Supporting Information

Discovery of FAHFA-Containing Triacylglycerols and Their Metabolic Regulation

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Supporting Information

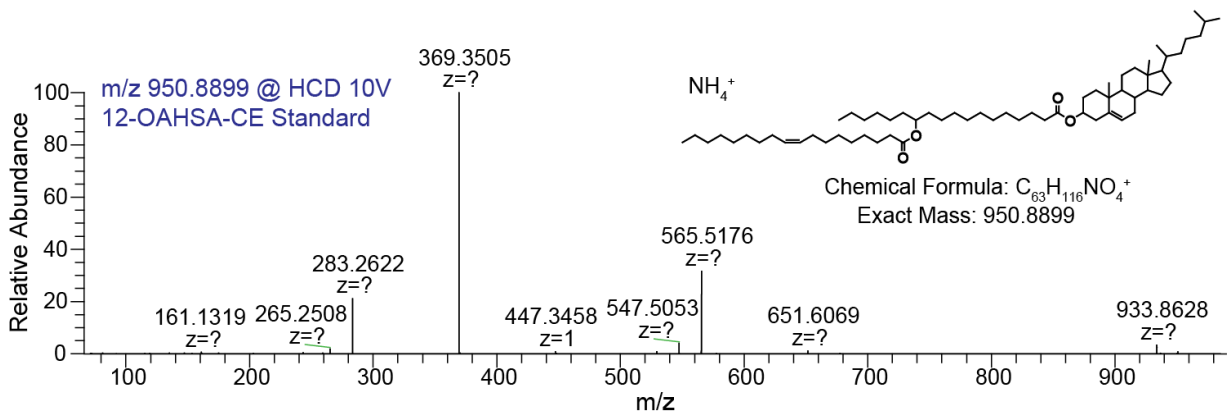


Figure S1. High energy collisional dissociation (HCD) spectrum of the ammonium adduct of synthetic 12-OAHSA-CE.

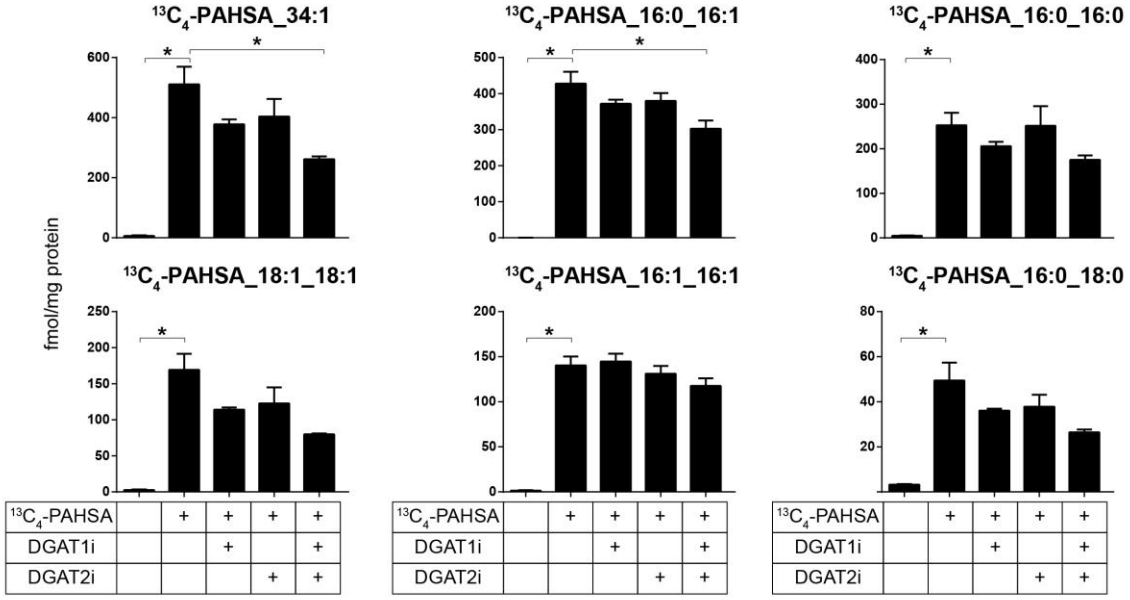


Figure S2. Various $^{13}C_4$-PAHSA-containing triacylglycerols with different combination of acyl chains were detected in 3T3-L1 adipocytes treated with 20 μM $^{13}C_4$-PAHSA for 24 hours. The cells were cultured in the absence or presence of DGAT1 inhibitor (DGAT1i) or/and DGAT2 inhibitor (DGAT2i). Quantification results were normalized to protein concentration. N = 3, *p < 0.05, data are means ± SEM.

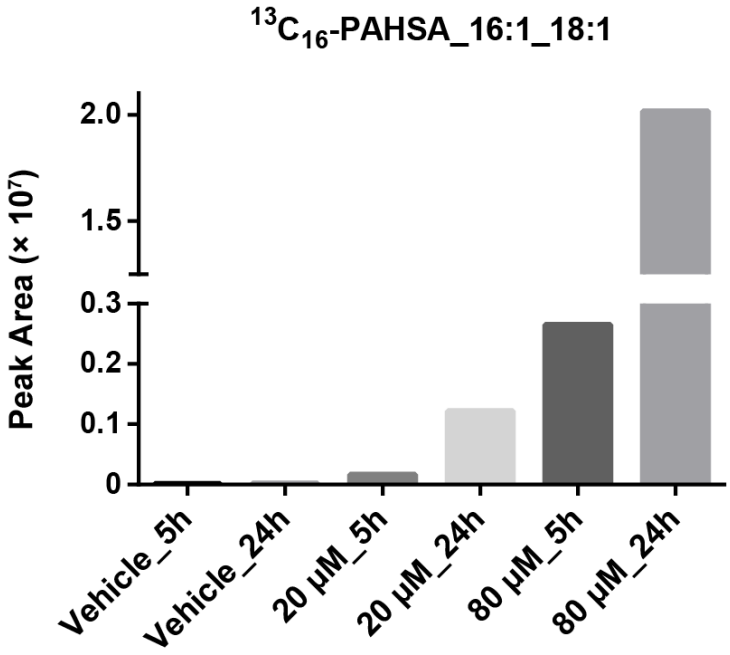


Figure S3. Differentiated 3T3-L1 adipocytes were treated with vehicle, 20 µM $^{13}C_{16}$-PAHSA, or 80 µM $^{13}C_{16}$-PAHSA for 5 or 24 hours. $^{13}C_{16}$-PAHSA_16:1_18:1-TG level was quantified using the transition corresponding to the loss of $^{13}C_{16}$-PAHSA plus ammonia (m/z 1149.1 > 577.5). N = 1.

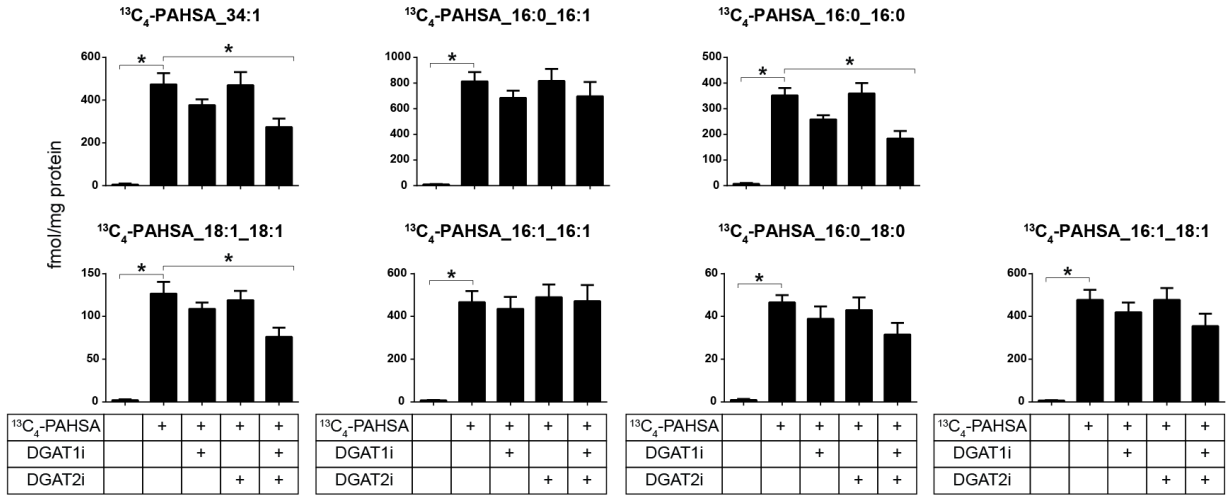


Figure S4. Levels of $^{13}C_4$-PAHSA-containing triacylglycerols with different acyl chains in 3T3-L1 adipocytes treated with 80 μM $^{13}C_4$-PAHSA in the absence or presence of 5 μM DGAT1 inhibitor (DGAT1i) or/and 5 μM DGAT2 inhibitor (DGAT1i) for 3 hours.

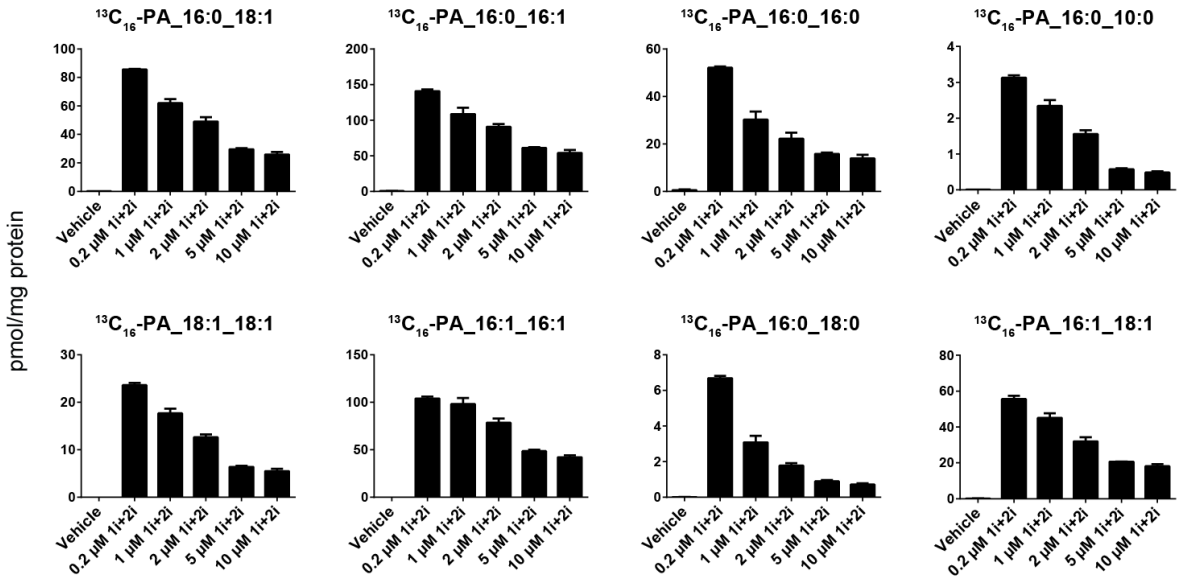


Figure S5. Levels of $^{13}C_{16}$-PA-containing triacylglycerols with different acyl chains in 3T3-L1 adipocytes treated with 80 μM $^{13}C_{16}$-PA in the presence of both DGAT1 inhibitor (1i) and DGAT2 inhibitor (1i) at various concentrations for 3 hours. For example, 5 μM 1i+2i represents 5 μM DGAT1 inhibitor and 5 μM DGAT2 inhibitor. Vehicle represents the cells were not treated with $^{13}C_{16}$-PA nor inhibitors.

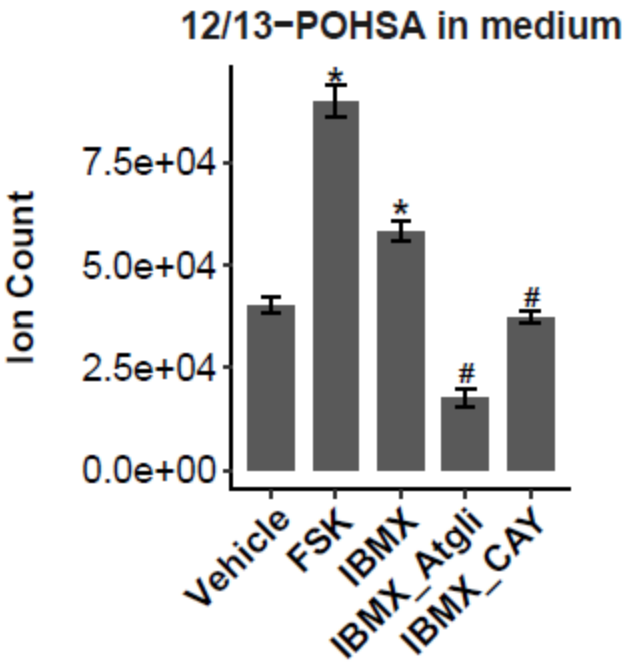


Figure S6. Quantification of 12/13-POHSA released into medium from 3T3-L1 adipocytes. N = 3, *p < 0.05 versus vehicle, #p < 0.05 versus IBMX, data are means ± SEM.

