

Reference Material 8231

Frozen Human Plasma Suite for Metabolomics

REFERENCE MATERIAL INFORMATION SHEET

Purpose: This Reference Material (RM) is intended to be used as quality assurance/quality control (QA/QC) materials for routine metabolomic measurements, differential studies, interlaboratory comparisons, laboratory and instrument qualifications, and trainings by the metabolomics community. RM 8231 can be used to assess comparability between studies and laboratories, or among different measurement approaches. RM 8231 can also be used to assess the confidence of metabolite annotation and identification.

Description: A unit of RM 8231 consists of two vials each of three phenotypes: Diabetic Plasma, Hypertriglyceridemic Plasma, and African-American Plasma pools. Each vial contains approximately 1.0 mL of frozen human plasma.

Non-Certified Values: Non-certified values do not provide metrological traceability to the International System of Units (SI) or other higher order reference system, however, represents the best estimation of the true value based upon the available data [1]. Non-certified metabolite identities (Metabolomics Standards Initiative [MSI] level 2 [2]) present in RM 8231 are listed in Tables 1–3. These tables are also available as a download from the details page https://shop.nist.gov/ccrz_ProductDetails?sku=8231&cccl=en_US. This information is the best metabolite annotation/identification estimate based on currently available information as determined by liquid chromatography tandem mass spectrometry (LC-MS/MS) analyses and comparison to the NIST 20 Mass Spectral Library, mzVault May 2019 Autoprocessed and mzVault May 2019 Reference databases; however, the evidence does not meet the NIST criteria for certification of chemical identity.

Period of Validity: The non-certified values are valid within the measurement uncertainty specified until **25 February 2030**. The metabolite identity assignments are nullified if the material is stored or used improperly, damaged, contaminated, or otherwise modified.

Maintenance of Non-Certified Values: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Reference Material Information Sheet. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (<https://www.nist.gov/srm>).

Safety: This is a human-source material. RM 8231 is a Biosafety Level 2 material and should be handled according to applicable federal, state, and/or local regulations and according to policies and procedures of recipient's organization. The supplier has reported that each donor unit of plasma used in the preparation of this product was tested by FDA-licensed tests and found to be negative for human immunodeficiency virus (HIV), HIV-1 antigen, hepatitis B, surface antigen, and hepatitis C.

Storage: RM 8231 should be stored at -80°C in the original unopened vials, until needed.

Additional Information: Methods used for the analysis of RM 8231 and additional information are provided in Appendix A.

Use: RM 8231 IS INTENDED FOR RESEARCH USE. RM 8231 is provided as frozen plasma that should be allowed to thaw at room temperature for no greater than 60 minutes prior to use. After the material is thawed, it should be used immediately. The contents of the vial should be gently mixed prior to removal of a test portion for analysis. Precautions should be taken to avoid exposure to strong UV light, direct sunlight and heat.

Index	Name	INCHIKEY
1	(2S)-2-(carbamoylamino)-4-(methylsulfanyl)butanoic acid	DEWDMTSMCKXBNP-BYPYZUCNSA-N
2	(3R,4R,5R)-1,3,4,5,6-Pentahydroxyhexan-2-one	BJHKXHVXCXFLS-PUFIMZNGSA-N
3	1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	STEYNUVPFMIUOY-UHFFFAOYSA-N
4	1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid	BWKMGYQJPOAASG-UHFFFAOYSA-N
5	1,2-Dioleoyl-3-trimethylammoniumpropane cation	FVXDQWZBHIXIEJ-LNDKUQBDSA-N
6	1,2-Dioleoyl-sn-glycero-3-phosphate	KWVJHCQQUFDPLU-YEUCEMRASA-N
7	1,2-Dipalmitoyl-sn-glycero-O-ethyl-3-phosphatidylcholine cation	VBZSUWNESITEBV-KHBQWKRXSA-N
8	1,4-Dibutyl benzene-1,4-dicarboxylate	LQLQDKBJAILIQ-UHFFFAOYSA-N
9	11-Hydroxy-12E,14Z-eicosadienoic acid	HDMIRVFIVOGVIC-YTLDOUCOSA-N
10	13-Docosenamide	UAUDZVJPLUQNMU-KTKRTIGZSA-N
11	13-Hydroxy-9Z,11E-octadecadienoic acid, cholesteryl ester	RZXYPYUQZUHPD-ZCNQENXSA-N
12	15-Hydroxy-11Z,13E-eicosadienoic acid	ZTRWPEHMGCHTIT-QWAPMFBSA-N
13	1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine	SIEDNCDNGMIKST-IYEJTHTFSA-N
14	1H-Indole-4-carboxaldehyde	JFDDFGLNZWNJTK-UHFFFAOYSA-N
15	1-O-Hexadecyl-2-arachidonoyl-sn-glycero-3-phosphocholine	DUUSFCFBREELS-LXDDVLOTSA-N
16	1-O-Hexadecyl-2-O-(2E-butenoyl)-sn-glyceryl-3-phosphocholine	SRZBVCCSIMMDOV-QPSGOUHRSA-N
17	1-O-Hexadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	RZNRKXGAJMGMLIM-RUZDIDTESA-N
18	1-Palmitoyl-2-lauroyl-sn-glycero-3-phosphorylcholine	OVRJLLUJKRFEBG-UUWRZSSWSA-N
19	1-Palmitoyl-3-oleoyl-sn-glycero-2-phosphoethanolamine	BLMYNJDXEOSYBR-OTMQOQLSA-N
20	2-(3-Carboxypropionylamino)-4-methylsulfanylbutyric acid	CZFFMUMOBXJDU-UHFFFAOYSA-N
21	2,4-Dihydroxybenzoic acid	UIAFKZKHHVMJGS-UHFFFAOYSA-N
22	2,6-Dihydroxybenzoic acid	AKEUNCKRJATALU-UHFFFAOYSA-N
23	2.alpha.-Mannobiose	HIWPGCMGAMJNRG-VXSGSMIHSAN
24	2-[(Dibenzylamino)carbonyl]benzoic acid	NVRSHPPQVYMIJAOV-UHFFFAOYSA-N
25	2-Aminoindan-2-carboxylic acid	UHQFXIWMMAQOCAN-UHFFFAOYSA-N
26	2-Methoxybenzoic acid	ILUJQPXNACGAN-UHFFFAOYSA-N
27	2-Pentenedioic acid, 2-octyl-	NIXDINZDFZJZHGLUAWRHEFSA-N
28	3-(2-Nitro-1-propenyl)indole	BPAQTDYDNBMYAM-SOFGYWHQSA-N
29	3-(Carboxymethyl)-1-.beta.-D-glucopyranosyl-1H-indole	MVSQEPAMLRIRW-YMILTQATSA-N
30	3,4-Dihydroxybenzenesulfonic acid	LTPDITODOAWRU-UHFFFAOYSA-N
31	3,5-Dichlorosalicylic acid	CNJGWCQEGROXEE-UHFFFAOYSA-N
32	3,5-Dihydroxybenzoic acid	UYEMGAFJOZZIFP-UHFFFAOYSA-N
33	3,5-Di-tert-butyl-2-hydroxybenzaldehyde	RRIQVLZDOZPJTH-UHFFFAOYSA-N
34	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	DOZRDZLFLOODMB-UHFFFAOYSA-N
35	3,6-Dichloro-2-hydroxybenzoic acid	FKIKPQHMMWFZEB-UHFFFAOYSA-N
36	3-Cyclohexyl-1,1-dimethylurea	PZWXRYRDNQYUIIU-UHFFFAOYSA-N
37	3-Cyclopentylalanine	KDYAKYRBGLKMAK-UHFFFAOYSA-N
38	3-Hydroxybutyric acid	WHBMMWSBFZVSSR-UHFFFAOYSA-N
39	3-Methoxybenzoic acid	XHQZJYCNDZAGLW-UHFFFAOYSA-N
40	3-Methoxysalicylic acid	AUZQQIPZESHNMG-UHFFFAOYSA-N
41	3-Succinoylpyridine	JGSUNMCABQUBOY-UHFFFAOYSA-N
42	4-(Methylamino)-4-(3-pyridyl)butyric acid	WERGLUDJRKXIV-UHFFFAOYSA-N
43	4.beta.-Hydroxycholesterol 4-acetate	CPAJTVKJFMIGFR-UOVLKSFCSA-N
44	4-Acetamidobenzoic acid	QCXJEYXVJIFCE-UHFFFAOYSA-N
45	4-Dodecylbenzenesulfonic Acid	KWXICGTUELOLSQ-UHFFFAOYSA-N
46	4-Hydroxybenzaldehyde	RGHHSNMVTDWUBI-UHFFFAOYSA-N
47	4-Hydroxybutyric acid	SIZRECIHVVDYJC-UHFFFAOYSA-N
48	4-Indolecarbaldehyde	JFDDFGLNZWNJTK-UHFFFAOYSA-N
49	4-Methoxysalicylic acid	MRIXVKKOHPPQFK-UHFFFAOYSA-N
50	4-Oxo-2-nonenal	SEPPVOUBHWNCAN-FNORWQNLISA-N
51	4-Oxo-L-proline	HFXAFXVXPMUQCQ-UHFFFAOYSA-N
52	4-Pyridoxic acid	HXACOUQIXZGNBF-UHFFFAOYSA-N
53	5.alpha.-Dihydrotestosterone sulfate	KYVPVJSGFKNNLD-ABEVXSGRSA-N
54	5.alpha.-Cholestanone	PESKGIQREUXSRR-UXIWKSVISA-N

