphosphate	1D-myo-Inositol 1, 2, 3, 4, 5, 6-hexakisphosphate, D-myo-Inositol 1, Inositol 1, Phytate, Phytic acid, myo-Inositol 1, myo-Inositol hexakisphosphate	C6H6O24P6	-12	Cytosol
minohp	myo-Inositol hexakisphosphate	1D-myo-Inositol 1, 2, 3, 4, 5, 6-hexakisphosphate, D-myo-Inositol 1, Inositol 1, Phytate, Phytic acid, myo-Inositol 1, myo-Inositol hexakisphosphate	C6H6O24P6	-12	Nucleus
mlthf	5,10-Methylenetetrahydrofolate	5,10-methylene-5,6,7,8-tetrahydrofolate, N5,N10-methylene-5,6,7,8-tetrahydrofolate, N5,N10-methylene-tetrahydrofolate	C20H21N7O6	-2	Cytosol
mlthf	5,10-Methylenetetrahydrofolate	5,10-methylene-5,6,7,8-tetrahydrofolate, N5,N10-methylene-5,6,7,8-tetrahydrofolate, N5,N10-methylene-tetrahydrofolate	C20H21N7O6	-2	Mitochondria
mma	monomethylamine	Methanamine, Methylamine	C1H6N	1	Cytosol
mmcoa-R	(R)-Methylmalonyl-CoA	(R)-2-Methyl-3-oxopropanoyl-CoA, (R)-2-Methyl-oxopropanoyl-CoA, (R)-3-Oxo-2-methylpropanoyl-CoA	C25H35N7O19P3S	-5	Mitochondria
mmcoa-S	(S)-Methylmalonyl-CoA	(S)-2-Methyl-3-oxopropanoyl-CoA, (S)-2-Methyl-oxopropanoyl-CoA, (S)-3-oxo-2-methylpropanoyl-CoA, (S)-Methylmalonyl-coenzyme A	C25H35N7O19P3S	-5	Cytosol
mmcoa-S	(S)-Methylmalonyl-CoA	(S)-2-Methyl-3-oxopropanoyl-CoA, (S)-2-Methyl-oxopropanoyl-CoA, (S)-3-oxo-2-methylpropanoyl-CoA, (S)-Methylmalonyl-coenzyme A	C25H35N7O19P3S	-5	Mitochondria
mmcoa-S	(S)-Methylmalonyl-CoA	(S)-2-Methyl-3-oxopropanoyl-CoA, (S)-2-Methyl-oxopropanoyl-CoA, (S)-3-oxo-2-methylpropanoyl-CoA, (S)-Methylmalonyl-coenzyme A	C25H35N7O19P3S	-5	Peroxisome
mn	beta-1,4-mannose-N-acetylglucosamine		C14H25NO11	0	Cytosol
mn	beta-1,4-mannose-N-acetylglucosamine		C14H25NO11	0	Lysosome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
mpdol_L	beta-D-Mannosyl diacetylchitobiosylidiphosphodolichol, human liver homolog	Man-beta1->4GlcNAc-PP-Dol, beta-1,4-D-Mannosylchitobiosylidiphosphodolichol	C1300H2128N20O220P20	-20	Cytosol
mpdol_U	beta-D-Mannosyl diacetylchitobiosylidiphosphodolichol, human uterine homolog	Man-beta1->4GlcNAc-PP-Dol, beta-1,4-D-Mannosylchitobiosylidiphosphodolichol	C1245H2040N20O220P20	-20	Cytosol
msa	Malonate semialdehyde	3-Oxopropanoate	C3H3O3	-1	Cytosol
msa	Malonate semialdehyde	3-Oxopropanoate	C3H3O3	-1	Mitochondria
mtgxl	Methylglyoxal	2-Ketopropionaldehyde, 2-Oxopropanal, Pyruvaldehyde, Pyruvic aldehyde	C3H4O2	0	Cytosol
mtgxl	Methylglyoxal	2-Ketopropionaldehyde, 2-Oxopropanal, Pyruvaldehyde, Pyruvic aldehyde	C3H4O2	0	Extracellular
myrsACP	Myristoyl-ACP (n-C14:0ACP)	Fatty acid C14:0 ACP, Tetradecanoyl-[acp], Tetradecanoyl-[acyl-carrier protein]	C25H47N2O8PRS	-1	Cytosol
n2m2masn	((N-acetyl-D-glucosaminy)2-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C50H83N4O35X	0	Golgi Apparatus
n2m2mn	de-Fuc, reducing GlcNAc removed, de-Sia, de-Gal form of PA6 (w/o peptide linkage)		C42H71N3O31	0	Lysosome
n2m2mn	n2m2masn (w/o peptide linkage)		C58H97N5O41	0	Cytosol
n2m2mn	n2m2masn (w/o peptide linkage)		C58H97N5O41	0	Lysosome
n2m2masn	N-Acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,3-(N-acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,6)-(N-acetyl-beta-D-glucosaminy-1,4)-beta-D-mannosyl-1,4-N-acetyl-beta-D-glucosaminy-R		C58H96N5O40X	0	Extracellular
n2m2masn	N-Acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,3-(N-acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,6)-(N-acetyl-beta-D-glucosaminy-1,4)-beta-D-mannosyl-1,4-N-acetyl-beta-D-glucosaminy-R		C58H96N5O40X	0	Golgi Apparatus
n2m2masn	N-Acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,3-(N-acetyl-beta-D-glucosaminy-1,2-alpha-D-mannosyl-1,6)-(N-acetyl-beta-D-glucosaminy-1,4)-beta-D-mannosyl-1,4-N-acetyl-beta-D-glucosaminy-R		C58H96N5O40X	0	Lysosome
n2m2mnn	reducing GlcNAc removed form of n2m2masn (w/o peptide)		C50H84N4O36	0	Cytosol
n2m2mnn	reducing GlcNAc removed form of n2m2masn (w/o peptide)		C50H84N4O36	0	Lysosome
n3m2masn	((N-acetyl-D-glucosaminy)3-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C58H96N5O40X	0	Golgi Apparatus
n4abutn	N4-Acetylaminobutanol		C6H11NO2	0	Cytosol
n4abutn	N4-Acetylaminobutanol		C6H11NO2	0	Mitochondria
n4m2masn	((N-acetyl-D-glucosaminy)4-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C66H109N6O45X	0	Golgi Apparatus
n5m2masn	((N-acetyl-D-glucosaminy)5-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C74H122N7O50X	0	Golgi Apparatus
na1	Sodium	Na, Natrium	Na	1	Cytosol
na1	Sodium	Na, Natrium	Na	1	Extracellular
na1	Sodium	Na, Natrium	Na	1	Golgi Apparatus
na1	Sodium	Na, Natrium	Na	1	Peroxisome
nac	Nicotinate	3-Pyridinecarboxylic acid, Niacin, Nicotinic acid	C6H4NO2	-1	Cytosol
nac	Nicotinate	3-Pyridinecarboxylic acid, Niacin, Nicotinic acid	C6H4NO2	-1	Extracellular
Nacasp	N-Acetyl-L-aspartate		C6H7NO5	-2	Cytosol
Nacasp	N-Acetyl-L-aspartate		C6H7NO5	-2	Mitochondria
Nacsertrn	N-Acetylsertrotin	N-Acetyl-5-hydroxytryptamine	C12H14N2O2	0	Cytosol
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Cytosol
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Extracellular
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Mitochondria
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Nucleus
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Endoplasmic Reticulum
nad	Nicotinamide adenine dinucleotide	NAD, NAD+, beta-Diphosphopyridine Nucleotide, beta-NAD, beta-Nicotinamide adenine dinucleotide	C21H26N7O14P2	-1	Peroxisome
nadh	Nicotinamide adenine dinucleotide - reduced	DPNH, NADH	C21H27N7O14P2	-2	Cytosol
nadh	Nicotinamide adenine dinucleotide - reduced	DPNH, NADH	C21H27N7O14P2	-2	Mitochondria
nadh	Nicotinamide adenine dinucleotide - reduced	DPNH, NADH	C21H27N7O14P2	-2	Endoplasmic Reticulum
nadh	Nicotinamide adenine dinucleotide - reduced	DPNH, NADH	C21H27N7O14P2	-2	Peroxisome
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Cytosol
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Extracellular
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Mitochondria
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Nucleus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Endoplasmic Reticulum
nadp	Nicotinamide adenine dinucleotide phosphate	NADP, NADP+, beta-Nicotinamide adenine dinucleotide phosphate	C21H25N7O17P3	-3	Peroxisome
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	NADPH, TPNH, beta-triphosphopyridine nucleotide	C21H26N7O17P3	-4	Cytosol
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	NADPH, TPNH, beta-triphosphopyridine nucleotide	C21H26N7O17P3	-4	Mitochondria
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	NADPH, TPNH, beta-triphosphopyridine nucleotide	C21H26N7O17P3	-4	Nucleus
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	NADPH, TPNH, beta-triphosphopyridine nucleotide	C21H26N7O17P3	-4	Endoplasmic Reticulum
nadph	Nicotinamide adenine dinucleotide phosphate - reduced	NADPH, TPNH, beta-triphosphopyridine nucleotide	C21H26N7O17P3	-4	Peroxisome
naclc2p_L	N-Acetyl-D-glucosaminyl-diphosphodolichol, human liver homolog	N-Acetyl-D-glucosaminyl-diphosphodolichol	C1160H1898N10O120P20	-20	Cytosol
naclc2p_U	N-Acetyl-D-glucosaminyl-diphosphodolichol, human uterin homolog		C1105H1810N10O120P20	-20	Cytosol
ncam	Nicotinamide	Niacinamide, Nicotinic acid amide, Vitamin PP	C6H6N2O	0	Cytosol
ncam	Nicotinamide	Niacinamide, Nicotinic acid amide, Vitamin PP	C6H6N2O	0	Extracellular
Ndmelys	Protein N6,N6-dimethyl-L-lysine	Protein N6,N6-dimethyl-L-lysine	C2H7X	2	Nucleus
nformanth	N-Formylanthranilate	2-(Formylamino)-benzoic acid, Formylanthranilate	C8H6NO3	-1	Cytosol
nh4	Ammonium	NH3	H4N	1	Cytosol
nh4	Ammonium	NH3	H4N	1	Extracellular
nh4	Ammonium	NH3	H4N	1	Mitochondria
nh4	Ammonium	NH3	H4N	1	Nucleus
nh4	Ammonium	NH3	H4N	1	Endoplasmic Reticulum
nh4	Ammonium	NH3	H4N	1	Peroxisome
nicrns	Nicotinate D-ribonucleoside		C11H13NO6	0	Cytosol
nicrnt	Nicotinate D-ribonucleotide	Nicotinate ribonucleotide, Nicotinic acid ribonucleotide, beta-Nicotinate D-ribonucleotide	C11H12NO9P	-2	Cytosol
nicrnt	Nicotinate D-ribonucleotide	Nicotinate ribonucleotide, Nicotinic acid ribonucleotide, beta-Nicotinate D-ribonucleotide	C11H12NO9P	-2	Mitochondria
nicrnt	Nicotinate D-ribonucleotide	Nicotinate ribonucleotide, Nicotinic acid ribonucleotide, beta-Nicotinate D-ribonucleotide	C11H12NO9P	-2	Nucleus
nifedipine	nifedipine	Adalat [MeSH: Nifedipine], Hexadilat, Introcar, Kordafen, Nifedidor, Oxcord, Procardia, Procardia [MeSH: Nifedipine], Tibricol, nifedipine [MeSH: Nifedipine]	C17H18N2O6	0	Cytosol
nifedipine	nifedipine	Adalat [MeSH: Nifedipine], Hexadilat, Introcar, Kordafen, Nifedidor, Oxcord, Procardia, Procardia [MeSH: Nifedipine], Tibricol, nifedipine [MeSH: Nifedipine]	C17H18N2O6	0	Extracellular
nm2masn	(N-acetyl-D-glucosaminyl-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C42H70N3O30X	0	Golgi Apparatus
nm4masn	(N-acetyl-D-glucosaminyl-(alpha-D-mannosyl)4-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)		C54H90N3O40X	0	Golgi Apparatus
Nimelys	Histone N6-methyl-L-lysine		CXH4	1	Nucleus
nmn	NMN	Nicotinamide D-ribonucleotide, Nicotinamide mononucleotide, Nicotinamide ribonucleotide	C11H14N2O8P	-1	Cytosol
nmn	NMN	Nicotinamide D-ribonucleotide, Nicotinamide mononucleotide, Nicotinamide ribonucleotide	C11H14N2O8P	-1	Mitochondria
nmn	NMN	Nicotinamide D-ribonucleotide, Nicotinamide mononucleotide, Nicotinamide ribonucleotide	C11H14N2O8P	-1	Nucleus
nmptc	N-Methylputrescine		C5H16N2	2	Cytosol
nmhsrtn	N-Methylserotonin		C11H15N2O	1	Cytosol
no	Nitric oxide	NO, Nitrogen monoxide	NO	0	Cytosol
no	Nitric oxide	NO, Nitrogen monoxide	NO	0	Extracellular
normete-L	L-Normetanephrine		C9H14NO3	1	Cytosol
npth	Naphthalene		C10H8	0	Cytosol
npth	Naphthalene		C10H8	0	Extracellular
nrpphr	Norepinephrine	2-benzenediol, 4-[(1R)-2-Amino-1-hydroxyethyl]-Arterenol, L-Noradrenaline, Noradrenaline	C8H12NO3	1	Cytosol
nrpphr	Norepinephrine	2-benzenediol, 4-[(1R)-2-Amino-1-hydroxyethyl]-Arterenol, L-Noradrenaline, Noradrenaline	C8H12NO3	1	Extracellular
nrpphrsf	Sulfate derivative of norepinephrine		C8H11NO6S	0	Cytosol
