

Supporting Information

for

High Coverage Profiling of Carboxylated Metabolites in HepG2 Cells Using Secondary Amine-Assisted Ultrahigh-Performance Liquid Chromatography Coupled to High-Resolution Mass Spectrometry

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The supporting information includes following items:

Page S3-S5	Additional experimental methods.
Page S6	Figure S1. ^1H NMR of d_3 -MPEA in $\text{DMSO-}d_6$.
Page S7	Figure S2. ^{13}C NMR of d_3 -MPEA in $\text{DMSO-}d_6$.
Page S8	Figure S3. Exact m/z of d_3 -MPEA.
Page S9	Figure S4. Workflow of the screening of carboxylic labeling reagents.
Page S10	Figure S5. MS intensity of labeled products of six carboxylic labeling reagents.
Page S11	Figure S6. Chromatograms of 4-AMBA-labeled polyCAs.
Page S12	Figure S7. Chromatograms of DmPA-labeled AAs.
Page S13-S16	Figure S8. MS^2 spectra of seven annotated carboxylated metabolites in HepG2 cell extracts.
Page S17	Figure S9. The RSDs of intensity ratios (light/heavy labeling) for 403 carboxylated metabolites.
Page S18-S21	Table S1. Detailed information of carboxylic acid standards.
Page S22	Table S2. Advantages and disadvantages of six carboxylic labeling reagents.
Page S23	Table S3. Reactivity of MPEA to metabolites containing other functional groups.
Page S24	Table S4. Detection sensitivity of carboxylic acids before and after MPEA labeling.
Page S25	Table S5. Labeling efficiency of MPEA in HepG2 cell extracts.
Page S26-S35	Table S6. Detected MPEA-labeled carboxylated metabolites in HepG2 cell extracts.
Page S36-S44	Table S7. Detected DmPA-labeled carboxylated metabolites in HepG2 cell extracts.
Page S45	Table S8. Investigation of the accuracy of relative quantitation.
Page S46-S50	Table S9. Carboxylated metabolites with significant difference between curcumin and control.
Page S51-S54	Table S10. Carboxylated metabolites with significant difference between <i>R</i> -3-HBA and control.
Page S55	References

Background of detection of carboxylated metabolites by LC-MS strategy

Mass spectrometry (MS) has become one of the most powerful techniques for detecting small molecular compounds owing to its high sensitivity and selectivity.^{S1} MS could couple with gas chromatography, liquid chromatography and other separation techniques to improve its separation capability.^{S2, 3} Gas chromatography-mass spectrometry (GC-MS) is suitable for the analysis of carboxylated metabolites with volatility and thermal stability;^{S4} while liquid chromatography-mass spectrometry (LC-MS) can be applied to a wider range of compounds.^{S5, 6} Many previous works were developed on LC-MS, aiming at providing effective methods for high coverage analysis of carboxylated metabolites in biological samples. For example, Yuan *et al.* used a hydrophilic interaction liquid chromatography (HILIC) column to detect SCFAs and TCA cycle intermediates in ESI-positive ion mode and AAs in ESI-negative ion mode, respectively. They realized the detection of hydrophilic carboxylated metabolites in pancreatic cancer cells.^{S5} Similarly, Lindsay *et al.* switched between positive and negative ion modes to detect AAs, TCA cycle intermediates and free fatty acids in human plasma on both HILIC and reversed-phase (RP) columns.^{S6} However, the MS response of carboxylated metabolites themselves was relatively poor in ESI-negative ion mode,^{S7} which was not conducive to high coverage analysis of carboxylated metabolites especially for those of low abundance.

Synthesis of *d*₃-MPEA

Briefly, 1.84 mmol of *N*-(2-phenylethyl)acetamide in THF (10 mL) were stirred until dissolved under anhydrous and anaerobic conditions. Next, sodium hydride (3.68 mmol) was added and stirred for 45 min followed by the addition of iodimethylene-*d*₃ (9.19 mmol).^{S8} The reaction process was monitored by TLC after overnight. Then, the reaction solvent was removed under vacuum and the residues were extracted with dichloromethane (3 × 30 mL). The obtained organic layer was washed with brine (3 × 30 mL), dried over Na₂SO₄ and concentrated under vacuum. Finally, the residues were purified by silica gel chromatography eluted with ethyl acetate/petroleum ether (10:1, v/v) to give the pure intermediate (172.4 mg, 0.96 mmol, liquid).

The intermediate was dissolved in 1,2-ethanediol (3 mL). Next, 0.2 mL 10% dilute HCl was added and the mixtures were refluxed for 24 h. After the reaction completed, the mixture was evaporated and adjusted to pH14 with saturated NaHCO₃ solution.^{S9} Then, the aqueous layer was extracted with dichloromethane (3 × 30 mL), and the organic layer was washed with brine and dried over anhydrous Na₂SO₄. The residues were purified by flash column chromatography on silica gel eluted with dichloromethane/MeOH/triethylamine (15: 1: 0.16, v/v/v). Finally, the product was obtained (63.1 mg, 0.46 mmol, liquid). The ¹H and ¹³C NMR spectra of *d*₃-MPEA were shown in Supporting Information (Figure S1-S2). The accurate molecular weight [M+H]⁺ of *d*₃-MPEA is 139.1305 Da (Figure S3).

Labeling results of 5 carboxylic labeling reagents

Besides MPEA, 5 previously reported carboxylic labeling reagents including 1-(2-pyrimidinyl)piperazine (2-PPM), *N*-(4-(aminomethyl)benzyl)aniline (4-AMBA), *N,N*-dimethylethylenediamine (DMED), 3-nitrophenylhydrazine (3-NPH) and *p*-dimethylaminophenacyl (DmPA) bromide, were also investigated for comparison. These labeling reactions were carried out under their optimal reaction conditions. The MS intensity of corresponding labeled products were presented in Figure S5.

2-PPM and MPEA are secondary amines, but the adjacent moieties of their secondary amine group are different. We investigated the reactivity of 2-PPM to various types of carboxylated metabolites. 2-PPM simultaneously labeled LCFAs (DA and PDA) and aromatic acids (PABA), but the labeled products of other carboxylic acids were hardly detected (Figure S5). It may be ascribed to the fact that the adjacent moiety attached to the secondary amine group of 2-PPM reduced its reactivity in the labeling reaction.

4-AMBA and DMED are primary amines, so they are expected to have similar reactivity toward carboxyl group. As shown in Figure S5, 4-AMBA can react with SCFAs, MCFs, LCFAs, and aromatic acids. Given that two benzene rings involved in the structure of 4-AMBA, the chromatographic retention of SCFAs on RP column is greatly enhanced. However, the MS intensity of 4-AMBA labelled polyCAs is relatively low compared with that of MPEA, which was attributed to side reactions. Taking citric acid as an example, singly, doubly and triply 4-AMBA-labeled citric acid were all detected and a by-product of intramolecular succinimide between two carboxylic groups of citric acid was also found (Figure S6). In addition, the MS intensity of 4-AMBA-labeled AAs is lower one order of magnitude than carboxylated metabolites without amino group. It may be attributed to that the reactivity of primary amine is not high enough toward AAs of relatively lower electrophilicity due to intermolecular hydrogen bond between primary amine and carboxyl groups. Therefore, 4-AMBA is not proper for the labeling of polyCAs and AAs. DMED can effectively label SCFAs, MCFAs, LCFAs and aromatic acids (Figure S5), but the labeled products of SCFAs are eluted at dead time on RP column due to their poor retention. When it came to polyCAs and AAs, similar labeling results happened on DMED compared with 4-AMBA due to their similar reactive groups. Therefore, due to the relatively low reactivity of primary amine labeling reagents such as 4-AMBA and DMED, they are not suitable for high coverage screening of carboxylated metabolites.

As shown in Figure S5, 3-NPH can react with MCFAs, LCFAs and aromatic acids under optimal conditions. However, other labeled products are hardly detected, such as SCFAs, AAs and polyCAs. As a result, the reactivity of 3-NPH to carboxylated metabolites is also relatively low so that it was not suitable for high coverage screening of carboxylated metabolites.

DmPA can react with SCFAs, MCFAs, LCFAs, polyCAs, AAs and aromatic acids under optimal reaction conditions (Figure S5), indicating its high reactivity to carboxylated metabolites. However, DmPA-labeled AAs exhibit double peaks in their chromatograms (Figure S7) and thus make the chromatograms complicated, which may be ascribed to the fact that DmPA simultaneously labeled the carboxyl and amino groups of AAs as mentioned above.

Labeling results of DmPA/¹³C₂-DmPA in HepG2 cell extracts

Furthermore, metabolites without carboxyl group, such as phenol, sulfhydryl and phosphate metabolites, cannot be detected after MPEA/*d*₃-MPEA labeling in this study, indicating that MPEA has high selectivity to carboxylated metabolites. For comparison, DmPA and ¹³C₂-DmPA were also used to label an aliquot of cell extracts, respectively. The procedures of experiments and data processing were similar with that of MPEA/*d*₃-MPEA. Totally, 998 potential metabolites were obtained by DmPA/¹³C₂-DmPA labeling (Table S7), which was more than that obtained using MPEA/*d*₃-MPEA labeling method. As for the types of identified metabolites, SCFAs (NO. 3 and 17 in Table S7), MCFAs (NO. 156 and 181 in Table S7), LCFAs (NO. 533 in Table S7), polyCAs (NO. 99 in Table S7), AAs (NO. 57 and 58 in Table S7) and aromatic acids (NO. 110 in Table S7), were all detected. However, the reactivity of DmPA was so high that amino (NO. 1, 19 and 20 in Table S7) and phenol (NO. 63 in Table S7) metabolites were also detected, which increased the difficulty in the identification of carboxylated metabolites to some degree (MS² spectra were not shown in the paper). Therefore, these results suggested that MPEA/*d*₃-MPEA labeling UHPLC-HRMS can achieve high coverage screening of carboxylated metabolites in HepG2 cells.

Figure S1. ^1H NMR of d_3 -MPEA in $\text{DMSO-}d_6$ (^1H NMR (400 MHz, DMSO) δ 7.39 – 7.20 (m, 5H), 3.10 (dd, $J = 10.2$, 6.2 Hz, 2H), 2.96 (dd, $J = 10.1$, 6.1 Hz, 2H)).

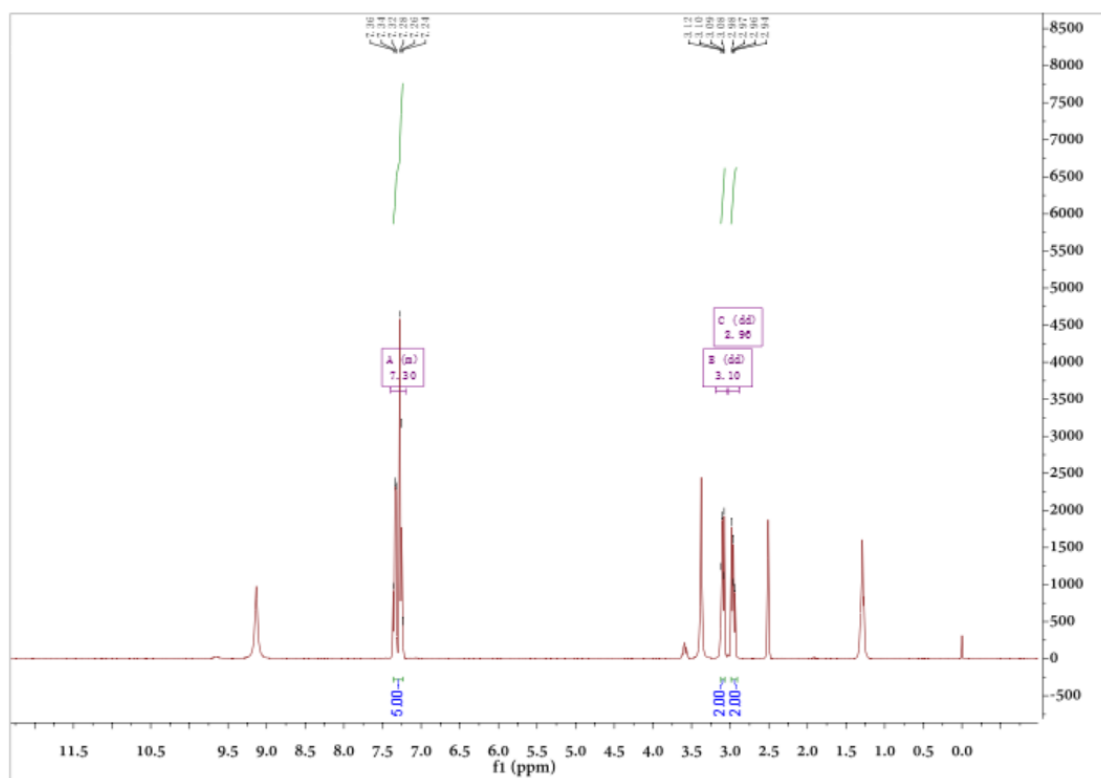


Figure S2. ^{13}C NMR of d_3 -MPEA in $\text{DMSO-}d_6$ (^{13}C NMR (101 MHz, DMSO) δ 137.70, 129.11, 129.09, 127.21, 53.64, 49.40, 31.86).

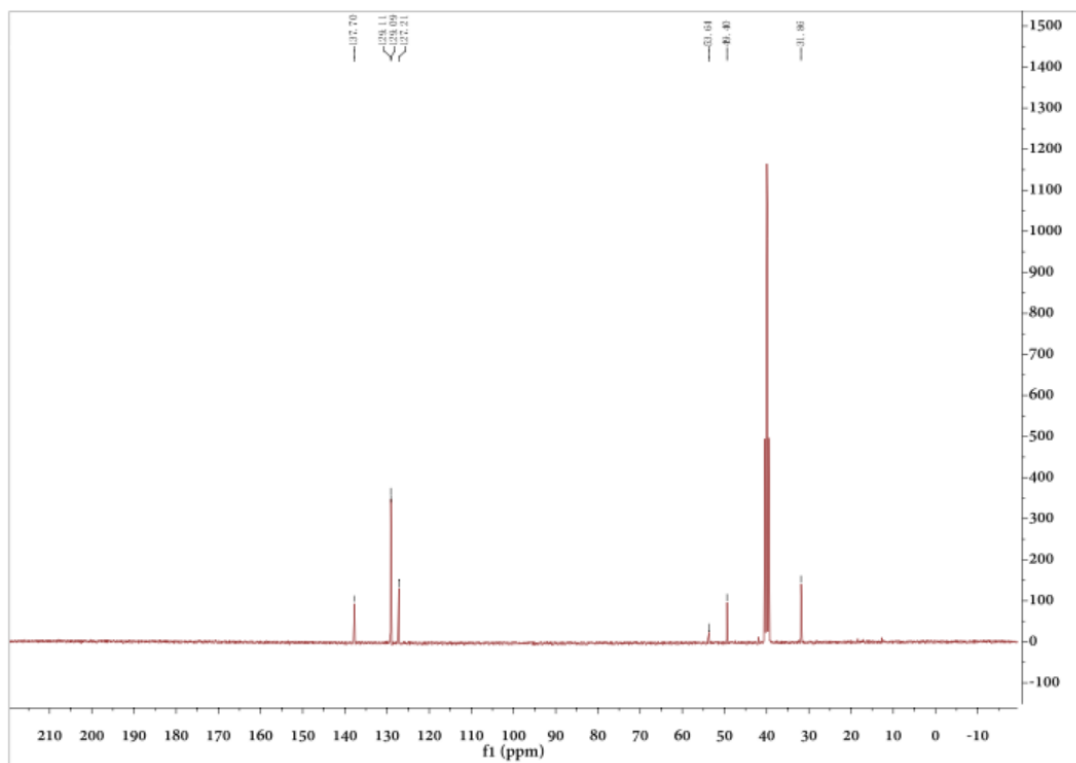


Figure S3. Exact m/z of d_3 -MPEA.

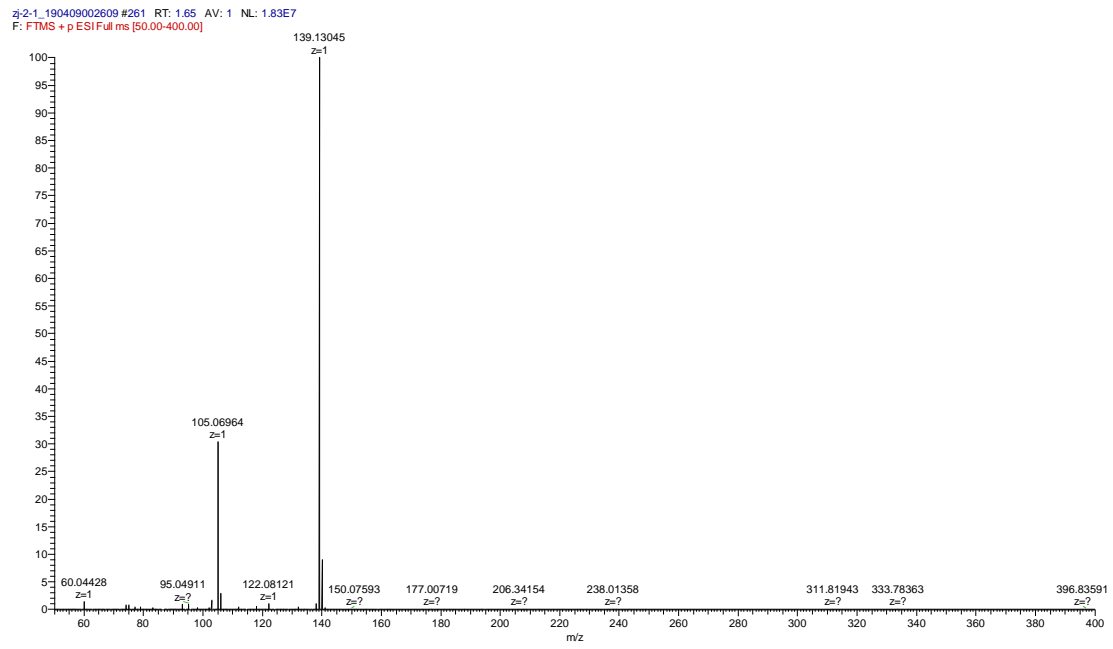


Figure S4. Workflow of the screening of carboxylic labeling reagents.

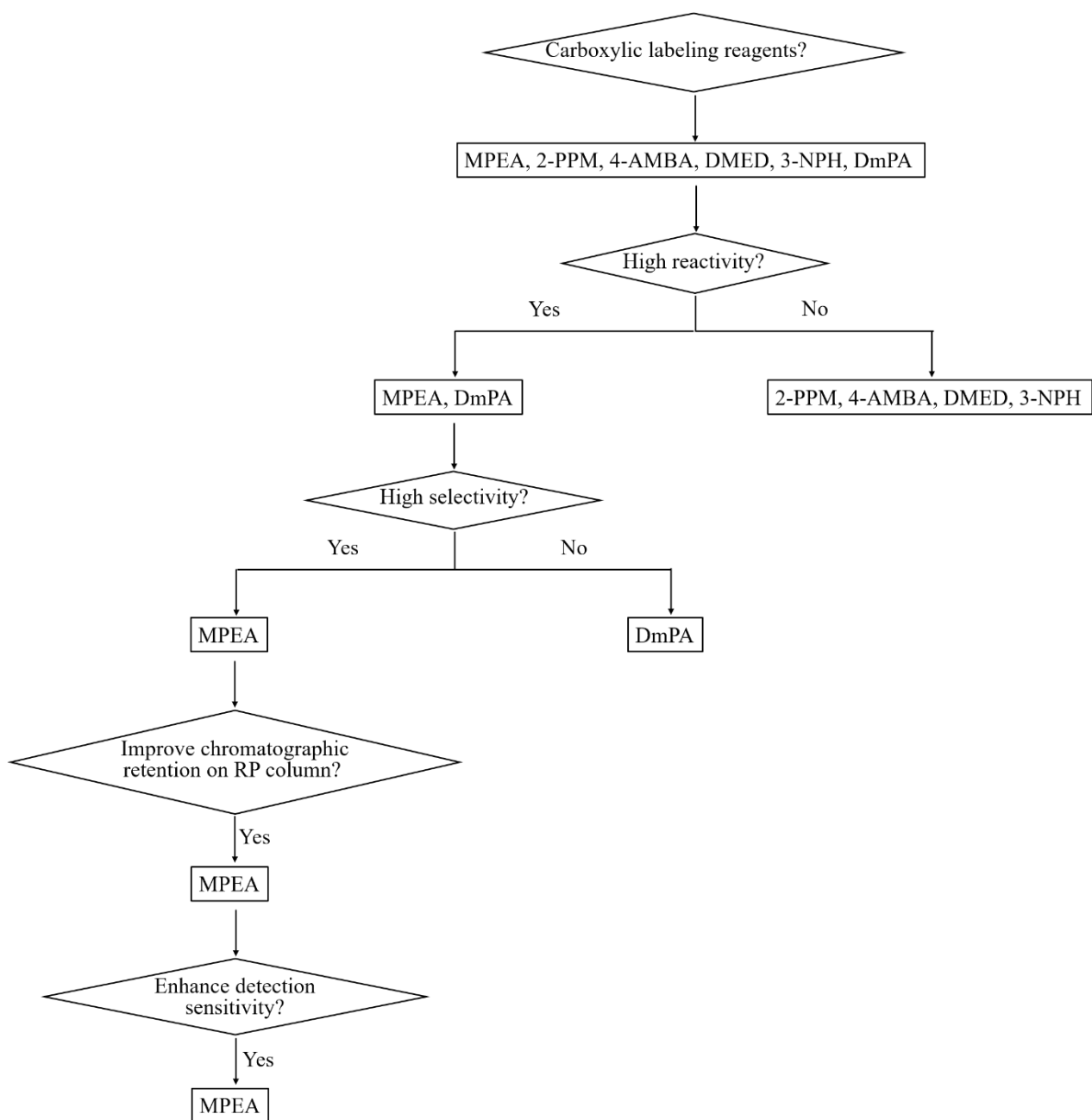


Figure S5. MS intensity of labeled products of six carboxylic labeling reagents. (Abbreviations of carboxylic acids: lactic acid (LA), propionic acid (PA), butyric acid (BA), succinic acid (SA), malic acid (MA), citric acid (CIT), 9-decenoic acid (DA), pentadecanoic acid (PDA), sebacic acid (SEA), α -alanine (α -Ala), leucine (Leu), tryptophan (Trp), proline (Pro), aspartic acid (Asp), β -alanine (β -Ala), γ -aminoisovaleric acid (γ -AIVA) and *p*-aminobenzoic acid (PABA)).

		MPEA	2-PPM	4-AMBA	DMED	3-NPH	DmPA	
SCFAs	LA	1.57E+06	5.94E+04	1.58E+06	2.06E+05	0.00E+00	5.24E+06	<p>Low</p> <p>High</p>
	PA	1.58E+07	1.88E+05	9.97E+06	1.47E+06	0.00E+00	2.31E+07	
	BA	1.23E+07	2.38E+05	1.12E+07	2.96E+06	0.00E+00	1.98E+07	
PolyCAs	SA (single)	1.56E+05	9.35E+05	8.79E+05	7.67E+05	2.32E+04	7.40E+06	
	SA (double)	1.07E+07	0.00E+00	3.33E+06	6.45E+04	0.00E+00	9.36E+06	
	MA (single)	0.00E+00	6.34E+05	3.53E+05	1.11E+05	0.00E+00	2.44E+06	
	MA (double)	1.81E+06	0.00E+00	9.63E+05	0.00E+00	0.00E+00	9.73E+04	
	CIT (single)	0.00E+00	0.00E+00	0.00E+00	1.84E+05	0.00E+00	0.00E+00	
	CIT (double)	1.42E+05	4.88E+04	0.00E+00	0.00E+00	0.00E+00	1.34E+05	
	CIT (triple)	1.74E+06	0.00E+00	3.66E+04	0.00E+00	0.00E+00	3.57E+05	
MCFAs LCFAs	DA	1.08E+07	2.58E+05	1.69E+07	1.46E+07	4.56E+05	1.74E+07	
	PDA	1.37E+07	2.92E+05	1.58E+07	1.40E+07	2.56E+05	1.91E+07	
	SEA (single)	7.45E+04	5.19E+05	7.03E+04	9.93E+04	1.74E+05	3.84E+06	
	SEA (double)	1.06E+07	0.00E+00	3.47E+06	1.71E+05	1.03E+05	6.63E+05	
AAs	α -Ala	1.03E+06	0.00E+00	2.53E+05	5.32E+04	0.00E+00	1.08E+05	
	Leu	2.34E+06	0.00E+00	6.20E+05	6.81E+04	0.00E+00	1.52E+06	
	Trp	3.26E+06	0.00E+00	5.10E+05	0.00E+00	0.00E+00	9.62E+05	
	Pro	5.00E+06	0.00E+00	2.33E+05	1.68E+05	0.00E+00	1.35E+06	
	Asp (single)	4.39E+05	0.00E+00	4.10E+05	0.00E+00	0.00E+00	2.90E+05	
	Asp (double)	1.65E+06	0.00E+00	7.38E+04	0.00E+00	0.00E+00	4.29E+04	
	β -Ala	2.28E+06	0.00E+00	2.93E+05	2.68E+05	0.00E+00	2.58E+06	
Aromatic acids	γ -AIVA	1.76E+06	4.32E+05	2.13E+05	8.57E+04	3.36E+04	3.50E+06	
	PABA	8.50E+06	0.00E+00	1.08E+06	9.20E+05	2.50E+05	1.09E+05	

Figure S6. Chromatograms of 4-AMBA-labeled polyCAs. (A) 4-AMBA-labeled SA; (B) 4-AMBA-labeled CIT.

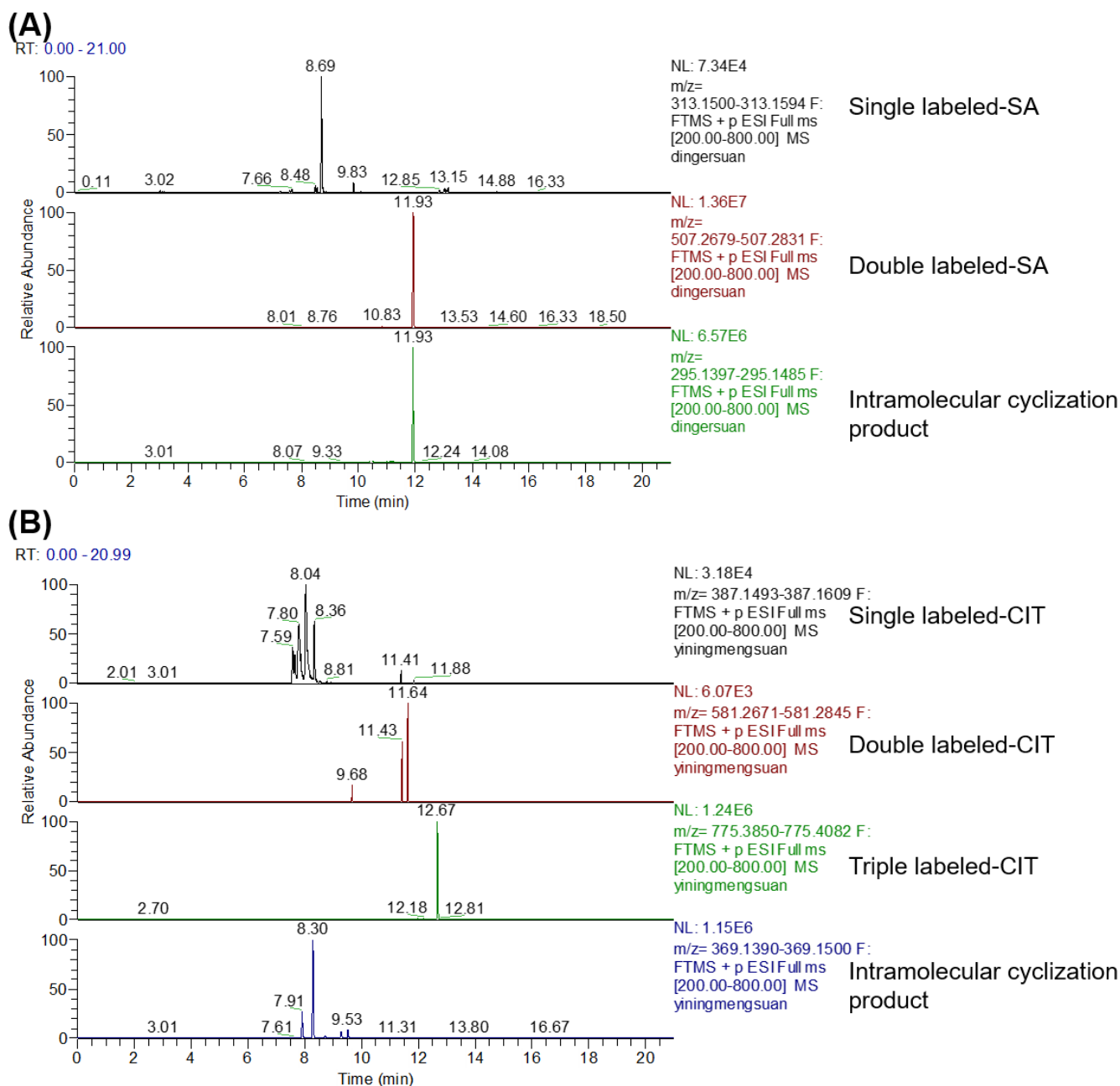


Figure S7. Chromatograms of DmPA-labeled AAs.

