

Num	Variable	Type	Len	Label
76	c17945	Num	8	biochemical: 2-hydroxystearate (chemid: 1239)
77	c1806	Num	8	biochemical: retinol (Vitamin A) (chemid: 498)
78	c18349	Num	8	biochemical: indolelactate (chemid: 100000463)
79	c18369	Num	8	biochemical: gamma-glutamylleucine (chemid: 1268)
80	c18374	Num	8	biochemical: methionine sulfoxide (chemid: 100000039)
81	c18392	Num	8	biochemical: theobromine (chemid: 100000445)
82	c18467	Num	8	biochemical: eicosapentaenoate (EPA; 20:5n3) (chemid: 2050)
83	c18476	Num	8	biochemical: glycocholate (chemid: 342)
84	c18494	Num	8	biochemical: taurochenodeoxycholate (chemid: 1629)
85	c1898	Num	8	biochemical: proline (chemid: 480)
86	c1899	Num	8	biochemical: quinolinate (chemid: 182)
87	c19130	Num	8	biochemical: 1,2-dipalmitoyl-GPC (16:0/16:0) (chemid: 100000657)
88	c19263	Num	8	biochemical: 1-palmitoyl-2-oleoyl-GPE (16:0/18:1) (chemid: 1526)
89	c19324	Num	8	biochemical: 1-stearoyl-GPI (18:0) (chemid: 100000656)
90	c19503	Num	8	biochemical: stearoyl sphingomyelin (d18:1/18:0) (chemid: 1538)
91	c20675	Num	8	biochemical: 1,5-anhydroglucitol (1,5-AG) (chemid: 100000580)
92	c20693	Num	8	biochemical: tartronate (hydroxymalonate) (chemid: 100000840)
93	c20694	Num	8	biochemical: oxalate (ethanedioate) (chemid: 100000841)
94	c20699	Num	8	biochemical: erythritol (chemid: 100000846)
95	c21184	Num	8	biochemical: 1-oleoylglycerol (18:1) (chemid: 100000924)
96	c2125	Num	8	biochemical: taurine (chemid: 512)
97	c2132	Num	8	biochemical: citrulline (chemid: 391)
98	c2137	Num	8	biochemical: biliverdin (chemid: 250)
99	c22001	Num	8	biochemical: 3-hydroxyoctanoate (chemid: 100000773)
100	c22036	Num	8	biochemical: 2-hydroxyoctanoate (chemid: 100000743)
101	c22053	Num	8	biochemical: 3-hydroxydecanoate (chemid: 100000997)
102	c22116	Num	8	biochemical: 4-methyl-2-oxopentanoate (chemid: 100000551)
103	c22130	Num	8	biochemical: phenyllactate (PLA) (chemid: 100000774)
104	c22137	Num	8	biochemical: homoarginine (chemid: 100000961)
105	c22176	Num	8	biochemical: cysteine s-sulfate (chemid: 100000808)
106	c22185	Num	8	biochemical: N-acetylaspartate (NAA) (chemid: 100000787)
107	c22842	Num	8	biochemical: cholate (chemid: 136)
108	c2342	Num	8	biochemical: serotonin (chemid: 504)
109	c2730	Num	8	biochemical: gamma-glutamylglutamine (chemid: 1140)
110	c2734	Num	8	biochemical: gamma-glutamyltyrosine (chemid: 1102)
111	c27513	Num	8	biochemical: indoleacetate (chemid: 100001034)
112	c2761	Num	8	biochemical: thyroxine (chemid: 1094)
113	c27665	Num	8	biochemical: 1-methylnicotinamide (chemid: 55)
114	c27672	Num	8	biochemical: 3-indoxyl sulfate (chemid: 100000467)

Num	Variable	Type	Len	Label
115	c27710	Num	8	biochemical: N-acetylglycine (chemid: 100001006)
116	c27718	Num	8	biochemical: creatine (chemid: 1221)
117	c27719	Num	8	biochemical: galactonate (chemid: 100001026)
118	c27738	Num	8	biochemical: threonate (chemid: 100001022)
119	c2829	Num	8	biochemical: N-formylmethionine (chemid: 194)
120	c30460	Num	8	biochemical: 1-methylhistidine (chemid: 100001051)
121	c3127	Num	8	biochemical: hypoxanthine (chemid: 171)
122	c3141	Num	8	biochemical: betaine (chemid: 799)
123	c3147	Num	8	biochemical: xanthine (chemid: 1004)
124	c3155	Num	8	biochemical: 3-ureidopropionate (chemid: 1053)
125	c31555	Num	8	biochemical: pyridoxate (chemid: 100001121)
126	c31591	Num	8	biochemical: androsterone sulfate (chemid: 100001073)
127	c31787	Num	8	biochemical: 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF) (chemid: 100001178)
128	c32197	Num	8	biochemical: 3-(4-hydroxyphenyl)lactate (HPLA) (chemid: 240)
129	c32198	Num	8	biochemical: acetylcarnitine (C2) (chemid: 100000802)
130	c32306	Num	8	biochemical: hydroxyproline (chemid: 1001)
131	c32328	Num	8	biochemical: hexanoylcarnitine (C6) (chemid: 100000781)
132	c32342	Num	8	biochemical: AMP (chemid: 209)
133	c32346	Num	8	biochemical: glycochenodeoxycholate (chemid: 1628)
134	c32350	Num	8	biochemical: 1-methyl-4-imidazoleacetate (chemid: 100001208)
135	c32397	Num	8	biochemical: 3-hydroxy-2-ethylpropionate (chemid: 100001170)
136	c32398	Num	8	biochemical: sebacate (C10-DC) (chemid: 100001211)
137	c32401	Num	8	biochemical: trigonelline (N'-methylnicotinate) (chemid: 100001092)
138	c32405	Num	8	biochemical: indolepropionate (chemid: 100001083)
139	c32412	Num	8	biochemical: butyrylcarnitine (C4) (chemid: 100001054)
140	c32418	Num	8	biochemical: myristoleate (14:1n5) (chemid: 100001198)
141	c32425	Num	8	biochemical: dehydroepiandrosterone sulfate (DHEA-S) (chemid: 100000792)
142	c32445	Num	8	biochemical: 3-methylxanthine (chemid: 100001108)
143	c32452	Num	8	biochemical: propionylcarnitine (C3) (chemid: 100001162)
144	c32457	Num	8	biochemical: 3-hydroxylaurate (chemid: 100001112)
145	c32489	Num	8	biochemical: caproate (6:0) (chemid: 926)
146	c32492	Num	8	biochemical: caprylate (8:0) (chemid: 932)
147	c32497	Num	8	biochemical: 10-undecenoate (11:1n1) (chemid: 100001197)
148	c32504	Num	8	biochemical: docosapentaenoate (DPA; 22:5n3) (chemid: 100001181)
149	c32553	Num	8	biochemical: phenol sulfate (chemid: 100001510)
150	c32562	Num	8	biochemical: pregnen-diol disulfate* (chemid: 100001993)
151	c32578	Num	8	biochemical: X - 11261
152	c32586	Num	8	biochemical: bilirubin (E,E)* (chemid: 100001950)
153	c32599	Num	8	biochemical: glycocholenate sulfate* (chemid: 100001989)