nrpphrsf	Sulfate derivative of norepinephrine		C8H11NO6S	0	Extracellular
nrvc	nervonic acid	(Z)-15-Tetracosenoic acid, Nervonic acid, tetracos-15-enoic acid	C24H45O2	-1	Cytosol
nrvc	nervonic acid	(Z)-15-Tetracosenoic acid, Nervonic acid, tetracos-15-enoic acid	C24H45O2	-1	Extracellular
nrvccoa	nervonyl coenzyme A		C45H76N7O17P3S	-4	Cytosol
nrvccoa	nervonyl coenzyme A		C45H76N7O17P3S	-4	Mitochondria
nrvccoa	nervonyl coenzyme A		C45H76N7O17P3S	-4	Peroxisome
nrvcnrm	Nervonyl carnitine	nervonic acid - carnitine	C31H59NO4	0	Cytosol
nrvcnrm	Nervonyl carnitine	nervonic acid - carnitine	C31H59NO4	0	Mitochondria
ntm2amep	N-Trimethyl-2-aminoethylphosphonate	2-Trimethylaminoethylphosphonate	C5H13NO3P	-1	Cytosol
Nimelys	Protein N6,N6,N6-trimethyl-L-lysine	Protein N6,N6,N6-trimethyl-L-lysine	C3H10X	3	Nucleus
Nimelys	Protein N6,N6,N6-trimethyl-L-lysine	Protein N6,N6,N6-trimethyl-L-lysine	C3H10X	3	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
nwharg	N-(omega)-Hydroxyarginine		C6H15N4O3	1	Cytosol
o2	O2	Oxygen, dioxygen	O2	0	Cytosol
o2	O2	Oxygen, dioxygen	O2	0	Extracellular
o2	O2	Oxygen, dioxygen	O2	0	Mitochondria
o2	O2	Oxygen, dioxygen	O2	0	Nucleus
o2	O2	Oxygen, dioxygen	O2	0	Endoplasmic Reticulum
o2	O2	Oxygen, dioxygen	O2	0	Peroxisome
o2s	Superoxide anion	O2 free radical, O2.-	O2	-1	Cytosol
o2s	Superoxide anion	O2 free radical, O2.-	O2	-1	Extracellular
o2s	Superoxide anion	O2 free radical, O2.-	O2	-1	Mitochondria
o2s	Superoxide anion	O2 free radical, O2.-	O2	-1	Nucleus
o2s	Superoxide anion	O2 free radical, O2.-	O2	-1	Peroxisome
oaa	Oxaloacetate	2-oxobutanedioic acid, Oxalacetic acid, Oxaloacetic acid, Oxosuccinic acid	C4H2O5	-2	Cytosol
oaa	Oxaloacetate	2-oxobutanedioic acid, Oxalacetic acid, Oxaloacetic acid, Oxosuccinic acid	C4H2O5	-2	Mitochondria
oaa	Oxaloacetate	2-oxobutanedioic acid, Oxalacetic acid, Oxaloacetic acid, Oxosuccinic acid	C4H2O5	-2	Peroxisome
oagd3_hs	9-O-Acetylated GD3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)1 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GD3, 9-O-Acetyl-GD3, 9-O-Acetylated GD3	C54H90N3O29FULLRCD60b	-2	Cytosol
oagd3_hs	9-O-Acetylated GD3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)1 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GD3, 9-O-Acetyl-GD3, 9-O-Acetylated GD3	C54H90N3O29FULLRCD60b	-2	Extracellular
oagd3_hs	9-O-Acetylated GD3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)1 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GD3, 9-O-Acetyl-GD3, 9-O-Acetylated GD3	C54H90N3O29FULLRCD60b	-2	Golgi Apparatus
oagt3_hs	9-O-Acetylated GT3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)2 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GT3, 9-O-Acetylated GT3	C65H106N4O37FULLRCD60b	-3	Cytosol
oagt3_hs	9-O-Acetylated GT3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)2 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GT3, 9-O-Acetylated GT3	C65H106N4O37FULLRCD60b	-3	Extracellular
oagt3_hs	9-O-Acetylated GT3 (homo sapiens)	[Gal]1 (Glc)1 (Neu5Ac)2 (Neu5Ac9Ac)1 (Cer)1, 9-O-Ac-GT3, 9-O-Acetylated GT3	C65H106N4O37FULLRCD60b	-3	Golgi Apparatus
occoa	Octanoyl-CoA (n-C8:0CoA)		C29H46N7O17P3S	-4	Cytosol
occoa	Octanoyl-CoA (n-C8:0CoA)		C29H46N7O17P3S	-4	Mitochondria
occoa	Octanoyl-CoA (n-C8:0CoA)		C29H46N7O17P3S	-4	Peroxisome
ocdca	octadecanoate (n-C18:0)	Octadecanoic acid, Stearate, Stearic acid	C18H35O2	-1	Cytosol
ocdca	octadecanoate (n-C18:0)	Octadecanoic acid, Stearate, Stearic acid	C18H35O2	-1	Extracellular
ocdcaACP	Octadecenoyl-ACP (n-C18:0ACP)	stearoyl-ACP	C29H55N2O8PRSS	-1	Cytosol
odcea	octadecenoate (n-C18:1)	(9Z)-Octadecenoic acid, (Z)-Octadec-9-enoic acid, Oleic acid, octadecenoic acid, oleate	C18H33O2	-1	Cytosol
odcea	octadecenoate (n-C18:1)	(9Z)-Octadecenoic acid, (Z)-Octadec-9-enoic acid, Oleic acid, octadecenoic acid, oleate	C18H33O2	-1	Extracellular
odcya	octadecadienoate (n-C18:2)	9,12-Octadecadienoic acid, octadecadienoic acid	C18H31O2	-1	Cytosol
odcyaACP	Octadecenoyl-ACP (n-C18:2ACP)		C29H51N2O8PRSS	-1	Cytosol
octa	octanoate (n-C8:0)	Caprylic acid, Octanoic acid, Octylic acid	C8H15O2	-1	Cytosol
octa	octanoate (n-C8:0)	Caprylic acid, Octanoic acid, Octylic acid	C8H15O2	-1	Extracellular
octeACP	cis-octadec-11-enoyl-[acyl-carrier protein] (n-C18:1)	Octadecenoyl-ACP (n-C18:1ACP), cis-vacc-11-enoyl-[acyl-carrier protein] (n-C18:1)	C29H53N2O8PRSS	-1	Cytosol
od2coa	trans-Octadec-2-enoyl-CoA	elaidic acid coenzyme A	C39H64N7O17P3S	-4	Cytosol
od2coa	trans-Octadec-2-enoyl-CoA	elaidic acid coenzyme A	C39H64N7O17P3S	-4	Mitochondria
oddecoa	Octadecenoyl-CoA (n-C18:1CoA)	Oleoyl-CoA	C39H64N7O17P3S	-4	Cytosol
oddecoa	Octadecenoyl-CoA (n-C18:1CoA)	Oleoyl-CoA	C39H64N7O17P3S	-4	Mitochondria
oddecoa	Octadecenoyl-CoA (n-C18:1CoA)	Oleoyl-CoA	C39H64N7O17P3S	-4	Peroxisome
odcern	octadecenoyl carnitine		C25H47N04	0	Cytosol
odcern	octadecenoyl carnitine		C25H47N04	0	Mitochondria
oh1	hydroxide ion	HO-, OH-	HO	-1	Cytosol
oh1	hydroxide ion	HO-, OH-	HO	-1	Extracellular
oh1	hydroxide ion	HO-, OH-	HO	-1	Mitochondria
omeprazole	omeprazole	Demeprazol, Dudencer, Emeproton, Epirazole, Gastrimut, Gastroloc, Gibnancer, Indurgan, Inhibitron, omeprazole [MeSH: Omeprazole]	C17H19N3O3S	0	Cytosol
omeprazole	omeprazole	Demeprazol, Dudencer, Emeproton, Epirazole, Gastrimut, Gastroloc, Gibnancer, Indurgan, Inhibitron, omeprazole [MeSH: Omeprazole]	C17H19N3O3S	0	Extracellular
onpthl	naphthalene epoxide		C10H8O	0	Cytosol
onpthl	naphthalene epoxide		C10H8O	0	Extracellular
oretin	4-oxo-retonic acid		C20H27O3	-1	Cytosol
oretin	4-oxo-retonic acid		C20H27O3	-1	Nucleus
orn	Ornithine	2,5-Diaminopentanoate, 2,5-Diaminopentanoic acid, 2,5-Diaminovaleric acid, L-Ornithine	CSH13N2O2	1	Cytosol
orn	Ornithine	2,5-Diaminopentanoate, 2,5-Diaminopentanoic acid, 2,5-Diaminovaleric acid, L-Ornithine	CSH13N2O2	1	Extracellular
orn	Ornithine	2,5-Diaminopentanoate, 2,5-Diaminopentanoic acid, 2,5-Diaminovaleric acid, L-Ornithine	CSH13N2O2	1	Mitochondria
om-D	D-Ornithine		CSH13N2O2	1	Peroxisome
orot	Orotate	Orotic acid, Uracil-6-carboxylic acid	CSH3N2O4	-1	Cytosol
oro5p	Orotidine 5'-phosphate	Orotidylic acid	C10H10N2O11P	-3	Cytosol
oxa	Oxalate	Ethanedioic acid, Oxalic acid	C2O4	-2	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
oxa	Oxalate	Ethanedioic acid, Oxalic acid	C2O4	-2	Extracellular
oxa	Oxalate	Ethanedioic acid, Oxalic acid	C2O4	-2	Peroxisome
pa_hs	phosphatidic acid (homo sapiens)	phosphatidate	C3H5O4PFULLR2CO2FULLR2C O2	-2	Cytosol
pa_hs	phosphatidic acid (homo sapiens)	phosphatidate	C3H5O4PFULLR2CO2FULLR2C O2	-2	Golgi Apparatus
pa_hs	phosphatidic acid (homo sapiens)	phosphatidate	C3H5O4PFULLR2CO2FULLR2C O2	-2	Mitochondria
pa_hs	phosphatidic acid (homo sapiens)	phosphatidate	C3H5O4PFULLR2CO2FULLR2C O2	-2	Nucleus
pa_hs	phosphatidic acid (homo sapiens)	phosphatidate	C3H5O4PFULLR2CO2FULLR2C O2	-2	Endoplasmic Reticulum
pac	Phenylacetic acid	Benzeneacetic acid, Benzylformic acid, Phenylacetate	C8H7O2	-1	Cytosol
pacald	Phenylacetaldehyde	alpha-Tolualdehyde	C8H8O	0	Cytosol
paf_hs	1-alkyl-2-acteylglycerol 3-phosphocholine (homo sapiens)	1-Alkyl-2-acetyl-sn-glycero-3-phosphocholine, PA platelet activating factor	C11H23O4NPFULLR2CO2	0	Cytosol
paf_hs	1-alkyl 2-acteylglycerol 3-phosphocholine (homo sapiens)	1-Alkyl-2-acetyl-sn-glycero-3-phosphocholine, PA platelet activating factor	C11H23O4NPFULLR2CO2	0	Extracellular
pail_hs	phosphatidylinositol (homo sapiens)	PtdIns	C9H16O9PFULLR2CO2FULLR2 CO2	-1	Cytosol
pail_hs	phosphatidylinositol (homo sapiens)	PtdIns	C9H16O9PFULLR2CO2FULLR2 CO2	-1	Nucleus
pail_hs	phosphatidylinositol (homo sapiens)	PtdIns	C9H16O9PFULLR2CO2FULLR2 CO2	-1	Endoplasmic Reticulum
pail345p_hs	phosphatidylinositol-3,4,5-trisphosphate (Homo sapiens)	PIP3, PtdIns(3,4,5)P3	C9H13O18P4FULLR2CO2FULLR 2CO2	-7	Cytosol
pail345p_hs	phosphatidylinositol-3,4,5-trisphosphate (Homo sapiens)	PIP3, PtdIns(3,4,5)P3	C9H13O18P4FULLR2CO2FULLR 2CO2	-7	Nucleus
pail34p_hs	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)		C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Cytosol
pail34p_hs	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)		C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Nucleus
pail34p_hs	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)		C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Endoplasmic Reticulum
pail35p_hs	phosphatidylinositol-3,5-bisphosphate (Homo sapiens)		C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Cytosol
pail35p_hs	phosphatidylinositol-3,5-bisphosphate (Homo sapiens)		C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Endoplasmic Reticulum
pail3p_hs	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Cytosol
pail3p_hs	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Nucleus
pail3p_hs	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Endoplasmic Reticulum
pail45p_hs	phosphatidylinositol 4,5-bisphosphate (Homo sapiens)	PIP2, PtdIns(4,5)P2, phosphatidylinositol disphosphate	C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Cytosol
pail45p_hs	phosphatidylinositol 4,5-bisphosphate (Homo sapiens)	PIP2, PtdIns(4,5)P2, phosphatidylinositol disphosphate	C9H14O15P3FULLR2CO2FULLR 2CO2	-5	Nucleus
pail4p_hs	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	PIP, PtdIns4P	C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Cytosol
pail4p_hs	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	PIP, PtdIns4P	C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Nucleus
pail4p_hs	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	PIP, PtdIns4P	C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Endoplasmic Reticulum
pail5p_hs	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Cytosol
pail5p_hs	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Nucleus
pail5p_hs	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)		C9H15O12P2FULLR2CO2FULLR 2CO2	-3	Endoplasmic Reticulum