Table 1. Non-Certified Values for Metabolite Identifications of Pooled Plasma 1, Diabetic Plasma		
Index	Name	INCHIKEY
55	5-Bromotryptophan	KZDNJQUJBMHDJW-UHFFFAOYSA-N
56	5-Methoxysalicylic acid	IZZIIWIAOVZOLBF-UHFFFAOYSA-N
57	6 alpha-Mannobiose	AYRXSINWFIIFAE-JGLDSSWSA-N
58	8-Dehydrocholesterol	VUKORTMHZDZZFR-AEBZCZTFSA-N
59	8-Oxononanoic acid	KNPGTJGXMGNBAY-UHFFFAOYSA-N
60	9-(2,3-Dihydroxypropoxy)-9-oxononanoic acid	BQRISQXLSXCXSC-UHFFFAOYSA-N
61	9,10-Epoxysearic acid	IMYZYCNQZDBZBQ-UHFFFAOYSA-N
62	9-Hydroxy-10E,12Z-octadecadienoic acid, cholesteryl ester	ALWABJCAEDQEGO-SGAXLBQASA-N
63	Acetylcarnosine	BKAYIFDRRZZKNF-VIFPVQESA-N
64	alpha-Guanidinoglutaric acid	RHVVRMJOHATSPD-VKHMYHEASA-N
65	alpha-Tocopherol	GVJHHUAWPYXKBD-IEOSBIPESA-N
66	Androstenediol 3-sulfate	HXJFCUUBVWOORF-LOVVWNRFA-N
67	Androsterone sulfate	ZMITXKRGXGRMKS-LUJQEAJASA-N
68	Asymmetric dimethylarginine	YDGMGEXADBMOJL-LURJTMIESA-N
69	Azelaic acid	BDJRBEYXGNGYIS-UHFFFAOYSA-N
70	Benzocaine	BLFLLBZGZJTVJG-UHFFFAOYSA-N
71	Benzoyl ecgonine	GVGYEFKIHJTNQZ-YIYPIFLZSA-N
72	beta-Gentiobiose	DLRVVLDZNNYCBX-LIZSDCNHSA-N
73	Betaine	KWIUHFFTVRNATP-UHFFFAOYSA-N
74	Bis(2-ethylhexyl) phthalate	BJQHLKABXJIVAM-UHFFFAOYSA-N
75	Carglumic acid	LCQLHJZYVOQKHU-VKHMYHEASA-N
76	Cer(d18:1/24:1(15Z))	VJSNBBSZJDKB-KPEYJIHVSA-N
77	Chenodeoxycholic acid glycine conjugate	GHCZAUBVMUEKPK-XROMFQGDSDA-N
78	Cholesterol	HVYWMOMLDMFJA-DPAQBDIFSA-N
79	Cholesterol sulfate	BHYOQNUELFTYRT-DPAQBDIFSA-N
80	Choline	OEYIOHPDSNJKLS-UHFFFAOYSA-N
81	cis,cis-9,12-Octadecadien-1-ol	JXNPEDYJTDQORS-HZJYTRNSA-N
82	Citraconic acid	HNEGQIOMVPPMNR-IHWYPQMZSA-N
83	Citrulline	RHGKLRLOHDJDR-UHFFFAOYSA-N
84	Cotinine	UIKROCXWUNQSPJ-VIFPVQESA-N
85	Creatine	CVSVTCORWBXHQV-UHFFFAOYSA-N
86	Cyclo(isoleucylpropyl)	ZDACRNZBFJOLTC-UHFFFAOYSA-N
87	D-2-Hydroxyglutaric acid	HWXBTNAVRSUOJR-VKHMYHEASA-N
88	Dehydroepiandrosterone sulfate	CZWCKYRVOZZJNM-USOAJAOKSA-N
89	Deoxyinosine	VGONTNSXDCQUGY-JXBZBNISA-N
90	D-Fructose	RFSUNEUAIZKAJO-ARQDHWQXSA-N
91	DG(16:0/18:1(9Z)/0:0)	YEJYLHKQOBOSCP-OZKTZCCCSA-N
92	DG(16:0/18:2(9Z,12Z)/0:0)	SVXWJFFKLMLOHO-BCTRXSSUSA-N
93	DG(18:1(9Z)/16:0/0:0)	DOZKMFVMCATMEH-ZCXUNETKSA-N
94	DG(18:1(9Z)/18:1(9Z)/0:0)	AFSHUZFNMVJNKX-LLWMBQKSA-N
95	DG(18:1(9Z)/18:2(9Z,12Z)/0:0)	BLZVZPYMHLXLHG-RQOIEFAZSA-N
96	DG(18:2(9Z,12Z)/18:1(9Z)/0:0)	FQNNBQJKEBDPQS-LTEAFHAISA-N
97	D-Glucose	WQZGKKKJIFFOK-GASJEMHNSA-N
98	Dibenzylamine	BWLUMTFWVZZND-UHFFFAOYSA-N
99	Dihomo-alpha-linolenic acid	AHANXAKGNAKFSK-PDBXOOCHSA-N
100	Diethyl phthalate	MQUIGAXCHLFZKX-UHFFFAOYSA-N
101	DL-2-Aminooctanoic acid	AKVBCGOVQXPRLD-UHFFFAOYSA-N
102	DL-Isoleucine	AGPKZVBTJNPAG-UHFFFAOYSA-N
103	DL-Norleucine	LRQKBLKVPFOOQJ-UHFFFAOYSA-N
104	DL-Phenylalanine	COLNVLDHVKWLRT-UHFFFAOYSA-N
105	DL-Threonine	AYFVYJQAPQTCCC-UHFFFAOYSA-N
106	DL-Valine	KZSNJWFQEVHDMF-UHFFFAOYSA-N
107	Dodecadienoic acid	HQSBWLQFLLMKPC-BNFZFUHLSA-N
108	D-Tyrosine tert-butyl ester	DIGHFXIWRPMGSA-LLVKDONJSA-N
109	Formylanthranilic acid	LLLPDUXGHXIXIW-UHFFFAOYSA-N
110	gamma-Glutamylalanine	WQXXXVRAFAKQJM-WHFBIKZSA-N
111	gamma-Glutamylleucine	MYFMARDICOWMQP-UHFFFAOYSA-N
112	Glutaconic acid	XVOUNQNXGKGMMA-OWOJBTEDSA-N
113	Glutamylthreonine	JSIQVRIXMINMTA-ZDLURKLDASA-N
114	Glutamyltyrosine	YSWHPLCDIMUKFE-UHFFFAOYSA-N

Table 1. Non-Certified Values for Metabolite Identifications of Pooled Plasma 1, Diabetic Plasma

Index	Name	INCHIKEY
115	Glutamylvaline	SITLTJHOQZFGG-XPUUQOCRSA-N
116	Glycerophosphocholine	SUHOQUVVVLNYQR-MRVPVSSYSA-N
117	Glycoprotein-phospho-D-mannose	GZCGUPFRVQAUEE-KCDKBNATSA-N
118	Gly-Gly-Leu	XPJBQTCXPJNIFE-ZETCQYMHSA-N
119	Heptaethylene glycol	XPJRQAIZZQMSCM-UHFFFAOYSA-N
120	Hexanoylcarnitine	VVPRQWYTSNDTEA-UHFFFAOYSA-N
121	Hippuric acid	QIAFMBKCNZACKA-UHFFFAOYSA-N
122	Hydroxytyrosol	JUUBCHWRXWPFH-UHFFFAOYSA-N
123	Hypoxanthine	FDGQSTZJBFJUBT-UHFFFAOYSA-N
124	Indoleacetic acid	SEOVTRFCIGRIMH-UHFFFAOYSA-N
125	Indoleacrylic acid	SXOUMVOMIGLHO-AATRIKPKSA-N
126	Indolelactic acid	XGILAAAMKEQUXLS-UHFFFAOYSA-N
127	Indoxyl sulfate	BXFFHSIDQOFMLE-UHFFFAOYSA-N
128	Inosine	UGQMRVRMYASKQ-KQYNXXCUSA-N
129	Isoleucyl-Phenylalanine	WMDZARFSMZOO-UHTWSYAYSA-N
130	Isopropyl (9Z,12Z)-9,12-octadecadienoate	XEIOPEQGDYSYOH-MURFETPASA-N
131	Isovanillic acid	LBKFGYZQBSGRHY-UHFFFAOYSA-N
132	Itaconic acid	LVBHYZANLWSRM-UHFFFAOYSA-N
133	Kynurenic acid	HCZHHEIFKROPDY-UHFFFAOYSA-N
134	L,L-Cyclo(leucylprolyl)	SZJNCZMRZAUNQT-UHFFFAOYSA-N
135	L-Acetylcarnitine	RDHQFKQIGNGIED-MRVPVSSYSA-N
136	L-Arginine	ODKSFYDXXFIFQN-UHFFFAOYSA-N
137	Lathosterol	IZVFFXVYBHFHY-SKCNUYALSA-N
138	Laurylsulfuric acid	MOTZDAYCYVMXPC-UHFFFAOYSA-N
139	Lenticin	AOHCBEAZXHZMOR-UHFFFAOYSA-N
140	Leucyl-Arginine	SENJXOPIZNYLHU-BDAKNGLRSA-N
141	Leucylphenylalanine	KFKWRHQBZQICHA-CHWSQXEYSA-N
142	L-Glutamic acid	WHUUTDBJXJRKMK-VKHYHEASA-N
143	L-Glutamine	ZDXPYRJPNDTMRX-GSVOUGTGSA-N
144	L-Histidine	HNDVDQJICIGZPNO-YFKPBYRVSA-N
145	L-Homoserine	UKAUYYFTDYCKQA-UHFFFAOYSA-N
146	Linoleic acid	OYHQOLUKZRVURQ-AVQMFFATSA-N
147	Lisinopril	RLAWWYSOJDYHDC-FQECFTEESA-N
148	L-Kynurenine	YGPSJZOEDVAXAB-QMMMGPBSA-N
149	L-Leucine	ROHFNLRQFUQHCH-YFKPBYRVSA-N
150	L-Lysine	KDXKERNBIXSRK-YFKPBYRVSA-N
151	L-Methionine	FFEARJCKVFRZRR-BYPYZUCNSA-N
152	L-Proline	ONIBWKKTOPOVIA-SCSAIBSYSA-N
153	L-Tryptophan	QIVBCDIJAJPQS-SECBINFSA-N
154	L-Tyrosine	OUYCCCASQSFEME-UHFFFAOYSA-N
155	L-Tyrosine tert-butyl ester	DIGHFXIWRPMGSA-NSHDSACASA-N
156	L-Tyrosine, O-(1,1-dimethylethyl)-	SNZIFNXFAFKRKT-NSHDSACASA-N
157	LysoPA(16:0/0:0)	YNDYKPRNFWPPFU-GOSISDBHSA-N
158	LysoPA(18:1(9Z)/0:0)	WRGQSWVCFNIUNZ-GDCKJWNLSA-N
159	LysoPC(0:0/18:2(9Z,12Z))	LSUXCWJOIAWGOU-UTJQPWESSA-N
160	LysoPC(16:0/0:0)	ASWBKNKHCZGQVJV-HSZRJPASA-N
161	LysoPC(17:0/0:0)	SRRQPVVYXBTRQK-XMMPPIXPASA-N
162	LysoPC(18:0/0:0)	IHNKQIMGVNPMTC-RUZDIDTESA-N
163	LysoPC(18:1(9Z)/0:0)	YAMUFBLWGFICM-PTGWMXDISA-N
164	LysoPC(18:2(9Z,12Z)/0:0)	SPJFYJXNPEZDW-UTJQPWESSA-N
165	LysoPC(O-18:0/0:0)	XKBJVQHMEXMFDZ-AREMUKBSSA-N
166	LysoPC(P-18:0/0:0)	WBOMIOWRFPZMC-AYICAFKVSA-N
167	LysoPE(16:0/0:0)	YVYMBNSKXOXSKW-HXUWFJHSA-N
168	LysoPI(18:2(9Z,12Z)/0:0)	SAHCQBPGXQFTRA-MTWZWNHSA-N
169	Malic acid	BJEYPKJPYRNKOW-UWTATZPHSA-N
170	Malioxamycin	KXQRAPMNPXYGT-VDTYLAMSSA-N
171	Methionine sulfoxide	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
172	Methyl linoleate	WTTJVINHCBLGX-NQLNTRDSA-N
173	Methylcysteine	IDIDJDIHTAOVLG-VKHYHEASA-N
174	MG(18:1(9Z)/0:0/0:0)	RZRNAYUHWVFMIP-MDZDMXLPSA-N