Num	Variable	Type	Len	Label
154	c32619	Num	8	biochemical: pregnenediol sulfate (C ₂₁ H ₃₄ O ₅ S)* (chemid: 100002067)
155	c32620	Num	8	biochemical: glycolithocholate sulfate* (chemid: 100001657)
156	c32807	Num	8	biochemical: taurocholenate sulfate* (chemid: 100001990)
157	c32827	Num	8	biochemical: andro steroid monosulfate C ₁₉ H ₂₈ O ₆ S (1)* (chemid: 100002152)
158	c33009	Num	8	biochemical: homostachydrine* (chemid: 100001550)
159	c33132	Num	8	biochemical: X - 11787
160	c33140	Num	8	biochemical: X - 11795
161	c33228	Num	8	biochemical: 1-arachidonoyl-GPC* (20:4)* (chemid: 100001551)
162	c33230	Num	8	biochemical: 1-palmitoleoyl-GPC* (16:1)* (chemid: 100001511)
163	c33364	Num	8	biochemical: gamma-glutamylthreonine (chemid: 100001314)
164	c33422	Num	8	biochemical: gamma-glutamylphenylalanine (chemid: 100000491)
165	c33441	Num	8	biochemical: isobutyrylcarnitine (C4) (chemid: 100001055)
166	c33442	Num	8	biochemical: pseudouridine (chemid: 821)
167	c33447	Num	8	biochemical: palmitoleate (16:1n7) (chemid: 452)
168	c33935	Num	8	biochemical: piperine (chemid: 100001267)
169	c33936	Num	8	biochemical: octanoylcarnitine (C8) (chemid: 100001247)
170	c33937	Num	8	biochemical: alpha-hydroxyisovalerate (chemid: 100001300)
171	c33939	Num	8	biochemical: N-acetylthreonine (chemid: 100001274)
172	c33941	Num	8	biochemical: decanoylcarnitine (C10) (chemid: 100001251)
173	c33942	Num	8	biochemical: N-acetylasparagine (chemid: 100001257)
174	c33946	Num	8	biochemical: N-acetylhistidine (chemid: 100001293)
175	c33949	Num	8	biochemical: gamma-glutamylglycine (chemid: 100001294)
176	c33950	Num	8	biochemical: N-acetylphenylalanine (chemid: 100001256)
177	c33952	Num	8	biochemical: myristoylcarnitine (C14) (chemid: 100001270)
178	c33953	Num	8	biochemical: N-acetylarginine (chemid: 100001266)
179	c33955	Num	8	biochemical: 1-palmitoyl-GPC (16:0) (chemid: 100001263)
180	c33959	Num	8	biochemical: N-acetyltryptophan (chemid: 100001254)
181	c33961	Num	8	biochemical: 1-stearoyl-GPC (18:0) (chemid: 100001271)
182	c33968	Num	8	biochemical: 5-dodecenoate (12:1n7) (chemid: 100001232)
183	c33969	Num	8	biochemical: stearidonate (18:4n3) (chemid: 100001229)
184	c33971	Num	8	biochemical: 10-heptadecenoate (17:1n7) (chemid: 100001278)
185	c33972	Num	8	biochemical: 10-nonadecenoate (19:1n9) (chemid: 100001277)
186	c33973	Num	8	biochemical: epiandrosterone sulfate (chemid: 100001287)
187	c34035	Num	8	biochemical: linolenate (18:3n3 or 3n6) (chemid: 100001337)
188	c34093	Num	8	biochemical: hyocholate (chemid: 100001279)
189	c34214	Num	8	biochemical: 1-arachidonoyl-GPI* (20:4)* (chemid: 100001654)
190	c34390	Num	8	biochemical: 7-methylxanthine (chemid: 100001396)
191	c34396	Num	8	biochemical: phosphocholine (chemid: 267)
192	c34407	Num	8	biochemical: isovalerylcarnitine (C5) (chemid: 100001393)