palmACP	Palmitoyl-ACP (n-C16:0ACP)	Hexadecanoyl-[acyl], Hexadecanoyl-[acyl-carrier protein], fa8-ACP, hexadecanoyl-ACP	C27H51N2O8PRS	-1	Cytosol
pan4p	Pantetheine 4'-phosphate	4'-Phosphopantetheine, Phosphopantetheine	C11H21N2O7PS	-2	Cytosol
pap	Adenosine 3',5'-bisphosphate	3'-Phosphoadenylylate, PAP, Phosphoadenosine phosphate	C10H11N5O10P2	4	Cytosol
pap	Adenosine 3',5'-bisphosphate	3'-Phosphoadenylylate, PAP, Phosphoadenosine phosphate	C10H11N5O10P2	4	Golgi Apparatus
paps	3'-Phosphoadenylyl sulfate	3'-Phospho-5'-adenylyl sulfate, 3'- Phosphoadenosine 5'-phosphosulfate, PAPS	C10H11N5O13P2S	-4	Cytosol
paps	3'-Phosphoadenylyl sulfate	3'-Phospho-5'-adenylyl sulfate, 3'- Phosphoadenosine 5'-phosphosulfate, PAPS	C10H11N5O13P2S	-4	Golgi Apparatus
pchol_hs	Phosphatidylcholine (homo sapiens)		C8H18NO4PFULLR2CO2FULLR 2CO2	0	Cytosol
pchol_hs	Phosphatidylcholine (homo sapiens)		C8H18NO4PFULLR2CO2FULLR 2CO2	0	Extracellular
pchol_hs	Phosphatidylcholine (homo sapiens)		C8H18NO4PFULLR2CO2FULLR 2CO2	0	Golgi Apparatus
pchol_hs	Phosphatidylcholine (homo sapiens)		C8H18NO4PFULLR2CO2FULLR 2CO2	0	Mitochondria
pchol_hs	Phosphatidylcholine (homo sapiens)		C8H18NO4PFULLR2CO2FULLR 2CO2	0	Endoplasmic Reticulum
pcollg5hlys	Procollagen 5-hydroxy-L-lysine		C6H14N2O3	0	Cytosol
pcollglys	Procollagen L-lysine		C7H14N3O2R2	1	Cytosol
pcreat	Phosphocreatine		C4H9N3O5P	-1	Cytosol
pcreat	Phosphocreatine		C4H9N3O5P	-1	Mitochondria
pcrn	propionyl-carnitine		C10H19NO4	0	Cytosol
pcrn	propionyl-carnitine		C10H19NO4	0	Mitochondria
pcrn	propionyl-carnitine		C10H19NO4	0	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
pd3	Previtamin D3		C27H44O	0	Cytosol
pdx5p	Pyridoxine 5'-phosphate	Pyridoxine 5-phosphate, Pyridoxine phosphate	C8H10NO6P	-2	Cytosol
pe_hs	phosphatidylethanolamine (homo sapiens)		C5H12NO4PFULLR2CO2	0	Cytosol
pe_hs	phosphatidylethanolamine (homo sapiens)		C5H12NO4PFULLR2CO2	0	Extracellular
pe_hs	phosphatidylethanolamine (homo sapiens)		C5H12NO4PFULLR2CO2	0	Golgi Apparatus
pe_hs	phosphatidylethanolamine (homo sapiens)		C5H12NO4PFULLR2CO2	0	Mitochondria
pe_hs	phosphatidylethanolamine (homo sapiens)		C5H12NO4PFULLR2CO2	0	Endoplasmic Reticulum
peamn	Phenethylamine	2-Phenylethylamine, Phenethylamine, Phenylethylamine, beta-Phenylethylamine	C8H12N	1	Cytosol
pegon	pseudoecgonine		C9H14NO3	-1	Endoplasmic Reticulum
pegoncoa	Pseudoecgonyl-CoA		C30H46N8O18P3S	-3	Endoplasmic Reticulum
pep	Phosphoenolpyruvate	PEP, Phosphoenolpyruvic acid	C3H2O6P	-3	Cytosol
pep	Phosphoenolpyruvate	PEP, Phosphoenolpyruvic acid	C3H2O6P	-3	Mitochondria
peplys	Peptidyl-L-lysine	L-Lysine-protein, Protein lysine	XH	0	Extracellular
peplys	Peptidyl-L-lysine	L-Lysine-protein, Protein lysine	XH	0	Nucleus
pepslys	peptide sans lysine	peptide without lysine (cleaved)	X	0	Endoplasmic Reticulum
peracd	Perillic acid		C10H13O2	-1	Cytosol
peracd	Perillic acid		C10H13O2	-1	Mitochondria
perillyl	Perillyl alcohol	(-)-Perillyl alcohol, Perillyl alcohol	C10H16O	0	Cytosol
perillyl	Perillyl alcohol	(-)-Perillyl alcohol, Perillyl alcohol	C10H16O	0	Extracellular
pglyc_hs	phosphatidylglycerol (homo sapiens)		C6H12O6PFULLR2CO2	-1	Cytosol
pglyc_hs	phosphatidylglycerol (homo sapiens)		C6H12O6PFULLR2CO2	-1	Extracellular
pgp_hs	phosphatidyl glycerol phosphate (homo sapiens)		C6H11O9P2FULLR2CO2	-3	Cytosol
phaccoa	Phenylacetyl-CoA		C29H38N7O17P3S	-4	Cytosol
pheacgln	alpha-N-Phenylacetyl-L-glutamine		C13H16N2O4	0	Cytosol
pheacgln	alpha-N-Phenylacetyl-L-glutamine		C13H16N2O4	0	Extracellular
phe-L	L-Phenylalanine	(S)-Phenylalanine, (S)-alpha-amino-beta-phenylpropionic acid, 3-phenylalanine	C9H11NO2	0	Cytosol
phe-L	L-Phenylalanine	(S)-Phenylalanine, (S)-alpha-amino-beta-phenylpropionic acid, 3-phenylalanine	C9H11NO2	0	Extracellular
phe-L	L-Phenylalanine	(S)-Phenylalanine, (S)-alpha-amino-beta-phenylpropionic acid, 3-phenylalanine	C9H11NO2	0	Mitochondria
pheme	Protoheme	Haem, Heme, Heme B, hemeB	C34H30FeN4O4	-2	Cytosol
pheme	Protoheme	Haem, Heme, Heme B, hemeB	C34H30FeN4O4	-2	Extracellular
pheme	Protoheme	Haem, Heme, Heme B, hemeB	C34H30FeN4O4	-2	Mitochondria
phom	O-Phospho-L-homoserine		C4H8NO6P	-2	Cytosol
phpyr	Phenylpyruvate	3-Phenyl-2-oxopropanoate, Phenylpyruvic acid, alpha-Ketohydrocinnamic acid, keto-Phenylpyruvate	C9H7O3	-1	Cytosol
phpyr	Phenylpyruvate	3-Phenyl-2-oxopropanoate, Phenylpyruvic acid, alpha-Ketohydrocinnamic acid, keto-Phenylpyruvate	C9H7O3	-1	Mitochondria
phyQ	Phylloquinone	2-Methyl-3-phytyl-1,4-naphthoquinone, Phylloquinone, Phytonadione, Vitamin K1	C31H46O2	0	Cytosol
phyQ	Phylloquinone	2-Methyl-3-phytyl-1,4-naphthoquinone, Phylloquinone, Phytonadione, Vitamin K1	C31H46O2	0	Extracellular
phyt	phytanic acid	Phytanate, Phytanic acid	C20H39O2	-1	Cytosol
phyt	phytanic acid	Phytanate, Phytanic acid	C20H39O2	-1	Extracellular
phyt	phytanic acid	Phytanate, Phytanic acid	C20H39O2	-1	Peroxisome
phyt2ohcoa	2-Hydroxyphytanoyl-CoA		C41H70N7O18P3S	-4	Peroxisome
phytcoa	phytanoyl coa	Phytanoyl-CoA, phytanic acid coenzyme a, phytanyl coa, phytanyl coenzyme a	C41H70N7O17P3S	-4	Cytosol
phytcoa	phytanoyl coa	Phytanoyl-CoA, phytanic acid coenzyme a, phytanyl coa, phytanyl coenzyme a	C41H70N7O17P3S	-4	Peroxisome
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Cytosol
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Extracellular
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Golgi Apparatus
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Lysosome
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Mitochondria
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Nucleus
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Endoplasmic Reticulum
pi	Phosphate	Orthophosphate, Phosphoric acid, Pi	HO4P	-2	Peroxisome
pmtcoa	Palmitoyl-CoA (n-C16:0CoA)	Hexadecanoyl-CoA	C37H62N7O17P3S	-4	Cytosol
pmtcoa	Palmitoyl-CoA (n-C16:0CoA)	Hexadecanoyl-CoA	C37H62N7O17P3S	-4	Mitochondria
pmtcoa	Palmitoyl-CoA (n-C16:0CoA)	Hexadecanoyl-CoA	C37H62N7O17P3S	-4	Peroxisome
pmtcrn	L-Palmitoylcarnitine		C23H45NO4	0	Cytosol
pmtcrn	L-Palmitoylcarnitine		C23H45NO4	0	Mitochondria
pnto-R	(R)-Pantothenate	D-Pantothenate, Pantothenate, Pantothenic acid	C9H16NO5	-1	Cytosol
pnto-R	(R)-Pantothenate	D-Pantothenate, Pantothenate, Pantothenic acid	C9H16NO5	-1	Extracellular
pnto-R	(R)-Pantothenate	D-Pantothenate, Pantothenate, Pantothenic acid	C9H16NO5	-1	Mitochondria
ppa	Propionate (n-C3:0)	Propanoate, Propanoic acid, Propionic acid	C3H5O2	-1	Cytosol
ppa	Propionate (n-C3:0)	Propanoate, Propanoic acid, Propionic acid	C3H5O2	-1	Extracellular

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ppa	Propionate (n-C3:0)	Propanoate, Propanoic acid, Propionic acid	C3H5O2	-1	Mitochondria
ppbng	Porphobilinogen		C10H13N2O4	-1	Cytosol
ppcoa	Propionyl-CoA	Propionyl coenzyme A, Propionyl-CoA	C24H36N7O17P3S	-4	Cytosol
ppcoa	Propionyl-CoA	Propionyl coenzyme A, Propionyl-CoA	C24H36N7O17P3S	-4	Mitochondria
ppcoa	Propionyl-CoA	Propionyl coenzyme A, Propionyl-CoA	C24H36N7O17P3S	-4	Peroxisome
ppi	Diphosphate	PPi, Pyrophosphate, Pyrophosphoric acid	HO7P2	-3	Cytosol
ppi	Diphosphate	PPi, Pyrophosphate, Pyrophosphoric acid	HO7P2	-3	Mitochondria
ppi	Diphosphate	PPi, Pyrophosphate, Pyrophosphoric acid	HO7P2	-3	Nucleus
ppi	Diphosphate	PPi, Pyrophosphate, Pyrophosphoric acid	HO7P2	-3	Endoplasmic Reticulum
ppi	Diphosphate	PPi, Pyrophosphate, Pyrophosphoric acid	HO7P2	-3	Peroxisome
ppmi12346p	5-Diphosphoinositol pentakisphosphate	5-PP-InsP5	C6H6O27P7	-13	Cytosol
ppmi12346p	5-Diphosphoinositol pentakisphosphate	5-PP-InsP5	C6H6O27P7	-13	Nucleus
ppmi1346p	Diphosphoinositol tetrakisphosphate		C6H7O24P6	-11	Cytosol
ppmi1346p	Diphosphoinositol tetrakisphosphate		C6H7O24P6	-11	Nucleus
ppp9	Protoporphyrin	Protoporphyrin IX, Protoporphyrin IX	C34H32N4O4	-2	Mitochondria
pppg9	Protoporphyrinogen IX		C34H38N4O4	-2	Cytosol
pppg9	Protoporphyrinogen IX		C34H38N4O4	-2	Mitochondria
pppi	Inorganic triphosphate		HO10P3	-4	Cytosol
pppi	Inorganic triphosphate		HO10P3	-4	Mitochondria
pppi	Inorganic triphosphate		HO10P3	-4	Nucleus
pram	5-Phospho-beta-D-riboseylamine	5-Phospho-D-riboseylamine, 5-Phosphoribosyl-1-amine, 5-Phosphoribosylamine	C5H11NO7P	-1	Cytosol
pre_prot	glycophosphatidylinositol (GPI)-anchored protein precursor		XY	0	Endoplasmic Reticulum
prgnlone	Pregnenolone	3beta-Hydroxypregn-5-en-20-one, 5-Pregnen-3beta-ol-20-one	C21H32O2	0	Cytosol
prgnlone	Pregnenolone	3beta-Hydroxypregn-5-en-20-one, 5-Pregnen-3beta-ol-20-one	C21H32O2	0	Mitochondria
prgnlone	Pregnenolone	3beta-Hydroxypregn-5-en-20-one, 5-Pregnen-3beta-ol-20-one	C21H32O2	0	Endoplasmic Reticulum
prgnlones	pregnenolone sulfate	3beta-Hydroxypregn-5-en-20-one sulfate, 5-Pregnen-3beta-ol-20-one sulfate	C21H31O5S	-1	Cytosol
prgnlones	pregnenolone sulfate	3beta-Hydroxypregn-5-en-20-one sulfate, 5-Pregnen-3beta-ol-20-one sulfate	C21H31O5S	-1	Endoplasmic Reticulum
prgstn	Progesterone	4-Pregnene-3,20-dione	C21H30O2	0	Cytosol
prgstn	Progesterone	4-Pregnene-3,20-dione	C21H30O2	0	Endoplasmic Reticulum
prist	pristanic acid	pristanic acid	C19H37O2	-1	Cytosol
prist	pristanic acid	pristanic acid	C19H37O2	-1	Peroxisome
pristanal	pristanal		C19H38O	0	Cytosol
pristanal	pristanal		C19H38O	0	Peroxisome
pristcoa	pristanoyl coa	pristanic acid coenzyme a, pristanoyl coa, pristanoyl coenzyme a	C40H68N7O17P3S	-4	Cytosol
pristcoa	pristanoyl coa	pristanic acid coenzyme a, pristanoyl coa, pristanoyl coenzyme a	C40H68N7O17P3S	-4	Peroxisome
pro-D	D-Proline	D-Pyrrolidine-2-carboxylic acid	C5H9NO2	0	Cytosol
pro-D	D-Proline	D-Pyrrolidine-2-carboxylic acid	C5H9NO2	0	Extracellular
pro-D	D-Proline	D-Pyrrolidine-2-carboxylic acid	C5H9NO2	0	Lysosome
pro-D	D-Proline	D-Pyrrolidine-2-carboxylic acid	C5H9NO2	0	Peroxisome
pro-L	L-Proline	2-Pyrrolidinecarboxylic acid, Pro	C5H9NO2	0	Cytosol
pro-L	L-Proline	2-Pyrrolidinecarboxylic acid, Pro	C5H9NO2	0	Extracellular
pro-L	L-Proline	2-Pyrrolidinecarboxylic acid, Pro	C5H9NO2	0	Lysosome
pro-L	L-Proline	2-Pyrrolidinecarboxylic acid, Pro	C5H9NO2	0	Mitochondria
pro-L	L-Proline	2-Pyrrolidinecarboxylic acid, Pro	C5H9NO2	0	Endoplasmic Reticulum