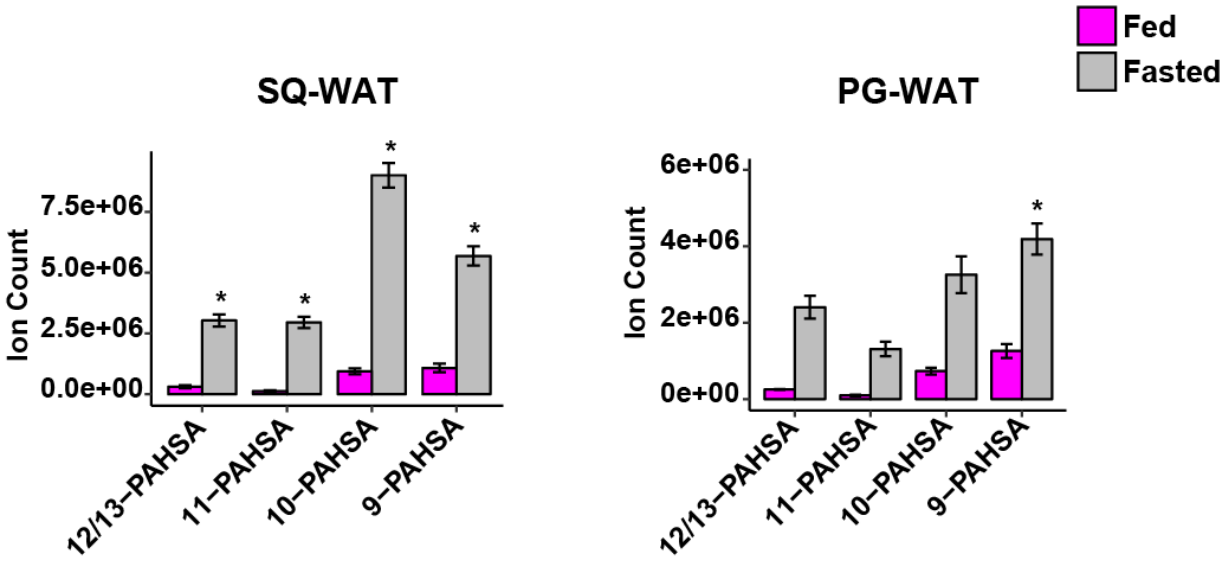


Figure S7. Nonesterified FAHFA levels in SQ-WAT and PG-WAT of fed or fasted mice. Mice were ad lib fed or fasted for 18 hours before they were sacrificed for tissue collection. N = 3-5, *p < 0.05, data are means ± SEM.

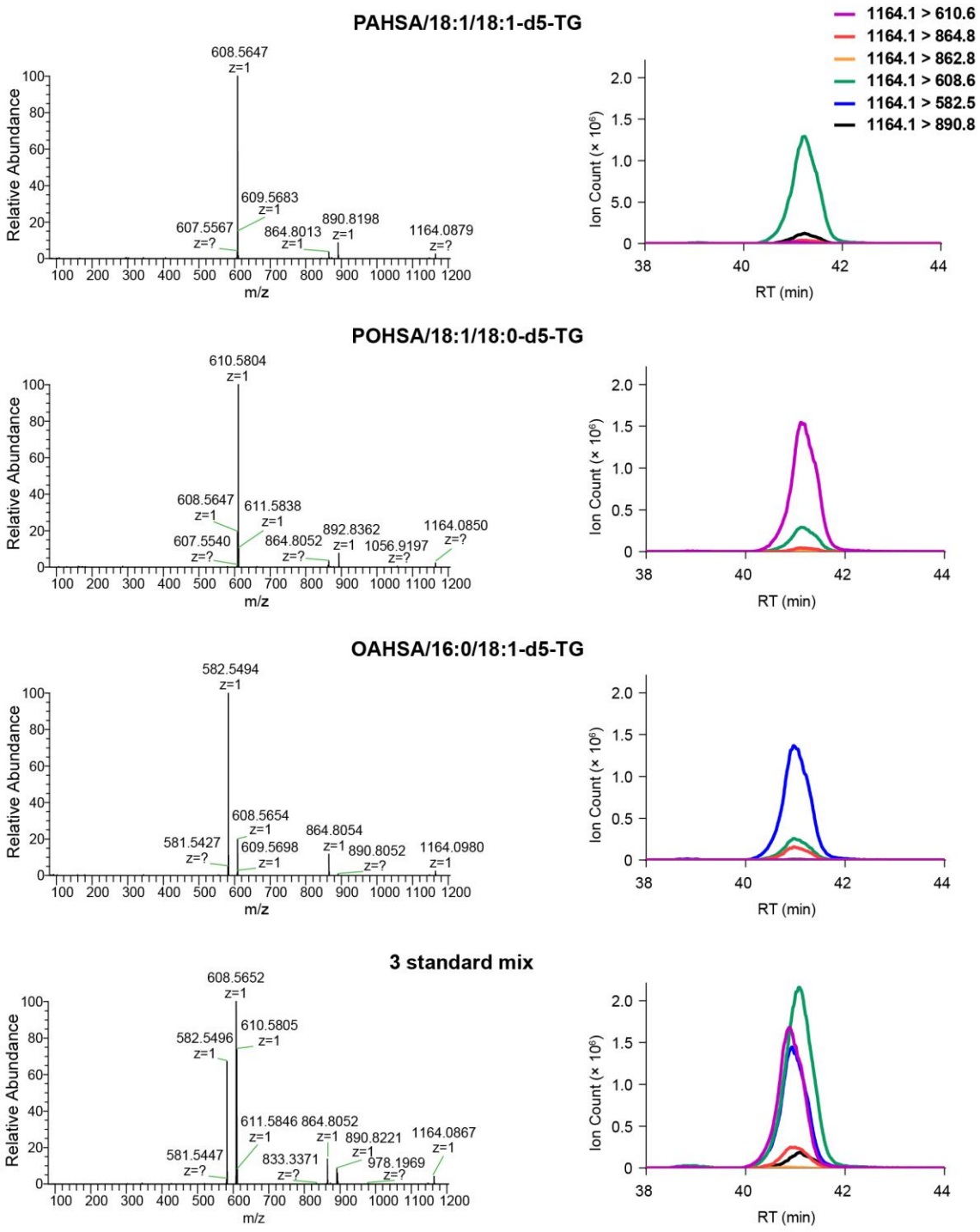


Figure S8. Representative MS/MS spectra and extracted ion chromatograms for multiple transitions of synthetic PAHSA/18:1/18:1-d5-TG, POHSA/18:1/18:0-d5-TG, OAHSA/16:0/18:1-d5-TG, and their 1:1:1 mixture. d5-TG, triacylglycerols with five hydrogen atoms on the glycerol backbone replaced by deuterium atoms.

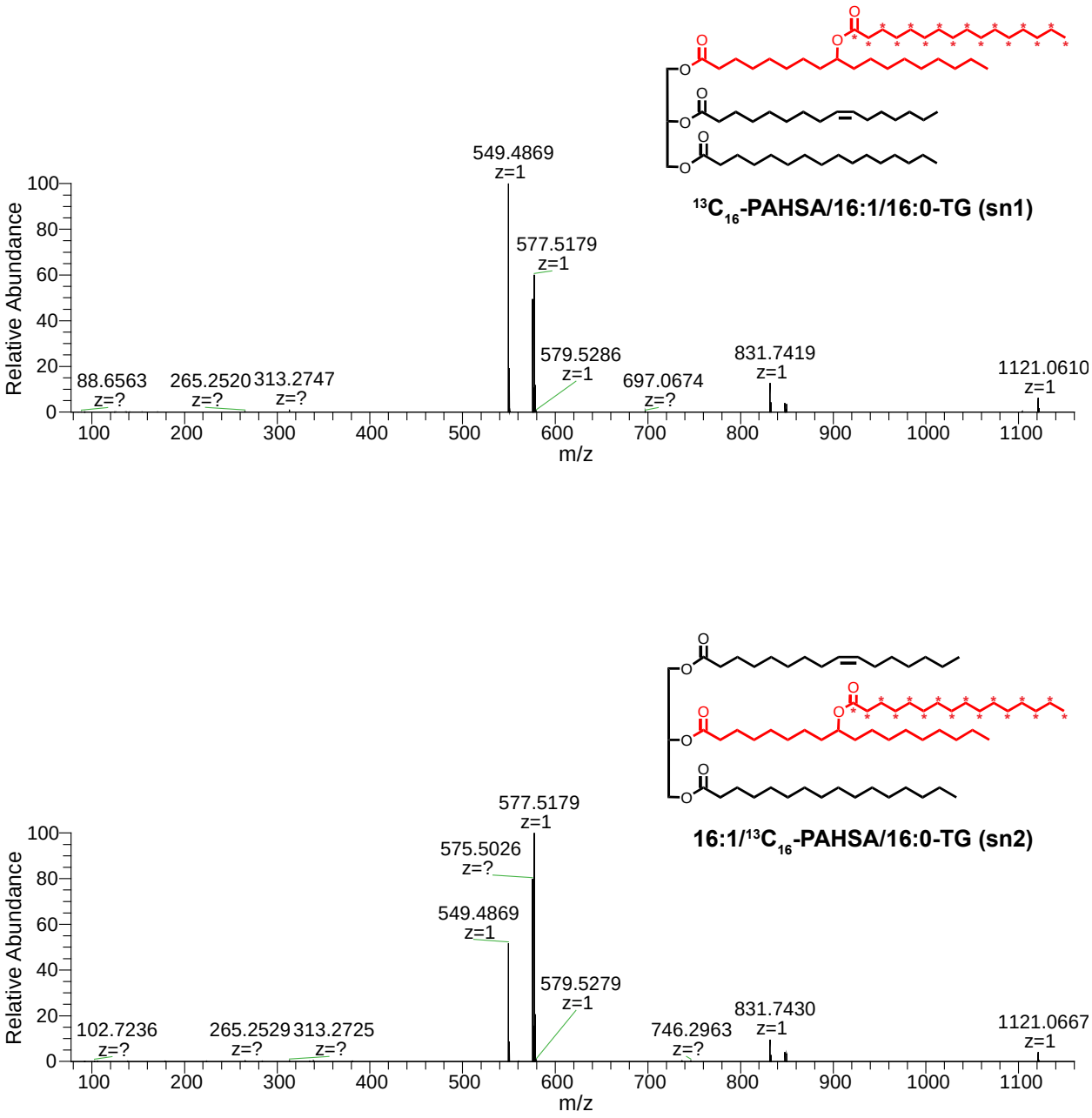


Figure S9. Relative intensity of fragment ions varies between $^{13}C_{16}$-PAHSA/16:1/16:0-TG and 16:1/$^{13}C_{16}$-PAHSA/16:0-TG. The $^{13}C_{16}$-PAHSA moiety is shown in red. Heavy labeled carbon atoms are highlighted by asterisks. When $^{13}C_{16}$-PAHSA is at sn1 position, the most intense fragment ion corresponds to the loss of $^{13}C_{16}$-PAHSA (m/z 549.4869). When $^{13}C_{16}$-PAHSA is at sn2 position, the most intense fragment corresponds to the simultaneous loss of the 16:1 moiety from the glycerol backbone and the $^{13}C_{16}$-PA moiety from $^{13}C_{16}$-PAHSA (m/z 577.5179).

FAHFA-TGs and 12-OAHSA-CE Synthetic Procedures

General Information

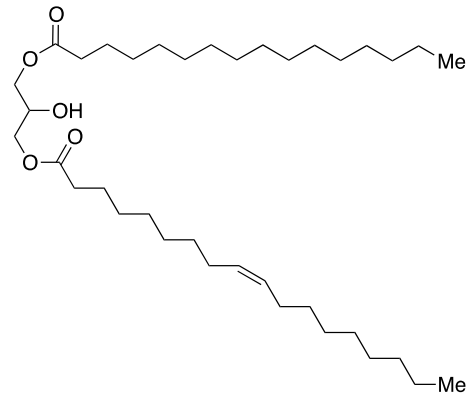
All reactions were performed in flame- or oven-dried glassware sealed with rubber septa and under nitrogen atmosphere, unless otherwise indicated. Air- and/or moisture-sensitive liquids or solutions were transferred by cannula or syringe. Organic solutions were concentrated by rotary evaporator at 30 millibar with the water bath heated to not more than 50°C, unless specified otherwise. Tetrahydrofuran (THF), diethyl ether (Et_2O), and dichloromethane (DCM) were purified with a Pure-Solve MD-5 Solvent Purification System (Innovative Technology). Thin-layer chromatography (TLC) was performed using 0.2 mm commercial silica gel plates (silica gel 60, F254, EMD Chemicals) and visualized with an aqueous potassium permanganate (KMnO4) stain. Nuclear Magnetic Resonance (NMR) spectra were recorded on a Varian (^{1}H NMR: $CDCl_3$ (7.26) at 600 MHz; ^{13}C NMR: $CDCl_3$ (77.16) at 151 MHz). All spectra were taken in $CDCl_3$ with shifts reported in parts per million (ppm) referenced to protium or carbon of the solvent (7.26 or 77.16, respectively). Coupling constants are reported in Hertz (Hz). Data for ^{1}H-NMR are reported as follows: chemical shift (ppm, reference to protium; s = single, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). High Resolution Mass Spectra (HRMS) were acquired on an Agilent 6230 High Resolution time-of-flight mass spectrometer and reported as m/z for the molecular ion [M+Na]+, [M+H]+.