Num	Variable	Type	Len	Label
193	c34419	Num	8	biochemical: 1-linoleoyl-GPC (18:2) (chemid: 100001395)
194	c34424	Num	8	biochemical: 5-acetylamino-6-amino-3-methyluracil (chemid: 100001403)
195	c34445	Num	8	biochemical: sphingosine 1-phosphate (chemid: 100000626)
196	c34456	Num	8	biochemical: gamma-glutamylisoleucine* (chemid: 100001485)
197	c34534	Num	8	biochemical: laurylearnitine (C12) (chemid: 100001392)
198	c35114	Num	8	biochemical: 7-methylguanine (chemid: 100001456)
199	c35126	Num	8	biochemical: phenylacetylglutamine (chemid: 100001417)
200	c35127	Num	8	biochemical: prolylhydroxyproline (chemid: 100001167)
201	c35136	Num	8	biochemical: 5-methyluridine (ribothymidine) (chemid: 100001446)
202	c35137	Num	8	biochemical: N2,N2-dimethylguanosine (chemid: 100001412)
203	c35157	Num	8	biochemical: N6-carbamoylthreonyladosine (chemid: 100001415)
204	c35160	Num	8	biochemical: oleoylcarnitine (C18:1) (chemid: 100001501)
205	c35172	Num	8	biochemical: orotidine (chemid: 100001416)
206	c35186	Num	8	biochemical: 1-arachidonoyl-GPE (20:4n6)* (chemid: 100001571)
207	c35320	Num	8	biochemical: catechol sulfate (chemid: 100001605)
208	c35527	Num	8	biochemical: 4-hydroxyhippurate (chemid: 100001423)
209	c35628	Num	8	biochemical: 1-oleoyl-GPE (18:1) (chemid: 100001569)
210	c35631	Num	8	biochemical: 1-palmitoyl-GPE (16:0) (chemid: 100001567)
211	c35635	Num	8	biochemical: 3-(3-hydroxyphenyl)propionate (chemid: 100001624)
212	c35637	Num	8	biochemical: cysteinylglycine (chemid: 278)
213	c35665	Num	8	biochemical: N-acetyl-aspartyl-glutamate (NAAG) (chemid: 100001612)
214	c35675	Num	8	biochemical: 2-hydroxypalmitate (chemid: 100001579)
215	c35678	Num	8	biochemical: hexadecanedioate (C16) (chemid: 100001614)
216	c35718	Num	8	biochemical: dihomolinolenate (20:3n3 or 3n6) (chemid: 100001739)
217	c36098	Num	8	biochemical: 4-vinylphenol sulfate (chemid: 100001755)
218	c36099	Num	8	biochemical: 4-ethylphenyl sulfate (chemid: 100001756)
219	c36103	Num	8	biochemical: p-cresol sulfate (chemid: 100001315)
220	c36594	Num	8	biochemical: 1-linoleoyl-GPI* (18:2)* (chemid: 100001778)
221	c36600	Num	8	biochemical: 1-linoleoyl-GPE (18:2)* (chemid: 100001570)
222	c36738	Num	8	biochemical: gamma-glutamylglutamate (chemid: 331)
223	c36746	Num	8	biochemical: 2-hydroxy-3-methylvalerate (chemid: 100001541)
224	c36747	Num	8	biochemical: deoxycarnitine (chemid: 100001662)
225	c36752	Num	8	biochemical: N6-acetyllysine (chemid: 100001734)
226	c36754	Num	8	biochemical: octadecanedioate (C18) (chemid: 100001615)
227	c36776	Num	8	biochemical: 7-HOCA (chemid: 100001609)
228	c36803	Num	8	biochemical: 3beta,7alpha-dihydroxy-5-cholestenoate (chemid: 100001611)
229	c36808	Num	8	biochemical: dimethylarginine (ADMA + SDMA) (chemid: 100001810)
230	c36850	Num	8	biochemical: tauroolithocholate 3-sulfate (chemid: 100001658)
231	c37058	Num	8	biochemical: succinylcarnitine (C4-DC) (chemid: 100001948)