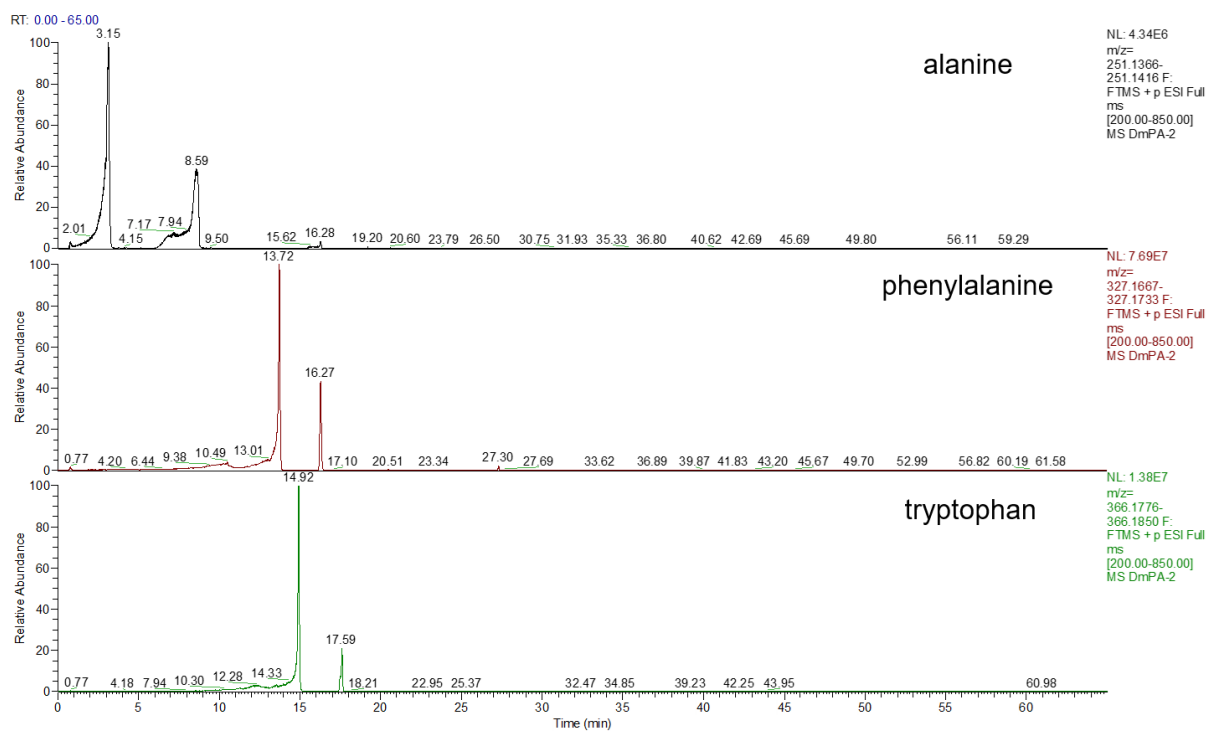
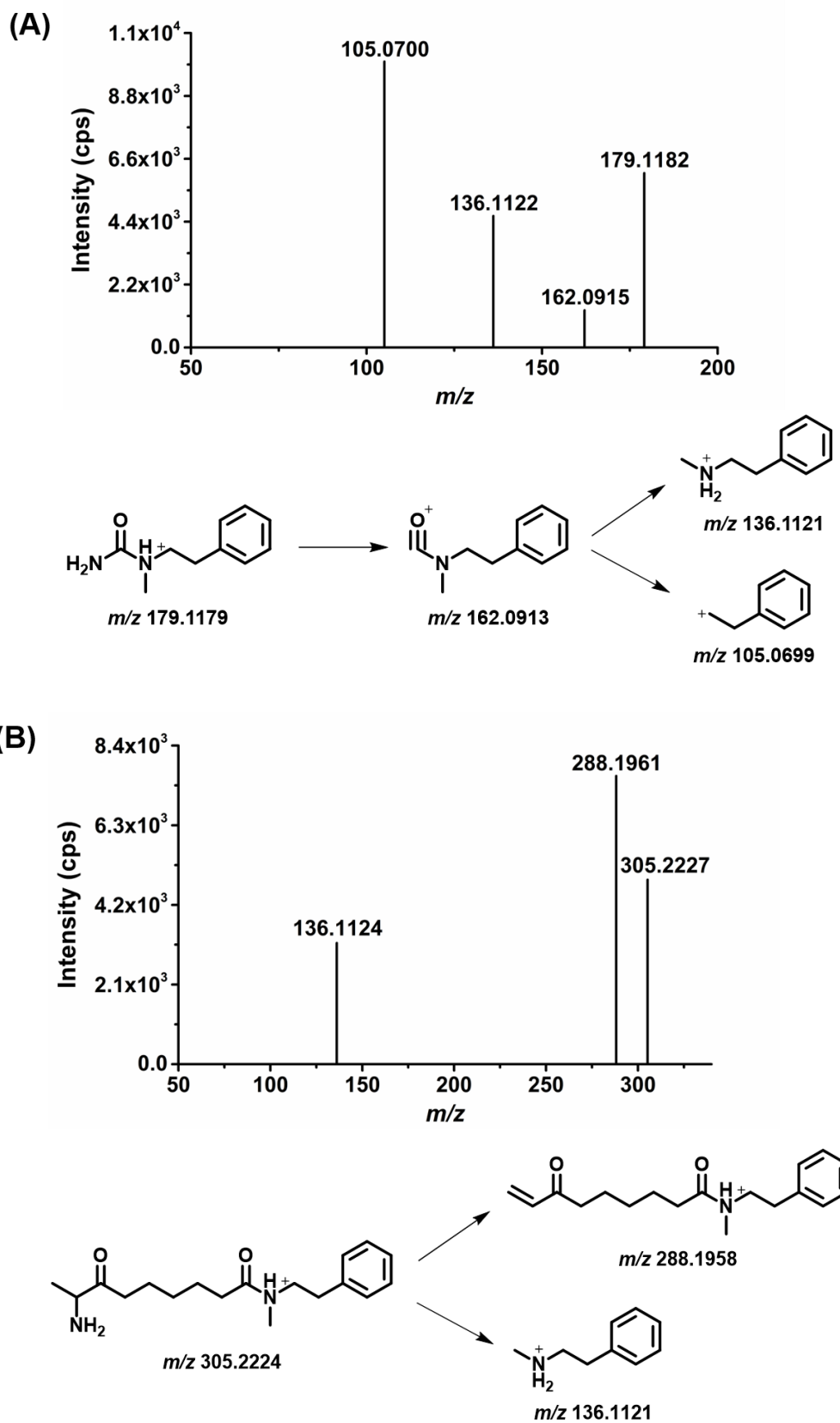
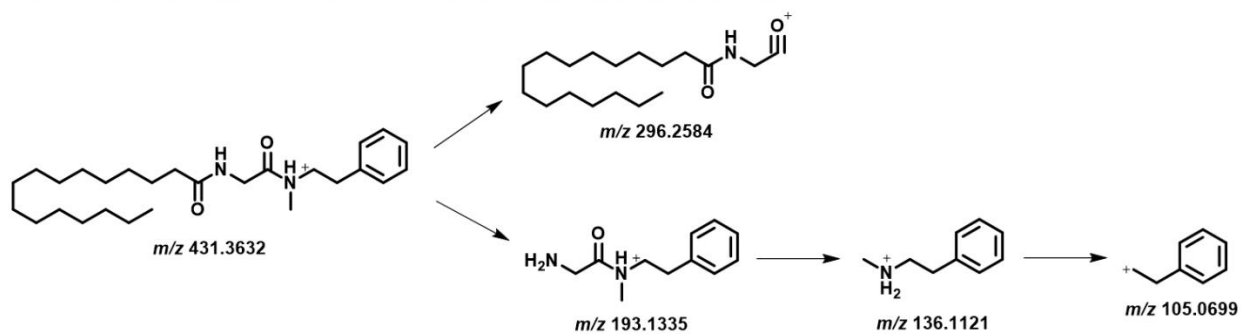
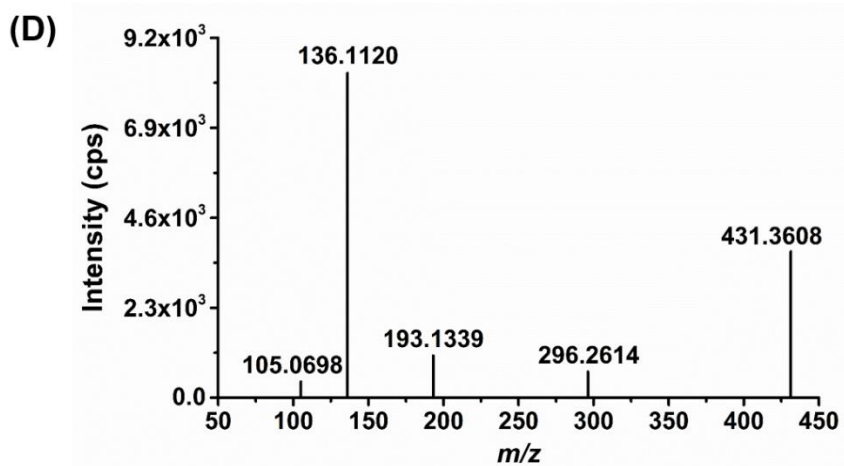
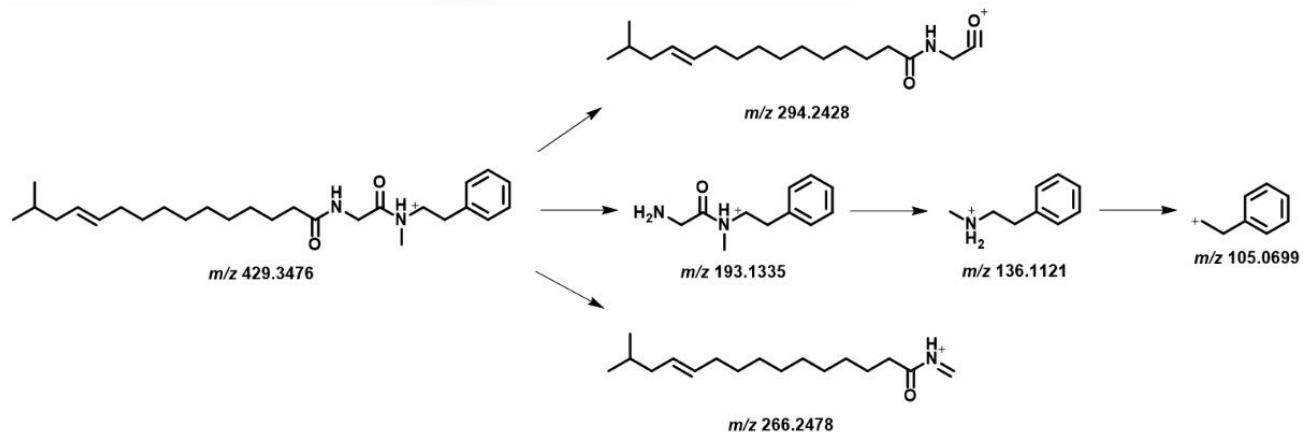
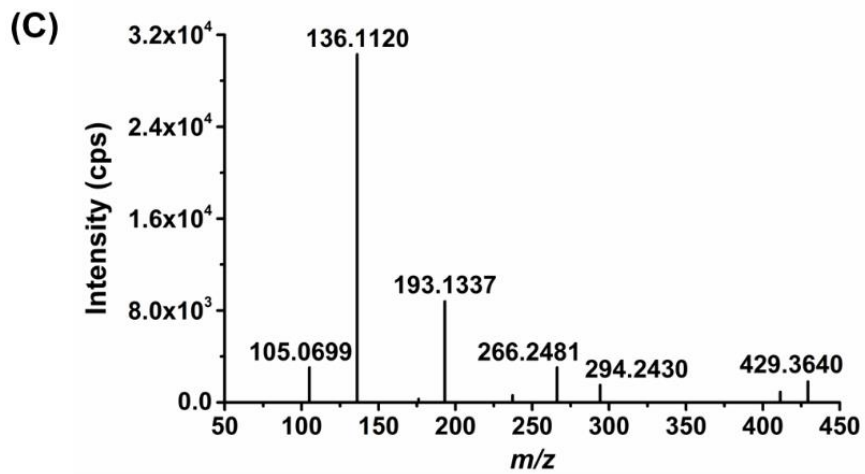
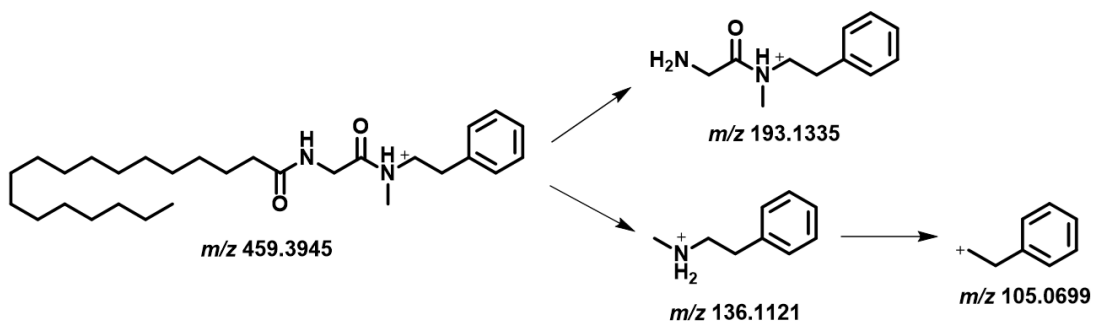
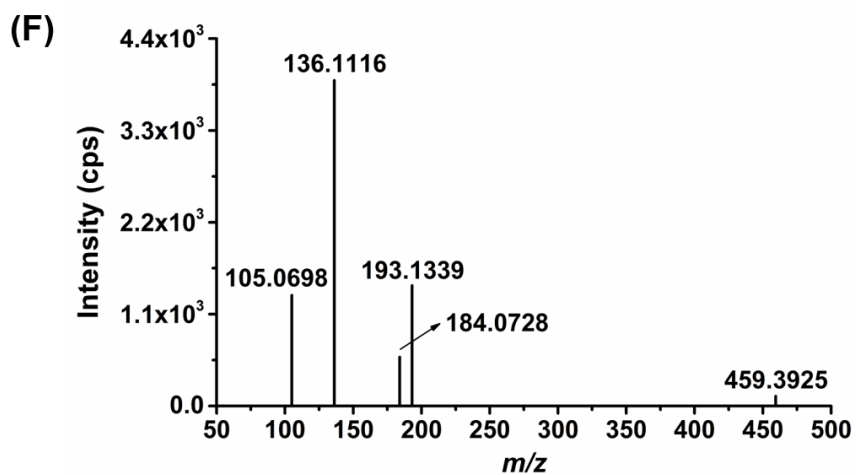
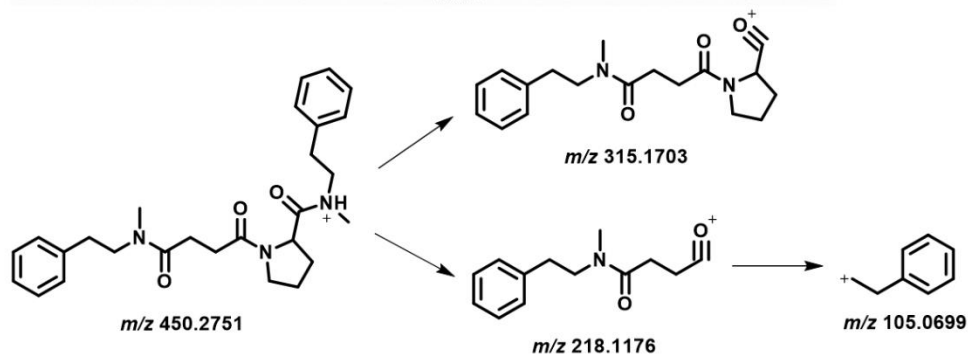
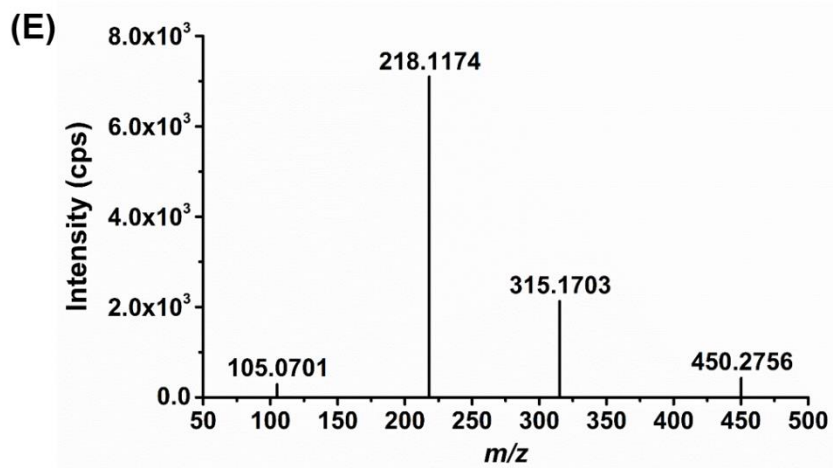


Figure S8. MS² spectra of seven annotated carboxylated metabolites in HepG2 cell extracts. (A) Carbamic acid; (B) 8-Amino-7-oxononanoic acid; (C) 2-(14-Methylpentadec-11-enoylamino)acetic acid; (D) Palmitoylglycine; (E) *N*-Succinyl proline; (F) Glycine stearamide; (G) *N*-Palmitoyl-phenylalanine.







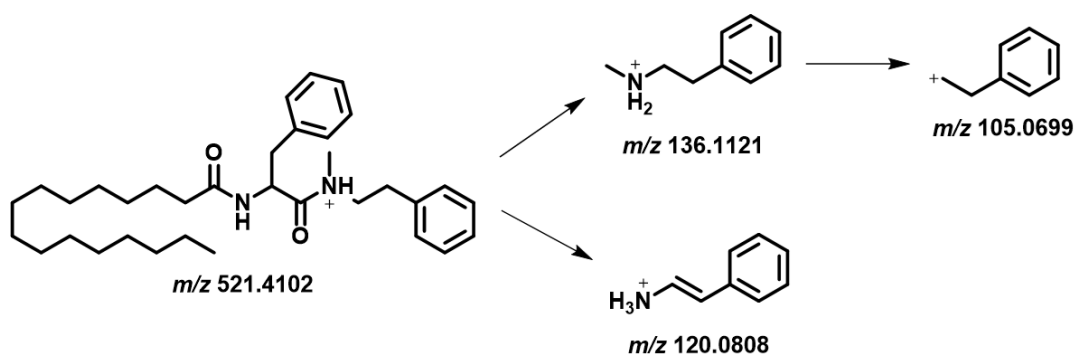
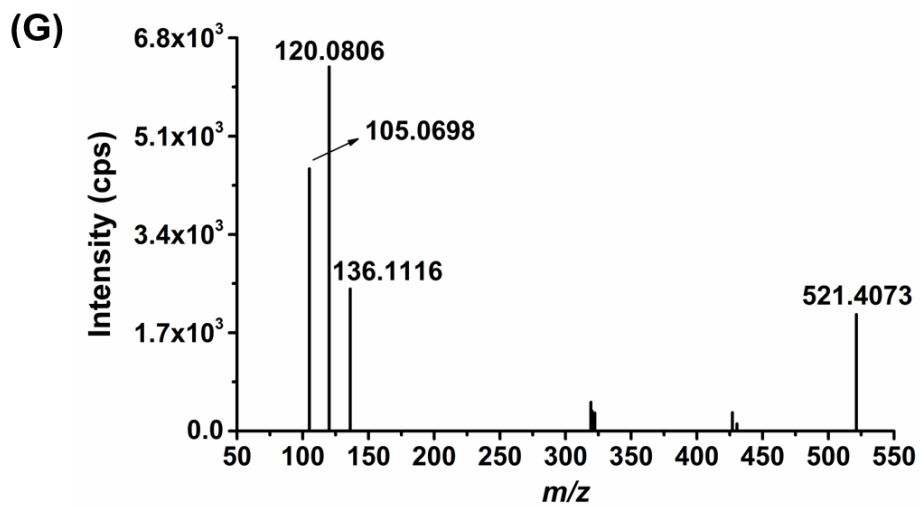


Figure S9. The RSDs of intensity ratios (light/heavy labeling) for 403 carboxylated metabolites (n = 3).

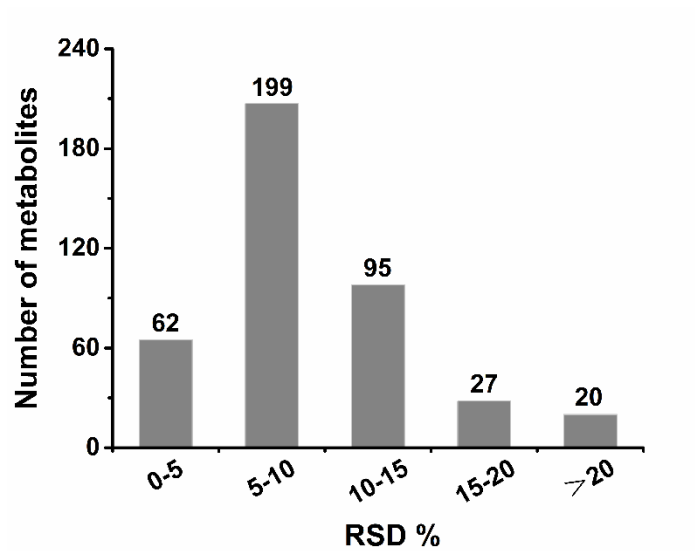


Table S1. Detailed information of carboxylic acid standards.

Name	CAS No.	Molecular Formula	Molecular weight
Glycine	56-40-6	C2H5O2N	75.0320
Alanine	302-72-7	C3H7O2N	89.0477
Serine	302-84-1	C3H7NO3	105.0426
Proline	29795-82-2	C5H9NO2	115.0633
Valine	516-06-3	C5H11O2N	117.0790
Threonine	72-19-5	C4H9NO3	119.0582
Isoleucine	443-79-8	C6H13O2N	131.0946
Leucine	328-39-2	C6H13O2N	131.0946
Methionine	59-51-8	C5H11O2NS	149.0510
Phenylalanine	150-30-1	C9H11O2N	165.0790
DL-Tyrosine	556-03-6	C9H11O3N	181.0739
DL-Tryptophan	73-22-3	C11H12O2N2	204.0899
Lactic acid	10326-41-7	C3H6O3	90.0317
3-Hydroxybutyric acid	600-15-7	C4H8O3	104.0473
16-Hydroxyhexadecanoic acid	506-13-8	C16H32O3	272.2351
3-Hydroxyoctadecanoic acid	17773-34-1	C18H36O3	300.2664
Formic acid	64-18-6	CH2O2	46.0055
Acetic acid	64-19-7	C2H4O2	60.0211
Propionic acid	79-09-4	C3H6O2	74.0368
Butyric acid	107-92-6	C4H8O2	88.0524
Isobutyric acid	79-31-2	C4H8O2	88.0524
Valeric acid	109-52-4	C5H10O2	102.0681
2-Methylbutyric acid	116-53-0	C5H10O2	102.0681
Isovaleric acid	503-74-2	C5H10O2	102.0681
Hexanoic acid	142-62-1	C6H12O2	116.0837
Heptanoic acid	111-14-8	C7H14O2	130.0994
Caprylic acid	124-07-2	C8H16O2	144.1150
Pelargonic acid	112-05-0	C9H18O2	158.1307
Capric acid	334-48-5	C10H20O2	172.1463
Hendecanoic acid	112-37-8	C11H22O2	186.1620
Dodecanoic acid	143-07-7	C12H24O2	200.1776
Tridecanoic acid	638-53-9	C13H26O2	214.1933
Myristic acid	544-63-8	C14H28O2	228.2089
Pentadecanoic acid	1002-84-2	C15H30O2	242.2246
Palmitic acid	57-10-3	C16H32O2	256.2402
Heptadecanoic acid	506-12-7	C17H34O2	270.2559
Stearic acid	57-11-4	C18H36O2	284.2715
Nonadecanoic acid	646-30-0	C19H38O2	298.2872
Arachidic acid	506-30-9	C20H40O2	312.3028
Fumaric acid	110-17-8	C4H4O4	116.0110
Succinic acid	110-15-6	C4H6O4	118.0266
Malic acid	97-67-6	C4H6O5	134.0215
Myristoleic acid	544-64-9	C14H26O2	226.1933
Palmitelaidic acid	10030-73-6	C16H30O2	254.2246
α -Linolenic acid	463-40-1	C18H30O2	278.2246
Linoleic acid	60-33-3	C18H32O2	280.2402
Eicosapentaenoic acid	10417-94-4	C20H30O2	302.2246

Arachidonic acid	506-32-1	C20H32O2	304.2402
Dihomo- γ -linolenic acid	1783-84-2	C20H34O2	306.2559

Continued table

Name	CAS No.	Molecular Formula	Molecular weight
Docosahexaenoic acid	6217-54-5	C22H32O2	328.2402
Docosapentaenoic acid	24880-45-3	C22H34O2	330.2559
Erucic acid	112-86-7	C22H42O2	338.3185
<i>cis</i> -Vaccenic acid	506-17-2	C18H34O2	282.2559
<i>N</i> -Formyl-DL-phenylalanine	4289-95-6	C10H11NO3	193.0739
<i>N</i> -Acetyl- β -alanine	3025-95-4	C5H9NO3	131.0582
<i>N</i> -Benzoyl-DL-alanine	1205-02-3	C10H11NO3	193.0739
<i>N</i> -Acetyl-DL-aspartic acid	2545-40-6	C6H9NO5	175.0481
Adipic acid	124-04-9	C6H10O4	146.0579
2-Methylsuccinic acid	498-21-5	C5H8O4	132.0423
5-Methylhexanoic acid	628-46-6	C7H14O2	130.0994
2-Methylheptanoic acid	1188-02-9	C8H16O2	144.1150
4-Methylnonanoic acid	45019-28-1	C10H20O2	172.1463
<i>trans</i> -2-Dodecenoic acid	32466-54-9	C12H22O2	198.1620
<i>N</i> -Oleoysarcosine	110-25-8	C21H39NO3	353.2930
Betamipron	3440-28-6	C10H11NO	161.0841
Glutaconic acid	1724-02-3	C5H6O4	130.0266
Glutaric acid	110-94-1	C5H8O4	132.0423
3-Methylglutaric acid	626-51-7	C6H10O4	146.0579
2-Methylhexanoic acid	4536-23-6	C7H14O2	130.0994
Sodium 2-ethylhexanoate	19766-89-3	C8H16O2	144.1150
2-Methylnonanoic acid	24323-21-5	C10H20O2	172.1463
4-Ethyloctanoic acid	16493-80-4	C10H20O2	172.1463
3-Hydroxybutyric acid	625-71-8	C4H8O3	104.0473
4-Hydroxybutyric acid	591-81-1	C4H8O3	104.0473
2-Hydroxyhexanoic acid	6064-63-7	C6H12O3	132.0786
2-Methylbutyric acid	116-53-0	C5H10O2	102.0681
Isovaleric acid	503-74-2	C5H10O2	102.0681
Valproic acid	99-66-1	C8H16O2	144.1150
<i>cis</i> -5-Dodecenoic acid	2430-94-6	C12H22O2	198.1620
2-Hydroxyhexadecanoic acid		C16H32O3	272.2351
6-Hydroxyhexadecanoic acid	58763-57-8	C16H32O3	272.2351
8-Hydroxyhexadecanoic acid	83921-07-7	C16H32O3	272.2351
9-Hydroxyhexadecanoic acid	17833-52-2	C16H32O3	272.2351
12-Hydroxyhexadecanoic acid	83646-62-2	C16H32O3	272.2351
13-Hydroxyhexadecanoic acid	59642-39-6	C16H32O3	272.2351
16-Hydroxyhexadecanoic acid	506-13-8	C16H32O3	272.2351
2-Hydroxyoctadecanoic acid		C18H36O3	300.2664
3-Hydroxyoctadecanoic acid	45261-96-9	C18H36O3	300.2664
9-Hydroxyoctadecanoic acid	3384-24-5	C18H36O3	300.2664
10-Hydroxyoctadecanoic acid	638-26-6	C18H36O3	300.2664
12-Hydroxyoctadecanoic acid	106-14-9	C18H36O3	300.2664
13-Hydroxyoctadecanoic acid		C18H36O3	300.2664
<i>cis</i> -4-Eicosenoic acid		C20H38O2	310.2872
<i>cis</i> -11-Eicosenoic acid	5561-99-9	C20H38O2	310.2872
2-Hydroxy-4-methylpentanoic acid	498-36-2	C6H12O3	132.0786

Ricinoleic acid	141-22-0	C18H34O3	298.2508
6-Hydroxycaproic acid	1191-25-9	C6H12O3	132.0786
Benzoic acid	65-85-0	C7H6O2	122.1214

Continued table

Name	CAS No.	Molecular Formula	Molecular weight
3-Hydroxypropanoic acid	503-66-2	C3H6O3	90.0317
Sebacic acid	111-20-6	C10H18O4	202.1205
Azelaic acid	204-669-1	C9H16O4	188.1049
Crotonic acid	107-93-7	C4H6O2	86.0368
2-Methyl-4-pentenoic acid	1575-74-2	C6H10O2	114.0681
2-Methyl-2-pentenoic acid	3142-72-1	C6H10O2	114.0681
2-Oxovaleric acid	1821-02-9	C5H8O3	116.0473
Levulinic acid	123-76-2	C5H8O3	116.0473
3-Methyl-2-oxobutanoic acid	759-05-7	C5H8O3	116.0473
2-Methylvaleric acid	97-61-0	C6H12O2	116.0837
3-Hydroxyisovaleric acid	625-08-1	C5H10O3	118.0630
2-Hydroxy-3-methylbutyric acid	4026-18-0	C5H10O3	118.0630
4-Methyl-2-oxovaleric acid	816-66-0	C6H10O3	130.0630
5-Oxohexanoic acid	3128-06-1	C6H10O3	130.0630
2-Acetoxypropanoic acid	535-17-1	C5H8O4	132.0423
6-Hydroxyhexanoic acid	1191-25-9	C6H12O3	132.0786
4-Aminobenzoic acid	150-13-0	C7H7NO2	137.0477
Salicylic acid	69-72-7	C7H6O3	138.0317
3-(2-Furyl)propanoic acid	935-13-7	C7H8O3	140.0473
<i>trans</i> -2-Octenoic acid	1871-67-6	C8H14O2	142.0994
4-Acetamidobutanoic acid	3025-96-5	C6H11NO3	145.0739
Cinnamic acid	621-82-9	C9H8O2	148.0524
3-Phenylpropionic acid	501-52-0	C9H10O2	150.0681
2-Phenylpropionic acid	492-37-5	C9H10O2	150.0681
4-Methylphenylacetic acid	622-47-9	C9H10O2	150.0681
Mandelic acid	90-64-2	C8H8O3	152.0473
2-Nonenoic acid	3760-11-0	C9H16O2	156.1150
3-Nonenoic acid	4124-88-3	C9H16O2	156.1150
Succinylacetone	51568-18-4	C7H10O4	158.0579
Phenyllactic acid	20312-36-1	C9H10O3	166.0630
Homogentisic acid	451-13-8	C8H8O4	168.0423
9-Decenoic acid	14436-32-9	C10H18O2	170.1307
10-Undecenoic acid	112-38-9	C10H18O2	170.1307
3-Hydroxycapric acid	14292-26-3	C10H20O3	188.1412
1-Methyl-3-indoleacetic acid	1912-48-7	C11H11NO2	189.0790
3-Indolepropionic acid	830-96-6	C11H11NO2	189.0790
Phenylacetyl glycine	500-98-1	C10H11NO3	193.0739
Palmitoleic acid	373-49-9	C16H30O2	254.2246
γ -Linolenic acid	506-26-3	C18H30O2	278.2246
α -Linolenic acid	463-40-1	C18H30O2	278.2246
Linoelaidic acid	506-21-8	C18H32O2	280.2402
Linoleic acid	60-33-3	C18H32O2	280.2402
Vaccenic acid	693-72-1	C18H34O2	282.2559
Elaidic acid	112-79-8	C18H34O2	282.2559

Petroselinic acid	593-39-5	C18H34O2	282.2559
<i>cis</i> -11,14-Eicosadienoic acid	2091-39-6	C20H36O2	308.2715
<i>cis</i> -11-Eicosenoic acid	5561-99-9	C20H38O2	310.2872
Octadecanedioic acid	871-70-5	C18H34O4	314.2547

Continued table

Name	CAS No.	Molecular Formula	Molecular weight
Docosatrienoic acid	28845-86-5	C22H38O2	334.2872
3-Oxo-5 β -cholanolic acid	1553-56-6	C24H38O3	374.2821
5-Cholenic acid-3 β -ol	5255-17-4	C24H38O3	374.2821
Lithocholenic acid	1053-37-8	C24H38O3	374.2821
Isolithocholic acid	1534-35-6	C24H40O3	376.2977
Isoallolithocholic acid	2276-93-9	C24H40O3	376.2977
Lithocholic acid	434-13-9	C24H40O3	376.2977
Nordeoxycholic acid	53608-86-9	C23H38O4	378.2770
3,6-Diketocholanolic acid	6868-73-1	C24H36O4	388.2614
Apocholic acid	641-81-6	C24H38O4	390.2770
3 α -Hydroxy-7-oxo-5 β -cholanolic acid	4651-67-6	C24H38O4	390.2770
12-Ketolithocholic acid	5130-29-0	C24H38O4	390.2770
6-Ketolithocholic acid	2393-61-5	C24H38O4	390.2770
Ursodeoxycholic acid	128-13-2	C24H40O4	392.2927
3 β -Ursodeoxycholic acid	78919-26-3	C24H40O4	392.2927
Isodeoxycholic acid	566-17-6	C24H40O4	392.2927
Deoxycholic acid	83-44-3	C24H40O4	392.2927
β -Hyodeoxycholic acid	570-84-3	C24H40O4	392.2927
Hyodeoxycholic acid	83-49-8	C24H40O4	392.2927
Nor Cholic acid	60696-62-0	C23H38O5	394.2719
Dehydrocholic acid	81-23-2	C24H34O5	402.2406
3-Keto-7 α ,12 α -dihydroxy-5 β -cholanolic acid	2304-89-4	C24H38O5	406.2719
3 β -Cholic acid	3338-16-7	C24H40O5	408.2876
Cholic acid	81-25-4	C24H40O5	408.2876
Allocholic acid	2464-18-8	C24H40O5	408.2876
α -Muricholic acid	2393-58-0	C24H40O5	408.2876
Ursocholic acid	2955-27-3	C24H40O5	408.2876
Hyochoolic acid	547-75-1	C24H40O5	408.2876
ω -Muricholic acid	6830-03-1	C24H40O5	408.2876
β -Muricholic acid	2393-59-1	C24H40O5	408.2876
Docosapentaenoic acid (22n-3)	24880-45-3	C22H34O2	330.2559

Table S2. Advantages and disadvantages of six carboxylic labeling reagents.

		MPEA	PPM	4-AMBA	DMED	3-NPH	DmPA
Reactivity	SCFAs	√	×	√	√	×	√
	MCFAs	√	×	√	√	√	√
	LCFAs	√	√	√	√	√	√
	polyCAs	√	×	×	×	×	√
	AAs	√	×	×	×	×	√
	aromatic acids	√	×	√	√	√	√
Chromatographic retention on RP column	SCFAs	√	-	√	×	-	√
	MCFAs	√	-	√	√	√	√
	LCFAs	√	√	√	√	√	√
	polyCAs	√	-	-	-	-	√
	AAs	√	-	-	-	-	--
	aromatic acids	√	-	√	√	√	√
Selectivity	carboxylated metabolites	√		-	-	-	√
	amino metabolites	×		-	-	-	√

- null

-- double chromatographic peak

Table S3. Reactivity of MPEA to metabolites containing other functional groups.

Acidic metabolites	Name	Whether can be labeled by MPEA or not
	Serotonin	No
	Dopamine	No
Phenol metabolites	4-Ethylphenol	No
	4-Nitrophenol	No
	Hydrogen sulfide	No
Sulfhydryl metabolites	2-Mercaptoethylamine	No
	3-Mercapto-1-propanol	No
	Methyl 3-mercaptopropionate	No
	Glucose-1-phosphate	No
Phosphate metabolites	Fructose-6-phosphate	No
	Adenosine triphosphate	No

Table S4. Detection sensitivity of carboxylated acids before and after MPEA labeling (injection volume: 10 μ L).

Analytes	LODs (ng/mL)	
	Unlabeled	Labeled by MPEA
Valeric acid	30	0.1
Succinic acid	50	0.2
Citric acid	90	0.1
Capric acid	3	0.2
Nonadecanoic acid	2	0.2
Alanine	40	1
Tryptophan	12	1
Phenylalanine	36	2

Table S5. Labeling efficiency of MPEA in HepG2 cell extracts.

Analytes	Labeling efficiency (%)
Valeric acid	99
Succinic acid	95
9-Decenoic acid	99
Nonadecanoic acid	99
Alanine	98
Tryptophan	95
Phenylalanine	95

Table S6. Detected MPEA-labeled carboxylated metabolites in HepG2 cell extracts.