General Procedures

General procedure A: To a stirred solution of the starting alcohol (1 equiv.) in dichloromethane (1.5 mL/mmol alcohol) at 23 °C was added the appropriate acid (1 equiv.) in neat form and the reaction was stirred for 5 minutes. Solid DMAP (4.0 equiv.) and solid EDC (1.2 equiv.) were simultaneously added in a single portion to the reaction mixture. The mixture was stirred for 6 hours then diluted with dichloromethane (4 mL/mmol alcohol) and 10% w/w sodium chloride solution (2 mL/mmol alcohol). The layers, were extracted with dichloromethane (4 mL/mmol alcohol) twice and the combined organic extracts were dried over sodium sulfate, filtered and concentrated in vacuo.

General procedure B: To a stirred solution of the starting alcohol (1 equiv.) in dichloromethane (1.5 mL/mmol alcohol) at 23 °C was added the appropriate acid (1.02 equiv.) in neat form and the reaction was stirred for 5 minutes. Solid DMAP (3.0 equiv.) and EDC (1.2 equiv.) were simultaneously added in a single portion to the reaction mixture. The mixture was stirred for 18 hours then diluted with dichloromethane (4 mL/mmol alcohol) and 10% w/w sodium chloride solution (2 mL/mmol alcohol). The layers, were extracted with dichloromethane (4 mL/mmol alcohol) twice and the combined organic extracts were dried over sodium sulfate, filtered and concentrated in vacuo.

2-Hydroxy-3-(palmitoyloxy) propyl oleate (**1**)



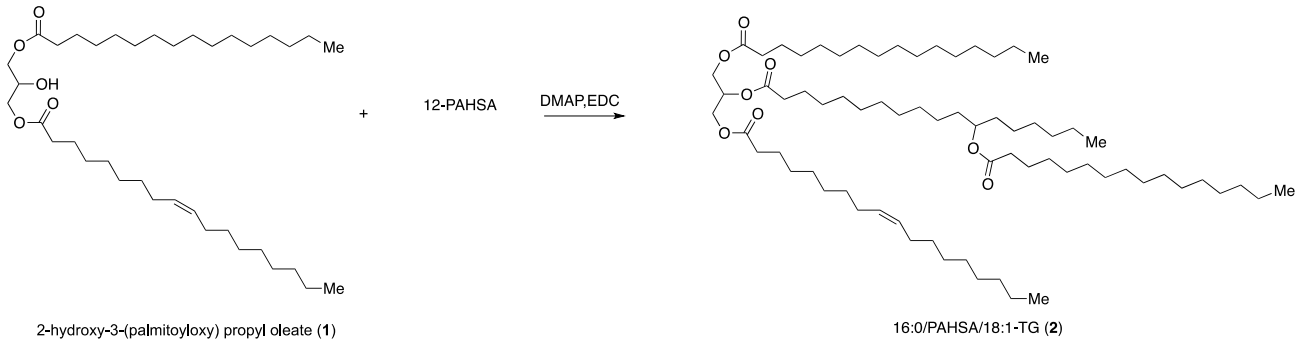
2-hydroxy-3-(palmitoyloxy) propyl oleate (**1**)

2,3-Dihydroxypropyl palmitate: Glycerol (37 mg, 0.390 mmol) and palmitic acid (100 mg, 0.390 mmol) were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (50 : 50) provided 2,3-dihydroxypropyl palmitate (84 mg, 0.253 mmol, 65%).

2-Hydroxy-3-(palmitoyloxy) propyl oleate (1): Neat 2,3-dihydroxypropyl palmitate (80 mg, 0.242 mmol) and oleic acid (70 mg, 0.247 mmol) were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (12 : 88) yielded 2-hydroxy-3-(palmitoyloxy) propyl oleate (**1**) (76 mg, 0.128 mmol, 53%).

$\mathbf{R_f}$ = 0.6 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.38 – 5.30 (m, 2H), 4.18 (dd, *J* = 11.5, 4.2 Hz, 2H), 4.15 – 4.11 (m, 2H), 4.11 – 4.06 (m, 1H), 2.44 (d, *J* = 4.5 Hz, 1H), 2.35 (t, *J* = 7.6 Hz, 4H), 2.05 – 1.98 (m, 4H), 1.66 – 1.59 (m, 4H), 1.35 – 1.24 (m, 44H), 0.88 (t, *J* = 7.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.09, 174.06, 130.13, 129.83, 68.45, 65.14, 34.22, 34.20, 32.05, 32.03, 29.89, 29.82, 29.81, 29.78, 29.73, 29.65, 29.58, 29.49, 29.45, 29.38, 29.28, 29.25, 29.21, 27.33, 27.28, 25.00, 24.99, 22.82, 14.26. **HRMS**: *m/z*: calcd for $C_{37}H_{70}O5Na$: 617.5115; found 617.5115 $[M + Na]^+$.

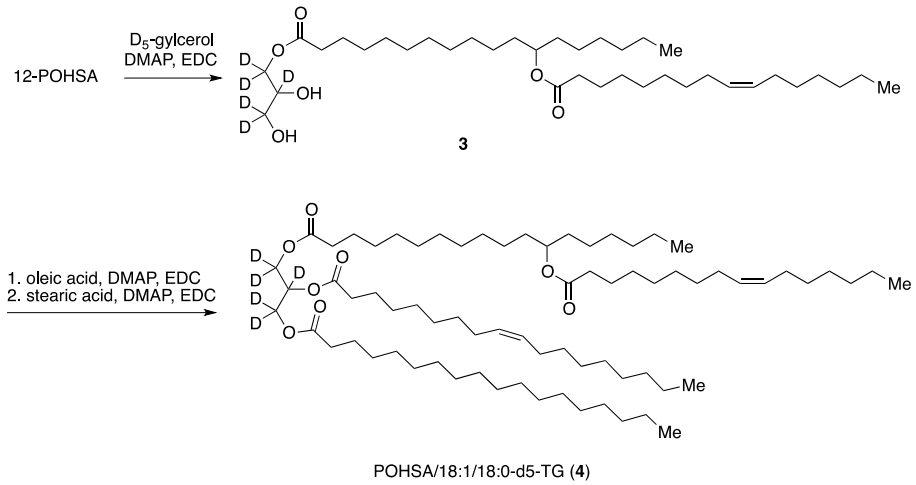
16:0/PAHSA/18:1-TG (**2**)



(16:0/PAHSA/18:1-TG) (2): Neat 2-hydroxy-3-(palmitoyloxy) propyl oleate (**1**) (35 mg, 0.059 mmol) and 12-PAHSA (32 mg, 0.06 mmol) were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (5 : 95) afforded 16:0/PAHSA/18:1-TG (**2**) as a clear colorless oil (58 mg, 0.052 mmol, 89%).

R_f = 0.6 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.37 – 5.28 (m, 2H), 5.27 – 5.22 (m, 1H), 4.85 (dd, *J* = 12.3, 5.8 Hz, 1H), 4.28 (dd, *J* = 11.9, 4.2 Hz, 2H), 4.12 (dd, *J* = 11.9, 5.9 Hz, 2H), 2.27 (dt, *J* = 20.9, 7.5 Hz, 8H), 1.99 (dd, *J* = 12.2, 6.2 Hz, 4H), 1.59 (s, 8H), 1.48 (d, *J* = 5.1 Hz, 4H), 1.35 – 1.12 (m, 90H), 0.86 (t, *J* = 7.0 Hz, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.76, 173.35, 173.32, 172.93, 130.08, 129.78, 74.09, 68.94, 62.17, 34.82, 34.28, 34.13, 34.11, 32.04, 32.02, 31.88, 29.87, 29.81, 29.78, 29.74, 29.67, 29.64, 29.63, 29.59, 29.49, 29.43, 29.41, 29.39, 29.32, 29.30, 29.29, 29.22, 29.19, 27.32, 27.27, 25.46, 25.39, 25.29, 24.99, 24.96, 24.94, 22.81, 22.70, 14.23, 14.18. **HRMS**: *m/z*: calcd for $C_{71}H_{134}O_8Na$: 1137.9971; found 1137.9964 $[M + Na]^+$.

POHSA/18:1/18:0-d5-TG (**4**)



2,3-dihydroxypropyl-1,1,2,3,3-d5-12-POHSA (3): Neat D_5-gylcerol (48 µL, 3.9 M, 0.187 mmol) and 12-POHSA (100 mg, 0.187 mmol) were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (40 : 60) provided **3** (61 mg, 0.099 mmol, 53%).

R_f = 0.4 (silica gel, 50:50 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.36 – 5.29 (m, 2H), 4.87 – 4.82 (m, 1H), 2.87 (s, 1H), 2.50 (s, 1H), 2.33 (dd, *J* = 14.0, 6.4 Hz, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.99 (dd, *J* = 12.4, 6.2 Hz, 4H), 1.60 (d, *J* = 5.4 Hz, 4H), 1.49 (d, *J* = 4.0 Hz, 4H), 1.32 – 1.22 (m, 38H), 0.86 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.50, 173.97, 130.09, 129.86, 74.25, 34.85, 34.26, 31.89, 31.87, 29.84, 29.81, 29.61, 29.59, 29.50, 29.37, 29.32, 29.27, 29.24, 29.20, 29.10, 27.32, 27.27, 25.43, 25.39, 25.28, 24.99, 22.77, 22.70, 14.23, 14.19. **HRMS**: *m/z*: calcd for $C_{37}H_{65}D_5O_6Na$: 638.5378; found 638.5373 $[M + Na]^+$.

1-((12-POHSA)-3-hydroxypropan-2-yl-1,1,2,3,3-d5 oleate):

Compound **3** (50 mg, 0.081 mmol) and oleic acid (23 mg, 0.081 mmol) in dichloromethane were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (13 : 87) yielded 1-((12-(((Z)-hexadec-9-enoyl)oxy)octadecanoyl)oxy)-3-hydroxypropan-2-yl-1,1,2,3,3-d5 oleate) (minor isomer on 2 position of glycerol)**:** (24 mg, 0.028 mmol, 34%) .

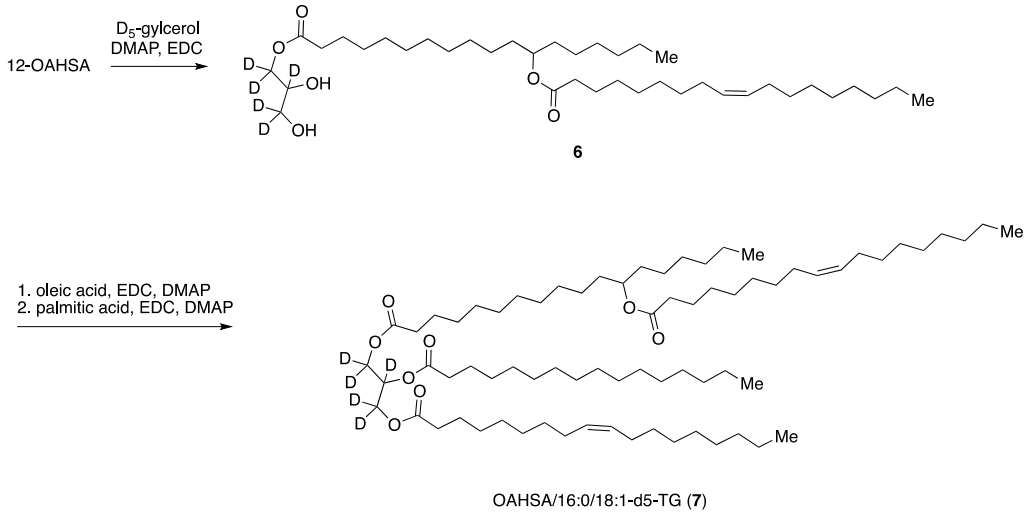
R_f = 0.5 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.38 – 5.31 (m, 4H), 4.89 – 4.83 (m, 1H), 2.36 – 2.31 (m, 5H), 2.27 (t, *J* = 7.5 Hz, 2H), 2.05 (d, *J* = 5.5 Hz, 1H), 2.01 (dd, *J* = 12.6, 6.5 Hz, 8H), 1.62 (d, *J* = 6.5 Hz, 4H), 1.50 (d, *J* = 5.5 Hz, 4H), 1.33 – 1.24 (m, 60H), 0.88 (m, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.10, 173.99, 173.57, 130.15, 130.11, 129.90, 129.88, 74.21, 34.86, 34.39, 34.28, 34.21, 32.03, 31.91, 31.89, 29.89, 29.86, 29.83, 29.79, 29.66, 29.56, 29.55, 29.50, 29.45, 29.38, 29.37, 29.34, 29.31,

29.29, 29.26, 29.24, 29.22, 29.12, 27.34, 27.29, 25.46, 25.41, 25.30, 25.04, 24.99, 22.82, 22.79, 22.71, 14.25, 14.22. **HRMS**: *m/z*: calcd for $C_{55}H_{97}D_5O_7Na$: 902.7827; found 902.7829 $[M + Na]^+$.