prostg1	(13E)-11alpha-Hydroxy-9,15-dioxoprost-13-enoate	(13E)-11alpha-Hydroxy-9,15-dioxoprost-13-enoate	C20H31O5	-1	Cytosol
prostg2	Prostaglandin D2	(5Z, 13-dienoate, 13E)-(15S)-9alpha, 15-Dihydroxy-11-oxoprost-5	C20H31O5	-1	Cytosol
prostg2	Prostaglandin D2	(5Z, 13-dienoate, 13E)-(15S)-9alpha, 15-Dihydroxy-11-oxoprost-5	C20H31O5	-1	Extracellular
prostg2	Prostaglandin D2	(5Z, 13-dienoate, 13E)-(15S)-9alpha, 15-Dihydroxy-11-oxoprost-5	C20H31O5	-1	Endoplasmic Reticulum
prostge1	Prostaglandin E1	(13E)-(15S)-11alpha,15-Dihydroxy-9-oxoprost-13-enoate, Alprostadi, Befar, Prink, Prostaglandin E1	C20H33O5	-1	Cytosol
prostge1	Prostaglandin E1	(13E)-(15S)-11alpha,15-Dihydroxy-9-oxoprost-13-enoate, Alprostadi, Befar, Prink, Prostaglandin E1	C20H33O5	-1	Extracellular
prostge2	Prostaglandin E2	(5Z, 13-dienoate, 13E)-(15S)-11alpha, 15-Dihydroxy-9-oxoprost-13-enoate, 15-Dihydroxy-9-oxoprost-5	C20H31O5	-1	Cytosol
prostge2	Prostaglandin E2	(5Z, 13-dienoate, 13E)-(15S)-11alpha, 15-Dihydroxy-9-oxoprost-13-enoate, 15-Dihydroxy-9-oxoprost-5	C20H31O5	-1	Extracellular
prostge2	Prostaglandin E2	(5Z, 13-dienoate, 13E)-(15S)-11alpha, 15-Dihydroxy-9-oxoprost-13-enoate, 15-Dihydroxy-9-oxoprost-5	C20H31O5	-1	Endoplasmic Reticulum
prostgf2	Prostaglandin F2alpha	(+)-Prostaglandin F2a, Amoglandin, Cyclosin, Dinoprost, Enzaprost, Enzaprost F, PGF2a, Panacelan, Prostaglandin F2, Prostaglandin F2a, Prostarmon F, Prostin F 2 alpha, Protamodin, U 14583	C20H33O5	-1	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
prostgf2	Prostaglandin F2alpha	(+)-Prostaglandin F2a, Amoglandin, Cyclostin, Dinoprost, Enzaprost, Enzaprost F, PGF2a, Panacelan, Prostaglandin F2, Prostaglandin F2a, Prostarmon F, Prostin F 2 alpha, Protamodin, U 14583	C20H33O5	-1	Extracellular
prostgh2	Prostaglandin H2	(5Z, 11alpha-Epidoxy-15-hydroxyprosta-5, 13-dienoate, 13E)-(15S)-9alpha	C20H31O5	-1	Cytosol
prostgh2	Prostaglandin H2	(5Z, 11alpha-Epidoxy-15-hydroxyprosta-5, 13-dienoate, 13E)-(15S)-9alpha	C20H31O5	-1	Endoplasmic Reticulum
prostgi2	Prostaglandin I2	Sdienoate, (5Z, 13-, 13E)-(15S)-6, 15-dihydroxyprosta-5, 9alpha-Epoxy-11alpha, PGI2, Prostacyclin	C20H31O5	-1	Endoplasmic Reticulum
prpncoa	Propenoyl-CoA	Acryloyl-CoA, Acrylyl-CoA	C24H34N7O17P3S	-4	Mitochondria
prpncoa	Propenoyl-CoA	Acryloyl-CoA, Acrylyl-CoA	C24H34N7O17P3S	-4	Peroxisome
prpp	5-Phospho-alpha-D-ribose 1-diphosphate	5-Phosphoribosyl 1-pyrophosphate, 5-Phosphoribosyl diphosphate, PRPP	C5H8O14P3	-5	Cytosol
ps_hs	phosphatidylserine (homo sapiens)	1,2-Diacyl-sn-glycerol 3-phospho-L-serine, 3-O-sn-Phosphatidyl-L-serine, O3-Phosphatidyl-L-serine, Phosphatidyl-L-serine	C6H11NO6FULLR2CO2FULLR2CO2	-1	Cytosol
ps_hs	phosphatidylserine (homo sapiens)	1,2-Diacyl-sn-glycerol 3-phospho-L-serine, 3-O-sn-Phosphatidyl-L-serine, O3-Phosphatidyl-L-serine, Phosphatidyl-L-serine	C6H11NO6FULLR2CO2FULLR2CO2	-1	Extracellular
ps_hs	phosphatidylserine (homo sapiens)	1,2-Diacyl-sn-glycerol 3-phospho-L-serine, 3-O-sn-Phosphatidyl-L-serine, O3-Phosphatidyl-L-serine, Phosphatidyl-L-serine	C6H11NO6FULLR2CO2FULLR2CO2	-1	Golgi Apparatus
ps_hs	phosphatidylserine (homo sapiens)	1,2-Diacyl-sn-glycerol 3-phospho-L-serine, 3-O-sn-Phosphatidyl-L-serine, O3-Phosphatidyl-L-serine, Phosphatidyl-L-serine	C6H11NO6FULLR2CO2FULLR2CO2	-1	Mitochondria
ps_hs	phosphatidylserine (homo sapiens)	1,2-Diacyl-sn-glycerol 3-phospho-L-serine, 3-O-sn-Phosphatidyl-L-serine, O3-Phosphatidyl-L-serine, Phosphatidyl-L-serine	C6H11NO6FULLR2CO2FULLR2CO2	-1	Endoplasmic Reticulum
pser-L	O-Phospho-L-serine	3-Phosphoserine	C3H6NO6P	-2	Cytosol
pdca	pentadecanoate	Pentadecanoic acid, n-Pentadecanoic Acid	C15H29O2	-1	Cytosol
pdca	pentadecanoate	Pentadecanoic acid, n-Pentadecanoic Acid	C15H29O2	-1	Extracellular
pdcacoa	pentadecanoyl Coenzyme A	Pentadecanoic acid coenzyme a, n-Pentadecanoic Acid coa	C36H60N7O17P3S	-4	Cytosol
pdcacoa	pentadecanoyl Coenzyme A	Pentadecanoic acid coenzyme a, n-Pentadecanoic Acid coa	C36H60N7O17P3S	-4	Mitochondria
pdcacrn	pentadenoyl carnitine	Pentadecanoic acid - carnitine, pentadecanoate carnitine	C22H43NO4	0	Cytosol
pdcacrn	pentadenoyl carnitine	Pentadecanoic acid - carnitine, pentadecanoate carnitine	C22H43NO4	0	Mitochondria
ptrc	Putrescine	1,4-Butanediamine, 1,4-Diaminobutane, Tetramethylenediamine	C4H14N2	2	Cytosol
ptrc	Putrescine	1,4-Butanediamine, 1,4-Diaminobutane, Tetramethylenediamine	C4H14N2	2	Mitochondria
pth	Pantetheine		C11H22N2O4S	0	Cytosol
pyam5p	Pyridoxamine 5'-phosphate	Pyridoxamine 5-phosphate, Pyridoxamine phosphate	C8H12N2O5P	-1	Cytosol
pyam5p	Pyridoxamine 5'-phosphate	Pyridoxamine 5-phosphate, Pyridoxamine phosphate	C8H12N2O5P	-1	Mitochondria
pydam	Pyridoxamine	PM	C8H13N2O2	1	Cytosol
pydam	Pyridoxamine	PM	C8H13N2O2	1	Extracellular
pydx	Pyridoxal		C8H9NO3	0	Cytosol
pydx	Pyridoxal		C8H9NO3	0	Extracellular
pydx5p	Pyridoxal 5'-phosphate	Pyridoxal 5-phosphate, Pyridoxal phosphate	C8H8NO6P	-2	Cytosol
pydx5p	Pyridoxal 5'-phosphate	Pyridoxal 5-phosphate, Pyridoxal phosphate	C8H8NO6P	-2	Mitochondria
pydxn	Pyridoxine	Pyridoxol, vitamin b6	C8H11NO3	0	Cytosol
pydxn	Pyridoxine	Pyridoxol, vitamin b6	C8H11NO3	0	Extracellular
pylald	Perillyl aldehyde	Perillaldehyde	C10H14O	0	Cytosol
pylald	Perillyl aldehyde	Perillaldehyde	C10H14O	0	Mitochondria
pyr	Pyruvate	2-Ketopropionic Acid, 2-Oxopropanoate, 2-Oxopropanoic acid, Pyroracemic acid, Pyruvic acid, alpha-Ketopropionic acid	C3H3O3	-1	Cytosol
pyr	Pyruvate	2-Ketopropionic Acid, 2-Oxopropanoate, 2-Oxopropanoic acid, Pyroracemic acid, Pyruvic acid, alpha-Ketopropionic acid	C3H3O3	-1	Extracellular
pyr	Pyruvate	2-Ketopropionic Acid, 2-Oxopropanoate, 2-Oxopropanoic acid, Pyroracemic acid, Pyruvic acid, alpha-Ketopropionic acid	C3H3O3	-1	Mitochondria
pyr	Pyruvate	2-Ketopropionic Acid, 2-Oxopropanoate, 2-Oxopropanoic acid, Pyroracemic acid, Pyruvic acid, alpha-Ketopropionic acid	C3H3O3	-1	Peroxisome
q10	Ubiquinone-10	ubidecarenone	C59H90O4	0	Cytosol
q10	Ubiquinone-10	ubidecarenone	C59H90O4	0	Mitochondria
q10h2	Ubiquinol-10		C59H92O4	0	Cytosol
q10h2	Ubiquinol-10		C59H92O4	0	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
quln	Quinolinate	2,3-Pyridinedicarboxylic acid, Pyridine-2,3-dicarboxylate, Quinolinic acid	C7H3NO4	-2	Cytosol
R1coa_hs	R group 1 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
R1coa_hs	R group 1 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Endoplasmic Reticulum
r1p	alpha-D-Ribose 1-phosphate	D-Ribose 1-phosphate, Ribose 1-phosphate	C5H9O8P	-2	Cytosol
R2coa_hs	R group 2 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
R2coa_hs	R group 2 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Endoplasmic Reticulum
R3coa_hs	R group 3 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
R4coa_hs	R group 4 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
R5coa_hs	R group 5 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
r5p	alpha-D-Ribose 5-phosphate	D-Ribose 5-phosphate, D-Ribose-5-phosphate, Ribose 5-phosphate	C5H9O8P	-2	Cytosol
r5p	alpha-D-Ribose 5-phosphate	D-Ribose 5-phosphate, D-Ribose-5-phosphate, Ribose 5-phosphate	C5H9O8P	-2	Mitochondria
R6coa_hs	R group 6 Coenzyme A homo sapiens		XC02C21H31N7O15P3S	-4	Cytosol
rib-D	D-Ribulose	D-Arabinoketose, D-Arabinulose, D-Erythro-2-pentulose, D-Riboketose	C5H10O5	0	Cytosol
rbt	Ribitol	Adonitol	C5H12O5	0	Cytosol
rbt	Ribitol	Adonitol	C5H12O5	0	Extracellular
retfa	fatty acid retinol		C20H29OFULLR2CO	0	Cytosol
retfa	fatty acid retinol		C20H29OFULLR2CO	0	Extracellular
retinal	Retinal	Retinene, Vitamin A aldehyde, all-trans-Retinal, all-trans-Retinene, all-trans-Vitamin A aldehyde	C20H28O	0	Cytosol
retinal-11-cis	cis-11-retinal	11-cis-Retinal, 11-cis-Retinene, 11-cis-Vitamin A aldehyde,	C20H28O	0	Cytosol
retinal-cis-13	cis-13-retinal		C20H28O	0	Cytosol
retinal-cis-9	cis-9-retinal		C20H28O	0	Cytosol
retinol	Retinol	Vitamin A, Vitamin A1, all-trans-Retinol	C20H30O	0	Cytosol
retinol	Retinol	Vitamin A, Vitamin A1, all-trans-Retinol	C20H30O	0	Extracellular
retinol-9-cis	9-cis-retinol		C20H30O	0	Cytosol
retinol-9-cis	9-cis-retinol		C20H30O	0	Extracellular
retinol-cis-11	cis-11-retinol		C20H30O	0	Cytosol
retinol-cis-11	cis-11-retinol		C20H30O	0	Extracellular
retinol-cis-13	cis-13-retinol		C20H30O	0	Cytosol
retn	Retinoate	(all-E)-, (all-E)-3, 2, 3, 4, 6, 6-trimethyl-1-cyclohexen-1-yl)-, 6-trimethyl-1-cyclohexen-1-yl)-6-trimethyl-1-cyclohexene-1-yl)-2, 7-Dimethyl-9-(7-dimethyl-9-(2, 8-Nonatetraenoic acid, 8-nonatetraenoic acid, 8-nonatetraenoic acid (ECL), AGN 100335, Acide retinoique (French) (DSL), German) (EINECS), Retin A, Retinoic acid, Ro 1-5488, Tretin M, Vitamin A acid, Vitamin A1 acid, all-(E)-Retinoic acid, all-trans-, all-trans-Retinoate, all-trans-Retinoic acid, all-trans-Tretinoin, all-trans-Vitamin A acid, all-trans-b-Retinoic acid, b-Retinoic acid, trans-Retinoic acid, tretinoin (English, tretinoine (French) (EINECS)	C20H27O2	-1	Cytosol
retn	Retinoate	(all-E)-, (all-E)-3, 2, 3, 4, 6, 6-trimethyl-1-cyclohexen-1-yl)-, 6-trimethyl-1-cyclohexen-1-yl)-6-trimethyl-1-cyclohexene-1-yl)-2, 7-Dimethyl-9-(7-dimethyl-9-(2, 8-Nonatetraenoic acid, 8-nonatetraenoic acid, 8-nonatetraenoic acid (ECL), AGN 100335, Acide retinoique (French) (DSL), German) (EINECS), Retin A, Retinoic acid, Ro 1-5488, Tretin M, Vitamin A acid, Vitamin A1 acid, all-(E)-Retinoic acid, all-trans-, all-trans-Retinoate, all-trans-Retinoic acid, all-trans-Tretinoin, all-trans-Vitamin A acid, all-trans-b-Retinoic acid, b-Retinoic acid, trans-Retinoic acid, tretinoin (English, tretinoine (French) (EINECS)	C20H27O2	-1	Extracellular
retn	Retinoate	(all-E)-, (all-E)-3, 2, 3, 4, 6, 6-trimethyl-1-cyclohexen-1-yl)-, 6-trimethyl-1-cyclohexen-1-yl)-6-trimethyl-1-cyclohexene-1-yl)-2, 7-Dimethyl-9-(7-dimethyl-9-(2, 8-Nonatetraenoic acid, 8-nonatetraenoic acid, 8-nonatetraenoic acid (ECL), AGN 100335, Acide retinoique (French) (DSL), German) (EINECS), Retin A, Retinoic acid, Ro 1-5488, Tretin M, Vitamin A acid, Vitamin A1 acid, all-(E)-Retinoic acid, all-trans-, all-trans-Retinoate, all-trans-Retinoic acid, all-trans-Tretinoin, all-trans-Vitamin A acid, all-trans-b-Retinoic acid, b-Retinoic acid, trans-Retinoic acid, tretinoin (English, tretinoine (French) (EINECS)	C20H27O2	-1	Nucleus