Table 1. Non-Certified Values for Metabolite Identifications of Pooled Plasma 1, Diabetic Plasma		
Index	Name	INCHIKEY
175	Mirtazapine	RONZAEMNMFQXRA-UHFFFAOYSA-N
176	Monoethylhexyl phthalic acid	DJDSLVSQSLW-UHFFFAOYSA-N
177	N-(.alpha.-Linolenoyl)tyrosine	DEQLZTQITSWABQ-GMOGWPNXSA-N
178	N-(2,4-Dinitrophenyl)-L-methionine	DOHZLJDJOSBJFP-UHFFFAOYSA-N
179	N-.alpha.-(tert-Butoxycarbonyl)-L-histidine	AYMLQYFMYHISQO-QMMMGPBSA-N
180	N-[1-Oxo-3-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)propyl]glycine	AHIZXACQJADRO-UHFFFAOYSA-N
181	N2-Acetylornithine	JRLGPAXAGHMNOL-LURJTMIESA-N
182	N-Acetyl-L-tyrosine	CAHKINHBCWCHCF-JTQLQIEISA-N
183	N-Acetylthreonine	PEDXUVCCGOLSNLQ-WUJLRWPWSA-N
184	N-Acetyltryptophan	DZTHIGRZJZPRDV-GFCCVEGCSA-N
185	Nipecotic acid	XLSEXAGTJCILF-UHFFFAOYSA-N
186	n-Octyl sulfate	UZZYXUGECOQHPU-UHFFFAOYSA-N
187	N-Phenylacetylphenylalanine	LIIPHJDKZNTNII-HNNXBMFYSA-N
188	PA(18:1(9Z)/18:1(9Z))	MHUWZNTUIIFHAS-DSSVUWSHSA-N
189	Paliperidone	PMXMIIMHBWHSKN-UHFFFAOYSA-N
190	p-Anisic acid	ZEYHEAKUIGZSGI-UHFFFAOYSA-N
191	Pantothenic acid	GHOKWGTUJEAQD-UHFFFAOYSA-N
192	Paracetamol sulfate	IGTYILLPRJOVYF-UHFFFAOYSA-N
193	PC(14:0/14:0)	CITHEXJVPOWHKC-UUWRZZSWSA-N
194	PC(14:0/16:0)	RFVFOQWKPSOBED-PSXMRANNSA-N
195	PC(15:0/15:0)	LJARBVLDOSWRJT-PSXMRANNSA-N
196	PC(16:0/14:0)	UIXXHROAQSBBOV-PSXMRANNSA-N
197	PC(16:0/16:0)	KILNVBDSWZSGLL-KXQOOQHDSA-N
198	PC(16:0/18:0)	PZNPLUBHRSSFHT-RRHRGVEJSA-N
199	PC(16:0/18:1(9Z))	WTJKGGKOPKCXLL-VYOBOKEJSA-N
200	PC(16:0/18:2(9Z,12Z))	JLPULHDHAOZNI-QTIMHPMXSA-N
201	PC(16:0/20:4(5Z,8Z,11Z,14Z))	IIZPXYDJKNOIY-JXPJXOSSA-N
202	PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	KLTHQSWIRFFBRI-KOQZQRJKA-N
203	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	IESVDEZGAHUQU-ZLBXKVHBSA-N
204	PC(16:1(9Z)/16:1(9Z))	GPWHCUUIQMDELX-VHQDNGOZSA-N
205	PC(18:0/14:0)	MZWGYEJOZNRLE-KXQOOQHDSA-N
206	PC(18:0/16:0)	BYSIMVBLIVBPA-RRHRGVEJSA-N
207	PC(18:0/18:1(9Z))	ATHVAFWAEPLPPQ-QPOMNCEOSA-N
208	PC(18:0/18:2(9Z,12Z))	FORFDCPQKJHEBF-VPUSDGANSAN
209	PC(18:0/20:4(5Z,8Z,11Z,14Z))	PSVRFUPOQYJOOZ-RYIOQAQXSA-N
210	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FAUYAENFVCNTAL-PFFNLMTBSA-N
211	PC(18:1(9Z)/14:0)	KIVAJCJTVPWSRJ-OQHNRNOKSA-N
212	PC(18:1(9Z)/16:0)	RRVPPYNAZJRZFR-VYOBOKEJSA-N
213	PC(18:1(9Z)/18:1(9Z))	SNKAWJBQDLSFF-NVKMUCNASA-N
214	PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	XXKFQJTOJZELMD-JICBSJGISA-N
215	PC(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	LZLVZIFMYXDKCN-QJWFYCHSA-N
216	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	AHWXJDWBIIDPKS-TZUVPVEASA-N
217	PC(O-16:0/20:3(8Z,11Z,14Z))	VYKSGWCIVDQIQR-GBDFIALSA-N
218	PC(O-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	YHSSHPWVFALMBA-IARQOZKNSA-N
219	PC(O-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	QQQQNYAHSSIZBU-HIQTUQZSA-N
220	PC(P-18:0/18:1(9Z))	DSWOVBIRJNAJAF-NVJOKYTBSA-N
221	PC(P-18:0/20:4(5Z,8Z,11Z,14Z))	FHHVIBVPBBRLOR-IYACIECVSA-N
222	PC(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	TXHZYNSTTCIWMJ-RXSQUPBBSA-N
223	p-Cresol sulfate	WGNAKZGUSRVWRH-UHFFFAOYSA-N
224	PE(16:0/18:1(9Z))	FHQVHHIBKUMWTI-OTMQOFLSA-N
225	PE(16:0/18:2(9Z,12Z))	HBZNVZIRJWODIB-NHCUFCNUSA-N
226	PE(16:0/20:4(5Z,8Z,11Z,14Z))	DRIVXEVMDCWLI-CAQMIEAISA-N
227	PE(18:0/18:2(9Z,12Z))	YDTWOEYVDRKKCR-KNERPIHNSA-N
228	PE(18:0/20:4(5Z,8Z,11Z,14Z))	ANRKEHNWKCXDB-BHFWLYLHSA-N
229	PE(P-18:0/18:1(9Z))	XVYPOHCSLJZFED-QZEVRLJSA-N
230	PE(P-18:0/20:4(5Z,8Z,11Z,14Z))	URPXXNCTXCOATD-FXMFQVEGSA-N
231	PE(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FIJPUAJUDAZEY-WAHBYMPSSA-N
232	Phenylacetylglutamine	JFLIEFSWGNOPJJ-JTQLQIEISA-N
233	Phenylalanylmethionine	PYOHODCEOHCZBM-RYUDHWPBSA-N
234	Phenylalanyltryptophan	JMCOUWKXLXDERB-WMZOPTSA-N

Index	Name	INCHIKEY
235	PI(16:0/18:1(9Z))	PDLAMJKMOKWLAJ-KTBSNPQYSA-N
236	PI(18:0/20:4(5Z,8Z,11Z,14Z))	KRTOMQDUKGRFDJ-ZAHDIMDSA-N
237	Pipecolic acid	HXEACLLIILLPRG-RXMQYKEDSA-N
238	Platelet-activating factor	HVAUUPRFYPCOCA-AREMUKBSSA-N
239	p-Octopamine	QHGUCRYDKWKLMG-UHFFFAOYSA-N
240	Polymaltose	DKXNBKWCZZMJT-WELRSGGNSA-N
241	Pregabalin	AYXYPKUFHZROOJ-ZETCQYMHSA-N
242	Pregnanolone sulfate	MENQCVHHONJLU-FZCSVUEKSA-N
243	Prolyl-Glutamine	SHAQGFGGJSLLE-BQBZGAKWSA-N
244	Prolylphenylalanine	IWIANZLCJVYEFX-RYUDHWBSSA-N
245	Prolylproline	RWCOTTLHDJWHRS-YUMQZZPRSA-N
246	Propionylcarnitine	UF AHZIUFPNSHSL-MRVPVSSYSA-N
247	Punicic acid	CUXYLFPMQMFGL-WPOADVJFSA-N
248	Pyroglutamic acid	ODHCTXKNWHXJC-GSVOUGTGSA-N
249	Ranitidine	VMXUWOKSQNHOC-AUKTHLTGXSA-N
250	SM(d18:1/12:0)	HZCLJRFPMKWHR-FEBLJDHQSA-N
251	SM(d18:1/16:0)	RWKUXQNLWDTSLQ-GWQJGLRPSA-N
252	SM(d18:1/18:0)	LKQLRGMMAHREN-NWBJSICCSA-N
253	SM(d18:1/18:1(9Z))	NBEADXWAAWCCDG-QDDWGVBSA-N
254	SM(d18:1/22:0)	FJJANLYCZUNFSE-TWKUQIQBSA-N
255	SM(d18:1/24:1(15Z))	WKZHECFHXLTLQJ-QYKFWSDDSA-N
256	Sodium Tetradecyl Sulfate	URLJMWZTXZTZR-UHFFFAOYSA-N
257	Stearolic acid	RGTIBVZDHOMOKC-UHFFFAOYSA-N
258	Suberic acid	TYFQFVWCELRYAO-UHFFFAOYSA-N
259	Symmetric dimethylarginine	HVPFXCBJHIIJGS-LURJTMIESA-N
260	Testosterone sulfate	WAQBISPOEAOCOG-DYKIFRCSA-N
261	TG(16:0/18:1(9Z)/18:2(9Z,12Z))	KGLAHZTWGPHKFF-FBSASISJSA-N
262	TG(18:1(9Z)/18:1(9Z)/18:1(9Z))	PHYFQTYBJUILEZ-IUPFWZBBSA-N
263	Tolycaine	UDKICLZCJWQTLQ-UHFFFAOYSA-N
264	Uric acid	LEHOTFFKMJEONL-UHFFFAOYSA-N
265	Vaccenic acid	UWHZIFQPPBDJPM-FPLPWBNSA-N
266	Vanillic acid	WKOLLVMJNQZCI-UHFFFAOYSA-N
267	Vitamin A	FPIPGXGPPQFEQ-HWCYFHEPSA-N

Table 2. Non-Certified Values for Metabolite Identifications of Pooled Plasma 2, Hypertriglyceridemia Plasma