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
1	164.1068	12.08	1.39E+08	167.1257	12.01	9.64E+07	100.0	C10H14ON	CH2O2	CLMD	Formic acid	64-18-6	Level 1
2	178.1225	13.56	7.06E+07	181.1414	13.48	8.76E+07	200.0	C11H16ON	C2H4O2	CLMD	Acetic acid	64-19-7	Level 1
3	192.1383	17.00	1.01E+07	195.1572	16.93	9.82E+06	300.0	C12H18ON	C3H6O2	CLMD	Propionic acid	79-09-4	Level 1
4	193.1335	3.04	6.73E+06	196.1524	3.00	3.83E+06		C11H17ON2	C2H5O2N	CLMD	Glycine	56-40-6	Level 1
5	206.1540	19.51	1.25E+06	209.1729	19.42	1.43E+06	384.6	C13H20ON	C4H8O2	CLMD	Isobutyric acid	79-31-2	Level 1
6	206.1540	19.97	4.78E+06	209.1729	19.88	3.78E+06	400.0	C13H20ON	C4H8O2	CLMD	Butyric acid	107-92-6	Level 1
7	207.1492	4.72	3.98E+06	210.1681	4.64	5.45E+06		C12H19ON2	C3H7O2N	CLMD	Alanine	302-72-7	Level 1
8	208.1336	13.19	1.14E+08	211.1525	13.10	1.13E+08	175.0	C12H18O2N	C3H6O3	CLMD	Lactic acid	10326-41-7	Level 1
9	220.1697	22.20	9.76E+05	223.1886	22.14	1.01E+06	476.4	C14H22ON	C5H10O2	CLMD	Ethylmethylacetic acid	116-53-0	Level 1
10	220.1697	22.89	4.46E+06	223.1886	22.82	4.67E+06	488.2	C14H22ON	C5H10O2	CLMD	Valeric acid	109-52-4	Level 1
11	220.1697	22.55	1.50E+06	223.1886	22.46	1.32E+06	500.0	C14H22ON	C5H10O2	CLMD	Pivalic acid	75-98-9	Level 1
12	222.1489	13.98	3.81E+06	225.1678	13.91	3.35E+06	212.2	C13H20O2N	C4H8O3	CLMD	3-Hydroxybutyric acid	300-85-6	Level 1
13	223.1441	3.00	4.45E+06	226.1630	2.98	5.21E+06		C12H19N2O2	C3H7NO3	CLMD	Serine	302-84-1	Level 1
14	233.1653	6.95	3.25E+06	236.1842	6.90	3.32E+06		C14H21N2O	C5H9NO2	CLMD	Proline	29795-82-2	Level 1
15	234.1849	25.85	4.26E+06	237.2038	25.78	5.26E+06	600.0	C15H24ON	C6H12O2	CLMD	Caproic acid	142-62-1	Level 1
16	235.1805	11.25	7.91E+06	238.1994	11.20	7.32E+07	43.5	C14H23ON2	C5H11O2N	CLMD	Valine	516-06-3	Level 1
17	236.1278	13.76	1.69E+07	239.1467	13.71	1.36E+07	205.9	C13H18O3N	C4H6O4	CLMD	Succinic acid	110-15-6	Level 1
18	237.1602	4.62	1.35E+06	240.1791	4.58	1.39E+06		C13H9NO3	C4H9NO3	CLMD	Threonine	72-19-5	Level 1
19	240.1380	21.87	3.39E+07	243.1569	21.79	2.83E+07	465.1	C16H18ON	C7H6O2	CLMD	Benzoic acid	65-85-0	Level 1
20	248.2003	28.60	2.25E+06	251.2192	28.53	1.96E+06	673.0	C16H26ON	C7H14O2	CLMD	Heptanoic acid	111-14-8	Level 1
21	248.2003	27.86	1.75E+06	251.2192	27.80	1.95E+06	700.0	C16H26ON	C7H14O2	CLMD	Isoheptanoic acid	628-46-6	Level 1
22	249.1594	12.05	9.86E+05	252.1783	11.96	1.05E+06	97.7	C14H21O2N2	C5H9O3N	CLMD	<i>N</i> -Acetyl-β-alanine	3025-95-4	Level 1
23	249.1961	13.78	2.86E+06	252.2150	13.72	2.36E+06	206.4	C15H25ON2	C6H13O2N	CLMD	Leucine	328-39-2	Level 1
24	249.1961	14.01	2.70E+07	252.2150	13.96	2.46E+07	213.1	C15H25ON2	C6H13O2N	CLMD	Isoleucine	443-79-8	Level 1
25	252.1218	11.05	1.30E+06	255.1407	10.99	1.17E+06	30.0	C13H18O4N	C4H6O5	CLMD	Malic acid	6915-15-7	Level 1
26	262.2163	31.23	1.83E+06	265.2352	31.16	1.29E+06	800.0	C17H28ON	C8H16O2	CLMD	Caprylic acid	124-07-2	Level 1

27	264.1592	16.37	2.91E+06	267.1781	16.31	3.51E+06	281.8	C15H22O3N	C6H10O4	CLMD	Adipic acid	124-04-9	Level 1
28	267.1526	12.43	3.50E+07	270.1715	12.37	4.20E+07	123.4	C14H23ON2S	C5H11O2NS	CLMD	Methionine	59-51-8	Level 1
29	276.2322	33.77	1.52E+07	279.2511	33.69	1.22E+07	900.0	C18H30ON	C9H18O2	CLMD	Pelargonic acid	112-05-0	Level 1
30	283.1805	15.83	3.40E+07	286.1994	15.76	2.53E+07	266.0	C18H23ON2	C9H11O2N	CLMD	Phenylalanine	150-30-1	Level 1
31	290.2474	36.24	5.54E+06	293.2663	36.15	6.03E+06	1000.0	C19H32ON	C10H20O2	CLMD	Capric acid	334-48-5	Level 1
32	293.1492	10.79	1.96E+07	296.1681	10.73	2.06E+07	12.3	C15H21O4N2	C6H9O5N	CLMD	N-Acetyl-aspartic acid	997-55-7	Level 1
33	299.1754	11.83	8.95E+06	302.1943	11.77	7.26E+06	82.8	C18H23O2N2	C9H11O3N	CLMD	Tyrosine	556-03-6	Level 1
34	304.2635	38.64	1.23E+06	307.2824	38.60	9.93E+05	1100.0	C20H34ON	C11H22O2	CLMD	Hendecanoic acid	112-37-8	Level 1
35	306.2063	21.91	5.43E+06	309.2252	21.83	4.63E+06	466.5	C18H28O3N	C9H16O4	CLMD	Azelaic acid	123-99-9	Level 1
36	316.2632	38.25	3.90E+06	319.2821	38.18	3.83E+06	1083.7	C21H34ON	C12H22O2	CLMD	9-Dodecenoic acid	21091-01-0	Level 1
37	318.2791	41.00	4.45E+07	321.2980	40.90	3.82E+07	1200.0	C21H36ON	C12H24O2	CLMD	Dodecanoic acid	143-07-7	Level 1
38	320.2219	26.53	1.31E+06	323.2408	26.47	1.50E+06	624.7	C19H30O3N	C10H18O4	CLMD	Sebacic acid	111-20-6	Level 1
39	322.1914	16.52	7.14E+06	325.2103	16.47	6.59E+06	286.0	C20H24ON3	C11H12O2N2	CLMD	Tryptophan	54-12-6	Level 1
40	332.2948	43.14	2.57E+06	335.3137	43.09	2.36E+06	1300.0	C22H38ON	C13H26O2	CLMD	n-Tridecanoic acid	638-53-9	Level 1
41	344.2946	42.03	1.54E+07	347.3135	41.98	1.47E+07	1248.2	C23H38ON	C14H26O2	CLMD	Tsuzuic acid	544-65-0	Level 1
42	346.3104	45.36	1.41E+08	349.3293	45.29	1.67E+08	1400.0	C23H40ON	C14H28O2	CLMD	Myristic acid	544-63-8	Level 1
43	360.3261	47.34	1.70E+07	363.3450	47.27	1.29E+07	1500.0	C24H42ON	C15H30O2	CLMD	Pentadecanoic acid	1002-84-2	Level 1
44	372.3261	46.04	1.16E+08	375.3450	45.95	8.33E+07	1434.2	C25H42ON	C16H30O2	CLMD	Hypogeic acid	2416-19-5	Level 1
45	374.3417	49.19	2.13E+08	377.3606	49.06	1.22E+08	1600.0	C25H44ON	C16H32O2	CLMD	Palmitic acid	57-10-3	Level 1
46	388.3574	50.83	2.75E+07	391.3763	50.77	1.47E+07	1700.0	C26H46ON	C17H34O2	CLMD	Heptadecanoic acid	506-12-7	Level 1
47	390.3367	36.54	2.57E+06	393.3556	36.51	4.92E+06	1012.6	C25H44O2N	C16H32O3	CLMD	16-Hydroxyhexadecanoic acid	506-13-8	Level 1
48	396.3261	44.50	6.95E+06	399.3450	44.44	8.04E+06	1361.0	C27H42ON	C18H30O2	CLMD	α -Linolenic acid	463-40-1	Level 1
49	398.3418	46.92	4.47E+07	401.3607	46.85	5.51E+07	1478.8	C27H44ON	C18H32O2	CLMD	Linoleic acid	60-33-3	Level 1
50	400.3574	49.44	4.67E+08	403.3763	49.35	3.88E+08	1615.5	C27H46ON	C18H34O2	CLMD	Oleic acid	112-80-1	Level 1
51	402.3730	52.80	3.08E+08	405.3919	52.70	3.63E+08	1800.0	C27H48ON	C18H36O2	CLMD	Stearic acid	57-11-4	Level 1
52	416.3886	54.33	1.98E+06	419.4075	54.30	1.98E+06	1900.0	C28H50ON	C19H38O2	CLMD	Nonadecanoic acid	646-30-0	Level 1
53	418.3679	48.65	5.68E+06	421.3868	48.57	3.51E+06	1570.9	C27H48O2N	C18H36O3	CLMD	3-Hydroxyoctadecanoic acid		Level 1
54	420.3261	44.04	4.87E+06	423.3450	43.98	5.18E+06	1340.6	C29H42ON	C20H30O2	CLMD	Eicosapentaenoic acid	10417-94-4	Level 1
55	422.3418	46.35	4.76E+07	425.3607	46.29	4.10E+07	1450.0	C29H44ON	C20H32O2	CLMD	Arachidonic acid	506-32-1	Level 1
56	424.3574	47.90	7.84E+06	427.3763	47.84	1.10E+07	1530.6	C29H46ON	C20H34O2	CLMD	5,8,11-Eicosatrienoic acid	20590-32-3	Level 1

57	426.3731	50.06	1.95E+07	429.3920	50.01	1.29E+07	1653.2	C29H48ON	C20H36O2	CLMD	11Z,14Z-Eicosadienoic acid	2091-39-6	Level 1
58	428.3887	52.94	2.87E+07	431.4076	52.93	3.02E+07	1809.1	C29H50ON	C20H38O2	CLMD	11Z-Eicosenoic acid	5561-99-9	Level 1
59	430.4042	58.25	2.00E+06	433.4231	58.20	2.14E+06	1986.5	C29H52ON	C20H40O2	CLMD	Arachidic acid	506-30-9	Level 1
60	446.3418	45.75	1.88E+07	449.3607	45.70	1.81E+07	1419.7	C31H44ON	C22H32O2	CLMD	Docosahexaenoic acid	6217-54-5	Level 1

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
61	448.3572	46.74	5.53E+06	451.3761	46.69	5.29E+06	1470.0	C31H46ON	C22H34O2	CLMD	Docosapentaenoic acid (22n-3)	24880-45-3	Level 1
62	450.3730	48.85	6.35E+06	453.3919	48.79	5.21E+06	1581.7	C31H48ON	C22H36O2	CLMD	7,10,13,16-Docosatetraenoic acid	28874-58-0	Level 1
63	456.4200	58.20	2.57E+06	459.4389	58.14	2.44E+06	2153.6	C31H54ON	C22H42O2	CLMD	Erucic acid	112-86-7	Level 1
64	351.2065	22.46	2.68E+06	357.2443	22.38	2.64E+06	485.2	C22H27O2N2	C4H4O4	CLMD	Fumaric acid	110-17-8	Level 1
65	353.2223	23.51	2.93E+08	359.2601	23.40	1.99E+08	520.8	C22H29O2N2	C4H6O4	CLMD	Succinic acid	110-15-6	Level 1
66	367.2381	24.08	8.21E+06	373.2759	23.99	7.28E+06	540.3	C23H31O2N2	C5H8O4	CLMD	Glutaric acid	110-94-1	Level 1
67	369.2174	21.91	2.76E+06	375.2552	21.81	3.48E+06	466.5	C22H29O3N2	C4H6O5	CLMD	Malic acid	6915-15-7	Level 1
68	410.2438	20.72	1.36E+07	416.2816	20.67	1.61E+07	425.7	C24H32O3N3	C6H9O5N	CLMD	2-Acetamidosuccinic acid	2545-40-6	Level 1
69	179.1169	11.11	5.82E+06	182.1358	11.02	9.50E+06	34.0	C10H15ON2	CH3O2N	HMDB	Carbamic acid	463-77-4	Level 2
70	305.2208	18.80	1.51E+06	308.2397	18.75	1.02E+06	360.7	C18H29O2N2	C9H17O3N	HMDB	8-Amino-7-oxononanoic acid	682799-71-9	Level 2
71	429.3475	41.48	1.14E+06	432.3664	41.45	1.25E+06	1222.8	C27H45O2N2	C18H33O3N	HMDB	2-(14-Methylpentadec-11-enoylamino)acetic acid		Level 2
72	431.3630	44.70	2.06E+06	434.3819	44.66	2.34E+06	1370.1	C27H47O2N2	C18H35O3N	HMDB	Palmitoylglycine	158305-64-7	Level 2
73	450.2751	22.91	6.10E+06	456.3129	22.82	7.17E+06	500.7	C27H36O3N3	C9H13O5N	Metlin	<i>N</i> -Succinyl proline	63250-32-8	Level 2
74	459.3945	48.41	7.88E+06	462.4134	48.38	7.34E+06	1558.1	C29H51O2N2	C20H39O3N	HMDB	Glycine stearamide	6333-54-6	Level 2
75	521.4100	48.62	2.69E+06	524.4289	48.55	2.25E+06	1569.3	C34H53O2N2	C25H41O3N	HMDB	<i>N</i> -Palmitoyl-phenylalanine		Level 2
76	207.1492	14.83	6.54E+06	210.1681	14.80	5.47E+06	236.9	C12H19ON2	C3H7O2N	Metlin	Sarcosine	107-97-1	Level 3
77	222.1489	15.33	2.75E+06	225.1678	15.26	2.56E+06	251.5	C13H20O2N	C4H8O3	HMDB	2-Hydroxybutyric acid	3347-90-8	Level 3
											4-Hydroxybutyric acid	591-81-1	
											2-Hydroxy-2-methylpropanoic acid	594-61-6	
78	233.1653	22.06	6.43E+06	236.1842	22.00	8.67E+06	471.6	C14H21N2O	C5H9NO2	HMDB	4-Amino-2-methylbutanoic acid	65370-67-4	Level 3
79	246.1123	15.52	2.87E+06	249.1312	15.45	2.86E+06	256.9	C14H16O3N	C5H4O4	HMDB	5-Hydroxy-2-furoic acid		Level 3

80	247.1441	11.96	6.65E+06	250.1630	11.92	6.39E+06	91.6	C14H19O2N2	C5H7O3N	Metlin	Pyrroline hydroxycarboxylic acid	22573-88-2	Level 3
81	247.1441	14.05	8.43E+05	250.1630	13.99	7.99E+05	214.3	C14H19O2N2	C5H7O3N	Metlin	Pyroglutamic acid	98-79-3	Level 3
											N-Acryloylglycine	24599-25-5	
											Pyrroline hydroxycarboxylic acid	22573-88-2	
											4-Oxoproline		
											1-Pyrroline-4-hydroxy-2-carboxylate	9054-77-7	
											2-Pyrrolidone-5-carboxylic acid	4042-36-8	
82	248.1280	14.08	4.58E+06	251.1469	14.02	4.41E+06	215.1	C14H18O3N	C5H6O4	HMDB	Citraconic acid	498-23-7	Level 3
											Itaconic acid	97-65-4	
											Glutaconic acid	1724-02-3	
83	248.2003	28.21	1.54E+06	251.2192	28.15	1.54E+06	685.7	C16H26ON	C7H14O2	HMDB	2-Methylhexanoic acid	4536-23-6	Level 3
											5-Methylhexanoic acid	628-46-6	
84	249.1594	12.97	8.90E+06	252.1783	12.91	7.85E+06	160.1	C14H21O2N2	C5H9O3N	HMDB	5-Aminolevulinic acid	106-60-5	Level 3
											2-Amino-5-oxopentanoic acid		
											5-Amino-5-oxopentanoic acid		
85	250.1799	16.53	1.12E+06	253.1988	16.47	9.64E+05	286.3	C15H24O2N	C6H12O3	HMDB	5-Hydroxyhexanoic acid	44843-89-2	Level 3
86	250.1799	19.66	1.35E+06	253.1988	19.61	1.31E+06	389.7	C15H24O2N	C6H12O3	HMDB	2-Hydroxycaproic acid	6064-63-7	Level 3
											Leucinic acid	498-36-2	
											3-Hydroxyhexanoic acid	10191-24-9	
											2-Hydroxy-3-methylpentanoic acid	488-15-3	
											6-Hydroxyhexanoic acid	1191-25-9	
87	260.2012	25.93	9.34E+05	263.2201	25.85	1.64E+06	602.9	C17H26ON	C8H14O2	HMDB	(E)-4-Octenoic acid	18776-92-6	Level 3
											2-Octenoic acid	1577-96-4	
											(3E)-2-Propylpent-3-enoic acid		
											cis-5-Octenoic acid	41653-97-8	
											4-ene-Valproic acid		
											2-ene-Valproic acid		
88	262.2163	30.05	1.36E+06	265.2352	29.98	1.46E+06	755.0	C17H28ON	C8H16O2	HMDB	6-Methylheptanoic acid	929-10-2	Level 3
											2-Methylenanthic acid	1188-02-9	
											2-Ethylhexanoic acid	149-57-5	

											Valproic acid	99-66-1	
89	264.1228	15.51	1.32E+06	267.1417	15.47	1.11E+06	256.8	C14H18O4N	C5H6O5	HMDB	Oxoglutaric acid	328-50-7	Level 3
											3-Oxoglutaric acid	542-05-2	
90	264.1592	18.01	1.67E+06	267.1781	17.96	1.76E+06	334.0	C15H22O3N	C6H10O4	HMDB	4-Ethoxy-4-oxobutanoic acid	1501-27-5	Level 3
91	264.1592	18.29	3.22E+06	267.1781	18.25	3.22E+06	343.5	C15H22O3N	C6H10O4	HMDB	2-Methylglutaric acid	617-62-9	Level 3
92	264.1592	19.76	4.86E+06	267.1781	19.81	4.86E+06	393.1	C15H22O3N	C6H10O4	HMDB	Methylglutaric acid	626-51-7	Level 3
											Monomethyl glutaric acid	1501-27-5	
93	265.1547	11.70	1.90E+06	268.1736	11.65	1.55E+06	74.0	C14H21O3N2	C5H9O4N	HMDB	DL-Glutamic acid	617-65-2	Level 3
94	270.1487	11.05	5.96E+06	273.1676	11.00	3.33E+06	29.9	C17H20O2N	C8H8O3	HMDB	4-Hydroxy-3-methylbenzoic acid	499-76-3	Level 3
95	270.1487	18.59	6.88E+06	273.1676	18.53	6.85E+06	353.7	C17H20O2N	C8H8O3	HMDB	2-Methoxybenzoic acid	579-75-9	Level 3

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
95	270.1487	18.59	6.88E+06	273.1676	18.53	6.85E+06	353.7	C17H20O2N	C8H8O3	HMDB	Mandelic acid	90-64-2	Level 3
											3-Methoxybenzoic acid	586-38-9	
96	275.1370	20.72	8.31E+06	278.1559	20.68	7.39E+06	425.8	C15H19O3N2	C6H7O4N	HMDB	2-Aminomuconic acid	4548-99-6	Level 3
97	277.1544	14.27	9.05E+06	280.1733	14.22	8.87E+06	220.8	C15H21O3N2	C6H9O4N	HMDB	4-Methyleneglutaric acid	16804-57-2	Level 3
											L-β-Aspartyl-L-glycine		
98	278.1750	20.29	1.55E+06	281.1939	20.21	1.52E+06	411.0	C16H24O3N	C7H12O4	HMDB	2-Ethylglutaric acid		Level 3
											2-Methyladipic acid	626-70-0	
											3-Methyladipic acid		
											Pimelic acid	111-16-0	
99	288.2318	33.58	8.11E+06	291.2507	20.41	8.15E+06	892.5	C19H30ON	C10H18O2	HMDB	5-Decenoic acid	85392-03-6	Level 3
100	288.2318	34.58	5.21E+06	291.2507	18.95	4.45E+06	932.8	C19H30ON	C10H18O2	HMDB	6-Decenoic acid	85392-04-7	Level 3
											3-Decenoic acid	15469-77-9	
											8-Methylnonenoate	59320-77-3	
											9-Decenoic acid	14436-32-9	
											Citronellic acid	502-47-6	
											<i>cis</i> -4-Decenoic acid	505-90-8	

											<i>trans</i> -Dec-2-enoic acid		
101	290.2474	34.82	9.31E+05	293.2663	34.74	1.15E+06	942.6	C19H32ON	C10H20O2	HMDB	4-Methylnonanoic acid	45019-28-1	Level 3
102	290.2474	35.70	1.54E+06	293.2663	35.60	2.10E+06	978.3	C19H32ON	C10H20O2	HMDB	4-Ethyl-octanoic acid	16493-80-4	Level 3
103	291.2046	19.89	3.21E+06	294.2235	19.83	3.21E+06	406.3	C17H27O2N2	C8H15O3N	HMDB	Hexanoylglycine	24003-67-6	Level 3
104	291.2046	20.15	1.10E+06	294.2235	20.11	9.02E+05	397.4	C17H27O2N2	C8H15O3N	HMDB	Hexanoylglycine	24003-67-6	Level 3
105	292.1905	19.97	1.98E+06	295.2094	19.91	1.05E+06	400.3	C17H26O3N	C8H14O4	HMDB	2,4-Dimethyladipic acid		
											2-Ethylsuberic acid	3971-33-3	
											3-Methylpimelic acid	10200-31-4	
											Suberic acid	505-48-6	
											2-Propylglutaric acid		
106	294.1335	14.36	2.43E+06	297.1524	14.32	3.04E+06	223.4	C15H20O5N	C6H8O6	HMDB	1,2,3-Propanetricarboxylic acid	99-14-9	Level 3
107	297.1595	19.06	9.11E+06	300.1784	19.02	8.34E+06	369.5	C18H21O2N2	C9H9O3N	HMDB	Hippuric acid	495-69-2	Level 3
108	304.1995	9.29	1.53E+06	307.2184	9.22	1.53E+06		C17H26O2N3	C8H14O3N2	HMDB	Prolylalanine		Level 3
109	304.1995	12.52	4.30E+06	307.2184	12.48	4.96E+06	129.6	C17H26O2N3	C8H14O3N2	HMDB	Prolylalanine		Level 3
110	304.2635	37.90	7.08E+05	307.2824	37.85	7.08E+05	1069.2	C20H34ON	C11H22O2	HMDB	9-Methyldecanoic acid	1119-63-7	Level 3
											4,6-Dimethylnonanoic acid	7540-70-7	
111	306.2063	24.38	4.40E+06	309.2252	24.29	4.83E+06	550.3	C18H28O3N	C9H16O4	HMDB	3-Methylsuberic acid		Level 3
											2,4-Dimethylpimelic acid		
112	307.1652	12.29	6.59E+06	310.1841	12.25	2.62E+06	114.0	C16H23O4N2	C7H11O5N	HMDB	<i>N</i> -Acetyl-DL-glutamic acid	1188-37-0	Level 3
113	308.1490	16.52	3.88E+06	311.1679	16.46	3.88E+06	286.0	C16H22O5N	C7H10O6	HMDB	3-Dehydroquinic acid		Level 3
114	308.1490	16.89	4.27E+06	311.1679	16.83	5.66E+06	296.8	C16H22O5N	C7H10O6	HMDB	2-Hydroxy-2-(2-oxopropyl)butanedioic acid		Level 3
115	311.1753	19.89	2.55E+06	314.1942	19.85	8.29E+06	397.5	C19H23O2N2	C10H11O3N	HMDB	<i>N</i> -Formylphenylalanine	13200-85-6	Level 3
116	316.2632	37.77	1.45E+06	319.2821	37.70	1.67E+06	1063.6	C21H34ON	C12H22O2	HMDB	11-Dodecenoic acid	65423-25-8	Level 3
117	316.2632	39.24	9.82E+06	319.2821	39.17	8.32E+06	1125.5	C21H34ON	C12H22O2	HMDB	<i>trans</i> -Dodec-2-enoic acid		Level 3
											5 <i>Z</i> -Dodecenoic acid	2430-94-6	
118	318.2791	39.62	8.11E+06	321.2980	39.57	9.87E+06	1141.7	C21H36ON	C12H24O2	Metlin	Isolauric acid	2724-56-3	Level 3
											2-Methyl-undecanoic acid	24323-25-9	
											3-Methyl-undecanoic acid	65781-38-6	
											4-Methyl-undecanoic acid		
											5-Methyl-undecanoic acid		

											6-Methyl-undecanoic acid		
											8-Methyl-undecanoic acid		
											9-Methyl-undecanoic acid		
119	320.2219	23.83	9.41E+05	323.2408	23.79	1.64E+06	531.6	C19H30O3N	C10H18O4	HMDB	2-Ethylsuberic acid	3971-33-3	Level 3
											3-Methylazelaic acid		
											Heptylmalonic acid		
120	320.2306	13.06	2.32E+06	323.2495	13.00	1.68E+06	166.2	C18H30O2N3	C9H18O3N2	Metlin	Alanyl-Isoleucine		Level 3
121	320.2306	13.42	1.88E+06	323.2495	13.36	1.38E+06	190.6	C18H30O2N3	C9H18O3N2	Metlin	Alanyl-Leucine		Level 3
122	320.2306	15.17	7.35E+06	323.2495	15.12	7.12E+06	246.8	C18H30O2N3	C9H18O3N2	Metlin	Isoleucyl-Alanine		Level 3
123	320.2306	16.54	3.16E+06	323.2495	16.50	4.76E+06	286.6	C18H30O2N3	C9H18O3N2	Metlin	Leucyl-Alanine	7298-84-2	Level 3
124	321.2172	20.04	8.19E+05	324.2361	20.01	1.20E+06	402.4	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3
125	321.2172	20.30	6.39E+06	324.2361	20.23	4.53E+06	411.4	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3
126	321.2172	20.58	1.07E+06	324.2361	20.53	1.41E+06	420.9	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3
127	332.2948	41.81	1.53E+06	335.3137	41.76	2.63E+06	1237.9	C22H38ON	C13H26O2	HMDB	9-Methyldodecanoic acid		Level 3
128	332.2948	42.31	1.17E+06	335.3137	42.26	1.34E+06	1261.3	C22H38ON	C13H26O2	HMDB	9-Methyldodecanoic acid		Level 3

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
129	332.2948	44.74	1.90E+06	335.3137	44.69	1.85E+06	1372.0	C22H38ON	C13H26O2	HMDB	9-Methyldodecanoic acid		Level 3
130	334.2376	25.75	3.52E+06	337.2565	25.70	4.52E+06	596.7	C20H32O3N	C11H20O4	HMDB	Undecanedioic acid	1852-04-6	Level 3
131	334.2376	28.66	1.24E+06	337.2565	28.59	1.47E+06	702.0	C20H32O3N	C11H20O4	HMDB	Undecanedioic acid	1852-04-6	Level 3
132	336.2255	13.17	6.39E+06	339.2444	13.12	4.61E+06	173.6	C18H30O3N3	C9H18O4N2	HMDB	SerinyI-Leucine		Level 3
133	336.2255	14.48	1.69E+06	339.2444	14.43	2.58E+06	226.8	C18H30O3N3	C9H18O4N2	HMDB	SerinyI-Isoleucine		Level 3
134	336.2255	15.31	3.05E+06	339.2444	15.27	2.94E+06	250.8	C18H30O3N3	C9H18O4N2	HMDB	Isoleucyl-Serine		Level 3
135	336.2255	15.66	4.76E+06	339.2444	15.61	4.76E+06	261.1	C18H30O3N3	C9H18O4N2	HMDB	Leucyl-Serine		Level 3
											ThreoninyI-Valine		
											Valyl-Threonine		
											Lysopine		
136	337.1573	18.10	4.76E+06	340.1762	18.03	4.76E+06	337.1	C20H21O3N2	C11H9O4N	Metlin	Methyl 2,6-dihydroxy-4-quinolinecarboxylate	66416-75-9	Level 3

137	337.1573	19.12	5.14E+06	340.1762	19.05	4.15E+06	371.5	C20H21O3N2	C11H9O4N	Metlin	5-Hydroxyindolepyruvate		Level 3
138	337.1573	25.76	1.89E+06	340.1762	25.70	3.21E+06	597.0	C20H21O3N2	C11H9O4N	Metlin	8-Methoxykynurenate		Level 3
139	339.2068	22.52	1.54E+06	345.2446	22.42	2.43E+06	487.3	C21H27O2N2	C3H4O4	HMDB	Hydroxypyruvic acid	1113-60-6	Level 3
											Malonic acid	141-82-2	
140	340.2019	14.64	2.10E+06	343.2208	14.61	3.33E+06	231.5	C20H26O2N3	C11H14O3N2	HMDB	Phenylalanylglycine	721-90-4	Level 3
141	340.2019	16.57	5.89E+06	343.2208	16.56	5.89E+06	287.5	C20H26O2N3	C11H14O3N2	HMDB	Glycyl-DL-phenylalanine		Level 3
142	344.2946	42.37	2.33E+06	347.3135	42.31	3.42E+06	1264.1	C23H38ON	C14H26O2	HMDB	7Z-Tetradecenoic acid		Level 3
143	344.2946	42.53	1.83E+06	347.3135	42.47	2.65E+06	1271.5	C23H38ON	C14H26O2	HMDB	9E-Tetradecenoic acid		Level 3
144	344.2946	42.73	2.09E+06	347.3135	42.67	2.68E+06	1280.9	C23H38ON	C14H26O2	HMDB	5Z-Tetradecenoic acid	5684-70-8	Level 3
145	344.2946	43.28	1.11E+06	347.3135	43.19	2.01E+06	1306.3	C23H38ON	C14H26O2	HMDB	<i>trans</i> -Tetra-dec-2-enoic acid		Level 3
146	344.2946	43.65	9.56E+05	347.3135	43.59	1.96E+06	1322.9	C23H38ON	C14H26O2	HMDB	Myristoleic acid	544-64-9	Level 3
147	346.3104	44.09	5.12E+06	349.3293	44.01	5.99E+06	1342.9	C23H40ON	C14H28O2	HMDB	10-Methyltridecanoic acid		Level 3
148	346.3104	44.86	1.12E+06	349.3293	44.79	1.65E+06	1377.4	C23H40ON	C14H28O2	HMDB	2,6,10-Trimethylundecanoic acid	1115-94-2	Level 3
											12-Methyltridecanoic acid	2724-57-4	
149	348.2645	16.52	4.90E+06	351.2834	16.46	4.90E+06	286.0	C20H34O2N3	C11H22O3N2	HMDB	Leucyl-Valine		Level 3
150	348.2645	18.66	1.99E+06	351.2834	18.63	2.53E+06	355.9	C20H34O2N3	C11H22O3N2	HMDB	Valyl-Leucine	3989-97-7	Level 3
151	349.2095	19.37	3.34E+06	352.2284	19.33	1.25E+06	379.8	C19H29O4N2	C10H17O5N	HMDB	<i>N</i> -Isovalerylglutamic acid	80154-63-8	Level 3
152	349.2095	19.98	2.68E+06	352.2284	19.78	2.85E+06	400.6	C19H29O4N2	C10H17O5N	HMDB	Suberylglycine	60317-54-6	Level 3
153	350.1863	14.78	9.54E+05	353.2052	14.77	1.25E+06	235.6	C21H24O2N3	C12H12O3N2	HMDB	Indole-3-acetyl glycine	13113-08-1	Level 3
											<i>N</i> -Formyl-tryptophan	16108-03-5	
154	351.2065	23.11	2.93E+06	357.2443	23.02	5.01E+06	507.4	C22H27O2N2	C4H4O4	HMDB	Maleic acid	110-16-7	Level 3
155	352.2020	16.13	2.12E+06	355.2209	16.10	2.67E+06	274.7	C21H26O2N3	C12H14O3N2	Metlin	5-Methoxy-DL-tryptophan	28052-84-8	Level 3
156	354.2176	15.05	2.45E+06	357.2365	15.00	3.35E+06	243.3	C21H28O2N3	C12H16O3N2	Metlin	Alanyl-Phenylalanine	1999-45-7	Level 3
157	354.2176	16.27	5.44E+06	357.2365	16.22	5.44E+06	278.8	C21H28O2N3	C12H16O3N2	Metlin	Phenylalanyl-Alanine		Level 3
158	354.2176	16.63	1.17E+06	357.2365	16.59	1.83E+06	289.2	C21H28O2N3	C12H16O3N2	Metlin			Level 3
159	354.2176	17.23	2.23E+06	357.2365	17.17	2.39E+06	307.8	C21H28O2N3	C12H16O3N2	Metlin			Level 3
160	358.3104	42.72	3.37E+06	361.3293	42.67	5.24E+06	1280.4	C24H40ON	C15H28O2	Metlin	2-Pentadecenoic acid		Level 3
161	358.3104	44.05	1.87E+06	361.3293	44.00	1.54E+06	1340.9	C24H40ON	C15H28O2	Metlin	14-Pentadecenoic acid		Level 3
162	358.3104	44.21	1.98E+06	361.3293	44.15	2.44E+06	1348.1	C24H40ON	C15H28O2	Metlin	10-Pentadecenoic acid		Level 3
163	358.3104	44.41	1.01E+06	361.3293	44.36	1.99E+06	1357.1	C24H40ON	C15H28O2	Metlin	6-Pentadecenoic acid		Level 3

164	358.3104	45.51	8.83E+05	361.3293	45.46	9.00E+05	1407.6	C24H40ON	C15H28O2	Metlin	2,5-Dimethyl-2E-tridecenoic acid		Level 3
											9-Pentadecenoic acid	15451-50-0	
165	360.3261	46.07	2.01E+06	363.3450	46.12	3.33E+06	1435.9	C24H42ON	C15H30O2	Metlin	12-Methyl myristic acid	5502-94-3	Level 3
166	360.3261	46.68	1.63E+06	363.3450	46.62	3.03E+06	1466.8	C24H42ON	C15H30O2	Metlin	Isopentadecylic acid		Level 3
167	360.3261	46.84	2.51E+06	363.3450	46.79	2.75E+06	1474.9	C24H42ON	C15H30O2	Metlin	4,12-Dimethyl-tridecanoic acid		Level 3
168	360.3261	48.70	2.51E+06	363.3450	48.64	4.70E+06	1573.6	C24H42ON	C15H30O2	Metlin	2-Methyl-tetradecanoic acid	7620-57-7	Level 3
											3-Methyl-tetradecanoic acid		
											11-Methyl-tetradecanoic acid		
											2,6,10-Trimethyldodecanoic acid	168254-98-6	
											3,5-Dimethyltridecanoic acid		
169	365.2227	24.75	1.43E+06	371.2605	24.65	1.05E+06	562.9	C23H29O2N2	C5H6O4	HMDB	Glutaconic acid	1724-02-3	Level 3
											Citraconic acid	498-23-7	
											Itaconic acid	97-65-4	
											Mesaconic acid	498-24-8	
170	367.2381	25.06	2.52E+06	373.2759	24.95	2.72E+06	573.2	C23H31O2N2	C5H8O4	HMDB	Methylsuccinic acid	498-21-5	Level 3
											Ethylmalonic acid	601-75-2	
171	370.2125	12.67	7.53E+06	373.2314	12.60	7.53E+06	139.7	C21H28O3N3	C12H16O4N2	Metlin	Alanyl-Tyrosine		Level 3
172	370.2125	16.38	1.29E+06	373.2314	16.35	2.40E+06	282.0	C21H28O3N3	C12H16O4N2	Metlin	Phenylalanyl-Serine		Level 3
											Seriny-Phenylalanine		
											Tyrosyl-Alanine		

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
173	372.3261	46.25	5.36E+07	375.3450	46.46	3.57E+07	1445.0	C25H42ON	C16H30O2	HMDB	(E)-11-Hexadecenoic acid	73292-39-4	Level 3
174	372.3261	46.41	1.33E+07	375.3450	46.41	1.68E+07	1453.1	C25H42ON	C16H30O2	HMDB	(E)-6-Hexadecenoic acid	28290-76-8	Level 3
											(Z)-5-Hexadecenoic acid	7056-90-8	
											(Z)-13-Hexadecenoic acid		
											(E)-3-Hexadecenoic acid	1686-10-8	
											(Z)-14-Methyl-6-pentadecenoic acid	123739-73-1	

											Palmitelaidic acid	10030-73-6	
											Palmitoleic acid	373-49-9	
											<i>trans</i> -Hexa-dec-2-enoic acid		
175	374.3417	47.99	2.69E+06	377.3606	47.92	2.44E+06	1535.3	C25H44ON	C16H32O2	HMDB	Isopalmitic acid	4669-02-7	Level 3
176	374.3417	48.62	2.15E+06	377.3606	48.54	1.35E+06	1569.3	C25H44ON	C16H32O2	HMDB	Trimethyltridecanoic acid	10339-73-8	Level 3
177	375.3006	27.84	1.16E+06	378.3195	17.81	1.07E+06	672.3	C23H39O2N2	C14H27O3N	HMDB	<i>N</i> -Lauroylglycine		Level 3
178	375.3006	36.02	1.89E+06	378.3195	35.97	1.16E+06	991.1	C23H39O2N2	C14H27O3N	HMDB	<i>N</i> -Lauroylglycine		Level 3
179	381.2538	24.78	3.52E+06	387.2916	24.69	3.42E+06	563.9	C24H33O2N2	C6H10O4	HMDB	Adipic acid	124-04-9	Level 3
180	381.2538	25.07	1.00E+06	387.2916	25.00	1.08E+06	573.7	C24H33O2N2	C6H10O4	HMDB	Monomethyl glutaric acid	1501-27-5	Level 3
181	381.2538	25.59	1.00E+06	387.2916	25.49	1.08E+06	591.4	C24H33O2N2	C6H10O4	HMDB	Methylglutaric acid	626-51-7	Level 3
182	381.2538	26.89	1.30E+06	387.2916	26.78	1.40E+06	637.8	C24H33O2N2	C6H10O4	HMDB	2-Methylglutaric acid	617-62-9	Level 3
											4-Ethoxy-4-oxobutanoic acid		
183	382.2489	17.48	1.24E+06	385.2678	17.41	1.24E+06	316.2	C23H32O2N3	C14H20O3N2	Metlin	Valyl-Phenylalanine		Level 3
184	382.2489	17.91	4.32E+06	385.2678	17.87	5.64E+06	330.7	C23H32O2N3	C14H20O3N2	Metlin	Phenylalanyl-Valine	3918-92-1	Level 3
185	382.2489	19.11	1.80E+06	385.2678	19.09	2.44E+06	371.2	C23H32O2N3	C14H20O3N2	Metlin			Level 3
186	382.2489	19.51	1.73E+06	385.2678	19.44	1.73E+06	384.6	C23H32O2N3	C14H20O3N2	Metlin			Level 3
187	386.3417	47.85	2.28E+07	389.3606	47.79	3.53E+07	1527.7	C26H44ON	C17H32O2	Metlin	10-Methyl-9-hexadecenoic acid		Level 3
188	386.3417	48.27	1.32E+06	389.3606	49.52	1.82E+06	1550.4	C26H44ON	C17H32O2	Metlin	14-Methyl-8-hexadecenoic acid		Level 3
189	386.3417	48.96	1.06E+06	389.3606	48.96	1.18E+06	1587.6	C26H44ON	C17H32O2	Metlin	2-Heptadecylenic acid		Level 3
											9-Heptadecylenic acid		
											10-Heptadecenoic acid		
											16-Heptadecenoic acid		
											7-Heptadecenoic acid		
											8-Heptadecenoic acid		
											3-Heptadecenoic acid		
											7-Methyl-6-hexadecenoic acid		
											9,10-Methanohexadecanoic acid		
190	388.3574	50.24	1.57E+07	391.3763	50.18	1.23E+07	1664.1	C26H46ON	C17H34O2	HMDB	11-Methylhexadecanoic acid		Level 3
191	388.3574	50.39	8.37E+05	391.3763	50.34	7.27E+05	1673.2	C26H46ON	C17H34O2	HMDB	15-Methylhexadecanoic acid		Level 3
192	388.3574	52.24	1.25E+06	391.3763	52.16	2.30E+06	1771.6	C26H46ON	C17H34O2	HMDB	(<i>S</i>)-14-Methylhexadecanoic acid	5746-59-8	Level 3