Num	Variable	Type	Len	Label
232	c37063	Num	8	biochemical: gamma-glutamylalanine (chemid: 100001843)
233	c37076	Num	8	biochemical: N-acetylserine (chemid: 100001851)
234	c37097	Num	8	biochemical: tryptophan betaine (chemid: 100001743)
235	c37114	Num	8	biochemical: N6-methyladenosine (chemid: 213)
236	c37181	Num	8	biochemical: 4-allylphenol sulfate (chemid: 100001868)
237	c37186	Num	8	biochemical: 5alpha-androstan-3alpha,17beta-diol monosulfate (1) (chemid: 100002018)
238	c37190	Num	8	biochemical: 5alpha-androstan-3beta,17beta-diol disulfate (chemid: 100001987)
239	c37196	Num	8	biochemical: 5alpha-pregnan-3beta,20beta-diol monosulfate (1) (chemid: 100002009)
240	c37198	Num	8	biochemical: 5alpha-pregnan-3beta,20alpha-diol disulfate (chemid: 100001988)
241	c37200	Num	8	biochemical: 5alpha-pregnan-3beta,20alpha-diol monosulfate (2) (chemid: 100002014)
242	c37202	Num	8	biochemical: androstenediol (3beta,17beta) disulfate (1) (chemid: 100001992)
243	c37203	Num	8	biochemical: androstenediol (3beta,17beta) disulfate (2) (chemid: 100001994)
244	c37207	Num	8	biochemical: androstenediol (3alpha, 17alpha) monosulfate (2) (chemid: 100002026)
245	c37209	Num	8	biochemical: androstenediol (3alpha, 17alpha) monosulfate (3) (chemid: 100002027)
246	c37210	Num	8	biochemical: androstenediol (3beta,17beta) monosulfate (2) (chemid: 100002029)
247	c37211	Num	8	biochemical: androstenediol (3beta,17beta) monosulfate (1) (chemid: 100002028)
248	c37253	Num	8	biochemical: 2-hydroxyglutarate (chemid: 100002070)
249	c37431	Num	8	biochemical: N-methylproline (chemid: 100001956)
250	c37432	Num	8	biochemical: N-acetyl-beta-alanine (chemid: 100002102)
251	c37443	Num	8	biochemical: cysteine sulfinic acid (chemid: 100002113)
252	c37459	Num	8	biochemical: ergothioneine (chemid: 100002154)
253	c37478	Num	8	biochemical: docosapentaenoate (n6 DPA; 22:5n6) (chemid: 100001580)
254	c37496	Num	8	biochemical: N-acetylputrescine (chemid: 192)
255	c37506	Num	8	biochemical: palmitoyl sphingomyelin (d18:1/16:0) (chemid: 100002107)
256	c37529	Num	8	biochemical: sphingomyelin (d18:1/18:1, d18:2/18:0) (chemid: 100002106)
257	c37536	Num	8	biochemical: 12-HETE (chemid: 100002167)
258	c38168	Num	8	biochemical: 16a-hydroxy DHEA 3-sulfate (chemid: 100002126)
259	c38170	Num	8	biochemical: pregnenolone sulfate (chemid: 100002129)
260	c38178	Num	8	biochemical: cis-4-decenoylcarnitine (C10:1) (chemid: 100002259)
261	c38276	Num	8	biochemical: 2,3-dihydroxyisovalerate (chemid: 100002417)
262	c38395	Num	8	biochemical: 12,13-DiHOME (chemid: 62)
263	c38637	Num	8	biochemical: cinnamoylglycine (chemid: 100002253)
264	c38768	Num	8	biochemical: (14 or 15)-methylpalmitate (a17:0 or i17:0) (chemid: 100002945)
265	c39270	Num	8	biochemical: 1-(1-enyl-palmitoyl)-GPE (P-16:0)* (chemid: 100003000)
266	c39271	Num	8	biochemical: 1-(1-enyl-stearoyl)-GPE (P-18:0)* (chemid: 100003001)
267	c39379	Num	8	biochemical: glycooursodeoxycholate (chemid: 100002911)
268	c39592	Num	8	biochemical: S-methylcysteine (chemid: 100002749)
269	c396	Num	8	biochemical: glutarate (C5-DC) (chemid: 339)
270	c39600	Num	8	biochemical: 3-hydroxyhippurate (chemid: 100002122)

Num	Variable	Type	Len	Label
271	c39609	Num	8	biochemical: 16-hydroxypalmitate (chemid: 100002953)
272	c39831	Num	8	biochemical: eicosanedioate (C20-DC) (chemid: 100002951)
273	c39994	Num	8	biochemical: valylleucine (chemid: 100003210)
274	c40010	Num	8	biochemical: leucylalanine (chemid: 100003179)
275	c40045	Num	8	biochemical: leucylglycine (chemid: 100003185)
276	c40406	Num	8	biochemical: trimethylamine N-oxide (chemid: 100003397)
277	c40469	Num	8	biochemical: N1-Methyl-2-pyridone-5-carboxamide (chemid: 100001468)
278	c40473	Num	8	biochemical: hydantoin-5-propionate (chemid: 100002514)
279	c40708	Num	8	biochemical: pregnanediol-3-glucuronide (chemid: 100003470)
280	c40730	Num	8	biochemical: imidazole propionate (chemid: 100003434)
281	c42027	Num	8	biochemical: histidylalanine (chemid: 100003542)
282	c42109	Num	8	biochemical: phosphate (chemid: 461)
283	c42370	Num	8	biochemical: S-1-pyrroline-5-carboxylate (chemid: 35)
284	c42374	Num	8	biochemical: 2-aminobutyrate (chemid: 1128)
285	c42382	Num	8	biochemical: S-adenosylhomocysteine (SAH) (chemid: 197)
286	c42398	Num	8	biochemical: 1-stearoyl-GPE (18:0) (chemid: 100001461)
287	c42420	Num	8	biochemical: erythronate* (chemid: 100001320)
288	c42446	Num	8	biochemical: 1-palmitoyl-2-linoleoyl-GPC (16:0/18:2) (chemid: 1537)
289	c42448	Num	8	biochemical: 1-stearoyl-2-oleoyl-GPE (18:0/18:1) (chemid: 100001856)
290	c42449	Num	8	biochemical: 1-palmitoyl-2-linoleoyl-GPE (16:0/18:2) (chemid: 100001870)
291	c42450	Num	8	biochemical: 1-stearoyl-2-arachidonoyl-GPC (18:0/20:4) (chemid: 100001869)
292	c42459	Num	8	biochemical: sphingomyelin (d18:2/16:0, d18:1/16:1)* (chemid: 100004329)
293	c42463	Num	8	biochemical: sphingomyelin (d18:1/14:0, d16:1/16:0)* (chemid: 100004328)
294	c42489	Num	8	biochemical: 2-hydroxydecanoate (chemid: 100004089)
295	c42574	Num	8	biochemical: glycohyocholate (chemid: 100004083)
296	c43239	Num	8	biochemical: S-allylcysteine (chemid: 100004509)
297	c43249	Num	8	biochemical: N-delta-acetylornithine (chemid: 100004523)
298	c43255	Num	8	biochemical: N-acetyl-1-methylhistidine* (chemid: 100004299)
299	c43264	Num	8	biochemical: (R)-3-hydroxybutyrylcarnitine (chemid: 100003926)
300	c43266	Num	8	biochemical: 2-aminophenol sulfate (chemid: 100004322)
301	c43343	Num	8	biochemical: 2-aminooctanoate (chemid: 100004227)
302	c43374	Num	8	biochemical: indolin-2-one (chemid: 100004318)
303	c43400	Num	8	biochemical: 2-piperidinone (chemid: 100004295)
304	c43488	Num	8	biochemical: N-acetylcarnosine (chemid: 100004046)
305	c43761	Num	8	biochemical: 2-aminoheptanoate (chemid: 100004542)
306	c43807	Num	8	biochemical: bilirubin (chemid: 1090)
307	c43829	Num	8	biochemical: gamma-glutamylvaline (chemid: 100001126)
308	c443	Num	8	biochemical: aspartate (chemid: 234)
309	c44526	Num	8	biochemical: 3-methyl-2-oxobutyrate (chemid: 100000936)