POHSA/18:1/18:0-d5-TG (4): 1-((12-POHSA)-3-hydroxypropan-2-yl-1,1,2,3,3-d5 oleate) (above) (20 mg, 0.023 mmol) and stearic acid (6.6 mg, 0.023 mmol) in DCM were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (4 : 96) afforded the title compound POHSA/18:1/18:0-d5-TG (**4**) (23 mg, 0.020 mmol, 87%).

$\mathbf{R_f}$ = 0.7 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.38 – 5.30 (m, 4H), 4.88 – 4.84 (m, 1H), 2.32 – 2.27 (m, 8H), 2.00 (dd, *J* = 12.3, 6.3 Hz, 8H), 1.62 – 1.58 (m, 8H), 1.49 (d, *J* = 4.6 Hz, 4H), 1.31 – 1.23 (m, 86H), 0.89 – 0.86 (m, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.82, 173.46, 173.44, 173.00, 130.15, 130.10, 129.88, 129.81, 74.19, 34.86, 34.34, 34.32, 34.29, 34.18, 32.07, 32.05, 31.92, 31.90, 29.90, 29.85, 29.81, 29.77, 29.70, 29.67, 29.63, 29.60, 29.51, 29.47, 29.44, 29.42, 29.35, 29.30, 29.27, 29.22, 29.18, 29.13, 27.35, 27.30, 25.49, 25.42, 25.30, 25.04, 25.01, 24.99, 24.98, 22.84, 22.80, 22.73, 14.27, 14.22. **HRMS**: *m/z*: calcd for $C_{73}H_{131}D_5O_8Na$: 1169.0441; found 1169.0445 $[M + Na]^+$.

OAHSA/16:0/18:1-d5-TG (**7**)



2,3-dihydroxypropyl-1,1,2,3,3-d5 12-OAHSA (6): Neat D_5-glycerol (46 µL, 3.9 M, 0.179 mmol) and 12-OAHSA (100 mg, 0.179 mmol) in dichloromethane were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (35 : 65) provided **6** (63 mg, 0.098 mmol, 55%).

R_f = 0.4 (silica gel, 50:50 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.37 – 5.28 (m, 2H), 4.85 (dd, *J* = 12.3, 5.8 Hz, 1H), 2.32 (t, *J* = 7.6 Hz, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 2.00 – 1.97 (m, 2H), 1.59 (d, *J* = 6.6 Hz, 4H), 1.48 (d, *J* = 4.6 Hz, 4H), 1.31 – 1.21 (m, 46H), 0.85 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.47, 173.97, 130.07, 129.83, 74.24, 34.83, 34.23, 31.99, 31.84, 29.85, 29.79, 29.75, 29.61, 29.60, 29.58, 29.54, 29.49, 29.41, 29.31, 29.29, 29.24, 29.23, 29.19, 27.30, 27.25, 25.41, 25.36, 25.26, 24.97, 22.78, 22.67, 14.22, 14.18. **HRMS**: *m/z*: calcd for $C_{39}H_{69}D_5O_6Na$: 666.5691; found 666.5688 $[M + Na]^+$.

2-hydroxy-3-((12-(oleoyloxy) octadecanoyl)oxy)propyl-1,1,2,3,3-d5 oleate: Compound **6** (58 mg, 0.09 mmol) and oleic acid (25 mg, 0.09 mmol) in dichloromethane were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (14 : 86) provided **2**-hydroxy-3-((12-(oleoyloxy) octadecanoyl)oxy)propyl-1,1,2,3,3-d5 oleate (39 mg, 0.043 mmol, 48%).

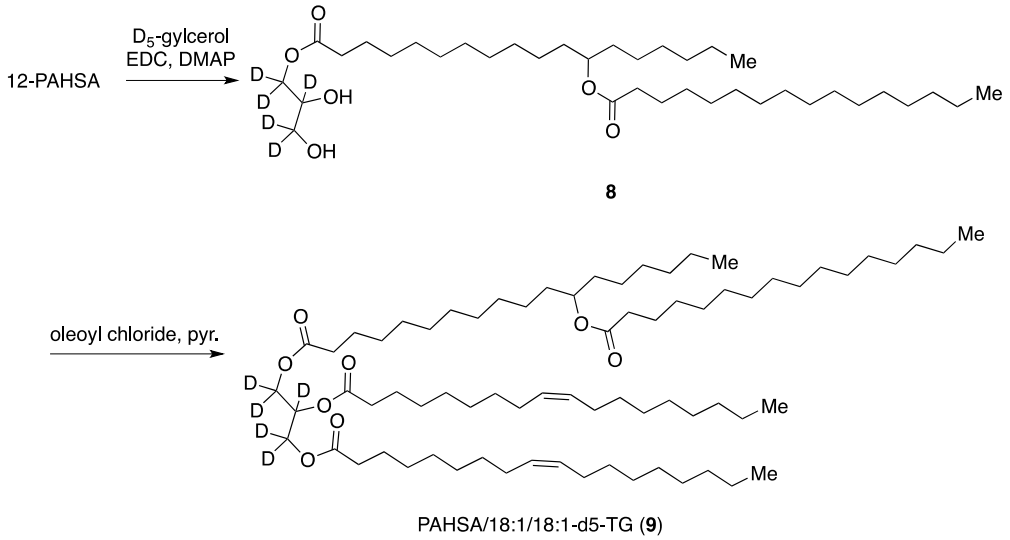
R_f = 0.6 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.38 – 5.28 (m, 4H), 4.87 – 4.83 (m, 1H), 2.33 (t, *J* = 7.5 Hz, 4H), 2.26 (t, *J* = 7.4 Hz, 2H), 2.07 – 1.94 (m, 8H), 1.60 (d, *J* = 5.1 Hz, 8H), 1.49 (d, *J* = 4.0 Hz, 4H), 1.26 (dd, *J* = 21.0, 8.6 Hz, 61H), 0.87 (m, 9H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.07, 174.05, 173.87, 130.12, 130.09, 129.86, 129.82, 74.20, 34.84, 34.27, 34.20, 32.02, 31.88, 29.88, 29.82, 29.80, 29.78, 29.69, 29.64, 29.58, 29.53, 29.44, 29.37, 29.35, 29.33, 29.28, 29.26, 29.23, 29.21, 29.17, 27.33, 27.28,

27.27, 25.45, 25.39, 25.28, 24.98, 22.80, 22.70, 14.25, 14.20. **HRMS**: *m/z*: calcd for $C_{57}H_{101}D_5O_7Na$: 930.8145; found 930.8136 $[M + Na]^+$.

OAHSA/16:0/18:1-d5-TG (7): Neat 2-hydroxy-3-((12-(oleoyloxy) octadecanoyl)oxy)propyl-1,1,2,3,3-d5 oleate (25 mg, 0.028 mmol) and palmitic acid (7.2 mg, 0.028 mmol) in dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (4 : 96) afforded the title compound OAHSA/16:0/18:1-d5-TG (**7**) (29 mg, 0.025 mmol, 91%).

R_f = 0.7 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.39 – 5.29 (m, 4H), 4.89 – 4.83 (m, 1H), 2.32 – 2.25 (m, 8H), 2.00 (dd, *J* = 12.3, 6.2 Hz, 8H), 1.60 (d, *J* = 6.4 Hz, 8H), 1.49 (d, *J* = 3.5 Hz, 4H), 1.33 – 1.22 (m, 86H), 0.89 – 0.85 (m, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.82, 173.44, 173.43, 173.03, 130.13, 130.10, 129.87, 129.83, 74.18, 34.85, 34.33, 34.31, 34.29, 34.16, 32.06, 32.04, 31.90, 29.90, 29.84, 29.81, 29.80, 29.78, 29.70, 29.66, 29.64, 29.60, 29.51, 29.46, 29.43, 29.42, 29.35, 29.32, 29.30, 29.27, 29.26, 29.25, 29.22, 29.21, 27.35, 27.30, 25.49, 25.41, 25.30, 25.03, 24.97, 22.83, 22.82, 22.72, 14.26, 14.22. **HRMS**: *m/z*: calcd for $C_{73}H_{131}D_5O_8Na$: 1169.0441; found 1169.0444 $[M + Na]^+$.

PAHSA/18:1/18:1-d5-TG (**9**)



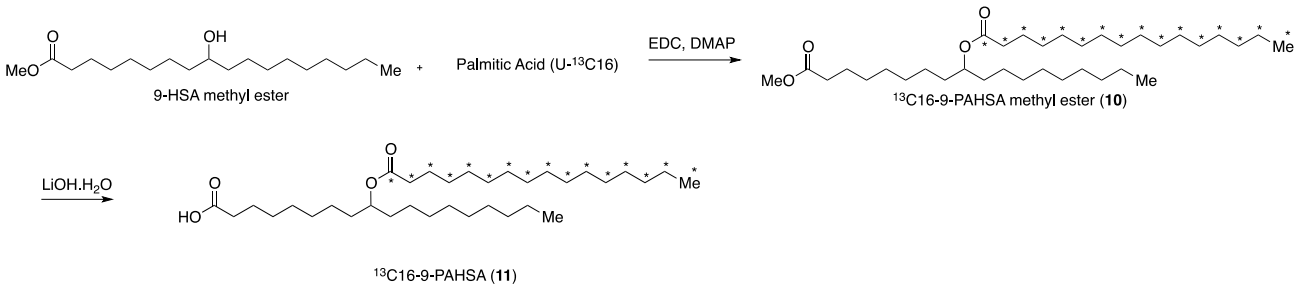
2,3-dihydroxypropyl-1,1,2,3,3-d5 12-PAHSA (8): Neat D_5-glycerol (38 µL, 3.9 M, 0.148 mmol) and 12-PAHSA (80 mg, 0.148 mmol) in dichloromethane were subjected to **General procedure A**. Purification by column chromatography using EtOAc: Hexane (35 : 65) provided compound **8** (55 mg, 0.089 mmol, 60%).

R_f = 0.55 (silica gel, 50:50 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 4.85 (dd, *J* = 12.1, 5.8 Hz, 1H), 2.32 (t, *J* = 7.5 Hz, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.59 (d, *J* = 5.5 Hz, 4H), 1.48 (d, *J* = 4.6 Hz, 4H), 1.24 (d, *J* = 21.2 Hz, 48H), 0.85 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.47, 174.01, 74.24, 34.86, 34.26, 34.24, 32.03, 31.86, 29.80, 29.79, 29.77, 29.73, 29.61, 29.58, 29.50, 29.47, 29.41, 29.37, 29.32, 29.31, 29.29, 29.24, 29.20, 25.42, 25.38, 25.29, 24.98, 22.80, 22.69, 14.23, 14.18. **HRMS**: *m/z*: calcd for $C_{37}H_{67}D_5O_6Na$: 640.5535; found 640.5529 $[M + Na]^+$.

PAHSA/18:1/18:1-d5-TG (9): A dry 10 mL round-bottom flask equipped with stir bar, under nitrogen atmosphere, and sealed with a rubber septum was charged with compound **8** (50 mg, 0.081 mmol, 1.0 equiv.) and dry dichloromethane (1.9 mL). Dry pyridine (33 µL, 0.405 mmol, 5.0 equiv.) was added via syringe. The reaction vessel was submerged in an ice water bath and aged 5 minutes. Oleoyl chloride (59 µL, 0.178 mmol, 2.2 equiv.) was added dropwise via syringe. The reaction was allowed to warm to ambient temperature and stirred 12 hours. The reaction was quenched with deionized water (1.0 mL). The biphasic mixture was transferred to a separatory funnel. The layers were partitioned and separated. The organic layer was saved while the aqueous layer was extracted with dichloromethane (2 X 4.0 mL). Organics were combined and washed with 0.5 M aqueous hydrochloric acid (2.0 mL), saturate aqueous sodium bicarbonate (2.0 mL), and brine (2.0 mL), dried (sodium sulfate), filtered, and concentrated. The crude product was purified by silica column chromatography, eluting with hexanes: EtOAc (95 : 5) afforded the title compound (**9**) (86 mg, 0.075 mmol, 93%) as oil.

R_f = 0.7 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.39 – 5.29 (m, 4H), 4.88 – 4.83 (m, 1H), 2.29 (ddd, *J* = 20.2, 11.2, 5.5 Hz, 8H), 2.06 – 1.95 (m, 8H), 1.60 (d, *J* = 6.5 Hz, 8H), 1.49 (d, *J* = 5.0 Hz, 4H), 1.36 – 1.17 (m, 86H), 0.87 (m, 12H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.83, 173.42, 173.41, 172.98, 130.13, 130.12, 129.82, 129.80, 74.15, 34.86, 34.30, 34.29, 34.14, 32.06, 32.04, 31.89, 29.89, 29.83, 29.79, 29.75, 29.68, 29.66, 29.64, 29.61, 29.59, 29.50, 29.46, 29.41, 29.34, 29.32, 29.31, 29.25, 29.24, 29.21, 29.17, 27.34, 27.29, 25.48, 25.41, 25.31, 25.00, 24.96, 22.82, 22.72, 14.25, 14.21. **HRMS**: *m/z*: calcd for $C_{73}H_{131}D_5O_8Na$: 1169.0441; found 1169.0444 $[M + Na]^+$.