193	389.3527	46.91	2.11E+06	392.3716	46.85	1.53E+06	1478.5	C25H45ON2	C16H33O2N	Metlin	2-Aminohexadecanoic acid		Level 3
194	390.3367	36.15	1.56E+06	393.3556	36.12	2.27E+06	996.5	C25H44O2N	C16H32O3	HMDB	7-Hydroxyhexadecanoic acid	16899-02-8	Level 3
195	390.3367	36.67	1.25E+06	393.3556	36.64	1.25E+06	1018.1	C25H44O2N	C16H32O3	HMDB	12-Hydroxyhexadecanoic acid	83646-62-2	Level 3
196	390.3367	37.12	1.23E+06	393.3556	37.09	1.10E+06	1036.8	C25H44O2N	C16H32O3	HMDB	10-Hydroxyhexadecanoic acid	23048-75-1	Level 3
197	390.3367	37.43	1.06E+06	393.3556	37.39	1.06E+06	1049.7	C25H44O2N	C16H32O3	HMDB	11-Hydroxyhexadecanoic acid	502-75-0	Level 3
198	390.3367	37.83	5.85E+06	393.3556	37.79	5.03E+06	1066.3	C25H44O2N	C16H32O3	HMDB	5-Hydroxyhexadecanoic acid	17369-53-8	Level 3
199	390.3367	38.26	1.02E+06	393.3556	38.23	1.12E+06	1084.2	C25H44O2N	C16H32O3	HMDB	9-Hydroxyhexadecanoic acid	17833-52-2	Level 3
200	390.3367	38.83	3.65E+06	393.3556	38.80	3.65E+06	1108.1	C25H44O2N	C16H32O3	HMDB	13-Hydroxyhexadecanoic acid	59642-39-6	Level 3
201	390.3367	39.39	8.28E+05	393.3556	39.36	1.26E+06	1131.8	C25H44O2N	C16H32O3	HMDB	8-Hydroxyhexadecanoic acid	83921-07-7	Level 3
											6-Hydroxyhexadecanoic acid	58763-57-8	
											3-Hydroxyhexadecanoic acid	83780-74-9	
											2-Hydroxyhexadecanoic acid	16452-52-1	
202	396.2646	15.16	4.40E+06	399.2835	15.15	6.58E+06	246.7	C24H34O2N3	C15H22O3N2	HMDB	Leucyl-Phenylalanine	3063-05-6	Level 3
203	396.2646	19.03	6.76E+06	399.2835	18.95	4.32E+06	368.4	C24H34O2N3	C15H22O3N2	HMDB	Isoleucyl-Phenylalanine		Level 3
204	396.2646	20.55	8.90E+05	399.2835	20.47	9.61E+05	420.0	C24H34O2N3	C15H22O3N2	HMDB			Level 3
205	396.3261	37.75	7.22E+05	399.3450	37.69	7.54E+05	1063.1	C27H42ON	C18H30O2	HMDB	γ -Linolenic acid	506-26-3	Level 3
206	396.3261	44.27	1.33E+06	399.3450	44.24	1.04E+06	1350.8	C27H42ON	C18H30O2	HMDB	Linolenalaidic acid	28290-79-1	Level 3
207	396.3261	44.89	1.69E+06	399.3450	44.82	1.69E+06	1378.7	C27H42ON	C18H30O2	HMDB			Level 3
208	396.3261	45.31	1.03E+06	399.3450	45.26	1.15E+06	1397.6	C27H42ON	C18H30O2	HMDB			Level 3
209	397.2488	24.71	1.40E+06	403.2866	24.61	1.15E+06	561.5	C24H33O3N2	C6H10O5	HMDB	2-Hydroxy-2-ethylsuccinic acid		Level 3
											3-Hydroxyadipic acid	14292-29-6	
											2-Hydroxyadipic acid	18294-85-4	
											3-Hydroxymethylglutaric acid	503-49-1	
210	398.3418	47.37	1.67E+07	401.3607	47.32	1.78E+07	1501.9	C27H44ON	C18H32O2	HMDB	Octadecadienoic acid		Level 3
											Mangiferic acid	18402-92-1	

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
210	398.3418	47.37	1.67E+07	401.3607	47.32	1.78E+07	1501.9	C27H44ON	C18H32O2	HMDB	6Z,9Z-Octadecadienoic acid	28290-77-9	Level 3

											Dihomolinoleic acid	7307-45-1	
											10E,12Z-Octadecadienoic acid	2420-56-6	
											Linoelaidic acid	506-21-8	
											Bovinic acid	2540-56-9	
											9E,11E-Octadecadienoic acid	1839-11-8	
211	399.1915	15.91	2.12E+06	402.2104	15.87	2.58E+06	268.2	C22H27O5N2	C13H15O6N	HMDB	4-Hydroxyphenylacetylglutamic acid	1029120-37-3	Level 3
212	400.3574	49.57	3.54E+08	403.3763	49.48	3.39E+08	1623.2	C27H46ON	C18H34O2	HMDB	(E)-13-Octadecenoic acid	693-71-0	Level 3
											Petroselinic acid	593-39-5	
											Octadec-9-enoic acid	2027-47-6	
											<i>cis</i> -Vaccenic acid	506-17-2	
											Vaccenic acid	693-72-1	
											(Z)-13-Octadecenoic acid	13126-39-1	
											Elaidic acid	112-79-8	
213	402.3730	51.65	1.47E+06	405.3919	51.57	1.47E+06	1741.6	C27H48ON	C18H36O2	Metlin	2,6-Dimethyl-hexadecanoic acid		Level 3
214	402.3730	51.90	1.60E+06	405.3919	51.69	1.90E+06	1754.2	C27H48ON	C18H36O2	Metlin	Isostearic acid	2724-58-5	Level 3
215	402.3730	52.20	2.97E+06	405.3919	52.12	1.65E+06	1769.5	C27H48ON	C18H36O2	Metlin	10-Methyl-heptadecanoic acid		Level 3
											4,8-Dimethyl-hexadecanoic acid		
											2,14-Dimethyl-hexadecanoic acid		
											4,14-Dimethyl-hexadecanoic acid		
											6,14-Dimethyl-hexadecanoic acid		
											14-Methyl-heptadecanoic acid		
											11,15-Dimethyl-hexadecanoic acid		
											15-Methyl-heptadecanoic acid		
216	410.2438	21.39	4.32E+06	416.2816	21.32	4.32E+06	448.7	C24H32O3N3	C6H9O5N	HMDB	<i>N</i> -Formyl-L-glutamic acid	1681-96-5	Level 3
											2-Amino-3-oxohexanedioic acid		
217	412.2231	13.46	1.93E+06	415.2420	13.41	1.68E+06	193.1	C23H30O4N3	C14H18O5N2	HMDB	L- γ -Glutamyl- β -phenyl- β -L-alanine	10275-84-0	Level 3
											Phenylalanylglutamic acid	3617-45-6	
218	414.3730	50.73	2.42E+06	417.3919	50.66	1.42E+06	1694.0	C28H48ON	C19H36O2	Metlin	2-Nonadecenoic acid		Level 3
219	414.3730	51.04	1.01E+07	417.3919	50.98	1.51E+07	1710.8	C28H48ON	C19H36O2	Metlin	17-Methyl-6Z-octadecenoic acid		Level 3
220	414.3730	51.32	1.52E+06	417.3919	51.26	1.82E+06	1724.9	C28H48ON	C19H36O2	Metlin	7-Nonadecenoic acid		Level 3

											Phytomonic acid	503-06-0	
											13-Cyclohexyltridecanoic acid		
											10Z-Nonadecenoic acid	73033-09-7	
											7E-Nonadecenoic acid		
221	416.3523	37.86	1.98E+06	419.3712	37.80	2.45E+06	1067.6	C27H46O2N	C18H34O3	HMDB	3-Oxooctadecanoic acid		Level 3
222	416.3523	38.24	4.07E+06	419.3712	38.17	3.48E+06	1083.4	C27H46O2N	C18H34O3	HMDB	5-Oxooctadecanoic acid	16694-31-8	Level 3
223	416.3523	39.00	1.44E+06	419.3712	38.94	2.30E+06	1115.3	C27H46O2N	C18H34O3	HMDB	9-Oxooctadecanoic acid	4114-74-3	Level 3
224	416.3523	41.35	5.24E+06	419.3712	41.28	7.12E+06	1216.5	C27H46O2N	C18H34O3	HMDB	11-Oxooctadecanoic acid	2388-83-2	Level 3
225	416.3523	41.80	9.03E+05	419.3712	41.74	8.42E+05	1237.6	C27H46O2N	C18H34O3	HMDB	10-Oxooctadecanoic acid	4158-12-7	Level 3
226	416.3523	42.58	2.68E+06	419.3712	42.52	2.68E+06	1273.9	C27H46O2N	C18H34O3	HMDB			Level 3
227	416.3523	42.99	4.23E+06	419.3712	42.93	3.28E+06	1293.0	C27H46O2N	C18H34O3	HMDB			Level 3
228	416.3523	43.40	9.03E+05	419.3712	43.36	1.51E+06	1311.8	C27H46O2N	C18H34O3	HMDB			Level 3
229	416.3523	43.99	1.19E+06	419.3712	43.96	1.71E+06	1338.4	C27H46O2N	C18H34O3	HMDB			Level 3
230	416.3886	55.26	2.36E+06	419.4075	55.18	3.98E+06	1961.3	C28H50ON	C19H38O2	HMDB	16-Methyloctadecanoic acid		Level 3
											Tuberculostearic acid	542-47-2	
											17-Methyloctadecanoic acid	2724-59-6	
											Pristanic acid	1189-37-3	
231	417.3840	50.26	1.51E+06	420.4029	50.20	1.22E+06	1665.5	C27H49ON2	C18H37O2N	Metlin	12-Amino-octadecanoic acid		Level 3
											2-Amino-octadecanoic acid		
232	418.3679	40.27	1.41E+06	421.3868	40.20	2.37E+06	1169.2	C27H48O2N	C18H36O3	HMDB	2-Hydroxystearic acid	629-22-1	Level 3
233	418.3679	40.64	8.90E+06	421.3868	40.57	5.72E+06	1184.8	C27H48O2N	C18H36O3	HMDB	5-Hydroxyoctadecanoic acid	2858-38-0	Level 3
234	418.3679	40.87	6.89E+06	421.3868	40.80	4.52E+06	1194.6	C27H48O2N	C18H36O3	HMDB	6-Hydroxyoctadecanoic acid	3158-47-2	Level 3
235	418.3679	41.12	4.82E+06	421.3868	41.04	2.77E+06	1205.7	C27H48O2N	C18H36O3	HMDB	7-Hydroxyoctadecanoic acid	3158-48-3	Level 3
236	418.3679	41.39	6.83E+06	421.3868	41.32	7.90E+06	1218.3	C27H48O2N	C18H36O3	HMDB	8-Hydroxyoctadecanoic acid	6807-91-6	Level 3
237	418.3679	41.73	4.21E+06	421.3868	41.65	4.21E+06	1234.2	C27H48O2N	C18H36O3	HMDB	9-Hydroxyoctadecanoic acid	3384-24-5	Level 3
238	418.3679	42.14	5.67E+06	421.3868	42.06	3.12E+06	1253.3	C27H48O2N	C18H36O3	HMDB	11-Hydroxyoctadecanoic acid	13419-91-5	Level 3
239	418.3679	48.16	3.56E+06	421.3868	48.08	4.87E+06	1544.5	C27H48O2N	C18H36O3	HMDB	13-Hydroxyoctadecanoic acid		Level 3
240	422.2074	25.72	1.65E+06	425.2263	20.14	1.05E+06	595.6	C24H28O4N3	C15H16O5N2	Metlin	Indole-3-acetylglutamic acid	57105-48-3	Level 3
241	422.2439	23.17	3.71E+06	428.2817	23.09	2.25E+06	509.4	C25H32O3N3	C7H9O5N	Metlin	N-Acryloyl aspartic acid	72064-86-9	Level 3
											α -(N-Acetylaminoethylene)succinic acid		

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
242	422.3418	45.65	2.25E+06	425.3607	45.58	2.45E+06	1414.6	C29H44ON	C20H32O2	HMDB	7,13-Eperudien-15-oic acid	14022-43-6	Level 3
243	422.3418	45.92	3.02E+06	425.3607	45.86	3.20E+06	1428.1	C29H44ON	C20H32O2	HMDB	<i>cis</i> -8,11,14,17-Eicosatetraenoic acid	2091-26-1	Level 3
244	422.3418	46.60	1.98E+06	425.3607	46.54	2.54E+06	1462.7	C29H44ON	C20H32O2	HMDB	Copalic acid	20257-75-4	Level 3
245	424.3574	47.33	1.84E+06	427.3763	47.27	1.21E+06	1499.6	C29H46ON	C20H34O2	HMDB	Dihomo- γ -linolenic acid	1783-84-2	Level 3
246	424.3574	48.19	2.35E+06	427.3763	48.11	3.34E+06	1546.1	C29H46ON	C20H34O2	HMDB	Dihomo- α -linolenic acid	17046-59-2	Level 3
247	424.3574	48.58	1.59E+06	427.3763	48.52	1.59E+06	1567.1	C29H46ON	C20H34O2	HMDB	Sciadonic acid	7019-85-4	Level 3
248	424.3574	48.79	6.22E+06	427.3763	48.74	6.67E+06	1578.3	C29H46ON	C20H34O2	HMDB			Level 3
249	426.3366	45.94	1.35E+06	429.3555	45.89	1.07E+06	1429.2	C28H44O2N	C19H32O3	HMDB	5-Butyl-3,4-dimethyl-2-furannonanoic acid	116627-46-4	Level 3
											3-Methyl-5-propyl-2-furanundecanoic acid	116627-49-7	
											5-Ethyl-3,4-dimethyl-2-furanundecanoic acid		
											3,4-Dimethyl-5-propyl-2-furandecanoic acid		
250	426.3731	50.30	1.43E+07	429.3920	50.23	1.46E+07	1667.7	C29H48ON	C20H36O2	Metlin	11Z,15Z-Eicosadienoic acid		Level 3
251	426.3731	50.70	1.32E+07	429.3920	50.66	1.26E+07	1692.1	C29H48ON	C20H36O2	Metlin	8Z,11Z-Eicosadienoic acid		Level 3
											11Z,14Z-Eicosadienoic acid	2091-39-6	
											8Z,14Z-Eicosadienoic acid	135498-07-6	
											8,11-Eicosadienoic acid		
											5Z,14Z-Eicosadienoic acid	122055-58-7	
252	428.3887	53.50	1.25E+07	431.4076	53.42	1.44E+07	1845.6	C29H50ON	C20H38O2	HMDB	9Z-Eicosenoic acid	29204-02-2	Level 3
											11-Eicosenoic acid	2462-94-4	
253	430.4042	56.32	1.96E+06	433.4231	56.27	2.78E+06	2030.4	C29H52ON	C20H40O2	Metlin	Phytanic acid	14721-66-5	Level 3
254	430.4042	56.61	1.36E+06	433.4231	56.56	1.36E+06	2049.4	C29H52ON	C20H40O2	Metlin	Isoarachidic acid	6250-72-2	Level 3
255	430.4042	57.28	1.34E+06	433.4231	57.22	9.80E+05	2093.3	C29H52ON	C20H40O2	Metlin	2,14-Dimethyl-octadecanoic acid		Level 3
											4,14-Dimethyl-octadecanoic acid		
											6,14-Dimethyl-octadecanoic acid		
											4,16-Dimethyl-octadecanoic acid		
											6,16-Dimethyl-octadecanoic acid		
											17-Methyl-nonadecanoic acid		

											3,7,11-Phytanic acid	31653-05-1	
											2,2,6,10,14-Pentamethylpentadecanoic acid	122706-67-6	
256	445.3790	44.17	7.54E+06	448.3979	44.10	6.53E+06	1346.3	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3
257	445.3790	44.45	4.61E+06	448.3979	44.37	4.61E+06	1358.9	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3
258	445.3790	45.82	1.85E+06	448.3979	45.78	1.23E+06	1423.0	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3
259	448.3572	47.90	3.59E+06	451.3761	47.84	3.46E+06	1530.5	C31H46ON	C22H34O2	HMDB	Docosapentaenoic acid (22n-6)	25448-00-4	Level 3
											4,8,12,15,19-Docosapentaenoic acid	2548-85-8	
260	450.3730	48.63	5.46E+06	453.3919	48.57	5.32E+06	1569.8	C31H48ON	C22H36O2	Metlin	4,7,10,13-Docosatetraenoic acid		Level 3
261	450.3730	50.15	4.38E+06	453.3919	50.07	3.53E+06	1658.6	C31H48ON	C22H36O2	Metlin	Adrenic acid	28874-58-0	Level 3
262	452.3887	50.08	1.13E+06	455.4076	50.03	1.18E+06	1654.3	C31H50ON	C22H38O2	Metlin	10,10-Dimethyl-5Z,8Z,11Z-eicosatrienoic acid		Level 3
263	452.3887	50.82	3.74E+06	455.4076	50.76	4.20E+06	1699.5	C31H50ON	C22H38O2	Metlin	7,7-Dimethyl-5Z,8Z,11Z-eicosatrienoic acid		Level 3
264	452.3887	51.17	7.34E+06	455.4076	51.11	8.20E+06	1717.2	C31H50ON	C22H38O2	Metlin	Docosatrienoic acid	28845-86-5	Level 3
											7Z,10Z,13Z-Docosatrienoic acid	28874-30-8	
											8,11,14-Docosatrienoic acid		
											13,16,19-Docosatrienoic acid		
											3Z,9Z,15Z-Docosatrienoic acid		
											5Z,11Z,17Z-Docosatrienoic acid		
265	456.4200	58.85	9.51E+05	459.4389	58.79	1.12E+06	2196.2	C31H54ON	C22H42O2	HMDB	Catelaicid acid	62600-37-7	Level 3
											Cetoleic acid	1002-96-6	
266	459.3945	45.74	5.78E+06	462.4134	45.70	4.71E+06	1419.1	C29H51O2N2	C20H39O3N	HMDB	<i>N</i> -Palmitoyl GABA		Level 3
267	471.3945	36.96	2.11E+06	474.4134	36.92	1.91E+06	1030.1	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Palmitoyl proline		Level 3
268	471.3945	45.23	4.71E+06	474.4134	45.19	4.71E+06	1394.0	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Oleoyl alanine		Level 3
269	471.3945	49.41	3.41E+06	474.4134	49.38	2.08E+06	1613.5	C30H51O2N2	C21H39O3N	Metlin			Level 3
270	474.3730	47.87	2.87E+06	477.3919	47.81	3.65E+06	1528.8	C33H48ON	C24H36O2	HMDB	Tetracosahexaenoic acid, n-3		Level 3
											Tetracosahexaenoic acid	81247-23-6	
271	476.3887	49.45	5.86E+06	479.4076	49.39	3.54E+06	1615.8	C33H50ON	C24H38O2	HMDB	Tetracosapentaenoic acid (24:5n-6)		Level 3
272	476.3887	49.81	1.56E+06	479.4076	49.75	1.55E+06	1637.9	C33H50ON	C24H38O2	HMDB	Tetracosapentaenoic acid (24:5n-3)		Level 3
273	494.3628	23.40	4.08E+06	497.3817	23.38	4.25E+06	517.1	C32H48O3N	C23H36O4	HMDB	9'-Carboxy- γ -chromanol	1215088-64-4	Level 3
274	499.4259	40.02	9.84E+06	502.4448	39.98	9.46E+06	1158.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3
275	499.4259	48.63	6.91E+06	502.4448	48.60	6.91E+06	1569.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3

276	499.4259	48.79	5.73E+06	502.4448	48.75	3.63E+06	1578.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3
277	499.4259	49.94	1.40E+06	502.4448	49.90	1.50E+06	1645.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3
278	501.4414	51.59	1.98E+06	504.4603	51.56	1.47E+06	1738.4	C32H57O2N2	C23H45O3N	Metlin	<i>N</i> -Stearoyl valine	Level 3
279	502.4022	50.23	1.68E+06	505.4211	50.21	1.90E+06	1663.6	C30H52O3N3	C21H40O4N2	Metlin	<i>N</i> -Palmitoyl glutamine	Level 3

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
280	518.3264	30.87	2.48E+06	521.3453	30.86	2.69E+06	786.2	C33H44O4N	C24H32O5	Metlin	3,7,12-Trioxo-5β- <i>chol</i> -1-en-24-oic acid 3,7,12-Trioxochol-4-en-24-oic acid 3,7,12-Trioxochol-5-en-24-oic acid		Level 3
281	549.4412	52.00	2.50E+06	552.4601	51.96	2.04E+06	1759.2	C36H57O2N2	C27H45O3N	HMDB	<i>N</i> -Stearoyl phenylalanine		Level 3
282	208.1331	2.51	2.33E+07	211.1520	2.49	2.63E+07		C12H18O2N	C3H6O3				Level 4
283	218.1174	13.90	1.26E+06	221.1363	13.83	2.24E+06	209.9	C13H16O2N	C4H4O3				Level 4
284	218.1174	23.50	4.10E+07	221.1363	23.40	3.26E+07	520.8	C13H16O2N	C4H4O3				Level 4
285	293.1492	11.63	2.52E+07	296.1681	11.57	2.48E+07	68.9	C15H21O4N2	C6H9O5N				Level 4
286	301.1366	23.89	3.89E+07	304.1555	23.80	4.20E+07	533.8	C14H23O4NS	C5H11O4S				Level 4
287	320.1943	12.76	1.25E+06	323.2132	14.26	1.03E+06	145.8	C17H26O3N3	C8H14O4N2				Level 4
288	322.1550	11.91	3.14E+06	325.1739	11.85	6.48E+06	88.1	C19H20O2N3	C10H8O3N2				Level 4
289	322.1914	27.17	2.09E+06	325.2103	27.11	2.87E+06	648.0	C20H24ON3	C11H12O2N2				Level 4
290	330.1438	19.95	2.56E+06	333.1627	19.87	2.10E+06	399.4	C17H20O4N3	C8H8O5N2				Level 4
291	332.2332	15.54	4.37E+06	335.2521	15.49	4.37E+06	257.6	C19H30O2N3	C10H18O3N2				Level 4
292	332.2332	15.86	1.37E+06	335.2521	15.83	8.16E+05	266.8	C19H30O2N3	C10H18O3N2				Level 4
293	333.1799	14.63	1.55E+07	336.1988	14.59	1.11E+07	231.2	C18H25O4N2	C9H13O5N				Level 4
294	335.1964	17.06	1.53E+06	338.2153	17.01	2.35E+06	302.0	C18H27O4N2	C9H15O5N				Level 4
295	335.1964	17.39	1.75E+06	338.2153	17.37	1.96E+06	313.3	C18H27O4N2	C9H15O5N				Level 4
296	338.1777	12.64	3.08E+06	341.1966	12.61	5.57E+06	137.8	C21H24O3N	C12H15O4				Level 4
297	339.2430	30.47	8.52E+05	342.2619	30.40	1.70E+06	771.0	C22H31ON2	C13H19O2N				Level 4
298	343.1836	31.58	3.52E+06	346.2025	31.52	4.46E+06	813.8	C23H23ON2	C14H11O2N				Level 4
299	350.1652	20.32	3.06E+06	353.1841	16.52	2.52E+06	412.1	C21H22O3N2	C12H10O4N				Level 4

300	351.1379	15.43	2.84E+06	354.1568	15.38	1.95E+06	254.4	C20H19O4N2	C11H7O5N	Level 4
301	351.1703	20.76	2.55E+06	354.1892	20.72	2.42E+06	427.1	C21H23O3N2	C12H11O4N	Level 4
302	351.1703	24.09	1.11E+06	354.1892	24.01	1.65E+06	540.5	C21H23O3N2	C12H11O4N	Level 4
303	353.1860	18.55	1.98E+06	356.2049	13.28	1.45E+06	352.3	C21H25O3N2	C12H13O4N	Level 4
304	358.1570	19.24	5.61E+06	361.1759	19.17	5.32E+06	375.5	C22H20O2N3	C13H12O3N2	Level 4
305	358.1570	20.62	4.04E+06	361.1759	20.58	7.71E+06	422.5	C22H20O2N3	C13H12O3N2	Level 4
307	360.2255	18.98	3.69E+06	363.2444	18.93	4.13E+06	366.8	C20H30O3N3	C11H18O4N2	Level 4
306	360.2255	19.28	2.31E+06	363.2444	19.23	1.82E+06	376.7	C20H30O3N3	C11H18O4N2	Level 4
308	361.2850	26.01	6.96E+06	364.3039	25.95	7.20E+06	606.0	C22H37O2N2	C13H25O3N	Level 4
309	403.3319	40.52	1.24E+06	406.3508	40.46	9.13E+05	1179.6	C25H43O2N2	C16H31O3N	Level 4
310	408.2079	14.78	1.38E+06	411.2268	14.79	1.11E+06	235.4	C27H26O3N3	C18H14O2N2	Level 4
311	408.2079	17.04	4.62E+06	411.2268	17.01	3.69E+06	301.3	C27H26O3N3	C18H14O2N2	Level 4
312	412.1816	20.36	2.89E+06	415.2005	20.36	2.78E+06	413.4	C26H24O3N2	C17H12O4N	Level 4
313	414.1976	20.95	2.31E+07	417.2165	20.93	1.73E+07	433.7	C26H26O3N2	C17H14O4N	Level 4
314	420.1541	20.22	2.22E+06	423.1730	20.22	1.91E+06	408.6	C23H22O5N3	C14H10O6N2	Level 4
315	420.1541	38.16	5.34E+06	423.1730	38.14	4.38E+06	1080.0	C23H22O5N3	C14H10O6N2	Level 4
316	421.2595	18.09	3.22E+06	424.2784	18.02	3.22E+06	336.8	C27H35O3N	C18H23O4	Level 4
317	421.2595	18.96	1.03E+06	424.2784	18.91	1.86E+06	366.2	C27H35O3N	C18H23O4	Level 4
318	429.3475	41.78	1.68E+06	432.3664	41.71	2.14E+06	1236.5	C27H45O2N2	C18H33O3N	Level 4
319	429.3475	42.06	2.54E+06	432.3664	41.98	2.22E+06	1249.6	C27H45O2N2	C18H33O3N	Level 4
320	430.1925	18.03	1.14E+06	433.2114	18.04	1.00E+06	334.9	C26H26O4N2	C17H14O5N	Level 4
321	430.1925	18.81	1.00E+06	433.2114	18.81	9.66E+05	360.9	C26H26O4N2	C17H14O5N	Level 4
322	430.1925	20.44	1.08E+06	433.2114	20.44	8.89E+05	416.4	C26H26O4N2	C17H14O5N	Level 4
323	430.1925	24.31	5.63E+06	433.2114	41.45	5.49E+06	548.1	C26H26O4N2	C17H14O5N	Level 4
324	430.2486	20.22	1.66E+06	433.2675	20.16	1.58E+06	408.8	C27H32O2N3	C18H20O3N2	Level 4
325	442.2520	30.51	1.61E+06	445.2709	30.45	1.33E+06	772.3	C25H34O5N2	C16H22O6N	Level 4
326	442.2520	30.94	9.36E+05	445.2709	30.89	1.34E+06	788.8	C25H34O5N2	C16H22O6N	Level 4
327	442.2520	31.27	4.15E+06	445.2709	31.20	5.69E+06	801.4	C25H34O5N2	C16H22O6N	Level 4
328	442.2520	31.59	1.40E+06	445.2709	31.52	2.70E+06	814.0	C25H34O5N2	C16H22O6N	Level 4
329	442.2520	31.74	1.04E+06	445.2709	31.66	1.08E+06	820.0	C25H34O5N2	C16H22O6N	Level 4

330	442.2520	32.02	8.89E+05	445.2709	31.96	1.09E+06	831.0	C25H34O5N2	C16H22O6N			Level 4
331	443.3629	33.45	3.12E+06	446.3818	33.38	3.96E+06	887.4	C28H47O2N2	C19H35O3N			Level 4
332	443.3629	42.64	1.80E+06	446.3818	42.56	2.67E+06	1276.7	C28H47O2N2	C19H35O3N			Level 4
333	443.3629	45.92	1.43E+06	446.3818	45.87	2.65E+06	1428.1	C28H47O2N2	C19H35O3N			Level 4
334	446.1896	26.21	1.53E+06	449.2085	26.16	1.36E+06	613.1	C29H24O2N3	C20H12O3N2			Level 4
335	446.1896	29.28	3.62E+06	449.2085	29.21	3.62E+06	725.7	C29H24O2N3	C20H12O3N2			Level 4
336	448.1591	23.78	1.29E+06	451.1780	23.78	9.47E+05	530.0	C29H22O4N	C20H10O5			Level 4
337	448.1591	24.19	1.18E+06	451.1780	24.19	1.09E+06	543.9	C29H22O4N	C20H10O5			Level 4
338	449.2990	19.86	4.09E+06	452.3179	19.85	2.59E+06	396.4	C25H41O5N2	C16H29O6N			Level 4

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₃ -MPEA-labeled)	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	Intensity (<i>d</i> ₃ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification
339	450.2751	18.40	9.03E+05	456.3129	18.32	1.00E+06	347.2	C27H36O3N3	C9H13O5N				Level 4
340	456.2670	32.59	3.92E+06	459.2859	32.52	2.47E+06	853.3	C29H34O2N3	C20H22O3N2				Level 4
341	456.2670	33.00	1.02E+06	459.2859	32.95	1.38E+06	869.8	C29H34O2N3	C20H22O3N2				Level 4
342	456.2670	33.32	8.63E+06	459.2859	33.26	9.56E+06	882.3	C29H34O2N3	C20H22O3N2				Level 4
343	456.2670	33.65	1.37E+06	459.2859	33.55	1.29E+06	895.1	C29H34O2N3	C20H22O3N2				Level 4
344	456.2670	34.25	4.32E+06	459.2859	34.18	3.62E+06	919.5	C29H34O2N3	C20H22O3N2				Level 4
345	458.2541	28.46	1.15E+06	461.2730	28.38	1.51E+06	694.8	C29H34O3N2	C20H22O4N				Level 4
346	511.3656	23.90	1.43E+06	514.3845	23.89	1.25E+06	534.1	C32H49O4N	C23H37O5				Level 4
347	512.3159	42.66	1.63E+06	515.3348	42.65	1.15E+06	1277.7	C34H42O3N	C25H30O4				Level 4
348	521.4100	48.76	1.33E+06	524.4289	48.74	2.45E+06	1576.8	C34H53O2N2	C25H41O3N				Level 4
349	521.4100	49.94	9.95E+05	524.4289	49.91	6.78E+05	1645.8	C34H53O2N2	C25H41O3N				Level 4
350	527.3587	27.67	1.20E+06	530.3776	27.67	1.25E+06	666.2	C32H49O5N	C23H37O6				Level 4
351	545.3488	20.72	1.10E+06	551.3866	20.65	1.76E+06	425.9	C30H47O6N3	C12H24O8N				Level 4
352	550.3161	25.00	6.04E+06	553.3350	24.93	5.31E+06	571.3	C35H41O3N3	C26H29O4N2				Level 4
353	550.3161	27.71	5.72E+06	553.3350	27.70	4.58E+06	667.7	C35H41O3N3	C26H29O4N2				Level 4
354	550.3161	29.14	1.81E+06	553.3350	29.16	1.49E+06	720.3	C35H41O3N3	C26H29O4N2				Level 4
355	568.2843	32.42	2.78E+06	571.3032	32.42	2.30E+06	846.7	C39H38O3N	C30H26O4				Level 4

356	596.3648	40.99	1.07E+06	599.3837	40.90	1.44E+06	1199.7	C38H48O4N2	C29H36O5N	Level 4
357	614.2366	25.78	1.51E+06	617.2555	25.75	1.13E+06	597.5	C42H32O4N	C33H20O5	Level 4
358	620.3932	38.29	1.53E+06	623.4121	38.29	1.16E+06	1085.4	C41H52O3N2	C32H40O4N	Level 4
359	624.3955	42.00	3.21E+06	627.4144	41.93	3.21E+06	1246.8	C40H52O4N2	C31H40O5N	Level 4
360	624.3955	44.05	9.83E+05	627.4144	43.98	1.24E+06	1340.9	C40H52O4N2	C31H40O5N	Level 4
361	624.3955	45.38	1.32E+06	627.4144	45.30	2.05E+06	1400.8	C40H52O4N2	C31H40O5N	Level 4
362	650.4120	46.03	1.47E+06	653.4309	45.96	2.24E+06	1434.0	C42H54O4N2	C33H42O5N	Level 4
363	650.4120	46.20	3.59E+06	653.4309	46.12	4.28E+06	1442.4	C42H54O4N2	C33H42O5N	Level 4
364	650.4120	46.46	6.92E+06	653.4309	46.38	5.49E+06	1455.6	C42H54O4N2	C33H42O5N	Level 4
365	652.4280	46.00	6.79E+06	655.4469	45.93	4.38E+06	1432.3	C45H54ON3	C36H42O2N2	Level 4
366	652.4280	48.00	6.59E+06	655.4469	47.93	6.59E+06	1535.8	C45H54ON3	C36H42O2N2	Level 4
367	652.4280	49.13	1.10E+06	655.4469	49.04	1.46E+06	1596.9	C45H54ON3	C36H42O2N2	Level 4
368	666.3831	40.91	3.70E+06	669.4020	42.23	2.80E+06	1196.3	C49H48ON	C40H36O2	Level 4
369	666.3831	41.13	5.78E+06	669.4020	41.05	4.82E+06	1206.2	C49H48ON	C40H36O2	Level 4
370	676.4279	46.92	3.04E+06	679.4468	46.86	4.00E+06	1478.8	C44H56O4N2	C35H44O5N	Level 4
371	680.4594	52.80	1.09E+06	683.4783	52.68	1.31E+06	1800.0	C47H58ON3	C35H46O2N2	Level 4
372	747.6760	45.97	5.38E+06	750.6949	45.90	7.35E+06	1430.8	C50H87O2N2	C41H75O3N	Level 4
373	747.6760	49.14	7.49E+06	750.6949	49.09	6.46E+06	1597.2	C50H87O2N2	C41H75O3N	Level 4
374	773.6925	47.84	2.57E+06	776.7114	47.77	2.57E+06	1527.2	C49H91O5N	C40H79O6	Level 4
375	773.6925	49.39	4.82E+06	776.7114	49.33	4.20E+06	1612.2	C49H91O5N	C40H79O6	Level 4
376	196.0884	23.51	2.23E+06	199.1073	23.41	1.72E+06	520.8			Level 5
377	205.0749	23.51	3.54E+06	208.0938	23.41	3.27E+06	520.8			Level 5
378	275.2475	19.22	1.06E+06	278.2664	19.21	1.23E+06	374.7			Level 5
379	275.2475	20.46	4.55E+06	278.2664	20.37	3.25E+06	416.9			Level 5
380	287.1210	20.46	1.36E+06	290.1399	20.39	1.25E+06	416.9			Level 5
381	309.1281	10.24	1.35E+06	312.1470	10.16	1.05E+06				Level 5
382	309.1281	13.32	2.48E+06	312.1470	13.24	2.68E+06	183.8			Level 5
383	318.2170	13.86	5.68E+06	321.2359	13.83	4.16E+06	208.7			Level 5
384	318.2170	14.64	6.90E+06	321.2359	14.62	6.90E+06	231.4			Level 5
385	318.2170	14.30	1.78E+06	321.2359	14.26	1.57E+06	221.5			Level 5

386	319.2205	13.87	7.65E+06	322.2394	13.82	7.16E+06	209.1								Level 5
387	333.2364	15.51	7.35E+06	336.2553	15.49	8.10E+06	256.7								Level 5
388	342.2244	22.47	2.67E+06	345.2433	22.42	2.43E+06	485.7								Level 5
389	349.3202	45.39	6.80E+06	352.3391	45.29	9.48E+06	1401.2								Level 5
390	366.1475	11.82	6.61E+06	369.1664	11.75	5.32E+06	82.1								Level 5
391	366.1475	13.48	8.91E+06	369.1664	13.44	5.40E+06	194.9								Level 5
392	368.1758	17.35	3.70E+06	371.1947	17.35	3.52E+06	311.8								Level 5
393	392.2130	17.62	1.74E+06	395.2319	17.63	1.57E+06	321.0								Level 5
394	392.2130	18.52	9.71E+05	395.2319	18.46	9.71E+05	351.3								Level 5
395	392.2130	19.69	1.62E+06	395.2319	19.69	1.53E+06	390.8								Level 5
396	400.2047	25.40	9.98E+05	403.2236	25.34	8.15E+05	584.9								Level 5
397	400.2047	26.18	1.98E+06	403.2236	26.12	1.67E+06	611.9								Level 5
398	400.2047	25.78	3.36E+06	403.2236	25.66	3.41E+06	597.5								Level 5
399	437.1748	23.51	9.77E+05	443.2126	23.40	8.81E+05	520.9								Level 5

Continued table

No.	<i>m/z</i> (MPEA-labeled)	Rt (min) (MPEA-labeled)	Intensity (MPEA-labeled)	<i>m/z</i> (<i>d</i> ₅ -MPEA-labeled)	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	Intensity (<i>d</i> ₅ -MPEA-labeled)	RI	Formula (MPEA-labeled)	Database	Formula (unlabeled)	Name	CAS No.	Identification	
400	470.1498	23.51	1.96E+06	476.1876	23.41	1.72E+06	521.0							Level 5
401	498.1446	23.51	8.88E+05	504.1824	23.40	1.08E+06	520.9							Level 5
402	546.4105	51.65	1.33E+06	549.4294	51.61	1.25E+06	1741.6							Level 5
403	653.2905	23.54	1.53E+06	659.3283	23.39	8.33E+05	522.1							Level 5
395	392.2130	19.69	1.62E+06	395.2319	19.69	1.53E+06	390.8							Level 5
396	400.2047	25.40	9.98E+05	403.2236	25.34	8.15E+05	584.9							Level 5
397	400.2047	26.18	1.98E+06	403.2236	26.12	1.67E+06	611.9							Level 5
398	400.2047	25.78	3.36E+06	403.2236	25.66	3.41E+06	597.5							Level 5
399	437.1748	23.51	9.77E+05	443.2126	23.40	8.81E+05	520.9							Level 5
400	470.1498	23.51	1.96E+06	476.1876	23.41	1.72E+06	521.0							Level 5
401	498.1446	23.51	8.88E+05	504.1824	23.40	1.08E+06	520.9							Level 5
402	546.4105	51.65	1.33E+06	549.4294	51.61	1.25E+06	1741.6							Level 5

Table S7. Detected DmPA-labeled carboxylated metabolites in HepG2 cell extracts.