Num	Variable	Type	Len	Label
310	c44656	Num	8	biochemical: isovalerate (C5) (chemid: 100000708)
311	c44664	Num	8	biochemical: glutarylcarnitine (C5-DC) (chemid: 100001593)
312	c44675	Num	8	biochemical: docosahexaenoate (DHA; 22:6n3) (chemid: 100000665)
313	c44681	Num	8	biochemical: palmitoylcarnitine (C16) (chemid: 100000776)
314	c44872	Num	8	biochemical: gamma-glutamylmethionine (chemid: 100001313)
315	c44876	Num	8	biochemical: gamma-CEHC (chemid: 100002094)
316	c44877	Num	8	biochemical: N-palmitoyl-sphingosine (d18:1/16:0) (chemid: 1518)
317	c44878	Num	8	biochemical: methionine sulfone (chemid: 100004635)
318	c45095	Num	8	biochemical: 2-methylbutyrylcarnitine (C5) (chemid: 100001509)
319	c45413	Num	8	biochemical: O-sulfo-L-tyrosine (chemid: 100005384)
320	c45428	Num	8	biochemical: N-acetylmethionine sulfoxide (chemid: 100005463)
321	c45951	Num	8	biochemical: 1-linolenoyl-GPC (18:3)* (chemid: 100005350)
322	c46111	Num	8	biochemical: guaiacol sulfate (chemid: 100004208)
323	c46115	Num	8	biochemical: 21-hydroxypregnenolone disulfate (chemid: 100001999)
324	c46142	Num	8	biochemical: mannitol/sorbitol (chemid: 100001740)
325	c46146	Num	8	biochemical: 4-methylcatechol sulfate (chemid: 100004111)
326	c46165	Num	8	biochemical: 3-methyl catechol sulfate (1) (chemid: 100004112)
327	c46172	Num	8	biochemical: 5alpha-pregnan-diol disulfate (chemid: 100002015)
328	c46223	Num	8	biochemical: linoleoylcarnitine (C18:2)* (chemid: 100003151)
329	c46225	Num	8	biochemical: pyroglutamine* (chemid: 100001540)
330	c46259	Num	8	biochemical: X - 21258
331	c46266	Num	8	biochemical: X - 15486
332	c46283	Num	8	biochemical: X - 15461
333	c46295	Num	8	biochemical: X - 21286
334	c46347	Num	8	biochemical: X - 11381
335	c46354	Num	8	biochemical: X - 21310
336	c46356	Num	8	biochemical: X - 21312
337	c46363	Num	8	biochemical: X - 21319
338	c46364	Num	8	biochemical: X - 12847
339	c46384	Num	8	biochemical: X - 21339
340	c46390	Num	8	biochemical: X - 11308
341	c46398	Num	8	biochemical: X - 21353
342	c46409	Num	8	biochemical: X - 21364
343	c46417	Num	8	biochemical: X - 13866
344	c46428	Num	8	biochemical: X - 21383
345	c46460	Num	8	biochemical: X - 11444
346	c46466	Num	8	biochemical: X - 11843
347	c46486	Num	8	biochemical: X - 21441
348	c46507	Num	8	biochemical: X - 11850

Num	Variable	Type	Len	Label
349	c46510	Num	8	biochemical: X - 12544
350	c46512	Num	8	biochemical: X - 21467
351	c46515	Num	8	biochemical: X - 21470
352	c46516	Num	8	biochemical: X - 21471
353	c46517	Num	8	biochemical: X - 16946
354	c46521	Num	8	biochemical: X - 11852
355	c46548	Num	8	biochemical: 3-methylglutarylcarnitine (2) (chemid: 100005850)
356	c46590	Num	8	biochemical: X - 07765
357	c46592	Num	8	biochemical: X - 11299
358	c46594	Num	8	biochemical: X - 11372
359	c46601	Num	8	biochemical: X - 11470
360	c46602	Num	8	biochemical: X - 11478
361	c46607	Num	8	biochemical: X - 11849
362	c46608	Num	8	biochemical: X - 11880
363	c46613	Num	8	biochemical: X - 12216
364	c46616	Num	8	biochemical: X - 12411
365	c46623	Num	8	biochemical: X - 12729
366	c46624	Num	8	biochemical: X - 12798
367	c46632	Num	8	biochemical: X - 14056
368	c46633	Num	8	biochemical: X - 12844
369	c46636	Num	8	biochemical: X - 12849
370	c46640	Num	8	biochemical: X - 15469
371	c46645	Num	8	biochemical: X - 13728
372	c46646	Num	8	biochemical: X - 13835
373	c46657	Num	8	biochemical: X - 14939
374	c46661	Num	8	biochemical: X - 15245
375	c46662	Num	8	biochemical: X - 15492
376	c46666	Num	8	biochemical: X - 15728
377	c46673	Num	8	biochemical: X - 16576
378	c46674	Num	8	biochemical: X - 21607
379	c46681	Num	8	biochemical: X - 16935
380	c46683	Num	8	biochemical: X - 16944
381	c46685	Num	8	biochemical: X - 16964
382	c46690	Num	8	biochemical: X - 18901
383	c46695	Num	8	biochemical: X - 18913
384	c46700	Num	8	biochemical: X - 18922
385	c46701	Num	8	biochemical: X - 19141
386	c46710	Num	8	biochemical: X - 17690
387	c46799	Num	8	biochemical: oleoyl-linoleoyl-glycerol (18:1/18:2) [2] (chemid: 100002990)