$^{13}C_{16}$-9-PAHSA (**11**)



$^{13}C_{16}$-9-PAHSA methyl ester (10): Neat 9-hydroxy stearic acid methyl ester (80.0 mg, 0.254 mmol) and palmitic-$^{13}C_{16}$ acid (71 mg, 0.259 mmol) in dry dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (6 : 94) provided $^{13}C_{16}$-9-PAHSA methyl ester (**10**) (128 mg, 0.225 mmol, 88%).

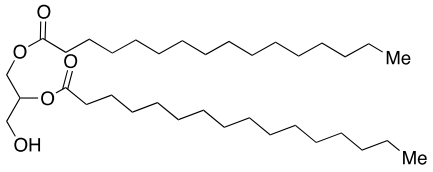
Rf = 0.6 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 4.86 (s, 1H), 3.66 (s, 3H), 2.38 (s, 1H), 2.29 (t, *J* = 7.6 Hz, 2H), 2.16 (d, *J* = 2.6 Hz, 1H), 1.71 (s, 1H), 1.60 (d, *J* = 6.1 Hz, 2H), 1.50 (s, 5H), 1.38 – 1.13 (m, 46H), 1.01 – 0.95 (m, 1.5H), 0.87 (t, *J* = 7.0 Hz, 3H), 0.80 – 0.74 (m, 1.5H). **HRMS**: *m/z*: calcd for $C_{19}{}^{13}C_{16}H_{68}O_4Na$: 591.5547; found 591.5546 $[M + Na]^+$.

$^{13}C_{16}$-9-PAHSA (11): To a stirred solution of $^{13}C_{16}$-9-PAHSA methyl ester (**10**) (120 mg, 0.211 mmol, 1.0 equiv.) in THF (1.1 mL) at 25°C was added an aqueous solution of lithium hydroxide (0.422 mL, 1.0 M, 0.422 mmol, 2.0 equiv.). The reaction mixture was stirred for 24 hours and quenched with 2N hydrogen chloride (4.0 mL), extract with ether (3 X 15 mL). The combined ether layers dried over sodium sulfate and concentrated. This crude product was purified via silica gel column chromatography using EtOAc: Hexane: AcOH (8 : 91 : 1) to give the $^{13}C_{16}$-9-PAHSA (**11**) (106 mg, 0.191 mmol, 91%).

R_f = 0.3 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 4.88 – 4.82 (m, 1H), 2.36 (ddd, *J* = 23.2, 11.0, 5.7 Hz, 3H), 2.21 – 2.12 (m, 1H), 1.71 (s, 1H), 1.65 – 1.59 (m, 2H), 1.49 (d, *J* = 5.0 Hz, 5H), 1.40 – 1.13 (m, 47H), 1.01 – 0.94 (m, 1.5H), 0.87 (t, *J* = 7.0 Hz, 3H), 0.77 (m, 1.5H). **HRMS**: *m/z*: calcd for $C_{18}{}^{13}C_{16}H_{67}O_4$: 555.5571; found 555.5566 $[M + H]^+$.

DGs **12** and **13**

12



13

Neat 2,3-dihydroxypropyl palmitate (150 mg, 0.454 mmol) and palmitic acid (119 mg, 0.463 mmol) in DCM were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (10 : 90) providing compound **12** (124 mg, 0.218 mmol, 48%) and **13** (77 mg, 0.136 mmol, 30%).

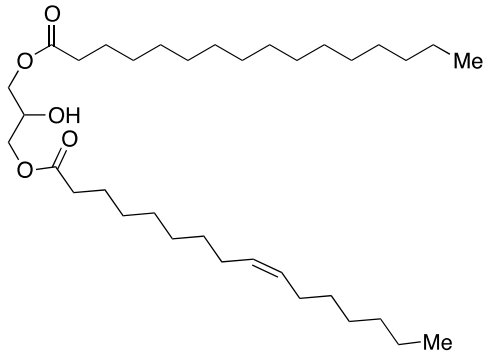
2-hydroxypropane-1, 3-dipalmitate (12)

R_f = 0.65 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 4.17 (dd, *J* = 11.5, 4.3 Hz, 2H), 4.12 (dd, *J* = 11.5, 5.9 Hz, 2H), 4.10 – 4.05 (m, 1H), 2.56 (d, *J* = 4.9 Hz, 1H), 2.34 (t, *J* = 7.6 Hz, 4H), 1.61 (dd, *J* = 14.4, 7.2 Hz, 4H), 1.31 – 1.22 (m, 48H), 0.87 (t, *J* = 7.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.07, 68.45, 65.15, 34.22, 32.06, 29.83, 29.81, 29.79, 29.74, 29.59, 29.50, 29.39, 29.25, 25.01, 22.83, 14.26. **HRMS**: *m/z*: calcd for $C_{35}H_{68}O_5Na$: 591.4959; found 591.4954 $[M + Na]^+$.

3-hydroxypropane-1, 2-dipalmitate (13)

R_f = 0.6 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (599 MHz, $CDCl_3$) δ 5.12 – 5.05 (m, 1H), 4.31 (dd, *J* = 11.9, 4.4 Hz, 1H), 4.22 (dd, *J* = 11.9, 5.7 Hz, 1H), 3.72 (s, 2H), 2.37 – 2.29 (m, 4H), 2.20 (s, 1H), 1.61 (dd, *J* = 14.4, 7.2 Hz, 4H), 1.32 – 1.23 (m, 48H), 0.87 (t, *J* = 7.0 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.97, 173.60, 72.20, 62.15, 61.61, 34.41, 34.23, 32.06, 29.84, 29.80, 29.76, 29.62, 29.50, 29.41, 29.25, 29.22, 25.06, 25.01, 22.83, 14.26. **HRMS**: *m/z*: calcd for $C_{35}H_{68}O_5Na$: 591.4959; found 591.4950 $[M + Na]^+$.

DGs **14** and **15**



14

15

Neat 2,3-dihydroxypropyl palmitate (140 mg, 0.424 mmol) and palmitoleic acid (110 mg, 0.432 mmol) in dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (11 : 89) yielded compound **14** (122 mg, 0.216 mmol, 51%) and compound **15** (70 mg, 0.123 mmol, 29%).

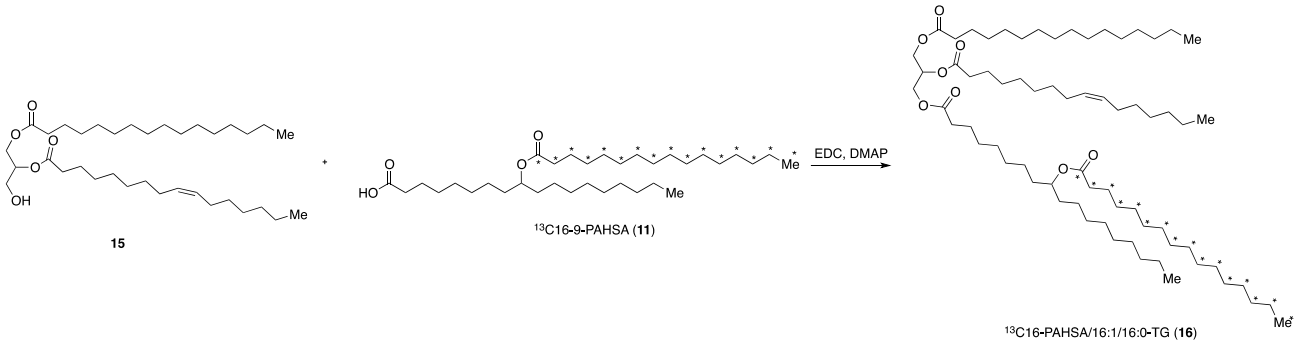
2-hydroxy-3-(palmitoyloxy)propyl (Z)-hexadec-9-enoate (14)

R_f = 0.6 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.38 – 5.30 (m, 2H), 4.18 (dd, *J* = 11.5, 4.2 Hz, 2H), 4.13 (dd, *J* = 11.6, 5.8 Hz, 2H), 4.09 (dd, *J* = 8.6, 3.6 Hz, 1H), 2.46 (d, *J* = 4.4 Hz, 1H), 2.34 (t, *J* = 7.6 Hz, 4H), 2.01 (dd, *J* = 12.7, 6.6 Hz, 4H), 1.63 (dd, *J* = 14.0, 7.3 Hz, 4H), 1.34 – 1.24 (m, 40H), 0.88 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.08, 174.05, 130.10, 129.81, 68.36, 65.11, 34.19, 34.18, 32.03, 31.88, 29.82, 29.80, 29.78, 29.76, 29.73, 29.71, 29.56, 29.47, 29.36, 29.26, 29.22, 29.19, 29.09, 27.31, 27.25, 24.98, 24.96, 22.80, 22.76, 14.23, 14.22. **HRMS**: *m/z*: calcd for $C_{35}H_{66}O_5Na$: 589.4802; found 589.4796 $[M + Na]^+$.

1-hydroxy-3-(palmitoyloxy)propan-2-yl (Z)-hexadec-9-enoate (15)

R_f = 0.55 (silica gel, 80:20 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.38 – 5.31 (m, 2H), 5.12 – 5.05 (m, 1H), 4.31 (dd, *J* = 11.9, 4.6 Hz, 1H), 4.24 (dd, *J* = 11.9, 5.6 Hz, 1H), 3.73 (s, 2H), 2.33 (dt, *J* = 13.3, 7.6 Hz, 4H), 2.01 (dd, *J* = 12.6, 6.6 Hz, 4H), 1.62 (dd, *J* = 14.4, 7.2 Hz, 4H), 1.35 – 1.24 (m, 41H), 0.88 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 174.10, 173.62, 130.10, 129.81, 72.17, 68.33, 65.10, 62.19, 61.50, 34.38, 34.19, 34.18, 32.02, 31.88, 29.79, 29.76, 29.72, 29.58, 29.56, 29.46, 29.37, 29.22, 29.18, 29.08, 27.31, 27.25, 25.02, 24.97, 22.79, 22.76, 14.22, 14.21. **HRMS**: *m/z*: calcd for $C_{35}H_{66}O_5Na$: 589.4802; found 589.4795 $[M + Na]^+$.

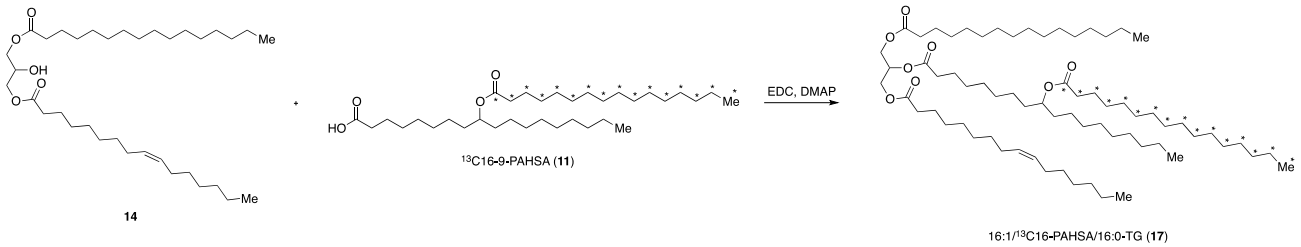
$^{13}C_{16}$-PAHSA/16:1/16:0-TG (**16**)



$^{13}C_{16}$-PAHSA/16:1/16:0-TG (16): Compound **15** (20 mg, 0.035 mmol) and $^{13}C_{16}$-9-PAHSA (**11**) (20 mg, 0.036 mmol) in dry dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (4: 96) to yield the compound $^{13}C_{16}$-PAHSA/16:1/16:0-TG (**16**) (32 mg, 0.029 mmol, 83%).

R_f = 0.6 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.38 – 5.30 (m, 2H), 5.28 – 5.24 (m, 1H), 4.88 – 4.83 (m, 1H), 4.29 (ddd, *J* = 11.9, 4.0, 2.8 Hz, 2H), 4.14 (dd, *J* = 11.9, 6.0 Hz, 2H), 2.38 (dd, *J* = 7.1, 3.9 Hz, 1H), 2.31 (ddd, *J* = 11.1, 7.4, 3.7 Hz, 6H), 2.16 (dd, *J* = 7.0, 3.7 Hz, 1H), 2.01 (dd, *J* = 12.7, 6.6 Hz, 4H), 1.71 (s, 1H), 1.59 (d, *J* = 6.2 Hz, 6H), 1.49 (d, *J* = 5.6 Hz, 5H), 1.38 – 1.14 (m, 86H), 0.98 (m, 1.5H), 0.87 (m, 9H), 0.79 – 0.74 (m, 1.5H). **HRMS**: *m/z*: calcd for $C_{53}{}^{13}C_{16}H_{130}O_8Na$: 1126.0195; found 1126.0205 $[M + Na]^+$.