Index	Name	INCHIKEY
1	(2S)-2-(carbamoylamino)-4-(methylsulfanyl)butanoic acid	DEWDMTSMCKXBNP-BYPYZUCNSA-N
2	(2S)-2-[[[(1S)-1-Carboxy-3-methylbutyl]carbamoylamino]glutaric acid	BSGWCSGMXAVYRT-YUMQZZPRSA-N
3	(E,Z)-2,4-Heptadienal	SATICYAWWYRAM-VNKDHWASSA-N
4	1-(1',3'-Benzodioxol-5'-yl)-2-butanamine	VHMRXGAIDDCGDU-UHFFFAOYSA-N
5	1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	STEYNUVPFMIUOY-UHFFFAOYSA-N
6	1-(4-Bromophenyl)-2-(9H-purin-6-ylsulfanyl)ethanol	AJWAPHOSPGHEJW-UHFFFAOYSA-N
7	1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid	BWKMGYQJPOAASG-UHFFFAOYSA-N
8	1,2-Dioleoyl-3-trimethylammoniumpropane cation	KWVJHCQQUFDPLU-YUECEMRASA-N
9	1,2-Dipalmitoyl-sn-glycero-O-ethyl-3-phosphatidylcholine cation	VBZSUWNESITEBV-KHBQWKRXSA-N
10	1,3-Dihydro-(2H)-indol-2-one	JYGFTBXVXVMTGB-UHFFFAOYSA-N
11	1,4-Dibutyl benzene-1,4-dicarboxylate	LQLQDKBJAIIQ-UHFFFAOYSA-N
12	11-Hydroxy-12E,14Z-eicosadienoic acid	HDMIRVFFVOGVIC-YLDOUCOSA-N
13	13-Docosenamide	UAUDZVJPLUQNMU-KTKRTIGZSA-N
14	17-Octadecyanoic acid	DZIIJLFGADWDKMF-UHFFFAOYSA-N
15	1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine	SIEDNCDNGMIKST-IEYJTHTFSA-N
16	1H-Indol-2-ol	JHFAEUCJHBVHB-UHFFFAOYSA-N
17	1H-Indol-3-yl 6-O-((2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yl)-beta-D-glucopyranoside	PCEVWHNBXIFFPJ-OTCFHACESA-N
18	1-O-Hexadecyl-2-arachidonoyl-sn-glycero-3-phosphocholine	DUUSFCFZBREELS-LXDDVLOTS-N
19	1-O-Hexadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	RZNRKXGAJMGJLIM-RUZDIDTESA-N
20	1-Palmitoyl-2-lauroyl-sn-glycero-3-phosphorylcholine	OVRJLLUJKRFEBG-UUWRZZSWSA-N
21	1-Palmitoyl-3-oleoyl-sn-glycero-2-phosphoethanolamine	BLMYNJDXEOSYBR-OTMQOFLSA-N
22	2-(1,3-Dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7H-purin-7-yl)-N-(4-isopropylphenyl)acetamide	HEQDZPHDVAOBLN-UHFFFAOYSA-N
23	2-(3-Carboxypropionylamino)-4-methylsulfanylbutyric acid	CZFFMUMOBXJDU-UHFFFAOYSA-N
24	2,4-Dihydroxybenzoic acid	UIAFKZKHVVMJGS-UHFFFAOYSA-N
25	2,6-Dihydroxybenzoic acid	AKEUNCKRJATALU-UHFFFAOYSA-N
26	2-[(Dibenzylamino)carbonyl]benzoic acid	NVRSHPQVYVMJOAW-UHFFFAOYSA-N
27	2-Aminoindan-2-carboxylic acid	UHQFXIWMQOCAN-UHFFFAOYSA-N
28	2'-Hydroxyacetanilide	ADVGVKWPZRIDURE-UHFFFAOYSA-N
29	2-Methylbutyrylcarnitine	IHCPCBBYTYJYIL-QVDQXJPCSA-N
30	2-Pentenedioic acid, 2-octyl-	NIXDINZDFZJZHGLUAWRHEFSA-N
31	3,4-Dihydroxybenzenesulfonic acid	LTPDITOEDOAWRU-UHFFFAOYSA-N
32	3,5-Di-tert-butyl-2-hydroxybenzaldehyde	RRIQVLZDOZPJTH-UHFFFAOYSA-N
33	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	DOZRDZLFLOODMB-UHFFFAOYSA-N
34	3-Cyclohexyl-1,1-dimethylurea	PZWXYRDNQYUIIU-UHFFFAOYSA-N
35	3-Cyclopentylalanine	KDYAKYRBGLKMAK-UHFFFAOYSA-N
36	3-Hexenoic acid	XXHDAWYDNSXJQM-ONEGZSNKSA-N
37	3-Hydroxybutyric acid	WHBMMWSBFZVSSR-UHFFFAOYSA-N
38	3-Hydroxy-L-proline	BJBUEDPLEOHJGE-IMJSDKUSA-N
39	4.beta.-Hydroxycholesterol 4-acetate	CPAJTVKFMIGFR-UOVLKSFCSA-N
40	4-[3,4,5-Trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzaldehyde	OLZAGZCCJJBKNZ-SYLKREKUSA-N
41	4-Dodecylbenzenesulfonic Acid	KWXICGTUELOLSQ-UHFFFAOYSA-N
42	4-Hydroxybenzaldehyde	RGHHSNMVTDWUBI-UHFFFAOYSA-N
43	4-Hydroxyproline	PMMYEEVYMWASQN-QWVWVQMSA-N
44	4-Oxo-L-proline	HFXAFXVXPMUQCQ-UHFFFAOYSA-N
45	4-Pyridoxic acid	HXACOUQIXZGNBF-UHFFFAOYSA-N
46	5-Acetylamino-6-amino-3-methyluracil	POQOTWQIYYNXAT-UHFFFAOYSA-N
47	5-Acetylamino-6-formylamino-3-methyluracil	RDZNZFGKEVDNPK-UHFFFAOYSA-N
48	5a-Dihydrotestosterone sulfate	KYVPWJSGFKNLD-ABEVXSGRSA-N
49	5alpha-Cholestanone	PESKJQREUXSRR-UXIWKSIUSA-N
50	6-Heptynoic acid	OFCPMJGTZUVUSM-UHFFFAOYSA-N
51	8-Dehydrocholesterol	VUKORTMHZDZZFR-AEBZCZTFSA-N
52	9-(2,3-Dihydroxypropoxy)-9-oxononanoic acid	BQRISQXLSXCXSC-UHFFFAOYSA-N
53	9,10-Epoxyoctadecenoic acid	FBUKMFQXMRGRB-XKJZPPASA-N
54	9,10-Epoxy stearic acid	IMYZYCNQZDBZBQ-UHFFFAOYSA-N
55	Acetaminophen	RZVAJINKPMORJF-UHFFFAOYSA-N
56	Acetaminophen glucuronide	IPROLSVTVHAQLE-BYNIDDHOSA-N
57	Acetylcarnosine	BKAYIFDRRZZKNF-VIFPVQESA-N
58	Allopurinol	OFNXPDPARWPKPPY-UHFFFAOYSA-N

Table 2. Non-Certified Values for Metabolite Identifications of Pooled Plasma 2, Hypertriglyceridemia Plasma

Index	Name	INCHIKEY
59	alpha-Guanidinoglutaric acid	RHVVRMJOHATSPD-VKHMVHEASA-N
60	alpha-Tocopherol	GVJHHUAWPYXKBD-IEOSBIPESA-N
61	Androstenediol 3-sulfate	HXJFCUUBVWOORF-LOVVWNRFSAN-N
62	Androsterone sulfate	ZMITXKRGXGRMKS-LUJOEAJASAN-N
63	Arachidonic acid	YZXBAPSDXZZRGB-DOFZRALJSA-N
64	Asymmetric dimethylarginine	YDGMGEXADBMOMJ-LURJTMIESAN-N
65	Azelaic acid	BDJRBEYXGGNYIS-UHFFFAOYSA-N
66	beta-Ala-Phe	FLJLAJANCPPHDW-JTQLQIEISAN-N
67	beta-Gentiobiose	DLRVVLDZNNYCBX-LIZSDCNHSA-N
68	Betaine	KWIUHFFTVRNATP-UHFFFAOYSA-N
69	Bis(2-ethylhexyl) phthalate	BJQHKLKABXJIVAM-UHFFFAOYSA-N
70	Caffeine	RYYVLZVUVIUVGH-UHFFFAOYSA-N
71	Carglumic acid	LCQLHJZYVOQKHU-VKHMVHEASA-N
72	Cer(d18:1/16:0)	YDNKGFDKCRUKPY-TURZORIXSAN-N
73	Cer(d18:1/24:1(15Z))	VJSBNBOSZJDKB-KPEYJHVSAN-N
74	Chenodeoxycholic acid glycine conjugate	GHCZAUBVMUEKKP-XROMFQGDASAN-N
75	Cholesterol	HVYWMOMLDMIFJA-DPAQBDIFSAN-N
76	Cholesterol sulfate	BHYOQNUELFTYRT-DPAQBDIFSAN-N
77	Choline	OEYIOHPDSNJKLS-UHFFFAOYSA-N
78	cis,cis-9,12-Octadecadien-1-ol	JXNPEDYJTDQORS-HZJYTTRNSAN-N
79	Citraconic acid	HNEGQIOMVPPMNR-IHWYPMQZSAN-N
80	Citric acid	KRKNYBCHXYNGOX-UHFFFAOYSA-N
81	Citrulline	RHGKLRLOHDJJDR-UHFFFAOYSA-N
82	Cotinine	UIKROCXWUNQSPJ-VIFPVBQESAN-N
83	Creatine	CVSVTCORWBXHQV-UHFFFAOYSA-N
84	Cyclo(isoleucylprolyl)	ZDACRNZBFJOLT-UHFFFAOYSA-N
85	D-.alpha.-Cyclohexylglycine	WAMWSIDTKSNDU-SSDOTTSWSAN-N
86	Dehydroepiandrosterone sulfate	CZWCKYRVOZZJNM-USOAJAOKSAN-N
87	DG(16:0/18:1(9Z)/0:0)	YEJYLHKQOBOSCP-OZKTZCCCSAN-N
88	DG(16:0/18:2(9Z,12Z)/0:0)	SVXWJFFKMLLOHO-BCTRXSSUSAN-N
89	DG(18:1(9Z)/18:1(9Z)/0:0)	AFSHUZFNMVJNKX-LLWMBQOKSAN-N
90	DG(18:1(9Z)/18:2(9Z,12Z)/0:0)	BLZVZPYMHLXLHG-RQOIEFAZSAN-N
91	DG(18:2(9Z,12Z)/18:1(9Z)/0:0)	FQNNBQJKEBDPQS-LTEAFHAISAN-N
92	D-Glucose	WQZGKKKJJFFOK-GASJEMHNSAN-N
93	Dibenzylamine	BWLUMTFVWZZND-UHFFFAOYSA-N
94	Dibutyl phthalate	DOIRQSBPFJWKBE-UHFFFAOYSA-N
95	Dihomo-gamma-linolenic acid methyl ester	QHATYOWJCAQINT-JPFHKJGASAN-N
96	Diisobutyl phthalate	MGWAUVDBGNNKXQV-UHFFFAOYSA-N
97	Dioctyl phthalate	MQUIGAXCHLFZKX-UHFFFAOYSA-N
98	DL-2-Aminooctanoic acid	AKVBCGQVQXPRLD-UHFFFAOYSA-N
99	Dodecadienoic acid	HQSBWLQFLMPKC-BNFZFUHLSAN-N
100	Dodecyl phosphate	TVACALAUQMRDF-UHFFFAOYSA-N
101	Epsilon-caprolactam	JBKVHLHDHXXQEQU-UHFFFAOYSA-N
102	Ethyl glucuronide	IWJBVMJWSPZJH-UQGZVRACSAN-N
103	Formylanthranilic acid	LLLDPDUXGHXIXIW-UHFFFAOYSA-N
104	Gal-alpha1,2-Gal	HIWPGCMGAMINRG-VXSGSMIHSAN-N
105	gamma-Glutamylalanine	WQXXVRAFAKQJM-WHFBIKZSAN-N
106	gamma-Glutamylleucine	MYFMARDICOWMQP-UHFFFAOYSA-N
107	Glutamylphenylalanine	XMBSYZWANAQXEV-GHMZBOCLSAN-N
108	Glutarylcarntine	NXJAXUYOQLTISD-SECBINFHSAN-N
109	Glycerophosphocholine	SUHOQUVVVLNYQR-MRVPVSSYSAN-N
110	Glycoprotein-phospho-D-mannose	GZCGUPFRVQAUEE-KCDKBNATSAN-N
111	Gly-Phe-Phe	FEUPVVCGLNXNP-IRXDYDNUSAN-N
112	Heptaethylene glycol	XPJRQAIZZQMCSM-UHFFFAOYSA-N
113	Hexaethylene glycol	IIRDTKBZINWQAW-UHFFFAOYSA-N
114	Hexanoylcarnitine	VVPRQWYTSNDTEA-UHFFFAOYSA-N
115	Hippuric acid	QIAFMBKCNZACKA-UHFFFAOYSA-N
116	Hypoxanthine	FDGQSTZJBFJUBT-UHFFFAOYSA-N
117	Indole-4-carboxaldehyde	JFDDFGLNZWNJTK-UHFFFAOYSA-N
118	Indoleacetyl glutamine	DVJJIAYHBZALO-LBPRGKRZSAN-N

Table 2. Non-Certified Values for Metabolite Identifications of Pooled Plasma 2, Hypertriglyceridemia Plasma

