

Table 3: Rows of the stoichiometric matrix (metabolites). Ordered list of rows of the stoichiometric matrix used in the debugging simulations (SI Table 2).

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1	286c	10fthf(c)	10-Formyltetrahydrofolate	Cytosol
2	20786c	10fthf5glu(c)	10-formyltetrahydrofolate-[Glu](5)	Cytosol
3	20787c	10fthf6glu(c)	10-formyltetrahydrofolate-[Glu](6)	Cytosol
4	20788c	10fthf7glu(c)	10-formyltetrahydrofolate-[Glu](7)	Cytosol
5	22812c	11-cis-retfa(c)	fatty acid 11-cis-retinol	Cytosol
6	3407c	11doctsl(c)	11-Deoxycortisol	Cytosol
7	2404c	11doctstrn(c)	11-Deoxycorticosterone	Cytosol
8	3552c	12HPET(c)	12-Hydroperoxyeicosa-5,8,10,14-tetraenoate	Cytosol
9	20144c	12RHPET(c)	12R-Hydroperoxyeicosatetraenoate	Cytosol
10	2181c	12ppd-R(c)	(R)-Propane-1,2-diol	Cytosol
11	1889c	12ppd-S(c)	(S)-Propane-1,2-diol	Cytosol
12	22815c	13-cis-oretn(c)	13-cis-oxo-retinoic acid	Cytosol
13	22814c	13-cis-retn(c)	13-cis-retinoate	Cytosol
14	22816c	13-cis-retnql(c)	13-cis-retinoyl glucuronide	Cytosol
15	812c	13dampp(c)	1,3-Diaminopropane	Cytosol
16	288c	13dpg(c)	3-Phospho-D-glyceroyl phosphate	Cytosol
17	4422c	15HPET(c)	15-Hydroperoxyeicosatetraenoic acid	Cytosol
18	3713c	17ahprgnlone(c)	17alpha-Hydroxypregnenolone	Cytosol
19	769c	17ahprgstrn(c)	17alpha-Hydroxyprogesterone	Cytosol
20	18732c	1mncam(c)	1-Methylnicotinamide	Cytosol
21	4589c	1mpyr(c)	1-Methylpyrrolinium	Cytosol
22	2994c	1pyr5c(c)	1-Pyrroline-5-carboxylate	Cytosol
23	4195c	23doguln(c)	2,3-Dioxo-L-gulonate	Cytosol
24	5576c	23dpg(c)	2,3-Disphospho-D-glycerate	Cytosol
25	20023c	2425dhvitd2(c)	24R,25-Dihydroxyvitamin D2	Cytosol
26	20024c	2425dhvitd3(c)	24R,25-Dihydroxyvitamin D3	Cytosol
27	20412c	24nph(c)	2,4 dihydroxy nitrophenol	Cytosol
28	3554c	25aics(c)	(S)-2-[5-Amino-1-(5-phospho-D-riboseyl)imidazole-4-carboxamido]succinate	Cytosol
29	20014c	25hvitd2(c)	25-Hydroxyvitamin D2	Cytosol
30	20012c	25hvitd3(c)	25-Hydroxyvitamin D3	Cytosol
31	1585c	2amac(c)	2-Aminoacrylate	Cytosol
32	2735c	2ameph(c)	(2-Aminoethyl)phosphonate	Cytosol
33	11252c	2c23dh56dhoxin(c)	2-Carboxy-2,3-dihydro-5,6-dihydroxyindole	Cytosol
34	4321c	2coum(c)	cis-2-Hydroxy cinnamate	Cytosol
35	446c	2dr1p(c)	2-Deoxy-D-ribose 1-phosphate	Cytosol
36	447c	2dr5p(c)	2-Deoxy-D-ribose 5-phosphate	Cytosol
37	4433c	2hb(c)	2-Hydroxybutyrate	Cytosol
38	4332c	2hyoxplac(c)	2-Hydroxyphenylacetate	Cytosol
39	5757c	2kmb(c)	2-keto-4-methylthiobutyrate	Cytosol
40	3219c	2mcaen(c)	cis-2-Methylaconitate	Cytosol
41	1591c	2mcit(c)	2-Methylcitrate	Cytosol
42	1071c	2obut(c)	2-Oxobutanoate	Cytosol
43	9002c	2oxoadp(c)	2-Oxoadipate	Cytosol
44	1120c	2pg(c)	D-Glycerate 2-phosphate	Cytosol
45	813c	2pglyc(c)	2-Phosphoglycolate	Cytosol
46	787c	34dhcinm(c)	3,4-Dihydroxy-trans-cinnamate	Cytosol
47	3465c	34dhmald(c)	3,4-Dihydroxymandelaldehyde	Cytosol
48	4121c	34dhoxmand(c)	3,4-Dihydroxymandelate	Cytosol
49	3464c	34dhoxpeg(c)	3,4-Dihydroxyphenylethyleneglycol	Cytosol
50	3087c	34dhpac(c)	3,4-Dihydroxyphenylacetaldehyde	Cytosol
51	916c	34dhpha(c)	3,4-Dihydroxyphenylacetate	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
52	190c	34dhphe(c)	3,4-Dihydroxy-L-phenylalanine	Cytosol
53	772c	34hpp(c)	3-(4-Hydroxyphenyl)pyruvate	Cytosol
54	9005c	35cgm(c)	3',5'-Cyclic GMP	Cytosol
55	693c	35dioty(c)	3,5-Diiodo-L-tyrosine	Cytosol
56	2457c	3aib(c)	L-3-Amino-isobutanoate	Cytosol
57	2444c	3aib-D(c)	D-3-Amino-isobutanoate	Cytosol
58	1111c	3dhgln(c)	3-Dehydro-L-gulonate	Cytosol
59	8537c	3dsphgn(c)	3-Dehydrosphinganine	Cytosol
60	9007c	3hanthrn(c)	3-Hydroxyanthranilate	Cytosol
61	4184c	3hpcoa(c)	3-Hydroxypropionyl-CoA	Cytosol
62	7127c	3hpp(c)	3-Hydroxypropanoate	Cytosol
63	7135c	3htmelys(c)	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine	Cytosol
64	4156c	3hxkynam(c)	3-Hydroxykynurenamine	Cytosol
65	1810c	3ityr-L(c)	3-Iodo-L-tyrosine	Cytosol
66	4123c	3m4hpga(c)	3-Methoxy-4-hydroxyphenylglycolaldehyde	Cytosol
67	10891c	3mlda(c)	3-Methylimidazoleacetic acid	Cytosol
68	4313c	3mldz(c)	3-Methylimidazole acetaldehyde	Cytosol
69	225c	3mob(c)	3-Methyl-2-oxobutanoate	Cytosol
70	445c	3mop(c)	(S)-3-Methyl-2-oxopentanoate	Cytosol
71	4124c	3mox4hoxm(c)	3-Methoxy-4-hydroxymandelate	Cytosol
72	4122c	3mox4hpac(c)	3-Methoxy-4-hydroxyphenylacetaldehyde	Cytosol
73	4126c	3moxytyr(c)	3-Methoxytyramine	Cytosol
74	4211c	3padsel(c)	3'-Phosphoadenylylselenate	Cytosol
75	259c	3pg(c)	3-Phospho-D-glycerate	Cytosol
76	9544c	3php(c)	3-Phosphohydroxypyruvate	Cytosol
77	1105c	3sala(c)	3-Sulfino-L-alanine	Cytosol
78	3427c	3snpyr(c)	3-Sulfonopyruvate	Cytosol
79	15766c	3spyr(c)	3-Sulfopyruvate	Cytosol
80	10517c	3uib(c)	3-Ureidoisobutyrate	Cytosol
81	4163c	42A3HP24DB(c)	4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoate	Cytosol
82	9128c	44mctr(c)	4,4-dimethylcholesta-8,14,24-trienol	Cytosol
83	4159c	46dhoxquin(c)	4,6-Dihydroxyquinoline	Cytosol
84	4157c	48dhoxquin(c)	4,8-Dihydroxyquinoline	Cytosol
85	7924c	4aabutn(c)	4-Acetamidobutanoate	Cytosol
86	176c	4abut(c)	4-Aminobutanoate	Cytosol
87	376c	4abutn(c)	4-Aminobutanal	Cytosol
88	7132c	4aphdob(c)	4-(2-Aminophenyl)-2,4-dioxobutanoate	Cytosol
89	9008c	4fumacac(c)	4-Fumarylacetoacetate	Cytosol
90	896c	4h2oglt(c)	4-Hydroxy-2-oxoglutarate	Cytosol
91	20409c	4hdebrisoquine(c)	4 hydroxy debrisoquine	Cytosol
92	2887c	4hoxpacd(c)	4-Hydroxyphenylacetaldehyde	Cytosol
93	1127c	4hphac(c)	4-Hydroxyphenylacetate	Cytosol
94	2826c	4izp(c)	4-Imidazolone-5-propanoate	Cytosol
95	9010c	4mlacac(c)	4-Maleylacetoacetate	Cytosol
96	285c	4mop(c)	4-Methyl-2-oxopentanoate	Cytosol
97	20411c	4mtolbutamide(c)	4 hydroxy tolbutamide	Cytosol
98	730c	4nph(c)	4-Nitrophenol	Cytosol
99	21119c	4nphsf(c)	4-Nitrophenyl sulfate	Cytosol
100	2022c	4ppan(c)	D-4'-Phosphopantothenate	Cytosol
101	2645c	4ppcys(c)	N-(R)-4-Phosphopantothenoyl-L-cysteine	Cytosol
102	717c	4pyrdx(c)	4-Pyridoxate	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
103	908c	4tmeabut(c)	4-Trimethylammoniobutanal	Cytosol
104	7131c	4tmeabutn(c)	4-Trimethylammoniobutanoate	Cytosol
105	7551c	56dihindlcrbxlt(c)	5,6-Dihydroxyindole-2-carboxylate	Cytosol
106	751c	56dthm(c)	5,6-Dihydrothymine	Cytosol
107	423c	56dura(c)	5,6-dihydrouracil	Cytosol
108	3862c	5HPET(c)	5-Hydroperoxy-6-trans-8,11,14-cis-eicosatetraenoate	Cytosol
109	10712c	5adtststerone(c)	5alpha-Dihydrotestosterone	Cytosol
110	22786c	5adtststeroneglc(c)	5alpha-Dihydrotestosterone glucuronide	Cytosol
111	26487c	5adtststerones(c)	5alpha-Dihydrotestosterone sulfate	Cytosol
112	10916c	5aizc(c)	5-amino-1-(5-phospho-D-ribose)imidazole-4-carboxylate	Cytosol
113	424c	5aop(c)	5-Amino-4-oxopentanoate	Cytosol
114	20783c	5dhf(c)	pentaglutamyl folate (DHF)	Cytosol
115	440c	5forthf(c)	5-Formiminotetrahydrofolate	Cytosol
116	11866c	5fthf(c)	5-Formyltetrahydrofolate	Cytosol
117	20405c	5homeprazole(c)	5 hydroxy omeprazole	Cytosol
118	4155c	5hoxindact(c)	5-Hydroxyindoleacetaldehyde	Cytosol
119	11161c	5hoxindoa(c)	5-Hydroxyindoleacetate	Cytosol
120	4166c	5hoxnfkyn(c)	5-Hydroxy-N-formylkynurenine	Cytosol
121	831c	5htrp(c)	5-Hydroxy-L-tryptophan	Cytosol
122	4169c	5hxkyn(c)	5-Hydroxykynurenine	Cytosol
123	4158c	5hxkynam(c)	5-Hydroxykynurenamine	Cytosol
124	3193c	5mdr1p(c)	5-Methylthio-5-deoxy-D-ribose 1-phosphate	Cytosol
125	3277c	5mdru1p(c)	5-Methylthio-5-deoxy-D-ribulose 1-phosphate	Cytosol
126	4178c	5moxact(c)	5-Methoxyindoleacetate	Cytosol
127	243c	5mta(c)	5-Methylthioadenosine	Cytosol
128	431c	5mthf(c)	5-Methyltetrahydrofolate	Cytosol
129	14013c	5oxpro(c)	5-Oxoproline	Cytosol
130	20780c	5thf(c)	pentaglutamyl folate (THF)	Cytosol
131	20784c	6dhf(c)	hexaglutamyl folate (DHF)	Cytosol
132	4162c	6hoxmelatn(c)	6-Hydroxymelatonin	Cytosol
133	20402c	6htststerone(c)	6 beta hydroxy testosterone	Cytosol
134	182c	6pgc(c)	6-Phospho-D-gluconate	Cytosol
135	963c	6pgl(c)	6-phospho-D-glucono-1,5-lactone	Cytosol
136	11000c	6pthp(c)	6-Pyruvoyl-5,6,7,8-tetrahydropterin	Cytosol
137	20781c	6thf(c)	hexaglutamyl folate (THF)	Cytosol
138	834c	7dhchsterol(c)	7-Dehydrocholesterol	Cytosol
139	20785c	7dhf(c)	heptaglutamyl folate (DHF)	Cytosol
140	20782c	7thf(c)	heptaglutamyl folate (THF)	Cytosol
141	22811c	9-cis-retfa(c)	fatty acid 9-cis-retinol	Cytosol
142	69c	ACP(c)	acyl carrier protein	Cytosol
143	7546c	L-dpchrn(c)	L-Dopachrome	Cytosol
144	9011c	L2aadp(c)	L-2-Amino adipate	Cytosol
145	7588c	L2aadp6sa(c)	L-2-Amino adipate 6-semialdehyde	Cytosol
146	120c	Lcyst(c)	L-Cysteate	Cytosol
147	105c	Lcystin(c)	L-Cystine	Cytosol
148	7641c	Lfmkynr(c)	L-Formylkynurenine	Cytosol
149	9013c	Lkynr(c)	L-Kynurenine	Cytosol
150	679c	Nacasp(c)	N-Acetyl-L-aspartate	Cytosol
151	10790c	Nacsertn(c)	N-Acetylserotonin	Cytosol
152	18469c	R1coa_hs(c)	R group 1 Coenzyme A homo sapiens	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
153	18470c	R2coa_hs(c)	R group 2 Coenzyme A homo sapiens	Cytosol
154	18471c	R3coa_hs(c)	R group 3 Coenzyme A homo sapiens	Cytosol
155	18493c	R4coa_hs(c)	R group 4 Coenzyme A homo sapiens	Cytosol
156	18494c	R5coa_hs(c)	R group 5 Coenzyme A homo sapiens	Cytosol
157	20277c	R6coa_hs(c)	R group 6 Coenzyme A homo sapiens	Cytosol
158	18523c	Rtotal(c)	R total	Cytosol
159	18525c	Rtotal2(c)	R total 2 position	Cytosol
160	22166c	Rtotal2coa(c)	R total 2 coenzyme A	Cytosol
161	22470c	Rtotal2crn(c)	R total 2 carnitine	Cytosol
162	18526c	Rtotal3(c)	R total 3 position	Cytosol
163	22167c	Rtotal3coa(c)	R total 3 Coenzyme A	Cytosol
164	22471c	Rtotal3crn(c)	R total 3 carnitine	Cytosol
165	22165c	Rtotalcoa(c)	R total Coenzyme A	Cytosol
166	22469c	Rtotalcrn(c)	R total carnitine	Cytosol
167	9015c	Sfglutth(c)	S-Formylglutathione	Cytosol
168	656c	T4hcinm(c)	trans-4-Hydroxycinnamate	Cytosol
169	18059c	Tyr-ggn(c)	Tyr-194 of apo-glycogenin protein (primer for glycogen synthesis)	Cytosol
170	174c	aacoa(c)	Acetoacetyl-CoA	Cytosol
171	1533c	aact(c)	Aminoacetone	Cytosol
172	360c	abt(c)	L-Arabinitol	Cytosol
173	319c	ac(c)	Acetate	Cytosol
174	5509c	acACP(c)	Acetyl-ACP	Cytosol
175	9016c	acac(c)	Acetoacetate	Cytosol
176	1052c	acald(c)	Acetaldehyde	Cytosol
177	11537c	accoa(c)	Acetyl-CoA	Cytosol
178	3775c	acetol(c)	Acetol	Cytosol
179	266c	acetone(c)	Acetone	Cytosol
180	19739c	acgagbside_hs(c)	alpha GalNAc globoside (homo sapiens)	Cytosol
181	899c	acgal(c)	N-Acetyl-D-galactosamine	Cytosol
182	19195c	acgal1p(c)	N-Acetyl-D-galactosamine 1-phosphate	Cytosol
183	22669c	acgalfucgalacgalfuc12gal14acglcgalgluside_hs(c)	Type IIIA glycolipid	Cytosol
184	22681c	acgalfucgalacgalfucgalacglcgal14acglcgalgluside_hs(c)	Type IIIAb	Cytosol
185	224c	acgam(c)	N-Acetyl-D-glucosamine	Cytosol
186	3247c	acgam1p(c)	N-Acetyl-D-glucosamine 1-phosphate	Cytosol
187	192c	acgam6p(c)	N-Acetyl-D-glucosamine 6-phosphate	Cytosol
188	19740c	acgbgbside_hs(c)	beta GalNAc globoside (homo sapiens)	Cytosol
189	7147c	acgpail_hs(c)	N-Acetyl-D-glucosaminylphosphatidylinositol	Cytosol
190	1617c	ach(c)	Acetylcholine	Cytosol
191	1129c	acmana(c)	N-Acetyl-D-mannosamine	Cytosol
192	11865c	acmanap(c)	N-Acetyl-D-mannosamine 6-phosphate	Cytosol
193	19741c	acn13acngalgsbside_hs(c)	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Cytosol
194	19742c	acn23acngalgsbside_hs(c)	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Cytosol
195	22662c	acnacngal14acglcgalgluside_hs(c)	3',8'-LD1	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
196	19738c	acnacngalgbside_h s(c)	disialyl galactosylgloboside (homo sapiens)	Cytosol
197	134c	acnam(c)	N-Acetylneuraminate	Cytosol
198	4637c	acnamp(c)	N-Acetylneuraminate 9-phosphate	Cytosol
199	22682c	acngalacglcgal14ac glcgalgluside_hs(c)	VI3NeuAc-nLc6Cer	Cytosol
200	428c	acorn(c)	N2-Acetyl-L-ornithine	Cytosol
201	7471c	acrn(c)	O-Acetylcarnitine	Cytosol
202	228c	ade(c)	Adenine	Cytosol
203	18534c	adhap_hs(c)	acyl-dihydroxyacetone phosphate	Cytosol
204	270c	adn(c)	Adenosine	Cytosol
205	471c	adp(c)	ADP	Cytosol
206	112c	adpglc(c)	ADPglucose	Cytosol
207	17282c	adpman(c)	ADPmannose	Cytosol
208	2434c	adprbp(c)	ADPribose 2'-phosphate	Cytosol
209	151c	adprib(c)	ADPribose	Cytosol
210	18463c	adrn(c)	adrenic acid	Cytosol
211	18484c	adrncoa(c)	adrenyl coenzyme A	Cytosol
212	25984c	adrncrn(c)	Adrenyl carnitine	Cytosol
213	641c	adrnl(c)	Adrenaline	Cytosol
214	11113c	adsel(c)	Adenylylselenate	Cytosol
215	20413c	aflatoxin(c)	aflatoxin B1	Cytosol
216	247c	agm(c)	Agmatine	Cytosol
217	20819c	ahandrostanglc(c)	Etiocholan-3alpha-ol-17-one 3-glucuronide	Cytosol
218	310c	ahcys(c)	S-Adenosyl-L-homocysteine	Cytosol
219	3611c	ahdt(c)	2-Amino-4-hydroxy-6-(erythro-1,2,3- trihydroxypropyl)dihydropteridine triphosphate	Cytosol
220	3340c	aicar(c)	5-Amino-1-(5-Phospho-D-riboseyl)imidazole-4- carboxamide	Cytosol
221	1941c	air(c)	5-amino-1-(5-phospho-D-riboseyl)imidazole	Cytosol
222	19360c	ak2g_hs(c)	1-alkyl 2-acylglycerol	Cytosol
223	19363c	ak2gchol_hs(c)	1-alkyl 2-acylglycerol 3-phosphocholine	Cytosol
224	19359c	ak2gp_hs(c)	1-alkyl 2-acylglycerol 3-phosphate	Cytosol
225	19361c	ak2gpe_hs(c)	1-alkyl 2-acylglycerol 3-phosphoethanolamine	Cytosol
226	19364c	ak2lgchol_hs(c)	1-alkyl 2-lysoglycerol 3-phosphocholine	Cytosol
227	19357c	akdhap_hs(c)	1-alkyldihydroxyacetone phosphate	Cytosol
228	314c	akg(c)	2-Oxoglutarate	Cytosol
229	19358c	akgp_hs(c)	1-alkylglycerol 3-phosphate (homo sapiens)	Cytosol
230	1063c	ala-B(c)	beta-Alanine	Cytosol
231	1093c	ala-D(c)	D-Alanine	Cytosol
232	11412c	ala-L(c)	L-Alanine	Cytosol
233	73c	alac-S(c)	(S)-2-Acetolactate	Cytosol
234	1447c	aldstrn(c)	Aldosterone	Cytosol
235	18535c	alpa_hs(c)	lysophosphatidic acid (homo sapiens)	Cytosol
236	7642c	am6sa(c)	2-Aminomuconate 6-semialdehyde	Cytosol
237	1086c	amet(c)	S-Adenosyl-L-methionine	Cytosol
238	903c	ametam(c)	S-Adenosylmethioninamine	Cytosol
239	309c	amp(c)	AMP	Cytosol
240	7645c	amuco(c)	2-Aminomuconate	Cytosol
241	352c	andrstrn(c)	Androsterone	Cytosol
242	20815c	andrstrnglc(c)	androsterone glucuronide	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
243	1070c	anth(c)	Anthranilate	Cytosol
244	20406c	antipyrene(c)	antipyrene	Cytosol
245	8976c	ap4a(c)	P1,P4-Bis(5'-adenosyl) tetraphosphate	Cytosol
246	2071c	apnnox(c)	alpha-Pinene-oxide	Cytosol
247	22737c	apoC(c)	Apocarboxylase (no lys residue)	Cytosol
248	22735c	apoC-Lys(c)	Apocarboxylase (Lys residue)	Cytosol
249	22736c	apoC-Lys_btn(c)	Holocarboxylase (biotin covalent bound to Lys residue of apoC)	Cytosol
250	4033c	appnn(c)	(+)-alpha-Pinene	Cytosol
251	3086c	aprgstrn(c)	20alpha-Hydroxyprogesterone	Cytosol
252	7649c	aprut(c)	N-Acetylputrescine	Cytosol
253	279c	aps(c)	Adenosine 5'-phosphosulfate	Cytosol
254	816c	aqcobal(c)	Aquacob(III)alamin	Cytosol
255	307c	arab-L(c)	L-Arabinose	Cytosol
256	5355c	arach(c)	Arachidic acid	Cytosol
257	18483c	arachcoa(c)	arachidyl coenzyme A	Cytosol
258	25967c	arachcrn(c)	arachidyl carnitine	Cytosol
259	11890c	arachd(c)	arachidonic acid	Cytosol
260	11887c	arachdcoa(c)	C20:4-CoA	Cytosol
261	11889c	arachdcrn(c)	C20:4 carnitine	Cytosol
262	337c	arg-L(c)	L-Arginine	Cytosol
263	1962c	argsuc(c)	N(omega)-(L-Arginino)succinate	Cytosol
264	11279c	ascb-L(c)	L-Ascorbate	Cytosol
265	232c	asn-L(c)	L-Asparagine	Cytosol
266	10519c	asp-D(c)	D-Aspartate	Cytosol
267	330c	asp-L(c)	L-Aspartate	Cytosol
268	465c	atp(c)	ATP	Cytosol
269	20142c	avite1(c)	alpha-Tocopherol	Cytosol
270	20141c	avite2(c)	alpha-Tocotrienol	Cytosol
271	4182c	bamppald(c)	beta-Aminopropion aldehyde	Cytosol
272	4322c	bdg2hc(c)	cis-beta-D-Glucosyl-2-hydroxycinnamate	Cytosol
273	392c	betald(c)	Betaine aldehyde	Cytosol
274	870c	bhb(c)	(R)-3-Hydroxybutanoate	Cytosol
275	4279c	bildglcur(c)	Bilirubin beta-diglucuronide	Cytosol
276	1942c	bilglcur(c)	Bilirubin monoglucuronide	Cytosol
277	101c	bilirub(c)	Bilirubin	Cytosol
278	114c	biliverd(c)	Biliverdin	Cytosol
279	4297c	biocyt(c)	Biocytin	Cytosol
280	4584c	btamp(c)	Biotinyl-5'-AMP	Cytosol
281	1079c	btn(c)	Biotin	Cytosol
282	294c	but(c)	Butyrate (n-C4:0)	Cytosol
283	20143c	bvite(c)	beta-tocopherol	Cytosol
284	10989c	bz(c)	Benzoate	Cytosol
285	11888c	c226coa(c)	cervonyl coenzyme A	Cytosol
286	11883c	c226crn(c)	cervonyl carnitine	Cytosol
287	346c	ca2(c)	Calcium	Cytosol
288	11003c	cala(c)	N-Carbamoyl-beta-alanine	Cytosol
289	8980c	camp(c)	cAMP	Cytosol
290	14010c	carn(c)	L-Carnosine	Cytosol
291	19576c	caro(c)	beta-Carotene	Cytosol
292	798c	carveol(c)	(E)-carveol	Cytosol
293	429c	cbasp(c)	N-Carbamoyl-L-aspartate	Cytosol
294	365c	cbl2(c)	Cob(II)alamin	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
295	11004c	cbp(c)	Carbamoyl phosphate	Cytosol
296	20077c	cca_d3(c)	Calcitroic acid (D3)	Cytosol
297	1073c	cdp(c)	CDP	Cytosol
298	9018c	cdpchol(c)	CDPcholine	Cytosol
299	19105c	cdpdag_hs(c)	CDP diacylglycerol (homo sapiens)	Cytosol
300	387c	cdpea(c)	CDPethanolamine	Cytosol
301	7908c	cgly(c)	Cys-Gly	Cytosol
302	14998c	chito2pdol_L(c)	N,N'-Diacylchitobiosyldiphosphodolichol, human liver homolog	Cytosol
303	14999c	chito2pdol_U(c)	N,N'-Diacylchitobiosyldiphosphodolichol, human uterine homolog	Cytosol
304	1075c	chol(c)	Choline	Cytosol
305	457c	cholate(c)	Cholate	Cytosol
306	9019c	cholp(c)	Choline phosphate	Cytosol
307	252c	chsterol(c)	Cholesterol	Cytosol
308	26330c	chsterols(c)	cholesterol sulfate	Cytosol
309	19243c	chtn(c)	chitin	Cytosol
310	236c	cit(c)	Citrate	Cytosol
311	169c	citr-L(c)	L-Citrulline	Cytosol
312	5268c	cl(c)	Chloride	Cytosol
313	19386c	clpn_hs(c)	cardiolipin (homo sapiens)	Cytosol
314	18467c	clpnd(c)	clupanodonic acid	Cytosol
315	18488c	clpndcoa(c)	clupanodonyl CoA	Cytosol
316	25990c	clpndcrn(c)	clupanodonyl carnitine	Cytosol
317	11376c	cmp(c)	CMP	Cytosol
318	4188c	cmp2amep(c)	CMP-2-aminoethylphosphonate	Cytosol
319	1088c	cmpacna(c)	CMP-N-acetylneuraminate	Cytosol
320	4189c	cmpntm2amep(c)	CMP-N-trimethyl-2-aminoethylphosphonate	Cytosol
321	7644c	cmusa(c)	2-Amino-3-carboxymuconate semialdehyde	Cytosol
322	12152c	co(c)	Carbon monoxide	Cytosol
323	474c	co2(c)	CO2	Cytosol
324	473c	coa(c)	Coenzyme A	Cytosol
325	4331c	coumarin(c)	coumarin	Cytosol
326	2442c	cpppg3(c)	Coproporphyrinogen III	Cytosol
327	150c	creat(c)	Creatine	Cytosol
328	19478c	crm_hs(c)	ceramide (homo sapiens)	Cytosol
329	2222c	crmp_hs(c)	Ceramide 1-phosphate	Cytosol
330	163c	crn(c)	L-Carnitine	Cytosol
331	643c	crtn(c)	Creatinine	Cytosol
332	11268c	crtsl(c)	Cortisol	Cytosol
333	1737c	crtstrn(c)	Corticosterone	Cytosol
334	11891c	crvnc(c)	cervonic acid, C22:6 n-3	Cytosol
335	212c	csn(c)	Cytosine	Cytosol
336	338c	ctp(c)	CTP	Cytosol
337	245c	cyan(c)	Hydrogen cyanide	Cytosol
338	1062c	cys-L(c)	L-Cysteine	Cytosol
339	14975c	cysam(c)	Cysteamine	Cytosol
340	1150c	cyst-L(c)	L-Cystathionine	Cytosol
341	92c	cytd(c)	Cytidine	Cytosol
342	380c	dad-2(c)	Deoxyadenosine	Cytosol
343	265c	dadp(c)	dADP	Cytosol
344	18537c	dag_hs(c)	diacylglycerol (homo sapiens)	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
345	19362c	dak2gpe_hs(c)	1-alkenyl 2-acylglycerol 3-phosphoethanolamine plasmalogen (homo sapiens)	Cytosol
346	193c	damp(c)	dAMP	Cytosol
347	1091c	datp(c)	dATP	Cytosol
348	3803c	dcacoa(c)	Decanoyl-CoA (n-C10:0CoA)	Cytosol
349	2908c	dcamp(c)	N6-(1,2-Dicarboxyethyl)-AMP	Cytosol
350	5272c	dcdp(c)	dCDP	Cytosol
351	290c	dcmp(c)	dCMP	Cytosol
352	18466c	dcsptn1(c)	docosa-4,7,10,13,16-pentaenoic acid (n-6)	Cytosol
353	18487c	dcsptn1coa(c)	docosa-4,7,10,13,16-pentaenoyl coenzyme A	Cytosol
354	25989c	dcsptn1crn(c)	docosa-4,7,10,13,16-pentaenoyl carnitine	Cytosol
355	78c	dctp(c)	dCTP	Cytosol
356	10918c	dcyt(c)	Deoxycytidine	Cytosol
357	1919c	ddca(c)	Dodecanoate (n-C12:0)	Cytosol
358	10497c	ddcaACP(c)	Dodecanoyl-ACP (n-C12:0ACP)	Cytosol
359	1383c	ddcacoa(c)	Dodecanoyl-CoA (n-C12:0CoA)	Cytosol
360	20408c	debrisoquine(c)	debrisoquine	Cytosol
361	12883c	decdp(c)	all trans Decaprenyl diphosphate	Cytosol
362	15096c	dedol_L(c)	Dehydrodolichol, human liver homolog	Cytosol
363	15100c	dedol_U(c)	Dehydrodolichol, human uterine homolog	Cytosol
364	15085c	dedoldp_L(c)	Dehydrodolichol diphosphate, human liver homolog	Cytosol
365	15086c	dedoldp_U(c)	Dehydrodolichol diphosphate, human uterine homolog	Cytosol
366	15093c	dedolp_L(c)	Dehydrodolichol phosphate, human liver homolog	Cytosol
367	15099c	dedolp_U(c)	Dehydrodolichol phosphate, human uterine homolog	Cytosol
368	3387c	dgchol(c)	Chenodeoxyglycocholate	Cytosol
369	194c	dgdpc(c)	dGDP	Cytosol
370	195c	dgmpp(c)	dGMP	Cytosol
371	172c	dgsn(c)	Deoxyguanosine	Cytosol
372	143c	dgtpp(c)	dGTP	Cytosol
373	251c	dha(c)	Dihydroxyacetone	Cytosol
374	1072c	dhap(c)	Dihydroxyacetone phosphate	Cytosol
375	133c	dhbpt(c)	6,7-Dihydrobiopterin	Cytosol
376	19477c	dhcrm_hs(c)	dihydroceramide (homo sapiens)	Cytosol
377	421c	dhdascb(c)	Dehydroascorbate	Cytosol
378	956c	dhea(c)	Dehydroepiandrosterone	Cytosol
379	3998c	dheas(c)	Dehydroepiandrosterone sulfate	Cytosol
380	10505c	dhf(c)	7,8-Dihydrofolate	Cytosol
381	177c	dhor-S(c)	(S)-Dihydroorotate	Cytosol
382	1032c	didp(c)	dIDP	Cytosol
383	4544c	digalsgalside_hs(c)	Digalactosylceramidesulfate	Cytosol
384	19810c	digalside_hs(c)	Digalactosylceramide	Cytosol
385	9639c	dimp(c)	dIMP	Cytosol
386	3417c	din(c)	Deoxyinosine	Cytosol
387	1033c	ditp(c)	dITP	Cytosol
388	8766c	dkmpp(c)	2,3-diketo-5-methylthio-1-phosphopentane	Cytosol
389	2431c	dlnlca(c)	dihomo-gamma-linolenic acid (n-6)	Cytosol
390	18491c	dlnlccoa(c)	dihomo-gamma-linolenyl coenzyme A	Cytosol
391	25979c	dlnlcgrn(c)	dihomo-gamma-linolenyl carnitine	Cytosol

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392	20407c	dmantipyrine(c)	demethylated antipyrine	Cytosol
393	840c	dmgly(c)	N,N-Dimethylglycine	Cytosol