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
1	207.1493	2.94	1.40E+07	209.1560	2.94	9.72E+06	Methylamine	61	254.0848	15.31	1.41E+06	256.0916	15.31	1.50E+06	
2	207.1494	12.00	1.08E+06	209.1561	12.00	9.25E+05		62	254.1573	15.48	8.28E+05	256.1644	15.48	5.28E+05	
3	208.0969	14.85	1.43E+08	210.1037	14.85	9.48E+07	Formic acid	63	256.1334	27.93	1.43E+06	258.1401	27.93	1.43E+06	Phenol
4	209.1560	2.94	9.72E+06	211.1628	2.94	6.32E+06		64	261.1600	13.34	2.94E+07	263.1667	13.34	2.96E+07	
5	210.0585	20.84	3.35E+05	212.0653	20.83	3.56E+05		65	261.1600	7.15	1.23E+07	263.1667	7.15	9.82E+06	
6	210.0948	19.41	6.39E+07	212.1015	19.41	5.35E+07		66	263.1392	3.63	1.65E+07	265.1459	3.63	1.23E+07	
7	212.0473	18.18	1.08E+08	214.0542	18.18	1.07E+08		67	263.1392	13.21	9.85E+05	265.1459	13.21	7.36E+05	
8	214.0631	2.64	1.31E+06	216.0698	2.64	1.10E+06		68	263.1392	3.12	5.40E+06	265.1459	3.12	5.40E+06	
9	214.0631	18.87	1.23E+06	216.0698	18.87	6.86E+05		69	263.1392	8.95	2.25E+06	265.1459	8.95	4.28E+06	
10	217.1338	10.11	1.33E+06	219.1405	10.11	1.18E+06		70	263.1392	15.78	5.54E+05	265.1459	15.78	5.54E+05	
11	217.1338	16.95	3.21E+06	219.1405	16.95	3.21E+06		71	263.1627	15.92	2.89E+06	265.1696	15.92	2.13E+06	
12	219.0953	7.83	1.23E+06	221.1019	7.83	1.03E+06		72	263.1627	15.48	4.22E+06	265.1696	15.48	3.11E+06	
13	219.1129	2.42	3.93E+06	221.1196	2.41	3.41E+06		73	264.0923	19.25	3.55E+06	266.0991	19.25	2.02E+06	
14	220.1572	12.00	1.50E+06	222.1639	12.00	1.47E+06		74	264.1532	11.82	1.21E+06	266.1599	11.82	1.87E+06	
15	221.1111	10.82	5.95E+06	223.1178	10.83	6.90E+06		75	264.1596	25.79	6.38E+06	266.1664	25.79	5.45E+06	Valeric acid
16	221.1111	6.69	2.13E+06	223.1178	6.69	2.13E+06		76	265.1183	12.68	5.40E+05	267.1252	12.67	3.63E+05	
17	222.1124	16.33	4.13E+08	224.1189	16.33	3.53E+08	Acetic acid	77	265.1372	10.11	1.40E+06	267.1439	10.11	1.34E+06	
18	222.1124	16.02	4.66E+08	224.1189	16.02	4.25E+08		78	266.1388	15.84	2.42E+06	268.1456	15.84	2.43E+06	
19	223.1442	2.26	4.78E+07	225.1508	2.26	5.65E+07	Ethanol amine	79	267.1343	2.65	2.23E+07	269.1408	2.65	2.24E+07	
20	223.1442	2.44	1.24E+07	225.1508	2.44	6.96E+06		80	267.1343	5.65	4.77E+06	269.1408	5.65	4.77E+06	Serine peak 1
21	224.1433	23.44	3.25E+06	226.1501	23.44	2.50E+06		81	267.1343	5.92	3.28E+06	269.1408	5.92	1.70E+06	Serine peak 2
22	224.1433	13.72	2.04E+06	226.1501	13.72	1.48E+06		82	270.1967	16.59	1.90E+06	272.2031	16.59	1.91E+06	
23	231.1492	5.17	3.95E+07	233.1559	5.17	3.64E+07		83	270.1967	16.26	3.67E+06	272.2031	16.26	4.38E+06	
24	232.1811	11.00	1.99E+06	234.1878	11.00	2.08E+06		84	270.1967	15.00	1.15E+06	272.2031	15.00	1.15E+06	
25	233.1649	21.05	1.64E+06	235.1718	21.05	1.16E+06		85	273.1058	22.07	2.65E+07	275.1125	22.07	4.17E+07	
26	233.1649	7.15	1.66E+07	235.1718	7.15	1.46E+07		86	274.1188	11.72	3.13E+07	276.1253	11.72	2.74E+07	

27	233.1649	12.00	1.95E+06	235.1718	12.00	1.70E+06		87	274.1188	9.78	5.72E+06	276.1253	9.78	4.64E+06	
28	235.0903	11.22	8.03E+06	237.0970	11.22	7.15E+06		88	275.1755	16.82	1.65E+07	277.1820	16.82	1.67E+07	
29	235.0903	4.62	3.67E+06	237.0970	4.62	3.67E+06		89	275.1755	17.29	3.96E+07	277.1820	17.29	4.02E+07	
30	235.0903	11.70	1.64E+06	237.0970	11.70	3.12E+06		90	275.1755	11.01	2.69E+06	277.1820	11.01	2.69E+06	
31	235.1442	14.99	1.68E+06	237.1511	14.99	9.54E+05		91	275.1755	11.90	5.47E+06	277.1820	11.90	5.47E+06	
32	235.1442	3.15	5.40E+05	237.1511	3.15	6.89E+05		92	277.1335	26.85	2.04E+06	279.1403	26.85	1.52E+06	
33	235.1442	12.55	3.26E+06	237.1511	12.55	4.72E+06		93	277.1547	5.17	6.87E+08	279.1612	5.17	4.94E+08	Proline
34	235.1442	15.33	1.87E+06	237.1511	15.33	2.64E+06		94	277.1547	10.50	2.21E+06	279.1612	10.49	2.66E+06	
35	236.0741	26.00	1.69E+06	238.0809	25.99	2.32E+06		95	278.1025	17.33	3.79E+05	280.1085	17.33	2.71E+05	
36	236.0741	12.66	7.83E+05	238.0809	12.66	5.64E+05		96	278.1753	28.77	1.39E+06	280.1819	28.77	1.31E+06	Caproic acid
37	236.1281	19.65	2.36E+05	238.1348	19.65	2.36E+05	Propionic acid	97	279.1702	7.15	3.35E+08	281.1768	7.15	2.94E+08	Valine peak 1
38	237.1058	3.90	3.71E+06	239.1125	3.90	3.03E+06		98	279.1702	13.13	2.16E+08	281.1768	13.13	2.15E+08	Valine peak 2
39	237.1234	2.77	7.93E+06	239.1302	2.77	8.03E+06		99	280.1182	15.59	3.42E+06	282.1248	15.59	3.08E+06	Succinic acid
40	237.1234	5.35	3.76E+06	239.1302	5.35	4.76E+06		100	280.1333	23.14	4.93E+06	282.1404	23.14	3.10E+06	
41	237.1234	5.55	1.65E+06	239.1302	5.55	1.65E+06		101	280.1808	15.02	4.28E+06	282.1876	15.02	5.26E+06	
42	244.0169	20.03	7.29E+09	246.0224	20.03	4.39E+09		102	281.0958	10.61	5.31E+06	283.1024	10.61	4.62E+06	
43	246.1967	13.89	4.71E+06	248.2034	13.89	4.93E+06		103	281.0958	11.51	3.78E+06	283.1024	11.51	3.78E+06	
44	247.1442	3.08	5.08E+06	249.1509	3.08	5.81E+06		104	281.1497	3.14	5.10E+07	283.1564	3.14	4.42E+07	
45	247.1442	2.93	3.27E+06	249.1509	2.93	2.23E+06		105	281.1497	8.92	3.88E+07	283.1564	8.92	3.65E+07	
46	247.1442	14.47	6.48E+05	249.1509	14.47	6.48E+05		106	281.1647	13.72	8.56E+06	283.1714	13.72	7.74E+06	
47	247.1805	11.04	1.02E+07	249.1871	11.04	1.09E+07		107	281.1647	23.45	1.47E+06	283.1714	23.43	9.39E+05	
48	247.1805	11.87	1.18E+07	249.1871	11.87	1.09E+07		108	283.1114	13.82	1.15E+06	285.1180	13.82	1.06E+06	
49	247.1805	22.53	3.21E+06	249.1871	22.53	1.86E+06		109	284.0954	13.63	1.78E+06	286.1020	13.63	1.78E+06	
50	247.1805	22.67	4.64E+06	249.1871	22.67	3.43E+06		110	284.1283	26.00	9.80E+05	286.1349	26.00	9.63E+05	
51	248.1104	26.77	1.83E+06	250.1171	26.77	1.39E+06		111	284.1393	4.14	1.38E+07	286.1461	4.14	1.46E+07	
52	249.1058	11.73	1.40E+06	251.1124	11.73	1.61E+06		112	284.1393	3.92	1.40E+07	286.1461	3.92	1.50E+07	
53	249.1472	15.08	1.72E+06	251.1541	15.08	1.09E+06		113	285.1236	18.03	6.84E+05	287.1301	18.03	7.06E+05	
54	249.1472	15.60	1.13E+06	251.1541	15.61	6.30E+05		114	288.1532	14.44	1.08E+06	290.1598	14.44	1.16E+06	
55	250.1440	22.97	3.93E+06	252.1506	22.97	3.32E+06	Butyric acid	115	290.0044	20.06	1.92E+08	292.0111	20.06	1.38E+08	
56	251.1391	16.28	1.11E+06	253.1459	16.28	9.55E+05		116	290.0044	18.81	1.98E+08	292.0111	18.81	2.15E+08	

57	251.1391	3.22	8.21E+07	253.1459	3.22	6.74E+07	Alanine peak 1	117	291.1339	14.63	2.40E+07	293.1407	14.63	2.16E+07
58	251.1391	8.62	5.13E+07	253.1459	8.62	4.99E+07	Alanine peak 2	118	291.1339	11.45	3.61E+06	293.1407	11.45	2.96E+06
59	252.1232	14.77	4.73E+08	254.1295	14.77	4.61E+08		119	291.1339	7.52	2.46E+06	293.1407	7.52	2.46E+06
60	253.1008	12.64	3.55E+06	255.1074	12.64	3.79E+06		120	291.2432	17.67	2.88E+07	293.2496	17.67	5.45E+07

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
121	291.2432	17.95	5.65E+06	293.2496	17.95	5.65E+06		181	320.2223	36.14	6.00E+06	322.2284	36.14	6.16E+06	Nonanoic acid
122	292.1544	26.68	1.48E+06	294.1610	26.68	1.98E+06		182	321.2173	12.21	5.90E+05	323.2242	12.20	4.71E+05	
123	292.1910	31.37	4.43E+05	294.1977	31.36	3.97E+05	Heptylic acid	183	322.1760	11.04	6.33E+05	324.1827	11.04	6.39E+05	
124	293.1287	22.38	1.47E+06	295.1354	22.38	1.18E+06		184	322.1760	5.35	1.56E+06	324.1827	5.35	1.22E+06	
125	293.1319	15.75	1.44E+07	295.1386	15.75	1.50E+07		185	323.1604	14.18	3.40E+05	325.1669	14.18	2.93E+05	
126	293.1319	10.14	8.74E+05	295.1386	10.14	4.73E+05		186	323.1967	9.63	1.62E+07	325.2035	9.60	1.45E+07	
127	293.1408	14.64	4.64E+05	295.1485	14.64	7.94E+05		187	324.1378	9.85	1.14E+06	326.1446	9.85	1.26E+06	
128	293.1495	17.57	5.76E+05	295.1562	17.59	4.82E+05		188	325.1217	14.10	9.39E+06	327.1284	14.10	9.75E+06	
129	293.1495	14.92	5.62E+06	295.1562	14.92	5.37E+06		189	325.1217	17.29	4.53E+06	327.1284	17.29	4.53E+06	
130	293.1495	3.58	1.13E+06	295.1562	3.58	1.13E+06		190	325.1548	12.08	1.37E+07	327.1614	12.08	1.36E+07	
131	293.1857	15.19	3.46E+08	295.1919	15.19	3.67E+08		191	325.1548	9.17	4.59E+06	327.1614	9.17	4.59E+06	
132	293.1857	11.01	3.29E+08	295.1920	11.01	3.03E+08		192	325.1759	8.47	8.01E+07	327.1824	8.45	5.22E+07	
133	293.1857	11.90	4.76E+08	295.1920	11.90	4.38E+08		193	327.1700	16.27	2.00E+08	329.1763	16.27	1.96E+08	Phenylalanine peak 1
134	293.1857	15.50	4.25E+08	295.1922	15.50	2.24E+08		194	327.1700	13.72	5.06E+08	329.1763	13.72	5.03E+08	Phenylalanine peak 2
135	294.1702	22.58	1.84E+06	296.1768	22.58	1.63E+06		195	327.1700	27.30	4.81E+07	329.1763	27.30	4.81E+07	
136	295.1114	13.31	1.56E+07	297.1182	13.31	1.76E+07		196	329.0777	29.42	2.50E+06	331.0844	29.42	2.48E+06	
137	295.1114	11.73	1.57E+07	297.1182	11.73	1.68E+07		197	334.2381	38.37	3.54E+06	336.2446	38.37	3.13E+06	Capric acid
138	296.1761	11.12	6.12E+05	298.1825	11.11	6.99E+05		198	334.2381	37.71	3.22E+06	336.2446	37.71	3.22E+06	
139	297.1459	9.94	3.20E+06	299.1525	9.94	2.75E+06		199	334.2381	37.92	1.18E+06	336.2446	37.92	8.77E+05	
140	297.1459	8.08	3.70E+06	299.1525	8.08	2.83E+06		200	335.1966	15.61	6.57E+05	337.2034	15.61	5.44E+05	
141	297.1459	6.01	1.77E+06	299.1525	6.01	1.23E+06		201	335.1966	15.15	9.75E+05	337.2034	15.15	9.75E+05	

142	297.1599	13.72	1.10E+06	299.1666	13.72	1.34E+06		202	336.1921	12.13	9.60E+05	338.1989	12.13	8.57E+05	
143	297.1599	9.15	2.96E+06	299.1666	9.15	2.72E+06		203	336.1921	14.45	5.32E+05	338.1989	14.45	5.32E+05	
144	297.1599	20.6	3.98E+05	299.1666	20.6	5.99E+05		204	336.2027	2.24	3.25E+05	338.2096	2.24	2.80E+05	
145	297.1961	16.15	5.32E+07	299.2027	16.15	2.99E+07		205	341.1495	20.76	7.91E+05	343.1564	20.76	5.52E+05	
146	297.1961	15.89	1.16E+07	299.2027	15.89	8.74E+06		206	343.1653	9.16	2.21E+08	345.1714	9.16	1.99E+08	
147	298.1300	11.68	1.23E+08	300.1365	11.68	9.87E+07		207	343.1653	13.84	6.76E+07	345.1714	13.71	9.36E+07	
148	298.1300	10.60	2.34E+08	300.1365	10.60	1.62E+08		208	347.1443	16.11	2.03E+06	349.1511	16.11	1.96E+06	
149	298.1300	11.01	7.64E+07	300.1365	11.01	4.36E+07		209	347.1443	16.32	1.16E+06	349.1511	16.32	8.98E+05	
150	302.1864	13.24	2.91E+05	304.1933	13.26	3.46E+05		210	347.1443	25.73	7.38E+05	349.1511	25.73	7.38E+05	
151	304.1808	17.69	2.78E+06	306.1877	17.69	2.91E+06		211	348.1708	15.92	3.20E+06	350.1774	15.93	3.29E+06	
152	305.1649	29.61	1.31E+06	307.1717	29.61	1.34E+06		212	348.2533	39.86	5.47E+05	350.2600	39.86	2.79E+05	Undecanoic acid
153	305.2099	12.34	2.79E+06	307.2162	12.33	1.71E+06		213	348.2533	40.52	1.33E+06	350.2600	40.52	1.01E+06	
154	306.2067	33.32	9.80E+05	308.2133	33.32	1.26E+06		214	350.2076	8.50	1.59E+06	352.2142	8.50	1.88E+06	
155	306.2067	33.61	4.79E+05	308.2133	33.61	4.79E+05		215	350.2076	16.60	1.03E+06	352.2142	16.60	9.31E+05	
156	306.2067	33.80	1.17E+06	308.2133	33.80	1.17E+06	Octanoic acid	216	350.2076	14.70	1.40E+06	352.2142	14.70	1.37E+06	
157	307.1113	18.06	4.11E+06	309.1181	18.07	3.65E+06		217	350.2076	13.44	4.26E+06	352.2142	13.44	3.80E+06	
158	308.1606	5.96	3.35E+06	310.1675	5.96	2.94E+06		218	350.2076	12.04	1.13E+06	352.2142	12.04	1.13E+06	
159	308.1606	5.70	4.03E+06	310.1675	5.70	3.25E+06		219	353.1166	18.30	7.66E+05	355.1235	18.30	4.28E+05	
160	309.1270	15.63	6.20E+06	311.1337	15.63	6.43E+06		220	353.1529	19.26	7.98E+06	355.1597	19.26	6.29E+06	
161	309.1270	13.31	1.25E+06	311.1337	13.31	2.26E+06		221	359.2124	19.89	3.06E+06	361.2198	19.89	2.79E+06	
162	309.1447	12.62	1.09E+06	311.1513	12.62	1.05E+06		222	360.2534	40.02	3.82E+06	362.2601	40.03	3.34E+06	
163	309.1598	18.99	2.17E+07	311.1665	18.99	2.34E+07		223	360.2534	39.62	1.05E+06	362.2601	39.63	9.60E+05	
164	309.1598	13.72	6.80E+06	311.1665	13.72	6.54E+06		224	361.3212	30.14	2.33E+05	363.3279	30.14	2.44E+05	
165	309.1812	13.82	1.38E+06	311.1878	13.82	1.24E+06		225	362.2148	37.47	3.09E+05	364.2221	37.46	4.73E+05	
166	309.1812	22.42	8.08E+05	311.1878	22.42	7.22E+05		226	362.2690	42.59	3.31E+07	364.2755	42.59	3.13E+07	Dodecanoic acid
167	310.1305	15.66	2.23E+06	312.1371	15.65	1.52E+06		227	364.2232	10.80	7.81E+05	366.2299	10.80	8.48E+05	
168	310.1587	15.64	2.62E+06	312.1653	15.64	2.71E+06		228	364.2232	14.44	1.79E+06	366.2299	14.44	1.59E+06	
169	311.1064	13.45	9.04E+05	313.1130	13.45	1.00E+06		229	364.2232	16.79	3.47E+06	366.2299	16.79	3.19E+06	
170	311.1425	13.24	7.65E+05	313.1491	13.24	5.25E+05		230	364.2232	11.33	1.19E+06	366.2299	11.33	9.01E+05	
171	311.1425	14.07	1.24E+08	313.1491	14.07	1.15E+08		231	364.2232	15.27	6.50E+05	366.2299	15.27	6.50E+05	

172	311.1425	10.14	1.62E+08	313.1491	10.11	1.46E+08		232	365.2074	12.80	2.22E+06	367.2139	12.80	1.91E+06	
173	311.1964	6.78	3.94E+08	313.2029	6.78	3.15E+08		233	366.1813	17.59	1.96E+07	368.1876	17.59	1.92E+07	Tryptophan peak 1
174	314.1249	11.85	7.99E+06	316.1315	11.85	6.57E+06		234	366.1813	14.92	8.93E+07	368.1876	14.92	8.73E+07	Tryptophan peak 2
175	314.1249	11.19	6.05E+07	316.1315	11.19	4.85E+07		235	366.2021	14.22	2.51E+05	368.2088	14.22	2.26E+05	
176	314.1249	8.83	2.17E+07	316.1315	8.83	1.66E+07		236	367.1874	36.16	5.00E+06	369.1942	36.17	5.34E+06	
177	315.0836	10.29	9.01E+05	317.0901	10.29	1.74E+06		237	367.1874	36.89	5.84E+06	369.1942	36.89	1.06E+07	
178	316.1445	26.42	3.76E+05	318.1516	26.42	3.05E+05		238	369.1840	12.42	2.73E+06	371.1910	12.42	3.54E+06	
179	320.1759	13.70	1.15E+06	322.1826	13.70	1.25E+06		239	369.1840	11.19	1.43E+06	371.1910	11.19	1.43E+06	
180	320.1759	14.92	3.26E+06	322.1826	14.92	3.14E+06		240	369.1840	10.08	9.41E+05	371.1910	10.08	5.38E+05	

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
241	371.1635	13.48	1.15E+06	373.1702	13.47	1.54E+06		301	400.1870	12.70	4.36E+05	402.1939	12.70	3.94E+05	
242	372.2466	19.43	1.24E+08	374.2533	19.43	6.38E+07		302	400.1870	14.66	6.98E+05	402.1939	14.66	8.97E+05	
243	375.3372	31.24	3.63E+06	377.3438	31.24	3.72E+06		303	400.1870	8.43	1.57E+06	402.1939	8.43	2.00E+06	
244	375.3372	32.75	5.20E+05	377.3438	32.75	5.84E+05		304	400.1870	10.44	1.90E+06	402.1939	10.44	1.90E+06	
245	376.2229	13.17	1.31E+06	378.2295	13.17	1.27E+06		305	402.3006	45.21	3.38E+06	404.3073	45.19	2.72E+06	
246	376.2846	43.91	9.96E+05	378.2914	43.91	8.87E+05		306	403.3683	34.55	2.94E+06	405.3752	34.55	3.00E+06	
247	376.2846	44.53	1.61E+06	378.2914	44.53	1.36E+06	Tridecanoic acid	307	403.3683	35.84	3.03E+06	405.3752	35.83	3.34E+06	
248	377.1539	24.57	1.36E+06	379.1606	24.55	2.38E+06		308	404.3159	48.04	3.49E+07	406.3222	48.04	3.03E+07	Pentadecylic acid
249	377.1539	18.90	3.67E+06	379.1606	18.90	1.88E+06		309	404.3159	47.45	3.75E+06	406.3222	47.45	5.38E+06	
250	378.2386	16.29	1.94E+06	380.2454	16.28	1.83E+06		310	404.3159	47.63	1.66E+06	406.3222	47.63	2.23E+06	
251	378.2386	13.28	6.27E+05	380.2454	13.28	6.24E+05		311	405.2752	28.15	1.13E+06	407.2820	28.15	1.03E+06	
252	378.2638	36.29	2.88E+05	380.2704	36.28	2.73E+05		312	405.3480	30.33	1.57E+06	407.3549	30.33	1.36E+06	
253	380.2181	16.31	1.45E+06	382.2250	16.31	1.68E+06		313	405.3480	29.00	8.88E+05	407.3549	29.00	8.88E+05	
254	380.2181	13.08	6.09E+05	382.2250	13.09	6.16E+05		314	406.1611	12.68	8.30E+05	408.1682	12.68	6.32E+05	
255	380.2181	14.29	1.24E+06	382.2250	14.29	1.06E+06		315	406.2702	16.45	1.05E+06	408.2768	16.29	1.39E+06	
256	380.2181	14.75	1.88E+06	382.2250	14.75	1.88E+06		316	406.2702	19.44	1.44E+06	408.2768	19.42	2.04E+06	
257	380.2181	16.07	8.45E+05	382.2250	16.07	5.32E+05		317	406.2702	19.09	7.41E+05	408.2768	19.09	5.93E+05	

258	381.1348	2.01	5.28E+05	383.1413	2.01	7.58E+05		318	406.2702	16.30	6.59E+05	408.2768	16.30	6.59E+05
259	381.2019	16.28	2.93E+06	383.2088	16.28	2.79E+06		319	406.2953	34.52	7.11E+05	408.3020	34.51	6.26E+05
260	382.1793	12.21	4.96E+05	384.1862	12.21	2.79E+05		320	406.2953	40.64	2.85E+05	408.3020	40.64	2.54E+05
261	382.1793	11.56	7.66E+05	384.1862	11.56	6.39E+05		321	407.2289	16.18	3.34E+05	409.2352	16.18	5.98E+05
262	383.1823	27.91	3.46E+05	385.1888	27.92	3.42E+05		322	407.2289	13.34	7.66E+05	410.2021	13.34	7.10E+05
263	383.1823	27.43	7.59E+05	385.1888	27.43	7.59E+05		323	408.2282	16.20	1.61E+06	410.2344	16.19	2.03E+06
264	384.1917	12.53	1.59E+06	386.1987	12.53	1.38E+06		324	408.2282	18.71	2.29E+07	410.2344	18.70	2.21E+07
265	384.1917	14.37	7.69E+05	386.1987	14.37	7.24E+05		325	409.2335	12.64	5.08E+05	411.2401	12.65	4.77E+05
266	384.1917	15.21	6.38E+05	386.1987	15.21	6.38E+05		326	409.2335	16.17	3.68E+05	411.2401	16.17	5.42E+05
267	385.1792	11.23	1.94E+06	387.1859	11.23	1.82E+06		327	410.2105	16.69	8.94E+05	412.2163	16.69	4.62E+05
268	387.1296	26.00	9.03E+05	389.1366	26.00	6.26E+05		328	410.2105	13.26	4.37E+05	412.2163	13.26	3.26E+05
269	387.2306	22.88	3.44E+05	389.2368	22.88	2.42E+05		329	410.2347	18.70	2.21E+07	412.2420	18.70	2.03E+07
270	388.1269	26.00	3.13E+05	390.1331	25.99	2.07E+05		330	410.2347	16.21	1.32E+06	412.2420	16.21	2.62E+06
271	388.2387	22.89	5.72E+05	390.2455	22.89	5.66E+05		331	412.2851	43.37	4.27E+05	414.2916	43.35	3.89E+05
272	388.2847	43.41	3.68E+07	390.2912	43.41	3.25E+07		332	414.2025	16.97	7.33E+05	416.2089	16.97	6.16E+05
273	388.2847	43.94	6.74E+06	390.2912	43.94	7.90E+06		333	414.2025	14.79	6.54E+05	416.2089	14.79	6.44E+05
274	388.2847	44.28	5.49E+06	390.2912	44.28	4.13E+06		334	414.2025	14.95	2.65E+05	416.2089	14.95	4.37E+05
275	389.1693	36.18	4.80E+05	391.1761	36.18	5.16E+05		335	414.2025	15.33	9.87E+05	416.2089	15.33	9.87E+05
276	389.1693	36.86	8.91E+05	391.1762	36.86	1.68E+06		336	414.3003	45.45	4.46E+06	416.3070	45.44	3.80E+06
277	390.2387	15.49	1.99E+06	392.2453	15.49	1.93E+06		337	414.3003	44.88	1.24E+06	416.3070	44.88	6.65E+05
278	390.3003	46.36	2.75E+08	392.3073	46.36	2.46E+08	Tetradecanoic acid	338	414.3003	44.72	2.32E+06	416.3070	44.72	2.32E+06
279	390.3003	45.41	3.31E+06	392.3073	45.41	2.99E+06		339	414.3003	37.38	1.29E+06	416.3070	37.38	7.85E+05
280	390.3003	45.92	2.87E+06	392.3073	45.92	1.48E+06		340	414.3003	43.90	4.85E+05	416.3070	43.90	4.85E+05
281	391.3320	40.05	7.55E+05	393.3388	40.05	5.81E+05		341	416.3156	46.85	6.45E+08	418.3228	46.85	5.91E+08
282	391.3320	29.59	8.83E+06	393.3388	29.59	8.39E+06		342	416.3156	41.26	4.60E+05	418.3228	41.26	3.19E+05
283	391.3320	46.61	4.38E+06	393.3388	46.61	5.90E+06		343	416.3156	47.16	5.67E+06	418.3228	47.16	3.26E+06
284	392.2548	18.08	3.80E+06	394.2615	18.07	4.01E+06		344	416.3156	39.33	2.41E+06	418.3228	39.33	2.41E+06
285	392.2548	17.57	4.54E+05	394.2615	17.56	4.04E+05		345	416.3156	40.08	1.16E+07	418.3228	40.08	8.86E+06
286	392.2548	15.33	1.46E+06	394.2615	15.33	1.42E+06		346	417.3843	36.54	5.27E+05	419.3910	36.54	5.74E+05
287	392.2548	14.55	6.49E+05	394.2615	14.55	4.72E+05		347	417.3843	37.30	8.90E+05	419.3910	37.30	8.90E+05

288	392.2548	18.08	2.27E+06	394.2615	18.08	1.77E+06		348	417.3843	49.24	1.76E+06	419.3910	49.24	2.25E+06	
289	392.2548	27.51	4.62E+06	394.2615	27.51	4.62E+06		349	418.3314	49.55	5.14E+08	420.3378	49.55	4.56E+08	Palmitic acid
290	394.2340	16.76	1.20E+06	396.2407	16.76	1.22E+06		350	418.3314	48.77	4.54E+07	420.3378	48.77	4.54E+07	
291	394.2340	14.35	7.17E+05	396.2407	14.35	6.44E+05		351	418.3314	49.17	2.13E+07	420.3378	49.17	1.14E+07	
292	394.2340	14.59	4.53E+05	396.2407	14.59	3.62E+05		352	419.2332	36.36	3.48E+05	421.2396	36.35	3.06E+05	
293	394.2340	14.86	2.67E+05	396.2407	14.86	4.36E+05		353	419.2332	36.71	8.73E+05	421.2396	36.71	8.73E+05	
294	394.2340	16.56	5.89E+05	396.2407	16.56	4.27E+05		354	419.3635	45.04	7.47E+06	421.3703	45.02	5.38E+06	
295	394.2340	10.50	1.67E+05	396.2407	10.50	1.67E+05		355	419.3635	50.31	1.41E+06	421.3703	50.31	1.08E+06	
296	396.1954	13.52	4.27E+05	398.2021	13.52	4.79E+05		356	419.3635	32.94	7.80E+05	421.3703	32.94	1.17E+06	
297	396.1954	13.14	8.36E+05	398.2021	13.14	6.21E+05		357	420.2471	4.43	4.15E+06	422.2540	4.42	2.62E+06	
298	398.2078	13.27	5.31E+05	400.2145	13.27	4.75E+05		358	424.6635	17.91	2.73E+05	426.6700	17.90	4.80E+05	
299	398.2078	17.90	6.89E+05	400.2145	17.90	7.32E+05		359	426.0872	13.72	5.43E+05	428.0940	13.72	6.39E+05	
300	398.2694	41.36	2.87E+06	400.2757	41.36	2.46E+06		360	426.2393	18.75	1.90E+06	428.2463	18.74	1.61E+06	

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
361	426.2393	15.96	7.14E+05	428.2464	15.96	5.73E+05		421	444.3470	49.79	6.70E+08	446.3532	49.77	6.00E+08	
362	426.2393	15.21	3.58E+05	428.2458	15.20	5.26E+05		422	444.3470	43.22	4.12E+08	446.3532	43.22	2.22E+08	
363	428.3643	37.66	4.45E+05	430.3706	37.67	4.03E+05		423	444.3470	50.46	1.95E+07	446.3532	50.46	1.95E+07	
364	428.3643	48.63	6.69E+05	430.3706	48.63	6.69E+05		424	445.3795	33.50	5.20E+05	447.3859	33.50	5.22E+05	
365	430.1722	11.53	1.61E+07	432.1788	11.53	1.72E+07		425	445.3795	33.91	7.98E+05	447.3859	33.91	8.23E+05	
366	430.1722	15.04	2.13E+07	432.1788	15.04	1.78E+07		426	445.3795	35.45	1.66E+06	447.3859	35.45	2.25E+06	
367	430.3316	48.42	8.62E+07	432.3381	48.42	7.64E+07		427	445.4158	39.32	9.79E+05	447.4221	39.32	1.04E+06	
368	430.3316	48.73	2.58E+07	432.3381	48.73	2.58E+07		428	445.4158	38.94	6.53E+05	447.4221	38.94	3.99E+05	
369	431.4001	38.65	5.54E+06	433.4069	38.65	6.12E+06		429	446.3636	52.81	1.80E+08	448.3699	52.81	1.62E+08	Octadecanoic acid
370	431.4001	37.54	1.03E+06	433.4068	37.53	1.05E+06		430	446.3636	51.69	7.61E+07	448.3699	51.69	5.22E+07	
371	432.3114	36.23	1.50E+06	434.3182	36.23	1.26E+06		431	446.3636	51.89	1.24E+07	448.3699	51.89	1.24E+07	
372	432.3114	40.29	6.86E+05	434.3182	40.29	4.62E+05		432	446.3636	52.28	8.99E+06	448.3699	52.28	8.99E+06	
373	432.3114	41.07	9.67E+05	434.3182	41.07	7.23E+05		433	447.2350	11.00	6.10E+06	449.2418	11.00	3.79E+06	