Index	Name	INCHIKEY
119	Indolelactic acid	XGILAAAMKEQUXLS-UHFFFAOYSA-N
120	Indoxyl sulfate	BXFFHSIDQOFMLE-UHFFFAOYSA-N
121	Isoleucyl-Phenylalanine	WMDZARSFSMZOO-UHTWSYAYSA-N
122	Isopropyl (9Z,12Z)-9,12-octadecadienoate	XEIOPEQGDYSYOH-MURFETPASA-N
123	Isovalerylcarnitine	IGQBPDJNUXPEMT-SNVBAGLBSA-N
124	Itaconic acid	LVHBHZANLOWSRM-UHFFFAOYSA-N
125	Kynurenic acid	HCZHHEIFKROPDY-UHFFFAOYSA-N
126	L,L-Cyclo(leucylpropyl)	SZJNCZMRZAUNQT-UHFFFAOYSA-N
127	L-Acetylcarnitine	RDHQFKQINGIED-UHFFFAOYSA-N
128	L-Arginine	ODKSFYDXXFQFN-UHFFFAOYSA-N
129	Lathosterol	IZVFFXVYBHFHY-SKCNUYALSA-N
130	Laurylsulfuric acid	MOTZDAYCYVMXPC-UHFFFAOYSA-N
131	Lenticin	AOHCBEAZXHZMOR-UHFFFAOYSA-N
132	Leucyl-Arginine	SENJXOPIZNYLHU-BDAKNGLRSA-N
133	Leucylphenylalanine	KFKWRHQBZQICHA-CHWSQXEVSAN
134	L-Glutamic acid	WHUUTDBJXRKMK-VKHMHEASAN
135	L-Glutamine	ZDXPYRPNMTMRX-GSVOUGTGSAN
136	L-Histidine	HNDVDQJICGZPNO-YFKPBYRVSAN
137	Linoleic acid	OYHQOLUKZRVURQ-AVQMFFATSAN
138	Lisinopril	RLAWWYSOJDYHDC-FQECFTEESAN
139	DL-Isoleucine	AGPKZVBTJNPAG-UHFFFAOYSA-N
140	L-Leucine	ROHFNLRQFUQHCH-YFKPBYRVSAN
141	L-Methionine	FFEARJCKVFRZRR-BYPYZUCNSAN
142	L-Norleucine	LRQKBLKVPFOOQJ-UHFFFAOYSA-N
143	L-Phenylalanine	COLNVLDHVKWLRT-QMMMGPOBSAN
144	L-Proline	ONIBWKKTOPOVIA-SCSAIBSYSAN
145	L-Tryptophan	QIVBCDIJAJPQS-SECBINFHSAN
146	L-Tyrosine	OUYCCASQSFEME-UHFFFAOYSA-N
147	L-Tyrosine tert-butyl ester	DIGHFXIWRPMGSA-NSHDSACASAN
148	L-Tyrosine, O-(1,1-dimethylethyl)-	SNZIFNXFAFKRKT-NSHDSACASAN
149	LysoPA(18:1(9Z)/0:0)	WRGQSWVCFNIUNZ-GDCKJWNLSAN
150	LysoPC(0:0/18:2(9Z,12Z))	LSUXCWJOIAGOU-UTJQPWESSAN
151	LysoPC(15:0/0:0)	RJZVWDTYEWCUAR-JOCHJYFZSAN
152	LysoPC(16:0/0:0)	ASWBNKHCZGQVJV-HSZRJFAPSAN
153	LysoPC(17:0/0:0)	SRRQPVVYXBTRQK-XMMPXPASAN
154	LysoPC(18:0/0:0)	IHNKQIMGVNPMT-PTZDIDTESAN
155	LysoPC(18:1(9Z)/0:0)	YAMUFBLWGFICM-PTGWMXDISAN
156	LysoPC(18:2(9Z,12Z)/0:0)	SPJFYIJXNPEZDW-UTJQPWESSAN
157	LysoPC(20:0/0:0)	UATOAILWGVYRQS-HHHXNRCGSAN
158	LysoPC(24:0/0:0)	SKJMUADLQLZAGH-WJOKGBTCASAN
159	LysoPC(O-18:0/0:0)	XKBJVQHMEXMFDZ-AREMUKBSSAN
160	LysoPC(P-18:0/0:0)	WBOMIOWRFPZMC-AYICAFKVSAN
161	LysoPE(18:1(9Z)/0:0)	PYVVRVFLRNJLY-MZMPXXGTSAN
162	LysoPI(18:2(9Z,12Z)/0:0)	SAHCQBPXQFTRA-MTWZWNHSAN
163	Metacetamol	QLNWXBAGRTUKKI-UHFFFAOYSA-N
164	Methionine sulfoxide	QEFRNWVLZKMPFJ-YGVKFDHGSAN
165	Methyl linoleate	WTTJVINHCBCLGX-NQLNTRKDSAN
166	Methyleysteine	IDIDJDIHTAOVLG-VKHMHEASAN
167	MG(0:0/18:2(9Z,12Z)/0:0)	IEPGNWMPFDNSD-HZJYTTRNSAN
168	MG(0:0/20:4(5Z,8Z,11Z,14Z)/0:0)	RCRCBTLIHCHWDZ-DOFZRALJSAN
169	MG(18:1(9Z)/0:0/0:0)	RZRNAYUHVWFMP-MDZDMXLPSAN
170	MG(20:4(5Z,8Z,11Z,14Z)/0:0/0:0)	DCPCOKIYJYGMND-DOFZRALJSAN
171	Monoethylhexyl phthalic acid	DJDSLBSVSSOQLW-UHFFFAOYSA-N
172	Monoethyl phthalate	PKIYFBCNICNGJ-UHFFFAOYSA-N
173	N-.alpha.-(tert-Butoxycarbonyl)-L-histidine	AYMLQYFMYHISQO-QMMMGPOBSAN
174	N-[1-Oxo-3-(4-oxo-1,2,3-benzotriazin-3(4H)-yl)propyl]glycine	AIIZXACQGJADRO-UHFFFAOYSA-N
175	N1-Methyl-2-pyridone-5-carboxamide	JLQSSXWTCJPCBC-UHFFFAOYSA-N
176	N2-Acetylorithine	JRLGPAXAGHMNOL-LURJTMIESAN
177	N-Acetyl-L-phenylalanine	CBQISKKFNMDLON-SNVBAGLBSAN
178	N-Acetyl-L-tyrosine	CAHKNHBCWCHCF-JTQLQIEISAN

Table 2. Non-Certified Values for Metabolite Identifications of Pooled Plasma 2, Hypertriglyceridemia Plasma

Index	Name	INCHIKEY
179	N-Acetyltryptophan	DZTHIGRZJZPRDV-GFCCVEGCSA-N
180	NA-Tyr 18:3(9Z,12Z,15Z)	DEQLZTQITSWABQ-GMOGWPNXSA-N
181	Niacinamide	DFFPAKSUCGFBDDE-UHFFFAOYSA-N
182	Oxypurinol	HXNFUBHNUDHIGC-UHFFFAOYSA-N
183	PA(18:1(9Z)/18:1(9Z))	MHUWZNTUIHFHAS-DSSVUWWSHA-N
184	Palmitic amide	HSEMFIZWXHQJAE-UHFFFAOYSA-N
185	Paraxanthine	QUNWUDVFRNGTGO-UHFFFAOYSA-N
186	PC(14:0/14:0)	CITHEXJVPOWHKC-UUWRZSWSA-N
187	PC(14:0/16:0)	RFVVFQQWKPSEB-PSXMRANNSA-N
188	PC(15:0/15:0)	LJARBVLDOSWRJT-PSXMRANNSA-N
189	PC(16:0/14:0)	UIXXHROAQSBBOV-PSXMRANNSA-N
190	PC(16:0/16:0)	KILNVBDSWZSGLL-KXQOOQHDSA-N
191	PC(16:0/18:1(9Z))	WTJKGGKOPKXLL-VYOBKEXSA-N
192	PC(16:0/18:2(9Z,12Z))	JLPULHDHAOZNLQI-ZTIMHPMXSA-N
193	PC(16:0/20:4(5Z,8Z,11Z,14Z))	IIZPXVDJLKNQIY-JXPKJXOSSA-N
194	PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	KLTHQSWIRFFBRI-KOQZQRJKSA-N
195	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	IESVDEZGAHUQUJ-ZLBKXVHBSA-N
196	PC(16:1(9Z)/16:1(9Z))	GPWHCUUIQMGELX-VHQDNGOZSA-N
197	PC(18:0/14:0)	MZWGYEJOZNLQE-KXQOOQHDSA-N
198	PC(18:0/18:1(9Z))	ATHVAWFAEPLPPQ-VRDBWYNSSA-N
199	PC(18:0/18:2(9Z,12Z))	FORFDCPQJHEBF-VPUISDANSAN-N
200	PC(18:0/20:4(5Z,8Z,11Z,14Z))	PSVRFUPOQYJOOZ-RYIOQAQXSA-N
201	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FAUYAENFVCNTAL-PFFNLMTBSA-N
202	PC(18:1(9Z)/14:0)	KIVAJCJTVPWSRJ-OQHNROKXSA-N
203	PC(18:1(9Z)/16:0)	RRVPPYNAJZRFR-VYOBKEXSA-N
204	PC(18:1(9Z)/18:1(9Z))	SNKAWBJQDLSFF-NVMUCNANSA-N
205	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	FVXDQWZBHIXIEJ-LNDKQBDSA-N
206	PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))	XXXFQTJOJZELMD-JICBSJGISA-N
207	PC(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	LZLVZIFMYXDKCN-QJWFYCHSA-N
208	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	AHWWJDWBIIDPKS-TZUVPEASA-N
209	PC(O-16:0/20:3(8Z,11Z,14Z))	VYKSGWCIVDQIQR-GBDFTIALSA-N
210	PC(O-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	YHSSHPWVVALMBA-IARQOZKNSA-N
211	PC(O-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	QQQQNYAHSSIZBU-HIQXTUQZSA-N
212	PC(P-18:0/18:1(9Z))	DSWOVBIRNAJAF-NVJOKYTBSA-N
213	PC(P-18:0/20:4(5Z,8Z,11Z,14Z))	FHHVIBPVBBRLOR-IYACIECVSA-N
214	PC(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	TXHZYNSTTCIWMJ-RXSQUPBGSA-N
215	p-Cresol glucuronide	JPAUCQAJHLSMQW-XPORZQOISA-N
216	p-Cresol sulfate	WGNKAZGUSRVWRH-UHFFFAOYSA-N
217	PE(16:0/18:1(9Z))	FHQVHHIBKUMWTI-OTMQOQLSA-N
218	PE(16:0/18:2(9Z,12Z))	HBZNVZIRJWODIB-NHCUFNCUSA-N
219	PE(16:0/20:4(5Z,8Z,11Z,14Z))	DRIVXEVMDCWFLI-CAQMIEAISA-N
220	PE(18:0/18:1(9Z))	JQKOHRZNEOQJNE-DJEJVYNPSA-N
221	PE(18:0/18:2(9Z,12Z))	YDTWEOEYVDRKKCR-KNERPIHNSA-N
222	PE(18:0/20:4(5Z,8Z,11Z,14Z))	ANRKEHNWXKXDB-BHFWLYLHSA-N
223	PE(P-18:0/18:1(9Z))	XVYPOHCSLJZFED-QZEVRLJSA-N
224	PE(P-18:0/20:4(5Z,8Z,11Z,14Z))	URPXXNCTXCOATD-FXMFQVEGSA-N
225	PE(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FIFPUAJUDAZEY-WAHBYMPSSA-N
226	Phenylacetylglutamine	JFLIEFSWGNOPJJ-JTQLQIEISA-N
227	Phenylalanyltryptophan	JMCOUWKXLXDERB-WMZOPITSA-N
228	PI(16:0/18:1(9Z))	PDLAMJMKOKWLAI-KTBSNPQYSA-N
229	PI(18:0/20:4(5Z,8Z,11Z,14Z))	KRTOMQDUKGRFDJ-ZAHDIIMDSA-N
230	Platelet-activating factor	HVAUUPRFYPCOCA-AREMUKBSSA-N
231	Pregnanolone sulfate	MENQCIVHHONJLU-FZCSVUEKSA-N
232	Pregnenolone sulfate	DIJBBUIOWGGQOP-QGVNFLTSA-N
233	Prolyl-Glutamine	SHAQFGGJSLLE-BQBZGAKWSA-N
234	Prolylphenylalanine	IWIANZLCJVEYFX-RYUDHWBWSA-N
235	Prolylproline	RWCOTTLHDJWHRS-YUMQZZPRSA-N
236	Punicic acid	CUXYLFPMQMGFPL-WPOADVJFSA-N
237	Pyroglutamic acid	ODHCTXKNWHXJC-GSVOUGTGSA-N
238	Quetiapine Sulfoxide	FXJNLPUSSHEDON-UHFFFAOYSA-N

Table 2. Non-Certified Values for Metabolite Identifications of Pooled Plasma 2, Hypertriglyceridemia Plasma