394	21977c	dmhptcoa(c)	2,6 dimethylheptanoyl-CoA	Cytosol
395	26488c	dmhptcrn(c)	2,6 dimethylheptanoyl carnitine	Cytosol
396	21959c	dmnoncoa(c)	4,8 dimethylnonanoyl-CoA	Cytosol
397	38c	dmpp(c)	Dimethylallyl diphosphate	Cytosol
398	724c	dnad(c)	Deamino-NAD+	Cytosol
399	14992c	dolglcp_L(c)	Dolichyl beta-D-glucosyl phosphate, human liver homolog	Cytosol
400	14993c	dolglcp_U(c)	Dolichyl beta-D-glucosyl phosphate, human uterine homolog	Cytosol
401	14986c	dolichol_L(c)	Dolichol, human liver homolog	Cytosol
402	14987c	dolichol_U(c)	Dolichol, human uterine homolog	Cytosol
403	14994c	dolmanp_L(c)	Dolichyl phosphate D-mannose, human liver homolog	Cytosol
404	14995c	dolmanp_U(c)	Dolichyl phosphate D-mannose, human uterine homolog	Cytosol
405	14988c	dolp_L(c)	Dolichol phosphate, human liver homolog	Cytosol
406	14989c	dolp_U(c)	Dolichol phosphate, human uterine homolog	Cytosol
407	2882c	dopa(c)	Dopamine	Cytosol
408	11025c	dopaqn(c)	Dopaquinone	Cytosol
409	21114c	dopasf(c)	Dopamine 3-O-sulfate	Cytosol
410	737c	dpcoa(c)	Dephospho-CoA	Cytosol
411	1462c	drib(c)	Deoxyribose	Cytosol
412	196c	dtdp(c)	dTDP	Cytosol
413	453c	dtdp4d6dg(c)	dTDP-4-dehydro-6-deoxy-D-glucose	Cytosol
414	11394c	dtdp4d6dm(c)	dTDP-4-dehydro-6-deoxy-L-mannose	Cytosol
415	712c	dtdpglu(c)	dTDPglucose	Cytosol
416	2288c	dtdprmn(c)	dTDP-L-rhamnose	Cytosol
417	197c	dtmp(c)	dTMP	Cytosol
418	132c	dtc(c)	Dithiothreitol	Cytosol
419	10551c	dttoX(c)	Oxidized dithiothreitol	Cytosol
420	79c	dttp(c)	dTTP	Cytosol
421	1034c	dudp(c)	dUDP	Cytosol
422	198c	dump(c)	dUMP	Cytosol
423	355c	duri(c)	Deoxyuridine	Cytosol
424	80c	dutp(c)	dUTP	Cytosol
425	18064c	dxtrn(c)	phosphorylase-limit dextrin (glycogenin-1,6{4[1,4-Glc], 4[1,4-Glc]})	Cytosol
426	8301c	e4hglu(c)	L-erythro-4-Hydroxyglutamate	Cytosol
427	10791c	e4p(c)	D-Erythrose 4-phosphate	Cytosol
428	20414c	eaflatoxin(c)	8,9 epxoy aflatoxin B1	Cytosol
429	20367c	ebastine(c)	ebastine	Cytosol
430	20368c	ebastineoh(c)	hydroxylated ebastine	Cytosol
431	18506c	eicostet(c)	eicosatetranoic acid	Cytosol
432	18507c	eicostetcoa(c)	eicosatetranoyl coenzyme A	Cytosol
433	25980c	eicostetcrn(c)	Eicosatetranoyl carnitine	Cytosol
434	588c	elaid(c)	elaidic acid	Cytosol
435	25972c	elaidcrn(c)	Elaidic carnitine	Cytosol
436	1653c	eryth(c)	L-Erythrulose	Cytosol
437	706c	estradiol(c)	Estradiol	Cytosol
438	20817c	estradiolglc(c)	estradiol glucuronide	Cytosol
439	3904c	estriol(c)	estriol	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
440	3415c	estriolglc(c)	16-Glucuronide-estriol	Cytosol
441	86c	estrone(c)	Estrone	Cytosol
442	20814c	estroneglc(c)	estrone glucuronide	Cytosol
443	2601c	estrones(c)	Estrone 3-sulfate	Cytosol
444	254c	etha(c)	Ethanolamine	Cytosol
445	9020c	ethamp(c)	Ethanolamine phosphate	Cytosol
446	87c	etoh(c)	Ethanol	Cytosol
447	2235c	f1p(c)	D-Fructose 1-phosphate	Cytosol
448	441c	f26bp(c)	D-Fructose 2,6-bisphosphate	Cytosol
449	4165c	f5hoxkyn(c)	Formyl-5-hydroxykynurenamine	Cytosol
450	1053c	f6p(c)	D-Fructose 6-phosphate	Cytosol
451	478c	fad(c)	Flavin adenine dinucleotide oxidized	Cytosol
452	42c	fadh2(c)	Flavin adenine dinucleotide reduced	Cytosol
453	340c	fald(c)	Formaldehyde	Cytosol
454	189c	fdp(c)	D-Fructose 1,6-bisphosphate	Cytosol
455	312c	fe2(c)	Fe2+	Cytosol
456	2663c	fgam(c)	N2-Formyl-N1-(5-phospho-D-ribosyl)glycinamide	Cytosol
457	336c	fmn(c)	FMN	Cytosol
458	4161c	fna5moxam(c)	Formyl-N-acetyl-5-methoxykynurenamine	Cytosol
459	118c	fol(c)	Folate	Cytosol
460	334c	for(c)	Formate	Cytosol
461	430c	forglu(c)	N-Formimidoyl-L-glutamate	Cytosol
462	11122c	formcoa(c)	Formyl-CoA	Cytosol
463	3319c	fpram(c)	2-(Formamido)-N1-(5-phospho-D-ribosyl)acetamide	Cytosol
464	3486c	fprica(c)	5-Formamido-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide	Cytosol
465	10388c	frdp(c)	Farnesyl diphosphate	Cytosol
466	1061c	fru(c)	D-Fructose	Cytosol
467	833c	fuc-L(c)	L-Fucose	Cytosol
468	22691c	fuc13galacglgal14acglgalgluside_hs(c)	III3Fuc-nLc6Cer	Cytosol
469	22658c	fuc14galacglgalgluside_hs(c)	Lea glycolipid	Cytosol
470	2240c	fuc1p-L(c)	L-Fucose 1-phosphate	Cytosol
471	22657c	fucacgalfucgalacglcggluside_hs(c)	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Cytosol
472	22663c	fucacngal14acglgalgluside_hs(c)	IV3-a-NeuAc,III3-a-Fuc-nLc4Cer	Cytosol
473	22655c	fucacngalacglgalgluside_hs(c)	IV3-a-Neu5Ac,III4-a-Fuc-Lc4Cer	Cytosol
474	22665c	fucfuc12gal14acglgalgluside_hs(c)	Ley glycolipid	Cytosol
475	22693c	fucfuc132galacglgal14acglgalgluside_hs(c)	V3Fuc,III3Fuc-nLc6Cer	Cytosol
476	22690c	fucfucfucgalacglc13galacglgal14acglcggluside_hs(c)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
477	22685c	fucfucfucgalacglgal14acglcgalgluside_hs(c)	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1	Cytosol
478	22650c	fucfucgalacglcgalgluside_hs(c)	Leb glycolipid	Cytosol
479	22660c	fucgal14acglcgalgluside_hs(c)	Lacto-N-fucopentaosyl III ceramide	Cytosol
480	22652c	fucgalfucgalacglgalgluside_hs(c)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Cytosol
481	19746c	fucgalgbside_hs(c)	fucosyl galactosylgloboside (homo sapiens)	Cytosol
482	1081c	fum(c)	Fumarate	Cytosol
483	1066c	glp(c)	D-Glucose 1-phosphate	Cytosol
484	438c	g3p(c)	Glyceraldehyde 3-phosphate	Cytosol
485	444c	g3pc(c)	sn-Glycero-3-phosphocholine	Cytosol
486	765c	g6p(c)	D-Glucose 6-phosphate	Cytosol
487	19963c	gacpail_hs(c)	glucosaminy-acylphosphatidylinositol	Cytosol
488	1083c	gal(c)	D-Galactose	Cytosol
489	434c	gal1p(c)	alpha-D-Galactose 1-phosphate	Cytosol
490	19744c	galacglcgalgbside_hs(c)	Gal-GlcNAc-Gal globoside (homo sapiens)	Cytosol
491	22670c	galfuc12gal14acglgalgluside_hs(c)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	Cytosol
492	22683c	galfucgalacglgal14acglcgalgluside_hs(c)	(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	Cytosol
493	22676c	galgalfucfucgalacglcgalacglgal14acglcgalgluside_hs(c)	(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	Cytosol
494	19735c	galgalgalthcrm_hs(c)	Gal-Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Cytosol
495	19619c	galgluside_hs(c)	galactosyl glucosyl ceramide	Cytosol
496	19614c	galside_hs(c)	galactocerebroside (homo sapiens)	Cytosol
497	1377c	galt(c)	Galactitol	Cytosol
498	171c	gam(c)	D-Glucosamine	Cytosol
499	187c	gam6p(c)	D-Glucosamine 6-phosphate	Cytosol
500	10804c	gar(c)	N1-(5-Phospho-D-ribose)glycinamide	Cytosol
501	19624c	gbside_hs(c)	globoside (homo sapiens)	Cytosol
502	10800c	gcald(c)	Glycolaldehyde	Cytosol
503	1554c	gchola(c)	glycocholate	Cytosol
504	19757c	gd1b2_hs(c)	GD1beta (homo sapiens)	Cytosol
505	19754c	gd1c_hs(c)	GD1c (homo sapiens)	Cytosol
506	19759c	gd3_hs(c)	GD3 (homo sapiens)	Cytosol
507	11524c	gdchola(c)	glycochenodeoxycholate	Cytosol
508	321c	gdp(c)	GDP	Cytosol
509	952c	gdppdman(c)	GDP-4-dehydro-6-deoxy-D-mannose	Cytosol
510	168c	gdpfuc(c)	GDP-L-fucose	Cytosol
511	9064c	gdpmann(c)	GDP-D-mannose	Cytosol
512	188c	ggdp(c)	Geranylgeranyl diphosphate	Cytosol
513	18060c	ggn(c)	primed glycogenin (glycogenin-8[1,4-Glc])	Cytosol
514	18308c	glac(c)	D-glucurono-6,3-lactone	Cytosol
515	318c	glc-D(c)	D-Glucose	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
516	632c	glcr(c)	D-Glucarate	Cytosol
517	256c	glcur(c)	D-Glucuronate	Cytosol
518	3887c	glcur1p(c)	D-Glucuronate 1-phosphate	Cytosol
519	11299c	gln-L(c)	L-Glutamine	Cytosol
520	313c	glu-L(c)	L-Glutamate	Cytosol
521	761c	glu5sa(c)	L-Glutamate 5-semialdehyde	Cytosol
522	443c	glucys(c)	gamma-L-Glutamyl-L-cysteine	Cytosol
523	19613c	gluside_hs(c)	glucocerebroside (homo sapiens)	Cytosol
524	329c	glx(c)	Glyoxylate	Cytosol
525	323c	gly(c)	Glycine	Cytosol
526	393c	glyald(c)	D-Glyceraldehyde	Cytosol
527	503c	glyb(c)	Glycine betaine	Cytosol
528	1077c	glyc(c)	Glycerol	Cytosol
529	306c	glyc-R(c)	(R)-Glycerate	Cytosol
530	18741c	glyc-S(c)	(S)-Glycerate	Cytosol
531	55c	glyc3p(c)	Glycerol 3-phosphate	Cytosol
532	237c	glyclt(c)	Glycolate	Cytosol
533	18061c	glygn1(c)	glycogen, structure 1 (glycogenin-11[1,4-Glc])	Cytosol
534	18062c	glygn2(c)	glycogen, structure 2 (glycogenin-1,6-{7[1,4-Glc], 4[1,4-Glc]})	Cytosol
535	18071c	glygn3(c)	glycogen, structure 3 (glycogenin-7[1,4-Glc])	Cytosol
536	226c	gmp(c)	GMP	Cytosol
537	19768c	gp1c_hs(c)	GP1c (homo sapiens)	Cytosol
538	19976c	gp1calpha_hs(c)	GP1c alpha (homo sapiens)	Cytosol
539	3238c	gpail_hs(c)	D-glucosaminylphosphatidylinositol	Cytosol
540	19763c	gq1b_hs(c)	GQ1b (homo sapiens)	Cytosol
541	19771c	gq1balpha_hs(c)	GQ1balpha (homo sapiens)	Cytosol
542	179c	grdp(c)	Geranyl diphosphate	Cytosol
543	5279c	gsn(c)	Guanosine	Cytosol
544	19749c	gt1a_hs(c)	GT1a (homo sapiens)	Cytosol
545	19764c	gt3_hs(c)	GT3 (homo sapiens)	Cytosol
546	1087c	gthox(c)	Oxidized glutathione	Cytosol
547	11388c	gthrd(c)	Reduced glutathione	Cytosol
548	327c	gtp(c)	GTP	Cytosol
549	291c	gua(c)	Guanine	Cytosol
550	10039c	gudac(c)	Guanidinoacetate	Cytosol
551	677c	gullac(c)	L-Gulono-1,4-lactone	Cytosol
552	650c	guln(c)	L-Gulonate	Cytosol
553	1049c	h(c)	H+	Cytosol
554	3c	h2co3(c)	carbonic acid	Cytosol
555	317c	h2o(c)	H2O	Cytosol
556	315c	h2o2(c)	Hydrogen peroxide	Cytosol
557	7643c	hLkynr(c)	3-Hydroxy-L-kynurenine	Cytosol
558	144c	hco3(c)	Bicarbonate	Cytosol
559	20383c	hcoumarin(c)	hydroxy coumarin	Cytosol
560	3844c	hcys-L(c)	L-Homocysteine	Cytosol
561	297c	hdca(c)	Hexadecanoate (n-C16:0)	Cytosol
562	5725c	hdcea(c)	Hexadecenoate (n-C16:1)	Cytosol
563	21857c	hdcecrn(c)	Hexadecenoyl carnitine	Cytosol
564	8780c	hdcoa(c)	Hexadecenoyl-CoA (n-C16:1CoA)	Cytosol
565	3801c	hdd2coa(c)	trans-Hexadec-2-enoyl-CoA	Cytosol
566	26402c	hdd2crn(c)	trans-Hexadec-2-enoyl carnitine	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
567	10496c	hdeACP(c)	cis-hexadec-9-enoyl-[acyl-carrier protein] (n-C16:1)	Cytosol
568	20384c	hestratriol(c)	4,17 dihydroxy estradiol	Cytosol
569	9242c	hexc(c)	hexacosanoate (n-C26:0)	Cytosol
570	11013c	hexccoa(c)	Hexacosanoyl-CoA (n-C26:0CoA)	Cytosol
571	25969c	hexccrn(c)	hexacosanoyl carnitine	Cytosol
572	9021c	hgentis(c)	Homogentisate	Cytosol
573	4128c	hi(c)	HI	Cytosol
574	11120c	his-L(c)	L-Histidine	Cytosol
575	15080c	hista(c)	Histamine	Cytosol
576	838c	hmbil(c)	Hydroxymethylbilane	Cytosol
577	191c	hmgcoa(c)	Hydroxymethylglutaryl-CoA	Cytosol
578	20400c	hnifedipine(c)	hydroxy nifedipine	Cytosol
579	131c	hom-L(c)	L-Homoserine	Cytosol
580	11270c	homoval(c)	Homovanillate	Cytosol
581	6306c	hpdca(c)	heptadecanoate	Cytosol
582	22502c	hpdccoa(c)	heptadecanoyl coa	Cytosol
583	22758c	hpdccarn(c)	heptadecanoyl carnitine	Cytosol
584	242c	hpyr(c)	Hydroxypyruvate	Cytosol
585	20388c	hretn(c)	4 hydroxy retinoic acid	Cytosol
586	20376c	htaxol(c)	hydroxylated taxol	Cytosol
587	218c	hxan(c)	Hypoxanthine	Cytosol
588	349c	hypaur(c)	Hypotaurine	Cytosol
589	464c	i(c)	Iodide	Cytosol
590	158c	icit(c)	Isocitrate	Cytosol
591	1125c	id3acald(c)	Indole-3-acetaldehyde	Cytosol
592	5392c	idour(c)	L-Iduronate	Cytosol
593	1067c	idp(c)	IDP	Cytosol
594	410c	ile-L(c)	L-Isoleucine	Cytosol
595	2132c	im4ac(c)	Imidazole-4-acetate	Cytosol
596	3706c	im4act(c)	Imidazole-4-acetaldehyde	Cytosol
597	1090c	imp(c)	IMP	Cytosol
598	9022c	ind3ac(c)	Indole-3-acetate	Cytosol
599	223c	inost(c)	myo-Inositol	Cytosol
600	147c	ins(c)	Inosine	Cytosol
601	534c	iodine(c)	Iodine	Cytosol
602	1089c	ipdp(c)	Isopentenyl diphosphate	Cytosol
603	1050c	itp(c)	ITP	Cytosol
604	289c	k(c)	potassium	Cytosol
605	19184c	kdn(c)	2-keto-3-deoxy-D-glycero-D-galactonic acid	Cytosol
606	19185c	kdn(c)	2-keto-3-deoxy-D-glycero-D-galactonic acid 9-phosphate	Cytosol
607	10998c	kynate(c)	4-Hydroxy-2-quinolinecarboxylic acid	Cytosol
608	15670c	l2n2m2mn(c)	de-Fuc, reducing GlcNAc removed, de-Sia form of PA6 (w/o peptide linkage)	Cytosol
609	304c	lac-D(c)	D-Lactate	Cytosol
610	10931c	lac-L(c)	L-Lactate	Cytosol
611	491c	lald-D(c)	D-Lactaldehyde	Cytosol
612	420c	lald-L(c)	L-Lactaldehyde	Cytosol
613	597c	lanost(c)	Lanosterol	Cytosol
614	292c	lcts(c)	Lactose	Cytosol
615	1082c	leu-L(c)	L-Leucine	Cytosol
616	755c	leuktrA4(c)	Leukotriene A4	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
617	1752c	leuktrB4(c)	Leukotriene B4	Cytosol
618	17887c	leuktrC4(c)	Leukotriene C4	Cytosol
619	4410c	leuktrD4(c)	Leukotriene D4	Cytosol
620	26338c	leuktrE4(c)	leukotriene E4	Cytosol
621	26339c	leuktrF4(c)	leukotriene F4	Cytosol
622	18473c	lgnc(c)	lignoceric acid	Cytosol
623	18490c	lgnccoa(c)	lignocericyl coenzyme A	Cytosol
624	25968c	lgncrn(c)	lignoceryl carnitine	Cytosol
625	2477c	lgt-S(c)	(R)-S-Lactoylglutathione	Cytosol
626	10371c	limnen(c)	Limonene	Cytosol
627	11278c	lipoate(c)	Lipoate	Cytosol
628	18461c	lneldc(c)	linoelaidic acid (all trans C18:2)	Cytosol
629	22137c	lneldcACP(c)	linoelaidic acid ACP (all trans)	Cytosol
630	18482c	lneldcoa(c)	linoelaidyl coenzyme A	Cytosol
631	25975c	lneldcrn(c)	Linoelaidyl carnitine	Cytosol
632	11172c	lnlc(c)	linoleic acid (all cis C18:2) n-6	Cytosol
633	22136c	lnlcACP(c)	linoleic acid ACP (all cis)	Cytosol
634	18481c	lnlccoa(c)	linoleic coenzyme A	Cytosol
635	25976c	lnlccrn(c)	Linoleyl carnitine	Cytosol
636	11152c	lnlnca(c)	alpha-Linolenic acid, C18:3, n-3	Cytosol
637	18480c	lnlncacoa(c)	alpha-Linolenoyl-CoA	Cytosol
638	25978c	lnlnacrn(c)	alpha-linolenyl carnitine	Cytosol
639	5356c	lnlncg(c)	gamma-linolenic acid	Cytosol
640	2277c	lnlncgcoa(c)	gamma-linolenoyl-CoA	Cytosol
641	25977c	lnlncgrn(c)	gamma-linolenyl carnitine	Cytosol
642	19382c	lpchol_hs(c)	lysophosphatidylcholine (homo sapiens)	Cytosol
643	19998c	lum3(c)	Lumisterol 3	Cytosol
644	328c	lys-L(c)	L-Lysine	Cytosol
645	4198c	lyxnt(c)	L-lyxonate	Cytosol
646	15002c	m1mpdol_L(c)	alpha-D-mannosyl-beta-D-mannosyl-diacylchitobiosyldiphosphodolichol, human liver homolog	Cytosol
647	15003c	m1mpdol_U(c)	alpha-D-mannosyl-beta-D-mannosyl-diacylchitobiosyldiphosphodolichol, human uterine homolog	Cytosol
648	15672c	m2mn(c)	(alpha-D-mannosyl)2-beta-D-mannosyl-N-acetylglucosamine	Cytosol
649	15004c	m2mpdol_L(c)	(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Cytosol
650	15005c	m2mpdol_U(c)	(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Cytosol
651	15006c	m3mpdol_L(c)	(alpha-D-mannosyl)3-beta-D-mannosyl-diacetylchitodiphosphodolichol, human liver homolog	Cytosol
652	15007c	m3mpdol_U(c)	(alpha-D-mannosyl)3-beta-D-mannosyl-diacetylchitodiphosphodolichol, human uterine homolog	Cytosol
653	15008c	m4mpdol_L(c)	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
654	15009c	m4mpdol_U(c)	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Cytosol
655	18539c	mag_hs(c)	monoacylglycerol 2 (homo sapiens)	Cytosol
656	230c	mal-L(c)	L-Malate	Cytosol
657	50c	malACP(c)	Malonyl-[acyl-carrier protein]	Cytosol
658	11267c	malcoa(c)	Malonyl-CoA	Cytosol
659	267c	malt(c)	Maltose	Cytosol
660	1284c	malttr(c)	Maltotriose	Cytosol
661	11018c	man(c)	D-Mannose	Cytosol
662	2920c	man1p(c)	D-Mannose 1-phosphate	Cytosol
663	137c	man6p(c)	D-Mannose 6-phosphate	Cytosol
664	4139c	melanin(c)	Melanin	Cytosol
665	1013c	melatn(c)	Melatonin	Cytosol
666	1092c	meoh(c)	Methanol	Cytosol
667	11265c	mepi(c)	Metanephrine	Cytosol
668	4310c	mercplac(c)	3-Mercaptolactate	Cytosol
669	26412c	mercplaccys(c)	3-mercaptolactate-cysteine disulfide	Cytosol
670	794c	mercppy(c)	Mercaptopyruvate	Cytosol
671	343c	met-L(c)	L-Methionine	Cytosol
672	433c	methf(c)	5,10-Methenyltetrahydrofolate	Cytosol
673	3703c	mhista(c)	N-Methylhistamine	Cytosol
674	996c	mi13456p(c)	1D-myo-Inositol 1,3,4,5,6-pentakisphosphate	Cytosol
675	7140c	mi1345p(c)	1D-myo-Inositol 1,3,4,5-tetrakisphosphate	Cytosol
676	11398c	mi1346p(c)	1D-myo-Inositol 1,3,4,6-tetrakisphosphate	Cytosol
677	969c	mi134p(c)	1D-myo-Inositol 1,3,4-trisphosphate	Cytosol
678	3100c	mi13p(c)	1D-myo-Inositol 1,3-bisphosphate	Cytosol
679	8995c	mi145p(c)	1D-myo-Inositol 1,4,5-trisphosphate	Cytosol
680	950c	mi14p(c)	1D-myo-Inositol 1,4-bisphosphate	Cytosol
681	8983c	mi1p-D(c)	1D-myo-Inositol 1-phosphate	Cytosol
682	3981c	mi3456p(c)	1D-myo-Inositol 3,4,5,6-tetrakisphosphate	Cytosol
683	10518c	mi34p(c)	1D-myo-Inositol 3,4-bisphosphate	Cytosol
684	2866c	mi3p-D(c)	1D-myo-Inositol 3-phosphate	Cytosol
685	11166c	mi4p-D(c)	1D-myo-Inositol 4-phosphate	Cytosol
686	3284c	micit(c)	methylisocitrate	Cytosol
687	938c	minohp(c)	myo-Inositol hexakisphosphate	Cytosol
688	11043c	mlthf(c)	5,10-Methylenetetrahydrofolate	Cytosol
689	13998c	mma(c)	monomethylamine	Cytosol
690	451c	mmcoa-S(c)	(S)-Methylmalonyl-CoA	Cytosol
691	15673c	mn(c)	beta-1,4-mannose-N-acetylglucosamine	Cytosol
692	15000c	mpdol_L(c)	beta-D-Mannosyldiacetylchitobiosyldiphosphodolichol, human liver homolog	Cytosol
693	15001c	mpdol_U(c)	beta-D-Mannosyldiacetylchitobiosyldiphosphodolichol, human uterine homolog	Cytosol
694	277c	msa(c)	Malonate semialdehyde	Cytosol
695	370c	mthgx(c)	Methylglyoxal	Cytosol
696	10495c	myrsACP(c)	Myristoyl-ACP (n-C14:0ACP)	Cytosol
697	15681c	n2m2nm(c)	n2m2nmasn (w/o peptide linkage)	Cytosol
698	15682c	n2m2nmn(c)	reducing GlcNAc removed form of n2m2nmasn (w/o peptide)	Cytosol
699	7923c	n4abutn(c)	N4-Acetylaminobutanal	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
700	1023c	na1(c)	Sodium	Cytosol
701	301c	nac(c)	Nicotinate	Cytosol
702	466c	nad(c)	Nicotinamide adenine dinucleotide	Cytosol
703	467c	nadh(c)	Nicotinamide adenine dinucleotide - reduced	Cytosol
704	469c	nadp(c)	Nicotinamide adenine dinucleotide phosphate	Cytosol
705	468c	nadph(c)	Nicotinamide adenine dinucleotide phosphate - reduced	Cytosol
706	14996c	naglc2p_L(c)	N-Acetyl-D-glucosaminylidiphosphodolichol, human liver homolog	Cytosol
707	14997c	naglc2p_U(c)	N-Acetyl-D-glucosaminylidiphosphodolichol, human uterine homolog	Cytosol
708	233c	ncam(c)	Nicotinamide	Cytosol
709	4171c	nformanth(c)	N-Formylanthranilate	Cytosol
710	476c	nh4(c)	Ammonium	Cytosol
711	10883c	nicrns(c)	Nicotinate D-ribonucleoside	Cytosol
712	776c	nicrnt(c)	Nicotinate D-ribonucleotide	Cytosol
713	20399c	nifedipine(c)	nifedipine	Cytosol
714	77c	nmn(c)	NMN	Cytosol
715	2047c	nmptrc(c)	N-Methylputrescine	Cytosol
716	4614c	nmthsrtn(c)	N-Methylserotonin	Cytosol
717	361c	no(c)	Nitric oxide	Cytosol
718	4127c	normete-L(c)	L-Normetanephrine	Cytosol
719	668c	npthl(c)	Naphthalene	Cytosol
720	371c	nrpphr(c)	Norepinephrine	Cytosol
721	21117c	nrpphrsfc(c)	Sulfate derivative of norepinephrine	Cytosol
722	18464c	nrvc(c)	nervonic acid	Cytosol
723	18485c	nrvnccoac(c)	nervonyl coenzyme A	Cytosol
724	25974c	nrvnccrn(c)	Nervonyl carnitine	Cytosol
725	5380c	ntm2amep(c)	N-Trimethyl-2-aminoethylphosphonate	Cytosol
726	4397c	nwharg(c)	N-(omega)-Hydroxyarginine	Cytosol
727	470c	o2(c)	O2	Cytosol
728	461c	o2s(c)	Superoxide anion	Cytosol
729	322c	oaa(c)	Oxaloacetate	Cytosol
730	20055c	oagd3_hs(c)	9-O-Acetylated GD3 (homo sapiens)	Cytosol
731	20056c	oagt3_hs(c)	9-O-Acetylated GT3 (homo sapiens)	Cytosol
732	10688c	occoa(c)	Octanoyl-CoA (n-C8:0CoA)	Cytosol
733	1249c	ocdca(c)	octadecanoate (n-C18:0)	Cytosol
734	5936c	ocdcaACP(c)	Octadecanoyl-ACP (n-C18:0ACP)	Cytosol
735	8769c	ocdcea(c)	octadecenoate (n-C18:1)	Cytosol
736	8770c	ocdcya(c)	octadecadienoate (n-C18:2)	Cytosol
737	8790c	ocdcyaACP(c)	Octadecynoyl-ACP (n-C18:2ACP)	Cytosol
738	5354c	octa(c)	octanoate (n-C8:0)	Cytosol
739	5871c	octeACP(c)	cis-octadec-11-enoyl-[acyl-carrier protein] (n-C18:1)	Cytosol
740	8401c	od2coa(c)	trans-Octadec-2-enoyl-CoA	Cytosol
741	8782c	odecoa(c)	Octadecenoyl-CoA (n-C18:1CoA)	Cytosol
742	11885c	odecrn(c)	octadecenoyl carnitine	Cytosol
743	1021c	oh1(c)	hydroxide ion	Cytosol
744	20404c	omeprazole(c)	omeprazole	Cytosol
745	20401c	onpthl(c)	naphthalene epoxide	Cytosol
746	22810c	oretn(c)	4-oxo-retonoic acid	Cytosol
747	1304c	orn(c)	Ornithine	Cytosol
748	148c	orot(c)	Orotate	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
749	881c	orot5p(c)	Orotidine 5'-phosphate	Cytosol
750	10901c	oxa(c)	Oxalate	Cytosol
751	18536c	pa_hs(c)	phosphatidic acid (homo sapiens)	Cytosol
752	9657c	pac(c)	Phenylacetic acid	Cytosol
753	1100c	pacald(c)	Phenylacetaldehyde	Cytosol
754	19365c	paf_hs(c)	1-alkyl 2-acteylglycerol 3-phosphocholine (homo sapiens)	Cytosol
755	4431c	pail345p_hs(c)	phosphatidylinositol-3,4,5-trisphosphate (Homo sapiens)	Cytosol
756	19605c	pail34p_hs(c)	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)	Cytosol
757	19704c	pail35p_hs(c)	phosphatidylinositol-3,5-bisphosphate (Homo sapiens)	Cytosol
758	3992c	pail3p_hs(c)	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)	Cytosol
759	19333c	pail45p_hs(c)	phosphatidylinositol 4,5-bisphosphate (Homo sapiens)	Cytosol
760	19332c	pail4p_hs(c)	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	Cytosol
761	19479c	pail5p_hs(c)	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)	Cytosol
762	19327c	pail_hs(c)	phosphatidylinositol (homo sapiens)	Cytosol
763	5870c	palACP(c)	Palmitoyl-ACP (n-C16:0ACP)	Cytosol
764	900c	pan4p(c)	Pantetheine 4'-phosphate	Cytosol
765	333c	pap(c)	Adenosine 3',5'-bisphosphate	Cytosol
766	332c	paps(c)	3'-Phosphoadenylyl sulfate	Cytosol
767	19051c	pchol_hs(c)	Phosphatidylcholine (homo sapiens)	Cytosol
768	7124c	pcollg5hlys(c)	Procollagen 5-hydroxy-L-lysine	Cytosol
769	2265c	pcollglys(c)	Procollagen L-lysine	Cytosol
770	10038c	pcreat(c)	Phosphocreatine	Cytosol
771	15675c	pcrn(c)	propionyl-carnitine	Cytosol
772	19999c	pd3(c)	Previtamin D3	Cytosol
773	1116c	pdx5p(c)	Pyridoxine 5'-phosphate	Cytosol
774	19050c	pe_hs(c)	phosphatidylethanolamine (homo sapiens)	Cytosol
775	9637c	peamn(c)	Phenethylamine	Cytosol
776	344c	pep(c)	Phosphoenolpyruvate	Cytosol
777	19700c	peracd(c)	Perillic acid	Cytosol