Num	Variable	Type	Len	Label
388	c46902	Num	8	biochemical: X - 21733
389	c46905	Num	8	biochemical: X - 21736
390	c46909	Num	8	biochemical: X - 21740
391	c46932	Num	8	biochemical: X - 12104
392	c46957	Num	8	biochemical: gulonate* (chemid: 100001586)
393	c46960	Num	8	biochemical: sulfate* (chemid: 100002528)
394	c46972	Num	8	biochemical: X - 21796
395	c46977	Num	8	biochemical: X - 15503
396	c46997	Num	8	biochemical: X - 12822
397	c47006	Num	8	biochemical: X - 21829
398	c47013	Num	8	biochemical: X - 16570
399	c47112	Num	8	biochemical: etiocholanolone glucuronide (chemid: 100005403)
400	c47118	Num	8	biochemical: 2-palmitoleoyl-GPC* (16:1)* (chemid: 100001561)
401	c47153	Num	8	biochemical: sphingomyelin (d18:1/24:1, d18:2/24:0)* (chemid: 100005986)
402	c47154	Num	8	biochemical: sphingomyelin (d18:2/14:0, d18:1/14:1)* (chemid: 100005985)
403	c47301	Num	8	biochemical: X - 18887
404	c47417	Num	8	biochemical: X - 22162
405	c47439	Num	8	biochemical: X - 13507
406	c47642	Num	8	biochemical: X - 12101
407	c47664	Num	8	biochemical: X - 13658
408	c47670	Num	8	biochemical: X - 18899
409	c47671	Num	8	biochemical: X - 18921
410	c47673	Num	8	biochemical: X - 19299
411	c47687	Num	8	biochemical: X - 12100
412	c47708	Num	8	biochemical: X - 12283
413	c47783	Num	8	biochemical: X - 22519
414	c47802	Num	8	biochemical: X - 16397
415	c47804	Num	8	biochemical: X - 16580
416	c47872	Num	8	biochemical: X - 17340
417	c47886	Num	8	biochemical: bilirubin (E,Z or Z,E)* (chemid: 100001951)
418	c47905	Num	8	biochemical: X - 12026
419	c47929	Num	8	biochemical: X - 12707
420	c47959	Num	8	biochemical: X - 13553
421	c48001	Num	8	biochemical: X - 17351
422	c48047	Num	8	biochemical: X - 18886
423	c48076	Num	8	biochemical: X - 22771
424	c48152	Num	8	biochemical: glucose (chemid: 572)
425	c48153	Num	8	biochemical: mannose (chemid: 803)
426	c48182	Num	8	biochemical: myristoleoylcarnitine (C14:1)* (chemid: 100006051)

Num	Variable	Type	Len	Label
427	c48195	Num	8	biochemical: fructose (chemid: 878)
428	c48255	Num	8	biochemical: arabonate/xylonate (chemid: 100006115)
429	c48258	Num	8	biochemical: 1-oleoyl-GPC (18:1) (chemid: 100001272)
430	c48351	Num	8	biochemical: N1-methylinosine (chemid: 100001409)
431	c48425	Num	8	biochemical: phenylacetylcarnitine (chemid: 100006108)
432	c48429	Num	8	biochemical: methyl-4-hydroxybenzoate sulfate (chemid: 100006116)
433	c48441	Num	8	biochemical: 4-hydroxychlorothalonil (chemid: 100006082)
434	c48448	Num	8	biochemical: 3-hydroxypyridine sulfate (chemid: 100006098)
435	c48490	Num	8	biochemical: sphingomyelin (d18:1/20:0, d16:1/22:0)* (chemid: 100006290)
436	c48491	Num	8	biochemical: sphingomyelin (d18:1/20:1, d18:2/20:0)* (chemid: 100006292)
437	c48492	Num	8	biochemical: behenoyl sphingomyelin (d18:1/22:0)* (chemid: 100006294)
438	c48493	Num	8	biochemical: sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)* (chemid: 100006295)
439	c485	Num	8	biochemical: spermidine (chemid: 50)
440	c48698	Num	8	biochemical: 6-hydroxyindole sulfate (chemid: 100006260)
441	c48763	Num	8	biochemical: 3-methoxycatechol sulfate (1) (chemid: 100006375)
442	c48782	Num	8	biochemical: C-glycosyltryptophan (chemid: 100006379)
443	c48841	Num	8	biochemical: p-cresol glucuronide* (chemid: 100006191)
444	c48885	Num	8	biochemical: arabitol/xylitol (chemid: 100006430)
445	c48990	Num	8	biochemical: pyruvate (chemid: 823)
446	c49463	Num	8	biochemical: X - 23587
447	c49466	Num	8	biochemical: X - 23590
448	c49469	Num	8	biochemical: X - 23593
449	c49515	Num	8	biochemical: X - 23639
450	c49517	Num	8	biochemical: X - 23641
451	c49521	Num	8	biochemical: X - 23644
452	c49536	Num	8	biochemical: X - 23659
453	c49557	Num	8	biochemical: X - 23680
454	c49592	Num	8	biochemical: X - 11315
455	c49617	Num	8	biochemical: 1-lignoceroyl-GPC (24:0) (chemid: 100002873)
456	c49637	Num	8	biochemical: X - 23739
457	c49679	Num	8	biochemical: X - 23780
458	c49681	Num	8	biochemical: X - 23782
459	c49883	Num	8	biochemical: X - 23974
460	c5086	Num	8	biochemical: dimethylglycine (chemid: 806)
461	c512	Num	8	biochemical: asparagine (chemid: 917)
462	c513	Num	8	biochemical: creatinine (chemid: 275)
463	c514	Num	8	biochemical: cytidine (chemid: 827)
464	c52234	Num	8	biochemical: glycosyl-N-stearoyl-sphingosine (d18:1/18:0) (chemid: 100001882)
465	c52281	Num	8	biochemical: 2-hydroxybutyrate/2-hydroxyisobutyrate (chemid: 100008928)