Index	Name	INCHIKEY
239	Quinine	LOUPRKONTZGTKE-USWSZDBUSA-N
240	Serylproline	WBAXJMCUFIXCNI-WDSKDSINSA-N
241	SM(d18:1/12:0)	HZCLJRFPMKWHR-FEBLJDHQSA-N
242	SM(d18:1/16:0)	RWKUXQNLWDTLO-GWQJGLRPSA-N
243	SM(d18:1/18:0)	LKQLRGMMMAHREN-NWBJSICCSA-N
244	SM(d18:1/18:1(9Z))	NBEADXWAAWCCDG-QDDWGVBSA-N
245	SM(d18:1/22:0)	FJANLYCZUNFSE-TWKUQIBSA-N
246	SM(d18:1/24:1(15Z))	WKZHECFHXLTLJ-QYKFWSDSSA-N
247	Sodium Tetradecyl Sulfate	URLJMZWXTZRR-UHFFFAOYSA-N
248	Suberic acid	TYFQVWCELRYAO-UHFFFAOYSA-N
249	Symmetric dimethylarginine	HVPFXCBJHJGS-LURJTMIESA-N
250	Testosterone sulfate	WAQBISPOEAOCOG-DYKIFRCSA-N
251	TG(16:0/18:1(9Z)/18:2(9Z,12Z))	KGLAHZTWGPHKFF-FBSASISJSA-N
252	TG(18:1(9Z)/18:1(9Z)/18:1(9Z))	PHYFQTYBUJLEZ-IUPFWZBJSAN
253	Theophylline	ZFXYFBGIUFBOJW-UHFFFAOYSA-N
254	Tolycaine	UDKICLZCJWQTLN-UHFFFAOYSA-N
255	Uric acid	LEHOTFFKMJEONL-UHFFFAOYSA-N
256	Vaccenic acid	UWHZIFQPPBDJPM-FPLPWBNSA-N
257	Vitamin A	FPIPGXGPPQFEQ-HWCYFHEPSA-N
258	Xanthine	LRFVTYWOQMYALW-UHFFFAOYSA-N

Table 3. Non-Certified Values for Metabolite Identifications of Pooled Plasma 3, African-American Plasma

Index	Name	INCHIKEY
1	(2-Oxo-4-morpholinyl)acetic acid	RCYMJALINOFPDJ-UHFFFAOYSA-N
2	(2S)-2-(carbamoylamino)-4-(methylsulfanyl)butanoic acid	DEWDMTSMCKXBNP-BYPYZUCNSA-N
3	(E,Z)-2,4-Heptadienal	SATICYYAWWYRAM-VNKDHWASSA-N
4	1-(1',3'-Benzodioxol-5'-yl)-2-butanamine	VHMRXGAIDDCGDU-UHFFFAOYSA-N
5	1-(2-Hydroxyethyl)-2,2,6,6-tetramethyl-4-piperidinol	STEYNUVPFMIUOY-UHFFFAOYSA-N
6	1-(4-Bromophenyl)-2-(9H-purin-6-ylsulfanyl)ethanol	AJWAPHOSPGHEJW-UHFFFAOYSA-N
7	1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid	BWKMGYQJPOAASG-UHFFFAOYSA-N
8	1,2,3-cyclopropanetricarboxylic acid	UVIRSBTTXOHPDA-UHFFFAOYSA-N
9	1,2-Dioleoyl-3-trimethylammoniumpropane cation	KWVJHCQQUFDEPLU-YEUCEMRASA-N
10	1,2-Dipalmitoyl-sn-glycero-O-ethyl-3-phosphatidylcholine cation	VBZSUWNESITEBV-KHBQWKRXSA-N
11	1,4-Dibutyl benzene-1,4-dicarboxylate	LQLQDKBJAIIQ-UHFFFAOYSA-N
12	11(R)-HETE	GCZRCCHPLVMMJE-RLZWZWKOSA-N
13	12-HETE	ZNHVWPKMFKADKW-LQWMCKPYSA-N
14	13-Docosenamide	UAUDZVJPLUQNNU-KTKRTIGZSA-N
15	14R,15S-EpETE	JBSCUHKPLGKXKH-ILYOTBPNSA-N
16	16(R)-HETE	JEKNPVYFNMRJG-IFOZKBMWSA-N
17	1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine	SIEDNCDNGMIKST-IYEJTHTFSA-N
18	1-O-Hexadecyl-2-arachidonoyl-sn-glycero-3-phosphocholine	DUUSFCFZBREELS-LXDDVLOTSAN
19	1-O-Hexadecyl-2-O-butanoyl-sn-glyceryl-3-phosphocholine	UVHUBDICYDPLIO-UHFFFAOYSA-N
20	1-O-Hexadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	RZNRKXGAJMLIM-RUZDIDTESA-N
21	1-O-Hexadecyl-sn-glycero-3-phosphocholine	VLBPIWYTPAXCFJ-XMMPXPASA-N
22	1-Palmitoyl-2-lauroyl-sn-glycero-3-phosphorylcholine	OVRJLLUJRFEBG-UUWRZSSWSA-N
23	1-Palmitoyl-3-oleoyl-sn-glycero-2-phosphoethanolamine	BLMYNJDXEOSYBR-OTMQOQLSA-N
24	2-(3-Carboxypropionylamino)-4-methylsulfanylbutyric acid	CZFFMUMOBIDXJU-UHFFFAOYSA-N
25	2,2'-(2-Hydroxyethylazanediyl)diacetic acid	JYXGKAKDAARW-UHFFFAOYSA-N
26	2,4-Dihydroxybenzoic acid	UIAFKZKHHVMJGS-UHFFFAOYSA-N
27	2-[(Dibenzylamino)carbonyl]benzoic acid	NVRSHQPQVYMOAW-UHFFFAOYSA-N
28	2-[1-[4,5-Dihydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]indol-3-yl]acetic acid	ISMUGWMKUVABAZ-XRNKWDJSA-N
29	2-Aminonicotinic acid	KPIVDNYJNOPGEB-UHFFFAOYSA-N
30	2-Methylbutyroylearnitine	IHCPCBBYTYJYL-QVDQXJPCSA-N
31	2-Pentenedioic acid, 2-octyl-	NIXDINZDFZJZHGLUAWRHEFSA-N
32	3-(Carboxymethyl)-1-β-D-glucopyranosyl-1H-indole	MVSQEPAOMLRIRW-YMLTQATSA-N
33	3,4-Dihydroxybenzenesulfonic acid	LTPDITOEAOAWRU-UHFFFAOYSA-N
34	3,5-Dichlorosalicylic acid	CNJGWCQEGROXEE-UHFFFAOYSA-N
35	3,6-Dichloro-2-hydroxybenzoic acid	FKIKPQHMWFZFE-UHFFFAOYSA-N
36	3-[5-(2-Methylpropyl)-3,6-dioxopiperazin-2-yl]propanoic acid	CSRXCVLPMJBQIM-UHFFFAOYSA-N
37	3-Cyclopentylalanine	KDYAKYRBGLKMAK-UHFFFAOYSA-N
38	3-Hydroxybutyric acid	WHBMMWSBFZVSSR-UHFFFAOYSA-N
39	3-Succinoylpyridine	JGSUNMCABQBOUY-UHFFFAOYSA-N
40	4-(Methylamino)-4-(3-pyridyl)butyric acid	WERGJLUDJRKXIV-UHFFFAOYSA-N
41	4.β-Hydroxycholesterol 4-acetate	CPAJTVKFMIGFR-UOVLKSFCSA-N
42	4-Acetamidobenzoic acid	QCXJEYXVJFCE-UHFFFAOYSA-N
43	4-Formyl-2-hydroxybenzoic acid	JQSSYLDZHPASJO-UHFFFAOYSA-N
44	4-Hydroxybenzaldehyde	RGHHSNMVTDWUBI-UHFFFAOYSA-N
45	4-Oxo-L-proline	HFXAFXVXPMUQCQ-UHFFFAOYSA-N
46	5α-Dihydrotestosterone sulfate	KYVPWJSGFKNLND-ABEVXSGRSA-N
47	5α-Cholestanone	PESKGJQREUXSRR-UXIWSIVSA-N
48	5-Bromotryptophan	KZDNJQUJBMHDJW-UHFFFAOYSA-N
49	6-Phenylthiomorpholin-3-one	RTCSYBNOEYGSSX-UHFFFAOYSA-N
50	8-Dehydrocholesterol	VUKORTMHZDZZFR-ABZCZTFSA-N
51	9,10-Epoxy stearic acid	IMZYCNQZDBZBQ-UHFFFAOYSA-N
52	Acetylcarnosine	BKAYIFDRRZZKNF-VIFPVQESA-N
53	Allopurinol	OFCNXPDRARWPPY-UHFFFAOYSA-N
54	α-Guanidinoglutamic acid	RHVVRMJOHATSPD-VKHMVHEASA-N
55	Androstenediol 3-sulfate	HXJFCUUBVWOORF-LOVVWNRFSA-N
56	Androsterone sulfate	ZMITXKRGXGRMKS-LUJOEAJASA-N
57	Asparaginylisoleucine	MQLZLIYFPDIDMZ-SHYZEUOFSAN
58	Asparaginyllucine	HXWUJJADFMXNKA-RQJHMYQMSA-N

Table 3. Non-Certified Values for Metabolite Identifications of Pooled Plasma 3, African-American Plasma