778	2536c	perillyl(c)	Perillyl alcohol	Cytosol
779	19385c	pglyc_hs(c)	phosphatidylglycerol (homo sapiens)	Cytosol
780	19384c	pgp_hs(c)	phosphatidyl glycerol phosphate (homo sapiens)	Cytosol
781	397c	phaccoa(c)	Phenylacetyl-CoA	Cytosol
782	1048c	phe-L(c)	L-Phenylalanine	Cytosol
783	2972c	pheacgln(c)	alpha-N-Phenylacetyl-L-glutamine	Cytosol
784	11520c	pheme(c)	Protoheme	Cytosol
785	10564c	phom(c)	O-Phospho-L-homoserine	Cytosol
786	240c	phpyr(c)	Phenylpyruvate	Cytosol
787	10509c	phyQ(c)	Phylloquinone	Cytosol
788	1308c	phyt(c)	phytanic acid	Cytosol
789	21953c	phytcoa(c)	phytanyl coa	Cytosol
790	472c	pi(c)	Phosphate	Cytosol
791	11029c	pmtcoa(c)	Palmitoyl-CoA (n-C16:0CoA)	Cytosol
792	2244c	pmtcrn(c)	L-Palmitoylcarnitine	Cytosol
793	10928c	pnto-R(c)	(R)-Pantothenate	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
794	238c	ppa(c)	Propionate (n-C3:0)	Cytosol
795	487c	ppbng(c)	Porphobilinogen	Cytosol
796	1064c	ppcoa(c)	Propanoyl-CoA	Cytosol
797	475c	ppi(c)	Diphosphate	Cytosol
798	19580c	ppmi12346p(c)	5-Diphosphoinositol pentakisphosphate	Cytosol
799	19581c	ppmi1346p(c)	Diphosphoinositol tetrakisphosphate	Cytosol
800	864c	pppg9(c)	Protoporphyrinogen IX	Cytosol
801	2452c	pppi(c)	Inorganic triphosphate	Cytosol
802	2325c	pram(c)	5-Phospho-beta-D-ribosylamine	Cytosol
803	10681c	prgnlone(c)	Pregnenolone	Cytosol
804	26331c	prgnlones(c)	pregnenolone sulfate	Cytosol
805	10510c	prgstrn(c)	Progesterone	Cytosol
806	21954c	prist(c)	pristanic acid	Cytosol
807	21957c	pristanal(c)	pristanal	Cytosol
808	21955c	pristcoa(c)	pristanoyl coa	Cytosol
809	629c	pro-D(c)	D-Proline	Cytosol
810	229c	pro-L(c)	L-Proline	Cytosol
811	3331c	prostg1(c)	(13E)-11 alpha-Hydroxy-9,15-dioxoprost-13-enoate	Cytosol
812	11382c	prostgd2(c)	Prostaglandin D2	Cytosol
813	3492c	prostge1(c)	Prostaglandin E1	Cytosol
814	398c	prostge2(c)	Prostaglandin E2	Cytosol
815	1126c	prostgf2(c)	Prostaglandin F2alpha	Cytosol
816	422c	prostgh2(c)	Prostaglandin H2	Cytosol
817	1078c	prpp(c)	5-Phospho-alpha-D-ribose 1-diphosphate	Cytosol
818	19052c	ps_hs(c)	phosphatidylserine (homo sapiens)	Cytosol
819	824c	pser-L(c)	O-Phospho-L-serine	Cytosol
820	6304c	ptdca(c)	pentadecanoate	Cytosol
821	22500c	ptdcacoa(c)	pentadecanoyl Coenzyme A	Cytosol
822	22757c	ptdcacrn(c)	pentadenoyl carnitine	Cytosol
823	1094c	ptrc(c)	Putrescine	Cytosol
824	670c	pth(c)	Pantetheine	Cytosol
825	1130c	pyam5p(c)	Pyridoxamine 5'-phosphate	Cytosol
826	362c	pydam(c)	Pyridoxamine	Cytosol
827	298c	pydx(c)	Pyridoxal	Cytosol
828	479c	pydx5p(c)	Pyridoxal 5'-phosphate	Cytosol
829	160c	pydxn(c)	Pyridoxine	Cytosol
830	1851c	pylald(c)	Perillyl aldehyde	Cytosol
831	311c	pyr(c)	Pyruvate	Cytosol
832	406c	q10(c)	Ubiquinone-10	Cytosol
833	11879c	q10h2(c)	Ubiquinol-10	Cytosol
834	2854c	quln(c)	Quinolate	Cytosol
835	10390c	r1p(c)	alpha-D-Ribose 1-phosphate	Cytosol
836	1999c	r5p(c)	alpha-D-Ribose 5-phosphate	Cytosol
837	156c	rbl-D(c)	D-Ribulose	Cytosol
838	91c	rbt(c)	Ribitol	Cytosol
839	22806c	retfa(c)	fatty acid retinol	Cytosol
840	208c	retinal(c)	Retinal	Cytosol
841	19631c	retinal-11-cis(c)	cis-11-retinal	Cytosol
842	22820c	retinal-cis-13(c)	cis-13-retinal	Cytosol
843	19630c	retinal-cis-9(c)	cis-9-retinal	Cytosol
844	90c	retinol(c)	Retinol	Cytosol
845	19628c	retinol-9-cis(c)	9-cis-retinol	Cytosol
846	19629c	retinol-cis-11(c)	cis-11-retinol	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
847	22819c	retinol-cis-13(c)	cis-13-retinol	Cytosol
848	11153c	retn(c)	Retinoate	Cytosol
849	22809c	retncoa(c)	retinoyl CoA	Cytosol
850	20818c	retnglc(c)	retinoyl glucuronide	Cytosol
851	1080c	rib-D(c)	D-Ribose	Cytosol
852	303c	ribflv(c)	Riboflavin	Cytosol
853	2368c	rnam(c)	N-Ribosylnicotinamide	Cytosol
854	261c	ru5p-D(c)	D-Ribulose 5-phosphate	Cytosol
855	15667c	s2l2n2m2m(c)	de-Fuc form of PA6 (w/o peptide linkage)	Cytosol
856	15669c	s2l2n2m2mn(c)	de-Fuc, reducing GlcNAc removed form of PA6 (w/o peptide linkage)	Cytosol
857	140c	s7p(c)	Sedoheptulose 7-phosphate	Cytosol
858	271c	sarcs(c)	Sarcosine	Cytosol
859	645c	sbt-D(c)	D-Sorbitol	Cytosol
860	4207c	seahcys(c)	Se-Adenosylselenohomocysteine	Cytosol
861	4301c	seasmeth(c)	Se-Adenosylselenomethionine	Cytosol
862	4212c	sel(c)	Selenate	Cytosol
863	4389c	selcys(c)	Selenocysteine	Cytosol
864	4214c	selcyst(c)	Selenocystathionine	Cytosol
865	4213c	selhcys(c)	Selenohomocysteine	Cytosol
866	3846c	selmeth(c)	Selenomethionine	Cytosol
867	1247c	seln(c)	Selenide	Cytosol
868	3734c	selnp(c)	Selenophosphate	Cytosol
869	512c	ser-D(c)	D-Serine	Cytosol
870	339c	ser-L(c)	L-Serine	Cytosol
871	19615c	sgalside_hs(c)	sulfatide galactocerebroside (homo sapiens)	Cytosol
872	15786c	sl-L(c)	L-sulfolactate	Cytosol
873	1060c	so3(c)	Sulfite	Cytosol
874	335c	so4(c)	Sulfate	Cytosol
875	26303c	spc_hs(c)	sphingosylphosphorylcholine (homo sapiens)	Cytosol
876	9025c	sph1p(c)	Sphinganine 1-phosphate	Cytosol
877	708c	sphgn(c)	Sphinganine	Cytosol
878	10703c	sphings(c)	Sphingosine	Cytosol
879	19618c	sphmyln_hs(c)	sphingomyelin (homo sapiens)	Cytosol
880	4541c	sphs1p(c)	Sphingosine 1-phosphate	Cytosol
881	161c	spmd(c)	Spermidine	Cytosol
882	518c	sprm(c)	Spermine	Cytosol
883	638c	srtn(c)	Serotonin	Cytosol
884	8781c	stcoa(c)	Stearoyl-CoA (n-C18:0CoA)	Cytosol
885	11884c	stcrm(c)	stearoylcarnitine	Cytosol
886	18462c	strdnc(c)	stearidonic acid C18:4, n-3	Cytosol
887	18492c	strdncoa(c)	stearidonyl coenzyme A	Cytosol
888	25985c	strdnccrn(c)	stearidonyl carnitine	Cytosol
889	325c	succ(c)	Succinate	Cytosol
890	26271c	tag1p-D(c)	D-Tagatose 1-phosphate	Cytosol
891	18538c	tag_hs(c)	triacylglycerol (homo sapiens)	Cytosol
892	646c	tagat-D(c)	D-Tagatose	Cytosol
893	293c	taur(c)	Taurine	Cytosol
894	20374c	taxol(c)	paclitaxel	Cytosol
895	3700c	tchola(c)	taurocholic acid	Cytosol
896	1428c	tcynt(c)	Thiocyanate	Cytosol
897	3390c	tdchola(c)	taurochenodeoxycholate	Cytosol
898	1862c	tdcoa(c)	Tetradecanoyl-CoA (n-C14:0CoA)	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
899	5939c	tdeACP(c)	cis-tetradec-7-enoyl-[acyl-carrier protein] (n-C14:1)	Cytosol
900	18514c	tethex3(c)	tetracosahexaenoic acid, n-3	Cytosol
901	18515c	tethex3coa(c)	tetracosahexaenoyl coenzyme A	Cytosol
902	18512c	tetpent3(c)	tetracosapentaenoic acid, n-3	Cytosol
903	18513c	tetpent3coa(c)	tetracosapentaenoyl coenzyme A, n-3	Cytosol
904	25991c	tetpent3crn(c)	tetracosapentaenoyl carnitine	Cytosol
905	18508c	tetpent6(c)	tetracosapentaenoic acid, n-6	Cytosol
906	18509c	tetpent6coa(c)	tetracosapentaenoyl coenzyme A, n-6	Cytosol
907	25992c	tetpent6crn(c)	tetracosapentaenoyl carnitine	Cytosol
908	18510c	tettet6(c)	tetracosatetraenoic acid n-6	Cytosol
909	18511c	tettet6coa(c)	tetracosatetraenoyl coenzyme A	Cytosol
910	25986c	tettet6crn(c)	Tetracosatetraenoyl carnitine	Cytosol
911	135c	thbpt(c)	Tetrahydrobiopterin	Cytosol
912	22636c	thbpt4acam(c)	Tetrahydrobiopterin-4a-carbinolamine	Cytosol
913	19623c	thcrm_hs(c)	trihexosyl ceramide (homo sapiens)	Cytosol
914	1483c	thcys(c)	Thiocysteine	Cytosol
915	1065c	thf(c)	5,6,7,8-Tetrahydrofolate	Cytosol
916	210c	thm(c)	Thiamin	Cytosol
917	866c	thmmp(c)	Thiamin monophosphate	Cytosol
918	341c	thmpp(c)	Thiamine diphosphate	Cytosol
919	2271c	thmtp(c)	Thiamin triphosphate	Cytosol
920	75c	thp2c(c)	2,3,4,5-Tetrahydropyridine-2-carboxylate	Cytosol
921	253c	thr-L(c)	L-Threonine	Cytosol
922	1481c	thrnt(c)	L-Threonate	Cytosol
923	246c	thym(c)	Thymine	Cytosol
924	5269c	thymd(c)	Thymidine	Cytosol
925	1482c	thyox-L(c)	L-Thyroxine	Cytosol
926	2907c	tmlys(c)	N6,N6,N6-Trimethyl-L-lysine	Cytosol
927	18465c	tmndnc(c)	timnodonic acid C20:5, n-3	Cytosol
928	18486c	tmndnccoac(c)	timnodonyl coenzyme A	Cytosol
929	25988c	tmndnccrn(c)	Timnodonyl carnitine	Cytosol
930	20410c	tolbutamide(c)	tolbutamide	Cytosol
931	181c	trdox(c)	Oxidized thioredoxin	Cytosol
932	180c	trdrd(c)	Reduced thioredoxin	Cytosol
933	867c	tre(c)	Trehalose	Cytosol
934	2543c	triodythy(c)	Triiodothyronine	Cytosol
935	21120c	triodythysuf(c)	Triiodothyronine sulfate	Cytosol
936	1047c	trp-L(c)	L-Tryptophan	Cytosol
937	405c	trypta(c)	Tryptamine	Cytosol
938	20000c	ts3(c)	Tachysterol 3	Cytosol
939	10622c	tststerone(c)	Testosterone	Cytosol
940	20816c	tststeroneglc(c)	testosterone glucuronide	Cytosol
941	26486c	tststerones(c)	testosterone sulfate	Cytosol
942	164c	tsul(c)	Thiosulfate	Cytosol
943	12382c	ttc-ggdp(c)	trans,trans,cis-Geranylgeranyl diphosphate	Cytosol
944	6302c	ttcca(c)	tetradecanoate (n-C14:0)	Cytosol
945	8772c	ttcca(c)	tetradecenoate (n-C14:1)	Cytosol
946	26814c	ttcrn(c)	tetradecanoyl carnitine	Cytosol
947	1777c	txa2(c)	Thromboxane A2	Cytosol
948	100c	tym(c)	Tyramine	Cytosol
949	21118c	tymsf(c)	Tyramine O-sulfate	Cytosol
950	1051c	tyr-L(c)	L-Tyrosine	Cytosol

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
951	326c	uacgam(c)	UDP-N-acetyl-D-glucosamine	Cytosol
952	477c	udp(c)	UDP	Cytosol
953	10912c	udpacgal(c)	UDP-N-acetyl-D-galactosamine	Cytosol
954	316c	udpg(c)	UDPglucose	Cytosol
955	331c	udpgal(c)	UDPgalactose	Cytosol
956	241c	udpglcur(c)	UDP-D-glucuronate	Cytosol
957	255c	udpxyl(c)	UDP-D-xylose	Cytosol
958	1068c	ump(c)	UMP	Cytosol
959	687c	uppg3(c)	Uroporphyrinogen III	Cytosol
960	1069c	ura(c)	Uracil	Cytosol
961	199c	urate(c)	Urate	Cytosol
962	640c	urcan(c)	Urocanate	Cytosol
963	1054c	urea(c)	Urea	Cytosol
964	10727c	uri(c)	Uridine	Cytosol
965	345c	utp(c)	UTP	Cytosol
966	18459c	vacc(c)	vaccenic acid	Cytosol
967	18479c	vacccoa(c)	vaccenyl coenzyme A	Cytosol
968	25973c	vaccern(c)	Vaccenyl carnitine	Cytosol
969	250c	val-L(c)	L-Valine	Cytosol
970	20013c	vitd2(c)	Vitamin D2	Cytosol
971	20001c	vitd3(c)	Vitamin D3	Cytosol
972	20811c	whddca(c)	omega hydroxy dodecanoate (n-C12:0)	Cytosol
973	20813c	whhdca(c)	omega hydroxy hexadecanoate (n-C16:0)	Cytosol
974	20403c	whststerone(c)	w hydroxy testosterone	Cytosol
975	20812c	whtdca(c)	omega hydroxy tetradecanoate (n-C14:0)	Cytosol
976	216c	xan(c)	Xanthine	Cytosol
977	436c	xmp(c)	Xanthosine 5'-phosphate	Cytosol
978	3380c	xol7ah(c)	7alpha-Hydroxy-5beta-cholestan-3-one	Cytosol
979	3381c	xol7ah2(c)	3alpha,7alpha-Dihydroxy-5beta-cholestane	Cytosol
980	11535c	xol7aone(c)	7alpha-Hydroxycholest-4-en-3-one	Cytosol
981	3384c	xoldiolone(c)	7alpha,12alpha-Dihydroxycholest-4-en-3-one	Cytosol
982	3382c	xoldioloneh(c)	7alpha,12alpha-Dihydroxy-5beta-cholestan-3-one	Cytosol
983	22732c	xolest2_hs(c)	cholesterol ester (from FULLR2)	Cytosol
984	2593c	xolest_hs(c)	cholesterol ester	Cytosol
985	17068c	xoltri24(c)	7-alpha,24(S)-Dihydroxycholesterol	Cytosol
986	17067c	xoltri25(c)	7-alpha,25-Dihydroxycholesterol	Cytosol
987	4061c	xoltri27(c)	7-alpha,27-Dihydroxycholesterol	Cytosol
988	3383c	xoltriol(c)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	Cytosol
989	459c	xtp(c)	XTP	Cytosol
990	10906c	xtsn(c)	Xanthosine	Cytosol
991	22281c	xu1p-D(c)	D-Xylulose 1-phosphate	Cytosol
992	283c	xu5p-D(c)	D-Xylulose 5-phosphate	Cytosol
993	248c	xyl-D(c)	D-Xylose	Cytosol
994	4197c	xylnt(c)	L-Xylonate	Cytosol
995	211c	xylt(c)	Xylitol	Cytosol
996	157c	xylu-D(c)	D-Xylulose	Cytosol
997	159c	xylu-L(c)	L-Xylulose	Cytosol
998	20140c	yvite(c)	gamma-Tocopherol	Cytosol
999	286e	10fthf(e)	10-Formyltetrahydrofolate	Extra-organism
1000	20786e	10fthf5glu(e)	10-formyltetrahydrofolate-[Glu](5)	Extra-organism
1001	20787e	10fthf6glu(e)	10-formyltetrahydrofolate-[Glu](6)	Extra-organism
1002	20788e	10fthf7glu(e)	10-formyltetrahydrofolate-[Glu](7)	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1003	22812e	11-cis-retfa(e)	fatty acid 11-cis-retinol	Extra-organism
1004	22816e	13-cis-retnglc(e)	13-cis-retinoyl glucuronide	Extra-organism
1005	22325e	1glyc_hs(e)	1 acyl phosphoglycerol	Extra-organism
1006	18732e	1mncam(e)	1-Methylnicotinamide	Extra-organism
1007	20023e	2425dhvitd2(e)	24R,25-Dihyoxyvitamin D2	Extra-organism
1008	20024e	2425dhvitd3(e)	24R,25-Dihydroxyvitamin D3	Extra-organism
1009	20412e	24nph(e)	2,4 dihydroxy nitrophenol	Extra-organism
1010	20014e	25hvitd2(e)	25-Hydroxyvitamin D2	Extra-organism
1011	20012e	25hvitd3(e)	25-Hydroxyvitamin D3	Extra-organism
1012	4433e	2hb(e)	2-Hydroxybutyrate	Extra-organism
1013	1591e	2mctit(e)	2-Methylcitrate	Extra-organism
1014	3464e	34dhoxpeg(e)	3,4-Dihydroxyphenylethyleneglycol	Extra-organism
1015	190e	34dhphe(e)	3,4-Dihydroxy-L-phenylalanine	Extra-organism
1016	9005e	35cgmp(e)	3',5'-Cyclic GMP	Extra-organism
1017	2457e	3aib(e)	L-3-Amino-isobutanoate	Extra-organism
1018	2444e	3aib-D(e)	D-3-Amino-isobutanoate	Extra-organism
1019	10891e	3mlda(e)	3-Methylimidazoleacetic acid	Extra-organism
1020	176e	4abut(e)	4-Aminobutanoate	Extra-organism
1021	20409e	4hdebrisoquine(e)	4 hydroxy debrisoquine	Extra-organism
1022	1127e	4hphac(e)	4-Hydroxyphenylacetate	Extra-organism
1023	20411e	4mtolbutamide(e)	4 hydroxy tolbutamide	Extra-organism
1024	730e	4nph(e)	4-Nitrophenol	Extra-organism
1025	21119e	4nphsf(e)	4-Nitrophenyl sulfate	Extra-organism
1026	717e	4pyrdx(e)	4-Pyridoxate	Extra-organism
1027	10712e	5adtststerone(e)	5alpha-Dihydrotestosterone	Extra-organism
1028	22786e	5adtststeroneglc(e)	5alpha-Dihydrotestosterone glucuronide	Extra-organism
1029	26487e	5adtststerones(e)	5alpha-Dihydrotestosterone sulfate	Extra-organism
1030	20783e	5dhf(e)	pentaglutamyl folate (DHF)	Extra-organism
1031	11866e	5fthf(e)	5-Formyltetrahydrofolate	Extra-organism
1032	20405e	5homeprazole(e)	5 hydroxy omeprazole	Extra-organism
1033	831e	5htrp(e)	5-Hydroxy-L-tryptophan	Extra-organism
1034	431e	5mthf(e)	5-Methyltetrahydrofolate	Extra-organism
1035	20780e	5thf(e)	pentaglutamyl folate (THF)	Extra-organism
1036	20784e	6dhf(e)	haxglutamyl folate (DHF)	Extra-organism
1037	20402e	6htststerone(e)	6 beta hydroxy testosterone	Extra-organism
1038	20781e	6thf(e)	hexaglutamyl folate (THF)	Extra-organism
1039	20785e	7dhf(e)	heptaglutamyl folate (DHF)	Extra-organism
1040	20782e	7thf(e)	heptaglutamyl folate (THF)	Extra-organism
1041	22811e	9-cis-retfa(e)	fatty acid 9-cis-retinol	Extra-organism
1042	105e	Lcystin(e)	L-Cystine	Extra-organism
1043	18523e	Rtotal(e)	R total	Extra-organism
1044	18525e	Rtotal2(e)	R total 2 position	Extra-organism
1045	18526e	Rtotal3(e)	R total 3 position	Extra-organism
1046	18059e	Tyr-ggn(e)	Tyr-194 of apo-glycogenin protein (primer for glycogen synthesis)	Extra-organism
1047	360e	abt(e)	L-Arabinitol	Extra-organism
1048	319e	ac(e)	Acetate	Extra-organism
1049	9016e	acac(e)	Acetoacetate	Extra-organism
1050	1052e	acald(e)	Acetaldehyde	Extra-organism
1051	266e	acetone(e)	Acetone	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1052	22669e	acgalfucgalacgalfuc12gal14acglcgalgluside_hs(e)	Type IIIA glycolipid	Extra-organism
1053	22681e	acgalfucgalacgalfucgalacglcgal14acglcgalgluside_hs(e)	Type IIIAb	Extra-organism
1054	224e	acgam(e)	N-Acetyl-D-glucosamine	Extra-organism
1055	1617e	ach(e)	Acetylcholine	Extra-organism
1056	19741e	acn13acngalgsbside_hs(e)	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Extra-organism
1057	19742e	acn23acngalgsbside_hs(e)	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Extra-organism
1058	22662e	acnacngal14acglcgalgluside_hs(e)	3',8'-LD1	Extra-organism
1059	19738e	acnacngalgsbside_hs(e)	disialyl galactosylgloboside (homo sapiens)	Extra-organism
1060	22682e	acngalacglcgal14acglcgalgluside_hs(e)	VI3NeuAc-nLc6Cer	Extra-organism
1061	228e	ade(e)	Adenine	Extra-organism
1062	270e	adn(e)	Adenosine	Extra-organism
1063	471e	adp(e)	ADP	Extra-organism
1064	2434e	adprbp(e)	ADPribose 2'-phosphate	Extra-organism
1065	151e	adprib(e)	ADPribose	Extra-organism
1066	18463e	adrn(e)	adrenic acid	Extra-organism
1067	641e	adrnl(e)	Adrenaline	Extra-organism
1068	20413e	aflatoxin(e)	aflatoxin B1	Extra-organism
1069	20819e	ahandrostanglc(e)	Etiocholan-3alpha-ol-17-one 3-glucuronide	Extra-organism
1070	19364e	ak2lgchol_hs(e)	1-alkyl 2-lysglycerol 3-phosphocholine	Extra-organism
1071	314e	akg(e)	2-Oxoglutarate	Extra-organism
1072	1063e	ala-B(e)	beta-Alanine	Extra-organism
1073	1093e	ala-D(e)	D-Alanine	Extra-organism
1074	11412e	ala-L(e)	L-Alanine	Extra-organism
1075	1447e	aldstrn(e)	Aldosterone	Extra-organism
1076	309e	amp(e)	AMP	Extra-organism
1077	352e	andrstrn(e)	Androsterone	Extra-organism
1078	20815e	andrstrnglc(e)	androsterone glucuronide	Extra-organism
1079	20406e	antipyrene(e)	antipyrene	Extra-organism
1080	2071e	apnnox(e)	alpha-Pinene-oxide	Extra-organism
1081	4033e	appnn(e)	(+)-alpha-Pinene	Extra-organism
1082	3086e	aprgstrn(e)	20alpha-Hydroxyprogesterone	Extra-organism
1083	816e	aqcobal(e)	Aquacob(III)alamin	Extra-organism
1084	307e	arab-L(e)	L-Arabinose	Extra-organism
1085	5355e	arach(e)	Arachidic acid	Extra-organism
1086	11890e	arachd(e)	arachidonic acid	Extra-organism
1087	337e	arg-L(e)	L-Arginine	Extra-organism
1088	11279e	ascb-L(e)	L-Ascorbate	Extra-organism
1089	232e	asn-L(e)	L-Asparagine	Extra-organism
1090	10519e	asp-D(e)	D-Aspartate	Extra-organism
1091	330e	asp-L(e)	L-Aspartate	Extra-organism
1092	465e	atp(e)	ATP	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1093	20142e	avite1(e)	alpha-Tocopherol	Extra-organism
1094	20141e	avite2(e)	alpha-Tocotrienol	Extra-organism
1095	870e	bhb(e)	(R)-3-Hydroxybutanoate	Extra-organism
1096	4279e	bilg1cur(e)	Bilirubin beta-diglycuronide	Extra-organism
1097	1942e	bilg1cur(e)	Bilirubin monoglycuronide	Extra-organism
1098	101e	bilirub(e)	Bilirubin	Extra-organism
1099	4297e	biocyt(e)	Biocytin	Extra-organism
1100	1079e	btn(e)	Biotin	Extra-organism
1101	294e	but(e)	Butyrate (n-C4:0)	Extra-organism
1102	20143e	bvite(e)	beta-tocopherol	Extra-organism
1103	10989e	bz(e)	Benzoate	Extra-organism
1104	346e	ca2(e)	Calcium	Extra-organism
1105	8980e	camp(e)	cAMP	Extra-organism
1106	19576e	caro(e)	beta-Carotene	Extra-organism
1107	798e	carveol(e)	(E)-carveol	Extra-organism
1108	20077e	cca_d3(e)	Calcitroic acid (D3)	Extra-organism
1109	7908e	cgly(e)	Cys-Gly	Extra-organism
1110	1075e	chol(e)	Choline	Extra-organism
1111	457e	cholate(e)	Cholate	Extra-organism
1112	252e	chsterol(e)	Cholesterol	Extra-organism
1113	19243e	chtn(e)	chitin	Extra-organism
1114	236e	cit(e)	Citrate	Extra-organism
1115	5268e	cl(e)	Chloride	Extra-organism
1116	18467e	clpnd(e)	clupanodonic acid	Extra-organism
1117	11376e	cmp(e)	CMP	Extra-organism
1118	12152e	co(e)	Carbon monoxide	Extra-organism
1119	474e	co2(e)	CO2	Extra-organism
1120	4331e	coumarin(e)	coumarin	Extra-organism
1121	150e	creat(e)	Creatine	Extra-organism
1122	2222e	crmp_hs(e)	Ceramide 1-phosphate	Extra-organism
1123	163e	crn(e)	L-Carnitine	Extra-organism
1124	11891e	crvnc(e)	cervonic acid, C22:6 n-3	Extra-organism
1125	212e	csn(e)	Cytosine	Extra-organism
1126	20541e	cspg_a(e)	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	Extra-organism
1127	20599e	cspg_b(e)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S) proteoglycan	Extra-organism
1128	20545e	cspg_c(e)	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	Extra-organism
1129	20554e	cspg_d(e)	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	Extra-organism
1130	20549e	cspg_e(e)	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	Extra-organism
1131	245e	cyan(e)	Hydrogen cyanide	Extra-organism
1132	1062e	cys-L(e)	L-Cysteine	Extra-organism
1133	92e	cytd(e)	Cytidine	Extra-organism
1134	380e	dad-2(e)	Deoxyadenosine	Extra-organism
1135	3751e	dad-5(e)	5'-Deoxyadenosine	Extra-organism
1136	18537e	dag_hs(e)	diacylglycerol (homo sapiens)	Extra-organism
1137	18466e	dcsptn1(e)	docosa-4,7,10,13,16-pentaenoic acid (n-6)	Extra-organism
1138	10918e	dcyt(e)	Deoxycytidine	Extra-organism
1139	20408e	debrisoquine(e)	debrisoquine	Extra-organism
1140	3387e	dgchol(e)	Chenodeoxyglycocholate	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1141	172e	dgsn(e)	Deoxyguanosine	Extra-organism
1142	421e	dhdascb(e)	Dehydroascorbate	Extra-organism
1143	3998e	dheas(e)	Dehydroepiandrosterone sulfate	Extra-organism
1144	10505e	dhf(e)	7,8-Dihydrofolate	Extra-organism
1145	4544e	digalsgalside_hs(e)	Digalactosylceramidesulfate	Extra-organism
1146	3417e	din(e)	Deoxyinosine	Extra-organism
1147	2431e	dnlcg(e)	dihomo-gamma-linolenic acid (n-6)	Extra-organism
1148	20407e	dmantipyrine(e)	demethylated antipyrine	Extra-organism
1149	26488e	dmhptcrn(e)	2,6 dimethylheptanoyl carnitine	Extra-organism
1150	2882e	dopa(e)	Dopamine	Extra-organism
1151	21114e	dopasf(e)	Dopamine 3-O-sulfate	Extra-organism
1152	1462e	drib(e)	Deoxyribose	Extra-organism
1153	355e	duri(e)	Deoxyuridine	Extra-organism
1154	20414e	eaflatoxin(e)	8,9 epoxy aflatoxin B1	Extra-organism
1155	20367e	ebastine(e)	ebastine	Extra-organism
1156	20368e	ebastineoh(e)	hydroxylated ebastine	Extra-organism
1157	18506e	eicostet(e)	eicosatetraenoic acid	Extra-organism
1158	588e	elaid(e)	elaidic acid	Extra-organism
1159	20817e	estradiolglc(e)	estradiol glucuronide	Extra-organism
1160	3415e	estriolglc(e)	16-Glucuronide-estriol	Extra-organism
1161	20814e	estroneglc(e)	estrone glucuronide	Extra-organism
1162	2601e	estrones(e)	Estrone 3-sulfate	Extra-organism
1163	87e	etoh(e)	Ethanol	Extra-organism
1164	312e	fe2(e)	Fe2+	Extra-organism
1165	5267e	fe3(e)	Fe3+	Extra-organism
1166	118e	fol(e)	Folate	Extra-organism
1167	334e	for(e)	Formate	Extra-organism
1168	1061e	fru(e)	D-Fructose	Extra-organism
1169	833e	fuc-L(e)	L-Fucose	Extra-organism
1170	22691e	fuc13galacglcg14 acglcggluside_hs(e)	III3Fuc-nLc6Cer	Extra-organism
1171	22658e	fuc14galacglcg1 uside_hs(e)	Lea glycolipid	Extra-organism
1172	22657e	fucacgalfucgalacgl cggluside_hs(e)	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Extra-organism