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
retn	Retinoate	(all-E)-, (all-E)-3, 2, 3, 4, 6, 6-trimethyl-1-cyclohexen-1-yl)-, 6-trimethyl-1-cyclohexen-1-yl)-, 6-trimethyl-1-cyclohexene-1-yl)-2, 7-Dimethyl-9-(7-dimethyl-9-(2, 8-Nonatetraenoic acid, 8-nonatetraenoic acid, 8-nonatetraenoic acid (ECL), AGN 100335, Acide retinoique (French) (DSL), German) (EINECS), Retin A, Retinoic acid, Ro 1-5488, Tretin M, Vitamin A acid, Vitamin A1 acid, all-(E)-Retinoic acid, all-trans-, all-trans-Retinoate, all-trans-Retinoic acid, all-trans-Tretinoin, all-trans-Vitamin A acid, all-trans-b-Retinoic acid, b-Retinoic acid, trans-Retinoic acid, tretinoin (English, tretinoine (French) (EINECS)	C20H27O2	-1	Endoplasmic Reticulum
retcoa	retinoyl CoA		C41H58N7O17P3S	-4	Cytosol
retnglc	retinoyl glucuronide	all-trans-Retinoyl-beta-glucuronide, retinoate glucuronide	C26H35O8	-1	Cytosol
retnglc	retinoyl glucuronide	all-trans-Retinoyl-beta-glucuronide, retinoate glucuronide	C26H35O8	-1	Extracellular
retnglc	retinoyl glucuronide	all-trans-Retinoyl-beta-glucuronide, retinoate glucuronide	C26H35O8	-1	Endoplasmic Reticulum
retpalm [deleted 10/09/2005 06:18:49 PM]	Retinyl palmitate	Aquasol A (TN), Retinol palmitate, Retinyl palmitate, Vitamin A palmitate, all-trans-Retinyl palmitate;	C36H60O2	0	Extracellular
rib-D	D-Ribose		C5H10O5	0	Cytosol
rib-D	D-Ribose		C5H10O5	0	Extracellular
ribflv	Riboflavin	7,8-Dimethyl-10-ribitylisoalloxazine, Lactoflavin, Vitamin B2	C17H20N4O6	0	Cytosol
ribflv	Riboflavin	7,8-Dimethyl-10-ribitylisoalloxazine, Lactoflavin, Vitamin B2	C17H20N4O6	0	Extracellular
rmam	N-Ribosylmicosinamide		C11H15N2O5	-1	Cytosol
Rtotal	R total		CO2FULLR	-1	Cytosol
Rtotal	R total		CO2FULLR	-1	Extracellular
Rtotal	R total		CO2FULLR	-1	Lysosome
Rtotal	R total		CO2FULLR	-1	Peroxisome
Rtotal2	R total 2 position		CO2FULLR2	-1	Cytosol
Rtotal2	R total 2 position		CO2FULLR2	-1	Extracellular
Rtotal2coa	R total 2 coenzyme A		CO2FULLR2C21H31N7O15P3S	-4	Cytosol
Rtotal2coa	R total 2 coenzyme A		CO2FULLR2C21H31N7O15P3S	-4	Mitochondria
Rtotal2crn	R total 2 carnitine		CO2FULLR2C7H14NO2	0	Cytosol
Rtotal2crn	R total 2 carnitine		CO2FULLR2C7H14NO2	0	Mitochondria
Rtotal3	R total 3 position		CO2FULLR3	-1	Cytosol
Rtotal3	R total 3 position		CO2FULLR3	-1	Extracellular
Rtotal3coa	R total 3 Coenzyme A		CO2FULLR3C21H31N7O15P3S	-4	Cytosol
Rtotal3coa	R total 3 Coenzyme A		CO2FULLR3C21H31N7O15P3S	-4	Mitochondria
Rtotal3crn	R total 3 carnitine		CO2FULLR3C7H14NO2	0	Cytosol
Rtotal3crn	R total 3 carnitine		CO2FULLR3C7H14NO2	0	Mitochondria
Rtotalcoa	R total Coenzyme A		CO2FULLRC21H31N7O15P3S	-4	Cytosol
Rtotalcoa	R total Coenzyme A		CO2FULLRC21H31N7O15P3S	-4	Mitochondria
Rtotalcoa	R total Coenzyme A		CO2FULLRC21H31N7O15P3S	-4	Peroxisome
Rtotalcrn	R total carnitine		CO2FULLRC7H14NO2	0	Cytosol
Rtotalcrn	R total carnitine		CO2FULLRC7H14NO2	0	Mitochondria
ru5p-D	D-Ribulose 5-phosphate		C5H9O8P	-2	Cytosol
ru5p-D	D-Ribulose 5-phosphate		C5H9O8P	-2	Endoplasmic Reticulum
s2l2fm2m2masn	PA6	HpxB1	C90H145N6O65X	-2	Extracellular
s2l2fm2m2masn	PA6	HpxB1	C90H145N6O65X	-2	Lysosome
s2l2fm2m2masn	PA6	HpxB1	C90H145N6O65X	-2	Lysosome
s2l2n2m2m	de-Fuc form of PA6 (w/o peptide linkage)		C84H136N6O62	-2	Cytosol
s2l2n2m2m	de-Fuc form of PA6 (w/o peptide linkage)		C84H136N6O62	-2	Lysosome
s2l2n2m2masn	de-Fuc form of PA6		C84H135N6O61X	-2	Extracellular
s2l2n2m2masn	de-Fuc form of PA6		C84H135N6O61X	-2	Lysosome
s2l2n2m2mn	de-Fuc, reducing GlcNAc removed form of PA6 (w/o peptide linkage)		C76H123N5O57	-2	Cytosol
s2l2n2m2mn	de-Fuc, reducing GlcNAc removed form of PA6 (w/o peptide linkage)		C76H123N5O57	-2	Lysosome
s7p	Sedoheptulose 7-phosphate	altro-Heptulose 7-phosphate	C7H13O10P	-2	Cytosol
sacrcp-L	L-Saccharopine	N6-(L-1,3-Dicarboxypropyl)-L-lysine, Saccharopin	C11H19N2O6	-1	Mitochondria
sarcs	Sarcosine	N-Methylglycine	C3H7NO2	0	Cytosol
sarcs	Sarcosine	N-Methylglycine	C3H7NO2	0	Extracellular
sarcs	Sarcosine	N-Methylglycine	C3H7NO2	0	Mitochondria
sarcs	Sarcosine	N-Methylglycine	C3H7NO2	0	Peroxisome
sbt-D	D-Sorbitol	Clucitol, D-Glucitol, D-Sorbit, D-Sorbitol, Glucitol, Gulitol, L-gulitol, Sorbit	C6H14O6	0	Cytosol
seahcys	Se-Adenosylselenohomocysteine		C14H20N6O5Se	0	Cytosol
seahcys	Se-Adenosylselenohomocysteine		C14H20N6O5Se	0	Nucleus
seasmet	Se-Adenosylselenomethionine		C15H23N6O5Se	1	Cytosol
seasmet	Se-Adenosylselenomethionine		C15H23N6O5Se	1	Nucleus
sel	Selenate	Selenate, Selenic acid	O4Se	-2	Cytosol
sel	Selenate	Selenate, Selenic acid	O4Se	-2	Extracellular
selcys	Selenocysteine		C3H7NO2Se	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
selcyst	Selenocystathionine	Selenocystathionine	C7H14N2O4Se	0	Cytosol
selhcys	Selenohomocysteine		C4H9NO2Se	0	Cytosol
selmeth	Selenomethionine	Selenomethionine	C5H11NO2Se	0	Cytosol
seln	Selenide	Hydrogen selenide, Selenide	HSe	-1	Cytosol
selnp	Selenophosphate	Selenophosphate	H2O3PSe	-1	Cytosol
Ser/Thr	protein-linked serine or threonine residue (O-glycosylation site)		XH	0	Golgi Apparatus
Ser/Thr	protein-linked serine or threonine residue (O-glycosylation site)		XH	0	Lysosome
ser-D	D-Serine	D-2-Amino-3-hydroxypropanoic acid	C3H7NO3	0	Cytosol
ser-D	D-Serine	D-2-Amino-3-hydroxypropanoic acid	C3H7NO3	0	Extracellular
Ser-Gly/Ala-X-Gly	protein-linked serine residue (glycosaminoglycan attachment site)		XH	0	Lysosome
Ser-Gly/Ala-X-Gly	protein-linked serine residue (glycosaminoglycan attachment site)		XH	0	Endoplasmic Reticulum
ser-L	L-Serine	L-2-Amino-3-hydroxypropionic acid, L-3-Hydroxyalanine, Ser	C3H7NO3	0	Cytosol
ser-L	L-Serine	L-2-Amino-3-hydroxypropionic acid, L-3-Hydroxyalanine, Ser	C3H7NO3	0	Extracellular
ser-L	L-Serine	L-2-Amino-3-hydroxypropionic acid, L-3-Hydroxyalanine, Ser	C3H7NO3	0	Mitochondria
ser-L	L-Serine	L-2-Amino-3-hydroxypropionic acid, L-3-Hydroxyalanine, Ser	C3H7NO3	0	Peroxisome
Sfgluth	S-Formylglutathione		C11H16N3O7S	-1	Cytosol
sgalside_hs	sulfatide galactocerebroside (homo sapiens)	galactocerebroside 3-sulfate	C24H45NO10SFULLRCO	-1	Cytosol
sgalside_hs	sulfatide galactocerebroside (homo sapiens)	galactocerebroside 3-sulfate	C24H45NO10SFULLRCO	-1	Golgi Apparatus
sgalside_hs	sulfatide galactocerebroside (homo sapiens)	galactocerebroside 3-sulfate	C24H45NO10SFULLRCO	-1	Lysosome
sl-L	L-sulfolactate	(S)-3-sulfolactate	C3H4O6S	-2	Cytosol
sl-L	L-sulfolactate	(S)-3-sulfolactate	C3H4O6S	-2	Extracellular
sl-L	L-sulfolactate	(S)-3-sulfolactate	C3H4O6S	-2	Mitochondria
so3	Sulfite	Sulfurous acid	O3S	-2	Cytosol
so3	Sulfite	Sulfurous acid	O3S	-2	Mitochondria
so4	Sulfate	Sulfuric acid	O4S	-2	Cytosol
so4	Sulfate	Sulfuric acid	O4S	-2	Extracellular
so4	Sulfate	Sulfuric acid	O4S	-2	Lysosome
so4	Sulfate	Sulfuric acid	O4S	-2	Mitochondria
so4	Sulfate	Sulfuric acid	O4S	-2	Endoplasmic Reticulum
spe_hs	sphingosylphosphorylcholine (homo sapiens)		C23H50N2O5P	1	Cytosol
spe_hs	sphingosylphosphorylcholine (homo sapiens)		C23H50N2O5P	1	Extracellular
sph1p	Sphinganine 1-phosphate	Dihydrosphingosine 1-phosphate	C18H39NO5P	-1	Cytosol
sph1p	Sphinganine 1-phosphate	Dihydrosphingosine 1-phosphate	C18H39NO5P	-1	Extracellular
sph1p	Sphinganine 1-phosphate	Dihydrosphingosine 1-phosphate	C18H39NO5P	-1	Endoplasmic Reticulum
sphgn	Sphinganine	2-Amino-1, 3-dihydroxyoctadecane, Dihydrosphingosine	C18H40NO2	1	Cytosol
sphgn	Sphinganine	2-Amino-1, 3-dihydroxyoctadecane, Dihydrosphingosine	C18H40NO2	1	Endoplasmic Reticulum
sphings	Sphingosine	Sphingene, Sphingoid	C18H38NO2	1	Cytosol
sphings	Sphingosine	Sphingene, Sphingoid	C18H38NO2	1	Lysosome
sphings	Sphingosine	Sphingene, Sphingoid	C18H38NO2	1	Endoplasmic Reticulum
sphmyln_hs	sphingomyelin (homo sapiens)		C23H48N2O5PFULLRCO	0	Cytosol
sphmyln_hs	sphingomyelin (homo sapiens)		C23H48N2O5PFULLRCO	0	Golgi Apparatus
sphmyln_hs	sphingomyelin (homo sapiens)		C23H48N2O5PFULLRCO	0	Lysosome
sphs1p	Sphingosine 1-phosphate	Sphing-4-enine 1-phosphate, Sphingosine 1-phosphate	C18H37NO5P	-1	Cytosol
sphs1p	Sphingosine 1-phosphate	Sphing-4-enine 1-phosphate, Sphingosine 1-phosphate	C18H37NO5P	-1	Extracellular
sphs1p	Sphingosine 1-phosphate	Sphing-4-enine 1-phosphate, Sphingosine 1-phosphate	C18H37NO5P	-1	Endoplasmic Reticulum
spmd	Spermidine	N-(3-Aminopropyl)-1,4-butane-diamine	C7H22N3	3	Cytosol
spmr	Spermine	4-butanediamine, N, N'-Bis(3-aminopropyl)-1	C10H30N4	4	Cytosol
sql	Squalene	Spinacene, Supraene	C30H50	0	Endoplasmic Reticulum
srin	Serotonin	3-(2-Aminoethyl)-1H-indol-5-ol, 5-Hydroxytryptamine, Enteramine	C10H13N2O	1	Cytosol
srin	Serotonin	3-(2-Aminoethyl)-1H-indol-5-ol, 5-Hydroxytryptamine, Enteramine	C10H13N2O	1	Extracellular
Ssq23epx	(S)-Squalene-2,3-epoxide	(S)-2, 3-Epoxy-squalene, 3-epoxide, 3-oxide, Squalene 2	C30H50O	0	Endoplasmic Reticulum
sT_antigen	sialyl-T antigen	alpha-N-Acetylneuraminyl-2,3-beta-D-galactosyl-1,3-N-acetyl-alpha-D-galactosaminyl-R	C25H40N2O18X	-1	Golgi Apparatus
stcoa	Stearoyl-CoA (n-C18:0CoA)	Octadecanoyl-CoA, Stearyl-CoA	C39H66N7O17P3S	-4	Cytosol
stcoa	Stearoyl-CoA (n-C18:0CoA)	Octadecanoyl-CoA, Stearyl-CoA	C39H66N7O17P3S	-4	Mitochondria
stcoa	Stearoyl-CoA (n-C18:0CoA)	Octadecanoyl-CoA, Stearyl-CoA	C39H66N7O17P3S	-4	Peroxisome
stcrn	stearoylcarnitine		C25H49NO4	0	Cytosol
stcrn	stearoylcarnitine		C25H49NO4	0	Mitochondria
sTn_antigen	sialyl-Tn antigen	Glycano-(2,6-alpha-N-acetylneuraminyl)-(N-acetyl-D-galactosaminyl)-glycoprotein	C19H30N2O13X	-1	Golgi Apparatus
strch1	starch, structure 1 (1,6-[7[1,4-Glc], 4[1,4-Glc]])		C66H112O56	0	Extracellular
strch2	starch, structure 2 (1,6-[2[1,4-Glc], 1,4-Glc]])		C18H32O16	0	Extracellular
strdnc	stearidonic acid C18:4, n-3	Stearidonic acid, octadeca-6,9,12,15-tetraenoic acid	C18H27O2	-1	Cytosol