Index	Name	INCHIKEY
59	Betaine	KWIUHFFTVRNPATP-UHFFFAOYSA-N
60	Bis(2-ethylhexyl) phthalate	BJQHLKABXJIVAM-UHFFFAOYSA-N
61	Carglumic acid	LCQLHJZYVOQKHU-VKHMVHEASA-N
62	Cer(d18:1/24:1(15Z))	VJSBNBOSZJDKB-KPEYJHVSAN
63	Cholesterol	HVYWMOMLDIMFJA-DPAQBDFSA-N
64	cis,cis-9,12-Octadecadien-1-ol	JXNPEDYJTDQORS-HZJYTTRNSA-N
65	cis-Aconitic acid	GTZCVFVGUGFEME-IWQZZHSRSA-N
66	Citraconic acid	HNEGQIOMVPPMNR-IHWYPQMZSA-N
67	Citric acid	KRKNYBCHXYNGOX-UHFFFAOYSA-N
68	Cotinine	UIKROCXWUNQSPJ-VIFPVBQESA-N
69	Creatine	CVSVTCORWBXHQV-UHFFFAOYSA-N
70	Dehydroepiandrosterone sulfate	CZWCKYRVOZZJNM-USOAJAOKSA-N
71	DG(16:0/18:1(9Z)/0:0)	YEJYLHKQOBOSCP-OZKTZCCCSA-N
72	DG(16:0/18:2(9Z,12Z)/0:0)	SVXWJFFKLMLOHO-BCTRXSSUSA-N
73	DG(18:1(9Z)/18:1(9Z)/0:0)	AFSHUZFNMVJNKX-LLWMBQOKSA-N
74	DG(18:1(9Z)/18:2(9Z,12Z)/0:0)	BLZVZPYMHLXLHG-RQOIEFAZSA-N
75	DG(18:2(9Z,12Z)/18:1(9Z)/0:0)	FQNNBQJKEBDPQS-LTEAFHAISA-N
76	D-Glucose	WQZGKKKJIFFOK-GASJEMHNSA-N
77	Dibenzylamine	BWLUMTFWVZZND-UHFFFAOYSA-N
78	Dibutyl phthalate	DOIRQSBPFJWKBE-UHFFFAOYSA-N
79	Dicyclohexyl phthalate	VOWAEIGWURALJQ-UHFFFAOYSA-N
80	Dihydro-5-propyl-2(3H)-furanone	VLSVVMPLPMNWBH-UHFFFAOYSA-N
81	Diisobutyl phthalate	MGWAVDBGNNKXQV-UHFFFAOYSA-N
82	Diisooctyl phthalate	IJFPVINAQGWBRJ-UHFFFAOYSA-N
83	Dioctyl phthalate	MQUIGAXCHLFZKX-UHFFFAOYSA-N
84	DL-2-Aminooctanoic acid	AKVBCGQVQXPRLD-UHFFFAOYSA-N
85	Dodecadienoic acid	HQSBWLQFLLMPKC-BNFZFUHLSA-N
86	Dodecyl phosphate	TVACALAUIMRDF-UHFFFAOYSA-N
87	D-Tyrosine tert-butyl ester	DIGHFXIWRPMGSA-LLVKDONJSA-N
88	Edetic Acid	KCXVZYZYPLLWCC-UHFFFAOYSA-N
89	gamma-Glutamylleucine	MYFMARDICOWMQP-UHFFFAOYSA-N
90	Glutaconic acid	XVOUMQNXGKGMMA-OWOJBTEDSA-N
91	Glutaminylisoleucine	XITLYYAIPBBHPX-LKEWCRSYSA-N
92	Glutamylleucine	ARPVSMCNIQAQBO-SFYZADRCSA-N
93	Glutamylphenylalanine	XMBSYZWANAQXEV-GHMZBOCLSA-N
94	Glycerophosphocholine	SUHOQUVVVLLNYQR-MRVPVSSYSA-N
95	Glycoprotein-phospho-D-mannose	GZCGUPFRVQAUEE-KCDKBNATSA-N
96	Glycylleucine	DKEXFJVMVGETOO-LURJTMIESA-N
97	Gly-Gly-Leu	XPJBQTCXPJNIFE-ZETCQYMMSA-N
98	Gly-Phe-Phe	FEUPVVCGLNXPXN-IRXDYDNUSA-N
99	Hexanoylcarnitine	VVPRQWTYSNDTEA-UHFFFAOYSA-N
100	Hippuric acid	QIAFMBKCNZACKA-UHFFFAOYSA-N
101	Histidylleucine	MMFKFJORZBJVNF-UWVGGRQHSA-N
102	Hypoxanthine	FDGQSTZJBFJUBT-UHFFFAOYSA-N
103	Indole-4-carboxaldehyde	JFDDFGLNZWNJTK-UHFFFAOYSA-N
104	Indoleacetic acid	SEOVTRFCIGRIMH-UHFFFAOYSA-N
105	Indoleacrylic acid	SXOUMVOMIGLHO-AATRIKPKSA-N
106	Indolelactic acid	XGILAAAMKEQXLS-UHFFFAOYSA-N
107	Indoxyl sulfate	BXFFHSIDQOFMLE-UHFFFAOYSA-N
108	Inosine	UGQMRVRMYASKQ-KQYNXXCUSA-N
109	Isoleucyl-Arginine	HYXQKVOADYPQEA-XHNCKOQMSA-N
110	Isoleucyl-Histidine	QNBVCZTZNVDMI-FXBDBTDDSA-N
111	Isoleucyl-Leucine	JWBXCSQZLLIOCI-LPEHRKFASA-N
112	Isoleucyl-Phenylalanine	WMDZARSFSMZOOQ-UHTWSYAYSA-N
113	Isoleucyl-Threonine	DRCKHKZYDLJYFQ-YWIQCBGSA-N
114	Isoleucyl-Valine	BCXBIONYYJCSDF-CIUDSAMLSA-N
115	Isopropyl (9Z,12Z)-9,12-octadecadienoate	XEIOPEQGDSYOIH-MURFETPASA-N
116	Isovalerylcarnitine	IGQBPDJNUXPEMT-SNVBAGLBSA-N
117	Itaconic acid	LVHBBZHANLWSRM-UHFFFAOYSA-N
118	Kynurenic acid	HCZHHEIFKROPDY-UHFFFAOYSA-N

Table 3. Non-Certified Values for Metabolite Identifications of Pooled Plasma 3, African-American Plasma

Index	Name	INCHIKEY
119	L-Acetylcarnitine	RDHQFKQIGNGIED-MRVPVSSYSA-N
120	L-Arginine	ODKSFYDXXFIFQN-UHFFFAOYSA-N
121	Lathosterol	IZVFFXVYBHFIHY-SKCNUYALSA-N
122	Laurylsulfuric acid	MOTZDAYCYVMXPC-UHFFFAOYSA-N
123	Lenticin	AOHCBEAZXHZMOR-UHFFFAOYSA-N
124	Leucyl-Arginine	SENJXOPIZNYLHU-BDAKNGLRSA-N
125	Leucyl-Histidine	XWOBNBRUDDUEEY-NXEZACHSA-N
126	Leucyl-Isoleucine	AZLASBBHSLQDB-IVZWLZJFSA-N
127	Leucylleucine	LCPYQJKPJDLB-ZJUJUUORDSA-N
128	Leucylphenylalanine	KFKWRHQBZQICHA-CHWSQXEVSA-N
129	Leucyl-Threonine	LRKCBUIDWAXNEG-CSMHCCOUSA-N
130	L-Glutamic acid	WHUUTDBJXRKMK-VKHMYHEASA-N
131	L-Glutamine	ZDXPYRJPNDTMRX-UHFFFAOYSA-N
132	L-Histidine	HNDVDQJGICZPNO-YFKPBYRVSA-N
133	Linoleic acid	OYHQOLUKZRVRURQ-AVQMFFATSA-N
134	DL-Isoleucine	AGPKZVBTJNPAG-UHFFFAOYSA-N
135	L-Leucine	ROHFNLRQFUQHCH-YFKPBYRVSA-N
136	L-Methionine	FFEARJCKVFRZRR-BYPYUZCNSA-N
137	L-Norleucine	LRQKBLKVPFOOQJ-UHFFFAOYSA-N
138	L-Phenylalanine	COLNVLDHVKWLRT-QMMMGPBSA-N
139	L-Proline	ONIBWKKTOPOVIA-UHFFFAOYSA-N
140	L-Tryptophan	QIVBCDIJAJPQS-UHFFFAOYSA-N
141	L-Tyrosine	OUYCCASQSFEME-UHFFFAOYSA-N
142	L-Tyrosine tert-butyl ester	DIGHFXIWRPMGSA-NSHDSACASA-N
143	L-Tyrosine, O-(1,1-dimethylethyl)-	SNZIFNXFAFKRKT-NSHDSACASA-N
144	LysoPA(18:1(9Z)/0:0)	WRGQSWVCFNIUNZ-GDCKJWNLSA-N
145	LysoPC(0:0/18:2(9Z,12Z))	LSUXCWJOIAGWOU-UTJQPWESSA-N
146	LysoPC(16:0/0:0)	ASWBNKHCZGQVJV-HSZRJFAPSA-N
147	LysoPC(17:0/0:0)	SRRQPVVYXBTRQK-XMMPXPASA-N
148	LysoPC(18:0/0:0)	IHNKQIMGVNPMTG-RUZDIDTESA-N
149	LysoPC(18:1(9Z)/0:0)	YAMUFBLWGFICM-PTGWMXDISA-N
150	LysoPC(18:2(9Z,12Z)/0:0)	SPJFYJXNPEZDW-UTJQPWESSA-N
151	LysoPC(20:0/0:0)	UATOAILWGVYRQS-HHHXNRCGSA-N
152	LysoPC(O-18:0/0:0)	XKBJVQHMEXMFDZ-AREMUKBSSA-N
153	LysoPC(P-16:0/0:0)	HTZINLFXLXRBC-CQLBITFSA-N
154	LysoPC(P-18:0/0:0)	WBOMIOWRFSPZMC-AYICAFKVSA-N
155	LysoPE(18:1(9Z)/0:0)	PYVRVRFVLRNLY-MZMPXXGTSAN
156	LysoPI(18:2(9Z,12Z)/0:0)	SAHCQBPQGQFTRA-MTWZWNHSA-N
157	Malic acid	BJEPYKJPYRNKOW-UHFFFAOYSA-N
158	Malioxamycin	KXQRAPMNPUXYGT-VDTYLAMSSA-N
159	Methionine sulfoxide	QEFRNWWLZKMPFJ-YGVKFDHGSA-N
160	Methyl linoleate	WTTJVINHCBLGX-NQLNTRKDSA-N
161	Methylcysteine	IDIDJDIHTAOVLG-VKHMYHEASA-N
162	MG(18:1(9Z)/0:0/0:0)	RZRNAVUHVWFMP-MDZDMLPASA-N
163	Monoethylhexyl phthalic acid	DJDSLVSQSLW-UHFFFAOYSA-N
164	Monoethyl phthalate	PKIYFICNICNGJ-UHFFFAOYSA-N
165	N-(.alpha.-Linolenoyl)tyrosine	DEQLZTQITSWABQ-GMOGWPNXSA-N
166	N-(2,4-Dinitrophenyl)-L-methionine	DOHZIIDJOSBJFP-UHFFFAOYSA-N
167	N-.alpha.-(tert-Butoxycarbonyl)-L-histidine	AYMLQYFMYHISQO-QMMMGPBSA-N
168	N-Acetylglycine methyl ester	RFNODQARGNZURK-UHFFFAOYSA-N
169	N-Acetyl-L-alanine	KTHDTJVBEPMMGL-UHFFFAOYSA-N
170	N-Acetyl-L-phenylalanine	CBQSKKFNMDLON-SNVBAGLBSA-N
171	N-Acetyl-L-tyrosine	CAHKINHBCWCHCF-JTQLQIEISA-N
172	N-Acetyltryptophan	DZTHIGRZJZPRDV-UHFFFAOYSA-N
173	Niacinamide	DFPAKSUCGFBDDF-UHFFFAOYSA-N
174	Nipescotic acid	XJLSEXAGTJILF-UHFFFAOYSA-N
175	N-Phenylacetylphenylalanine	LIIPHJDKZNTNII-HNNXBMFYSA-N
176	PA(18:1(9Z)/18:1(9Z))	MHUWZNTUIIFHAS-DSSVUWSHSA-N
177	PC(14:0/14:0)	CITHEXJVPOWHKC-UUWRZZSWSA-N
178	PC(14:0/16:0)	RFVFAQWKPQSOBEB-PSXMRANNSA-N

Table 3. Non-Certified Values for Metabolite Identifications of Pooled Plasma 3, African-American Plasma