1173	22663e	fucacngal14acglcga lgluside_hs(e)	IV3-a-NeuAc,III3-a-Fuc-nLc4Cer	Extra-organism
1174	22655e	fucacngalacglcgalg luside_hs(e)	IV3-a-Neu5Ac,III4-a-Fuc-Lc4Cer	Extra-organism
1175	22665e	fucfuc12gal14acglc galgluside_hs(e)	Ley glycolipid	Extra-organism
1176	22693e	fucfuc132galacglcg al14acglcggluside _hs(e)	V3Fuc,III3Fuc-nLc6Cer	Extra-organism
1177	22690e	fucfucfucgalacglc1 3galacglcg14acgl cggluside_hs(e)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1178	22685e	fucfucfucgalacglcgal14acglcgalgluside_hs(e)	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1	Extra-organism
1179	22650e	fucfucgalacglcgalgluside_hs(e)	Leb glycolipid	Extra-organism
1180	22660e	fucgal14acglcgalgluside_hs(e)	Lacto-N-fucopentaosyl III ceramide	Extra-organism
1181	22652e	fucgalfucgalacglcgalgluside_hs(e)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Extra-organism
1182	19746e	fucgalgbside_hs(e)	fucosyl galactosylglobside (homo sapiens)	Extra-organism
1183	1083e	gal(e)	D-Galactose	Extra-organism
1184	19744e	galacglcgalgbside_hs(e)	Gal-GlcNAc-Gal globoside (homo sapiens)	Extra-organism
1185	22670e	galfuc12gal14acglcgalgluside_hs(e)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	Extra-organism
1186	22683e	galfucgalacglcgal14acglcgalgluside_hs(e)	(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	Extra-organism
1187	22676e	galgalfucfucgalacglcgalacglcgal14acglcgalgluside_hs(e)	(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	Extra-organism
1188	19735e	galgalgalthcrm_hs(e)	Gal-Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Extra-organism
1189	171e	gam(e)	D-Glucosamine	Extra-organism
1190	19624e	gbside_hs(e)	globside (homo sapiens)	Extra-organism
1191	1554e	gchola(e)	glycocholate	Extra-organism
1192	19757e	gd1b2_hs(e)	GD1beta (homo sapiens)	Extra-organism
1193	19754e	gd1c_hs(e)	GD1c (homo sapiens)	Extra-organism
1194	11524e	gdchola(e)	glycochenodeoxycholate	Extra-organism
1195	321e	gdp(e)	GDP	Extra-organism
1196	318e	glc-D(e)	D-Glucose	Extra-organism
1197	11299e	gln-L(e)	L-Glutamine	Extra-organism
1198	313e	glu-L(e)	L-Glutamate	Extra-organism
1199	7925e	gluala(e)	5-L-Glutamyl-L-alanine	Extra-organism
1200	323e	gly(e)	Glycine	Extra-organism
1201	503e	glyb(e)	Glycine betaine	Extra-organism
1202	1077e	glyc(e)	Glycerol	Extra-organism
1203	18741e	glyc-S(e)	(S)-Glycerate	Extra-organism
1204	18062e	glygn2(e)	glycogen, structure 2 (glycogenin-1,6-{7[1,4-Glc], 4[1,4-Glc]})	Extra-organism
1205	18142e	glygn4(e)	glycogen, structure 4 (glycogenin-1,6-{2[1,4-Glc], [1,4-Glc]})	Extra-organism
1206	18148e	glygn5(e)	glycogen, structure 5 (glycogenin-2[1,4-Glc])	Extra-organism
1207	226e	gmp(e)	GMP	Extra-organism
1208	19768e	gp1c_hs(e)	GP1c (homo sapiens)	Extra-organism
1209	19976e	gp1calpha_hs(e)	GP1c alpha (homo sapiens)	Extra-organism
1210	19763e	gq1b_hs(e)	GQ1b (homo sapiens)	Extra-organism
1211	19771e	gq1balpha_hs(e)	GQ1balpha (homo sapiens)	Extra-organism
1212	5279e	gsn(e)	Guanosine	Extra-organism
1213	19749e	gt1a_hs(e)	GT1a (homo sapiens)	Extra-organism
1214	1087e	gthox(e)	Oxidized glutathione	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1215	11388e	gthrd(e)	Reduced glutathione	Extra-organism
1216	327e	gtp(e)	GTP	Extra-organism
1217	291e	gua(e)	Guanine	Extra-organism
1218	1049e	h(e)	H+	Extra-organism
1219	317e	h2o(e)	H2O	Extra-organism
1220	315e	h2o2(e)	Hydrogen peroxide	Extra-organism
1221	9554e	ha(e)	hyaluronan	Extra-organism
1222	22610e	ha_pre1(e)	hyaluronan biosynthesis, precursor 1	Extra-organism
1223	144e	hco3(e)	Bicarbonate	Extra-organism
1224	20383e	hcoumarin(e)	hydroxy coumarin	Extra-organism
1225	297e	hdca(e)	Hexadecanoate (n-C16:0)	Extra-organism
1226	5725e	hdcea(e)	Hexadecenoate (n-C16:1)	Extra-organism
1227	20384e	hestratriol(e)	4,17 dihydroxy estradiol	Extra-organism
1228	9242e	hexc(e)	hexacosanoate (n-C26:0)	Extra-organism
1229	11120e	his-L(e)	L-Histidine	Extra-organism
1230	15080e	hista(e)	Histamine	Extra-organism
1231	131e	hom-L(e)	L-Homoserine	Extra-organism
1232	6306e	hpdca(e)	heptadecanoate	Extra-organism
1233	20638e	hspg(e)	heparan sulfate proteoglycan	Extra-organism
1234	20376e	htaxol(e)	hydroxylated taxol	Extra-organism
1235	218e	hxan(e)	Hypoxanthine	Extra-organism
1236	464e	i(e)	Iodide	Extra-organism
1237	1067e	idp(e)	IDP	Extra-organism
1238	410e	ile-L(e)	L-Isoleucine	Extra-organism
1239	1090e	imp(e)	IMP	Extra-organism
1240	223e	inost(e)	myo-Inositol	Extra-organism
1241	147e	ins(e)	Inosine	Extra-organism
1242	289e	k(e)	potassium	Extra-organism
1243	20192e	ksi(e)	keratan sulfate I	Extra-organism
1244	22553e	ksi_deg1(e)	keratan sulfate I, degradation product 1	Extra-organism
1245	20156e	ksii_core2(e)	keratan sulfate II (core 2-linked)	Extra-organism
1246	20342e	ksii_core4(e)	keratan sulfate II (core 4-linked)	Extra-organism
1247	304e	lac-D(e)	D-Lactate	Extra-organism
1248	10931e	lac-L(e)	L-Lactate	Extra-organism
1249	292e	lcts(e)	Lactose	Extra-organism
1250	1082e	leu-L(e)	L-Leucine	Extra-organism
1251	17887e	leuktrC4(e)	Leukotriene C4	Extra-organism
1252	18473e	lgnc(e)	lignoceric acid	Extra-organism
1253	10371e	limnen(e)	Limonene	Extra-organism
1254	11278e	lipoate(e)	Lipoate	Extra-organism
1255	18461e	lneldc(e)	linoelaidic acid (all trans C18:2)	Extra-organism
1256	11172e	lnlc(e)	linoleic acid (all cis C18:2) n-6	Extra-organism
1257	11152e	lnlnca(e)	alpha-Linolenic acid, C18:3, n-3	Extra-organism
1258	5356e	lnlncg(e)	gamma-linolenic acid	Extra-organism
1259	19382e	lpchol_hs(e)	lysophosphatidylcholine (homo sapiens)	Extra-organism
1260	328e	lys-L(e)	L-Lysine	Extra-organism
1261	18539e	mag_hs(e)	monoacylglycerol 2 (homo sapiens)	Extra-organism
1262	267e	malt(e)	Maltose	Extra-organism
1263	1284e	malttr(e)	Maltotriose	Extra-organism
1264	11018e	man(e)	D-Mannose	Extra-organism
1265	137e	man6p(e)	D-Mannose 6-phosphate	Extra-organism
1266	1092e	meoh(e)	Methanol	Extra-organism
1267	11265e	mepi(e)	Metanephrine	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1268	26412e	mercplaccys(e)	3-mercaptolactate-cysteine disulfide	Extra-organism
1269	343e	met-L(e)	L-Methionine	Extra-organism
1270	370e	mthgxl(e)	Methylglyoxal	Extra-organism
1271	3649e	n2m2nmasn(e)	N-Acetyl-beta-D-glucosaminyl-1,2-alpha-D-mannosyl-1,3-(N-acetyl-beta-D-glucosaminyl-1,2-alpha-D-mannosyl-1,6)-(N-acetyl-beta-D-glucosaminyl-1,4)-beta-D-mannosyl-1,4-N-acetyl-beta-D-glucosaminyl-R	Extra-organism
1272	1023e	na1(e)	Sodium	Extra-organism
1273	301e	nac(e)	Nicotinate	Extra-organism
1274	466e	nad(e)	Nicotinamide adenine dinucleotide	Extra-organism
1275	469e	nadp(e)	Nicotinamide adenine dinucleotide phosphate	Extra-organism
1276	233e	ncam(e)	Nicotinamide	Extra-organism
1277	476e	nh4(e)	Ammonium	Extra-organism
1278	20399e	nifedipine(e)	nifedipine	Extra-organism
1279	361e	no(e)	Nitric oxide	Extra-organism
1280	668e	npthl(e)	Naphthalene	Extra-organism
1281	371e	nrpphr(e)	Norepinephrine	Extra-organism
1282	21117e	nrpphrs(e)	Sulfate derivative of norepinephrine	Extra-organism
1283	18464e	nrvc(e)	nervonic acid	Extra-organism
1284	470e	o2(e)	O2	Extra-organism
1285	461e	o2s(e)	Superoxide anion	Extra-organism
1286	20055e	oagd3_hs(e)	9-O-Acetylated GD3 (homo sapiens)	Extra-organism
1287	20056e	oagt3_hs(e)	9-O-Acetylated GT3 (homo sapiens)	Extra-organism
1288	1249e	ocdca(e)	octadecanoate (n-C18:0)	Extra-organism
1289	8769e	ocdcea(e)	octadecenoate (n-C18:1)	Extra-organism
1290	5354e	octa(e)	octanoate (n-C8:0)	Extra-organism
1291	1021e	oh1(e)	hydroxide ion	Extra-organism
1292	20404e	omeprazole(e)	omeprazole	Extra-organism
1293	20401e	onpthl(e)	naphthalene epoxide	Extra-organism
1294	1304e	orn(e)	Ornithine	Extra-organism
1295	10901e	oxa(e)	Oxalate	Extra-organism
1296	19365e	paf_hs(e)	1-alkyl 2-acteylglycerol 3-phosphocholine (homo sapiens)	Extra-organism
1297	19051e	pchol_hs(e)	Phosphatidylcholine (homo sapiens)	Extra-organism
1298	19050e	pe_hs(e)	phosphatidylethanolamine (homo sapiens)	Extra-organism
1299	5307e	peplys(e)	Peptidyl-L-lysine	Extra-organism
1300	2536e	perillyl(e)	Perillyl alcohol	Extra-organism
1301	19385e	pglyc_hs(e)	phosphatidylglycerol (homo sapiens)	Extra-organism
1302	1048e	phe-L(e)	L-Phenylalanine	Extra-organism
1303	2972e	pheacgln(e)	alpha-N-Phenylacetyl-L-glutamine	Extra-organism
1304	11520e	pHEME(e)	Protoheme	Extra-organism
1305	10509e	phyQ(e)	Phylloquinone	Extra-organism
1306	1308e	phyt(e)	phytanic acid	Extra-organism
1307	472e	pi(e)	Phosphate	Extra-organism
1308	10928e	pnto-R(e)	(R)-Pantothenate	Extra-organism
1309	238e	ppa(e)	Propionate (n-C3:0)	Extra-organism
1310	629e	pro-D(e)	D-Proline	Extra-organism
1311	229e	pro-L(e)	L-Proline	Extra-organism
1312	11382e	prostgd2(e)	Prostaglandin D2	Extra-organism
1313	3492e	prostge1(e)	Prostaglandin E1	Extra-organism
1314	398e	prostge2(e)	Prostaglandin E2	Extra-organism
1315	1126e	prostgf2(e)	Prostaglandin F2alpha	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1316	19052e	ps_hs(e)	phosphatidylserine (homo sapiens)	Extra-organism
1317	6304e	ptdca(e)	pentadecanoate	Extra-organism
1318	362e	pydam(e)	Pyridoxamine	Extra-organism
1319	298e	pydx(e)	Pyridoxal	Extra-organism
1320	160e	pydxn(e)	Pyridoxine	Extra-organism
1321	311e	pyr(e)	Pyruvate	Extra-organism
1322	91e	rbt(e)	Ribitol	Extra-organism
1323	22806e	retfa(e)	fatty acid retinol	Extra-organism
1324	90e	retinol(e)	Retinol	Extra-organism
1325	19628e	retinol-9-cis(e)	9-cis-retinol	Extra-organism
1326	19629e	retinol-cis-11(e)	cis-11-retinol	Extra-organism
1327	11153e	retn(e)	Retinoate	Extra-organism
1328	20818e	retnglc(e)	retinoyl glucuronide	Extra-organism
1329	19574e	retpalm [deleted 10/09/2005 06:18:49 PM](e)	Retinyl palmitate	Extra-organism
1330	1080e	rib-D(e)	D-Ribose	Extra-organism
1331	303e	ribflv(e)	Riboflavin	Extra-organism
1332	15207e	s2l2fn2m2masn(e)	PA6	Extra-organism
1333	15665e	s2l2n2m2masn(e)	de-Fuc form of PA6	Extra-organism
1334	271e	sarcs(e)	Sarcosine	Extra-organism
1335	4212e	sel(e)	Selenate	Extra-organism
1336	512e	ser-D(e)	D-Serine	Extra-organism
1337	339e	ser-L(e)	L-Serine	Extra-organism
1338	15786e	sl-L(e)	L-sulfolactate	Extra-organism
1339	335e	so4(e)	Sulfate	Extra-organism
1340	26303e	spc_hs(e)	sphingosylphosphorylcholine (homo sapiens)	Extra-organism
1341	9025e	sph1p(e)	Sphinganine 1-phosphate	Extra-organism
1342	4541e	sphs1p(e)	Sphingosine 1-phosphate	Extra-organism
1343	638e	srtn(e)	Serotonin	Extra-organism
1344	18126e	strch1(e)	starch, structure 1 (1,6-{7[1,4-Glc], 4[1,4-Glc]})	Extra-organism
1345	18141e	strch2(e)	starch, structure 2 (1,6-{2[1,4-Glc], [1,4-Glc]})	Extra-organism
1346	18462e	strdnc(e)	stearidonic acid C18:4, n-3	Extra-organism
1347	325e	succ(e)	Succinate	Extra-organism
1348	1056e	sucr(e)	Sucrose	Extra-organism
1349	18538e	tag_hs(e)	triacylglycerol (homo sapiens)	Extra-organism
1350	646e	tagat-D(e)	D-Tagatose	Extra-organism
1351	293e	taur(e)	Taurine	Extra-organism
1352	20374e	taxol(e)	paclitaxel	Extra-organism
1353	3700e	tchola(e)	taurocholic acid	Extra-organism
1354	1428e	tcynt(e)	Thiocyanate	Extra-organism
1355	3390e	tdchola(e)	taurochenodeoxycholate	Extra-organism
1356	18514e	tethex3(e)	tetracosahexaenoic acid, n-3	Extra-organism
1357	18512e	tetpent3(e)	tetracosapentaenoic acid, n-3	Extra-organism
1358	18508e	tetpent6(e)	tetracosapentaenoic acid, n-6	Extra-organism
1359	18510e	tettet6(e)	tetracosatetraenoic acid n-6	Extra-organism
1360	1065e	thf(e)	5,6,7,8-Tetrahydrofolate	Extra-organism
1361	210e	thm(e)	Thiamin	Extra-organism
1362	866e	thmmp(e)	Thiamin monophosphate	Extra-organism
1363	2271e	thmtp(e)	Thiamin triphosphate	Extra-organism
1364	253e	thr-L(e)	L-Threonine	Extra-organism
1365	246e	thym(e)	Thymine	Extra-organism
1366	5269e	thymd(e)	Thymidine	Extra-organism

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1367	1482e	thyox-L(e)	L-Thyroxine	Extra-organism
1368	18465e	tmndnc(e)	timnodonic acid C20:5, n-3	Extra-organism
1369	20410e	tolbutamide(e)	tolbutamide	Extra-organism
1370	867e	tre(e)	Trehalose	Extra-organism
1371	2543e	triodythy(e)	Triiodothyronine	Extra-organism
1372	21120e	triodythysuf(e)	Triiodothyronine sulfate	Extra-organism
1373	1047e	trp-L(e)	L-Tryptophan	Extra-organism
1374	20816e	ttststeroneglc(e)	testosterone glucuronide	Extra-organism
1375	26486e	ttststerones(e)	testosterone sulfate	Extra-organism
1376	164e	tsul(e)	Thiosulfate	Extra-organism
1377	6302e	ttdca(e)	tetradecanoate (n-C14:0)	Extra-organism
1378	1777e	txa2(e)	Thromboxane A2	Extra-organism
1379	21118e	tymsf(e)	Tyramine O-sulfate	Extra-organism
1380	1051e	tyr-L(e)	L-Tyrosine	Extra-organism
1381	477e	udp(e)	UDP	Extra-organism
1382	1068e	ump(e)	UMP	Extra-organism
1383	1069e	ura(e)	Uracil	Extra-organism
1384	199e	urate(e)	Urate	Extra-organism
1385	1054e	urea(e)	Urea	Extra-organism
1386	10727e	uri(e)	Uridine	Extra-organism
1387	345e	utp(e)	UTP	Extra-organism
1388	18459e	vacc(e)	vaccenic acid	Extra-organism
1389	250e	val-L(e)	L-Valine	Extra-organism
1390	20013e	vitd2(e)	Vitamin D2	Extra-organism
1391	20001e	vitd3(e)	Vitamin D3	Extra-organism
1392	20811e	whddca(e)	omega hydroxy dodecanoate (n-C12:0)	Extra-organism
1393	20813e	whhdca(e)	omega hydroxy hexadecanoate (n-C16:0)	Extra-organism
1394	20403e	whststerone(e)	w hydroxy testosterone	Extra-organism
1395	20812e	whtdca(e)	omega hydroxy tetradecanoate (n-C14:0)	Extra-organism
1396	22732e	xolest2_hs(e)	cholesterol ester (from FULLR2)	Extra-organism
1397	2593e	xolest_hs(e)	cholesterol ester	Extra-organism
1398	17068e	xoltri24(e)	7-alpha,24(S)-Dihydroxycholesterol	Extra-organism
1399	17067e	xoltri25(e)	7-alpha,25-Dihydroxycholesterol	Extra-organism
1400	4061e	xoltri27(e)	7-alpha,27-Dihydroxycholesterol	Extra-organism
1401	248e	xyl-D(e)	D-Xylose	Extra-organism
1402	211e	xylt(e)	Xylitol	Extra-organism
1403	20140e	yvite(e)	gamma-Tocopherol	Extra-organism
1404	9005g	35cgmp(g)	3',5'-Cyclic GMP	Golgi Apparatus
1405	15787g	Ser/Thr(g)	protein-linked serine or threonine residue (O-glycosylation site)	Golgi Apparatus
1406	15792g	T_antigen(g)	T antigen (core 1)	Golgi Apparatus
1407	15788g	Tn_antigen(g)	Tn antigen	Golgi Apparatus
1408	319g	ac(g)	Acetate	Golgi Apparatus
1409	11537g	accoa(g)	Acetyl-CoA	Golgi Apparatus
1410	19739g	acgagbside_hs(g)	alpha GalNAc globoside (homo sapiens)	Golgi Apparatus
1411	899g	acgal(g)	N-Acetyl-D-galactosamine	Golgi Apparatus
1412	22666g	acgalfuc12gal14acglcgalgluside_hs(g)	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	Golgi Apparatus
1413	22669g	acgalfucgalacgalfuc12gal14acglcgalgluside_hs(g)	Type IIIA glycolipid	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1414	22681g	acgalfucgalacgalfu cgalacglcgal14acgl cgalgluside_hs(g)	Type IIIAb	Golgi Apparatus
1415	22678g	acgalfucgalacglcgal 14acglcgalgluside_ hs(g)	(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	Golgi Apparatus
1416	22656g	acgalfucgalacglcgal gluside_hs(g)	Type IA glycolipid	Golgi Apparatus
1417	19740g	acgbgbside_hs(g)	beta GalNAc globoside (homo sapiens)	Golgi Apparatus
1418	22686g	acglc13galacglcgal 14acglcgalgluside_ hs(g)	nLc7Cer	Golgi Apparatus
1419	22671g	acglcgal14acglcgal gluside_hs(g)	nLc5Cer	Golgi Apparatus
1420	22673g	acglcgalacglcgal14 acglcgalgluside_hs(g)	(Gal)3 (Glc)1 (GlcNAc)3 (Cer)1	Golgi Apparatus
1421	19743g	acglcgalgbside_hs(g)	GlcNAc-Gal globoside (homo sapiens)	Golgi Apparatus
1422	22647g	acglcgalgluside_hs(g)	(Gal)1 (Glc)1 (GlcNAc)1 (Cer)1	Golgi Apparatus
1423	19741g	acn13acngalgbside _hs(g)	sialyl (1,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Golgi Apparatus
1424	19742g	acn23acngalgbside _hs(g)	sialyl (2,3) sialyl (2,6) galactosylgloboside (homo sapiens)	Golgi Apparatus
1425	22662g	acnacngal14acglcg algluside_hs(g)	3',8'-LD1	Golgi Apparatus
1426	19738g	acnacngalgbside_h s(g)	disialyl galactosylgloboside (homo sapiens)	Golgi Apparatus
1427	22661g	acngal14acglcgalgl uside_hs(g)	Sialyl-3-paragloboside	Golgi Apparatus
1428	22682g	acngalacglcgal14ac glcgalgluside_hs(g)	VI3NeuAc-nLc6Cer	Golgi Apparatus
1429	22654g	acngalacglcgalglusi de_hs(g)	(Gal)3 (Glc)1 (GlcNAc)1 (Cer)1	Golgi Apparatus
1430	19737g	acngalgbside_hs(g)	sialyl galactosylgloboside (homo sapiens)	Golgi Apparatus
1431	309g	amp(g)	AMP	Golgi Apparatus
1432	8980g	camp(g)	cAMP	Golgi Apparatus
1433	1075g	chol(g)	Choline	Golgi Apparatus
1434	9019g	cholp(g)	Choline phosphate	Golgi Apparatus
1435	252g	chsterol(g)	Cholesterol	Golgi Apparatus
1436	11376g	cmp(g)	CMP	Golgi Apparatus
1437	1088g	cmpacna(g)	CMP-N-acetylneuraminate	Golgi Apparatus
1438	474g	co2(g)	CO2	Golgi Apparatus
1439	473g	coa(g)	Coenzyme A	Golgi Apparatus
1440	15793g	core2(g)	Core 2	Golgi Apparatus
1441	15796g	core3(g)	Core 3	Golgi Apparatus
1442	15797g	core4(g)	Core 4	Golgi Apparatus
1443	15887g	core5(g)	Core 5	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1444	15798g	core6(g)	Core 6	Golgi Apparatus
1445	15888g	core7(g)	Core 7	Golgi Apparatus
1446	15886g	core8(g)	Core 8	Golgi Apparatus
1447	19478g	crm_hs(g)	ceramide (homo sapiens)	Golgi Apparatus
1448	20499g	cs_hs_linkage(g)	chondroitin sulfate/heparan sulfate linkage region (GlcA-(Gal)2-Xyl-L-Ser (protein))	Golgi Apparatus
1449	20538g	cs_a,b,e_pre1(g)	chondroitin sulfate A (GalNAc4S-GlcA), B (IdoA2S-GalNAc4S), and E (GalNAc4,6diS-GlcA), precursor 1	Golgi Apparatus
1450	20539g	cs_a,b_pre2(g)	chondroitin sulfate A (GalNAc4S-GlcA) and B (IdoA2S-GalNAc4S), precursor 2	Golgi Apparatus
1451	20540g	cs_a,b_pre3(g)	chondroitin sulfate A (GalNAc4S-GlcA) and B (IdoA2S-GalNAc4S), precursor 3	Golgi Apparatus
1452	20597g	cs_b_pre4(g)	chondroitin sulfate B (IdoA2S-GalNAc4S), precursor 4	Golgi Apparatus
1453	20598g	cs_b_pre5(g)	chondroitin sulfate B (IdoA2S-GalNAc4s), precursor 5	Golgi Apparatus
1454	20542g	cs_c,d,e_pre1(g)	chondroitin sulfate C (GalNAc6S-GlcA) and D (GlcNAc6S-GlcA2S), precursor 1	Golgi Apparatus
1455	20543g	cs_c_pre2(g)	chondroitin sulfate C (GalNAc6S-GlcA), precursor 2	Golgi Apparatus
1456	20544g	cs_c_pre3(g)	chondroitin sulfate C (GalNAc6S-GlcA), precursor 3	Golgi Apparatus
1457	20550g	cs_d_pre2(g)	chondroitin sulfate D (GlcNAc6S-GlcA2S) precursor 2	Golgi Apparatus
1458	20551g	cs_d_pre3(g)	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 3	Golgi Apparatus
1459	20552g	cs_d_pre4(g)	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 4	Golgi Apparatus
1460	20553g	cs_d_pre5(g)	chondroitin sulfate D (GlcNAc6S-GlcA2S), precursor 5	Golgi Apparatus
1461	20546g	cs_e_pre2(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 2	Golgi Apparatus
1462	20547g	cs_e_pre3(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 3	Golgi Apparatus
1463	20548g	cs_e_pre4(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 4	Golgi Apparatus
1464	20591g	cs_e_pre5a(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5a	Golgi Apparatus
1465	20594g	cs_e_pre5b(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5b	Golgi Apparatus
1466	20537g	cs_pre(g)	chondroitin sulfate precursor (GalNAc-GlcA-(Gal)2-Xyl-L-Ser (protein))	Golgi Apparatus
1467	20541g	cspg_a(g)	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	Golgi Apparatus
1468	20599g	cspg_b(g)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S) proteoglycan	Golgi Apparatus
1469	20545g	cspg_c(g)	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	Golgi Apparatus
1470	20554g	cspg_d(g)	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	Golgi Apparatus
1471	20549g	cspg_e(g)	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1472	4544g	digalsgalside_hs(g)	Digalactosylceramidesulfate	Golgi Apparatus
1473	19810g	digalside_hs(g)	Digalactosylceramide	Golgi Apparatus
1474	14993g	dolglcp_U(g)	Dolichyl beta-D-glucosyl phosphate, human uterine homolog	Golgi Apparatus
1475	14989g	dolp_U(g)	Dolichol phosphate, human uterine homolog	Golgi Apparatus
1476	15795g	dsT_antigen(g)	disialyl-T antigen	Golgi Apparatus
1477	15885g	f1a(g)	F1alpha	Golgi Apparatus
1478	15195g	fn2m2masn(g)	N4-{N-Acetyl-beta-D-glucosaminyl-(1,2)-alpha-D-mannosyl-(1,3)-[N-acetyl-beta-D-glucosaminyl-(1,2)-alpha-D-mannosyl-(1,6)]-beta-D-mannosyl-(1,4)-N-acetyl-beta-D-glucosaminyl-(1,4)-[alpha-L-fucosyl-(1,6)]-N-acetyl-beta-D-glucosaminyl} asparagine	Golgi Apparatus
1479	22664g	fuc12gal14acglcgalgluside_hs(g)	Type IIIH glycolipid	Golgi Apparatus
1480	22692g	fuc132galacglcgal14acglcgalgluside_hs(g)	V3Fuc-nLc6Cer	Golgi Apparatus
1481	22691g	fuc13galacglcgal14acglcgalgluside_hs(g)	III3Fuc-nLc6Cer	Golgi Apparatus
1482	22658g	fuc14galacglcgalgluside_hs(g)	Lea glycolipid	Golgi Apparatus
1483	22657g	fucacgalfucgalacglcgalgluside_hs(g)	(Gal)2 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Golgi Apparatus
1484	22663g	fucacngal14acglcgalgluside_hs(g)	IV3-a-NeuAc,III3-a-Fuc-nLc4Cer	Golgi Apparatus
1485	22655g	fucacngalacglcgalgluside_hs(g)	IV3-a-Neu5Ac,III4-a-Fuc-Lc4Cer	Golgi Apparatus
1486	22665g	fucfuc12gal14acglcgalgluside_hs(g)	Ley glycolipid	Golgi Apparatus
1487	22693g	fucfuc132galacglcgal14acglcgalgluside_hs(g)	V3Fuc,III3Fuc-nLc6Cer	Golgi Apparatus
1488	22690g	fucfucfucgalacglc13galacglcgal14acglcgalgluside_hs(g)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)3 (Cer)1	Golgi Apparatus
1489	22685g	fucfucfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)3 (Cer)1	Golgi Apparatus
1490	22689g	fucfucgalacglc13galacglcgal14acglcgalgluside_hs(g)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	Golgi Apparatus
1491	22684g	fucfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)3 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	Golgi Apparatus