374	432.3114	41.67	2.37E+05	434.3182	41.67	3.61E+05		434	447.2350	11.67	2.96E+06	449.2420	11.66	2.58E+06
375	432.3114	44.54	1.79E+05	434.3182	44.54	2.37E+05		435	447.3219	39.78	2.88E+05	449.3289	39.78	2.83E+05
376	432.3114	46.57	3.87E+05	434.3182	46.57	5.37E+05		436	447.3586	31.96	5.19E+05	449.3651	31.96	4.82E+05
377	432.3114	39.13	5.82E+05	434.3182	39.13	4.37E+05		437	447.3586	49.79	9.89E+05	449.3651	49.79	9.89E+05
378	432.3474	50.54	1.49E+07	434.3541	50.53	1.27E+07		438	447.3949	36.02	5.29E+05	449.4016	36.02	5.22E+05
379	432.3474	51.04	1.68E+07	434.3541	51.04	1.08E+07	Heptadecanoic acid	439	447.3949	54.46	2.70E+06	449.4016	54.46	2.52E+06
380	433.3433	30.35	1.25E+06	435.3499	30.35	1.13E+06		440	447.3949	35.83	8.97E+05	449.4016	35.83	6.57E+05
381	433.3433	48.41	5.83E+05	435.3499	48.41	5.83E+05		441	447.3949	49.73	2.57E+05	449.4016	49.73	1.45E+05
382	433.3788	47.41	4.29E+05	435.3860	47.42	3.12E+05		442	448.3064	37.16	9.83E+05	450.3127	37.15	8.97E+05
383	433.3788	39.09	3.36E+05	435.3860	39.09	3.36E+05		443	449.2837	43.70	5.13E+05	451.2904	43.70	4.70E+05
384	434.3271	39.32	8.00E+05	436.3336	39.33	7.33E+05		444	449.2837	42.69	4.21E+05	451.2904	42.69	8.23E+05
385	434.3271	40.08	9.38E+05	436.3336	40.07	8.49E+05		445	449.2837	42.27	2.68E+05	451.2904	42.27	2.68E+05
386	434.3271	45.48	3.67E+05	436.3336	45.48	3.56E+05		446	451.3689	34.37	8.91E+05	453.3756	34.37	7.93E+05
387	434.3271	44.65	3.31E+05	436.3336	44.66	3.46E+05		447	451.3689	50.40	5.48E+05	453.3756	50.40	4.38E+05
388	434.3271	38.42	3.93E+06	436.3336	38.42	3.46E+06		448	454.3311	47.60	1.87E+06	456.3377	47.60	1.50E+06
389	434.3271	38.06	1.57E+06	436.3336	38.06	2.42E+06		449	454.3311	50.50	4.21E+05	456.3377	50.50	3.89E+05
390	434.3271	47.29	8.86E+05	436.3336	47.29	5.88E+05		450	454.3311	51.04	2.18E+05	456.3377	51.04	2.18E+05
391	434.3271	38.77	4.80E+05	436.3336	38.77	6.66E+05		451	456.2495	17.54	3.89E+05	458.2561	17.54	3.35E+05
392	435.1565	36.19	3.40E+05	437.1629	36.18	4.10E+05		452	456.2495	13.50	6.73E+05	458.2561	13.50	7.82E+05
393	435.3585	29.36	7.51E+05	437.3653	29.33	6.71E+05		453	456.2495	15.82	9.56E+05	458.2561	15.82	6.34E+05
394	435.3585	28.85	1.76E+06	437.3653	28.85	2.22E+06		454	456.3953	40.30	8.98E+05	458.4023	40.30	7.75E+05
395	435.3585	27.77	2.65E+06	437.3653	27.77	4.32E+06		455	456.3953	51.81	4.88E+05	458.4023	51.81	5.22E+05
396	435.3585	50.53	8.71E+05	437.3653	50.53	6.33E+05		456	458.3630	51.21	2.07E+07	460.3696	51.21	1.78E+07
397	440.2185	12.19	2.72E+05	442.2246	12.20	1.95E+05		457	458.3630	50.89	5.70E+06	460.3696	50.89	4.24E+06
398	440.2436	38.40	7.18E+06	442.2506	38.40	6.62E+06		458	458.3630	51.74	2.35E+06	460.3696	51.74	2.35E+06
399	440.2436	19.13	5.12E+06	442.2506	19.13	3.78E+06		459	459.3410	49.96	8.26E+05	461.3477	49.96	8.29E+05
400	440.2436	37.98	3.81E+06	442.2506	37.98	2.99E+06		460	459.3410	39.27	4.59E+05	461.3477	39.27	3.72E+05
401	440.2548	19.78	1.10E+05	442.2614	19.79	1.20E+05		461	459.3585	31.28	2.59E+06	461.3651	31.28	2.33E+06
402	440.2548	17.80	4.00E+05	442.2614	17.80	3.26E+05		462	459.3585	31.70	8.49E+05	461.3651	31.70	9.33E+05
403	440.2548	17.13	8.45E+05	442.2614	17.13	4.61E+05		463	459.4312	40.23	1.26E+06	461.4381	40.23	1.27E+06

404	440.2548	20.66	4.26E+05	442.2614	20.66	3.61E+05		464	460.3250	50.65	1.16E+06	462.3319	50.65	1.71E+06	
405	440.2548	21.05	7.52E+05	442.2614	21.05	7.52E+05		465	460.3250	50.27	7.84E+05	462.3319	50.27	6.39E+05	
406	440.2548	21.28	8.43E+05	442.2614	21.28	5.72E+05		466	460.3427	39.87	2.19E+06	462.3493	39.87	1.98E+06	
407	440.3164	45.45	1.48E+07	442.3231	45.45	1.33E+07		467	460.3427	39.57	4.53E+05	462.3493	39.57	3.88E+05	
408	440.3164	45.67	5.77E+06	442.3231	45.67	4.38E+06		468	460.3427	40.33	6.22E+05	462.3493	40.33	6.22E+05	
409	440.3164	46.00	2.15E+06	442.3231	46.00	2.15E+06		469	460.3427	42.77	4.13E+05	462.3493	42.77	2.37E+05	
410	440.3164	46.20	1.64E+06	442.3231	46.20	8.59E+05		470	460.3427	43.14	2.99E+05	462.3493	43.14	1.56E+05	
411	440.3164	46.56	7.89E+05	442.3231	46.56	6.34E+05		471	460.3427	43.46	6.74E+05	462.3493	43.46	3.90E+05	
412	440.3164	49.51	5.32E+05	442.3231	49.51	4.71E+05		472	460.3427	43.69	4.88E+05	462.3493	43.69	3.22E+05	
413	442.3316	47.58	2.46E+08	444.3377	47.58	2.06E+08		473	460.3427	43.98	7.85E+05	462.3493	43.98	7.85E+05	
414	442.3316	46.81	8.97E+05	444.3377	46.76	7.25E+05		474	460.3427	45.22	4.77E+05	462.3493	45.22	4.22E+05	
415	442.3316	40.40	5.21E+05	444.3377	40.39	3.44E+05		475	460.3427	45.44	2.77E+05	462.3493	45.44	4.36E+05	
416	442.3316	47.89	3.56E+07	444.3377	47.89	4.78E+07		476	460.3427	45.94	6.74E+05	462.3493	45.94	4.38E+05	
417	442.3316	48.25	4.70E+06	444.3377	48.25	3.28E+06		477	460.3427	46.09	4.88E+05	462.3493	46.09	9.28E+05	
418	442.3316	41.26	1.53E+06	444.3377	41.26	8.42E+05		478	460.3427	46.70	1.26E+06	462.3493	46.70	1.26E+06	
419	442.3316	48.51	6.52E+05	444.3377	48.51	6.52E+05		479	460.3792	54.22	2.92E+06	462.3858	54.22	2.09E+06	
420	444.2068	11.31	8.43E+06	446.2136	11.31	7.83E+06		480	460.3792	55.00	1.65E+06	462.3858	55.00	8.81E+05	Nonadecanoic acid

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
481	460.3903	37.83	7.11E+05	462.3971	37.83	5.26E+05		541	484.3792	51.74	6.39E+05	486.3858	51.74	5.62E+05	
482	461.2765	14.31	3.61E+05	463.2851	14.31	3.05E+05		542	486.3946	55.13	2.94E+06	488.4011	55.13	2.69E+06	
483	461.2765	19.94	5.87E+05	463.2851	19.94	5.87E+05		543	487.2995	31.58	1.38E+06	489.3065	31.58	1.46E+06	
484	461.2765	26.27	1.67E+06	463.2851	26.27	1.67E+06		544	487.2995	31.10	3.57E+06	489.3065	31.10	1.46E+06	
485	461.3742	33.00	5.30E+05	463.3809	33.00	4.43E+05		545	487.2995	44.88	7.00E+05	489.3065	44.88	1.06E+06	
486	461.3742	33.53	1.11E+07	463.3809	33.53	1.05E+07		546	487.3728	53.42	1.58E+06	489.3786	53.42	1.35E+06	
487	461.3742	35.36	3.55E+05	463.3809	35.36	3.07E+05		547	487.3728	42.11	1.19E+06	489.3786	42.11	1.19E+06	
488	461.3742	33.21	1.46E+06	463.3809	33.21	1.46E+06		548	487.3976	55.12	1.03E+06	489.4046	55.11	8.09E+05	
489	461.3742	35.38	2.43E+06	463.3809	35.38	1.37E+06		549	488.3133	46.93	3.66E+06	490.3199	46.93	3.23E+06	

490	461.3742	48.23	8.65E+05	463.3809	48.23	5.42E+05	550	488.3133	46.41	1.85E+06	490.3199	46.41	1.85E+06
491	461.3742	47.77	3.78E+05	463.3809	47.77	3.78E+05	551	488.3133	46.62	1.14E+06	490.3199	46.62	8.96E+05
492	461.3742	51.20	9.84E+05	463.3809	51.20	6.73E+05	552	488.3133	47.19	5.86E+05	490.3199	47.19	4.82E+05
493	462.3008	43.82	2.19E+06	464.3074	43.82	2.05E+06	553	488.3571	54.46	7.26E+06	490.3628	54.46	4.41E+06
494	462.3008	43.05	1.54E+06	464.3074	43.05	1.54E+06	554	488.4218	40.45	1.39E+06	490.4286	40.45	1.03E+06
495	462.3008	46.00	5.93E+05	464.3074	46.00	8.42E+05	555	489.4052	51.41	8.59E+04	491.4126	51.41	5.82E+04
496	462.3008	46.55	1.69E+06	464.3074	46.55	1.69E+06	556	489.4052	36.56	1.66E+05	491.4126	36.56	2.23E+05
497	462.3585	48.18	3.17E+05	464.3648	48.18	2.89E+05	557	489.4052	35.75	3.70E+05	491.4126	35.75	3.70E+05
498	462.3585	41.86	9.29E+05	464.3648	41.86	9.01E+05	558	490.3320	46.08	9.30E+07	492.3382	46.08	8.30E+07
499	462.3585	43.23	1.11E+06	464.3648	43.23	1.07E+06	559	490.3320	48.38	2.37E+07	492.3382	48.38	1.86E+07
500	462.3585	42.26	1.24E+06	464.3648	42.26	6.66E+05	560	492.3474	47.31	2.80E+07	494.3539	47.31	2.56E+07
501	462.3585	42.65	5.36E+05	464.3648	42.65	3.33E+05	561	492.3474	47.62	7.64E+06	494.3539	47.62	7.64E+06
502	462.3585	47.84	3.46E+05	464.3648	47.84	5.63E+05	562	492.3474	48.02	5.83E+06	494.3539	48.02	3.77E+06
503	462.3585	48.19	1.79E+05	464.3648	48.19	3.22E+05	563	492.3474	50.31	1.69E+06	494.3539	50.31	1.69E+06
504	462.3585	48.84	3.58E+05	464.3648	48.84	3.72E+05	564	494.3607	52.91	1.10E+06	496.3674	52.91	1.00E+06
505	462.3585	50.30	1.88E+05	464.3648	50.30	1.88E+05	565	494.3607	48.97	2.26E+06	496.3674	48.97	2.26E+06
506	463.3897	34.45	1.39E+06	465.3963	34.45	1.31E+06	566	494.3607	49.34	4.72E+06	496.3674	49.34	2.65E+06
507	464.3161	44.88	3.57E+07	466.3229	44.88	3.27E+07	567	494.3607	50.01	9.85E+05	496.3674	50.01	9.85E+05
508	464.3161	45.14	1.14E+07	466.3229	45.14	6.79E+07	568	500.4102	57.97	3.30E+06	502.4172	57.96	2.95E+06
509	464.3161	47.90	2.42E+06	466.3229	47.90	2.42E+06	569	500.4102	58.44	1.13E+06	502.4172	58.44	9.88E+06
510	466.3314	49.79	6.45E+06	468.3380	49.79	4.16E+06	570	501.3154	35.10	3.71E+05	503.3221	35.10	3.44E+05
511	466.3314	46.92	7.64E+07	468.3380	46.92	6.78E+07	571	502.4368	34.50	5.28E+05	504.4438	34.50	5.40E+05
512	466.3314	30.90	1.57E+07	468.3380	30.90	8.87E+06	572	505.3460	50.73	1.66E+06	507.3529	50.73	3.24E+06
513	466.3314	47.19	5.27E+06	468.3380	47.19	3.51E+06	573	505.3460	49.97	5.78E+06	507.3529	49.97	4.91E+06
514	466.3314	46.42	2.53E+06	468.3380	46.42	1.33E+06	574	505.3460	49.73	1.57E+06	507.3529	49.73	1.57E+06
515	466.3314	46.62	6.80E+05	468.3380	46.62	6.80E+05	575	514.3291	48.01	2.70E+05	516.3365	48.01	2.49E+05
516	468.3480	48.36	4.18E+07	470.3541	48.36	3.69E+07	576	514.3291	47.29	1.94E+06	516.3365	47.29	1.73E+06
517	468.3480	47.81	1.26E+06	470.3541	47.81	1.21E+06	577	518.3632	48.19	1.02E+07	520.3698	48.19	9.17E+06
518	468.3480	48.58	5.65E+06	470.3541	48.58	3.46E+06	578	518.3632	48.47	6.58E+06	520.3698	48.47	3.45E+06
519	468.3480	49.02	3.43E+06	470.3541	49.02	3.43E+06	579	519.3255	40.18	1.47E+06	521.3324	40.18	1.60E+06

520	468.3480	49.34	1.68E+06	470.3541	49.34	9.99E+05		580	519.3255	40.44	7.87E+05	521.3324	40.44	4.67E+05
521	468.3480	52.85	2.66E+06	470.3541	52.85	2.66E+06		581	519.3255	48.65	4.44E+05	521.3324	48.65	6.58E+05
522	470.2107	25.78	3.15E+05	472.2171	25.78	2.68E+05		582	520.3785	49.68	7.01E+06	522.3853	49.68	6.35E+06
523	470.2107	26.13	2.38E+05	472.2171	26.13	3.62E+05		583	520.3785	49.97	5.85E+06	522.3853	49.97	3.82E+06
524	470.3270	46.69	2.41E+05	472.3338	46.70	4.22E+05		584	521.3410	43.28	1.91E+07	523.3477	43.28	2.04E+07
525	470.3631	49.47	6.69E+05	472.3697	49.47	6.28E+05		585	521.3777	43.86	1.09E+06	523.3840	43.86	8.67E+05
526	470.3631	50.31	2.09E+07	472.3697	50.31	1.93E+07		586	521.3777	45.79	6.80E+05	523.3840	45.79	5.42E+05
527	470.3631	50.47	6.59E+06	472.3697	50.47	4.63E+06		587	521.3777	46.09	1.79E+05	523.3840	46.09	1.79E+05
528	470.3631	50.82	1.55E+06	472.3697	50.82	1.55E+06		588	521.3777	49.96	2.34E+06	523.3840	49.96	1.54E+06
529	471.2603	11.70	2.34E+06	473.2672	11.70	2.39E+06		589	522.3945	51.48	6.03E+05	524.4012	51.48	5.26E+05
530	471.2603	14.94	8.50E+05	473.2672	14.94	6.58E+05		590	527.3279	49.97	1.06E+05	529.3351	49.97	1.20E+05
531	472.3787	52.97	1.01E+08	474.3851	52.95	8.97E+07		591	527.3279	15.47	2.79E+05	529.3351	15.47	4.13E+05
532	474.3220	38.62	5.94E+05	476.3284	38.62	5.28E+05		592	527.3279	15.92	4.79E+05	529.3351	15.92	4.99E+05
533	474.3947	57.91	1.31E+06	476.4012	57.91	1.19E+06	Eicosanoic acid	593	527.3279	50.76	2.68E+05	529.3351	50.76	2.68E+05
534	474.3947	56.17	6.71E+05	476.4012	56.17	6.71E+05		594	528.2874	46.09	4.77E+05	530.2947	46.09	4.20E+05
535	475.4264	38.85	6.37E+05	477.4330	38.85	6.24E+05		595	528.2874	24.84	7.65E+05	530.2947	24.84	7.65E+05
536	477.3146	47.51	2.21E+06	479.3211	47.51	1.89E+06		596	530.4680	37.48	3.02E+05	532.4752	37.47	3.19E+05
537	477.3146	46.68	1.74E+06	479.3211	46.68	1.48E+06		597	546.3947	50.36	1.26E+06	548.4014	50.36	1.15E+06
538	477.3146	46.32	5.65E+05	479.3211	46.32	4.79E+05		598	547.3569	43.82	6.27E+06	549.3638	43.82	6.59E+06
539	477.3688	29.18	2.08E+05	479.3746	29.17	1.74E+05		599	547.3569	43.96	4.23E+06	549.3638	43.96	4.23E+06
540	484.2829	43.78	4.02E+05	486.2893	43.78	3.63E+05		600	549.3724	46.93	4.23E+05	551.3799	46.93	4.44E+05

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
601	553.3392	31.22	2.23E+06	555.3457	31.22	1.98E+06		661	665.3929	36.55	8.36E+05	667.3999	36.55	6.59E+05	
602	553.3392	23.92	5.42E+05	555.3457	23.92	4.90E+05		662	665.3929	36.99	4.54E+05	667.3999	36.99	4.54E+05	
603	556.2222	26.00	1.75E+05	558.2292	26.00	2.84E+05		663	677.3978	18.13	2.81E+05	679.4046	18.13	2.69E+05	
604	556.2222	31.84	4.23E+05	558.2292	31.84	2.67E+05		664	677.3978	30.55	5.48E+05	679.4046	30.55	4.62E+05	
605	559.2916	21.07	1.67E+06	561.2988	21.07	1.21E+06		665	687.3774	34.41	2.52E+06	689.3834	34.41	2.95E+06	

606	559.2916	26.80	8.57E+05	561.2988	26.80	6.38E+05	666	687.3774	34.02	1.41E+06	689.3834	34.01	1.51E+06
607	561.4263	37.35	6.46E+05	563.4333	37.35	6.15E+05	667	689.3928	34.94	2.49E+05	691.3992	34.94	2.54E+05
608	569.3777	41.87	4.87E+06	571.3848	41.87	4.43E+06	668	689.3928	35.37	3.10E+05	691.3992	35.37	3.56E+05
609	569.3777	50.34	1.49E+06	571.3848	50.34	8.47E+05	669	708.4530	38.88	6.01E+05	710.4587	38.88	7.17E+05
610	571.5568	45.79	5.85E+05	573.5632	45.79	6.11E+05	670	361.1490	15.42	2.49E+07	365.1623	15.42	1.78E+07
611	573.3214	23.76	1.08E+06	575.3284	23.76	9.81E+05	671	361.1490	26.37	1.13E+07	365.1623	26.37	9.87E+06
612	573.3214	29.74	5.40E+05	575.3284	29.74	3.78E+05	672	361.1490	26.97	6.77E+06	365.1623	26.97	6.77E+06
613	578.3303	15.41	1.52E+06	580.3368	15.41	1.41E+06	673	365.2338	17.55	5.29E+06	369.2471	17.55	4.18E+06
614	578.4210	45.81	2.80E+06	580.4272	45.81	2.51E+06	674	366.2177	16.94	4.46E+07	370.2312	16.94	3.89E+07
615	579.2775	11.52	2.49E+06	581.2842	11.52	2.97E+06	675	366.2177	18.19	2.32E+07	370.2312	18.19	2.32E+07
616	582.4385	47.59	8.17E+05	584.4439	47.58	7.61E+05	676	368.1793	15.64	4.90E+05	372.1925	15.64	5.04E+05
617	587.3713	15.49	1.31E+07	589.3776	15.49	6.85E+06	677	368.1793	17.94	1.00E+07	372.1925	17.94	1.43E+07
618	587.3713	15.20	6.55E+06	589.3776	15.20	9.77E+06	678	368.1793	14.64	6.55E+06	372.1925	14.64	4.22E+06
619	587.3713	11.88	3.29E+06	589.3776	11.88	4.77E+06	679	368.2332	19.43	2.00E+08	372.2466	19.43	1.24E+08
620	587.3713	11.01	1.17E+06	589.3776	11.01	8.88E+05	680	368.2332	18.47	4.69E+06	372.2466	18.47	3.03E+06
621	589.4583	39.99	4.59E+05	591.4650	39.99	4.31E+05	681	371.1427	29.08	5.71E+05	375.1561	29.07	3.22E+05
622	590.3088	11.69	1.33E+06	592.3154	11.69	2.34E+06	682	371.1787	18.44	1.17E+06	375.1922	18.44	7.24E+05
623	590.3088	11.03	6.73E+05	592.3154	11.03	4.54E+05	683	373.1583	21.09	7.54E+05	377.1712	21.09	1.13E+06
624	599.5881	47.35	6.08E+05	601.5945	47.35	6.35E+05	684	375.1470	24.55	3.60E+06	379.1606	24.55	2.38E+06
625	612.2515	7.19	2.03E+06	614.2581	7.19	1.05E+06	685	375.1470	25.36	1.30E+06	379.1606	25.36	8.91E+05
626	613.3617	32.85	9.33E+05	615.3687	32.85	9.31E+05	686	375.1470	18.90	2.35E+06	379.1606	18.90	2.35E+06
627	613.3617	33.41	1.45E+06	615.3687	33.41	1.59E+06	687	377.1443	24.55	1.05E+06	381.1573	24.55	7.78E+05
628	613.3617	33.65	3.57E+06	615.3687	33.65	2.51E+06	688	377.1443	25.37	1.57E+06	381.1573	25.37	1.57E+06
629	613.3617	33.89	1.15E+06	615.3687	33.89	1.15E+06	689	377.1443	25.53	2.42E+06	381.1573	25.53	1.24E+06
630	615.3776	36.34	1.48E+06	617.3843	36.34	1.56E+06	690	377.1443	26.93	5.44E+06	381.1573	26.93	3.43E+06
631	615.3776	35.70	4.82E+05	617.3843	35.70	4.82E+05	691	377.1443	18.90	1.12E+06	381.1573	18.90	1.12E+06
632	615.4734	40.25	2.98E+05	617.4802	40.25	3.12E+05	692	378.1633	27.54	1.97E+06	382.1768	27.54	9.90E+05
633	617.4891	42.35	4.06E+05	619.4962	42.35	3.87E+05	693	380.1967	17.45	3.54E+06	384.2102	17.45	2.52E+06
634	624.3699	31.96	2.73E+05	626.3763	31.96	3.12E+05	694	381.2286	16.18	1.43E+06	385.2420	16.18	1.04E+06
635	630.4381	46.10	5.07E+05	632.4449	46.09	4.86E+05	695	382.1945	19.58	1.51E+06	386.2080	19.58	8.48E+05

636	639.3774	34.65	8.01E+05	641.3839	34.65	9.00E+05		696	382.2490	20.24	3.35E+06	386.2623	20.24	3.15E+06
637	639.3774	34.11	5.34E+05	641.3839	34.11	5.74E+05		697	383.1970	14.31	6.62E+05	387.2106	14.31	3.84E+05
638	639.3774	35.38	1.78E+06	641.3839	35.38	1.54E+06		698	383.1970	19.57	4.88E+05	387.2106	19.57	7.44E+05
639	640.2827	11.02	1.36E+06	642.2890	11.02	7.88E+05		699	384.1742	12.85	5.84E+06	388.1874	12.84	5.01E+06
640	640.2827	11.87	6.83E+05	642.2890	11.87	5.86E+05		700	384.2281	17.08	8.63E+08	388.2411	17.08	7.44E+08
641	641.3929	37.21	7.35E+06	643.3996	37.21	8.12E+06		701	385.1227	25.97	3.45E+05	389.1366	25.97	6.26E+05
642	641.3929	36.64	2.07E+06	643.3996	36.64	1.89E+06		702	391.2496	19.08	6.38E+05	395.2637	19.06	6.26E+05
643	641.3929	36.44	1.54E+06	643.3996	36.44	1.11E+06		703	392.2335	18.79	2.50E+05	396.2472	18.79	4.95E+05
644	641.3929	37.05	8.85E+05	643.3996	37.05	1.09E+06		704	393.2649	21.35	1.32E+07	397.2783	21.35	1.07E+07
645	641.6350	49.36	4.34E+05	643.6418	49.36	4.30E+05		705	394.1587	28.42	2.07E+06	398.1721	28.41	1.79E+06
646	643.4088	40.35	1.16E+06	645.4156	40.35	1.20E+06		706	394.1953	20.27	4.66E+05	398.2083	20.27	8.12E+05
647	643.4088	39.70	6.90E+05	645.4156	39.70	5.49E+05		707	394.2487	21.29	2.21E+06	398.2629	21.28	1.66E+06
648	643.4088	43.77	9.98E+05	645.4156	43.77	9.98E+05		708	394.2487	20.20	7.76E+05	398.2629	20.19	5.82E+05
649	653.3011	13.87	3.62E+05	655.3074	13.87	6.95E+05		709	394.2487	19.00	5.53E+05	398.2629	19.01	6.35E+05
650	656.3422	32.42	6.50E+05	658.3494	32.42	7.11E+05		710	396.1743	18.74	5.45E+06	400.1877	18.74	3.10E+06
651	656.3422	13.72	1.59E+06	658.3494	13.72	1.22E+06		711	396.1743	21.92	5.43E+06	400.1877	21.92	3.25E+06
652	656.3422	16.26	9.96E+05	658.3494	16.26	9.96E+05		712	396.1743	23.33	3.22E+06	400.1877	23.33	3.22E+06
653	656.3422	32.59	2.54E+06	658.3494	32.59	2.54E+06		713	396.2287	19.53	9.26E+05	400.2418	19.53	1.04E+06
654	661.3620	32.22	3.00E+05	663.3687	32.22	2.96E+05		714	396.2287	22.84	1.27E+06	400.2418	22.84	1.27E+06
655	661.3620	32.64	3.63E+05	663.3687	32.64	4.38E+05		715	396.2287	23.94	2.14E+06	400.2418	23.94	2.14E+06
656	663.3774	34.62	2.27E+06	665.3842	34.62	2.60E+06		716	396.2648	20.78	2.26E+06	400.2780	20.78	2.64E+06
657	663.3774	34.19	1.79E+06	665.3842	34.18	1.82E+06		717	396.2648	21.98	9.60E+06	400.2780	21.98	7.95E+06
658	663.3774	37.21	5.75E+05	665.3842	37.21	6.82E+05		718	397.1583	25.04	1.45E+06	401.1717	25.04	9.61E+05
659	665.3929	35.53	2.25E+05	667.3999	35.53	2.43E+05		719	397.1583	26.34	1.96E+06	401.1717	26.34	1.48E+06
660	665.3929	36.02	5.79E+05	667.3999	36.02	3.47E+05		720	398.1900	19.08	1.95E+06	402.2030	19.08	1.04E+06

Continued table

No.	m/z (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	m/z (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	m/z (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	m/z (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
721	398.2075	17.90	5.39E+08	402.2205	17.90	4.64E+08		781	428.2096	21.20	1.38E+05	432.2241	21.20	1.38E+05	

722	398.2075	17.45	6.52E+07	402.2205	17.45	4.24E+07		782	428.2096	21.61	2.98E+05	432.2241	21.61	3.61E+05	
723	400.1694	23.11	2.27E+06	404.1826	23.11	2.51E+06		783	428.2181	17.62	5.35E+07	432.2314	17.62	3.80E+07	
724	400.1694	18.05	2.67E+06	404.1826	18.05	2.67E+06		784	428.2545	17.20	3.01E+06	432.2680	17.20	2.53E+06	
725	400.2052	18.54	7.55E+05	404.2186	18.54	7.97E+05		785	432.1953	16.91	1.87E+06	436.2087	16.91	1.63E+06	
726	400.2235	26.94	3.38E+05	404.2367	26.94	2.69E+05		786	438.2387	19.12	2.33E+08	442.2523	19.12	1.81E+08	Proline
727	403.1016	16.25	4.01E+06	407.1155	16.25	2.24E+06		787	439.2482	22.52	1.17E+06	443.2635	22.52	7.18E+05	
728	403.1016	27.25	3.24E+06	407.1155	27.25	2.34E+06		788	440.2183	24.09	1.20E+06	444.2317	24.09	7.86E+05	
729	403.1016	30.71	1.23E+06	407.1155	30.71	1.58E+06		789	440.2543	21.29	2.02E+08	444.2675	21.29	1.11E+08	
730	405.2650	21.92	7.63E+05	409.2787	21.92	1.13E+06		790	440.2543	21.06	4.92E+08	444.2675	21.04	3.57E+08	
731	407.2809	22.65	2.25E+07	411.2942	22.65	1.84E+07		791	441.2016	26.05	2.23E+06	445.2159	26.05	1.62E+06	Succinic acid
732	407.2809	23.03	1.13E+07	411.2942	23.03	1.13E+07		792	441.2653	23.29	1.75E+07	445.2787	23.28	1.56E+07	
733	408.2284	18.71	2.29E+07	411.2942	18.71	2.03E+07		793	442.1799	20.73	6.93E+05	446.1934	20.72	3.91E+05	
734	408.2284	16.21	1.10E+07	412.2420	16.21	1.10E+07		794	442.1799	25.36	1.24E+06	446.1934	25.36	2.14E+06	
735	408.2396	16.02	2.91E+05	412.2529	16.02	2.64E+05		795	442.1799	25.77	2.86E+06	446.1934	25.76	3.07E+06	
736	408.2647	22.45	8.50E+06	412.2779	22.45	6.39E+06		796	442.1799	26.40	3.72E+06	446.1934	26.40	2.46E+06	
737	408.2847	23.03	2.03E+06	412.2980	23.04	1.51E+06		797	442.1799	28.26	5.93E+05	446.1934	28.26	6.18E+05	
738	408.2847	22.65	1.13E+06	412.2980	22.65	1.13E+06		798	442.2336	18.87	1.13E+08	446.2470	18.87	8.50E+07	
739	410.1539	29.19	4.27E+05	414.1675	29.19	3.33E+05		799	442.2491	23.33	2.61E+06	446.2625	23.33	2.06E+06	
740	410.1539	27.06	8.65E+05	414.1675	27.06	7.65E+05		800	444.1953	18.31	4.20E+06	448.2088	18.31	3.27E+06	
741	410.1539	30.33	1.12E+06	414.1675	30.33	1.12E+06		801	444.1953	22.42	3.61E+05	448.2088	22.42	3.52E+05	
742	410.2441	17.27	1.13E+06	414.2573	17.26	1.40E+06		802	444.1953	18.90	8.76E+06	448.2088	18.90	5.48E+06	
743	410.2441	16.25	9.23E+05	414.2573	16.25	1.18E+06		803	444.2647	23.87	5.71E+05	448.2778	23.87	4.65E+05	
744	412.1691	28.47	2.12E+07	416.1823	28.47	1.90E+07		804	445.1795	24.09	1.15E+06	449.1931	24.09	1.06E+06	
745	412.1691	21.84	1.08E+07	416.1823	21.84	1.12E+07		805	445.2237	17.69	1.34E+06	449.2372	17.69	1.51E+06	
746	412.2231	18.43	1.72E+08	416.2361	18.43	1.12E+08	Alanine	806	446.1745	22.41	4.83E+05	450.1887	22.41	3.34E+05	
747	412.2231	18.18	2.46E+08	416.2361	18.18	1.79E+08		807	446.1745	21.47	1.23E+06	450.1887	21.47	1.43E+06	
748	413.2071	12.88	2.54E+05	417.2208	12.88	1.99E+05		808	448.1901	17.43	2.87E+07	452.2034	17.43	2.28E+07	
749	414.1672	25.79	5.42E+05	418.1805	25.79	6.30E+05		809	450.1838	17.43	9.35E+05	454.1973	17.42	9.45E+05	
750	414.1672	28.47	1.24E+06	418.1805	28.47	1.24E+06		810	450.1987	17.42	1.81E+06	454.2130	17.42	9.19E+05	
751	414.1849	16.91	3.42E+05	418.1982	16.91	2.95E+05		811	452.2183	23.95	4.44E+06	456.2317	23.95	3.41E+06	

752	414.1849	21.94	3.23E+07	418.1982	21.94	3.11E+07	812	452.3274	26.73	9.44E+05	456.3409	26.73	1.52E+06
753	414.1849	23.34	1.46E+07	418.1982	23.34	1.37E+07	813	454.2143	21.55	4.18E+05	458.2270	21.59	4.36E+05
754	414.2213	20.99	7.48E+05	418.2344	20.99	6.81E+05	814	454.2335	18.87	3.67E+06	458.2474	18.87	4.90E+06
755	415.1690	26.50	1.55E+06	419.1823	26.50	1.55E+06	815	454.2702	22.45	1.29E+09	458.2832	22.45	7.77E+08
756	415.1690	25.78	4.33E+06	419.1823	25.78	3.25E+06	816	454.2702	22.67	4.64E+08	458.2832	22.67	3.53E+08
757	415.1690	28.47	1.24E+06	419.1823	28.47	1.24E+06	817	455.2291	17.40	9.02E+06	459.2423	17.40	6.06E+06
758	416.1807	23.32	5.18E+05	420.1925	23.32	4.80E+05	818	455.2372	18.87	4.45E+06	459.2505	18.87	3.07E+06
759	417.1840	17.40	1.66E+06	421.1979	17.40	1.46E+06	819	456.0801	25.99	4.96E+05	460.0934	25.99	7.25E+05
760	417.1840	21.84	1.87E+06	421.1979	21.84	3.21E+06	820	456.1953	27.74	2.48E+07	460.2085	27.74	2.10E+07
761	420.1892	17.88	5.87E+06	424.2026	17.88	4.14E+06	821	457.1618	27.46	1.17E+06	461.1753	27.46	1.66E+06
762	423.2545	27.24	2.75E+05	427.2679	27.23	1.96E+05	822	457.2609	19.94	9.43E+06	461.2742	19.94	7.94E+06
763	424.1691	26.41	2.07E+06	428.1823	26.41	1.11E+06	823	458.2110	20.98	6.64E+05	462.2239	20.98	4.02E+05
764	424.2215	18.86	4.83E+05	428.2357	18.88	3.13E+05	824	458.2305	18.28	7.10E+05	462.2436	18.28	4.67E+05
765	424.2215	23.25	1.43E+07	428.2357	23.27	8.79E+06	825	458.2437	19.68	1.72E+06	462.2584	19.67	1.28E+06
766	425.2267	23.25	1.18E+05	429.2393	23.25	1.07E+05	826	458.2437	24.00	3.35E+06	462.2584	24.00	3.32E+06
767	425.2372	21.00	6.71E+06	429.2507	21.00	5.95E+06	827	459.2141	17.01	2.91E+06	463.2273	17.00	2.11E+06
768	425.2910	15.36	1.89E+06	429.3047	15.36	2.01E+06	828	459.2141	21.73	1.98E+08	463.2273	21.73	1.47E+08
769	425.2910	15.64	6.54E+05	429.3047	15.64	6.54E+05	829	459.2141	19.75	2.24E+07	463.2273	19.75	1.57E+07
770	425.2910	14.05	4.32E+05	429.3047	14.05	4.32E+05	830	461.2241	21.72	6.39E+05	465.2384	21.72	4.04E+05
771	426.1848	18.31	1.79E+06	430.1982	18.31	1.12E+06	831	470.2113	29.10	2.87E+06	474.2248	29.10	2.13E+06
772	426.1848	19.25	5.44E+07	430.1982	19.25	3.20E+07	832	470.2442	32.94	1.94E+06	474.2578	32.94	1.47E+06
773	426.1848	28.03	5.06E+05	430.1982	28.03	3.71E+05	833	472.2270	21.37	1.68E+08	476.2404	21.37	1.50E+08
774	426.1848	17.21	1.51E+06	430.1982	17.21	1.51E+06	834	472.2270	12.97	8.82E+06	476.2404	12.97	6.23E+06
775	426.2207	21.37	9.78E+05	430.2346	21.37	7.17E+05	835	472.2270	13.25	9.98E+06	476.2404	13.25	6.89E+06
776	426.2391	19.48	1.03E+06	430.2527	19.48	5.16E+05	836	472.2270	21.54	5.63E+06	476.2404	21.54	5.63E+06
777	426.2391	19.71	9.54E+05	430.2527	19.71	6.45E+05	837	474.2388	22.23	1.89E+06	478.2524	22.23	2.29E+06
778	426.2391	21.00	1.23E+06	430.2527	21.00	1.23E+06	838	475.2089	21.16	2.50E+07	479.2225	21.16	1.83E+07
779	428.1641	25.15	6.91E+05	432.1773	25.15	7.54E+05	839	475.2089	17.14	2.90E+06	479.2225	17.14	2.13E+06
780	428.2096	20.96	1.25E+05	432.2241	20.96	1.28E+05	840	476.1671	19.24	8.88E+05	480.1811	19.24	1.25E+06