Num	Variable	Type	Len	Label
466	c52282	Num	8	biochemical: 2-methylcitrate/homocitrate (chemid: 100008929)
467	c52285	Num	8	biochemical: oleate/vaccenate (18:1) (chemid: 100008930)
468	c52433	Num	8	biochemical: sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)* (chemid: 100006314)
469	c52434	Num	8	biochemical: palmitoyl dihydrosphingomyelin (d18:0/16:0)* (chemid: 100008954)
470	c52435	Num	8	biochemical: sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)* (chemid: 100008956)
471	c52436	Num	8	biochemical: tricosanoyl sphingomyelin (d18:1/23:0)* (chemid: 100008955)
472	c52438	Num	8	biochemical: 1-stearoyl-2-oleoyl-GPC (18:0/18:1) (chemid: 100008904)
473	c52446	Num	8	biochemical: 1-stearoyl-2-linoleoyl-GPE (18:0/18:2)* (chemid: 100008976)
474	c52447	Num	8	biochemical: 1-stearoyl-2-arachidonoyl-GPE (18:0/20:4) (chemid: 100008977)
475	c52449	Num	8	biochemical: 1-stearoyl-2-arachidonoyl-GPI (18:0/20:4) (chemid: 100000616)
476	c52450	Num	8	biochemical: 1-palmitoyl-2-linoleoyl-GPI (16:0/18:2) (chemid: 1528)
477	c52452	Num	8	biochemical: 1-stearoyl-2-linoleoyl-GPC (18:0/18:2)* (chemid: 100008980)
478	c52453	Num	8	biochemical: 1-oleoyl-2-linoleoyl-GPC (18:1/18:2)* (chemid: 100008981)
479	c52461	Num	8	biochemical: 1-palmitoyl-2-oleoyl-GPC (16:0/18:1) (chemid: 1539)
480	c52462	Num	8	biochemical: 1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6) (chemid: 100008914)
481	c52464	Num	8	biochemical: 1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)* (chemid: 100008990)
482	c52468	Num	8	biochemical: 1-stearoyl-2-linoleoyl-GPI (18:0/18:2) (chemid: 100008994)
483	c52470	Num	8	biochemical: 1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)* (chemid: 100008984)
484	c52475	Num	8	biochemical: 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* (chemid: 100008999)
485	c52477	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)* (chemid: 100009005)
486	c52478	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)* (chemid: 100009007)
487	c52483	Num	8	biochemical: X - 24295
488	c52495	Num	8	biochemical: sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)* (chemid: 100009025)
489	c52524	Num	8	biochemical: X - 24328
490	c52533	Num	8	biochemical: X - 24337
491	c52603	Num	8	biochemical: 1,2-dilinoeloyl-GPC (18:2/18:2) (chemid: 100008903)
492	c52605	Num	8	biochemical: sphinganine-1-phosphate (chemid: 100001876)
493	c52608	Num	8	biochemical: linoleoyl ethanolamide (chemid: 100006726)
494	c52614	Num	8	biochemical: 1-(1-enyl-stearoyl)-2-oleoyl-GPE (P-18:0/18:1) (chemid: 100008919)
495	c52615	Num	8	biochemical: sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0) (chemid: 100008920)
496	c52636	Num	8	biochemical: X - 24422
497	c52665	Num	8	biochemical: X - 24435
498	c52669	Num	8	biochemical: 1-palmitoyl-2-oleoyl-GPI (16:0/18:1)* (chemid: 100009066)
499	c52673	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)* (chemid: 100009002)
500	c52677	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-linoleoyl-GPE (P-16:0/18:2)* (chemid: 100009069)
501	c52682	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)* (chemid: 100009009)
502	c52689	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)* (chemid: 100009014)
503	c527	Num	8	biochemical: lactate (chemid: 482)
504	c52710	Num	8	biochemical: 1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)* (chemid: 100009131)