1492	22675g	fucfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1493	22650g	fucfucgalacglcgalgluside_hs(g)	Leb glycolipid	Golgi Apparatus
1494	22660g	fucgal14acglcgalgluside_hs(g)	Lacto-N-fucopentaosyl III ceramide	Golgi Apparatus
1495	22668g	fucgalacgalfuc12gal14acglcgalgluside_hs(g)	Type IIIH glycolipid	Golgi Apparatus
1496	22680g	fucgalacgalfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)2 (Cer)1	Golgi Apparatus
1497	22688g	fucgalacglc13galacglcgal14acglcgalgluside_hs(g)	(Gal)4 (Glc)1 (GlcNAc)3 (LFuc)1 (Cer)1	Golgi Apparatus
1498	22677g	fucgalacglcgal14acglcgalgluside_hs(g)	VI2Fuc-nLc6	Golgi Apparatus
1499	22649g	fucgalacglcgalgluside_hs(g)	Type IH glycolipid	Golgi Apparatus
1500	22652g	fucgalfucgalacglcgalgluside_hs(g)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)2 (Cer)1	Golgi Apparatus
1501	19746g	fucgalgbside_hs(g)	fucosyl galactosylglobside (homo sapiens)	Golgi Apparatus
1502	15443g	g1m6masnB1(g)	glucosyl-(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1503	15442g	g1m7masnB(g)	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)	Golgi Apparatus
1504	15441g	g1m7masnC(g)	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform C (protein)	Golgi Apparatus
1505	15142g	g1m8masn(g)	(alpha-D-Glucosyl)-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1506	15138g	g2m8masn(g)	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1507	15115g	g3m8masn(g)	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1508	15024g	g3m8mpdol_U(g)	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Golgi Apparatus
1509	19751g	ga1_hs(g)	GA1 (homo sapiens)	Golgi Apparatus
1510	19750g	ga2_hs(g)	GA2 (homo sapiens)	Golgi Apparatus
1511	22659g	gal14acglcgalgluside_hs(g)	Lactoneotetraosylceramide	Golgi Apparatus
1512	22667g	galacgalfuc12gal14acglcgalgluside_hs(g)	(Gal)3 (GalNAc)1 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	Golgi Apparatus
1513	22679g	galacgalfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)4 (GalNAc)1 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1514	22687g	galacglc13galacglcgal14acglcgalgluside_hs(g)	nLc8Cer	Golgi Apparatus
1515	22672g	galacglcgal14acglcgalgluside_hs(g)	i-antigen	Golgi Apparatus
1516	22674g	galacglcgalacglcgal14acglcgalgluside_hs(g)	I-antigen	Golgi Apparatus
1517	19744g	galacglcgalgbside_hs(g)	Gal-GlcNAc-Gal globoside (homo sapiens)	Golgi Apparatus
1518	22648g	galacglcgalgluside_hs(g)	Lc4Cer	Golgi Apparatus
1519	22670g	galfuc12gal14acglcgalgluside_hs(g)	(Gal)3 (Glc)1 (GlcNAc)1 (LFuc)1 (Cer)1	Golgi Apparatus
1520	22683g	galfucgalacglcgal14acglcgalgluside_hs(g)	(Gal)4 (Glc)1 (GlcNAc)2 (LFuc)1 (Cer)1	Golgi Apparatus
1521	22651g	galfucgalacglcgalgluside_hs(g)	Type IB glycolipid	Golgi Apparatus
1522	22676g	galgalfucfucgalacglcgalacglcgal14acglcgalgluside_hs(g)	(Gal)6 (Glc)1 (GlcNAc)3 (LFuc)2 (Cer)1	Golgi Apparatus
1523	19735g	galgalthcrm_hs(g)	Gal-Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Golgi Apparatus
1524	19734g	galgalthcrm_hs(g)	Gal-Gal-Gal-Gal-Glc-Cer (homo sapiens)	Golgi Apparatus
1525	19736g	galgbside_hs(g)	galactosylgloboside (homo sapiens)	Golgi Apparatus
1526	19619g	galgluside_hs(g)	galactosyl glucosyl ceramide	Golgi Apparatus
1527	19614g	galside_hs(g)	galactocerebroside (homo sapiens)	Golgi Apparatus
1528	19733g	galthcrm_hs(g)	Gal-Gal-Gal-Glc-Cer (homo sapiens)	Golgi Apparatus
1529	19624g	gbside_hs(g)	globoside (homo sapiens)	Golgi Apparatus
1530	19747g	gd1a_hs(g)	GD1a (homo sapiens)	Golgi Apparatus
1531	19769g	gd1alpha_hs(g)	GD1a (homo sapiens)	Golgi Apparatus
1532	19757g	gd1b2_hs(g)	GD1beta (homo sapiens)	Golgi Apparatus
1533	19761g	gd1b_hs(g)	GD1b (homo sapiens)	Golgi Apparatus
1534	19754g	gd1c_hs(g)	GD1c (homo sapiens)	Golgi Apparatus
1535	19760g	gd2_hs(g)	GD2 (homo sapiens)	Golgi Apparatus
1536	19759g	gd3_hs(g)	GD3 (homo sapiens)	Golgi Apparatus
1537	321g	gdp(g)	GDP	Golgi Apparatus
1538	168g	gdpfuc(g)	GDP-L-fucose	Golgi Apparatus
1539	318g	glc-D(g)	D-Glucose	Golgi Apparatus
1540	15438g	glc1man(g)	glucose-1,3-mannose oligosaccharide	Golgi Apparatus
1541	15437g	glc2man(g)	(2)[glucose-1,3]-mannose oligosaccharide	Golgi Apparatus
1542	15433g	glc3man(g)	glucose-1,2-(2)[glucose-1,3]-mannose oligosaccharide	Golgi Apparatus
1543	19613g	gluside_hs(g)	glucocerebroside (homo sapiens)	Golgi Apparatus
1544	19622g	gm1_hs(g)	ganglioside GM1 (homo sapiens)	Golgi Apparatus
1545	19756g	gm1a_hs(g)	GM1alpha (homo sapiens)	Golgi Apparatus
1546	19752g	gm1b_hs(g)	GM1b (homo sapiens)	Golgi Apparatus
1547	19621g	gm2_hs(g)	ganglioside GM2 (homo sapiens)	Golgi Apparatus
1548	19755g	gm2a_hs(g)	GM2alpha (homo sapiens)	Golgi Apparatus
1549	19620g	gm3_hs(g)	ganglioside GM3 (homo sapiens)	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1550	226g	gmp(g)	GMP	Golgi Apparatus
1551	15935g	gncore1(g)	GlcNAc-alpha-1,4-Core 1	Golgi Apparatus
1552	15932g	gncore2(g)	GlcNAc-alpha-1,4-Core 2	Golgi Apparatus
1553	19768g	gp1c_hs(g)	GP1c (homo sapiens)	Golgi Apparatus
1554	19976g	gp1calpha_hs(g)	GP1c alpha (homo sapiens)	Golgi Apparatus
1555	19763g	gq1b_hs(g)	GQ1b (homo sapiens)	Golgi Apparatus
1556	19771g	gq1balpha_hs(g)	GQ1balpha (homo sapiens)	Golgi Apparatus
1557	19767g	gq1c_hs(g)	GQ1c (homo sapiens)	Golgi Apparatus
1558	19749g	gt1a_hs(g)	GT1a (homo sapiens)	Golgi Apparatus
1559	19770g	gt1alpha_hs(g)	GT1alpha (homo sapiens)	Golgi Apparatus
1560	19762g	gt1b_hs(g)	GT1b (homo sapiens)	Golgi Apparatus
1561	19766g	gt1c_hs(g)	GT1c (homo sapiens)	Golgi Apparatus
1562	19765g	gt2_hs(g)	GT2 (homo sapiens)	Golgi Apparatus
1563	19764g	gt3_hs(g)	GT3 (homo sapiens)	Golgi Apparatus
1564	1049g	h(g)	H+	Golgi Apparatus
1565	317g	h2o(g)	H2O	Golgi Apparatus
1566	3844g	hcys-L(g)	L-Homocysteine	Golgi Apparatus
1567	20618g	hs_pre1(g)	heparan sulfate, precursor 1	Golgi Apparatus
1568	20627g	hs_pre10(g)	heparan sulfate, precursor 10	Golgi Apparatus
1569	20628g	hs_pre11(g)	heparan sulfate, precursor 11	Golgi Apparatus
1570	20629g	hs_pre12(g)	heparan sulfate, precursor 12	Golgi Apparatus
1571	20630g	hs_pre13(g)	heparan sulfate, precursor 13	Golgi Apparatus
1572	20718g	hs_pre14(g)	heparan sulfate, precursor 14	Golgi Apparatus
1573	20719g	hs_pre15(g)	heparan sulfate, precursor 15	Golgi Apparatus
1574	20619g	hs_pre2(g)	heparan sulfate, precursor 2	Golgi Apparatus
1575	20620g	hs_pre3(g)	heparan sulfate, precursor 3	Golgi Apparatus
1576	20621g	hs_pre4(g)	heparan sulfate, precursor 4	Golgi Apparatus
1577	20622g	hs_pre5(g)	heparan sulfate, precursor 5	Golgi Apparatus
1578	20623g	hs_pre6(g)	heparan sulfate, precursor 6	Golgi Apparatus
1579	20624g	hs_pre7(g)	heparan sulfate, precursor 7	Golgi Apparatus
1580	20625g	hs_pre8(g)	heparan sulfate, precursor 8	Golgi Apparatus
1581	20626g	hs_pre9(g)	heparan sulfate, precursor 9	Golgi Apparatus
1582	20638g	hspg(g)	heparan sulfate proteoglycan	Golgi Apparatus
1583	289g	k(g)	potassium	Golgi Apparatus
1584	20192g	ksi(g)	keratan sulfate I	Golgi Apparatus
1585	20131g	ksi_pre1(g)	keratan sulfate I biosynthesis, precursor 1	Golgi Apparatus
1586	20165g	ksi_pre10(g)	keratan sulfate I biosynthesis, precursor 10	Golgi Apparatus
1587	20166g	ksi_pre11(g)	keratan sulfate I biosynthesis, precursor 11	Golgi Apparatus
1588	20167g	ksi_pre12(g)	keratan sulfate I biosynthesis, precursor 12	Golgi Apparatus
1589	20168g	ksi_pre13(g)	keratan sulfate I biosynthesis, precursor 13	Golgi Apparatus
1590	20169g	ksi_pre14(g)	keratan sulfate I biosynthesis, precursor 14	Golgi Apparatus
1591	20170g	ksi_pre15(g)	keratan sulfate I biosynthesis, precursor 15	Golgi Apparatus
1592	20171g	ksi_pre16(g)	keratan sulfate I biosynthesis, precursor 16	Golgi Apparatus
1593	20172g	ksi_pre17(g)	keratan sulfate I biosynthesis, precursor 17	Golgi Apparatus
1594	20173g	ksi_pre18(g)	keratan sulfate I biosynthesis, precursor 18	Golgi Apparatus
1595	20174g	ksi_pre19(g)	keratan sulfate I biosynthesis, precursor 19	Golgi Apparatus
1596	20132g	ksi_pre2(g)	keratan sulfate I biosynthesis, precursor 2	Golgi Apparatus
1597	20175g	ksi_pre20(g)	keratan sulfate I biosynthesis, precursor 20	Golgi Apparatus
1598	20176g	ksi_pre21(g)	keratan sulfate I biosynthesis, precursor 21	Golgi Apparatus
1599	20177g	ksi_pre22(g)	keratan sulfate I biosynthesis, precursor 22	Golgi Apparatus
1600	20178g	ksi_pre23(g)	keratan sulfate I biosynthesis, precursor 23	Golgi Apparatus
1601	20179g	ksi_pre24(g)	keratan sulfate I biosynthesis, precursor 24	Golgi Apparatus
1602	20180g	ksi_pre25(g)	keratan sulfate I biosynthesis, precursor 25	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1603	20181g	ksi_pre26(g)	keratan sulfate I biosynthesis, precursor 26	Golgi Apparatus
1604	20182g	ksi_pre27(g)	keratan sulfate I biosynthesis, precursor 27	Golgi Apparatus
1605	20183g	ksi_pre28(g)	keratan sulfate I biosynthesis, precursor 28	Golgi Apparatus
1606	20184g	ksi_pre29(g)	keratan sulfate I biosynthesis, precursor 29	Golgi Apparatus
1607	20133g	ksi_pre3(g)	keratan sulfate I biosynthesis, precursor 3	Golgi Apparatus
1608	20185g	ksi_pre30(g)	keratan sulfate I biosynthesis, precursor 30	Golgi Apparatus
1609	20186g	ksi_pre31(g)	keratan sulfate I biosynthesis, precursor 31	Golgi Apparatus
1610	20187g	ksi_pre32(g)	keratan sulfate I biosynthesis, precursor 32	Golgi Apparatus
1611	20188g	ksi_pre33(g)	keratan sulfate I biosynthesis, precursor 33	Golgi Apparatus
1612	20189g	ksi_pre34(g)	keratan sulfate I biosynthesis, precursor 34	Golgi Apparatus
1613	20190g	ksi_pre35(g)	keratan sulfate I biosynthesis, precursor 35	Golgi Apparatus
1614	20191g	ksi_pre36(g)	keratan sulfate I biosynthesis, precursor 36	Golgi Apparatus
1615	20159g	ksi_pre4(g)	keratan sulfate I biosynthesis, precursor 4	Golgi Apparatus
1616	20160g	ksi_pre5(g)	keratan sulfate I biosynthesis, precursor 5	Golgi Apparatus
1617	20161g	ksi_pre6(g)	keratan sulfate I biosynthesis, precursor 6	Golgi Apparatus
1618	20162g	ksi_pre7(g)	keratan sulfate I biosynthesis, precursor 7	Golgi Apparatus
1619	20163g	ksi_pre8(g)	keratan sulfate I biosynthesis, precursor 8	Golgi Apparatus
1620	20164g	ksi_pre9(g)	keratan sulfate I biosynthesis, precursor 9	Golgi Apparatus
1621	20156g	ksii_core2(g)	keratan sulfate II (core 2-linked)	Golgi Apparatus
1622	20079g	ksii_core2_pre1(g)	keratan sulfate II biosynthesis, precursor 1	Golgi Apparatus
1623	20155g	ksii_core2_pre10(g)	keratan sulfate II biosynthesis, precursor 10	Golgi Apparatus
1624	20085g	ksii_core2_pre2(g)	keratan sulfate II biosynthesis, precursor 2	Golgi Apparatus
1625	20134g	ksii_core2_pre3(g)	keratan sulfate II biosynthesis, precursor 3	Golgi Apparatus
1626	20135g	ksii_core2_pre4(g)	keratan sulfate II biosynthesis, precursor 4	Golgi Apparatus
1627	20149g	ksii_core2_pre5(g)	keratan sulfate II biosynthesis, precursor 5	Golgi Apparatus
1628	20150g	ksii_core2_pre6(g)	keratan sulfate II biosynthesis, precursor 6	Golgi Apparatus
1629	20151g	ksii_core2_pre7(g)	keratan sulfate II biosynthesis, precursor 7	Golgi Apparatus
1630	20153g	ksii_core2_pre8(g)	keratan sulfate II biosynthesis, precursor 8	Golgi Apparatus
1631	20154g	ksii_core2_pre9(g)	keratan sulfate II biosynthesis, precursor 9	Golgi Apparatus
1632	20342g	ksii_core4(g)	keratan sulfate II (core 4-linked)	Golgi Apparatus
1633	20332g	ksii_core4_pre1(g)	keratan sulfate II biosynthesis, precursor 1	Golgi Apparatus
1634	20341g	ksii_core4_pre10(g)	keratan sulfate II biosynthesis, precursor 10	Golgi Apparatus
1635	20333g	ksii_core4_pre2(g)	keratan sulfate II biosynthesis, precursor 2	Golgi Apparatus
1636	20334g	ksii_core4_pre3(g)	keratan sulfate II biosynthesis, precursor 3	Golgi Apparatus
1637	20335g	ksii_core4_pre4(g)	keratan sulfate II biosynthesis, precursor 4	Golgi Apparatus
1638	20336g	ksii_core4_pre5(g)	keratan sulfate II biosynthesis, precursor 5	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1639	20337g	ksii_core4_pre6(g)	keratan sulfate II biosynthesis, precursor 6	Golgi Apparatus
1640	20338g	ksii_core4_pre7(g)	keratan sulfate II biosynthesis, precursor 7	Golgi Apparatus
1641	20339g	ksii_core4_pre8(g)	keratan sulfate II biosynthesis, precursor 8	Golgi Apparatus
1642	20340g	ksii_core4_pre9(g)	keratan sulfate II biosynthesis, precursor 9	Golgi Apparatus
1643	15198g	l2fn2m2masn(g)	{[galactosyl-(1,4)-N-Acetyl-glucosaminy-(1,2)-mannosyl-(1,3)-],[N-acetyl-glucosaminy-(1,2)-mannosyl-(1,6)-]mannosyl-(1,4)-N-acetyl-glucosaminy-(1,4)-[fucosyl-(1,6)]-N-acetyl-glucosaminy}asparagine	Golgi Apparatus
1644	20459g	l2xser(g)	(Gal)2-Xyl-L-Ser (protein)	Golgi Apparatus
1645	292g	lcts(g)	Lactose	Golgi Apparatus
1646	20364g	lxser(g)	Gal-Xyl-L-Ser (protein)	Golgi Apparatus
1647	15154g	m4masn(g)	(alpha-D-mannosyl)4-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1648	15170g	m5masnB1(g)	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1649	15171g	m5masnB2(g)	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1650	15161g	m5masnC(g)	(alpha-D-mannosyl)5-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1651	15167g	m6masnA(g)	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1652	15168g	m6masnB1(g)	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1653	15169g	m6masnB2(g)	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1654	15160g	m6masnC(g)	(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1655	15165g	m7masnA(g)	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform A (protein)	Golgi Apparatus
1656	15159g	m7masnB(g)	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)	Golgi Apparatus
1657	15166g	m7masnC(g)	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform C (protein)	Golgi Apparatus
1658	15144g	m8masn(g)	(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Golgi Apparatus
1659	11018g	man(g)	D-Mannose	Golgi Apparatus
1660	15192g	n2m2masn(g)	((N-acetyl-D-glucosaminy)2-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1661	3649g	n2m2nmasn(g)	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-L	Golgi Apparatus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1662	15212g	n3m2masn(g)	((N-acetyl-D-glucosaminy)3-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1663	15213g	n4m2masn(g)	((N-acetyl-D-glucosaminy)4-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1664	15214g	n5m2masn(g)	((N-acetyl-D-glucosaminy)5-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1665	1023g	na1(g)	Sodium	Golgi Apparatus
1666	4360g	nm2masn(g)	(N-acetyl-D-glucosaminy-(alpha-D-mannosyl)2-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1667	4358g	nm4masn(g)	(N-acetyl-D-glucosaminy-(alpha-D-mannosyl)4-beta-D-mannosyl-diacetylchitobiosyl)-L-asparagine (protein)	Golgi Apparatus
1668	20055g	oagd3_hs(g)	9-O-Acetylated GD3 (homo sapiens)	Golgi Apparatus
1669	20056g	oagt3_hs(g)	9-O-Acetylated GT3 (homo sapiens)	Golgi Apparatus
1670	18536g	pa_hs(g)	phosphatidic acid (homo sapiens)	Golgi Apparatus
1671	333g	pap(g)	Adenosine 3',5'-bisphosphate	Golgi Apparatus
1672	332g	paps(g)	3'-Phosphoadenylyl sulfate	Golgi Apparatus
1673	19051g	pchol_hs(g)	Phosphatidylcholine (homo sapiens)	Golgi Apparatus
1674	19050g	pe_hs(g)	phosphatidylethanolamine (homo sapiens)	Golgi Apparatus
1675	472g	pi(g)	Phosphate	Golgi Apparatus
1676	19052g	ps_hs(g)	phosphatidylserine (homo sapiens)	Golgi Apparatus
1677	15207g	s2l2fn2m2masn(g)	PA6	Golgi Apparatus
1678	15794g	sT_antigen(g)	sialyl-T antigen	Golgi Apparatus
1679	15789g	sTn_antigen(g)	sialyl-Tn antigen	Golgi Apparatus
1680	19615g	sgalside_hs(g)	sulfatide galactocerebroside (homo sapiens)	Golgi Apparatus
1681	19618g	sphmyln_hs(g)	sphingomyelin (homo sapiens)	Golgi Apparatus
1682	19623g	thcrm_hs(g)	trihexosyl ceramide (homo sapiens)	Golgi Apparatus
1683	326g	uacgam(g)	UDP-N-acetyl-D-glucosamine	Golgi Apparatus
1684	477g	udp(g)	UDP	Golgi Apparatus
1685	10912g	udpacgal(g)	UDP-N-acetyl-D-galactosamine	Golgi Apparatus
1686	316g	udpg(g)	UDPglucose	Golgi Apparatus
1687	331g	udpgal(g)	UDPgalactose	Golgi Apparatus
1688	241g	udpglcur(g)	UDP-D-glucuronate	Golgi Apparatus
1689	255g	udpxyl(g)	UDP-D-xylose	Golgi Apparatus
1690	1068g	ump(g)	UMP	Golgi Apparatus
1691	20363g	xser(g)	Xyl-L-Ser (protein)	Golgi Apparatus
1692	2861	10fthf(l)	10-Formyltetrahydrofolate	Lysosome
1693	207861	10fthf5glu(l)	10-formyltetrahydrofolate-[Glu](5)	Lysosome
1694	207871	10fthf6glu(l)	10-formyltetrahydrofolate-[Glu](6)	Lysosome
1695	207881	10fthf7glu(l)	10-formyltetrahydrofolate-[Glu](7)	Lysosome
1696	186041	3amp(l)	3'-AMP	Lysosome
1697	1761	4abut(l)	4-Aminobutanoate	Lysosome
1698	207831	5dhf(l)	pentaglutamyl folate (DHF)	Lysosome
1699	207801	5thf(l)	pentaglutamyl folate (THF)	Lysosome
1700	207841	6dhf(l)	hexaglutamyl folate (DHF)	Lysosome
1701	207811	6thf(l)	hexaglutamyl folate (THF)	Lysosome
1702	207851	7dhf(l)	heptaglutamyl folate (DHF)	Lysosome
1703	207821	7thf(l)	heptaglutamyl folate (THF)	Lysosome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1704	151021	Asn-X-Ser/Thr(l)	protein-linked asparagine residue (N-glycosylation site)	Lysosome
1705	185231	Rtotal(l)	R total	Lysosome
1706	203621	Ser-Gly/Ala-X-Gly(l)	protein-linked serine residue (glycosaminoglycan attachment site)	Lysosome
1707	157871	Ser/Thr(l)	protein-linked serine or threonine residue (O-glycosylation site)	Lysosome
1708	157881	Tn_antigen(l)	Tn antigen	Lysosome
1709	115371	accoa(l)	Acetyl-CoA	Lysosome
1710	197391	acgagbside_hs(l)	alpha GalNAc globoside (homo sapiens)	Lysosome
1711	8991	acgal(l)	N-Acetyl-D-galactosamine	Lysosome
1712	2241	acgam(l)	N-Acetyl-D-glucosamine	Lysosome
1713	197401	acgbgbside_hs(l)	beta GalNAc globoside (homo sapiens)	Lysosome
1714	1341	acnam(l)	N-Acetylneuraminate	Lysosome
1715	2281	ade(l)	Adenine	Lysosome
1716	2701	adn(l)	Adenosine	Lysosome
1717	10931	ala-D(l)	D-Alanine	Lysosome
1718	114121	ala-L(l)	L-Alanine	Lysosome
1719	3091	amp(l)	AMP	Lysosome
1720	90191	cholp(l)	Choline phosphate	Lysosome
1721	2521	chsterol(l)	Cholesterol	Lysosome
1722	113761	cmp(l)	CMP	Lysosome
1723	4731	coa(l)	Coenzyme A	Lysosome
1724	157981	core6(l)	Core 6	Lysosome
1725	194781	crm_hs(l)	ceramide (homo sapiens)	Lysosome
1726	225081	cs_a(l)	chondroitin sulfate A (GalNAc4S-GlcA), free chain	Lysosome
1727	225071	cs_a_deg1(l)	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 1	Lysosome
1728	225131	cs_a_deg2(l)	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 2	Lysosome
1729	225141	cs_a_deg3(l)	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 3	Lysosome
1730	225151	cs_a_deg4(l)	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 4	Lysosome
1731	225161	cs_a_deg5(l)	chondroitin sulfate A (GalNAc4S-GlcA), degradation product 5	Lysosome
1732	225111	cs_b(l)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), free chain	Lysosome
1733	225171	cs_b_deg1(l)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 1	Lysosome
1734	225181	cs_b_deg2(l)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 2	Lysosome
1735	225191	cs_b_deg3(l)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S), degradation product 3	Lysosome
1736	225091	cs_c(l)	chondroitin sulfate C (GalNAc6S-GlcA), free chain	Lysosome
1737	225201	cs_c_deg1(l)	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 1	Lysosome
1738	225211	cs_c_deg2(l)	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 2	Lysosome
1739	225221	cs_c_deg3(l)	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 3	Lysosome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1740	225231	cs_c_deg4(l)	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 4	Lysosome
1741	225241	cs_c_deg5(l)	chondroitin sulfate C (GalNAc6S-GlcA), degradation product 5	Lysosome
1742	225101	cs_d(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), free chain	Lysosome
1743	225251	cs_d_deg1(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 1	Lysosome
1744	225261	cs_d_deg2(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 2	Lysosome
1745	225271	cs_d_deg3(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 3	Lysosome
1746	225281	cs_d_deg4(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 4	Lysosome
1747	225291	cs_d_deg5(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 5	Lysosome
1748	225301	cs_d_deg6(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S), degradation product 6	Lysosome
1749	225121	cs_e(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), free chain	Lysosome
1750	225321	cs_e_deg1(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 1	Lysosome
1751	225331	cs_e_deg2(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 2	Lysosome
1752	225341	cs_e_deg3(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 3	Lysosome
1753	225351	cs_e_deg4(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 4	Lysosome
1754	225361	cs_e_deg5(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 5	Lysosome
1755	225371	cs_e_deg6(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 6	Lysosome
1756	225381	cs_e_deg7(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA), degradation product 7	Lysosome
1757	205411	cspg_a(l)	chondroitin sulfate A (GalNAc4S-GlcA) proteoglycan	Lysosome
1758	205991	cspg_b(l)	chondroitin sulfate B / dermatan sulfate (IdoA2S-GalNAc4S) proteoglycan	Lysosome
1759	205451	cspg_c(l)	chondroitin sulfate C (GalNAc6S-GlcA) proteoglycan	Lysosome
1760	205541	cspg_d(l)	chondroitin sulfate D (GlcNAc6S-GlcA2S) proteoglycan	Lysosome
1761	205491	cspg_e(l)	chondroitin sulfate E (GalNAc4,6diS-GlcA) proteoglycan	Lysosome