Index	Name	INCHIKEY
179	PC(15:0/15:0)	LJARBVLDOSWRJT-PSXMRANNSA-N
180	PC(16:0/14:0)	UIXXHROAQSBOV-PSXMRANNSA-N
181	PC(16:0/16:0)	KILNVBDSWZSGLL-UHFFFAOYSA-N
182	PC(16:0/18:1(9Z))	WTJKGGKOPKCXLL-VYOBOKEXSA-N
183	PC(16:0/18:2(9Z,12Z))	JLPULHDHAOZNQI-ZTIMHPMXSA-N
184	PC(16:0/20:4(5Z,8Z,11Z,14Z))	IIZPXJDJLKNQIY-JXPJKXOSSA-N
185	PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	KLTHQSWIRFFBRI-KOQZQRJKSA-N
186	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	IESVDEZGAHUQUJ-ZLBKXVHBSA-N
187	PC(16:1(9Z)/16:1(9Z))	GPWHCUUIQMGLX-VHQDNGOZSA-N
188	PC(18:0/14:0)	MZWGYEJOZNRLE-KXQOOQHDSA-N
189	PC(18:0/18:1(9Z))	ATHVAWFAEPLPQ-VRDBWYNSSA-N
190	PC(18:0/18:2(9Z,12Z))	FORFDCPQJHEBF-VPUUSDGANSAN
191	PC(18:0/20:4(5Z,8Z,11Z,14Z))	PSVRFUPOQYJOOZ-RYIOQAQXSA-N
192	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FAUYAENFVCNTAL-PFFNLMTBSA-N
193	PC(18:1(9Z)/14:0)	KIVAJCJTVPWSRJ-OQHNRNOKSA-N
194	PC(18:1(9Z)/16:0)	RRVPPYNAZJRZFR-VYOBOKEXSA-N
195	PC(18:1(9Z)/18:1(9Z))	SNKAWBJQDLSFF-NVKMUCNASAN
196	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	FVXDQWZBHIXIEJ-LNDKUQBDSA-N
197	PC(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	LZLVZIFMYXDKCN-QJWFYWCHSA-N
198	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	AHWXJDWBIDPKS-TZUVPVEASAN
199	PC(O-16:0/20:3(8Z,11Z,14Z))	VYKSGWCIVDQIQR-GBDFTIALSAN
200	PC(O-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	YHSSHPWVFALMBA-IARQOZKNSAN
201	PC(O-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	QQQQNYAHSSIZBU-HIQXTUQZSAN
202	PC(P-18:0/18:1(9Z))	DSWOVBIRJNAJAF-NVJOKYTBSAN
203	PC(P-18:0/20:4(5Z,8Z,11Z,14Z))	FHHVIBPVBBRLOR-IYACIECVSAN
204	PC(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	TXHZYNSTTCIWMJ-RXSQUPBGSAN
205	p-Cresol sulfate	WGNAKZGUSRVWRH-UHFFFAOYSAN
206	PE(16:0/18:1(9Z))	FHQVHHIBKUMWTI-OTMQOFLSAN
207	PE(16:0/18:2(9Z,12Z))	HBZNVZIRJWODIB-NHCUFNCUSAN
208	PE(16:0/20:4(5Z,8Z,11Z,14Z))	DRIVXEVMDCWLI-CAQMIEAISAN
209	PE(18:0/18:2(9Z,12Z))	YDTWOEYVDRKKCR-KNERPIHHSAN
210	PE(18:0/20:4(5Z,8Z,11Z,14Z))	ANRKEHNWXXCXDB-BHFWLYLHSAN
211	PE(P-18:0/18:1(9Z))	XVYPOHCSLJZFED-QZEVRLJJSAN
212	PE(P-18:0/20:4(5Z,8Z,11Z,14Z))	URPXXNCTXCOATD-FXMFQVEGASAN
213	PE(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FJFPUAJUDAZEY-WAHBYMPSSAN
214	Phenylacetylglutamine	JFLIEFSWGNOPJJ-JTQLQIEISAN
215	Phthalic acid	XNGIFLGASWRNHJ-UHFFFAOYSAN
216	Phthalic anhydride	LGRFSURHDFAJFT-UHFFFAOYSAN
186	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	IESVDEZGAHUQUJ-ZLBKXVHBSA-N
187	PC(16:1(9Z)/16:1(9Z))	GPWHCUUIQMGLX-VHQDNGOZSA-N
188	PC(18:0/14:0)	MZWGYEJOZNRLE-KXQOOQHDSA-N
189	PC(18:0/18:1(9Z))	ATHVAWFAEPLPQ-VRDBWYNSSA-N
190	PC(18:0/18:2(9Z,12Z))	FORFDCPQJHEBF-VPUUSDGANSAN
191	PC(18:0/20:4(5Z,8Z,11Z,14Z))	PSVRFUPOQYJOOZ-RYIOQAQXSA-N
192	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FAUYAENFVCNTAL-PFFNLMTBSA-N
193	PC(18:1(9Z)/14:0)	KIVAJCJTVPWSRJ-OQHNRNOKSA-N
194	PC(18:1(9Z)/16:0)	RRVPPYNAZJRZFR-VYOBOKEXSA-N
195	PC(18:1(9Z)/18:1(9Z))	SNKAWBJQDLSFF-NVKMUCNASAN
196	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	FVXDQWZBHIXIEJ-LNDKUQBDSA-N
197	PC(20:4(5Z,8Z,11Z,14Z)/20:4(5Z,8Z,11Z,14Z))	LZLVZIFMYXDKCN-QJWFYWCHSA-N
198	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	AHWXJDWBIDPKS-TZUVPVEASAN
199	PC(O-16:0/20:3(8Z,11Z,14Z))	VYKSGWCIVDQIQR-GBDFTIALSAN
200	PC(O-16:0/20:5(5Z,8Z,11Z,14Z,17Z))	YHSSHPWVFALMBA-IARQOZKNSAN
201	PC(O-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	QQQQNYAHSSIZBU-HIQXTUQZSAN
202	PC(P-18:0/18:1(9Z))	DSWOVBIRJNAJAF-NVJOKYTBSAN
203	PC(P-18:0/20:4(5Z,8Z,11Z,14Z))	FHHVIBPVBBRLOR-IYACIECVSAN
204	PC(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	TXHZYNSTTCIWMJ-RXSQUPBGSAN
205	p-Cresol sulfate	WGNAKZGUSRVWRH-UHFFFAOYSAN
206	PE(16:0/18:1(9Z))	FHQVHHIBKUMWTI-OTMQOFLSAN
207	PE(16:0/18:2(9Z,12Z))	HBZNVZIRJWODIB-NHCUFNCUSAN

Table 3. Non-Certified Values for Metabolite Identifications of Pooled Plasma 3, African-American Plasma

Index	Name	INCHIKEY
208	PE(16:0/20:4(5Z,8Z,11Z,14Z))	DRIVXEVMDCWLI-CAQMIEAISA-N
209	PE(18:0/18:2(9Z,12Z))	YDTWOEYVDRKKCR-KNERPIHSA-N
210	PE(18:0/20:4(5Z,8Z,11Z,14Z))	ANRKEHNWXKCDB-BHFWLYLHSA-N
211	PE(P-18:0/18:1(9Z))	XVYPOHCSLJZFED-QZEVRLJSA-N
212	PE(P-18:0/20:4(5Z,8Z,11Z,14Z))	URPXXNCTXCOATD-FXMFQVEGSA-N
213	PE(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	FIJFPUAJUDAZEY-WAHBYMPSSA-N
214	Phenylacetylglutamine	JFLIEFSWGNOPJJ-JTQLQIEISA-N
215	Phthalic acid	XNGIFLGASWRNHJ-UHFFFAOYSA-N
216	Phthalic anhydride	LGRFSURHDFAJT-UHFFFAOYSA-N
217	PI(16:0/18:1(9Z))	PDLAMJKMOKWLJAJ-KTBSNPQYSA-N
218	PI(18:0/20:4(5Z,8Z,11Z,14Z))	KRTOMQDUKGRFDJ-ZAHDIIIMDSA-N
219	Pipecolic acid	HXEACLLIILLPRG-UHFFFAOYSA-N
220	Platelet-activating factor	HVAUUPRFYPCOCA-AREMUKBSSA-N
221	Pregnanolone sulfate	MENQCIVHHONJLU-FZCSVUEKSA-N
222	Pregnenolone sulfate	DJBBUIOWGGQOP-QGVNFLTSA-N
223	Prolyl-Glutamine	SHAQGGGJSLLEH-BQBZGAKWSA-N
224	Prolylphenylalanine	IWIANZLCJVYEFX-RYUDHWBXSAN
225	Prolyl-Valine	AWJGUZSYVIVZGP-YUMQZZPRSA-N
226	Propanedioic acid, 2-(2-methylpropyl)-, 1,3-dimethyl ester	GAZFDPSEEIVCEX-UHFFFAOYSA-N

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APPENDIX A

Analytical Approach for Metabolite Identification (NIST): Metabolite identifications were determined by an untargeted liquid chromatography tandem mass spectrometry (LC-MS/MS), based metabolomics approach. Each phenotypic plasma pool Pooled Plasma 1, Diabetic Plasma; Pooled Plasma 2, Hypertriglyceridemic Plasma; and Pooled Plasma 3, African-American Plasma was extracted by two methods, a methanol precipitation and an ethanol precipitation. Triplicate samples of each phenotype were removed from storage at $-80\text{ }^{\circ}\text{C}$ and thawed at room temperature and protected from light. After gently mixing, approximately 0.100 g of each sample was extracted with 900 μL of solvent (methanol or ethanol) for a total sample volume of 1 mL. The samples were shaken at maximum speed for 20 min on an incubating shaker at room temperature and then placed in a $-80\text{ }^{\circ}\text{C}$ freezer for 1 hr to induce protein precipitation. Precipitate was centrifuged at 10,000 cfm for 10 min at $4\text{ }^{\circ}\text{C}$. The supernatant was removed and taken to dryness in a vacuum centrifuge, then stored at $-80\text{ }^{\circ}\text{C}$ until analysis. Five procedural blanks (1 mL of ethanol or methanol) were also processed along with the samples. All samples and blanks were reconstituted in 100 μL of 98 % water and 2 % methanol (volume fraction) prior to analysis. A gradient method with a 0.1 % formic acid in water/0.1 % formic acid in methanol mobile phase and a C18 column was used for LC MS/MS analysis in both positive and negative mode with a data dependent acquisition on two different high resolution MS instruments. The resulting tandem MS spectra were searched using HighChem-HighRes, HighChemDP, and NIST spectral library search algorithms with NIST20 and 2019 version of mzVault libraries. Putative metabolite identifications (MSI level 2) by spectral library matches and scores for each search algorithm, sample preparation, and instrument (54 total datasets) were filtered (match score ≥ 65) and combined. For the final list, the InChiKey values of the commonly identified compounds were converted to common nomenclature using RefMet [3].

Analysis: For qualitative measurands like metabolite identity, a conventional evaluation and expression of measurement uncertainty conforming to the JCGM GUM [4] cannot be used. Tables 1–3 list the identities of metabolites in the Diabetic, Hypertriglyceridemic, and African-American pools that have been established using identification methodology generally accepted by experts in the field. The identified metabolites in RM 8231 are a Metabolomics Standards Initiative (MSI) level 2 identity [2] and are inferred from untargeted metabolomics analysis (liquid chromatography mass spectrometry data dependent acquisition) using two different sample preparation protocols, methanol or ethanol precipitation. Samples from each preparation protocol were analyzed on two different high resolution mass spectrometer instruments and the resulting tandem MS spectra (MS/MS) were searched with three different mass spectral library search algorithms. Identified metabolites are included only when the following are met:

- 1) putatively identified with tandem MS spectra in both sample preparation methods,
- 2) putatively identified with tandem MS spectra from both instruments, and
- 3) putatively identified with tandem MS spectra with three mass spectral library search algorithms.

NIST is confident of the identity of the non-certified qualitative values of the metabolites listed in Tables 1–3 that met all criteria.

Source and Preparation: RM 8231 is created as a suite of phenotypically distinct human plasma. This RM was developed after an appropriate human subjects research determination by NIST.

Pooled Plasma 1, Diabetic Plasma: This specific plasma pool was designed to represent a Type 2 diabetic plasma material with glucose $>126\text{ mg/dL}$ and low/normal triglyceride ($<150\text{ mg/dL}$). Plasma was obtained from 11 individuals (six male and five female) who had undergone an overnight fast prior to blood draw by Solomon Park Research Laboratories, Inc. (Kirkland, WA). Lithium heparin was used as the anticoagulant. Age distribution of individuals was between 34 and 68 years old with a racial distribution of 55 % White, 36 % African-American or Black, 9% Asian.

Pooled Plasma 2, Hypertriglyceridemic Plasma: This specific plasma pool was designed as a hypertriglyceridemic plasma material with glucose $<100\text{ mg/dL}$ and triacylglycerols $>300\text{ mg/dL}$. Plasma was obtained from 11 male donors who had undergone an overnight fast prior to blood draw by Solomon Park Research Laboratories, Inc. (Kirkland, WA). Lithium heparin was used as the anticoagulant. Male donors were between 31 and 72 years of age with a racial demographic of 55 % White, 36 % African-American or Black, 9 % Hispanic.

Pooled Plasma 3, African-American Plasma: This specific plasma pool was created as a African-American plasma material. Plasma was collected from 16 individuals who had undergone an overnight fast prior to blood draw by Bioreclamation IVT (Westbury, NY). K2 ethylenediaminetetraacetic acid (EDTA) was used as an anticoagulant. Plasma from an equal number of men and women between 20 and 25 years of age was collected. Plasma samples were pooled and aliquoted by Solomon Park Research Laboratories, Inc. (Kirkland, WA).

***** End of Appendix A *****