strdnc	stearidonic acid C18:4, n-3	Stearidonic acid, octadeca-6,9,12,15-tetraenoic acid	C18H27O2	-1	Extracellular
strdncoa	stearidonyl coenzyme A	stearidonic acid CoA, stearidonic acid coenzyme A	C39H58N7O17P3S	-4	Cytosol
strdncoa	stearidonyl coenzyme A	stearidonic acid CoA, stearidonic acid coenzyme A	C39H58N7O17P3S	-4	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
strdncoa	stearidonyl coenzyme A	stearidonic acid CoA, stearidonic acid coenzyme A	C39H58N7O17P3S	-4	Peroxisome
strdnrcm	stearidonyl carnitine	stearidonic acid carnitine	C25H41NO4	0	Cytosol
strdnrcm	stearidonyl carnitine	stearidonic acid carnitine	C25H41NO4	0	Mitochondria
succ	Succinate	Butanedionic acid, Ethylenesuccinic acid, Succinic acid	C4H4O4	-2	Cytosol
succ	Succinate	Butanedionic acid, Ethylenesuccinic acid, Succinic acid	C4H4O4	-2	Extracellular
succ	Succinate	Butanedionic acid, Ethylenesuccinic acid, Succinic acid	C4H4O4	-2	Mitochondria
succ	Succinate	Butanedionic acid, Ethylenesuccinic acid, Succinic acid	C4H4O4	-2	Endoplasmic Reticulum
succ	Succinate	Butanedionic acid, Ethylenesuccinic acid, Succinic acid	C4H4O4	-2	Peroxisome
succoa	Succinyl-CoA	Succinyl coenzyme A, succino-1-yl-coenzymeA	C25H35N7O19P3S	-5	Mitochondria
sucr	Sucrose	1-alpha-D-glucopyranosyl-2-beta-D-fructofuranoside, Cane sugar, Saccharose, Sugar	C12H22O11	0	Extracellular
sucsal	Succinic semialdehyde	4-Oxobutanoate, Succinate semialdehyde	C4H5O3	-1	Mitochondria
T_antigen	T antigen (core 1)	Core 1, Glycoprotein D-galactosyl-1,3-N-acetyl-D-galactosamine, beta-D-Galactosyl-1,3-N-acetyl-D-galactosaminyl-R, beta-D-Galactosyl-1,3-N-acetyl-alpha-D-galactosaminyl-R	C14H24NO10X	0	Golgi Apparatus
t2m26dcoa	trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA		C31H46N7O17P3S	-4	Mitochondria
t2m26dcoa	trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA		C31H46N7O17P3S	-4	Peroxisome
T4hcinmm	trans-4-Hydroxycinnamate	4-Coumarate, 4-Hydroxycinnamate, 4-Hydroxycinnamic acid, p-Coumaric acid	C9H7O3	-1	Cytosol
T4hcinmm	trans-4-Hydroxycinnamate	4-Coumarate, 4-Hydroxycinnamate, 4-Hydroxycinnamic acid, p-Coumaric acid	C9H7O3	-1	Mitochondria
tag_hs	triacylglycerol (homo sapiens)		C3H5FULLR2CO2FULLR2CO2FULLR3CO2	0	Cytosol
tag_hs	triacylglycerol (homo sapiens)		C3H5FULLR2CO2FULLR2CO2FULLR3CO2	0	Extracellular
tag1p-D	D-Tagatose 1-phosphate		C6H11O9P	-2	Cytosol
tagat-D	D-Tagatose	lyxo-Hexulose	C6H12O6	0	Cytosol
tagat-D	D-Tagatose	lyxo-Hexulose	C6H12O6	0	Extracellular
taur	Taurine	2-Aminoethanesulfonic acid	C2H7NO3S	0	Cytosol
taur	Taurine	2-Aminoethanesulfonic acid	C2H7NO3S	0	Extracellular
taur	Taurine	2-Aminoethanesulfonic acid	C2H7NO3S	0	Peroxisome
taxol	paclitaxel	LipoPac, Onxol, Paxceed, TAXOL, Taxol A [MeSH: Paclitaxel], paclitaxel [MeSH: Paclitaxel]	C47H31NO14	0	Cytosol
taxol	paclitaxel	LipoPac, Onxol, Paxceed, TAXOL, Taxol A [MeSH: Paclitaxel], paclitaxel [MeSH: Paclitaxel]	C47H31NO14	0	Extracellular
tchola	taurocholic acid	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(2-sulphoethyl-amide), Cholytaurine, Taurocholate, Taurocholic acid, bile acid	C26H45NO7S	0	Cytosol
tchola	taurocholic acid	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(2-sulphoethyl-amide), Cholytaurine, Taurocholate, Taurocholic acid, bile acid	C26H45NO7S	0	Extracellular
tchola	taurocholic acid	5-beta-cholanic acid-3-alpha-7-alpha-12-alpha-trio-N-(2-sulphoethyl-amide), Cholytaurine, Taurocholate, Taurocholic acid, bile acid	C26H45NO7S	0	Peroxisome
tcynt	Thiocyanate	Thiocyanate, Thiocyanic acid	CNS	-1	Cytosol
tcynt	Thiocyanate	Thiocyanate, Thiocyanic acid	CNS	-1	Extracellular
tcynt	Thiocyanate	Thiocyanate, Thiocyanic acid	CNS	-1	Mitochondria
tdchola	taurochenodeoxycholate	Taurochenodeoxycholate, bile acid	C26H45NO6S	0	Cytosol
tdchola	taurochenodeoxycholate	Taurochenodeoxycholate, bile acid	C26H45NO6S	0	Extracellular
tdchola	taurochenodeoxycholate	Taurochenodeoxycholate, bile acid	C26H45NO6S	0	Peroxisome
tdcoa	Tetradecanoyl-CoA (n-C14:0CoA)	Myristoyl-CoA	C35H58N7O17P3S	-4	Cytosol
tdcoa	Tetradecanoyl-CoA (n-C14:0CoA)	Myristoyl-CoA	C35H58N7O17P3S	-4	Mitochondria
tdcoa	Tetradecanoyl-CoA (n-C14:0CoA)	Myristoyl-CoA	C35H58N7O17P3S	-4	Peroxisome
tdACP	cis-tetradec-7-enoyl-[acyl-carrier protein] (n-C14:1)	Tetradecenoyl-ACP (n-C14:1ACP), cis-myristol-7-enoyl-[acyl-carrier protein] (n-C14:1)	C25H45N2O8PRS	-1	Cytosol
tethex3	tetracosahexaenoic acid, n-3		C24H35O2	-1	Cytosol
tethex3	tetracosahexaenoic acid, n-3		C24H35O2	-1	Extracellular
tethex3coa	tetracosahexaenoyl coenzyme A		C45H66N7O17P3S	-4	Cytosol
tethex3coa	tetracosahexaenoyl coenzyme A		C45H66N7O17P3S	-4	Peroxisome
tetpent3	tetracosapentaenoic acid, n-3		C24H37O2	-1	Cytosol
tetpent3	tetracosapentaenoic acid, n-3		C24H37O2	-1	Extracellular
tetpent3coa	tetracosapentaenoyl coenzyme A, n-3		C45H68N7O17P3S	-4	Cytosol
tetpent3coa	tetracosapentaenoyl coenzyme A, n-3		C45H68N7O17P3S	-4	Mitochondria
tetpent3coa	tetracosapentaenoyl coenzyme A, n-3		C45H68N7O17P3S	-4	Peroxisome
tetpent3crn	tetracosapentaenoyl carnitine		C31H51NO4	0	Cytosol
tetpent3crn	tetracosapentaenoyl carnitine		C31H51NO4	0	Mitochondria
tetpent6	tetracosapentaenoic acid, n-6	tetracosapentaenoate, n-6, tetracosapentaenoic acid n-6	C24H37O2	-1	Cytosol
tetpent6	tetracosapentaenoic acid, n-6	tetracosapentaenoate, n-6, tetracosapentaenoic acid n-6	C24H37O2	-1	Extracellular
tetpent6coa	tetracosapentaenoyl coenzyme A, n-6		C45H68N7O17P3S	-4	Cytosol
tetpent6coa	tetracosapentaenoyl coenzyme A, n-6		C45H68N7O17P3S	-4	Mitochondria
tetpent6coa	tetracosapentaenoyl coenzyme A, n-6		C45H68N7O17P3S	-4	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
tetpent6crn	tetracosapentaenoyl carnitine		C31H51NO4	0	Cytosol
tetpent6crn	tetracosapentaenoyl carnitine		C31H51NO4	0	Mitochondria
tetet6	tetracosatetraenoic acid n-6		C24H39O2	-1	Cytosol
tetet6	tetracosatetraenoic acid n-6		C24H39O2	-1	Extracellular
tetet6coa	tetracosatetraenoyl coenzyme A		C45H70N7O17P3S	-4	Cytosol
tetet6coa	tetracosatetraenoyl coenzyme A		C45H70N7O17P3S	-4	Mitochondria
tetet6coa	tetracosatetraenoyl coenzyme A		C45H70N7O17P3S	-4	Peroxisome
tetet6crn	Tetracosatetraenoyl carnitine	tetracosatetraenoic acid carnitine	C31H53NO4	0	Cytosol
tetet6crn	Tetracosatetraenoyl carnitine	tetracosatetraenoic acid carnitine	C31H53NO4	0	Mitochondria
thbpt	Tetrahydrobiopterin	2-Amino-6-(1,2-dihydroxypropyl)-5,6,7,8-tetrahydro-4(1H)-pteridinone, 5,6,7,8-Tetrahydrobiopterin, Tetrahydrobiopterin	C9H15N5O3	0	Cytosol
thbpt	Tetrahydrobiopterin	2-Amino-6-(1,2-dihydroxypropyl)-5,6,7,8-tetrahydro-4(1H)-pteridinone, 5,6,7,8-Tetrahydrobiopterin, Tetrahydrobiopterin	C9H15N5O3	0	Nucleus
thbpt4acam	Tetrahydrobiopterin-4a-carbinolamine		C9H15N5O4	0	Cytosol
thcholoylcoa	3alpha,7alpha,24-Trihydroxy-5beta-cholestanoyl-CoA	3alpha,7alpha,24-Trihydroxy-5beta-cholestanoyl-CoA	C48H76N7O20P3S	-4	Peroxisome
thcholst	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestan-26-al	C27H46O4	0	Mitochondria
thcholstoic	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoic acid, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-oate, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	C27H45O5	-1	Mitochondria
thcholstoic	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoic acid, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-oate, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	C27H45O5	-1	Endoplasmic Reticulum
thcholstoic	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	3-alpha-7-alpha-12-alpha-trihydroxy-5-beta-cholestanoic acid, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-oate, 3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	C27H45O5	-1	Peroxisome
thcrm_hs	trihexoyl ceramide (homo sapiens)	Gal(alpha 1->4)-Gal(beta 1->4)-Glc-Cer, Gal-Gal-Glc-Cer, Gal-Gal-Glu-Cer	C36H66NO17FULLRCO	0	Cytosol
thcrm_hs	trihexoyl ceramide (homo sapiens)	Gal(alpha 1->4)-Gal(beta 1->4)-Glc-Cer, Gal-Gal-Glc-Cer, Gal-Gal-Glu-Cer	C36H66NO17FULLRCO	0	Golgi Apparatus
thcys	Thiocysteine	Thiocysteine	C3H7NO2S2	0	Cytosol
thf	5,6,7,8-Tetrahydrofolate	(6S)-THFA, (6S)-Tetrahydrofolate, (6S)-Tetrahydrofolic acid, THF, Tetrahydrofolate, Tetrahydrofolic acid	C19H21N7O6	-2	Cytosol
thf	5,6,7,8-Tetrahydrofolate	(6S)-THFA, (6S)-Tetrahydrofolate, (6S)-Tetrahydrofolic acid, THF, Tetrahydrofolate, Tetrahydrofolic acid	C19H21N7O6	-2	Extracellular
thf	5,6,7,8-Tetrahydrofolate	(6S)-THFA, (6S)-Tetrahydrofolate, (6S)-Tetrahydrofolic acid, THF, Tetrahydrofolate, Tetrahydrofolic acid	C19H21N7O6	-2	Lysosome
thf	5,6,7,8-Tetrahydrofolate	(6S)-THFA, (6S)-Tetrahydrofolate, (6S)-Tetrahydrofolic acid, THF, Tetrahydrofolate, Tetrahydrofolic acid	C19H21N7O6	-2	Mitochondria
thm	Thiamin	Aneurin, Antiberiberi factor, Thiamine, Vitamin B1	C12H17N4OS	1	Cytosol
thm	Thiamin	Aneurin, Antiberiberi factor, Thiamine, Vitamin B1	C12H17N4OS	1	Extracellular
thm	Thiamin	Aneurin, Antiberiberi factor, Thiamine, Vitamin B1	C12H17N4OS	1	Mitochondria
thmmp	Thiamin monophosphate	TMP, Thiamin phosphate, Thiamine monophosphate, Thiamine phosphate	C12H16N4O4PS	-1	Cytosol
thmmp	Thiamin monophosphate	TMP, Thiamin phosphate, Thiamine monophosphate, Thiamine phosphate	C12H16N4O4PS	-1	Extracellular
thmmp	Thiamin monophosphate	TMP, Thiamin phosphate, Thiamine monophosphate, Thiamine phosphate	C12H16N4O4PS	-1	Mitochondria
thmpp	Thiamine diphosphate	TPP, ThPP, Thiamin diphosphate, Thiamin pyrophosphate, cocarboxylase	C12H16N4O7P2S	-2	Cytosol
thmpp	Thiamine diphosphate	TPP, ThPP, Thiamin diphosphate, Thiamin pyrophosphate, cocarboxylase	C12H16N4O7P2S	-2	Mitochondria
thmtp	Thiamin triphosphate	Thiamine triphosphate	C12H16N4O10P3S	-3	Cytosol
thmtp	Thiamin triphosphate	Thiamine triphosphate	C12H16N4O10P3S	-3	Extracellular
thp2c	2,3,4,5-Tetrahydropyridine-2-carboxylate	(R)-2,3,4,5-Tetrahydropyridine-2-carboxylate, delta-6-Piperidine-2-L-carboxylate	C6H8NO2	-1	Cytosol
thp2c	2,3,4,5-Tetrahydropyridine-2-carboxylate	(R)-2,3,4,5-Tetrahydropyridine-2-carboxylate, delta-6-Piperidine-2-L-carboxylate	C6H8NO2	-1	Peroxisome