Num	Variable	Type	Len	Label
505	c52713	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)* (chemid: 100009160)
506	c52716	Num	8	biochemical: 1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)* (chemid: 100009162)
507	c52726	Num	8	biochemical: 1-stearoyl-2-oleoyl-GPI (18:0/18:1)* (chemid: 100009181)
508	c52748	Num	8	biochemical: 1-(1-enyl-stearoyl)-2-linoleoyl-GPE (P-18:0/18:2)* (chemid: 100009225)
509	c52772	Num	8	biochemical: X - 24455
510	c52773	Num	8	biochemical: X - 24456
511	c528	Num	8	biochemical: alpha-ketoglutarate (chemid: 93)
512	c52865	Num	8	biochemical: X - 24544
513	c52867	Num	8	biochemical: X - 24546
514	c52877	Num	8	biochemical: X - 24556
515	c52909	Num	8	biochemical: X - 24588
516	c52974	Num	8	biochemical: glycochenodeoxycholate 3-sulfate (chemid: 100006641)
517	c52975	Num	8	biochemical: glycodeoxycholate 3-sulfate (chemid: 100006642)
518	c52983	Num	8	biochemical: glycochenodeoxycholate glucuronide (1) (chemid: 100009264)
519	c52988	Num	8	biochemical: adipoylcarnitine (C6-DC) (chemid: 100006614)
520	c53	Num	8	biochemical: glutamine (chemid: 563)
521	c53013	Num	8	biochemical: glycosyl-N-palmitoyl-sphingosine (d18:1/16:0) (chemid: 100009272)
522	c53031	Num	8	biochemical: methylsuccinoylcarnitine (chemid: 100009275)
523	c531	Num	8	biochemical: 3-hydroxy-3-methylglutarate (chemid: 112)
524	c53127	Num	8	biochemical: X - 24699
525	c53176	Num	8	biochemical: 1-linoleoyl-2-linolenoyl-GPC (18:2/18:3)* (chemid: 100009343)
526	c53223	Num	8	biochemical: palmitoleoylcarnitine (C16:1)* (chemid: 100009406)
527	c53224	Num	8	biochemical: pimeloylcarnitine/3-methyladipoylcarnitine (C7-DC) (chemid: 100009407)
528	c53230	Num	8	biochemical: 3-hydroxyhexanoate (chemid: 100006367)
529	c53231	Num	8	biochemical: thioproline (chemid: 100009232)
530	c53257	Num	8	biochemical: palmitoleoylcholine (chemid: 100009334)
531	c53262	Num	8	biochemical: dihomo-linolenoyl-choline (chemid: 100009335)
532	c53263	Num	8	biochemical: docosahexaenoylcholine (chemid: 100009333)
533	c54	Num	8	biochemical: tryptophan (chemid: 565)
534	c54805	Num	8	biochemical: 3beta-hydroxy-5-cholestenoate (chemid: 100006370)
535	c54840	Num	8	biochemical: X - 24812
536	c54907	Num	8	biochemical: hexanoylglutamine (chemid: 100001733)
537	c54914	Num	8	biochemical: gamma-glutamylserine (chemid: 100009231)
538	c54923	Num	8	biochemical: beta-citrylglutamate (chemid: 100003271)
539	c54979	Num	8	biochemical: N-stearoyl-sphingosine (d18:1/18:0)* (chemid: 1547)
540	c55	Num	8	biochemical: beta-alanine (chemid: 244)
541	c55015	Num	8	biochemical: gamma-glutamyl-alpha-lysine (chemid: 100010901)
542	c55017	Num	8	biochemical: 4-hydroxyphenylacetylglutamine (chemid: 100010850)
543	c55072	Num	8	biochemical: 2-oxoarginine* (chemid: 100002784)

Num	Variable	Type	Len	Label
544	c554	Num	8	biochemical: adenine (chemid: 880)
545	c566	Num	8	biochemical: phenylpyruvate (chemid: 241)
546	c569	Num	8	biochemical: caffeine (chemid: 849)
547	c57	Num	8	biochemical: glutamate (chemid: 561)
548	c57330	Num	8	biochemical: lignoceroyl sphingomyelin (d18:1/24:0) (chemid: 100006298)
549	c57331	Num	8	biochemical: behenoyl dihydrosphingomyelin (d18:0/22:0)* (chemid: 100009026)
550	c57365	Num	8	biochemical: myristoyl dihydrosphingomyelin (d18:0/14:0)* (chemid: 100009038)
551	c57370	Num	8	biochemical: lactosyl-N-nervonoyl-sphingosine (d18:1/24:1)* (chemid: 100015620)
552	c57714	Num	8	biochemical: X - 24947
553	c57716	Num	8	biochemical: X - 24949
554	c57720	Num	8	biochemical: X - 24953
555	c58	Num	8	biochemical: glycine (chemid: 340)
556	c587	Num	8	biochemical: gluconate (chemid: 338)
557	c59	Num	8	biochemical: histidine (chemid: 355)
558	c590	Num	8	biochemical: hypotaurine (chemid: 358)
559	c594	Num	8	biochemical: nicotinamide (chemid: 432)
560	c60	Num	8	biochemical: leucine (chemid: 397)
561	c606	Num	8	biochemical: uridine (chemid: 535)
562	c607	Num	8	biochemical: trans-urocanate (chemid: 537)
563	c62636	Num	8	biochemical: X - 25343
564	c62664	Num	8	biochemical: X - 25371
565	c62716	Num	8	biochemical: X - 25419
566	c62717	Num	8	biochemical: X - 25420
567	c62719	Num	8	biochemical: X - 25422
568	c62963	Num	8	biochemical: X - 25519
569	c62964	Num	8	biochemical: X - 25520
570	c63	Num	8	biochemical: cholesterol (chemid: 266)
571	c63560	Num	8	biochemical: X - 25790
572	c63908	Num	8	biochemical: X - 25957
573	c64	Num	8	biochemical: phenylalanine (chemid: 460)

Data Set Name: metabolomics_meta_data.sas7bdat

Num	Variable	Type	Len	Format	Informat
1	sortorder	Num	8	BEST12.	BEST32.
2	biochemical	Char	54	\$54.	\$54.
3	superpath	Char	11	\$11.	\$11.
4	subpath	Char	49	\$49.	\$49.
5	chemid	Num	8	BEST12.	BEST32.
6	compound	Char	200		