1762	921	cytd(l)	Cytidine	Lysosome
1763	3801	dad-2(l)	Deoxyadenosine	Lysosome
1764	1931	damp(l)	dAMP	Lysosome
1765	2901	dcmp(l)	dCMP	Lysosome
1766	109181	dcyt(l)	Deoxycytidine	Lysosome
1767	1951	dgmp(l)	dGMP	Lysosome
1768	1721	dgsn(l)	Deoxyguanosine	Lysosome
1769	105051	dhf(l)	7,8-Dihydrofolate	Lysosome
1770	198101	digalside_hs(l)	Digalactosylceramide	Lysosome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1771	7371	dpcoa(l)	Dephospho-CoA	Lysosome
1772	1971	dtmp(l)	dTMP	Lysosome
1773	158851	f1a(l)	F1alpha	Lysosome
1774	3401	fald(l)	Formaldehyde	Lysosome
1775	8331	fuc-L(l)	L-Fucose	Lysosome
1776	10831	gal(l)	D-Galactose	Lysosome
1777	196191	galgluside_hs(l)	galactosyl glucosyl ceramide	Lysosome
1778	196141	galside_hs(l)	galactocerebroside (homo sapiens)	Lysosome
1779	196241	gbside_hs(l)	globoside (homo sapiens)	Lysosome
1780	3181	glc-D(l)	D-Glucose	Lysosome
1781	2561	glcur(l)	D-Glucuronate	Lysosome
1782	3131	glu-L(l)	L-Glutamate	Lysosome
1783	196131	gluside_hs(l)	glucocerebroside (homo sapiens)	Lysosome
1784	3231	gly(l)	Glycine	Lysosome
1785	2261	gmp(l)	GMP	Lysosome
1786	52791	gsn(l)	Guanosine	Lysosome
1787	10491	h(l)	H+	Lysosome
1788	3171	h2o(l)	H2O	Lysosome
1789	3151	h2o2(l)	Hydrogen peroxide	Lysosome
1790	95541	ha(l)	hyaluronan	Lysosome
1791	226111	ha_deg1(l)	hyaluronan degradation product 1	Lysosome
1792	226101	ha_pre1(l)	hyaluronan biosynthesis, precursor 1	Lysosome
1793	207961	hs(l)	heparan sulfate, free chain	Lysosome
1794	207551	hs_deg1(l)	heparan sulfate, degradation product 1	Lysosome
1795	207641	hs_deg10(l)	heparan sulfate, degradation product 10	Lysosome
1796	207651	hs_deg11(l)	heparan sulfate, degradation product 11	Lysosome
1797	207661	hs_deg12(l)	heparan sulfate, degradation product 12	Lysosome
1798	207671	hs_deg13(l)	heparan sulfate, degradation product 13	Lysosome
1799	207681	hs_deg14(l)	heparan sulfate, degradation product 14	Lysosome
1800	207691	hs_deg15(l)	heparan sulfate, degradation product 15	Lysosome
1801	207701	hs_deg16(l)	heparan sulfate, degradation product 16	Lysosome
1802	207711	hs_deg17(l)	heparan sulfate, degradation product 17	Lysosome
1803	207721	hs_deg18(l)	heparan sulfate, degradation product 18	Lysosome
1804	207731	hs_deg19(l)	heparan sulfate, degradation product 19	Lysosome
1805	207561	hs_deg2(l)	heparan sulfate, degradation product 2	Lysosome
1806	207741	hs_deg20(l)	heparan sulfate, degradation product 20	Lysosome
1807	207751	hs_deg21(l)	heparan sulfate, degradation product 21	Lysosome
1808	207761	hs_deg22(l)	heparan sulfate, degradation product 22	Lysosome
1809	207771	hs_deg23(l)	heparan sulfate, degradation product 23	Lysosome
1810	207951	hs_deg24(l)	heparan sulfate, degradation product 24	Lysosome
1811	207941	hs_deg25(l)	heparan sulfate, degradation product 25	Lysosome
1812	207571	hs_deg3(l)	heparan sulfate, degradation product 3	Lysosome
1813	207581	hs_deg4(l)	heparan sulfate, degradation product 4	Lysosome
1814	207591	hs_deg5(l)	heparan sulfate, degradation product 5	Lysosome
1815	207601	hs_deg6(l)	heparan sulfate, degradation product 6	Lysosome
1816	207611	hs_deg7(l)	heparan sulfate, degradation product 7	Lysosome
1817	207621	hs_deg8(l)	heparan sulfate, degradation product 8	Lysosome
1818	207631	hs_deg9(l)	heparan sulfate, degradation product 9	Lysosome
1819	206381	hspg(l)	heparan sulfate proteoglycan	Lysosome
1820	2181	hxan(l)	Hypoxanthine	Lysosome
1821	53921	idour(l)	L-Iduronate	Lysosome
1822	1471	ins(l)	Inosine	Lysosome
1823	201921	ksi(l)	keratan sulfate I	Lysosome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1824	225531	ksi_deg1(l)	keratan sulfate I, degradation product 1	Lysosome
1825	225621	ksi_deg10(l)	keratan sulfate I, degradation product 10	Lysosome
1826	225631	ksi_deg11(l)	keratan sulfate I, degradation product 11	Lysosome
1827	225641	ksi_deg12(l)	keratan sulfate I, degradation product 12	Lysosome
1828	225651	ksi_deg13(l)	keratan sulfate I, degradation product 13	Lysosome
1829	225661	ksi_deg14(l)	keratan sulfate I, degradation product 14	Lysosome
1830	225671	ksi_deg15(l)	keratan sulfate I, degradation product 15	Lysosome
1831	225751	ksi_deg16(l)	keratan sulfate I, degradation product 16	Lysosome
1832	225831	ksi_deg17(l)	keratan sulfate I, degradation product 17	Lysosome
1833	225681	ksi_deg18(l)	keratan sulfate I, degradation product 18	Lysosome
1834	225761	ksi_deg19(l)	keratan sulfate I, degradation product 19	Lysosome
1835	225541	ksi_deg2(l)	keratan sulfate I, degradation product 2	Lysosome
1836	225841	ksi_deg20(l)	keratan sulfate I, degradation product 20	Lysosome
1837	225691	ksi_deg21(l)	keratan sulfate I, degradation product 21	Lysosome
1838	225771	ksi_deg22(l)	keratan sulfate I, degradation product 22	Lysosome
1839	225851	ksi_deg23(l)	keratan sulfate I, degradation product 23	Lysosome
1840	225701	ksi_deg24(l)	keratan sulfate I, degradation product 24	Lysosome
1841	225781	ksi_deg25(l)	keratan sulfate I, degradation product 25	Lysosome
1842	225861	ksi_deg26(l)	keratan sulfate I, degradation product 26	Lysosome
1843	225711	ksi_deg27(l)	keratan sulfate I, degradation product 27	Lysosome
1844	225791	ksi_deg28(l)	keratan sulfate I, degradation product 28	Lysosome
1845	225871	ksi_deg29(l)	keratan sulfate I, degradation product 29	Lysosome
1846	225551	ksi_deg3(l)	keratan sulfate I, degradation product 3	Lysosome
1847	225721	ksi_deg30(l)	keratan sulfate I, degradation product 30	Lysosome
1848	225801	ksi_deg31(l)	keratan sulfate I, degradation product 31	Lysosome
1849	225881	ksi_deg32(l)	keratan sulfate I, degradation product 32	Lysosome
1850	225731	ksi_deg33(l)	keratan sulfate I, degradation product 33	Lysosome
1851	225811	ksi_deg34(l)	keratan sulfate I, degradation product 34	Lysosome
1852	225891	ksi_deg35(l)	keratan sulfate I, degradation product 35	Lysosome
1853	225741	ksi_deg36(l)	keratan sulfate I, degradation product 36	Lysosome
1854	225821	ksi_deg37(l)	keratan sulfate I, degradation product 37	Lysosome
1855	225901	ksi_deg38(l)	keratan sulfate I, degradation product 38	Lysosome
1856	225911	ksi_deg39(l)	keratan sulfate I, degradation product 39	Lysosome
1857	225561	ksi_deg4(l)	keratan sulfate I, degradation product 4	Lysosome
1858	225921	ksi_deg40(l)	keratan sulfate I, degradation product 40	Lysosome
1859	225931	ksi_deg41(l)	keratan sulfate I, degradation product 41	Lysosome
1860	225571	ksi_deg5(l)	keratan sulfate I, degradation product 5	Lysosome
1861	225581	ksi_deg6(l)	keratan sulfate I, degradation product 6	Lysosome
1862	225591	ksi_deg7(l)	keratan sulfate I, degradation product 7	Lysosome
1863	225601	ksi_deg8(l)	keratan sulfate I, degradation product 8	Lysosome
1864	225611	ksi_deg9(l)	keratan sulfate I, degradation product 9	Lysosome
1865	201561	ksii_core2(l)	keratan sulfate II (core 2-linked)	Lysosome
1866	225941	ksii_core2_deg1(l)	keratan sulfate II (core 2-linked), degradation product 1	Lysosome
1867	225951	ksii_core2_deg2(l)	keratan sulfate II (core 2-linked), degradation product 2	Lysosome
1868	225961	ksii_core2_deg3(l)	keratan sulfate II (core 2-linked), degradation product 3	Lysosome
1869	225971	ksii_core2_deg4(l)	keratan sulfate II (core 2-linked), degradation product 4	Lysosome
1870	225981	ksii_core2_deg5(l)	keratan sulfate II (core 2-linked), degradation product 5	Lysosome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1871	225991	ksii_core2_deg6(l)	keratan sulfate II (core 2-linked), degradation product 6	Lysosome
1872	226001	ksii_core2_deg7(l)	keratan sulfate II (core 2-linked), degradation product 7	Lysosome
1873	226011	ksii_core2_deg8(l)	keratan sulfate II (core 2-linked), degradation product 8	Lysosome
1874	226021	ksii_core2_deg9(l)	keratan sulfate II (core 2-linked), degradation product 9	Lysosome
1875	203421	ksii_core4(l)	keratan sulfate II (core 4-linked)	Lysosome
1876	226051	ksii_core4_deg1(l)	keratan sulfate II (core 4-linked), degradation product 1	Lysosome
1877	226061	ksii_core4_deg2(l)	keratan sulfate II (core 4-linked), degradation product 2	Lysosome
1878	226071	ksii_core4_deg3(l)	keratan sulfate II (core 4-linked), degradation product 3	Lysosome
1879	226081	ksii_core4_deg4(l)	keratan sulfate II (core 4-linked), degradation product 4	Lysosome
1880	156701	l2n2m2mn(l)	de-Fuc, reducing GlcNAc removed, de-Sia form of PA6 (w/o peptide linkage)	Lysosome
1881	2921	lcts(l)	Lactose	Lysosome
1882	156721	m2mn(l)	(alpha-D-mannosyl)2-beta-D-mannosyl-N-acetylglucosamine	Lysosome
1883	2671	malt(l)	Maltose	Lysosome
1884	12841	malttr(l)	Maltotriose	Lysosome
1885	110181	man(l)	D-Mannose	Lysosome
1886	10921	meoh(l)	Methanol	Lysosome
1887	156731	mn(l)	beta-1,4-mannose-N-acetylglucosamine	Lysosome
1888	156711	n2m2mn(l)	de-Fuc, reducing GlcNAc removed, de-Sia, de-Gal form of PA6 (w/o peptide linkage)	Lysosome
1889	156811	n2m2nm(l)	n2m2nmasn (w/o peptide linkage)	Lysosome
1890	36491	n2m2nmasn(l)	N-Acetyl-beta-D-glucosaminyl-1,2-alpha-D-mannosyl-1,3-(N-acetyl-beta-D-glucosaminyl-1,2-alpha-D-mannosyl-1,6)-(N-acetyl-beta-D-glucosaminyl-1,4)-beta-D-mannosyl-1,4-N-acetyl-beta-D-glucosaminyl-R	Lysosome
1891	156821	n2m2nmn(l)	reducing GlcNAc removed form of n2m2nmasn (w/o peptide)	Lysosome
1892	4721	pi(l)	Phosphate	Lysosome
1893	6291	pro-D(l)	D-Proline	Lysosome
1894	2291	pro-L(l)	L-Proline	Lysosome
1895	152071	s2l2fn2m2masn(l)	PA6	Lysosome
1896	156671	s2l2n2m2m(l)	de-Fuc form of PA6 (w/o peptide linkage)	Lysosome
1897	156651	s2l2n2m2masn(l)	de-Fuc form of PA6	Lysosome
1898	156691	s2l2n2m2mn(l)	de-Fuc, reducing GlcNAc removed form of PA6 (w/o peptide linkage)	Lysosome
1899	196151	sgalside_hs(l)	sulfatide galactocerebroside (homo sapiens)	Lysosome
1900	3351	so4(l)	Sulfate	Lysosome
1901	107031	sphings(l)	Sphingosine	Lysosome
1902	196181	sphmyln_hs(l)	sphingomyelin (homo sapiens)	Lysosome
1903	10651	thf(l)	5,6,7,8-Tetrahydrofolate	Lysosome
1904	52691	thymd(l)	Thymidine	Lysosome
1905	4771	udp(l)	UDP	Lysosome
1906	109121	udpacgal(l)	UDP-N-acetyl-D-galactosamine	Lysosome

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1907	1068l	ump(l)	UMP	Lysosome
1908	10727l	uri(l)	Uridine	Lysosome
1909	248l	xyl-D(l)	D-Xylose	Lysosome
1910	286m	10fthf(m)	10-Formyltetrahydrofolate	Mitochondria
1911	20786m	10fthf5glu(m)	10-formyltetrahydrofolate-[Glu](5)	Mitochondria
1912	20787m	10fthf6glu(m)	10-formyltetrahydrofolate-[Glu](6)	Mitochondria
1913	20788m	10fthf7glu(m)	10-formyltetrahydrofolate-[Glu](7)	Mitochondria
1914	3407m	11doctrsl(m)	11-Deoxycortisol	Mitochondria
1915	2404m	11doctrstrn(m)	11-Deoxycorticosterone	Mitochondria
1916	20075m	1a2425thvitd2(m)	1-alpha,24R,25-Trihydroxyvitamin D2	Mitochondria
1917	20076m	1a2425thvitd3(m)	1-alpha,24R,25-Trihydroxyvitamin D3	Mitochondria
1918	20018m	1a25dhvitd2(m)	1-alpha,25-Dihydroxyvitamin D2	Mitochondria
1919	20017m	1a25dhvitd3(m)	1-alpha,25-Dihydroxyvitamin D3	Mitochondria
1920	3261m	1p3h5c(m)	L-1-Pyrroline-3-hydroxy-5-carboxylate	Mitochondria
1921	2994m	1pyr5c(m)	1-Pyrroline-5-carboxylate	Mitochondria
1922	7532m	20ahchsterol(m)	20alpha-hydroxy cholesterol	Mitochondria
1923	20023m	2425dhvitd2(m)	24R,25-Dihydroxyvitamin D2	Mitochondria
1924	20024m	2425dhvitd3(m)	24R,25-Dihydroxyvitamin D3	Mitochondria
1925	20014m	25hvitd2(m)	25-Hydroxyvitamin D2	Mitochondria
1926	20012m	25hvitd3(m)	25-Hydroxyvitamin D3	Mitochondria
1927	2707m	2aobut(m)	L-2-Amino-3-oxobutanoate	Mitochondria
1928	19793m	2dp6mep(m)	2-Decaprenyl-6-methoxyphenol	Mitochondria
1929	19804m	2dp6mobq(m)	2-Decaprenyl-6-methoxy-1,4-benzoquinone	Mitochondria
1930	19805m	2dp6mobq_me(m)	2-Decaprenyl-3-methyl-6-methoxy-1,4-benzoquinone	Mitochondria
1931	19808m	2dpmhobq(m)	2-Decaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinone	Mitochondria
1932	2497m	2maacoa(m)	2-Methyl-3-acetoacetyl-CoA	Mitochondria
1933	2498m	2mb2coa(m)	trans-2-Methylbut-2-enoyl-CoA	Mitochondria
1934	844m	2mbcoa(m)	2-Methylbutanoyl-CoA	Mitochondria
1935	186m	2mop(m)	2-Methyl-3-oxopropanoate	Mitochondria
1936	2388m	2mp2coa(m)	2-Methylprop-2-enoyl-CoA	Mitochondria
1937	9002m	2oxoadp(m)	2-Oxoadipate	Mitochondria
1938	22485m	34hpl(m)	3-(4-Hydroxyphenyl)lactate	Mitochondria
1939	772m	34hpp(m)	3-(4-Hydroxyphenyl)pyruvate	Mitochondria
1940	2457m	3aib(m)	L-3-Amino-isobutanoate	Mitochondria
1941	2444m	3aib-D(m)	D-3-Amino-isobutanoate	Mitochondria
1942	19791m	3dpdhh(m)	3-Decaprenyl-4,5-dihydroxybenzoate	Mitochondria
1943	19792m	3dpdhh_me(m)	3-Decaprenyl-4-hydroxy-5-methoxybenzoate	Mitochondria
1944	19772m	3dphb(m)	3-Decaprenyl-4-hydroxybenzoate	Mitochondria
1945	19703m	3h26dm5coa(m)	3-Hydroxy-2,6-dimethyl-5-methylene-heptanoyl-CoA	Mitochondria
1946	905m	3hbcoa(m)	(S)-3-Hydroxybutanoyl-CoA	Mitochondria
1947	2736m	3hbcoa-R(m)	(R)-3-Hydroxybutanoyl-CoA	Mitochondria
1948	4444m	3hibutcoa(m)	(S)-3-Hydroxyisobutyryl-CoA	Mitochondria
1949	3162m	3hmbcoa(m)	(S)-3-Hydroxy-2-methylbutyryl-CoA	Mitochondria
1950	779m	3hmp(m)	3-Hydroxy-2-methylpropanoate	Mitochondria
1951	4184m	3hpcoa(m)	3-Hydroxypropionyl-CoA	Mitochondria
1952	7135m	3htmelys(m)	3-Hydroxy-N6,N6,N6-trimethyl-L-lysine	Mitochondria
1953	2308m	3mb2coa(m)	3-Methylbut-2-enoyl-CoA	Mitochondria
1954	2423m	3mgcoa(m)	3-Methylglutaconyl-CoA	Mitochondria
1955	225m	3mob(m)	3-Methyl-2-oxobutanoate	Mitochondria
1956	445m	3mop(m)	(S)-3-Methyl-2-oxopentanoate	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
1957	1105m	3sala(m)	3-Sulfino-L-alanine	Mitochondria
1958	3427m	3snpyr(m)	3-Sulfino-pyruvate	Mitochondria
1959	15766m	3spyr(m)	3-Sulfopyruvate	Mitochondria
1960	7924m	4aabutn(m)	4-Acetamidobutanoate	Mitochondria
1961	176m	4abut(m)	4-Aminobutanoate	Mitochondria
1962	896m	4h2oglt(m)	4-Hydroxy-2-oxoglutarate	Mitochondria
1963	234m	4hbz(m)	4-Hydroxybenzoate	Mitochondria
1964	22487m	4hbzcoa(m)	4-hydroxybenoyl-CoA	Mitochondria
1965	8300m	4hglusa(m)	L-4-Hydroxyglutamate semialdehyde	Mitochondria
1966	913m	4hpro-LT(m)	trans-4-Hydroxy-L-proline	Mitochondria
1967	285m	4mop(m)	4-Methyl-2-oxopentanoate	Mitochondria
1968	1711m	4mptnl(m)	4-Methylpentanal	Mitochondria
1969	2022m	4ppan(m)	D-4'-Phosphopantothenate	Mitochondria
1970	908m	4tmeabut(m)	4-Trimethylammonio-butanal	Mitochondria
1971	424m	5aop(m)	5-Amino-4-oxopentanoate	Mitochondria
1972	20783m	5dhf(m)	pentaglutamyl folate (DHF)	Mitochondria
1973	4155m	5hoxindact(m)	5-Hydroxyindoleacetaldehyde	Mitochondria
1974	11161m	5hoxindoa(m)	5-Hydroxyindoleacetate	Mitochondria
1975	20780m	5thf(m)	pentaglutamyl folate (THF)	Mitochondria
1976	20784m	6dhf(m)	hexaglutamyl folate (DHF)	Mitochondria
1977	20781m	6thf(m)	hexaglutamyl folate (THF)	Mitochondria
1978	20785m	7dhf(m)	heptaglutamyl folate (DHF)	Mitochondria
1979	20782m	7thf(m)	heptaglutamyl folate (THF)	Mitochondria
1980	69m	ACP(m)	acyl carrier protein	Mitochondria
1981	9011m	L2aadp(m)	L-2-Amino adipate	Mitochondria
1982	7588m	L2aadp6sa(m)	L-2-Amino adipate 6-semialdehyde	Mitochondria
1983	120m	Lcyst(m)	L-Cysteate	Mitochondria
1984	679m	Nacasp(m)	N-Acetyl-L-aspartate	Mitochondria
1985	22166m	Rtotal2coa(m)	R total 2 coenzyme A	Mitochondria
1986	22470m	Rtotal2crn(m)	R total 2 carnitine	Mitochondria
1987	22167m	Rtotal3coa(m)	R total 3 Coenzyme A	Mitochondria
1988	22471m	Rtotal3crn(m)	R total 3 carnitine	Mitochondria
1989	22165m	Rtotalcoa(m)	R total Coenzyme A	Mitochondria
1990	22469m	Rtotalcrn(m)	R total carnitine	Mitochondria
1991	656m	T4hcinnm(m)	trans-4-Hydroxycinnamate	Mitochondria
1992	174m	aacoa(m)	Acetoacetyl-CoA	Mitochondria
1993	1533m	aact(m)	Aminoacetone	Mitochondria
1994	319m	ac(m)	Acetate	Mitochondria
1995	9016m	acac(m)	Acetoacetate	Mitochondria
1996	1052m	acald(m)	Acetaldehyde	Mitochondria
1997	11537m	accoa(m)	Acetyl-CoA	Mitochondria
1998	266m	acetone(m)	Acetone	Mitochondria
1999	2957m	acg5p(m)	N-Acetyl-L-glutamyl 5-phosphate	Mitochondria
2000	975m	acg5sa(m)	N-Acetyl-L-glutamate 5-semialdehyde	Mitochondria
2001	1115m	acglu(m)	N-Acetyl-L-glutamate	Mitochondria
2002	7471m	acrn(m)	O-Acetylcarnitine	Mitochondria
2003	270m	adn(m)	Adenosine	Mitochondria
2004	10925m	adocbl(m)	Adenosylcobalamin	Mitochondria
2005	471m	adp(m)	ADP	Mitochondria
2006	151m	adprib(m)	ADPribose	Mitochondria
2007	18484m	adrncoa(m)	adrenyl coenzyme A	Mitochondria
2008	25984m	adrncrn(m)	Adrenyl carnitine	Mitochondria
2009	247m	agm(m)	Agmatine	Mitochondria

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2010	310m	ahcys(m)	S-Adenosyl-L-homocysteine	Mitochondria
2011	314m	akg(m)	2-Oxoglutarate	Mitochondria
2012	1063m	ala-B(m)	beta-Alanine	Mitochondria
2013	11412m	ala-L(m)	L-Alanine	Mitochondria
2014	1447m	aldstrn(m)	Aldosterone	Mitochondria
2015	18535m	alpa_hs(m)	lysophosphatidic acid (homo sapiens)	Mitochondria
2016	7690m	alpam(m)	S-aminomethylidihydroipoamide	Mitochondria
2017	10354m	alpro(m)	S-Aminomethylidihydroipoylprotein	Mitochondria
2018	1086m	amet(m)	S-Adenosyl-L-methionine	Mitochondria
2019	309m	amp(m)	AMP	Mitochondria
2020	22737m	apoC(m)	Apocboxylase (no lys residue)	Mitochondria
2021	22735m	apoC-Lys(m)	Apocboxylase (Lys residue)	Mitochondria
2022	22736m	apoC-Lys_btn(m)	Holocarboxylase (biotin covalent bound to Lys residue of apoC)	Mitochondria
2023	18483m	arachcoa(m)	arachidyl coenzyme A	Mitochondria
2024	25967m	arachcrn(m)	arachidyl carnitine	Mitochondria
2025	11887m	arachdcoa(m)	C20:4-CoA	Mitochondria
2026	11889m	arachdcrn(m)	C20:4 carnitine	Mitochondria
2027	337m	arg-L(m)	L-Arginine	Mitochondria
2028	232m	asn-L(m)	L-Asparagine	Mitochondria
2029	330m	asp-L(m)	L-Aspartate	Mitochondria
2030	465m	atp(m)	ATP	Mitochondria
2031	733m	b2coa(m)	Crotonoyl-CoA	Mitochondria
2032	4182m	bamppald(m)	beta-Aminopropion aldehyde	Mitochondria
2033	392m	betald(m)	Betaine aldehyde	Mitochondria
2034	870m	bhb(m)	(R)-3-Hydroxybutanoate	Mitochondria
2035	4297m	biocyt(m)	Biocytin	Mitochondria
2036	4584m	btamp(m)	Biotinyl-5'-AMP	Mitochondria
2037	222m	btcoa(m)	Butanoyl-CoA	Mitochondria
2038	1079m	btn(m)	Biotin	Mitochondria
2039	294m	but(m)	Butyrate (n-C4:0)	Mitochondria
2040	11888m	c226coa(m)	cervonyl coenzyme A	Mitochondria
2041	11883m	c226crn(m)	cervonyl carnitine	Mitochondria
2042	19701m	c2m26dcoa(m)	cis-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA	Mitochondria
2043	10988m	cbl1(m)	Cob(I)alamin	Mitochondria
2044	365m	cbl2(m)	Cob(II)alamin	Mitochondria
2045	11004m	cbp(m)	Carbamoyl phosphate	Mitochondria
2046	20077m	cca_d3(m)	Calcitroic acid (D3)	Mitochondria
2047	1073m	cdp(m)	CDP	Mitochondria
2048	19105m	cdpdag_hs(m)	CDP diacylglycerol (homo sapiens)	Mitochondria
2049	1075m	chol(m)	Choline	Mitochondria
2050	252m	chsterol(m)	Cholesterol	Mitochondria
2051	236m	cit(m)	Citrate	Mitochondria
2052	828m	citmcoa-L(m)	L-Citramalyl-CoA	Mitochondria
2053	169m	citr-L(m)	L-Citrulline	Mitochondria
2054	18488m	clpndcoa(m)	clupanodonyl CoA	Mitochondria
2055	25990m	clpndcrn(m)	clupanodonyl carnitine	Mitochondria
2056	11376m	cmp(m)	CMP	Mitochondria
2057	474m	co2(m)	CO2	Mitochondria
2058	473m	coa(m)	Coenzyme A	Mitochondria
2059	22486m	coucoa(m)	p-coumaroyl-CoA	Mitochondria
2060	150m	creat(m)	Creatine	Mitochondria
2061	163m	crn(m)	L-Carnitine	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2062	11268m	crtsl(m)	Cortisol	Mitochondria
2063	1737m	crtstrn(m)	Corticosterone	Mitochondria
2064	338m	ctp(m)	CTP	Mitochondria
2065	245m	cyan(m)	Hydrogen cyanide	Mitochondria
2066	1062m	cys-L(m)	L-Cysteine	Mitochondria
2067	92m	cytd(m)	Cytidine	Mitochondria
2068	265m	dadp(m)	dADP	Mitochondria
2069	1091m	datp(m)	dATP	Mitochondria
2070	5272m	dcdp(m)	dCDP	Mitochondria
2071	290m	dcmp(m)	dCMP	Mitochondria
2072	18487m	dcsptnlcoa(m)	docosa-4,7,10,13,16-pentaenoyl coenzyme A	Mitochondria
2073	25989m	dcsptnlcrn(m)	docosa-4,7,10,13,16-pentaenoyl carnitine	Mitochondria
2074	78m	dctp(m)	dCTP	Mitochondria
2075	10918m	dcyt(m)	Deoxycytidine	Mitochondria
2076	2416m	dd2coa(m)	trans-Dodec-2-enoyl-CoA	Mitochondria
2077	12055m	dd3coa(m)	3-dodecenoyl CoA	Mitochondria
2078	12883m	decdp(m)	all trans Decaprenyl diphosphate	Mitochondria
2079	194m	dgdpm(m)	dGDP	Mitochondria
2080	195m	dgm(m)	dGMP	Mitochondria
2081	172m	dgsn(m)	Deoxyguanosine	Mitochondria
2082	143m	dgt(m)	dGTP	Mitochondria
2083	3997m	dhcholestanate(m)	3alpha,7alpha-Dihydroxy-5beta-cholestanate	Mitochondria
2084	10505m	dhf(m)	7,8-Dihydrofolate	Mitochondria
2085	394m	dhlam(m)	Dihydrolipoamide	Mitochondria
2086	56m	dhlpro(m)	Dihydrolipolprotein	Mitochondria
2087	1032m	didp(m)	dIDP	Mitochondria
2088	1033m	ditp(m)	dITP	Mitochondria
2089	18491m	dlnlcgcoa(m)	dihomo-gamma-linolenyl coenzyme A	Mitochondria
2090	25979m	dlnlcgcrn(m)	dihomo-gamma-linolenyl carnitine	Mitochondria
2091	840m	dmgly(m)	N,N-Dimethylglycine	Mitochondria
2092	21977m	dnhptcoa(m)	2,6 dimethylheptanoyl-CoA	Mitochondria
2093	26488m	dnhptcrn(m)	2,6 dimethylheptanoyl carnitine	Mitochondria
2094	21959m	dmnoncoa(m)	4,8 dimethylnonanoyl-CoA	Mitochondria
2095	21976m	dmnoncrn(m)	4,8 dimethylnonanoyl carnitine	Mitochondria
2096	724m	dnad(m)	Deamino-NAD+	Mitochondria
2097	196m	dtdp(m)	dTDP	Mitochondria
2098	197m	dtmp(m)	dTMP	Mitochondria
2099	79m	dttp(m)	dTTP	Mitochondria
2100	1034m	dudp(m)	dUDP	Mitochondria
2101	198m	dump(m)	dUMP	Mitochondria
2102	355m	duri(m)	Deoxyuridine	Mitochondria
2103	80m	dutp(m)	dUTP	Mitochondria
2104	8301m	e4hglu(m)	L-erythro-4-Hydroxyglutamate	Mitochondria
2105	18507m	eicosetcoa(m)	eicosatetranoyl coenzyme A	Mitochondria
2106	25980m	eicosetcrn(m)	Eicosatetranoyl carnitine	Mitochondria
2107	25972m	elaidcrn(m)	Elaidic carnitine	Mitochondria