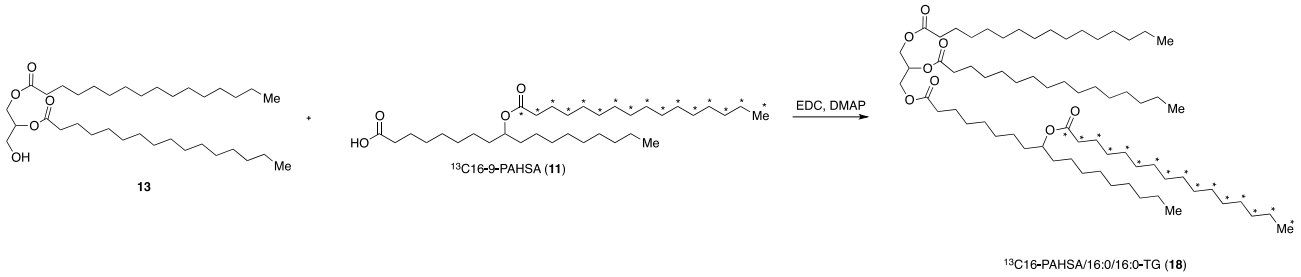
16:1/$^{13}C_{16}$-PAHSA/16:0-TG (**17**)



16:1/$^{13}C_{16}$-PAHSA/16:0-TG (17): Compound **14** (18 mg, 0.032 mmol) and $^{13}C_{16}$-9-PAHSA (**11**) (18 mg, 0.032 mmol) in dry dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (5 : 95) to yield 16:1/$^{13}C_{16}$-PAHSA/16:0-TG (**17**) (30 mg, 0.033 mmol, 86%).

R_f = 0.6 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.34 (d, *J* = 3.6 Hz, 2H), 5.26 (d, *J* = 4.6 Hz, 1H), 4.86 (s, 1H), 4.29 (dd, *J* = 11.7, 3.9 Hz, 2H), 4.14 (dd, *J* = 11.8, 5.8 Hz, 2H), 2.40 – 2.28 (m, 7H), 2.17 (s, 1H), 2.01 (d, *J* = 5.8 Hz, 4H), 1.71 (s, 1H), 1.60 (s, 6H), 1.50 (s, 5H), 1.25 (dd, *J* = 47.0, 29.2 Hz, 86H), 1.00 – 0.96 (m, 1.5H), 0.91 – 0.86 (m, 9H), 0.77 (m, 1.5H). **HRMS**: *m/z*: calcd for $C_{53}{}^{13}C_{16}H_{130}O_8Na$: 1126.0195; found 1126.0192 $[M + Na]^+$.

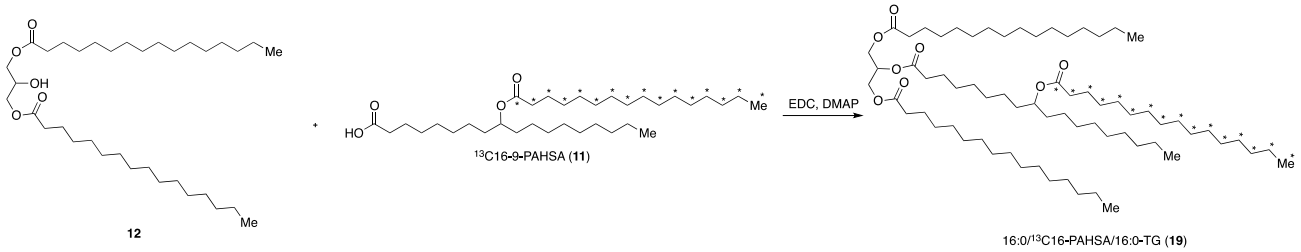
$^{13}C_{16}$-PAHSA/16:0/16:0-TG (**18**)



$^{13}C_{16}$-PAHSA/16:0/16:0-TG (18): Compound **13** (16 mg, 0.028 mmol) and $^{13}C_{16}$-9-PAHSA (**11**) (16 mg, 0.029 mmol) in dry dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (5 : 95) to yield $^{13}C_{16}$-PAHSA/16:0/16:0-TG (**18**) (26 mg, 0.024 mmol, 84%).

R_f = 0.5 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.29 – 5.24 (m, 1H), 4.88 – 4.82 (m, 1H), 4.31 – 4.26 (m, 2H), 4.14 (dd, *J* = 11.9, 6.0 Hz, 2H), 2.41 – 2.35 (m, 1H), 2.31 (ddd, *J* = 10.9, 7.3, 3.5 Hz, 6H), 2.20 – 2.13 (m, 1H), 1.69 (d, *J* = 20.7 Hz, 1H), 1.61 (dt, *J* = 6.7, 6.0 Hz, 6H), 1.49 (d, *J* = 5.7 Hz, 5H), 1.38 – 1.14 (m, 94H), 0.98 (m, 1.5H), 0.88 (t, *J* = 7.0 Hz, 9H), 0.79 – 0.75 (m, 1.5H). **HRMS**: *m/z*: calcd for $C_{53}{}^{13}C_{16}H_{132}O_8Na$: 1128.0351; found 1128.0353 $[M + Na]^+$.

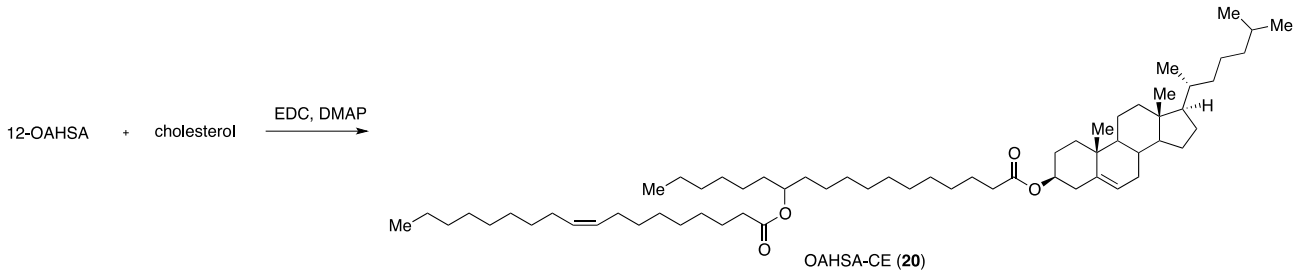
16:0/$^{13}C_{16}$-PAHSA/16:0-TG (**19**)



16:0/$^{13}C_{16}$-PAHSA/16:0-TG (19): Compound **12** (17 mg, 0.03 mmol) and $^{13}C_{16}$-9-PAHSA (**11**) (17 mg, 0.03 mmol) in dry dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (4: 96) afforded 16:0/$^{13}C_{16}$-PAHSA/16:0-TG (**19**) (26 mg, 0.024 mmol, 79%).

Rf = 0.5 (silica gel, 90:10 hexanes: EtOAc); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 5.27 (d, *J* = 4.2 Hz, 1H), 4.86 (s, 1H), 4.33 – 4.27 (m, 2H), 4.14 (dd, *J* = 10.8, 5.8 Hz, 2H), 2.38 (s, 1H), 2.31 (dd, *J* = 10.6, 4.3 Hz, 6H), 2.17 (s, 1H), 1.72 (s, 1H), 1.61 (d, *J* = 5.5 Hz, 5H), 1.50 (s, 5H), 1.37 – 1.16 (m, 95H), 1.02 – 0.95 (m, 1.5H), 0.90 – 0.86 (m, 9H), 0.81 – 0.75 (m, 1.5H). HRMS: *m/z*: calcd for $C_{53}{}^{13}C_{16}H_{132}O_8Na$: 1128.0351; found 1128.0351 $[M + Na]^+$.

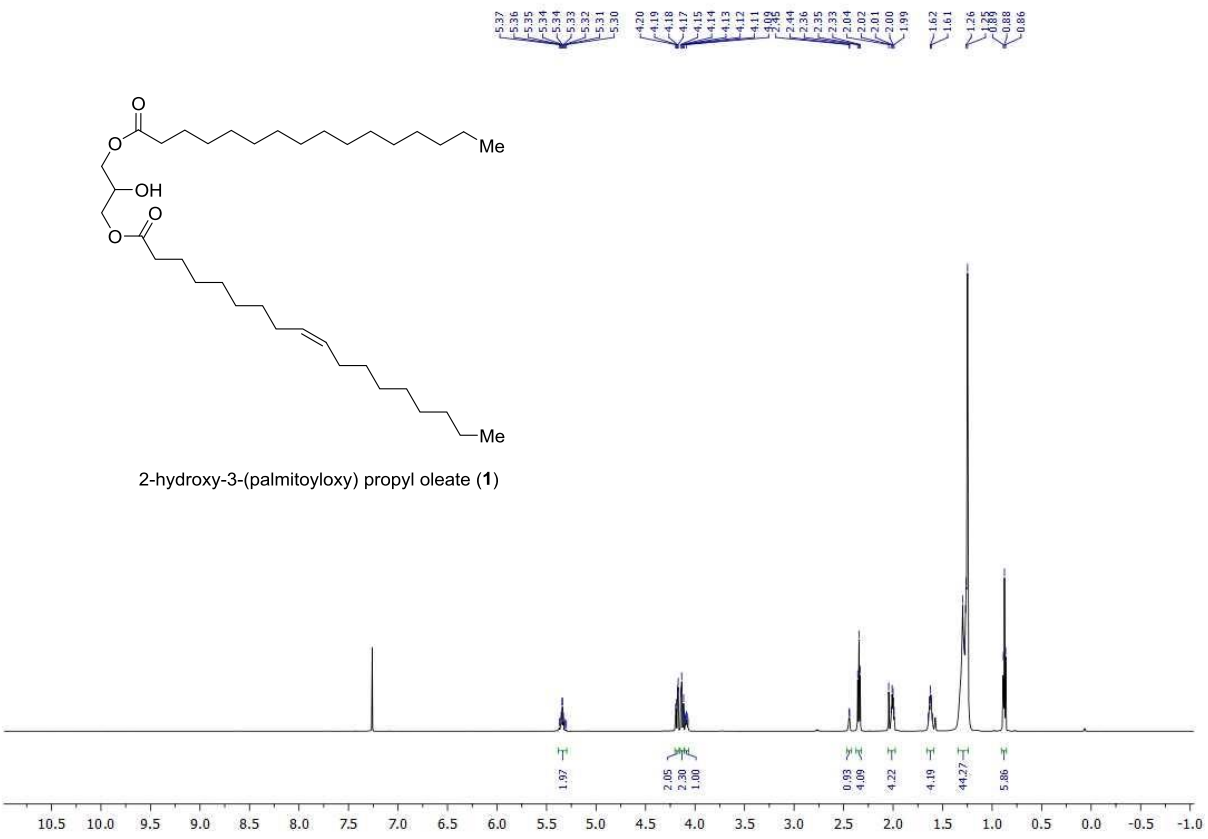
OAHSA-CE (**20**)



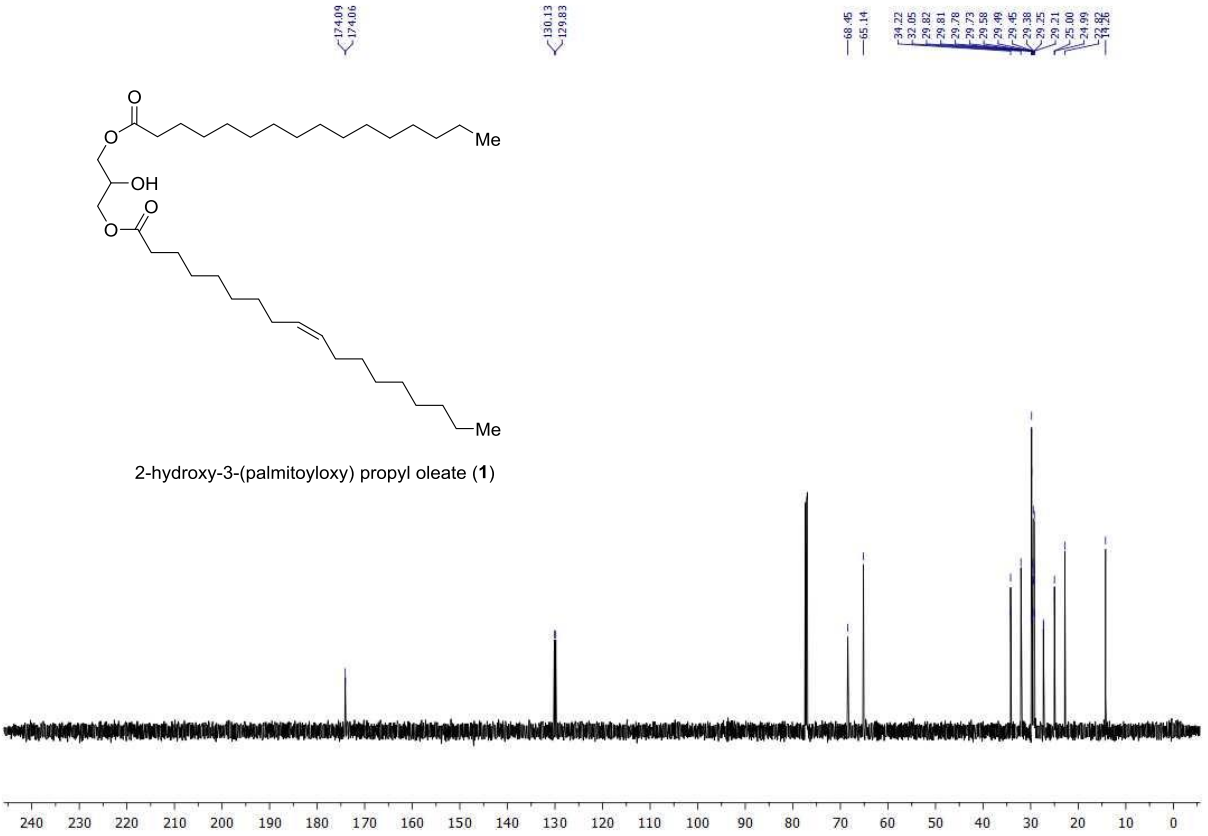
OAHSA-CE (20): Cholesterol (50 mg, 0.129 mmol) and 12-OAHSA (75 mg, 0.132 mmol) in dichloromethane were subjected to **General procedure B**. Purification by column chromatography using EtOAc: Hexane (4 : 9) provided OAHSA-CE (**20**) (91 mg, 0.097 mmol, 75%).