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
841	476.1671	19.46	1.15E+06	480.1811	19.46	1.23E+06		901	569.2793	22.18	6.07E+05	573.2924	22.18	5.33E+05	
842	478.2451	13.81	3.00E+06	482.2584	13.81	2.07E+06		902	571.1439	21.36	3.95E+05	575.1570	21.36	2.68E+05	
843	478.2451	14.50	1.06E+06	482.2584	14.50	6.62E+05		903	571.2944	22.40	2.47E+05	575.3090	22.40	1.83E+05	
844	478.2451	16.70	2.71E+06	482.2584	16.69	1.76E+06		904	577.4006	36.86	1.01E+06	581.4141	36.86	7.80E+05	
845	478.2451	16.94	3.73E+06	482.2584	16.94	3.71E+06		905	578.4678	40.91	5.43E+05	582.4821	40.91	4.66E+05	
846	480.2763	22.91	2.05E+06	484.2899	22.91	1.76E+06		906	578.4678	41.28	1.39E+06	582.4821	41.28	1.23E+06	
847	483.2606	18.30	1.15E+06	487.2744	18.30	9.14E+05		907	578.4678	40.67	1.47E+06	582.4821	40.67	1.32E+06	
848	486.2059	23.78	7.71E+06	490.2190	23.78	6.98E+06		908	579.4160	39.09	2.47E+06	583.4294	39.08	1.66E+06	
849	486.2059	12.27	6.62E+05	490.2190	12.27	4.28E+05		909	587.3232	24.10	4.16E+05	591.3364	24.10	3.12E+05	
850	486.2408	20.62	4.92E+05	490.2531	20.62	5.01E+05		910	590.3088	11.03	1.09E+06	594.3219	11.03	9.44E+05	
851	488.2217	17.68	1.74E+06	492.2351	17.68	1.34E+06		911	590.3088	11.67	1.33E+06	594.3219	11.67	1.07E+06	
852	488.2548	23.34	9.49E+08	492.2678	23.34	7.35E+08		912	591.2850	13.82	6.34E+05	595.2990	13.82	6.18E+05	
853	488.2548	23.44	4.62E+08	492.2678	23.44	3.21E+08		913	592.4837	42.35	3.25E+07	596.4969	42.35	2.87E+07	
854	492.2054	29.69	1.57E+06	496.2183	29.69	2.79E+06		914	597.2953	17.43	1.66E+06	601.3088	17.42	1.37E+06	
855	497.1246	17.91	2.05E+06	501.1376	17.90	1.38E+06		915	597.2953	26.50	3.21E+06	601.3088	26.50	3.21E+06	
856	497.2762	18.01	5.83E+05	501.2895	18.01	4.45E+05		916	601.3394	25.72	3.03E+05	605.3519	25.72	2.05E+05	
857	504.2494	20.62	1.94E+08	508.2623	20.62	1.48E+08		917	605.4315	39.41	4.55E+06	609.4449	39.41	3.25E+06	
858	504.2494	19.67	1.62E+08	508.2625	19.67	1.03E+08		918	606.4997	42.86	4.17E+05	610.5135	42.85	3.43E+05	
859	508.3901	34.88	7.16E+06	512.4035	34.88	7.91E+06		919	607.4473	41.51	6.18E+05	611.4607	41.51	3.72E+05	
860	509.2763	19.30	1.11E+06	513.2899	19.30	1.87E+06		920	608.3194	21.71	5.56E+06	612.3327	21.71	4.11E+06	
861	510.3441	13.93	7.97E+06	514.3575	13.93	5.35E+06		921	609.4128	12.35	1.12E+06	613.4254	12.34	5.97E+05	
862	510.3441	12.00	3.56E+06	514.3575	12.00	3.23E+06		922	622.4584	38.01	1.01E+06	626.4720	38.01	7.46E+05	
863	511.2915	18.44	6.25E+05	515.3050	18.44	4.02E+05		923	632.3448	20.37	1.90E+06	636.3578	20.37	1.49E+06	
864	511.2915	21.17	8.11E+05	515.3050	21.16	6.08E+05		924	646.4583	38.22	2.71E+05	650.4719	38.22	3.50E+05	
865	511.2915	18.12	6.22E+05	515.3050	18.12	3.55E+05		925	648.3837	39.45	1.21E+06	652.3970	39.46	9.92E+05	
866	511.2915	21.82	1.31E+06	515.3050	21.82	1.13E+06		926	648.3837	38.65	9.98E+05	652.3970	38.66	8.02E+05	
867	511.2915	19.82	1.82E+06	515.3050	19.82	1.47E+06		927	648.4739	40.33	5.61E+05	652.4876	40.33	6.57E+05	

868	511.2915	23.64	8.88E+05	515.3050	23.64	6.54E+05	928	653.3011	13.87	3.62E+05	657.3149	13.87	3.44E+05
869	514.2012	29.21	1.03E+06	518.2147	29.21	5.39E+05	929	666.4306	53.35	1.60E+06	670.4437	53.35	1.19E+06
870	514.2012	28.76	9.52E+05	518.2147	28.76	7.34E+05	930	674.3531	27.62	3.64E+05	678.3655	27.62	5.43E+05
871	519.1124	17.43	8.34E+05	523.1254	17.43	6.97E+05	931	674.4899	40.69	1.11E+06	678.5029	40.68	1.41E+06
872	525.3078	20.94	6.24E+05	529.3204	20.94	4.94E+05	932	680.4102	44.95	5.70E+05	684.4235	44.96	5.03E+05
873	525.3078	21.14	1.06E+06	529.3204	21.13	9.51E+05	933	682.4255	47.46	3.35E+06	686.4386	47.46	3.04E+06
874	525.3078	22.59	2.00E+06	529.3204	22.59	1.59E+06	934	693.2813	16.35	3.75E+05	697.2946	16.35	2.60E+05
875	525.3180	15.93	1.66E+06	529.3315	15.93	1.04E+06	935	693.2813	16.10	4.78E+05	697.2946	16.10	4.78E+05
876	525.3180	15.49	2.35E+06	529.3315	15.49	3.27E+06	936	694.4615	58.45	1.50E+06	698.4756	58.44	1.12E+06
877	527.2653	23.57	4.22E+07	531.2787	23.57	3.13E+07	937	704.4064	47.42	1.26E+06	708.4205	47.41	1.13E+06
878	527.2653	22.42	6.64E+07	531.2787	22.42	5.10E+07	938	774.4456	37.17	2.96E+06	778.4592	37.17	2.35E+06
879	529.2847	14.58	8.22E+05	533.2981	14.59	6.20E+05	939	774.4456	36.66	2.02E+06	778.4592	36.66	1.55E+06
880	529.2847	14.34	1.06E+06	533.2981	14.34	6.95E+05	940	774.4456	37.41	3.87E+06	778.4592	37.41	3.87E+06
881	536.4216	37.63	5.01E+06	540.4351	37.62	4.37E+06	941	774.4456	37.65	1.67E+06	778.4592	37.65	2.31E+06
882	537.3073	22.31	1.29E+06	541.3208	22.31	1.08E+06	942	776.4608	39.50	5.30E+05	780.4745	39.51	4.43E+05
883	538.2314	15.43	1.52E+06	542.2448	15.43	1.08E+06	943	776.4608	40.07	2.31E+06	780.4747	40.07	1.79E+06
884	539.3231	22.74	7.68E+05	543.3367	22.74	5.50E+05	944	800.4615	38.25	1.18E+06	804.4756	38.25	9.44E+05
885	541.2480	18.00	3.30E+05	545.2616	18.00	3.21E+05	945	800.4615	37.77	1.12E+06	804.4756	37.77	8.30E+05
886	541.3023	22.15	5.81E+05	545.3163	22.15	4.10E+05	946	802.4772	40.62	1.53E+07	806.4906	40.62	1.23E+07
887	543.1485	21.38	6.96E+05	547.1620	21.36	5.00E+05	947	802.4772	40.10	1.67E+07	806.4906	40.10	1.22E+07
888	543.2646	28.42	2.87E+05	547.2763	28.42	2.52E+05	948	802.4772	40.26	6.31E+06	806.4906	40.26	6.31E+06
889	545.2761	22.24	3.47E+05	549.2894	22.24	2.88E+05	949	802.4772	40.78	3.21E+06	806.4906	40.78	3.21E+06
890	545.2761	23.91	7.83E+05	549.2894	23.91	5.35E+05	950	804.4925	43.75	2.03E+06	808.5063	43.75	1.58E+06
891	545.2761	20.42	5.58E+05	549.2894	20.43	4.28E+05	951	804.4925	43.21	3.22E+06	808.5063	43.21	3.22E+06
892	545.2761	18.68	1.38E+06	549.2894	18.68	1.44E+06	952	814.4332	23.18	3.13E+05	818.4462	23.18	2.44E+05
893	550.4373	38.92	6.26E+05	554.4511	38.91	5.14E+05	953	822.4461	36.09	5.92E+05	826.4598	36.08	6.30E+05
894	550.4373	38.48	1.44E+06	554.4511	38.48	1.44E+06	954	822.4461	35.73	7.50E+05	826.4598	35.73	5.80E+05
895	551.3221	23.81	1.29E+06	555.3361	23.81	1.22E+06	955	824.4611	38.06	3.25E+06	828.4744	38.06	2.78E+06
896	559.2921	22.02	3.77E+05	563.3046	22.02	2.82E+05	956	824.4611	37.69	3.85E+06	828.4744	37.69	2.96E+06
897	561.1141	21.36	3.51E+05	565.1281	21.35	2.52E+05	957	824.4611	40.26	4.58E+06	828.4744	40.26	5.22E+06

898	564.4524	40.14	1.94E+07	568.4657	40.14	1.72E+07		958	824.4611	40.65	6.74E+06	828.4744	40.65	6.74E+06	
899	567.3540	24.71	8.56E+05	571.3677	24.70	6.18E+05		959	826.4772	40.39	4.50E+05	830.4896	40.39	3.19E+05	
900	568.3212	42.28	7.16E+05	572.3345	42.29	5.58E+05		960	826.4772	39.02	4.23E+05	830.4896	39.02	3.21E+05	

Continued table

No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name	No.	<i>m/z</i> (DmPA-labeled)	Rt (min) (DmPA-labeled)	Intensity (DmPA-labeled)	<i>m/z</i> (¹³ C ₂ -DmPA-labeled)	Rt (min) (¹³ C ₂ -DmPA-labeled)	Intensity (¹³ C ₂ -DmPA-labeled)	Name
961	826.4772	39.46	5.42E+05	830.4896	39.46	4.26E+05		980	615.3539	32.12	1.03E+08	621.3738	32.12	5.82E+07	
962	826.4772	43.74	7.83E+05	830.4896	43.74	7.83E+05		981	615.3539	34.58	2.94E+07	621.3738	34.59	1.71E+07	
963	559.2914	26.82	1.46E+08	565.3110	26.80	8.28E+07		982	617.2800	30.04	3.20E+05	623.2998	30.04	5.62E+05	
964	559.2914	25.08	1.48E+06	565.3110	25.09	9.15E+05		983	617.2800	29.17	3.89E+05	623.2998	29.18	6.16E+05	
965	561.2894	24.72	2.71E+06	567.3093	24.72	2.04E+06		984	619.2592	30.25	4.11E+06	625.2784	30.25	3.85E+06	
966	573.3073	26.51	4.81E+07	579.3274	26.51	2.57E+07		985	620.2988	24.20	2.03E+06	626.3190	24.20	1.26E+06	
967	573.3073	24.31	3.97E+05	579.3274	24.29	2.95E+05		986	633.3103	31.99	4.13E+07	639.3302	31.99	2.36E+07	
968	581.2730	26.80	1.55E+07	587.2928	26.80	8.34E+06		987	633.3103	21.38	3.72E+06	639.3302	21.38	4.33E+06	
969	587.3229	24.49	2.70E+05	593.3430	24.48	1.74E+05		988	633.3103	22.37	5.48E+06	639.3302	22.37	4.79E+06	
970	587.3229	28.97	2.69E+06	593.3430	28.97	3.20E+06		989	639.3294	25.76	5.89E+05	645.3492	25.76	2.98E+05	
971	589.3018	27.17	6.47E+06	595.3224	27.17	3.29E+06		990	649.3382	33.61	1.29E+08	655.3581	33.61	7.40E+07	
972	593.2793	25.26	3.20E+06	599.2996	25.26	2.42E+06		991	653.2894	24.38	7.96E+05	659.3085	24.38	4.34E+05	
973	599.3232	26.43	6.41E+05	605.3432	26.43	3.79E+05		992	653.2894	23.83	4.74E+05	659.3085	23.83	4.74E+05	
974	601.2480	33.72	9.45E+05	607.2680	33.72	7.19E+05		993	665.3331	28.96	5.87E+07	671.3535	28.96	3.32E+07	
975	601.3387	33.12	4.26E+07	607.3589	33.12	2.48E+07		994	665.3331	26.48	3.87E+05	671.3535	26.49	6.97E+05	
976	603.2645	31.86	3.57E+05	609.2839	31.85	3.18E+05		995	672.3761	30.54	1.44E+06	678.3959	30.54	9.49E+05	
977	603.2645	32.63	4.58E+05	609.2839	32.63	4.58E+05		996	672.3761	26.22	6.90E+05	678.3959	26.22	6.90E+05	
978	603.3183	29.57	7.54E+06	609.3383	29.57	4.53E+06		997	688.3493	31.03	1.70E+07	694.3692	31.03	9.33E+06	
979	605.2797	25.42	5.82E+06	611.2998	25.42	3.95E+06		998	706.3607	30.81	3.00E+05	712.3796	30.80	2.06E+05	

Table S8. Investigation of the accuracy of relative quantitation.

Analytes	Linear range (ng/mL)	Regression line		
		Slope	Intercept	R ²
Valeric acid	1-500	1.135	-0.02342	0.9989
Succinic acid	1-500	1.053	0.1337	0.9997
9-Decenoic acid	1-500	0.9554	0.08747	0.9996
Nonadecanoic acid	1-500	1.040	-0.06245	0.9964
Alanine	5-1000	0.9679	-0.04075	0.9979
Tryptophan	5-1000	1.171	-0.3718	0.9923
Phenylalanine	5-1000	1.105	-0.07414	0.9977

Table S9. Carboxylated metabolites with significant difference between curcumin and control.

No.	MPEA labeled m/z	Rt (min) (MPEA-labeled)	d ₅ -MPEA labeled m/z	Rt (min) (d ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
13	223.1441	3.00	226.1630	2.98		C12H19N2O2	C3H7NO3	CLMD	Serine	302-84-1	Level 1	2.65	1.75E-02
14	233.1653	6.95	236.1842	6.90		C14H21N2O	C5H9NO2	CLMD	Proline	29795-82-2	Level 1	3.70	1.66E-06
17	236.1278	13.76	239.1467	13.71	205.9	C13H18O3N	C4H6O4	CLMD	Succinic acid	110-15-6	Level 1	8.99	1.80E-03
25	252.1218	11.05	255.1407	10.99	30.0	C13H18O4N	C4H6O5	CLMD	Malic acid	6915-15-7	Level 1	2.05	2.52E-03
27	264.1592	16.37	267.1781	16.31	281.8	C15H22O3N	C6H10O4	CLMD	Adipic acid	124-04-9	Level 1	7.20	1.66E-03
32	293.1492	10.79	296.1681	10.73	12.3	C15H21O4N2	C6H9O5N	CLMD	<i>N</i> -Acetyl-aspartic acid	997-55-7	Level 1	4.26	4.23E-03
76	207.1492	14.83	210.1681	14.80	236.9	C12H19ON2	C3H7O2N	Metlin	Sarcosine	107-97-1	Level 3	2.99	1.20E-03
77	222.1489	15.33	225.1678	15.26	251.5	C13H20O2N	C4H8O3	HMDB	2-Hydroxybutyric acid	3347-90-8	Level 3	3.43	1.08E-03
									4-Hydroxybutyric acid	591-81-1			
									2-Hydroxy-2-methylpropanoic acid	594-61-6			
79	246.1123	15.52	249.1312	15.45	256.9	C14H16O3N	C5H4O4	HMDB	5-Hydroxy-2-furoic acid		Level 3	2.32	4.56E-04
83	248.2003	28.21	251.2192	28.15	685.7	C16H26ON	C7H14O2	HMDB	2-Methylhexanoic acid	4536-23-6	Level 3	2.50	5.42E-04
									5-Methylhexanoic acid	628-46-6			
89	264.1228	15.51	267.1417	15.47	256.8	C14H18O4N	C5H6O5	HMDB	Oxoglutaric acid	328-50-7	Level 3	3.21	7.21E-06
									3-Oxoglutaric acid	542-05-2			
100	288.2318	34.58	291.2507	18.95	932.8	C19H30ON	C10H18O2	HMDB	6-Decenoic acid	85392-04-7	Level 3	2.11	7.32E-04
									3-Decenoic acid	15469-77-9			
									8-Methylnonenoate	59320-77-3			
									9-Decenoic acid	14436-32-9			
									Citronellic acid	502-47-6			
									<i>cis</i> -4-Decenoic acid	505-90-8			
									<i>trans</i> -Dec-2-enoic acid				
111	306.2063	24.38	309.2252	24.29	550.3	C18H28O3N	C9H16O4	HMDB	3-Methylsuberic acid		Level 3	4.37	3.08E-03
									2,4-Dimethylpimelic acid				
112	307.1652	12.29	310.1841	12.25	114.0	C16H23O4N2	C7H11O5N	HMDB	<i>N</i> -Acetyl-DL-glutamic acid	1188-37-0	Level 3	2.17	1.83E-02
114	308.1490	16.89	311.1679	16.83	296.8	C16H22O5N	C7H10O6	HMDB	2-Hydroxy-2-(2-oxopropyl)butanedioic acid		Level 3	3.01	6.75E-04

									3-Dehydroquinic acid				
116	316.2632	37.77	319.2821	37.70	1063.6	C21H34ON	C12H22O2	HMDB	11-Dodecenoic acid	65423-25-8	Level 3	2.36	6.15E-03
117	316.2632	39.24	319.2821	39.17	1125.5	C21H34ON	C12H22O2	HMDB	<i>trans</i> -Dodec-2-enoic acid		Level 3	2.70	1.51E-03
									5Z-Dodecenoic acid	2430-94-6			
118	318.2791	39.62	321.2980	39.57	1141.7	C21H36ON	C12H24O2	Metlin	Isolauric acid	2724-56-3	Level 3	2.63	5.93E-04
									2-Methyl-undecanoic acid	24323-25-9			
									3-Methyl-undecanoic acid	65781-38-6			
									4-Methyl-undecanoic acid				
									5-Methyl-undecanoic acid				
									6-Methyl-undecanoic acid				
									8-Methyl-undecanoic acid				
									9-Methyl-undecanoic acid				
136	337.1573	18.10	340.1762	18.03	337.1	C20H21O3N2	C11H9O4N	Metlin	Methyl 2,6-dihydroxy-4-quinolinecarboxylate	66416-75-9	Level 3	3.36	2.34E-04
									5-Hydroxyindolepyruvate				
									8-Methoxykynurenate				
146	344.2946	43.65	347.3135	43.59	1322.9	C23H38ON	C14H26O2	HMDB	Myristoleic acid	544-64-9	Level 3	2.10	2.62E-03
									7Z-Tetradecenoic acid				
									9E-Tetradecenoic acid				
									5Z-Tetradecenoic acid	5684-70-8			
									<i>trans</i> -Tetra-dec-2-enoic acid				
147	346.3104	44.09	349.3293	44.01	1342.9	C23H40ON	C14H28O2	HMDB	10-Methyltridecanoic acid		Level 3	2.11	1.26E-04
									2,6,10-Trimethylundecanoic acid	1115-94-2			
									12-Methyltridecanoic acid	2724-57-4			
151	349.2095	19.37	352.2284	19.33	379.8	C19H29O4N2	C10H17O5N	HMDB	<i>N</i> -Isovalerylglutamic acid	80154-63-8	Level 3	2.62	1.04E-05
									Suberylglycine	60317-54-6			
155	352.2020	16.13	355.2209	16.10	274.7	C21H26O2N3	C12H14O3N2	Metlin	5-Methoxy-DL-tryptophan	28052-84-8	Level 3	10.18	2.87E-03
181	381.2538	25.59	387.2916	25.49	591.4	C24H33O2N2	C6H10O4	HMDB	Methylglutaric acid	626-51-7	Level 3	2.18	2.21E-02
									2-Methylglutaric acid	617-62-9			
									4-Ethoxy-4-oxobutanoic acid				
									Adipic acid	124-04-9			

									Monomethyl glutaric acid	1501-27-5			
191	388.3574	50.39	391.3763	50.34	1673.2	C26H46ON	C17H34O2	HMDB	15-Methylhexadecanoic acid		Level 3	4.06	3.94E-04
									(S)-14-Methylhexadecanoic acid	5746-59-8			
									11-Methylhexadecanoic acid		Level 3		
208	396.3261	45.31	399.3450	45.26	1397.6	C27H42ON	C18H30O2	HMDB	γ -Linolenic acid	506-26-3	Level 3	2.48	1.44E-02

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₃ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₃ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
208	396.3261	45.31	399.3450	45.26	1397.6	C27H42ON	C18H30O2	HMDB	Linolenic acid	28290-79-1	Level 3	2.48	1.44E-02
211	399.1915	15.91	402.2104	15.87	268.2	C22H27O5N2	C13H15O6N	HMDB	4-Hydroxyphenylacetylglutamic acid	1029120-37-3	Level 3	2.49	4.83E-03
217	412.2231	13.46	415.2420	13.41	193.1	C23H30O4N3	C14H18O5N2	HMDB	L- γ -Glutamyl- β -phenyl- β -L-alanine	10275-84-0	Level 3	2.21	9.68E-03
									Phenylalanylglutamic acid	3617-45-6			
282	208.1331	2.51	211.1520	2.49		C12H18O2N	C3H6O3				Level 4	2.00	2.43E-04
283	218.1174	13.90	221.1363	13.83	209.9	C13H16O2N	C4H4O3				Level 4	8.06	1.56E-03
285	293.1492	11.63	296.1681	11.57	68.9	C15H21O4N2	C6H9O5N				Level 4	2.74	4.65E-03
294	335.1964	17.06	338.2153	17.01	302.0	C18H27O4N2	C9H15O5N				Level 4	3.69	6.07E-04
295	335.1964	17.39	338.2153	17.37	313.3	C18H27O4N2	C9H15O5N				Level 4	2.07	2.39E-02
296	338.1777	12.64	341.1966	12.61	137.8	C21H24O3N	C12H15O4				Level 4	3.25	1.73E-02
303	353.1860	18.55	356.2049	13.28	352.3	C21H25O3N2	C12H13O4N				Level 4	4.16	6.31E-03
391	366.1475	13.48	369.1664	13.44	194.9						Level 5	2.59	3.21E-04
402	546.4105	51.65	549.4294	51.61	1741.6						Level 5	3.02	1.14E-04
7	207.1492	4.72	210.1681	4.64		C12H19ON2	C3H7O2N	CLMD	Alanine	302-72-7	Level 1	0.22	5.06E-03
16	235.1805	11.25	238.1994	11.20	43.5	C14H23ON2	C5H11O2N	CLMD	Valine	516-06-3	Level 1	0.29	2.11E-04
18	237.1602	4.62	240.1791	4.58		C13H9NO3	C4H9NO3	CLMD	Threonine	72-19-5	Level 1	0.30	2.95E-06
20	248.2003	28.60	251.2192	28.53	673.0	C16H26ON	C7H14O2	CLMD	Heptanoic acid	111-14-8	Level 1	0.49	1.89E-04
23	249.1961	13.78	252.2150	13.72	206.4	C15H25ON2	C6H13O2N	CLMD	Leucine	328-39-2	Level 1	0.27	8.31E-04
24	249.1961	14.01	252.2150	13.96	213.1	C15H25ON2	C6H13O2N	CLMD	Isoleucine	443-79-8	Level 1	0.29	7.00E-04
28	267.1526	12.43	270.1715	12.37	123.4	C14H23ON2S	C5H11O2NS	CLMD	Methionine	59-51-8	Level 1	0.48	3.60E-04
29	276.2322	33.77	279.2511	33.69	900.0	C18H30ON	C9H18O2	CLMD	Pelargonic acid	112-05-0	Level 1	0.47	4.54E-03

30	283.1805	15.83	286.1994	15.76	266.0	C18H23ON2	C9H11O2N	CLMD	Phenylalanine	150-30-1	Level 1	0.25	3.77E-04
33	299.1754	11.83	302.1943	11.77	82.8	C18H23O2N2	C9H11O3N	CLMD	Tyrosine	556-03-6	Level 1	0.29	4.60E-04
38	320.2219	26.53	323.2408	26.47	624.7	C19H30O3N	C10H18O4	CLMD	Sebacic acid	111-20-6	Level 1	0.44	9.18E-03
39	322.1914	16.52	325.2103	16.47	286.0	C20H24ON3	C11H12O2N2	CLMD	Tryptophan	54-12-6	Level 1	0.34	1.39E-04
43	360.3261	47.34	363.3450	47.27	1500.0	C24H42ON	C15H30O2	CLMD	Pentadecanoic acid	1002-84-2	Level 1	0.44	8.20E-04
46	388.3574	50.83	391.3763	50.77	1700.0	C26H46ON	C17H34O2	CLMD	Heptadecanoic acid	506-12-7	Level 1	0.47	1.66E-02
52	416.3886	54.33	419.4075	54.30	1900.0	C28H50ON	C19H38O2	CLMD	Nonadecanoic acid	646-30-0	Level 1	0.46	5.95E-04
53	418.3679	48.65	421.3868	48.57	1570.9	C27H48O2N	C18H36O3	CLMD	3-Hydroxyoctadecanoic acid		Level 1	0.38	4.09E-04
62	450.3730	48.85	453.3919	48.79	1581.7	C31H48ON	C22H36O2	CLMD	7,10,13,16-Docosatetraenoic acid	28874-58-0	Level 1	0.04	8.54E-04
70	305.2208	18.80	308.2397	18.75	360.7	C18H29O2N2	C9H17O3N	HMDB	8-Amino-7-oxononanoic acid	682799-71-9	Level 2	0.29	1.38E-04
71	429.3475	41.48	432.3664	41.45	1222.8	C27H45O2N2	C18H33O3N	HMDB	2-(14-Methylpentadec-11-enoylamino)acetic acid		Level 2	0.39	2.38E-02
72	431.3630	44.70	434.3819	44.66	1370.1	C27H47O2N2	C18H35O3N	HMDB	Palmitoylglycine	158305-64-7	Level 2	0.18	1.54E-02
73	450.2751	22.91	456.3129	22.82	500.7	C27H36O3N3	C9H13O5N	Metlin	<i>N</i> -Succinyl proline	63250-32-8	Level 2	0.29	5.97E-05
74	459.3945	48.41	462.4134	48.38	1558.1	C29H51O2N2	C20H39O3N	HMDB	Glycine stearamide	6333-54-6	Level 2	0.14	2.10E-02
75	521.4100	48.62	524.4289	48.55	1569.3	C34H53O2N2	C25H41O3N	HMDB	<i>N</i> -Palmitoyl-phenylalanine		Level 2	0.32	4.23E-03
78	233.1653	22.06	236.1842	22.00	471.6	C14H21N2O	C5H9NO2	HMDB	4-Amino-2-methylenebutanoic acid	65370-67-4	Level 3	0.31	2.21E-03
80	247.1441	11.96	250.1630	11.92	91.6	C14H19O2N2	C5H7O3N	Metlin	Pyroline hydroxycarboxylic acid	22573-88-2	Level 3	0.39	5.83E-05
									Pyroglutamic acid	98-79-3			
									<i>N</i> -Acryloylglycine	24599-25-5			
									Pyroline hydroxycarboxylic acid	22573-88-2			
									4-Oxoproline				
									1-Pyrroline-4-hydroxy-2-carboxylate	9054-77-7			
									2-Pyrrolidone-5-carboxylic acid	4042-36-8			
88	262.2163	30.05	265.2352	29.98	755.0	C17H28ON	C8H16O2	HMDB	6-Methylheptanoic acid	929-10-2	Level 3	0.17	3.06E-04
									2-Methylenanthic acid	1188-02-9			
									2-Ethylhexanoic acid	149-57-5			
									Valproic acid	99-66-1			
90	264.1592	18.01	267.1781	17.96	334.0	C15H22O3N	C6H10O4	HMDB	4-Ethoxy-4-oxobutanoic acid	1501-27-5	Level 3	0.09	4.69E-03
91	264.1592	18.29	267.1781	18.25	343.5	C15H22O3N	C6H10O4	HMDB	2-Methylglutaric acid	617-62-9	Level 3	0.15	7.78E-04
									Methylglutaric acid	626-51-7			

									Monomethyl glutaric acid	1501-27-5			
93	265.1547	11.70	268.1736	11.65	74.0	C14H21O3N2	C5H9O4N	HMDB	DL-Glutamic acid	617-65-2	Level 3	0.44	4.39E-04
103	291.2046	19.89	294.2235	19.83	406.3	C17H27O2N2	C8H15O3N	HMDB	Hexanoylglycine	24003-67-6	Level 3	0.35	9.51E-04
104	291.2046	20.15	294.2235	20.11	397.4	C17H27O2N2	C8H15O3N	HMDB	Hexanoylglycine	24003-67-6	Level 3	0.32	1.65E-03
121	320.2306	13.42	323.2495	13.36	190.6	C18H30O2N3	C9H18O3N2	Metlin	Alanyl-Leucine		Level 3	0.48	2.03E-03
									Isoleucyl-Alanine				
									Leucyl-Alanine	7298-84-2			
									Alanyl-Isoleucine				
124	321.2172	20.04	324.2361	20.01	402.4	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3	0.32	4.85E-03
126	321.2172	20.58	324.2361	20.53	420.9	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3	0.26	7.18E-03

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
132	336.2255	13.17	339.2444	13.12	173.6	C18H30O3N3	C9H18O4N2	HMDB	SerinyI-Leucine		Level 3	0.39	3.01E-03
133	336.2255	14.48	339.2444	14.43	226.8	C18H30O3N3	C9H18O4N2	HMDB	SerinyI-Isoleucine		Level 3	0.47	4.69E-03
									Isoleucyl-Serine				
									Leucyl-Serine				
									ThreonyI-Valine				
									Valyl-Threonine				
									Lysopine				
140	340.2019	14.64	343.2208	14.61	231.5	C20H26O2N3	C11H14O3N2	HMDB	PhenylalanyIglycine	721-90-4	Level 3	0.29	8.19E-06
									Glycyl-DL-phenylalanine				
148	346.3104	44.86	349.3293	44.79	1377.4	C23H40ON	C14H28O2	HMDB	2,6,10-Trimethylundecanoic acid	1115-94-2	Level 3	0.47	1.09E-02
									12-Methyltridecanoic acid	2724-57-4			
									10-Methyltridecanoic acid				
154	351.2065	23.11	357.2443	23.02	507.4	C22H27O2N2	C4H4O4	HMDB	Maleic acid	110-16-7	Level 3	0.27	5.08E-03
158	354.2176	16.63	357.2365	16.59	289.2	C21H28O2N3	C12H16O3N2	Metlin	Alanyl-Phenylalanine	1999-45-7	Level 3	0.44	6.69E-03
159	354.2176	17.23	357.2365	17.17	307.8	C21H28O2N3	C12H16O3N2	Metlin	PhenylalanyI-Alanine		Level 3	0.49	1.95E-02
167	360.3261	46.84	363.3450	46.79	1474.9	C24H42ON	C15H30O2	Metlin	4,12-Dimethyl-tridecanoic acid		Level 3	0.39	3.01E-02

									2-Methyl-tetradecanoic acid	7620-57-7			
									3-Methyl-tetradecanoic acid				
									11-Methyl-tetradecanoic acid				
									2,6,10-Trimethyldodecanoic acid	168254-98-6			
									3,5-Dimethyltridecanoic acid				
									12-Methyl myristic acid	5502-94-3			
									Isopentadecylic acid				
171	370.2125	12.67	373.2314	12.60	139.7	C21H28O3N3	C12H16O4N2	Metlin	Alanyl-Tyrosine		Level 3	0.47	6.78E-04
172	370.2125	16.38	373.2314	16.35	282.0	C21H28O3N3	C12H16O4N2	Metlin	Phenylalanyl-Serine		Level 3	0.48	3.61E-03
									Seriny-Phenylalanine				
									Tyrosyl-Alanine				
176	374.3417	48.62	377.3606	48.54	1569.3	C25H44ON	C16H32O2	HMDB	Trimethyltridecanoic acid	10339-73-8	Level 3	0.42	1.36E-04
									Isopalmitic acid	4669-02-7			
177	375.3006	27.84	378.3195	17.81	672.3	C23H39O2N2	C14H27O3N	HMDB	N-Lauroylglycine		Level 3	0.49	1.02E-02
178	375.3006	36.02	378.3195	35.97	991.1	C23H39O2N2	C14H27O3N	HMDB	N-Lauroylglycine		Level 3	0.30	6.67E-03
182	381.2538	26.89	387.2916	26.78	637.8	C24H33O2N2	C6H10O4	HMDB	2-Methylglutaric acid	617-62-9	Level 3	0.35	3.00E-04
									4-Ethoxy-4-oxobutanoic acid				
									Adipic acid	124-04-9			
									Monomethyl glutaric acid	1501-27-5			
									Methylglutaric acid	626-51-7			
183	382.2489	17.48	385.2678	17.41	316.2	C23H32O2N3	C14H20O3N2	Metlin	Valyl-Phenylalanine		Level 3	0.39	3.31E-02
184	382.2489	17.91	385.2678	17.87	330.7	C23H32O2N3	C14H20O3N2	Metlin	Phenylalanyl-Valine	3918-92-1	Level 3	0.41	3.93E-03
186	382.2489	19.51	385.2678	19.44	384.6	C23H32O2N3	C14H20O3N2	Metlin			Level 3	0.45	7.58E-04
188	386.3417	48.27	389.3606	49.52	1550.4	C26H44ON	C17H32O2	Metlin	10-Methyl-9-hexadecenoic acid		Level 3	0.49	2.24E-05
									14-Methyl-8-hexadecenoic acid				
									2-Heptadecylenic acid				
									9-Heptadecylenic acid				
									10-Heptadecenoic acid				
									16-Heptadecenoic acid				
									7-Heptadecenoic acid				