thr-L	L-Threonine	2-Amino-3-hydroxybutyric acid, Thr	C4H9NO3	0	Cytosol
thr-L	L-Threonine	2-Amino-3-hydroxybutyric acid, Thr	C4H9NO3	0	Extracellular
thrt	L-Threonate	L-Threonate	C4H7O5	-1	Cytosol
thym	Thymine	2,4-Dihydroxy-5-methylpyrimidine, T, Thy	CSH6N2O2	0	Cytosol
thym	Thymine	2,4-Dihydroxy-5-methylpyrimidine, T, Thy	CSH6N2O2	0	Extracellular
thymd	Thymidine	2'-Deoxythymidine, Deoxythymidine, dT	C10H14N2O5	0	Cytosol
thymd	Thymidine	2'-Deoxythymidine, Deoxythymidine, dT	C10H14N2O5	0	Extracellular
thymd	Thymidine	2'-Deoxythymidine, Deoxythymidine, dT	C10H14N2O5	0	Lysosome
thymd	Thymidine	2'-Deoxythymidine, Deoxythymidine, dT	C10H14N2O5	0	Mitochondria

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
thyox-L	L-Thyroxine	3,5,3',5'-Tetraiodo-L-thyronine, O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine, T4, Thyroxine, thyroid hormone	C15H11I4NO4	0	Cytosol
thyox-L	L-Thyroxine	3,5,3',5'-Tetraiodo-L-thyronine, O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine, T4, Thyroxine, thyroid hormone	C15H11I4NO4	0	Extracellular
tmlys	N6,N6,N6-Trimethyl-L-lysine	N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	0	Cytosol
tmlys	N6,N6,N6-Trimethyl-L-lysine	N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	0	Endoplasmic Reticulum
tmndnc	timnodonic acid C20:5, n-3	(5Z,8Z,11Z,14Z,17Z)-Eicosapentaenoate, 5,8,11,14,17-Eicosapentaenoic acid, (5Z,8Z,11Z,14Z,17Z)-, 5,8,11,14,17-Icosapentaenoic acid, Eicosapentaenoic acid, Icosapentaenoic acid, Icosapento, Icosapentum [INN-Latin], Timnodonic acid, cis-5,8,11,14,17-Eicosapentaenoic acid	C20H29O2	-1	Cytosol
tmndnc	timnodonic acid C20:5, n-3	(5Z,8Z,11Z,14Z,17Z)-Eicosapentaenoate, 5,8,11,14,17-Eicosapentaenoic acid, (5Z,8Z,11Z,14Z,17Z)-, 5,8,11,14,17-Icosapentaenoic acid, Eicosapentaenoic acid, Icosapentaenoic acid, Icosapento, Icosapentum [INN-Latin], Timnodonic acid, cis-5,8,11,14,17-Eicosapentaenoic acid	C20H29O2	-1	Extracellular
tmndncoa	timnodonyl coenzyme A		C41H60N7O17P3S	-4	Cytosol
tmndncoa	timnodonyl coenzyme A		C41H60N7O17P3S	-4	Mitochondria
tmndncoa	timnodonyl coenzyme A		C41H60N7O17P3S	-4	Peroxisome
tmndccrn	Timnodonyl carnitine	timnodonic acid carnitine	C27H43NO4	0	Cytosol
tmndccrn	Timnodonyl carnitine	timnodonic acid carnitine	C27H43NO4	0	Mitochondria
Tn_antigen	Tn antigen	Glycoprotein N-acetyl-D-galactosamine	C8H14NO5X	0	Golgi Apparatus
Tn_antigen	Tn antigen	Glycoprotein N-acetyl-D-galactosamine	C8H14NO5X	0	Lysosome
tolbutamide	tolbutamide	Aglicid, Arkozal, Artosin, Butamide [MeSH: Tolbutamide], Diabetamid, Diabetol [MeSH: Tolbutamide], Diabuton, Diasulfon, Dirastan, tolbutamide [MeSH: Tolbutamide]	C12H18N2O3S	0	Cytosol
tolbutamide	tolbutamide	Aglicid, Arkozal, Artosin, Butamide [MeSH: Tolbutamide], Diabetamid, Diabetol [MeSH: Tolbutamide], Diabuton, Diasulfon, Dirastan, tolbutamide [MeSH: Tolbutamide]	C12H18N2O3S	0	Extracellular
trdox	Oxidized thioredoxin		X	0	Cytosol
trdox	Oxidized thioredoxin		X	0	Mitochondria
trdrd	Reduced thioredoxin		XH2	0	Cytosol
trdrd	Reduced thioredoxin		XH2	0	Mitochondria
tre	Trehalose	alpha, alpha'-Trehalose; alpha, alpha-Trehalose	C12H22O11	0	Cytosol
tre	Trehalose	alpha, alpha'-Trehalose; alpha, alpha-Trehalose	C12H22O11	0	Extracellular
triodthy	Triiodothyronine	3,3',5'-Triiodo-L-thyronine, 3,5,3'-L-Triiodo-L-thyronine, 3,5,3'-Triiodothyronine, L-3,5,3'-Triiodothyronine, Liothyronine, T3	C15H12I3NO4	0	Cytosol
triodthy	Triiodothyronine	3,3',5'-Triiodo-L-thyronine, 3,5,3'-L-Triiodo-L-thyronine, 3,5,3'-Triiodothyronine, L-3,5,3'-Triiodothyronine, Liothyronine, T3	C15H12I3NO4	0	Extracellular
triodthsuf	Triiodothyronine sulfate	IUPAC Name: 2-amino-3-[3,5-diiodo-4-(3-iodo-4-sulfooxy-phenoxy)-phenyl]-propanoic acid, L-Tyrosine, 3,5-diiodo-O-(3-iodo-4-(sulfooxy)phenyl)-31135-55-4, Triiodothyronine sulfuric ester	C15H11I3NO7S	-1	Cytosol
triodthsuf	Triiodothyronine sulfate	IUPAC Name: 2-amino-3-[3,5-diiodo-4-(3-iodo-4-sulfooxy-phenoxy)-phenyl]-propanoic acid, L-Tyrosine, 3,5-diiodo-O-(3-iodo-4-(sulfooxy)phenyl)-31135-55-4, Triiodothyronine sulfuric ester	C15H11I3NO7S	-1	Extracellular
trp-L	L-Tryptophan	(S)-alpha-amino-beta-(3-indolyl)-propionic acid	C11H12N2O2	0	Cytosol
trp-L	L-Tryptophan	(S)-alpha-amino-beta-(3-indolyl)-propionic acid	C11H12N2O2	0	Extracellular
trypta	Tryptamine	3-(2-Aminoethyl)indole	C10H13N2	1	Cytosol
ts3	Tachysterol 3		C27H44O	0	Cytosol
tssterone	Testosterone	17beta-Hydroxy-4-androsten-3-one	C19H28O2	0	Cytosol
tssterone	Testosterone	17beta-Hydroxy-4-androsten-3-one	C19H28O2	0	Endoplasmic Reticulum
tssteroneglc	testosterone glucuronide		C25H36O8	0	Cytosol
tssteroneglc	testosterone glucuronide		C25H36O8	0	Extracellular
tssteroneglc	testosterone glucuronide		C25H36O8	0	Endoplasmic Reticulum
tssterones	testosterone sulfate	17beta-(Sulfooxy)androst-4-en-3-one, Testosterone-17-sulphate, Testosterone-17-sulfate	C19H27O5S	-1	Cytosol
tssterones	testosterone sulfate	17beta-(Sulfooxy)androst-4-en-3-one, Testosterone-17-sulphate, Testosterone-17-sulfate	C19H27O5S	-1	Extracellular
tsul	Thiosulfate	Hyposulfite	O3S2	-2	Cytosol
tsul	Thiosulfate	Hyposulfite	O3S2	-2	Extracellular
tsul	Thiosulfate	Hyposulfite	O3S2	-2	Mitochondria
ttcoa	tetracosanoyl-CoA (n-C24:0CoA)		C45H78N7O17P3S	-4	Peroxisome

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ttc-ggdp	trans,trans,cis-Geranylgeranyl diphosphate	trans,trans,cis-Geranylgeranyl pyrophosphate	C20H33O7P2	-3	Cytosol
ttca	tetradecanoate (n-C14:0)	1-tridecanecarboxylic acid; Myristate, Myristic Acid; Myristic acid, Tetradecanoate; crodacid; emery 655; hydrofol acid 1495; hystrene 9014, myristic acid, n-Tetradecanoic Acid, n-tetradecoic acid; neo-fat 14; univol u 3165;	C14H27O2	-1	Cytosol
ttca	tetradecanoate (n-C14:0)	1-tridecanecarboxylic acid; Myristate, Myristic Acid; Myristic acid, Tetradecanoate; crodacid; emery 655; hydrofol acid 1495; hystrene 9014, myristic acid, n-Tetradecanoic Acid, n-tetradecoic acid; neo-fat 14; univol u 3165;	C14H27O2	-1	Extracellular
ttcea	tetradecenoate (n-C14:1)	tetradecenoic acid	C14H25O2	-1	Cytosol
ttocrn	tetradecanoyl carnitine	myristic acid carnitine	C21H41NO4	0	Cytosol
ttocrn	tetradecanoyl carnitine	myristic acid carnitine	C21H41NO4	0	Mitochondria
txa2	Thromboxane A2	5S,13-dien-1-oid acid, Sdienoate, (5Z,13E)-(15S)-9alpha,11alpha-Epoxy-15-hydroxythromboxa-5,13, (5Z,9alpha,11alpha,13E,15S)-9,11-Epoxy-15-hydroxythromboxa-, Thromboxane A2	C20H31O5	-1	Cytosol
txa2	Thromboxane A2	5S,13-dien-1-oid acid, Sdienoate, (5Z,13E)-(15S)-9alpha,11alpha-Epoxy-15-hydroxythromboxa-5,13, (5Z,9alpha,11alpha,13E,15S)-9,11-Epoxy-15-hydroxythromboxa-, Thromboxane A2	C20H31O5	-1	Extracellular
txa2	Thromboxane A2	5S,13-dien-1-oid acid, Sdienoate, (5Z,13E)-(15S)-9alpha,11alpha-Epoxy-15-hydroxythromboxa-5,13, (5Z,9alpha,11alpha,13E,15S)-9,11-Epoxy-15-hydroxythromboxa-, Thromboxane A2	C20H31O5	-1	Endoplasmic Reticulum
tym	Tyramine	2-(p-Hydroxyphenyl)ethylamine	C8H12NO	1	Cytosol
tymf	Tyramine O-sulfate	IUPAC Name: 1-(2-aminoethyl)-4-sulfooxybenzene, Phenol, 4-(2-aminoethyl)-, hydrogen sulfate (ester)	C8H11NO4S	0	Cytosol
tymf	Tyramine O-sulfate	IUPAC Name: 1-(2-aminoethyl)-4-sulfooxybenzene, Phenol, 4-(2-aminoethyl)-, hydrogen sulfate (ester)	C8H11NO4S	0	Extracellular
Tyr-ggn	Tyr-194 of apo-glycogenin protein (primer for glycogen synthesis)		XOH	0	Cytosol
Tyr-ggn	Tyr-194 of apo-glycogenin protein (primer for glycogen synthesis)		XOH	0	Extracellular
tyr-L	L-Tyrosine	(S)-2-Amino-3-(p-hydroxyphenyl)propionic acid, (S)-3-(p-Hydroxyphenyl)alanine	C9H11NO3	0	Cytosol
tyr-L	L-Tyrosine	(S)-2-Amino-3-(p-hydroxyphenyl)propionic acid, (S)-3-(p-Hydroxyphenyl)alanine	C9H11NO3	0	Extracellular
tyr-L	L-Tyrosine	(S)-2-Amino-3-(p-hydroxyphenyl)propionic acid, (S)-3-(p-Hydroxyphenyl)alanine	C9H11NO3	0	Mitochondria
uacgam	UDP-N-acetyl-D-glucosamine	UDP-GlcNAc, UDP-N-acetylglucosamine, common abbr: UDP-NAcGlc	C17H25N3O17P2	-2	Cytosol
uacgam	UDP-N-acetyl-D-glucosamine	UDP-GlcNAc, UDP-N-acetylglucosamine, common abbr: UDP-NAcGlc	C17H25N3O17P2	-2	Golgi Apparatus
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Cytosol
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Extracellular
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Golgi Apparatus
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Lysosome
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Mitochondria
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Nucleus
udp	UDP	5'-uridylyate diphosphate, Uridine 5'-diphosphate, uridine diphosphate	C9H11N2O12P2	-3	Endoplasmic Reticulum
udpacgal	UDP-N-acetyl-D-galactosamine	UDP-GalNAc	C17H25N3O17P2	-2	Cytosol
udpacgal	UDP-N-acetyl-D-galactosamine	UDP-GalNAc	C17H25N3O17P2	-2	Golgi Apparatus
udpacgal	UDP-N-acetyl-D-galactosamine	UDP-GalNAc	C17H25N3O17P2	-2	Lysosome
udpacgal	UDP-N-acetyl-D-galactosamine	UDP-GalNAc	C17H25N3O17P2	-2	Endoplasmic Reticulum
udpg	UDPglucose	UDP-D-glucose	C15H22N2O17P2	-2	Cytosol
udpg	UDPglucose	UDP-D-glucose	C15H22N2O17P2	-2	Golgi Apparatus
udpg	UDPglucose	UDP-D-glucose	C15H22N2O17P2	-2	Endoplasmic Reticulum
udpgal	UDPgalactose	UDP-D-galactopyranose, UDP-D-galactose	C15H22N2O17P2	-2	Cytosol
udpgal	UDPgalactose	UDP-D-galactopyranose, UDP-D-galactose	C15H22N2O17P2	-2	Golgi Apparatus
udpglcur	UDP-D-glucuronate	UDP-GlcA, UDPglucuronate	C15H19N2O18P2	-3	Cytosol
udpglcur	UDP-D-glucuronate	UDP-GlcA, UDPglucuronate	C15H19N2O18P2	-3	Golgi Apparatus
udpglcur	UDP-D-glucuronate	UDP-GlcA, UDPglucuronate	C15H19N2O18P2	-3	Endoplasmic Reticulum
udpxyl	UDP-D-xylose	UDP-alpha-D-xylose, UDPxylose	C14H20N2O16P2	-2	Cytosol
udpxyl	UDP-D-xylose	UDP-alpha-D-xylose, UDPxylose	C14H20N2O16P2	-2	Golgi Apparatus
udpxyl	UDP-D-xylose	UDP-alpha-D-xylose, UDPxylose	C14H20N2O16P2	-2	Endoplasmic Reticulum

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Cytosol
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Extracellular
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Golgi Apparatus
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Lysosome