^{1}H NMR (599 MHz, $CDCl_3$) δ 5.40 – 5.30 (m, 3H), 4.87 (dd, *J* = 12.3, 5.9 Hz, 1H), 4.61 (dt, *J* = 11.6, 5.5 Hz, 1H), 2.28 (dt, *J* = 23.1, 7.5 Hz, 6H), 1.99 (dd, *J* = 21.5, 15.1 Hz, 6H), 1.88 – 1.79 (m, 3H), 1.64 – 1.41 (m, 16H), 1.28 (dd, *J* = 32.8, 12.7 Hz, 45H), 1.18 – 1.05 (m, 7H), 1.01 (s, 3H), 1.00 – 0.83 (m, 18H), 0.67 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 173.75, 173.36, 139.78, 130.07, 129.84, 122.69, 74.13, 73.74, 56.78, 56.22, 50.11, 42.40, 39.82, 39.62, 38.26, 37.10, 36.68, 36.29, 35.91, 34.82, 34.80, 34.29, 32.04, 32.00, 31.95, 31.89, 29.89, 29.82, 29.66, 29.64, 29.63, 29.55, 29.51, 29.45, 29.38, 29.34, 29.28, 29.26, 29.23, 28.35, 28.12, 27.91, 27.33, 27.28, 25.45, 25.41, 25.28, 25.16, 24.39, 23.94, 22.95, 22.82, 22.71, 22.68, 21.13, 19.43, 18.82, 14.25, 14.21, 11.96. **HRMS**: *m/z*: calcd for $C_{63}H_{112}O_4Na$: 955.8453; found 955.8446 $[M + Na]^+$.

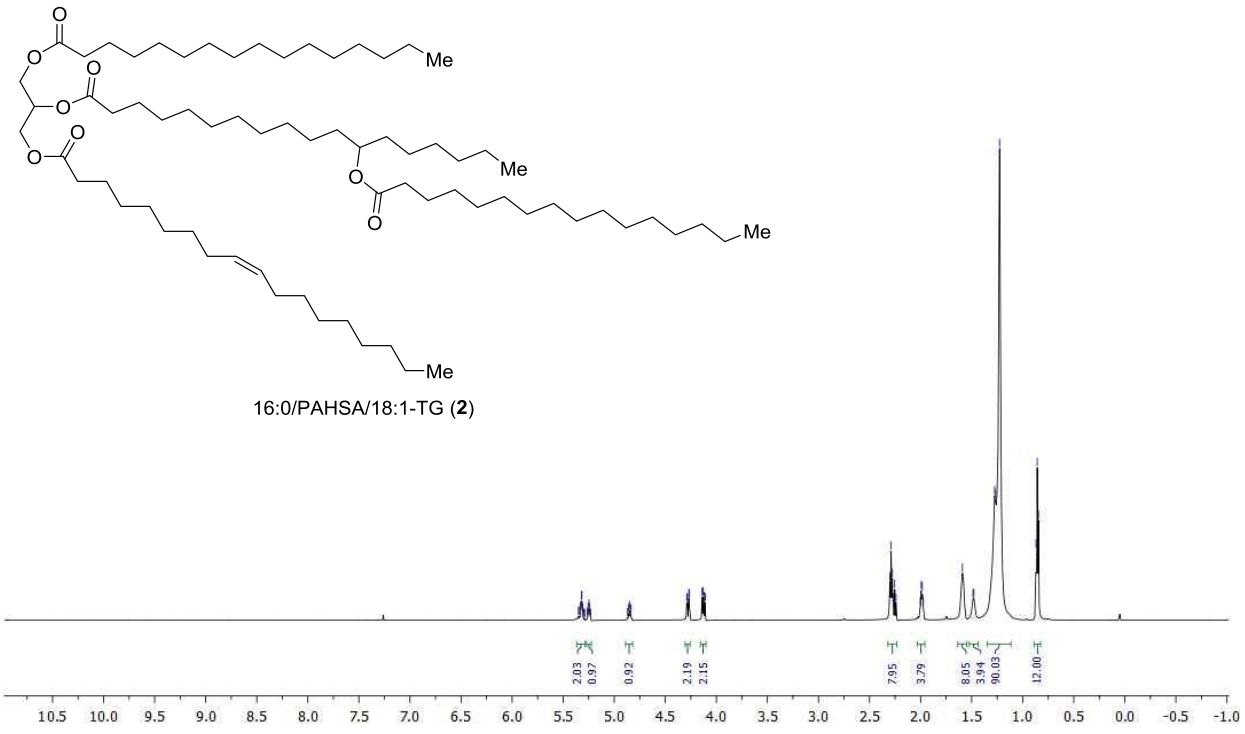
FAHFA-TGs and 12-OAHSA-CE Spectral Data



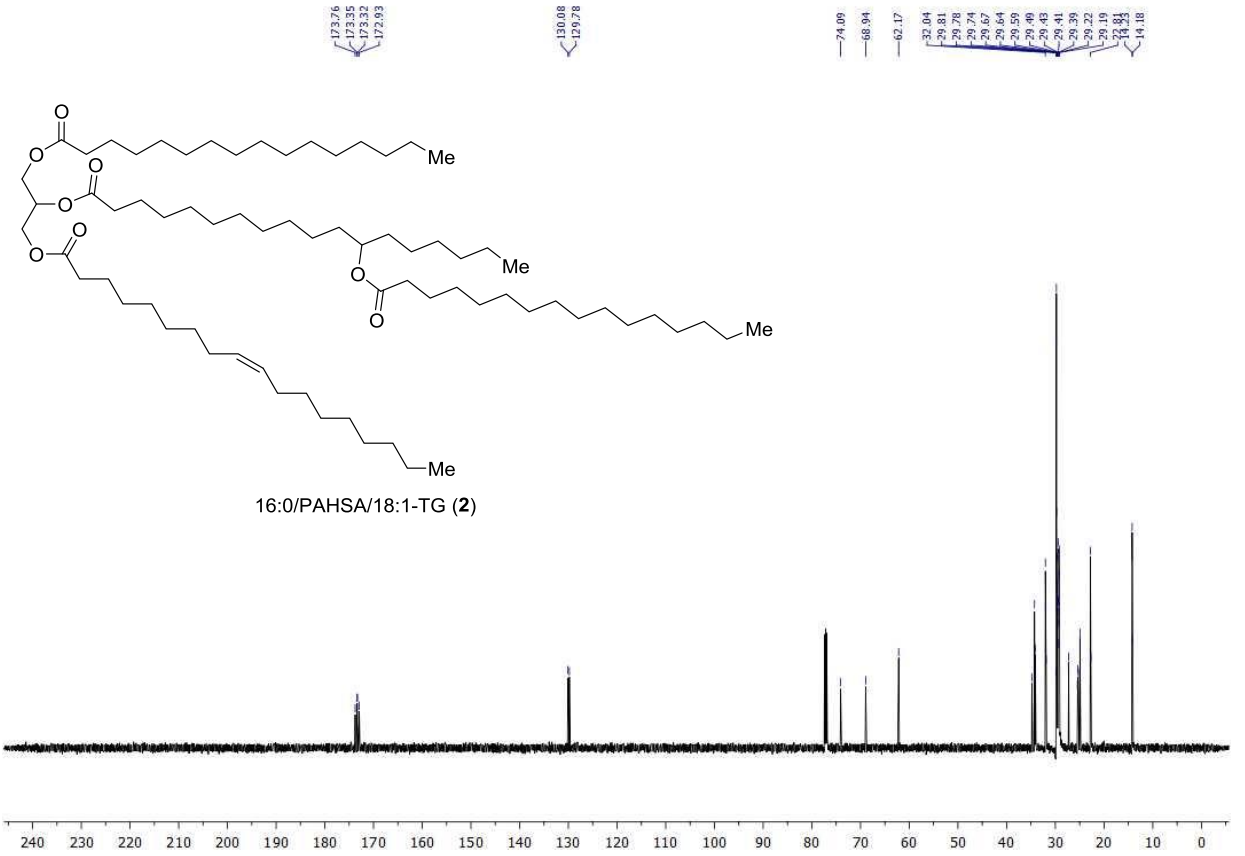
2-hydroxy-3-(palmitoyloxy) propyl oleate (**1**)



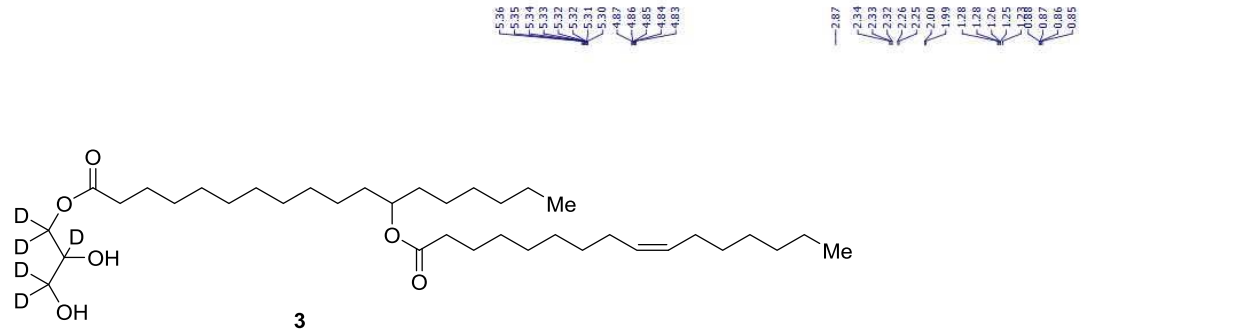
2-hydroxy-3-(palmitoyloxy) propyl oleate (**1**)



16:0/PAHSA/18:1-TG (**2**)



16:0/PAHSA/18:1-TG (**2**)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4.85
4.84
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2.87
2.34
2.33
2.32
2.26
2.25
2.00
1.99
1.28
1.28
1.26
1.25
1.23
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0.87
0.86
0.85
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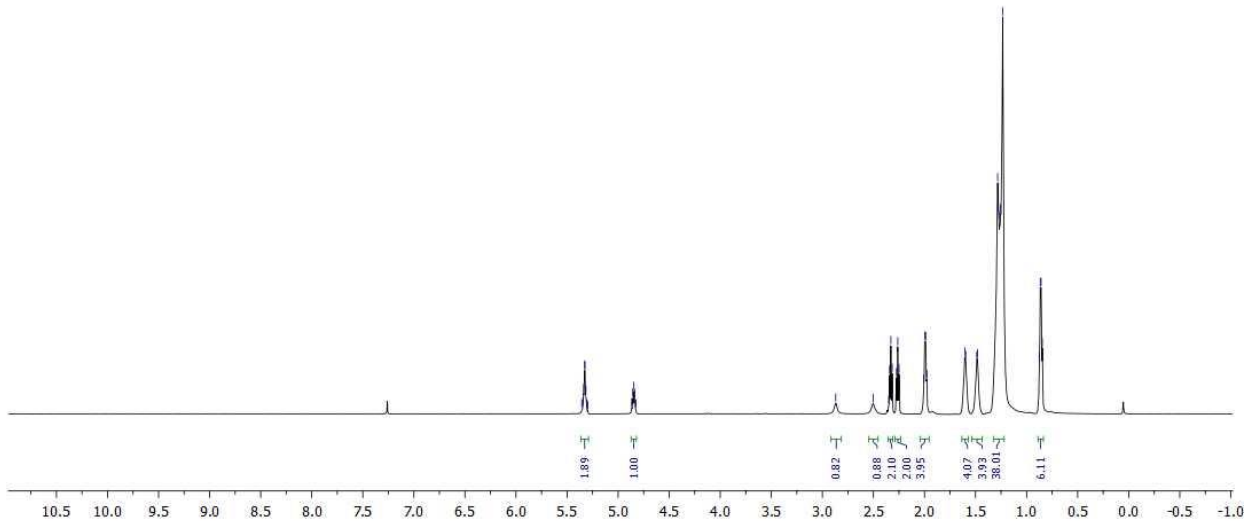
O
D
D
D
D
D
OH
OH
Me
O
O
Me