									8-Heptadecenoic acid				
									3-Heptadecenoic acid				
									7-Methyl-6-hexadecenoic acid				
									9,10-Methanohexadecanoic acid				
190	388.3574	50.24	391.3763	50.18	1664.1	C26H46ON	C17H34O2	HMDB	11-Methylhexadecanoic acid		Level 3	0.49	5.82E-05
									15-Methylhexadecanoic acid				
									(S)-14-Methylhexadecanoic acid	5746-59-8			
201	390.3367	39.39	393.3556	39.36	1131.8	C25H44O2N	C16H32O3	HMDB	7-Hydroxyhexadecanoic acid	16899-02-8	Level 3	0.48	2.23E-02
									12-Hydroxyhexadecanoic acid	83646-62-2			
									10-Hydroxyhexadecanoic acid	23048-75-1			
									11-Hydroxyhexadecanoic acid	502-75-0			
									5-Hydroxyhexadecanoic acid	17369-53-8			
									9-Hydroxyhexadecanoic acid	17833-52-2			
									8-Hydroxyhexadecanoic acid	83921-07-7			
									13-Hydroxyhexadecanoic acid	59642-39-6			

Continued table

No.	MPEA labeled m/z	Rt (min) (MPEA-labeled)	d ₃ -MPEA labeled m/z	Rt (min) (d ₃ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
201	390.3367	39.39	393.3556	39.36	1131.8	C25H44O2N	C16H32O3	HMDB	6-Hydroxyhexadecanoic acid	58763-57-8	Level 3	0.48	2.23E-02
									3-Hydroxyhexadecanoic acid	83780-74-9			
									2-Hydroxyhexadecanoic acid	16452-52-1			
203	396.2646	19.03	399.2835	18.95	368.4	C24H34O2N3	C15H22O3N2	HMDB	Leucyl-Phenylalanine	3063-05-6	Level 3	0.35	3.42E-04
204	396.2646	20.55	399.2835	20.47	420.0	C24H34O2N3	C15H22O3N2	HMDB	Isoleucyl-Phenylalanine		Level 3	0.33	1.81E-02
205	396.3261	37.75	399.3450	37.69	1063.1	C27H42ON	C18H30O2	HMDB	γ-Linolenic acid	506-26-3	Level 3	0.46	6.48E-03
									Linolenelaidic acid	28290-79-1			
215	402.3730	52.20	405.3919	52.12	1769.5	C27H48ON	C18H36O2	Metlin	2,6-Dimethyl-hexadecanoic acid		Level 3	0.47	3.51E-03
									Isostearic acid	2724-58-5			
									10-Methyl-heptadecanoic acid				
									4,8-Dimethyl-hexadecanoic acid				

									2,14-Dimethyl-hexadecanoic acid				
									4,14-Dimethyl-hexadecanoic acid				
									6,14-Dimethyl-hexadecanoic acid				
									14-Methyl-heptadecanoic acid				
									11,15-Dimethyl-hexadecanoic acid				
									15-Methyl-heptadecanoic acid				
216	410.2438	21.39	416.2816	21.32	448.7	C24H32O3N3	C6H9O5N	HMDB	<i>N</i> -Formyl-L-glutamic acid	1681-96-5	Level 3	0.35	5.21E-03
									2-Amino-3-oxohexanedioic acid				
218	414.3730	50.73	417.3919	50.66	1694.0	C28H48ON	C19H36O2	Metlin	2-Nonadecenoic acid		Level 3	0.45	8.01E-05
219	414.3730	51.04	417.3919	50.98	1710.8	C28H48ON	C19H36O2	Metlin	17-Methyl-6Z-octadecenoic acid		Level 3	0.44	4.12E-04
									7-Nonadecenoic acid				
									Phytomonic acid	503-06-0			
									13-Cyclohexyltridecanoic acid				
									10Z-Nonadecenoic acid	73033-09-7			
									7E-Nonadecenoic acid				
230	416.3886	55.26	419.4075	55.18	1961.3	C28H50ON	C19H38O2	HMDB	16-Methyloctadecanoic acid		Level 3	0.45	6.58E-03
									Tuberculostearic acid	542-47-2			
									17-Methyloctadecanoic acid	2724-59-6			
									Pristanic acid	1189-37-3			
240	422.2074	25.72	425.2263	20.14	595.6	C24H28O4N3	C15H16O5N2	Metlin	Indole-3-acetylglutamic acid	57105-48-3	Level 3	0.21	1.82E-02
241	422.2439	23.17	428.2817	23.09	509.4	C25H32O3N3	C7H9O5N	Metlin	<i>N</i> -Acryloyl aspartic acid	72064-86-9	Level 3	0.38	3.12E-04
									α -(<i>N</i> -Acetylamino)methylene)succinic acid				
258	445.3790	45.82	448.3979	45.78	1423.0	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3	0.13	6.58E-03
257	445.3790	44.45	448.3979	44.37	1358.9	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3	0.27	1.68E-04
260	450.3730	48.63	453.3919	48.57	1569.8	C31H48ON	C22H36O2	Metlin	4,7,10,13-Docosatetraenoic acid		Level 3	0.48	6.90E-03
									Adrenic acid	28874-58-0			
									8,12,16,19-Docosatetraenoic acid				
									<i>cis</i> -4,10,13,16-Docosatetraenoic acid	122068-08-0			
266	459.3945	45.74	462.4134	45.70	1419.1	C29H51O2N2	C20H39O3N	HMDB	<i>N</i> -Oleoyl alanine		Level 3	0.24	3.03E-03
267	471.3945	36.96	474.4134	36.92	1030.1	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Palmitoyl proline		Level 3	0.24	6.26E-03

269	471.3945	49.41	474.4134	49.38	1613.5	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Palmitoyl GABA	Level 3	0.19	1.38E-02
274	499.4259	40.02	502.4448	39.98	1158.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3	0.22	5.37E-03
275	499.4259	48.63	502.4448	48.60	1569.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3	0.18	3.25E-03
276	499.4259	48.79	502.4448	48.75	1578.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3	0.26	1.85E-03
277	499.4259	49.94	502.4448	49.90	1645.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline	Level 3	0.26	1.85E-03
278	501.4414	51.59	504.4603	51.56	1738.4	C32H57O2N2	C23H45O3N	Metlin	<i>N</i> -Stearoyl valine	Level 3	0.16	4.76E-03
281	549.4412	52.00	552.4601	51.96	1759.2	C36H57O2N2	C27H45O3N	HMDB	<i>N</i> -Stearoyl phenylalanine	Level 3	0.13	7.88E-03
304	358.1570	19.24	361.1759	19.17	375.5	C22H20O2N3	C13H12O3N2			Level 4	0.31	5.60E-03
305	358.1570	20.62	361.1759	20.58	422.5	C22H20O2N3	C13H12O3N2			Level 4	0.24	1.12E-02
308	361.2850	26.01	364.3039	25.95	606.0	C22H37O2N2	C13H25O3N			Level 4	0.32	2.28E-02
309	403.3319	40.52	406.3508	40.46	1179.6	C25H43O2N2	C16H31O3N			Level 4	0.30	9.00E-03
316	421.2595	18.09	424.2784	18.02	336.8	C27H35O3N	C18H23O4			Level 4	0.26	2.05E-05
317	421.2595	18.96	424.2784	18.91	366.2	C27H35O3N	C18H23O4			Level 4	0.44	5.53E-03
318	429.3475	41.78	432.3664	41.71	1236.5	C27H45O2N2	C18H33O3N			Level 4	0.42	5.75E-03
319	429.3475	42.06	432.3664	41.98	1249.6	C27H45O2N2	C18H33O3N			Level 4	0.37	4.13E-02
324	430.2486	20.22	433.2675	20.16	408.8	C27H32O2N3	C18H20O3N2			Level 4	0.43	3.14E-03
325	442.2520	30.51	445.2709	30.45	772.3	C25H34O5N2	C16H22O6N			Level 4	0.49	2.03E-03
329	442.2520	31.74	445.2709	31.66	820.0	C25H34O5N2	C16H22O6N			Level 4	0.45	2.28E-04
331	443.3629	33.45	446.3818	33.38	887.4	C28H47O2N2	C19H35O3N			Level 4	0.33	1.95E-03
332	443.3629	42.64	446.3818	42.56	1276.7	C28H47O2N2	C19H35O3N			Level 4	0.27	1.13E-02

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
335	446.1896	29.28	449.2085	29.21	725.7	C29H24O2N3	C20H12O3N2				Level 4	0.30	2.26E-03
339	450.2751	18.40	456.3129	18.32	347.2	C27H36O3N3	C9H13O5N				Level 4	0.38	2.78E-06
341	456.2670	33.00	459.2859	32.95	869.8	C29H34O2N3	C20H22O3N2				Level 4	0.33	6.19E-04
343	456.2670	33.65	459.2859	33.55	895.1	C29H34O2N3	C20H22O3N2				Level 4	0.34	8.22E-03
348	521.4100	48.76	524.4289	48.74	1576.8	C34H53O2N2	C25H41O3N				Level 4	0.16	6.68E-03
349	521.4100	49.94	524.4289	49.91	1645.8	C34H53O2N2	C25H41O3N				Level 4	0.19	4.50E-03

Highlighted in red represents the carboxylated metabolites exhibit significant increase in the curcumin-treated HepG2 cells compared to control.

Highlighted in blue represents the carboxylated metabolites exhibit significant decrease in the curcumin-treated HepG2 cells compared to control.

Table S10. Carboxylated metabolites with significant difference between *R*-3-HBA and control.

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
13	223.1441	3.00	226.1630	2.98		C12H19N2O2	C3H7NO3	CLMD	Serine	302-84-1	Level 1	2.71	9.47E-03
14	233.1653	6.95	236.1842	6.90		C14H21N2O	C5H9NO2	CLMD	Proline	29795-82-2	Level 1	3.87	4.20E-04
17	236.1278	13.76	239.1467	13.71	205.9	C13H18O3N	C4H6O4	CLMD	Succinic acid	110-15-6	Level 1	8.49	3.61E-04
27	264.1592	16.37	267.1781	16.31	281.8	C15H22O3N	C6H10O4	CLMD	Adipic acid	124-04-9	Level 1	10.60	4.59E-04
32	293.1492	10.79	296.1681	10.73	12.3	C15H21O4N2	C6H9O5N	CLMD	<i>N</i> -Acetyl-aspartic acid	997-55-7	Level 1	3.93	5.10E-04
41	344.2946	42.03	347.3135	41.98	1248.2	C23H38ON	C14H26O2	CLMD	Tsuzuic acid	544-65-0	Level 1	2.45	9.82E-04
76	207.1492	14.83	210.1681	14.80	236.9	C12H19ON2	C3H7O2N	Metlin	Sarcosine	107-97-1	Level 3	3.19	6.15E-03
									2-Hydroxybutyric acid	3347-90-8			
									4-Hydroxybutyric acid	591-81-1			
									2-Hydroxy-2-methylpropanoic acid	594-61-6			
83	248.2003	28.21	251.2192	28.15	685.7	C16H26ON	C7H14O2	HMDB	2-Methylhexanoic acid	4536-23-6	Level 3	2.43	5.23E-03
									5-Methylhexanoic acid	628-46-6			
87	260.2012	25.93	263.2201	25.85	602.9	C17H26ON	C8H14O2	HMDB	(<i>E</i>)-4-Octenoic acid	18776-92-6	Level 3	2.50	2.58E-03
									2-Octenoic acid	1577-96-4			
									(3 <i>E</i>)-2-Propylpent-3-enoic acid				
									<i>cis</i> -5-Octenoic acid	41653-97-8			
									4-ene-Valproic acid				
									2-ene-Valproic acid				
89	264.1228	15.51	267.1417	15.47	256.8	C14H18O4N	C5H6O5	HMDB	Oxoglutaric acid	328-50-7	Level 3	2.22	1.43E-03
									3-Oxoglutaric acid	542-05-2			
100	288.2318	34.58	291.2507	18.95	932.8	C19H30ON	C10H18O2	HMDB	5-Decenoic acid	85392-03-6	Level 3	2.06	1.43E-03
									6-Decenoic acid	85392-04-7			
									3-Decenoic acid	15469-77-9			
									8-Methylnonenoate	59320-77-3			
									9-Decenoic acid	14436-32-9			
									Citronellie acid	502-47-6			

									<i>cis</i> -4-Decenoic acid	505-90-8			
									<i>trans</i> -Dec-2-enoic acid				
111	306.2063	24.38	309.2252	24.29	550.3	C18H28O3N	C9H16O4	HMDB	3-Methylsuberic acid		Level 3	3.97	1.25E-04
									2,4-Dimethylpimelic acid				
113	308.1490	16.52	311.1679	16.46	286.0	C16H22O5N	C7H10O6	HMDB	3-Dehydroquinic acid		Level 3	3.65	4.26E-06
114	308.1490	16.89	311.1679	16.83	296.8	C16H22O5N	C7H10O6	HMDB	2-Hydroxy-2-(2-oxopropyl)butanedioic acid		Level 3	3.90	2.57E-03
116	316.2632	37.77	319.2821	37.70	1063.6	C21H34ON	C12H22O2	HMDB	11-Dodecenoic acid	65423-25-8	Level 3	3.07	5.11E-03
									<i>trans</i> -Dodec-2-enoic acid				
									5Z-Dodecenoic acid	2430-94-6			
118	318.2791	39.62	321.2980	39.57	1141.7	C21H36ON	C12H24O2	Metlin	Isolauroic acid	2724-56-3	Level 3	2.85	5.66E-08
									2-Methyl-undecanoic acid	24323-25-9			
									3-Methyl-undecanoic acid	65781-38-6			
									4-Methyl-undecanoic acid				
									5-Methyl-undecanoic acid				
									6-Methyl-undecanoic acid				
									8-Methyl-undecanoic acid				
									9-Methyl-undecanoic acid				
119	320.2219	23.83	323.2408	23.79	531.6	C19H30O3N	C10H18O4	HMDB	2-Ethylsuberic acid	3971-33-3	Level 3	2.13	2.68E-02
									3-Methylazelaic acid				
									Heptylmalonic acid				
143	344.2946	42.53	347.3135	42.47	1271.5	C23H38ON	C14H26O2	HMDB	7Z-Tetradecenoic acid		Level 3	2.07	6.52E-07
									9E-Tetradecenoic acid				
									5Z-Tetradecenoic acid	5684-70-8			
									<i>trans</i> -Tetra-dec-2-enoic acid				
									Myristoleic acid	544-64-9			
147	346.3104	44.09	349.3293	44.01	1342.9	C23H40ON	C14H28O2	HMDB	10-Methyltridecanoic acid		Level 3	2.18	1.69E-04
									2,6,10-Trimethylundecanoic acid	1115-94-2			
									12-Methyltridecanoic acid	2724-57-4			
151	349.2095	19.37	352.2284	19.33	379.8	C19H29O4N2	C10H17O5N	HMDB	<i>N</i> -Isovalerylglutamic acid	80154-63-8	Level 3	3.23	6.85E-03
									Suberylglycine	60317-54-6			

154	351.2065	23.11	357.2443	23.02	507.4	C22H27O2N2	C4H4O4	HMDB	Maleic acid	110-16-7	Level 3	2.18	1.65E-03
170	367.2381	25.06	373.2759	24.95	573.2	C23H31O2N2	C5H8O4	HMDB	Methylsuccinic acid	498-21-5	Level 3	2.29	4.78E-02
									Ethylmalonic acid	601-75-2			
181	381.2538	25.59	387.2916	25.49	591.4	C24H33O2N2	C6H10O4	HMDB	Adipic acid	124-04-9	Level 3	2.09	3.55E-03
									Monomethyl glutaric acid	1501-27-5			

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
181	381.2538	25.59	387.2916	25.49	591.4	C24H33O2N2	C6H10O4	HMDB	Methylglutaric acid	626-51-7	Level 3	2.09	3.55E-03
									2-Methylglutaric acid	617-62-9			
									4-Ethoxy-4-oxobutanoic acid				
191	388.3574	50.39	391.3763	50.34	1673.2	C26H46ON	C17H34O2	HMDB	11-Methylhexadecanoic acid		Level 3	4.95	1.44E-03
									15-Methylhexadecanoic acid				
									(<i>S</i>)-14-Methylhexadecanoic acid	5746-59-8			
198	390.3367	37.83	393.3556	37.79	1066.3	C25H44O2N	C16H32O3	HMDB	7-Hydroxyhexadecanoic acid	16899-02-8	Level 3	2.20	1.82E-03
									12-Hydroxyhexadecanoic acid	83646-62-2			
									10-Hydroxyhexadecanoic acid	23048-75-1			
									11-Hydroxyhexadecanoic acid	502-75-0			
									5-Hydroxyhexadecanoic acid	17369-53-8			
									9-Hydroxyhexadecanoic acid	17833-52-2			
									13-Hydroxyhexadecanoic acid	59642-39-6			
									8-Hydroxyhexadecanoic acid	83921-07-7			
									6-Hydroxyhexadecanoic acid	58763-57-8			
									3-Hydroxyhexadecanoic acid	83780-74-9			
									2-Hydroxyhexadecanoic acid	16452-52-1			
206	396.3261	44.27	399.3450	44.24	1350.8	C27H42ON	C18H30O2	HMDB	γ-Linolenic acid	506-26-3	Level 3	2.89	4.62E-02
208	396.3261	45.31	399.3450	45.26	1397.6	C27H42ON	C18H30O2	HMDB	Linolenelaidic acid	28290-79-1	Level 3	2.99	2.86E-03
211	399.1915	15.91	402.2104	15.87	268.2	C22H27O5N2	C13H15O6N	HMDB	4-Hydroxyphenylacetylglutamic acid	1029120-37-3	Level 3	3.10	4.00E-03
282	208.1331	2.51	211.1520	2.49		C12H18O2N	C3H6O3				Level 4	2.34	4.09E-04

283	218.1174	13.90	221.1363	13.83	209.9	C13H16O2N	C4H4O3				Level 4	7.15	6.40E-04
285	293.1492	11.63	296.1681	11.57	68.9	C15H21O4N2	C6H9O5N				Level 4	2.81	4.79E-03
294	335.1964	17.06	338.2153	17.01	302.0	C18H27O4N2	C9H15O5N				Level 4	3.77	2.09E-02
295	335.1964	17.39	338.2153	17.37	313.3	C18H27O4N2	C9H15O5N				Level 4	2.12	1.80E-02
296	338.1777	12.64	341.1966	12.61	137.8	C21H24O3N	C12H15O4				Level 4	2.39	2.11E-02
297	339.2430	30.47	342.2619	30.40	771.0	C22H31ON2	C13H19O2N				Level 4	2.55	1.94E-02
303	353.1860	18.55	356.2049	13.28	352.3	C21H25O3N2	C12H13O4N				Level 4	5.72	5.61E-03
360	624.3955	44.05	627.4144	43.98	1340.9	C40H52O4N2	C31H40O5N				Level 4	2.12	1.08E-02
402	546.4105	51.65	549.4294	51.61	1741.6						Level 5	2.84	3.26E-04
7	207.1492	4.72	210.1681	4.64		C12H19ON2	C3H7O2N	CLMD	Alanine	302-72-7	Level 1	0.23	4.89E-03
16	235.1805	11.25	238.1994	11.20	43.5	C14H23ON2	C5H11O2N	CLMD	Valine	516-06-3	Level 1	0.31	2.89E-04
18	237.1602	4.62	240.1791	4.58		C13H9NO3	C4H9NO3	CLMD	Threonine	72-19-5	Level 1	0.27	9.74E-10
23	249.1961	13.78	252.2150	13.72	206.4	C15H25ON2	C6H13O2N	CLMD	Leucine	328-39-2	Level 1	0.32	1.51E-03
24	249.1961	14.01	252.2150	13.96	213.1	C15H25ON2	C6H13O2N	CLMD	Isoleucine	443-79-8	Level 1	0.33	1.54E-03
29	276.2322	33.77	279.2511	33.69	900.0	C18H30ON	C9H18O2	CLMD	Pelargonic acid	112-05-0	Level 1	0.37	2.34E-04
30	283.1805	15.83	286.1994	15.76	266.0	C18H23ON2	C9H11O2N	CLMD	Phenylalanine	150-30-1	Level 1	0.29	4.70E-04
33	299.1754	11.83	302.1943	11.77	82.8	C18H23O2N2	C9H11O3N	CLMD	Tyrosine	556-03-6	Level 1	0.32	2.22E-03
35	306.2063	21.91	309.2252	21.83	466.5	C18H28O3N	C9H16O4	CLMD	Azelaic acid	123-99-9	Level 1	0.16	2.13E-05
39	322.1914	16.52	325.2103	16.47	286.0	C20H24ON3	C11H12O2N2	CLMD	Tryptophan	54-12-6	Level 1	0.33	1.07E-03
47	390.3367	36.54	393.3556	36.51	1012.6	C25H44O2N	C16H32O3	CLMD	16-Hydroxyhexadecanoic acid	506-13-8	Level 1	0.34	4.11E-04
53	418.3679	48.65	421.3868	48.57	1570.9	C27H48O2N	C18H36O3	CLMD	3-Hydroxyoctadecanoic acid		Level 1	0.42	1.50E-03
70	305.2208	18.80	308.2397	18.75	360.7	C18H29O2N2	C9H17O3N	HMDB	8-Amino-7-oxononanoic acid	682799-71-9	Level 2	0.42	1.14E-04
71	429.3475	41.48	432.3664	41.45	1222.8	C27H45O2N2	C18H33O3N	HMDB	2-(14-Methylpentadec-11-enoylamino)acetic acid		Level 2	0.42	2.53E-02
72	431.3630	44.70	434.3819	44.66	1370.1	C27H47O2N2	C18H35O3N	HMDB	Palmitoylglycine	158305-64-7	Level 2	0.18	1.57E-02
73	450.2751	22.91	456.3129	22.82	500.7	C27H36O3N3	C9H13O5N	Metlin	N-Succinyl proline	63250-32-8	Level 2	0.37	9.65E-05
74	459.3945	48.41	462.4134	48.38	1558.1	C29H51O2N2	C20H39O3N	HMDB	Glycine stearamide	6333-54-6	Level 2	0.16	2.06E-02
75	521.4100	48.62	524.4289	48.55	1569.3	C34H53O2N2	C25H41O3N	HMDB	N-Palmitoyl-phenylalanine		Level 2	0.46	1.89E-03
78	233.1653	22.06	236.1842	22.00	471.6	C14H21N2O	C5H9NO2	HMDB	4-Amino-2-methylenebutanoic acid	65370-67-4	Level 3	0.45	2.65E-03
80	247.1441	11.96	250.1630	11.92	91.6	C14H19O2N2	C5H7O3N	Metlin	Pyroline hydroxycarboxylic acid	22573-88-2	Level 3	0.33	9.76E-06
									Pyroglutamic acid	98-79-3			

									<i>N</i> -Acryloylglycine	24599-25-5			
									Pyrroline hydroxycarboxylic acid	22573-88-2			
									4-Oxoproline				
									1-Pyrroline-4-hydroxy-2-carboxylate	9054-77-7			
									2-Pyrrolidone-5-carboxylic acid	4042-36-8			
88	262.2163	30.05	265.2352	29.98	755.0	C17H28ON	C8H16O2	HMDB	6-Methylheptanoic acid	929-10-2	Level 3	0.17	2.82E-04
									2-Methylenanthic acid	1188-02-9			
									2-Ethylhexanoic acid	149-57-5			
									Valproic acid	99-66-1			
90	264.1592	18.01	267.1781	17.96	334.0	C15H22O3N	C6H10O4	HMDB	4-Ethoxy-4-oxobutanoic acid	1501-27-5	Level 3	0.12	5.44E-03

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
91	264.1592	18.29	267.1781	18.25	343.5	C15H22O3N	C6H10O4	HMDB	2-Methylglutaric acid	617-62-9	Level 3	0.15	2.24E-04
									Methylglutaric acid	626-51-7			
									Monomethyl glutaric acid	1501-27-5			
93	265.1547	11.70	268.1736	11.65	74.0	C14H21O3N2	C5H9O4N	HMDB	DL-Glutamic acid	617-65-2	Level 3	0.45	4.61E-03
94	270.1487	11.05	273.1676	11.00	29.9	C17H20O2N	C8H8O3	HMDB	4-Hydroxy-3-methylbenzoic acid	499-76-3	Level 3	0.43	3.12E-04
									2-Methoxybenzoic acid	579-75-9			
									Mandelic acid	90-64-2			
									3-Methoxybenzoic acid	586-38-9			
102	290.2474	35.70	293.2663	35.60	978.3	C19H32ON	C10H20O2	HMDB	4-Methylnonanoic acid	45019-28-1	Level 3	0.49	1.81E-02
									4-Ethyl octanoic acid	16493-80-4			
104	291.2046	20.15	294.2235	20.11	397.4	C17H27O2N2	C8H15O3N	HMDB	Hexanoylglycine	24003-67-6	Level 3	0.45	5.99E-04
121	320.2306	13.42	323.2495	13.36	190.6	C18H30O2N3	C9H18O3N2	Metlin	Alanyl-Isoleucine		Level 3	0.49	7.38E-03
									Alanyl-Leucine				
									Isoleucyl-Alanine				
									Leucyl-Alanine	7298-84-2			
124	321.2172	20.04	324.2361	20.01	402.4	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3	0.43	8.05E-03

126	321.2172	20.58	324.2361	20.53	420.9	C18H29O3N2	C9H17O4N	Metlin	L-Glutamic acid n-butyl ester	152726-66-4	Level 3	0.37	8.38E-03
132	336.2255	13.17	339.2444	13.12	173.6	C18H30O3N3	C9H18O4N2	HMDB	Seriny-L-leucine		Level 3	0.44	1.12E-02
									Seriny-L-iso-leucine				
									Isoleucyl-Serine				
									Leucyl-Serine				
									Threoniny-L-valine				
									Valyl-Threonine				
									Lysopine				
140	340.2019	14.64	343.2208	14.61	231.5	C20H26O2N3	C11H14O3N2	HMDB	Phenylalanylglycine	721-90-4	Level 3	0.34	1.09E-05
									Glycyl-DL-phenylalanine				
148	346.3104	44.86	349.3293	44.79	1377.4	C23H40O2N	C14H28O2	HMDB	10-Methyltridecanoic acid		Level 3	0.45	6.87E-04
									2,6,10-Trimethylundecanoic acid	1115-94-2			
									12-Methyltridecanoic acid	2724-57-4			
167	360.3261	46.84	363.3450	46.79	1474.9	C24H42O2N	C15H30O2	Metlin	12-Methyl myristic acid	5502-94-3	Level 3	0.48	4.52E-02
									Isopentadecylic acid				
									4,12-Dimethyl-tridecanoic acid				
									2-Methyl-tetradecanoic acid	7620-57-7			
									3-Methyl-tetradecanoic acid				
									11-Methyl-tetradecanoic acid				
									2,6,10-Trimethyldodecanoic acid	168254-98-6			
									3,5-Dimethyltridecanoic acid				
176	374.3417	48.62	377.3606	48.54	1569.3	C25H44O2N	C16H32O2	HMDB	Isopalmitic acid	4669-02-7	Level 3	0.44	6.45E-03
									Trimethyltridecanoic acid	10339-73-8	Level 3		
177	375.3006	27.84	378.3195	17.81	672.3	C23H39O2N2	C14H27O3N	HMDB	N-Lauroylglycine		Level 3	0.26	7.39E-03
178	375.3006	36.02	378.3195	35.97	991.1	C23H39O2N2	C14H27O3N	HMDB	N-Lauroylglycine		Level 3	0.42	1.16E-02
182	381.2538	26.89	387.2916	26.78	637.8	C24H33O2N2	C6H10O4	HMDB	Adipic acid	124-04-9	Level 3	0.39	1.47E-04
									Monomethyl glutaric acid	1501-27-5	Level 3		
									Methylglutaric acid	626-51-7	Level 3		
									2-Methylglutaric acid	617-62-9	Level 3		
									4-Ethoxy-4-oxobutanoic acid				

184	382.2489	17.91	385.2678	17.87	330.7	C23H32O2N3	C14H20O3N2	Metlin	Valyl-Phenylalanine		Level 3	0.47	1.52E-02
									Phenylalanyl-Valine	3918-92-1	Level 3		
203	396.2646	19.03	399.2835	18.95	368.4	C24H34O2N3	C15H22O3N2	HMDB	Leucyl-Phenylalanine	3063-05-6	Level 3	0.43	4.30E-03
204	396.2646	20.55	399.2835	20.47	420.0	C24H34O2N3	C15H22O3N2	HMDB	Isoleucyl-Phenylalanine		Level 3	0.44	1.85E-02
216	410.2438	21.39	416.2816	21.32	448.7	C24H32O3N3	C6H9O5N	HMDB	<i>N</i> -Formyl-L-glutamic acid	1681-96-5	Level 3	0.30	8.68E-04
									2-Amino-3-oxohexanedioic acid				
240	422.2074	25.72	425.2263	20.14	595.6	C24H28O4N3	C15H16O5N2	Metlin	Indole-3-acetylglutamic acid	57105-48-3	Level 3	0.15	2.55E-02
241	422.2439	23.17	428.2817	23.09	509.4	C25H32O3N3	C7H9O5N	Metlin	<i>N</i> -Acryloyl aspartic acid	72064-86-9	Level 3	0.43	1.28E-03
									α -(<i>N</i> -Acetylaminoethylene)succinic acid				
257	445.3790	44.45	448.3979	44.37	1358.9	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3	0.33	2.29E-04
258	445.3790	45.82	448.3979	45.78	1423.0	C28H49O2N2	C19H37O3N	Metlin	<i>N</i> -Palmitoyl alanine		Level 3	0.16	6.74E-03
268	459.3945	45.74	462.4134	45.70	1419.1	C29H51O2N2	C20H39O3N	HMDB	<i>N</i> -Palmitoyl GABA		Level 3	0.30	1.71E-03
266	471.3945	36.96	474.4134	36.92	1030.1	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Palmitoyl proline		Level 3	0.26	6.89E-03
269	471.3945	49.41	474.4134	49.38	1613.5	C30H51O2N2	C21H39O3N	Metlin	<i>N</i> -Oleoyl alanine		Level 3	0.23	1.50E-02
274	499.4259	40.02	502.4448	39.98	1158.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3	0.27	6.22E-03

Continued table

No.	MPEA labeled <i>m/z</i>	Rt (min) (MPEA-labeled)	<i>d</i> ₅ -MPEA labeled <i>m/z</i>	Rt (min) (<i>d</i> ₅ -MPEA-labeled)	RI	Molecular	Unlabeled	Database	Name	CAS	Identification	Fold change (curcumin/control)	P value
275	499.4259	48.63	502.4448	48.60	1569.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3	0.35	1.17E-03
276	499.4259	48.79	502.4448	48.75	1578.5	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3	0.35	1.17E-03
277	499.4259	49.94	502.4448	49.90	1645.8	C32H55O2N2	C23H43O3N	Metlin	<i>N</i> -Stearoyl proline		Level 3	0.21	2.79E-03
278	501.4414	51.59	504.4603	51.56	1738.4	C32H57O2N2	C23H45O3N	Metlin	<i>N</i> -Stearoyl valine		Level 3	0.19	4.21E-03
281	549.4412	52.00	552.4601	51.96	1759.2	C36H57O2N2	C27H45O3N	HMDB	<i>N</i> -Stearoyl phenylalanine		Level 3	0.17	7.19E-03
305	358.1570	20.62	361.1759	20.58	422.5	C22H20O2N3	C13H12O3N2				Level 4	0.30	1.68E-02
308	361.2850	26.01	364.3039	25.95	606.0	C22H37O2N2	C13H25O3N				Level 4	0.32	2.59E-02
309	403.3319	40.52	406.3508	40.46	1179.6	C25H43O2N2	C16H31O3N				Level 4	0.29	7.95E-03
316	421.2595	18.09	424.2784	18.02	336.8	C27H35O3N	C18H23O4				Level 4	0.33	3.07E-05
317	421.2595	18.96	424.2784	18.91	366.2	C27H35O3N	C18H23O4				Level 4	0.42	1.13E-02
318	429.3475	41.78	432.3664	41.71	1236.5	C27H45O2N2	C18H33O3N				Level 4	0.41	9.27E-03

319	429.3475	42.06	432.3664	41.98	1249.6	C27H45O2N2	C18H33O3N	Level 4	0.34	3.54E-02
324	430.2486	20.22	433.2675	20.16	408.8	C27H32O2N3	C18H20O3N2	Level 4	0.44	3.56E-03
331	443.3629	33.45	446.3818	33.38	887.4	C28H47O2N2	C19H35O3N	Level 4	0.44	7.11E-04
332	443.3629	42.64	446.3818	42.56	1276.7	C28H47O2N2	C19H35O3N	Level 4	0.36	1.76E-02
335	446.1896	29.28	449.2085	29.21	725.7	C29H24O2N3	C20H12O3N2	Level 4	0.28	2.34E-03
339	450.2751	18.40	456.3129	18.32	347.2	C27H36O3N3	C9H13O5N	Level 4	0.43	3.70E-03
341	456.2670	33.00	459.2859	32.95	869.8	C29H34O2N3	C20H22O3N2	Level 4	0.44	2.65E-03
343	456.2670	33.65	459.2859	33.55	895.1	C29H34O2N3	C20H22O3N2	Level 4	0.46	9.29E-03
348	521.4100	48.76	524.4289	48.74	1576.8	C34H53O2N2	C25H41O3N	Level 4	0.19	7.20E-03
349	521.4100	49.94	524.4289	49.91	1645.8	C34H53O2N2	C25H41O3N	Level 4	0.21	3.73E-03

Highlighted in red represents the carboxylated metabolites exhibit significant increase in the *R*-3-hydroxybutyric acid-treated HepG2 cells compared to control.

Highlighted in blue represents the carboxylated metabolites exhibit significant decrease in the *R*-3-hydroxybutyric acid-treated HepG2 cells compared to control.

REFERENCES:

- [S1] Elpa, D. P.; Prabhu, G. R. D.; Wu, S. P.; Tay, K. S.; Urban, P. L. *Talanta* 2020, 208, 120304.
- [S2] Zheng, F.; Zhao, X.; Zeng, Z.; Wang, L.; Lv, W.; Wang, Q.; Xu, G. *Nat. Protoc.* 2020, 1-19.
- [S3] Higashi, T.; Ogawa, S. *J. Pharmaceut. Biomed.* 2016, 130, 181-193.
- [S4] Tian, H.; Li, S.; Wen, H.; Zhang, X.; Li, J. *J. Chromatogr. A* 2020, 1614, 460717.
- [S5] Yuan, M.; Kremer, D. M.; Huang, H.; Breitkopf, S. B.; Ben-Sahra, I.; Manning, B. D.; Lyssiotis, C. A.; Asara, J. M. *Nat. Protoc.* 2019, 14, 313-330.
- [S6] Lindsay, K. L.; Hellmuth, C.; Uhl, O.; Buss, C.; Wadhwa, P. D.; Koletzko, B.; Entringer, S. *PloS one* 2015, 10, e0145794.
- [S7] Bollinger, J. G.; Thompson, W.; Lai, Y.; Oslund, R. C.; Hallstrand, T. S.; Sadilek, M.; Turecek, F.; Gelb, M. H. *Anal. Chem.* 2010, 82, 6790-6796.
- [S8] Zhu, M.; Zhang, C.; Nwachukwu, J. C.; Srinivasan, S.; Cavett, V.; Zheng, Y.; Carlson, K. E.; Dong, C.; Katzenellenbogen, J. A.; Nettles, K. W.; Zhou, H. B. *Org. Biomol. Chem.* 2012, 10, 8692-8700.
- [S9] Khalil, I. M.; Barker, D.; Copp, B. R. *J. Org. Chem.* 2016, 81, 282-289.