2108	20557m	etfox(m)	Electron transfer flavoprotein oxidized	Mitochondria
2109	20558m	etfrd(m)	Electron transfer flavoprotein reduced	Mitochondria
2110	478m	fad(m)	Flavin adenine dinucleotide oxidized	Mitochondria
2111	42m	fadh2(m)	Flavin adenine dinucleotide reduced	Mitochondria
2112	340m	fald(m)	Formaldehyde	Mitochondria
2113	312m	fe2(m)	Fe2+	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2114	10041m	ficytC(m)	Ferricytochrome c	Mitochondria
2115	1084m	ficytc(m)	Ferricytochrome c	Mitochondria
2116	10042m	foeytC(m)	Ferrocyclochrome C	Mitochondria
2117	1085m	foeytc(m)	Ferrocyclochrome c	Mitochondria
2118	334m	for(m)	Formate	Mitochondria
2119	1081m	fum(m)	Fumarate	Mitochondria
2120	10800m	gcald(m)	Glycolaldehyde	Mitochondria
2121	321m	gdp(m)	GDP	Mitochondria
2122	18308m	glac(m)	D-glucurono-6,3-lactone	Mitochondria
2123	632m	glcr(m)	D-Glucarate	Mitochondria
2124	661m	gln-D(m)	D-Glutamine	Mitochondria
2125	11299m	gln-L(m)	L-Glutamine	Mitochondria
2126	273m	glu-D(m)	D-Glutamate	Mitochondria
2127	313m	glu-L(m)	L-Glutamate	Mitochondria
2128	2458m	glu5p(m)	L-Glutamate 5-phosphate	Mitochondria
2129	761m	glu5sa(m)	L-Glutamate 5-semialdehyde	Mitochondria
2130	356m	glutcoa(m)	Glutaryl-CoA	Mitochondria
2131	329m	glx(m)	Glyoxylate	Mitochondria
2132	323m	gly(m)	Glycine	Mitochondria
2133	503m	glyb(m)	Glycine betaine	Mitochondria
2134	1077m	glyc(m)	Glycerol	Mitochondria
2135	55m	glyc3p(m)	Glycerol 3-phosphate	Mitochondria
2136	237m	glyclt(m)	Glycolate	Mitochondria
2137	226m	gmp(m)	GMP	Mitochondria
2138	5279m	gsn(m)	Guanosine	Mitochondria
2139	1087m	gthox(m)	Oxidized glutathione	Mitochondria
2140	11388m	gthrd(m)	Reduced glutathione	Mitochondria
2141	327m	gtp(m)	GTP	Mitochondria
2142	1049m	h(m)	H+	Mitochondria
2143	3m	h2co3(m)	carbonic acid	Mitochondria
2144	317m	h2o(m)	H2O	Mitochondria
2145	315m	h2o2(m)	Hydrogen peroxide	Mitochondria
2146	144m	hco3(m)	Bicarbonate	Mitochondria
2147	21857m	hdcecrn(m)	Hexadecenoyl carnitine	Mitochondria
2148	8780m	hdcoa(m)	Hexadecenoyl-CoA (n-C16:1CoA)	Mitochondria
2149	3801m	hdd2coa(m)	trans-Hexadec-2-enoyl-CoA	Mitochondria
2150	26402m	hdd2crn(m)	trans-Hexadec-2-enoyl carnitine	Mitochondria
2151	11013m	hexccoa(m)	Hexacosanoyl-CoA (n-C26:0CoA)	Mitochondria
2152	25969m	hexccrn(m)	hexacosanoyl carnitine	Mitochondria
2153	191m	hmgcoa(m)	Hydroxymethylglutaryl-CoA	Mitochondria
2154	22502m	hpdccoa(m)	heptadecanoyl coa	Mitochondria
2155	22758m	hpdccrn(m)	heptadecanoyl carnitine	Mitochondria
2156	242m	hpyr(m)	Hydroxypyruvate	Mitochondria
2157	1119m	ibcoa(m)	Isobutyryl-CoA	Mitochondria
2158	158m	icit(m)	Isocitrate	Mitochondria
2159	1125m	id3acald(m)	Indole-3-acetaldehyde	Mitochondria
2160	1067m	idp(m)	IDP	Mitochondria
2161	410m	ile-L(m)	L-Isoleucine	Mitochondria
2162	2132m	im4ac(m)	Imidazole-4-acetate	Mitochondria
2163	3706m	im4act(m)	Imidazole-4-acetaldehyde	Mitochondria
2164	1090m	imp(m)	IMP	Mitochondria
2165	9022m	ind3ac(m)	Indole-3-acetate	Mitochondria
2166	147m	ins(m)	Inosine	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2167	359m	itaccoa(m)	Itaconyl-CoA	Mitochondria
2168	104m	itacon(m)	Itaconate	Mitochondria
2169	1050m	itp(m)	ITP	Mitochondria
2170	1908m	ivcoa(m)	Isovaleryl-CoA	Mitochondria
2171	304m	lac-D(m)	D-Lactate	Mitochondria
2172	10931m	lac-L(m)	L-Lactate	Mitochondria
2173	491m	lald-D(m)	D-Lactaldehyde	Mitochondria
2174	420m	lald-L(m)	L-Lactaldehyde	Mitochondria
2175	1082m	leu-L(m)	L-Leucine	Mitochondria
2176	18490m	lgncco(m)	lignoceryyl coenzyme A	Mitochondria
2177	25968m	lgnccrn(m)	lignoceryl carnitine	Mitochondria
2178	2477m	lgt-S(m)	(R)-S-Lactoylglutathione	Mitochondria
2179	18482m	lnelcco(m)	linoelaidyl coenzyme A	Mitochondria
2180	25975m	lnelccrn(m)	Linoelaidyl carnitine	Mitochondria
2181	18481m	lnlcco(m)	linoleic coenzyme A	Mitochondria
2182	25976m	lnlccrn(m)	Linoleyl carnitine	Mitochondria
2183	18480m	lnlncco(m)	alpha-Linolenoyl-CoA	Mitochondria
2184	25978m	lnlnccrn(m)	alpha-linolenyl carnitine	Mitochondria
2185	2277m	lnlncgco(m)	gamma-linolenoyl-CoA	Mitochondria
2186	25977m	lnlncgcrn(m)	gamma-linolenyl carnitine	Mitochondria
2187	296m	lpam(m)	Lipoamide	Mitochondria
2188	1657m	lpro(m)	Lipoylprotein	Mitochondria
2189	328m	lys-L(m)	L-Lysine	Mitochondria
2190	230m	mal-L(m)	L-Malate	Mitochondria
2191	50m	malACP(m)	Malonyl-[acyl-carrier protein]	Mitochondria
2192	11267m	malco(m)	Malonyl-CoA	Mitochondria
2193	794m	mercppy(m)	Mercaptopyruvate	Mitochondria
2194	4468m	mesco(m)	Mesaconyl-CoA	Mitochondria
2195	1409m	mescon(m)	Mesaconate	Mitochondria
2196	433m	methf(m)	5,10-Methenyltetrahydrofolate	Mitochondria
2197	11043m	mlthf(m)	5,10-Methylenetetrahydrofolate	Mitochondria
2198	943m	mmcoa-R(m)	(R)-Methylmalonyl-CoA	Mitochondria
2199	451m	mmcoa-S(m)	(S)-Methylmalonyl-CoA	Mitochondria
2200	277m	msa(m)	Malonate semialdehyde	Mitochondria
2201	7923m	n4abutn(m)	N4-Acetylaminobutanal	Mitochondria
2202	466m	nad(m)	Nicotinamide adenine dinucleotide	Mitochondria
2203	467m	nadh(m)	Nicotinamide adenine dinucleotide - reduced	Mitochondria
2204	469m	nadp(m)	Nicotinamide adenine dinucleotide phosphate	Mitochondria
2205	468m	nadph(m)	Nicotinamide adenine dinucleotide phosphate - reduced	Mitochondria
2206	476m	nh4(m)	Ammonium	Mitochondria
2207	776m	nicrnt(m)	Nicotinate D-ribonucleotide	Mitochondria
2208	77m	nmn(m)	NMN	Mitochondria
2209	18485m	nrvncco(m)	nervonyl coenzyme A	Mitochondria
2210	25974m	nrvnccrn(m)	Nervonyl carnitine	Mitochondria
2211	470m	o2(m)	O2	Mitochondria
2212	461m	o2s(m)	Superoxide anion	Mitochondria
2213	322m	oaa(m)	Oxaloacetate	Mitochondria
2214	10688m	occoa(m)	Octanoyl-CoA (n-C8:0CoA)	Mitochondria
2215	8401m	od2coa(m)	trans-Octadec-2-enoyl-CoA	Mitochondria
2216	8782m	odecoa(m)	Octadecenoyl-CoA (n-C18:1CoA)	Mitochondria
2217	11885m	odecrn(m)	octadecenoyl carnitine	Mitochondria
2218	1021m	ohl(m)	hydroxide ion	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2219	1304m	orn(m)	Ornithine	Mitochondria
2220	18536m	pa_hs(m)	phosphatidic acid (homo sapiens)	Mitochondria
2221	19051m	pchol_hs(m)	Phosphatidylcholine (homo sapiens)	Mitochondria
2222	10038m	pcreat(m)	Phosphocreatine	Mitochondria
2223	15675m	pcrn(m)	propionyl-carnitine	Mitochondria
2224	19050m	pe_hs(m)	phosphatidylethanolamine (homo sapiens)	Mitochondria
2225	344m	pep(m)	Phosphoenolpyruvate	Mitochondria
2226	19700m	peracd(m)	Perillic acid	Mitochondria
2227	1048m	phe-L(m)	L-Phenylalanine	Mitochondria
2228	11520m	pHEME(m)	Protoheme	Mitochondria
2229	240m	phpyr(m)	Phenylpyruvate	Mitochondria
2230	472m	pi(m)	Phosphate	Mitochondria
2231	11029m	pmtcoa(m)	Palmitoyl-CoA (n-C16:0CoA)	Mitochondria
2232	2244m	pmtcrn(m)	L-Palmitoylcarnitine	Mitochondria
2233	10928m	pnto-R(m)	(R)-Pantothenate	Mitochondria
2234	238m	ppa(m)	Propionate (n-C3:0)	Mitochondria
2235	1064m	ppcoa(m)	Propanoyl-CoA	Mitochondria
2236	475m	ppi(m)	Diphosphate	Mitochondria
2237	1772m	ppp9(m)	Protoporphyrin	Mitochondria
2238	864m	pppg9(m)	Protoporphyrinogen IX	Mitochondria
2239	2452m	pppi(m)	Inorganic triphosphate	Mitochondria
2240	10681m	prgnlone(m)	Pregnenolone	Mitochondria
2241	229m	pro-L(m)	L-Proline	Mitochondria
2242	744m	prpcoa(m)	Propenoyl-CoA	Mitochondria
2243	19052m	ps_hs(m)	phosphatidylserine (homo sapiens)	Mitochondria
2244	22500m	ptdcacoa(m)	pentadecanoyl Coenzyme A	Mitochondria
2245	22757m	ptdcacr(m)	pentadecenoyl carnitine	Mitochondria
2246	1094m	ptrc(m)	Putrescine	Mitochondria
2247	1130m	pyam5p(m)	Pyridoxamine 5'-phosphate	Mitochondria
2248	479m	pydx5p(m)	Pyridoxal 5'-phosphate	Mitochondria
2249	1851m	pylald(m)	Perillyl aldehyde	Mitochondria
2250	311m	pyr(m)	Pyruvate	Mitochondria
2251	406m	q10(m)	Ubiquinone-10	Mitochondria
2252	11879m	q10h2(m)	Ubiquinol-10	Mitochondria
2253	1999m	r5p(m)	alpha-D-Ribose 5-phosphate	Mitochondria
2254	8994m	sacrcp-L(m)	L-Saccharopine	Mitochondria
2255	271m	sarcs(m)	Sarcosine	Mitochondria
2256	339m	ser-L(m)	L-Serine	Mitochondria
2257	15786m	sl-L(m)	L-sulfolactate	Mitochondria
2258	1060m	so3(m)	Sulfite	Mitochondria
2259	335m	so4(m)	Sulfate	Mitochondria
2260	8781m	stcoa(m)	Stearoyl-CoA (n-C18:0CoA)	Mitochondria
2261	11884m	stcrn(m)	stearoylcarnitine	Mitochondria
2262	18492m	strdncco(m)	stearidonyl coenzyme A	Mitochondria
2263	25985m	strdnccrn(m)	stearidonyl carnitine	Mitochondria
2264	325m	succ(m)	Succinate	Mitochondria
2265	1058m	succoa(m)	Succinyl-CoA	Mitochondria
2266	284m	sucsal(m)	Succinic semialdehyde	Mitochondria
2267	19702m	t2m26dcoa(m)	trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA	Mitochondria
2268	1428m	tcynt(m)	Thiocyanate	Mitochondria
2269	1862m	tdcoa(m)	Tetradecanoyl-CoA (n-C14:0CoA)	Mitochondria
2270	18513m	tetpent3coa(m)	tetracosapentaenoyl coenzyme A, n-3	Mitochondria
2271	25991m	tetpent3crn(m)	tetracosapentaenoyl carnitine	Mitochondria

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2272	18509m	tetpent6coa(m)	tetracosapentaenoyl coenzyme A, n-6	Mitochondria
2273	25992m	tetpent6crn(m)	tetracosapentaenoyl carnitine	Mitochondria
2274	18511m	tettet6coa(m)	tetracosatetraenoyl coenzyme A	Mitochondria
2275	25986m	tettet6crn(m)	Tetracosatetraenoyl carnitine	Mitochondria
2276	852m	thcholst(m)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestan-26-al	Mitochondria
2277	3477m	thcholstoic(m)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	Mitochondria
2278	1065m	thf(m)	5,6,7,8-Tetrahydrofolate	Mitochondria
2279	210m	thm(m)	Thiamin	Mitochondria
2280	866m	thmmp(m)	Thiamin monophosphate	Mitochondria
2281	341m	thmpp(m)	Thiamine diphosphate	Mitochondria
2282	5269m	thymd(m)	Thymidine	Mitochondria
2283	18486m	tmndnccoa(m)	timnodonyl coenzyme A	Mitochondria
2284	25988m	tmndnccrn(m)	Timnodonyl carnitine	Mitochondria
2285	181m	trdox(m)	Oxidized thioredoxin	Mitochondria
2286	180m	trdrd(m)	Reduced thioredoxin	Mitochondria
2287	164m	tsul(m)	Thiosulfate	Mitochondria
2288	26814m	ttocrn(m)	tetradecanoyl carnitine	Mitochondria
2289	1051m	tyr-L(m)	L-Tyrosine	Mitochondria
2290	477m	udp(m)	UDP	Mitochondria
2291	1068m	ump(m)	UMP	Mitochondria
2292	1054m	urea(m)	Urea	Mitochondria
2293	10727m	uri(m)	Uridine	Mitochondria
2294	345m	utp(m)	UTP	Mitochondria
2295	18479m	vacccoa(m)	vaccenyl coenzyme A	Mitochondria
2296	25973m	vaccrn(m)	Vaccenyl carnitine	Mitochondria
2297	250m	val-L(m)	L-Valine	Mitochondria
2298	20013m	vitd2(m)	Vitamin D2	Mitochondria
2299	20001m	vitd3(m)	Vitamin D3	Mitochondria
2300	4060m	xol27oh(m)	27-Hydroxycholesterol	Mitochondria
2301	3381m	xol7ah2(m)	3alpha,7alpha-Dihydroxy-5beta-cholestane	Mitochondria
2302	3375m	xol7ah2al(m)	3alpha,7alpha-Dihydroxy-5beta-cholestan-26-al	Mitochondria
2303	3374m	xol7ah3(m)	3alpha,7alpha,26-Trihydroxy-5beta-cholestane	Mitochondria
2304	3384m	xoldiolone(m)	7alpha,12alpha-Dihydroxycholest-4-en-3-one	Mitochondria
2305	3379m	xoltetrol(m)	3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane	Mitochondria
2306	3383m	xoltriol(m)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	Mitochondria
2307	22815n	13-cis-oretn(n)	13-cis-oxo-retinoic acid	Nucleus
2308	22814n	13-cis-retn(n)	13-cis-retinoate	Nucleus
2309	9005n	35cgm(n)	3',5'-Cyclic GMP	Nucleus
2310	11000n	6p(h)(n)	6-Pyruvoyl-5,6,7,8-tetrahydropterin	Nucleus
2311	4292n	Ndmelys(n)	Protein N6,N6-dimethyl-L-lysine	Nucleus
2312	10936n	Nmelys(n)	Histone N6-methyl-L-lysine	Nucleus
2313	4293n	Ntmelys(n)	Protein N6,N6,N6-trimethyl-L-lysine	Nucleus
2314	11537n	accoa(n)	Acetyl-CoA	Nucleus
2315	1617n	ach(n)	Acetylcholine	Nucleus
2316	134n	acnam(n)	N-Acetylneuraminic acid	Nucleus
2317	471n	adp(n)	ADP	Nucleus
2318	310n	ahcys(n)	S-Adenosyl-L-homocysteine	Nucleus
2319	3611n	ahdt(n)	2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl) dihydropteridine triphosphate	Nucleus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2320	1086n	amet(n)	S-Adenosyl-L-methionine	Nucleus
2321	465n	atp(n)	ATP	Nucleus
2322	4297n	biocyt(n)	Biocytin	Nucleus
2323	1079n	btn(n)	Biotin	Nucleus
2324	1073n	cdp(n)	CDP	Nucleus
2325	1075n	chol(n)	Choline	Nucleus
2326	11376n	cmp(n)	CMP	Nucleus
2327	1088n	cmpacna(n)	CMP-N-acetylneuramate	Nucleus
2328	474n	co2(n)	CO2	Nucleus
2329	473n	coa(n)	Coenzyme A	Nucleus
2330	338n	ctp(n)	CTP	Nucleus
2331	92n	cytd(n)	Cytidine	Nucleus
2332	265n	dadp(n)	dADP	Nucleus
2333	18537n	dag_hs(n)	diacylglycerol (homo sapiens)	Nucleus
2334	1091n	datp(n)	dATP	Nucleus
2335	5272n	dcdp(n)	dCDP	Nucleus
2336	290n	dcmp(n)	dCMP	Nucleus
2337	78n	dctp(n)	dCTP	Nucleus
2338	10918n	dcyt(n)	Deoxycytidine	Nucleus
2339	194n	dgdp(n)	dGDP	Nucleus
2340	143n	dgtp(n)	dGTP	Nucleus
2341	1032n	didp(n)	dIDP	Nucleus
2342	1033n	ditp(n)	dITP	Nucleus
2343	18424n	dna(n)	DNA	Nucleus
2344	18425n	dna5mtc(n)	DNA 5-methylcytosine	Nucleus
2345	724n	dnad(n)	Deamino-NAD+	Nucleus
2346	196n	dtdp(n)	dTDP	Nucleus
2347	79n	dttp(n)	dTTP	Nucleus
2348	1034n	dudp(n)	dUDP	Nucleus
2349	198n	dump(n)	dUMP	Nucleus
2350	355n	duri(n)	Deoxyuridine	Nucleus
2351	80n	dutp(n)	dUTP	Nucleus
2352	334n	for(n)	Formate	Nucleus
2353	321n	gdp(n)	GDP	Nucleus
2354	226n	gmp(n)	GMP	Nucleus
2355	327n	gtp(n)	GTP	Nucleus
2356	1049n	h(n)	H+	Nucleus
2357	317n	h2o(n)	H2O	Nucleus
2358	315n	h2o2(n)	Hydrogen peroxide	Nucleus
2359	20388n	hretn(n)	4 hydroxy retinoic acid	Nucleus
2360	1067n	idp(n)	IDP	Nucleus
2361	1050n	itp(n)	ITP	Nucleus
2362	328n	lys-L(n)	L-Lysine	Nucleus
2363	996n	mi13456p(n)	1D-myo-Inositol 1,3,4,5,6-pentakisphosphate	Nucleus
2364	7140n	mi1345p(n)	1D-myo-Inositol 1,3,4,5-tetrakisphosphate	Nucleus
2365	11398n	mi1346p(n)	1D-myo-Inositol 1,3,4,6-tetrakisphosphate	Nucleus
2366	19579n	mi1456p(n)	1D-myo-Inositol 1,4,5,6-tetrakisphosphate	Nucleus
2367	8995n	mi145p(n)	1D-myo-Inositol 1,4,5-trisphosphate	Nucleus
2368	950n	mi14p(n)	1D-myo-Inositol 1,4-bisphosphate	Nucleus
2369	8983n	mi1p-D(n)	1D-myo-Inositol 1-phosphate	Nucleus
2370	938n	minohp(n)	myo-Inositol hexakisphosphate	Nucleus
2371	466n	nad(n)	Nicotinamide adenine dinucleotide	Nucleus
2372	469n	nadp(n)	Nicotinamide adenine dinucleotide phosphate	Nucleus

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2373	468n	nadph(n)	Nicotinamide adenine dinucleotide phosphate - reduced	Nucleus
2374	476n	nh4(n)	Ammonium	Nucleus
2375	776n	nicrnt(n)	Nicotinate D-ribonucleotide	Nucleus
2376	77n	nmn(n)	NMN	Nucleus
2377	470n	o2(n)	O2	Nucleus
2378	461n	o2s(n)	Superoxide anion	Nucleus
2379	22810n	oretn(n)	4-oxo-retonoic acid	Nucleus
2380	18536n	pa_hs(n)	phosphatidic acid (homo sapiens)	Nucleus
2381	4431n	pail345p_hs(n)	phosphatidylinositol-3,4,5-trisphosphate (Homo sapiens)	Nucleus
2382	19605n	pail34p_hs(n)	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)	Nucleus
2383	3992n	pail3p_hs(n)	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)	Nucleus
2384	19333n	pail45p_hs(n)	phosphatidylinositol 4,5-bisphosphate (Homo sapiens)	Nucleus
2385	19332n	pail4p_hs(n)	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	Nucleus
2386	19479n	pail5p_hs(n)	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)	Nucleus
2387	19327n	pail_hs(n)	phosphatidylinositol (homo sapiens)	Nucleus
2388	5307n	peplys(n)	Peptidyl-L-lysine	Nucleus
2389	472n	pi(n)	Phosphate	Nucleus
2390	475n	ppi(n)	Diphosphate	Nucleus
2391	19580n	ppmi12346p(n)	5-Diphosphoinositol pentakisphosphate	Nucleus
2392	19581n	ppmi1346p(n)	Diphosphoinositol tetrakisphosphate	Nucleus
2393	2452n	pppi(n)	Inorganic triphosphate	Nucleus
2394	11153n	retn(n)	Retinoate	Nucleus
2395	4207n	seahcys(n)	Se-Adenosylselenohomocysteine	Nucleus
2396	4301n	seasmet(n)	Se-Adenosylselenomethionine	Nucleus
2397	135n	thbpt(n)	Tetrahydrobiopterin	Nucleus
2398	477n	udp(n)	UDP	Nucleus
2399	1068n	ump(n)	UMP	Nucleus
2400	10727n	uri(n)	Uridine	Nucleus
2401	345n	utp(n)	UTP	Nucleus
2402	3407r	11docrtsl(r)	11-Deoxycortisol	Endoplasmic Reticulum
2403	2404r	11docrtstrn(r)	11-Deoxycorticosterone	Endoplasmic Reticulum
2404	20447r	12harachd(r)	12 hydroxy arachidonic acid	Endoplasmic Reticulum
2405	22814r	13-cis-retn(r)	13-cis-retinoate	Endoplasmic Reticulum
2406	22816r	13-cis-retnglc(r)	13-cis-retinoyl glucuronide	Endoplasmic Reticulum
2407	3713r	17ahprgnlone(r)	17alpha-Hydroxyprogrenolone	Endoplasmic Reticulum
2408	769r	17ahprgstrn(r)	17alpha-Hydroxyprogesterone	Endoplasmic Reticulum
2409	20446r	18harachd(r)	18 hydroxy arachidonic acid	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2410	9128r	44mctr(r)	4,4-dimethylcholesta-8,14,24-trienol	Endoplasmic Reticulum
2411	3689r	44mzym(r)	4,4-dimethylzymosterol	Endoplasmic Reticulum
2412	913r	4hpro-LT(r)	trans-4-Hydroxy-L-proline	Endoplasmic Reticulum
2413	9129r	4mzym_int1(r)	4-Methylzymosterol intermediate 1	Endoplasmic Reticulum
2414	9130r	4mzym_int2(r)	4-Methylzymosterol intermediate 2	Endoplasmic Reticulum
2415	10712r	5adtststerone(r)	5alpha-Dihydrotestosterone	Endoplasmic Reticulum
2416	22786r	5adtststeroneglc(r)	5alpha-Dihydrotestosterone glucuronide	Endoplasmic Reticulum
2417	20402r	6htststerone(r)	6 beta hydroxy testosterone	Endoplasmic Reticulum
2418	182r	6pgc(r)	6-Phospho-D-gluconate	Endoplasmic Reticulum
2419	963r	6ppl(r)	6-phospho-D-glucono-1,5-lactone	Endoplasmic Reticulum
2420	834r	7dhchsterol(r)	7-Dehydrocholesterol	Endoplasmic Reticulum
2421	15102r	Asn-X-Ser/Thr(r)	protein-linked asparagine residue (N-glycosylation site)	Endoplasmic Reticulum
2422	4293r	Ntmelys(r)	Protein N6,N6,N6-trimethyl-L-lysine	Endoplasmic Reticulum
2423	18469r	R1coa_hs(r)	R group 1 Coenzyme A homo sapiens	Endoplasmic Reticulum
2424	18470r	R2coa_hs(r)	R group 2 Coenzyme A homo sapiens	Endoplasmic Reticulum
2425	20362r	Ser-Gly/Ala-X-Gly(r)	protein-linked serine residue (glycosaminoglycan attachment site)	Endoplasmic Reticulum
2426	689r	Ssq23epx(r)	(S)-Squalene-2,3-epoxide	Endoplasmic Reticulum
2427	1052r	acald(r)	Acetaldehyde	Endoplasmic Reticulum
2428	11537r	accoa(r)	Acetyl-CoA	Endoplasmic Reticulum
2429	7471r	acrn(r)	O-Acetylcarnitine	Endoplasmic Reticulum
2430	471r	adp(r)	ADP	Endoplasmic Reticulum
2431	2661r	ahandrostan(r)	3alpha-Hydroxy-5beta-androstan-17-one	Endoplasmic Reticulum
2432	20819r	ahandrostanglc(r)	Etiocholan-3alpha-ol-17-one 3-glucuronide	Endoplasmic Reticulum
2433	310r	ahcys(r)	S-Adenosyl-L-homocysteine	Endoplasmic Reticulum
2434	314r	akg(r)	2-Oxoglutarate	Endoplasmic Reticulum
2435	1086r	amet(r)	S-Adenosyl-L-methionine	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2436	309r	amp(r)	AMP	Endoplasmic Reticulum
2437	2893r	andrstandn(r)	androstanedione	Endoplasmic Reticulum
2438	17675r	andrstndn(r)	Androstenedione	Endoplasmic Reticulum
2439	352r	andrstrn(r)	Androsterone	Endoplasmic Reticulum
2440	20815r	andrstrnglc(r)	androsterone glucuronide	Endoplasmic Reticulum
2441	11890r	arachd(r)	arachidonic acid	Endoplasmic Reticulum
2442	465r	atp(r)	ATP	Endoplasmic Reticulum
2443	4279r	bildglcur(r)	Bilirubin beta-diglycuronide	Endoplasmic Reticulum
2444	1942r	bilglcur(r)	Bilirubin monoglycuronide	Endoplasmic Reticulum
2445	101r	bilirub(r)	Bilirubin	Endoplasmic Reticulum
2446	10989r	bz(r)	Benzoate	Endoplasmic Reticulum
2447	11004r	cbp(r)	Carbamoyl phosphate	Endoplasmic Reticulum
2448	3369r	chlstol(r)	Cholesta-7,24-dien-3beta-ol	Endoplasmic Reticulum
2449	1075r	chol(r)	Choline	Endoplasmic Reticulum
2450	3507r	cholcoar(r)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	Endoplasmic Reticulum
2451	17159r	cholcoas(r)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(S)	Endoplasmic Reticulum
2452	252r	chsterol(r)	Cholesterol	Endoplasmic Reticulum
2453	26330r	chsterols(r)	cholesterol sulfate	Endoplasmic Reticulum
2454	474r	co2(r)	CO2	Endoplasmic Reticulum
2455	473r	coa(r)	Coenzyme A	Endoplasmic Reticulum
2456	559r	coke(r)	cocaine	Endoplasmic Reticulum
2457	11168r	cortsn(r)	Cortisone	Endoplasmic Reticulum
2458	19478r	crm_hs(r)	ceramide (homo sapiens)	Endoplasmic Reticulum
2459	163r	crn(r)	L-Carnitine	Endoplasmic Reticulum
2460	11268r	crtsl(r)	Cortisol	Endoplasmic Reticulum
2461	1737r	crtstrn(r)	Corticosterone	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2462	18537r	dag_hs(r)	diacylglycerol (homo sapiens)	Endoplasmic Reticulum
2463	3688r	ddsmsterol(r)	7-Dehydrodesmosterol	Endoplasmic Reticulum
2464	20042r	dem2emgacpail_prot_hs(r)	deacylated-(phosphoethanolaminyldimannosyl),(phosphoethanolaminyl)-mannosyl-glucosaminyl-acylphosphatidylinositol	Endoplasmic Reticulum
2465	20041r	dgpi_prot_hs(r)	deacylated-glycophosphatidylinositol (GPI)-anchored protein	Endoplasmic Reticulum
2466	3997r	dhcholestanate(r)	3alpha,7alpha-Dihydroxy-5beta-cholestanate	Endoplasmic Reticulum
2467	3322r	dhcholestancoa(r)	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	Endoplasmic Reticulum
2468	3377r	dhcholoylcoa(r)	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	Endoplasmic Reticulum
2469	956r	dhea(r)	Dehydroepiandrosterone	Endoplasmic Reticulum
2470	3998r	dheas(r)	Dehydroepiandrosterone sulfate	Endoplasmic Reticulum
2471	14990r	doldp_L(r)	Dolichol diphosphate, human liver homolog	Endoplasmic Reticulum
2472	14991r	doldp_U(r)	Dolichol diphosphate, human uterine homolog	Endoplasmic Reticulum
2473	14992r	dolglcp_L(r)	Dolichyl beta-D-glucosyl phosphate, human liver homolog	Endoplasmic Reticulum
2474	14993r	dolglcp_U(r)	Dolichyl beta-D-glucosyl phosphate, human uterine homolog	Endoplasmic Reticulum
2475	14986r	dolichol_L(r)	Dolichol, human liver homolog	Endoplasmic Reticulum
2476	14987r	dolichol_U(r)	Dolichol, human uterine homolog	Endoplasmic Reticulum
2477	14994r	dolmanp_L(r)	Dolichyl phosphate D-mannose, human liver homolog	Endoplasmic Reticulum