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Mitochondria
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Nucleus
ump	UMP	5Uridylic acid, Uridine 5'-monophosphate, Uridine monophosphate, Uridylic acid	C9H11N2O9P	-2	Endoplasmic Reticulum
uppg3	Uroporphyrinogen III		C40H36N4O16	-8	Cytosol
ura	Uracil	2,4-(1H,3H)-Pyrimidinedione, 2,4-Dihydropyrimidine, 2,4-dioxypyrimidine, U	C4H4N2O2	0	Cytosol
ura	Uracil	2,4-(1H,3H)-Pyrimidinedione, 2,4-Dihydropyrimidine, 2,4-dioxypyrimidine, U	C4H4N2O2	0	Extracellular
urate	Urate	2,6,8-trioxypurine, 8-Hydroxyxanthine, Lithic acid Uric acid, Uric oxide	C5H4N4O3	0	Cytosol
urate	Urate	2,6,8-trioxypurine, 8-Hydroxyxanthine, Lithic acid Uric acid, Uric oxide	C5H4N4O3	0	Extracellular
urate	Urate	2,6,8-trioxypurine, 8-Hydroxyxanthine, Lithic acid Uric acid, Uric oxide	C5H4N4O3	0	Peroxisome
urcan	Urocanate	2-Propenoic acid, 4-Imidazoleacrylic acid, Urocanic acid	C6H5N2O2	-1	Cytosol
urea	Urea	Carbamide, Carbamimidic acid, Carbonyl diamine, Isourea, aquadrate	CH4N2O	0	Cytosol
urea	Urea	Carbamide, Carbamimidic acid, Carbonyl diamine, Isourea, aquadrate	CH4N2O	0	Extracellular
urea	Urea	Carbamide, Carbamimidic acid, Carbonyl diamine, Isourea, aquadrate	CH4N2O	0	Mitochondria
uri	Uridine		C9H12N2O6	0	Cytosol
uri	Uridine		C9H12N2O6	0	Extracellular
uri	Uridine		C9H12N2O6	0	Lysosome
uri	Uridine		C9H12N2O6	0	Mitochondria
uri	Uridine		C9H12N2O6	0	Nucleus
utp	UTP	5'-uridylylate triphosphate, Uridine 5'-triphosphate, Uridine triphosphate, rUTP	C9H11N2O15P3	-4	Cytosol
utp	UTP	5'-uridylylate triphosphate, Uridine 5'-triphosphate, Uridine triphosphate, rUTP	C9H11N2O15P3	-4	Extracellular
utp	UTP	5'-uridylylate triphosphate, Uridine 5'-triphosphate, Uridine triphosphate, rUTP	C9H11N2O15P3	-4	Mitochondria
utp	UTP	5'-uridylylate triphosphate, Uridine 5'-triphosphate, Uridine triphosphate, rUTP	C9H11N2O15P3	-4	Nucleus
vacc	vaccenic acid	(E)-Octadec-11-enoic acid, 11-Octadecenoic acid, (E)-, 11-octadecenoic acid	C18H33O2	-1	Cytosol
vacc	vaccenic acid	(E)-Octadec-11-enoic acid, 11-Octadecenoic acid, (E)-, 11-octadecenoic acid	C18H33O2	-1	Extracellular
vaccoa	vaccenyl coenzyme A	vaccenyl CoA	C39H64N7O17P3S	-4	Cytosol
vaccoa	vaccenyl coenzyme A	vaccenyl CoA	C39H64N7O17P3S	-4	Mitochondria
vacccm	Vaccenyl carnitine		C25H47NO4	0	Cytosol
vacccm	Vaccenyl carnitine		C25H47NO4	0	Mitochondria
val-L	L-Valine	2-Amino-3-methylbutyric acid, 2-Aminoisovaleric acid, Val	C5H11NO2	0	Cytosol
val-L	L-Valine	2-Amino-3-methylbutyric acid, 2-Aminoisovaleric acid, Val	C5H11NO2	0	Extracellular
val-L	L-Valine	2-Amino-3-methylbutyric acid, 2-Aminoisovaleric acid, Val	C5H11NO2	0	Mitochondria
vitd2	Vitamin D2	Calciferol (TN); Drisdol (TN), Ergocalciferol;	C28H44O	0	Cytosol
vitd2	Vitamin D2	Calciferol (TN); Drisdol (TN), Ergocalciferol;	C28H44O	0	Extracellular
vitd2	Vitamin D2	Calciferol (TN); Drisdol (TN), Ergocalciferol;	C28H44O	0	Mitochondria
vitd3	Vitamin D3		C27H44O	0	Cytosol
vitd3	Vitamin D3		C27H44O	0	Extracellular
vitd3	Vitamin D3		C27H44O	0	Mitochondria
wharachd	w-hydroxyl arachidonic acid	omega hydroxylated arachidonic acid	C20H31O3	-1	Endoplasmic Reticulum
whddca	omega hydroxy dodecanoate (n-C12:0)	omega hydroxy lauric acid	C12H23O3	-1	Cytosol
whddca	omega hydroxy dodecanoate (n-C12:0)	omega hydroxy lauric acid	C12H23O3	-1	Extracellular
whhdca	omega hydroxy hexadecanoate (n-C16:0)	omega hydroxy palmitic acid	C16H31O3	-1	Cytosol
whhdca	omega hydroxy hexadecanoate (n-C16:0)	omega hydroxy palmitic acid	C16H31O3	-1	Extracellular
whststerone	w hydroxy testosterone	omega hydroxy testosterone	C19H28O3	0	Cytosol
whststerone	w hydroxy testosterone	omega hydroxy testosterone	C19H28O3	0	Extracellular
whststerone	w hydroxy testosterone	omega hydroxy testosterone	C19H28O3	0	Endoplasmic Reticulum
whtdca	omega hydroxy tetradecanoate (n-C14:0)	omega hydroxy myristic acid	C14H27O3	-1	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
whttca	omega hydroxy tetradecanoate (n-C14:0)	omega hydroxy myristic acid	C14H27O3	-1	Extracellular
xan	Xanthine	2,6-Dioxopurine	C5H4N4O2	0	Cytosol
xan	Xanthine	2,6-Dioxopurine	C5H4N4O2	0	Peroxisome
xmp	Xanthosine 5'-phosphate	(9-D-Ribosylxanthine)-5'-phosphate, XMP, Xanthylic acid	C10H11N4O9P	-2	Cytosol
xol24oh	24-Hydroxycholesterol	Cerebrosterol, Cholest-5-ene-3,24-diol, Cholest-5-ene-3,24-diol, (3beta,24S)-	C27H46O2	0	Endoplasmic Reticulum
xol25oh	25-Hydroxycholesterol	5-Cholestene-3beta,25-diol, Cholest-5-ene-3beta,25-diol	C27H46O2	0	Endoplasmic Reticulum
xol27oh	27-Hydroxycholesterol	27-Hydroxycholesterol, 5-Cholesten-3beta,27-diol	C27H46O2	0	Mitochondria
xol27oh	27-Hydroxycholesterol	27-Hydroxycholesterol, 5-Cholesten-3beta,27-diol	C27H46O2	0	Endoplasmic Reticulum
xol7a	7 alpha-Hydroxycholesterol	7alpha-Hydroxycholesterol, Cholest-5-ene-3beta,7alpha-diol	C27H46O2	0	Endoplasmic Reticulum
xol7ah	7alpha-Hydroxy-5beta-cholestan-3-one	5-beta-cholestan-7-alpha-ol-3-one	C27H46O2	0	Cytosol
xol7ah2	3alpha,7alpha-Dihydroxy-5beta-cholestane	3alpha,7alpha-Dihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-diol, 5beta-cholestane-3alpha,7alpha-diol	C27H48O2	0	Cytosol
xol7ah2	3alpha,7alpha-Dihydroxy-5beta-cholestane	3alpha,7alpha-Dihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-diol, 5beta-cholestane-3alpha,7alpha-diol	C27H48O2	0	Mitochondria
xol7ah2	3alpha,7alpha-Dihydroxy-5beta-cholestane	3alpha,7alpha-Dihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-diol, 5beta-cholestane-3alpha,7alpha-diol	C27H48O2	0	Endoplasmic Reticulum
xol7ah2al	3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al	3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al	C27H46O3	0	Mitochondria
xol7ah3	3alpha,7alpha,26-Trihydroxy-5beta-cholestane	3alpha,7alpha,26-Trihydroxy-5beta-cholestane, 5beta-Cholestane-3alpha,7alpha,26-triol	C27H48O3	0	Mitochondria
xol7aone	7alpha-Hydroxycholest-4-en-3-one	4-cholesten-7-alpha-ol-3-one	C27H44O2	0	Cytosol
xol7aone	7alpha-Hydroxycholest-4-en-3-one	4-cholesten-7-alpha-ol-3-one	C27H44O2	0	Endoplasmic Reticulum
xoldiolone	7alpha,12alpha-Dihydroxycholest-4-en-3-one	4-cholestan-7-alpha-12-alpha-diol-3-one, 7alpha,12alpha-Dihydroxycholest-4-en-3-one	C27H44O3	0	Cytosol
xoldiolone	7alpha,12alpha-Dihydroxycholest-4-en-3-one	4-cholestan-7-alpha-12-alpha-diol-3-one, 7alpha,12alpha-Dihydroxycholest-4-en-3-one	C27H44O3	0	Mitochondria
xoldiolone	7alpha,12alpha-Dihydroxycholest-4-en-3-one	4-cholestan-7-alpha-12-alpha-diol-3-one, 7alpha,12alpha-Dihydroxycholest-4-en-3-one	C27H44O3	0	Endoplasmic Reticulum
xoldioloneh	7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one	5-beta-cholestan-7-alpha-12-alpha-3-one, 7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one	C27H46O3	0	Cytosol
xolest_hs	cholesterol ester	Cholesterol ester	C27H45XCO2	0	Cytosol
xolest_hs	cholesterol ester	Cholesterol ester	C27H45XCO2	0	Extracellular
xolest_hs	cholesterol ester	Cholesterol ester	C27H45XCO2	0	Endoplasmic Reticulum
xolest2_hs	cholesterol ester (from FULLR2)		C27H45FULLR2CO2	0	Cytosol
xolest2_hs	cholesterol ester (from FULLR2)		C27H45FULLR2CO2	0	Extracellular
xolletrol	3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane		C27H48O4	0	Mitochondria
xoltri24	7-alpha,24(S)-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 24(S)-triol	C27H46O3	0	Cytosol
xoltri24	7-alpha,24(S)-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 24(S)-triol	C27H46O3	0	Extracellular
xoltri24	7-alpha,24(S)-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 24(S)-triol	C27H46O3	0	Endoplasmic Reticulum
xoltri25	7-alpha,25-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 25-triol	C27H46O3	0	Cytosol
xoltri25	7-alpha,25-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 25-triol	C27H46O3	0	Extracellular
xoltri25	7-alpha,25-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 25-triol	C27H46O3	0	Endoplasmic Reticulum
xoltri27	7-alpha,27-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 27-triol	C27H46O3	0	Cytosol
xoltri27	7-alpha,27-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 27-triol	C27H46O3	0	Extracellular
xoltri27	7-alpha,27-Dihydroxycholesterol	5-Cholesten-3-beta, 7 alpha, 27-triol	C27H46O3	0	Endoplasmic Reticulum
xoltriol	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol	C27H48O3	0	Cytosol
xoltriol	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol	C27H48O3	0	Mitochondria
xoltriol	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane, 5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol	C27H48O3	0	Endoplasmic Reticulum
xser	Xyl-L-Ser (protein)		C5H9O4X	0	Golgi Apparatus
xser	Xyl-L-Ser (protein)		C5H9O4X	0	Endoplasmic Reticulum
xtp	XTP		C10H11N4O15P3	-4	Cytosol
xtsn	Xanthosine		C10H12N4O6	0	Cytosol
xu1p-D	D-Xylulose 1-phosphate		C5H9O8P	-2	Cytosol
xu5p-D	D-Xylulose 5-phosphate		C5H9O8P	-2	Cytosol
xyl-D	D-Xylose	Wood sugar	C5H10O5	0	Cytosol
xyl-D	D-Xylose	Wood sugar	C5H10O5	0	Extracellular
xyl-D	D-Xylose	Wood sugar	C5H10O5	0	Lysosome
xylnt	L-Xylonate	L-xylonic acid	C5H9O6	-1	Cytosol
xylt	Xylitol		C5H12O5	0	Cytosol
xylt	Xylitol		C5H12O5	0	Extracellular
xylu-D	D-Xylulose	D-L-xylulose, D-threo-Pentulose	C5H10O5	0	Cytosol
xylu-L	L-Xylulose	L-Lyxulose, L-threo-Pentulose	C5H10O5	0	Cytosol
yyite	gamma-Tocopherol	7,8-Dimethyltocol, 7,8-Dimethyltocolo-xylotocopherol, CCRIS 3610, CCRIS 4506, E-MD 80, Methyltolcols, TOCOPHEROL, gamma-Tokoferol, o-Xylotocopherol	C28H48O2	0	Cytosol

Abbreviation	Metabolite Name	Synonyms	Formula	Charge	Compartment
yyite	gamma-Tocopherol	7,8-Dimethyltocol, 7,8-Dimethyltolocol, 7,8-Dimethyltolocol, CCRIS 3610, CCRIS 4506, E-MIX 80, Methyltolocols, TOCOPHEROL, gamma-Tokoferol, o-Xylotocopherol	C28H48O2	0	Extracellular
zym_int2	zymosterol intermediate 2		C27H42O	0	Endoplasmic Reticulum
zymst	zymosterol	delta8,24-Cholestadien-3beta-ol	C27H44O	0	Endoplasmic Reticulum
zymstnl	Zymostenol	5alpha-Cholest-8-en-3beta-ol, Cholestenol, Lathosterol, Zymostenol	C27H46O	0	Endoplasmic Reticulum