2478	14995r	dolmanp_U(r)	Dolichyl phosphate D-mannose, human uterine homolog	Endoplasmic Reticulum
2479	14988r	dolp_L(r)	Dolichol phosphate, human liver homolog	Endoplasmic Reticulum
2480	14989r	dolp_U(r)	Dolichol phosphate, human uterine homolog	Endoplasmic Reticulum
2481	1463r	dsmsterol(r)	Desmosterol	Endoplasmic Reticulum
2482	3714r	eandrstrn(r)	epiandrosterone	Endoplasmic Reticulum
2483	20367r	ebastine(r)	ebastine	Endoplasmic Reticulum
2484	20368r	ebastineoh(r)	hydroxylated ebastine	Endoplasmic Reticulum
2485	19820r	ecgon(r)	ecgonine	Endoplasmic Reticulum
2486	19809r	egme(r)	ecgonine methyl ester	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2487	19995r	em2emgacpail_hs(r)	(phosphoethanolaminyldimannosyl),(phosphoethanolaminyl)-mannosyl-glucosaminyl-acylphosphatidylinositol (H7)	Endoplasmic Reticulum
2488	20040r	em2emgacpail_prot_hs(r)	(phosphoethanolaminyldimannosyl),(phosphoethanolaminyl)-mannosyl-glucosaminyl-acylphosphatidylinositol	Endoplasmic Reticulum
2489	19993r	em3gacpail_hs(r)	phosphoethanolaminyl-trimannosyl-glucosaminyl-acylphosphatidylinositol (H6')	Endoplasmic Reticulum
2490	19994r	emem2gacpail_hs(r)	(phosphoethanolaminyldimannosyl),(phosphoethanolaminyl)-dimannosyl-glucosaminyl-acylphosphatidylinositol (H7')	Endoplasmic Reticulum
2491	19989r	emgacpail_hs(r)	phosphoethanolaminyldimannosyl-glycosylaminyl-acylphosphatidylinositol (H5)	Endoplasmic Reticulum
2492	706r	estradiol(r)	Estradiol	Endoplasmic Reticulum
2493	20817r	estradiolglc(r)	estradiol glucuronide	Endoplasmic Reticulum
2494	3904r	estriol(r)	estriol	Endoplasmic Reticulum
2495	3415r	estriolglc(r)	16-Glucuronide-estriol	Endoplasmic Reticulum
2496	86r	estrone(r)	Estrone	Endoplasmic Reticulum
2497	20814r	estroneglc(r)	estrone glucuronide	Endoplasmic Reticulum
2498	2601r	estrones(r)	Estrone 3-sulfate	Endoplasmic Reticulum
2499	9020r	ethamp(r)	Ethanolamine phosphate	Endoplasmic Reticulum
2500	478r	fad(r)	Flavin adenine dinucleotide oxidized	Endoplasmic Reticulum
2501	42r	fadh2(r)	Flavin adenine dinucleotide reduced	Endoplasmic Reticulum
2502	334r	for(r)	Formate	Endoplasmic Reticulum
2503	10388r	frdp(r)	Farnesyl diphosphate	Endoplasmic Reticulum
2504	15443r	g1m6masnB1(r)	glucosyl-(alpha-D-mannosyl)6-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Endoplasmic Reticulum
2505	15442r	g1m7masnB(r)	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)	Endoplasmic Reticulum
2506	15441r	g1m7masnC(r)	glucosyl-(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform C (protein)	Endoplasmic Reticulum
2507	15142r	g1m8masn(r)	(alpha-D-Glucosyl)-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Endoplasmic Reticulum
2508	15019r	g1m8mpdol_L(r)	alpha-D-Glucosyl-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2509	15020r	g1m8mpdol_U(r)	alpha-D-Glucosyl-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2510	15138r	g2m8masn(r)	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Endoplasmic Reticulum
2511	15021r	g2m8mpdol_L(r)	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2512	15022r	g2m8mpdol_U(r)	(alpha-D-Glucosyl)2-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2513	15115r	g3m8masn(r)	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Endoplasmic Reticulum
2514	15023r	g3m8mpdol_L(r)	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2515	15024r	g3m8mpdol_U(r)	(alpha-D-Glucosyl)3-(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2516	765r	g6p(r)	D-Glucose 6-phosphate	Endoplasmic Reticulum
2517	19963r	gacpail_hs(r)	glucosaminyl-acylphosphatidylinositol	Endoplasmic Reticulum
2518	18308r	glac(r)	D-glucurono-6,3-lactone	Endoplasmic Reticulum
2519	318r	glc-D(r)	D-Glucose	Endoplasmic Reticulum
2520	256r	glcur(r)	D-Glucuronate	Endoplasmic Reticulum
2521	313r	glu-L(r)	L-Glutamate	Endoplasmic Reticulum
2522	19613r	gluside_hs(r)	glucocerebroside (homo sapiens)	Endoplasmic Reticulum
2523	19996r	gpi_hs(r)	glycophosphatidylinositol (GPI) anchor precursor (3-(phosphoethanolaminy-mannosyl)-glucosaminyl-acylphosphatidylinositol) (H8)	Endoplasmic Reticulum
2524	20035r	gpi_prot_hs(r)	glycophosphatidylinositol (GPI)-anchored protein	Endoplasmic Reticulum
2525	20039r	gpi_sig(r)	glycophosphatidylinositol (GPI) signal sequence (C-terminal peptide)	Endoplasmic Reticulum
2526	11388r	gthrd(r)	Reduced glutathione	Endoplasmic Reticulum
2527	677r	gullac(r)	L-Gulono-1,4-lactone	Endoplasmic Reticulum
2528	650r	guln(r)	L-Gulonate	Endoplasmic Reticulum
2529	1049r	h(r)	H+	Endoplasmic Reticulum
2530	317r	h2o(r)	H2O	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2531	297r	hdca(r)	Hexadecanoate (n-C16:0)	Endoplasmic Reticulum
2532	17864r	hemeBo(r)	Heme B oxidized	Endoplasmic Reticulum
2533	17865r	hemeBr(r)	Heme B reduced	Endoplasmic Reticulum
2534	20384r	hestratriol(r)	4,17 dihydroxy estradiol	Endoplasmic Reticulum
2535	191r	hmgcoa(r)	Hydroxymethylglutaryl-CoA	Endoplasmic Reticulum
2536	399r	hxdcal(r)	Hexadecanal	Endoplasmic Reticulum
2537	597r	lanost(r)	Lanosterol	Endoplasmic Reticulum
2538	755r	leuktrA4(r)	Leukotriene A4	Endoplasmic Reticulum
2539	1752r	leuktrB4(r)	Leukotriene B4	Endoplasmic Reticulum
2540	26340r	leuktrB4wcooh(r)	w-carboxy leukotriene B4	Endoplasmic Reticulum
2541	20365r	leuktrB4woh(r)	w-hydroxyl leukotriene B4	Endoplasmic Reticulum
2542	17887r	leuktrC4(r)	Leukotriene C4	Endoplasmic Reticulum
2543	4410r	leuktrD4(r)	Leukotriene D4	Endoplasmic Reticulum
2544	780r	lthstrl(r)	5alpha-Cholest-7-en-3beta-ol	Endoplasmic Reticulum
2545	20047r	m(em)3gacpail_hs(r)	mannosyl-3-(phosphoethanolaminy)-glucosaminyl-acylphosphatidylinositol (M4A)	Endoplasmic Reticulum
2546	20052r	m(em)3gacpail_prot_hs(r)	mannosyl-3-(phosphoethanolaminy)-glucosaminyl-acylphosphatidylinositol-Protein (M4A)	Endoplasmic Reticulum
2547	19991r	m2emgacpail_hs(r)	(dimannosyl),(phosphoethanolaminy)-mannosyl-glucosylaminy-acylphosphatidylinositol (H6)	Endoplasmic Reticulum
2548	19968r	m2gacpail_hs(r)	dimannosyl-glucosaminyl-acylphosphatidylinositol (H3)	Endoplasmic Reticulum
2549	20045r	m3emgacpail_hs(r)	(trimannosyl),(phosphoethanolaminy)-mannosyl-glucosaminyl-acylphosphatidylinositol (M4C)	Endoplasmic Reticulum
2550	19992r	m3gacpail_hs(r)	trimannosyl-glucosaminyl-acylphosphatidylinositol (H4)	Endoplasmic Reticulum
2551	15008r	m4mpdol_L(r)	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2552	15009r	m4mpdol_U(r)	(alpha-D-Mannosyl)4-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2553	15010r	m5mpdol_L(r)	(alpha-D-Mannosyl)5-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2554	15011r	m5mpdol_U(r)	(alpha-D-Mannosyl)5-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2555	15012r	m6mpdol_L(r)	(alpha-D-Mannosyl)6-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2556	15013r	m6mpdol_U(r)	(alpha-D-Mannosyl)6-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2557	15159r	m7masnB(r)	(alpha-D-mannosyl)7-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine, isoform B (protein)	Endoplasmic Reticulum
2558	15014r	m7mpdol_L(r)	(alpha-D-Mannosyl)7-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2559	15016r	m7mpdol_U(r)	(alpha-D-Mannosyl)7-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2560	15144r	m8masn(r)	(alpha-D-mannosyl)8-beta-D-mannosyl-diacetylchitobiosyl-L-asparagine (protein)	Endoplasmic Reticulum
2561	15017r	m8mpdol_L(r)	(alpha-D-Mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human liver homolog	Endoplasmic Reticulum
2562	15018r	m8mpdol_U(r)	(alpha-D-Mannosyl)8-beta-D-mannosyl-diacetylchitobiosyldiphosphodolichol, human uterine homolog	Endoplasmic Reticulum
2563	11018r	man(r)	D-Mannose	Endoplasmic Reticulum
2564	20046r	mem2emgacpail_hs(r)	({(mannosyl),(phosphoethanolaminy)}-dimannosyl},{phosphoethanolaminy})-mannosyl-glucosaminy-acylphosphatidylinositol (M4B)	Endoplasmic Reticulum
2565	20051r	mem2emgacpail_prot_hs(r)	({(mannosyl),(phosphoethanolaminy)}-dimannosyl},{phosphoethanolaminy})-mannosyl-glucosaminy-acylphosphatidylinositol-Protein (M4B)	Endoplasmic Reticulum
2566	19990r	memgacpail_hs(r)	(mannosyl),(phosphoethanolaminy)-mannosyl-glucosylaminy-acylphosphatidylinositol (B)	Endoplasmic Reticulum
2567	1092r	meoh(r)	Methanol	Endoplasmic Reticulum
2568	418r	mev-R(r)	(R)-Mevalonate	Endoplasmic Reticulum
2569	19966r	mgacpail_hs(r)	mannosyl-glucosaminy-acylphosphatidylinositol (H2)	Endoplasmic Reticulum
2570	466r	nad(r)	Nicotinamide adenine dinucleotide	Endoplasmic Reticulum
2571	467r	nadh(r)	Nicotinamide adenine dinucleotide - reduced	Endoplasmic Reticulum
2572	469r	nadp(r)	Nicotinamide adenine dinucleotide phosphate	Endoplasmic Reticulum
2573	468r	nadph(r)	Nicotinamide adenine dinucleotide phosphate - reduced	Endoplasmic Reticulum
2574	476r	nh4(r)	Ammonium	Endoplasmic Reticulum
2575	470r	o2(r)	O2	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2576	18536r	pa_hs(r)	phosphatidic acid (homo sapiens)	Endoplasmic Reticulum
2577	19605r	pail34p_hs(r)	phosphatidylinositol-3,4-bisphosphate (Homo sapiens)	Endoplasmic Reticulum
2578	19704r	pail35p_hs(r)	phosphatidylinositol-3,5-bisphosphate (Homo sapiens)	Endoplasmic Reticulum
2579	3992r	pail3p_hs(r)	1-Phosphatidyl-1D-myo-inositol 3-phosphate (Homo sapiens)	Endoplasmic Reticulum
2580	19332r	pail4p_hs(r)	1-Phosphatidyl-1D-myo-inositol 4-phosphate (Homo sapiens)	Endoplasmic Reticulum
2581	19479r	pail5p_hs(r)	1-Phosphatidyl-1D-myo-inositol 5-phosphate (Homo sapiens)	Endoplasmic Reticulum
2582	19327r	pail_hs(r)	phosphatidylinositol (homo sapiens)	Endoplasmic Reticulum
2583	19051r	pchol_hs(r)	Phosphatidylcholine (homo sapiens)	Endoplasmic Reticulum
2584	19050r	pe_hs(r)	phosphatidylethanolamine (homo sapiens)	Endoplasmic Reticulum
2585	19967r	pecgon(r)	pseudoecgonine	Endoplasmic Reticulum
2586	19969r	pecgoncoa(r)	Pseudoecgonyl-CoA	Endoplasmic Reticulum
2587	22613r	pepslys(r)	peptide sans lysine	Endoplasmic Reticulum
2588	472r	pi(r)	Phosphate	Endoplasmic Reticulum
2589	475r	ppi(r)	Diphosphate	Endoplasmic Reticulum
2590	20038r	pre_prot(r)	glycophosphatidylinositol (GPI)-anchored protein precursor	Endoplasmic Reticulum
2591	10681r	prgnlone(r)	Pregnenolone	Endoplasmic Reticulum
2592	26331r	prgnlones(r)	pregnenolone sulfate	Endoplasmic Reticulum
2593	10510r	prgstrn(r)	Progesterone	Endoplasmic Reticulum
2594	229r	pro-L(r)	L-Proline	Endoplasmic Reticulum
2595	11382r	prostgd2(r)	Prostaglandin D2	Endoplasmic Reticulum
2596	398r	prostge2(r)	Prostaglandin E2	Endoplasmic Reticulum
2597	422r	prostgh2(r)	Prostaglandin H2	Endoplasmic Reticulum
2598	856r	prostgi2(r)	Prostaglandin I2	Endoplasmic Reticulum
2599	19052r	ps_hs(r)	phosphatidylserine (homo sapiens)	Endoplasmic Reticulum
2600	11153r	retn(r)	Retinoate	Endoplasmic Reticulum
2601	20818r	retnqlc(r)	retinoyl glucuronide	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2602	261r	ru5p-D(r)	D-Ribulose 5-phosphate	Endoplasmic Reticulum
2603	335r	so4(r)	Sulfate	Endoplasmic Reticulum
2604	9025r	sph1p(r)	Sphinganine 1-phosphate	Endoplasmic Reticulum
2605	708r	sphgn(r)	Sphinganine	Endoplasmic Reticulum
2606	10703r	sphings(r)	Sphingosine	Endoplasmic Reticulum
2607	4541r	sphs1p(r)	Sphingosine 1-phosphate	Endoplasmic Reticulum
2608	519r	sql(r)	Squalene	Endoplasmic Reticulum
2609	325r	succ(r)	Succinate	Endoplasmic Reticulum
2610	3477r	thcholstoic(r)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	Endoplasmic Reticulum
2611	2907r	tmlys(r)	N6,N6,N6-Trimethyl-L-lysine	Endoplasmic Reticulum
2612	10622r	ttsterone(r)	Testosterone	Endoplasmic Reticulum
2613	20816r	ttsteroneglc(r)	testosterone glucuronide	Endoplasmic Reticulum
2614	1777r	txa2(r)	Thromboxane A2	Endoplasmic Reticulum
2615	477r	udp(r)	UDP	Endoplasmic Reticulum
2616	10912r	udpacgal(r)	UDP-N-acetyl-D-galactosamine	Endoplasmic Reticulum
2617	316r	udpg(r)	UDPglucose	Endoplasmic Reticulum
2618	241r	udpglcur(r)	UDP-D-glucuronate	Endoplasmic Reticulum
2619	255r	udpxyl(r)	UDP-D-xylose	Endoplasmic Reticulum
2620	1068r	ump(r)	UMP	Endoplasmic Reticulum
2621	20366r	wharachd(r)	w-hydroxyl arachidonic acid	Endoplasmic Reticulum
2622	20403r	whtsterone(r)	w hydroxy testosterone	Endoplasmic Reticulum
2623	17046r	xol24oh(r)	24-Hydroxycholesterol	Endoplasmic Reticulum
2624	17047r	xol25oh(r)	25-Hydroxycholesterol	Endoplasmic Reticulum
2625	4060r	xol27oh(r)	27-Hydroxycholesterol	Endoplasmic Reticulum
2626	11131r	xol7a(r)	7 alpha-Hydroxycholesterol	Endoplasmic Reticulum
2627	3381r	xol7ah2(r)	3alpha,7alpha-Dihydroxy-5beta-cholestane	Endoplasmic Reticulum

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2628	11535r	xol7aone(r)	7alpha-Hydroxycholest-4-en-3-one	Endoplasmic Reticulum
2629	3384r	xoldiolone(r)	7alpha,12alpha-Dihydroxycholest-4-en-3-one	Endoplasmic Reticulum
2630	2593r	xolest_hs(r)	cholesterol ester	Endoplasmic Reticulum
2631	17068r	xoltri24(r)	7-alpha,24(S)-Dihydroxycholesterol	Endoplasmic Reticulum
2632	17067r	xoltri25(r)	7-alpha,25-Dihydroxycholesterol	Endoplasmic Reticulum
2633	4061r	xoltri27(r)	7-alpha,27-Dihydroxycholesterol	Endoplasmic Reticulum
2634	3383r	xoltriol(r)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestane	Endoplasmic Reticulum
2635	20363r	xser(r)	Xyl-L-Ser (protein)	Endoplasmic Reticulum
2636	9132r	zym_int2(r)	zymosterol intermediate 2	Endoplasmic Reticulum
2637	3367r	zymst(r)	zymosterol	Endoplasmic Reticulum
2638	10801r	zymstnl(r)	Zymostenol	Endoplasmic Reticulum
2639	11156x	1p2cbxl(x)	1-Pyrroline-2-carboxylate	Peroxisome
2640	3121x	1pipdn2c(x)	delta1-Piperideine-2-carboxylate	Peroxisome
2641	19703x	3h26dm5coa(x)	3-Hydroxy-2,6-dimethyl-5-methylene-heptanoyl-CoA	Peroxisome
2642	905x	3hbcoa(x)	(S)-3-Hydroxybutanoyl-CoA	Peroxisome
2643	4184x	3hpcoa(x)	3-Hydroxypropionyl-CoA	Peroxisome
2644	3794x	3odcoa(x)	3-Oxodecanoyl-CoA	Peroxisome
2645	3792x	3oddcoa(x)	3-Oxododecanoyl-CoA	Peroxisome
2646	3788x	3ohdcoa(x)	3-Oxohexadecanoyl-CoA	Peroxisome
2647	8402x	3ohodcoa(x)	3-Oxoctadecanoyl-CoA	Peroxisome
2648	9236x	3ohxcoa(x)	3-Oxohexacosyl-CoA	Peroxisome
2649	3790x	3otdcoa(x)	3-Oxotetradecanoyl-CoA	Peroxisome
2650	10559x	5a2opntn(x)	5-Amino-2-oxopentanoate	Peroxisome
2651	10525x	5dpmev(x)	(R)-5-Diphosphomevalonate	Peroxisome
2652	2892x	5g2oxpt(x)	5-Guanidino-2-oxopentanoate	Peroxisome
2653	883x	5pmev(x)	(R)-5-Phosphomevalonate	Peroxisome
2654	2428x	6a2ohxnt(x)	6-Amino-2-oxohexanoate	Peroxisome
2655	411x	Lpipecol(x)	L-Pipecolate	Peroxisome
2656	18523x	Rtotal(x)	R total	Peroxisome
2657	22165x	Rtotalcoa(x)	R total Coenzyme A	Peroxisome
2658	174x	aacoa(x)	Acetoacetyl-CoA	Peroxisome
2659	9016x	acac(x)	Acetoacetate	Peroxisome
2660	1052x	acald(x)	Acetaldehyde	Peroxisome
2661	11537x	accoa(x)	Acetyl-CoA	Peroxisome
2662	7471x	acrn(x)	O-Acetylcarnitine	Peroxisome
2663	18534x	adhap_hs(x)	acyl-dihydroxyacetone phosphate	Peroxisome
2664	471x	adp(x)	ADP	Peroxisome
2665	18463x	adrn(x)	adrenic acid	Peroxisome
2666	18484x	adrncoa(x)	adrenyl coenzyme A	Peroxisome
2667	19357x	akdhap_hs(x)	1-alkyldihydroxyacetone phosphate	Peroxisome
2668	314x	akg(x)	2-Oxoglutarate	Peroxisome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2669	1093x	ala-D(x)	D-Alanine	Peroxisome
2670	11412x	ala-L(x)	L-Alanine	Peroxisome
2671	19356x	alkylR1oh(x)	hydroxy alkyl chain	Peroxisome
2672	309x	amp(x)	AMP	Peroxisome
2673	18483x	arachcoa(x)	arachidyl coenzyme A	Peroxisome
2674	11887x	arachdcoa(x)	C20:4-CoA	Peroxisome
2675	644x	arg-D(x)	D-Arginine	Peroxisome
2676	10519x	asp-D(x)	D-Aspartate	Peroxisome
2677	465x	atp(x)	ATP	Peroxisome
2678	733x	b2coa(x)	Crotonoyl-CoA	Peroxisome
2679	11888x	c226coa(x)	cervonyl coenzyme A	Peroxisome
2680	19701x	c2m26dcoa(x)	cis-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA	Peroxisome
2681	10881x	cholcoa(x)	Choloyl-CoA	Peroxisome
2682	3386x	cholcoads(x)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholest-24-enoyl-CoA	Peroxisome
2683	3391x	cholcoaone(x)	3alpha,7alpha,12alpha-Trihydroxy-5beta-24-oxocholestanoyl-CoA	Peroxisome
2684	3507x	cholcoar(x)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA	Peroxisome
2685	17159x	cholcoas(x)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoyl-CoA(S)	Peroxisome
2686	18488x	clpndcoa(x)	clupanodonyl CoA	Peroxisome
2687	474x	co2(x)	CO2	Peroxisome
2688	473x	coa(x)	Coenzyme A	Peroxisome
2689	163x	crn(x)	L-Carnitine	Peroxisome
2690	3803x	dcacoa(x)	Decanoyl-CoA (n-C10:0CoA)	Peroxisome
2691	3848x	dcholcoa(x)	chenodeoxycholoyl coenzyme a	Peroxisome
2692	18487x	dcsptn1coa(x)	docosa-4,7,10,13,16-pentaenoyl coenzyme A	Peroxisome
2693	1383x	ddcacoa(x)	Dodecanoyl-CoA (n-C12:0CoA)	Peroxisome
2694	3387x	dgchol(x)	Chenodeoxyglycocholate	Peroxisome
2695	11531x	dgcholcoa(x)	Chenodeoxyglycocholoyl-CoA	Peroxisome
2696	1072x	dhap(x)	Dihydroxyacetone phosphate	Peroxisome
2697	3997x	dhcholestanate(x)	3alpha,7alpha-Dihydroxy-5beta-cholestanate	Peroxisome
2698	3322x	dhcholestancoa(x)	3alpha,7alpha-Dihydroxy-5beta-cholestanoyl-CoA	Peroxisome
2699	3377x	dhcholoylcoa(x)	3alpha,7alpha-Dihydroxy-5beta-cholest-24-enoyl-CoA	Peroxisome
2700	3376x	dhocholoylcoa(x)	3alpha,7alpha,12alpha,26-Tetrahydroxy-5beta-cholestane	Peroxisome
2701	21959x	dmnoncoa(x)	4,8 dimethylnonanoyl-CoA	Peroxisome
2702	21976x	dmnoncrn(x)	4,8 dimethylnonanoyl carnitine	Peroxisome
2703	38x	dmpp(x)	Dimethylallyl diphosphate	Peroxisome
2704	87x	etoh(x)	Ethanol	Peroxisome
2705	478x	fad(x)	Flavin adenine dinucleotide oxidized	Peroxisome
2706	42x	fadh2(x)	Flavin adenine dinucleotide reduced	Peroxisome
2707	340x	fald(x)	Formaldehyde	Peroxisome
2708	11122x	formcoa(x)	Formyl-CoA	Peroxisome
2709	10388x	frdp(x)	Farnesyl diphosphate	Peroxisome
2710	1554x	gchola(x)	glycocholate	Peroxisome
2711	11524x	gdchola(x)	glycochenodeoxycholate	Peroxisome
2712	329x	glx(x)	Glyoxylate	Peroxisome
2713	323x	gly(x)	Glycine	Peroxisome
2714	237x	glyclt(x)	Glycolate	Peroxisome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2715	179x	grdp(x)	Geranyl diphosphate	Peroxisome
2716	1049x	h(x)	H+	Peroxisome
2717	317x	h2o(x)	H2O	Peroxisome
2718	315x	h2o2(x)	Hydrogen peroxide	Peroxisome
2719	297x	hdca(x)	Hexadecanoate (n-C16:0)	Peroxisome
2720	3801x	hdd2coa(x)	trans-Hexadec-2-enoyl-CoA	Peroxisome
2721	11013x	hexccoa(x)	Hexacosanoyl-CoA (n-C26:0CoA)	Peroxisome
2722	191x	hmgcoa(x)	Hydroxymethylglutaryl-CoA	Peroxisome
2723	242x	hpyr(x)	Hydroxypyruvate	Peroxisome
2724	218x	hxan(x)	Hypoxanthine	Peroxisome
2725	158x	icit(x)	Isocitrate	Peroxisome
2726	1089x	ipdp(x)	Isopentenyl diphosphate	Peroxisome
2727	18490x	lgnccoa(x)	lignocericyl coenzyme A	Peroxisome
2728	2277x	lnlncgcoa(x)	gamma-linolenoyl-CoA	Peroxisome
2729	328x	lys-L(x)	L-Lysine	Peroxisome
2730	11267x	malcoa(x)	Malonyl-CoA	Peroxisome
2731	418x	mev-R(x)	(R)-Mevalonate	Peroxisome
2732	451x	mmcoa-S(x)	(S)-Methylmalonyl-CoA	Peroxisome
2733	1023x	na1(x)	Sodium	Peroxisome
2734	466x	nad(x)	Nicotinamide adenine dinucleotide	Peroxisome
2735	467x	nadh(x)	Nicotinamide adenine dinucleotide - reduced	Peroxisome
2736	469x	nadp(x)	Nicotinamide adenine dinucleotide phosphate	Peroxisome
2737	468x	nadph(x)	Nicotinamide adenine dinucleotide phosphate - reduced	Peroxisome
2738	476x	nh4(x)	Ammonium	Peroxisome
2739	18485x	nrvnccoa(x)	nervonyl coenzyme A	Peroxisome
2740	470x	o2(x)	O2	Peroxisome
2741	461x	o2s(x)	Superoxide anion	Peroxisome
2742	322x	oaa(x)	Oxaloacetate	Peroxisome
2743	10688x	occoa(x)	Octanoyl-CoA (n-C8:0CoA)	Peroxisome
2744	8782x	odecoa(x)	Octadecenoyl-CoA (n-C18:1CoA)	Peroxisome
2745	19415x	orn-D(x)	D-Ornithine	Peroxisome
2746	10901x	oxa(x)	Oxalate	Peroxisome
2747	15675x	pcrn(x)	propionyl-carnitine	Peroxisome
2748	1308x	phyt(x)	phytanic acid	Peroxisome
2749	21956x	phyt2ohcoa(x)	2-Hydroxyphytanoyl-CoA	Peroxisome
2750	21953x	phytcoa(x)	phytanyl coa	Peroxisome
2751	472x	pi(x)	Phosphate	Peroxisome
2752	11029x	pmtcoa(x)	Palmitoyl-CoA (n-C16:0CoA)	Peroxisome
2753	1064x	ppcoa(x)	Propanoyl-CoA	Peroxisome
2754	475x	ppi(x)	Diphosphate	Peroxisome
2755	21954x	prist(x)	pristanic acid	Peroxisome
2756	21957x	pristanal(x)	pristanal	Peroxisome
2757	21955x	pristcoa(x)	pristanoyl coa	Peroxisome
2758	629x	pro-D(x)	D-Proline	Peroxisome
2759	744x	prpncoa(x)	Propenoyl-CoA	Peroxisome
2760	311x	pyr(x)	Pyruvate	Peroxisome
2761	271x	sarcs(x)	Sarcosine	Peroxisome
2762	339x	ser-L(x)	L-Serine	Peroxisome
2763	8781x	stcoa(x)	Stearoyl-CoA (n-C18:0CoA)	Peroxisome
2764	18492x	strdnccoa(x)	stearidonyl coenzyme A	Peroxisome
2765	325x	succ(x)	Succinate	Peroxisome
2766	19702x	t2m26dcoa(x)	trans-2-Methyl-5-isopropylhexa-2,5-dienoyl-CoA	Peroxisome

Row	Metabolite #	Abbreviation	Metabolite Name	Compartment
2767	293x	taur(x)	Taurine	Peroxisome
2768	3700x	tchola(x)	taurocholic acid	Peroxisome
2769	3390x	tdchola(x)	taurochenodeoxycholate	Peroxisome
2770	1862x	tdcoa(x)	Tetradecanoyl-CoA (n-C14:0CoA)	Peroxisome
2771	18515x	tethex3coa(x)	tetracosahexaenoyl coenzyme A	Peroxisome
2772	18513x	tetpent3coa(x)	tetracosapentaenoyl coenzyme A, n-3	Peroxisome
2773	18509x	tetpent6coa(x)	tetracosapentaenoyl coenzyme A, n-6	Peroxisome
2774	18511x	tettet6coa(x)	tetracosatetraenoyl coenzyme A	Peroxisome
2775	3378x	thcholoylcoa(x)	3alpha,7alpha,24-Trihydroxy-5beta-cholestanoyl-CoA	Peroxisome
2776	3477x	thcholstoic(x)	3alpha,7alpha,12alpha-Trihydroxy-5beta-cholestanoate	Peroxisome
2777	75x	thp2c(x)	2,3,4,5-Tetrahydropyridine-2-carboxylate	Peroxisome
2778	18486x	tmndncco(x)	timnodonyl coenzyme A	Peroxisome
2779	8904x	ttcoa(x)	tetracosanoyl-CoA (n-C24:0CoA)	Peroxisome
2780	199x	urate(x)	Urate	Peroxisome
2781	216x	xan(x)	Xanthine	Peroxisome