3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4.07
3.93
38.01
6.11
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0


174.50
173.97
130.09
129.86
74.25
34.26
31.89
31.87
29.84
29.81
29.61
29.59
29.32
29.27
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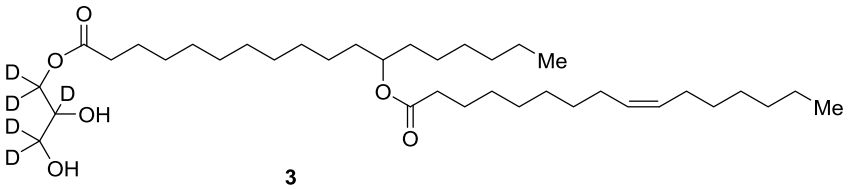
27.27
25.39
25.28
22.77
22.73
14.29
14.19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D
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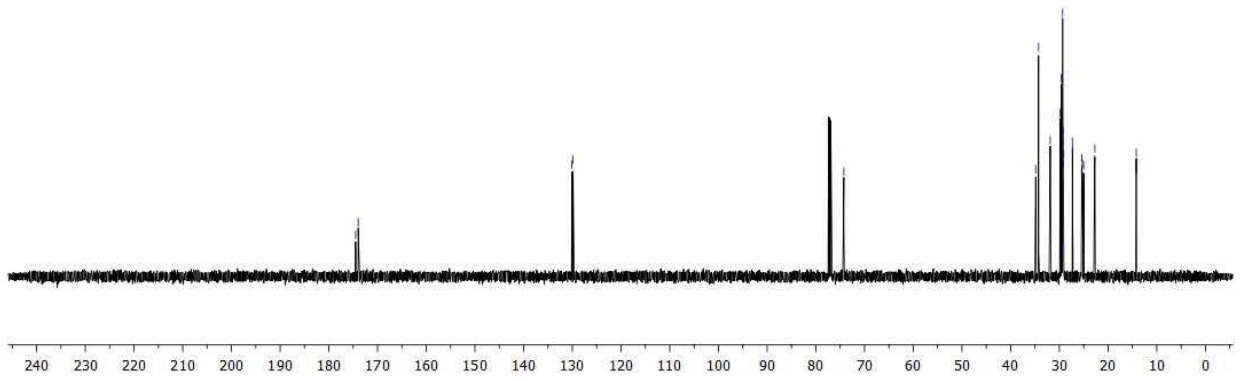
O
O
Me

3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160
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140
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120
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100
90
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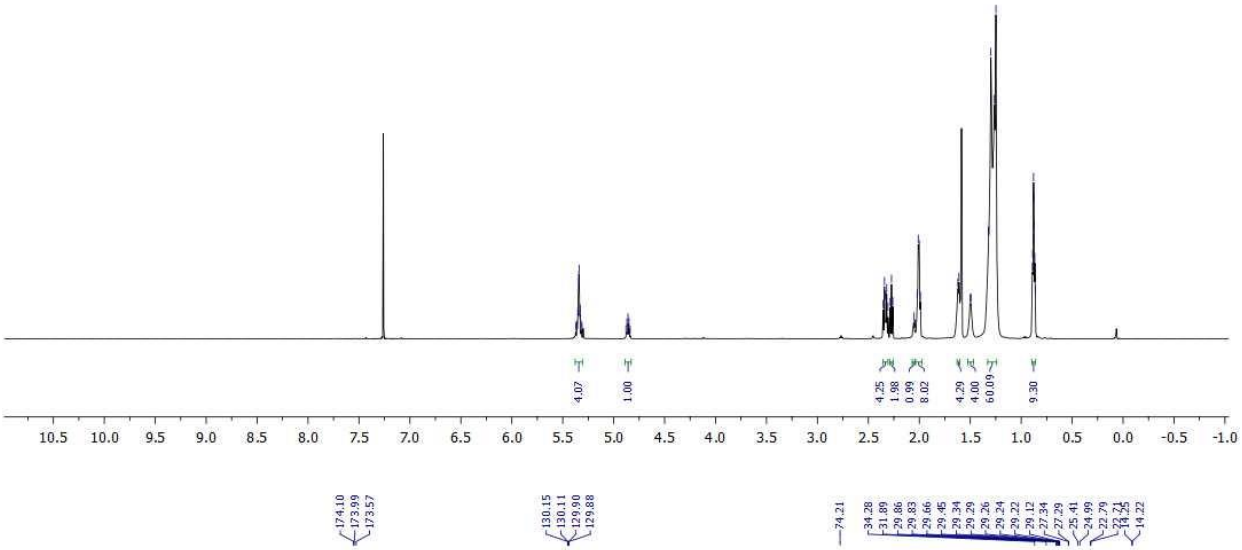
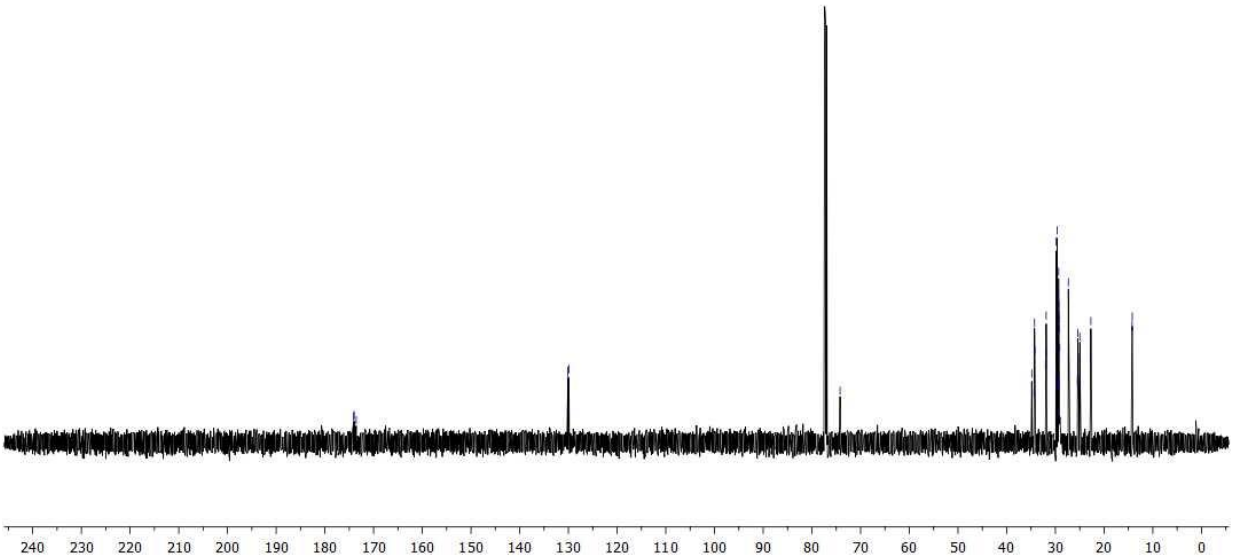
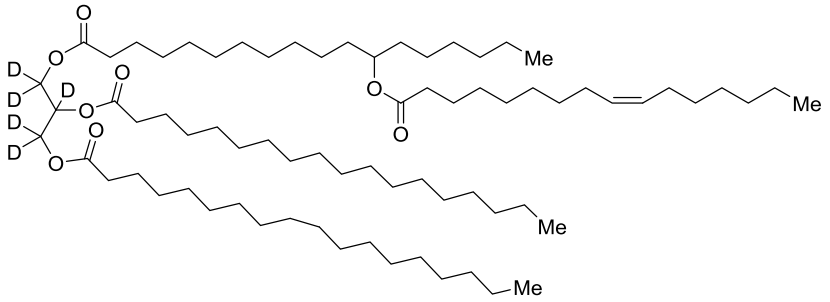
20
10
0

1-((12-POHSA)-3-hydroxypropan-2-yl-1,1,2,3,3-d5 oleate)

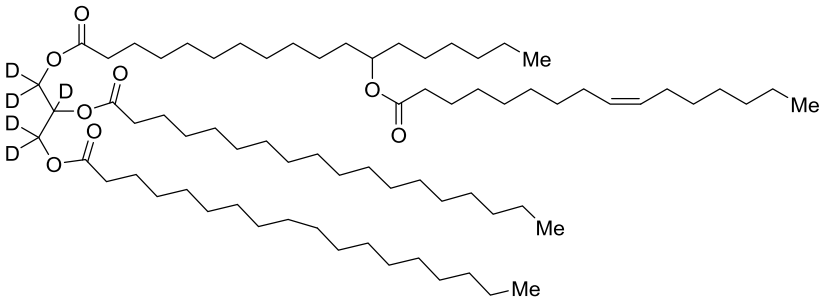


1-((12-POHSA)-3-hydroxypropan-2-yl-1,1,2,3,3-d5 oleate)

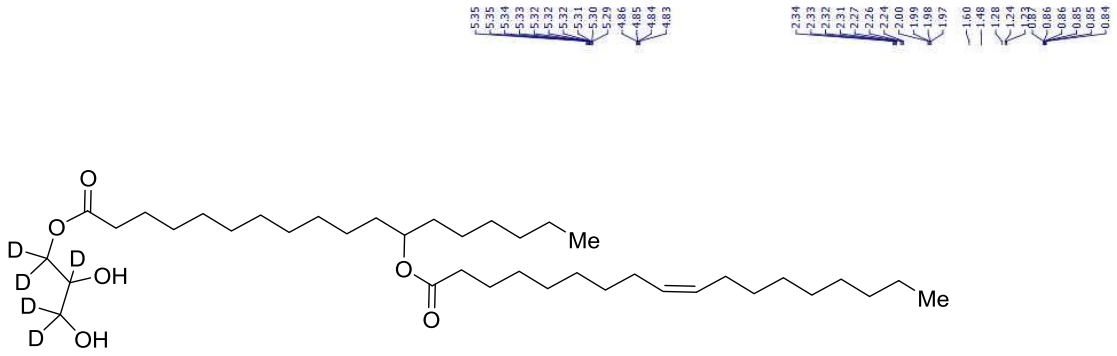




POHSA/18:1/18:0-d5-TG (**4**)



POHSA/18:1/18:0-d5-TG (**4**)



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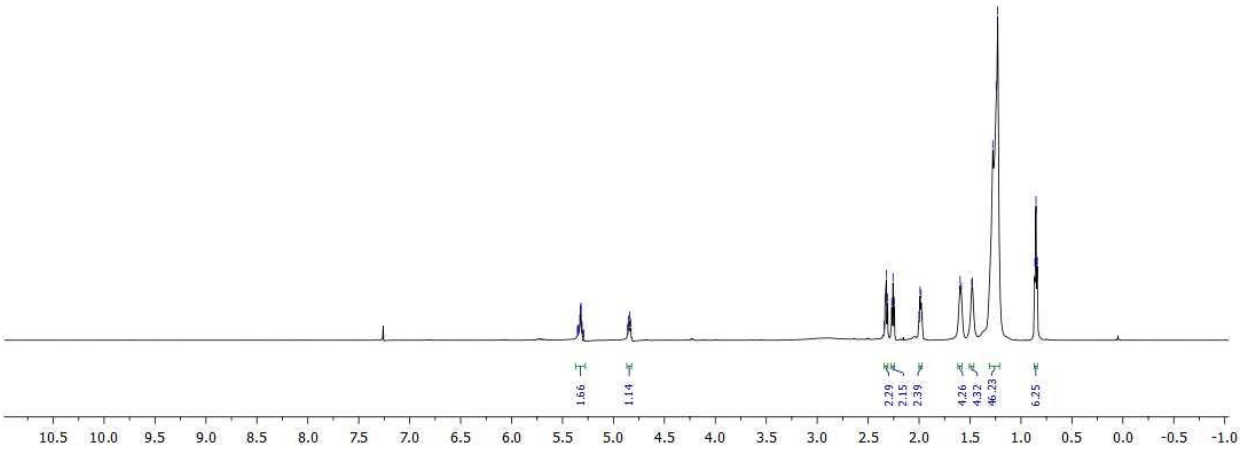
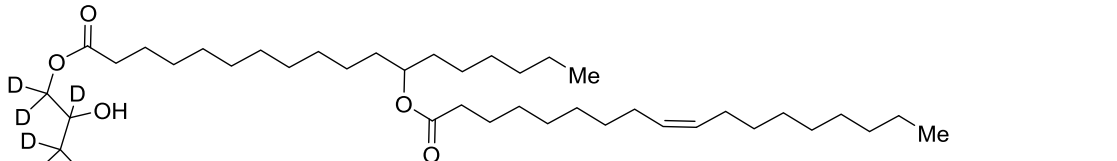
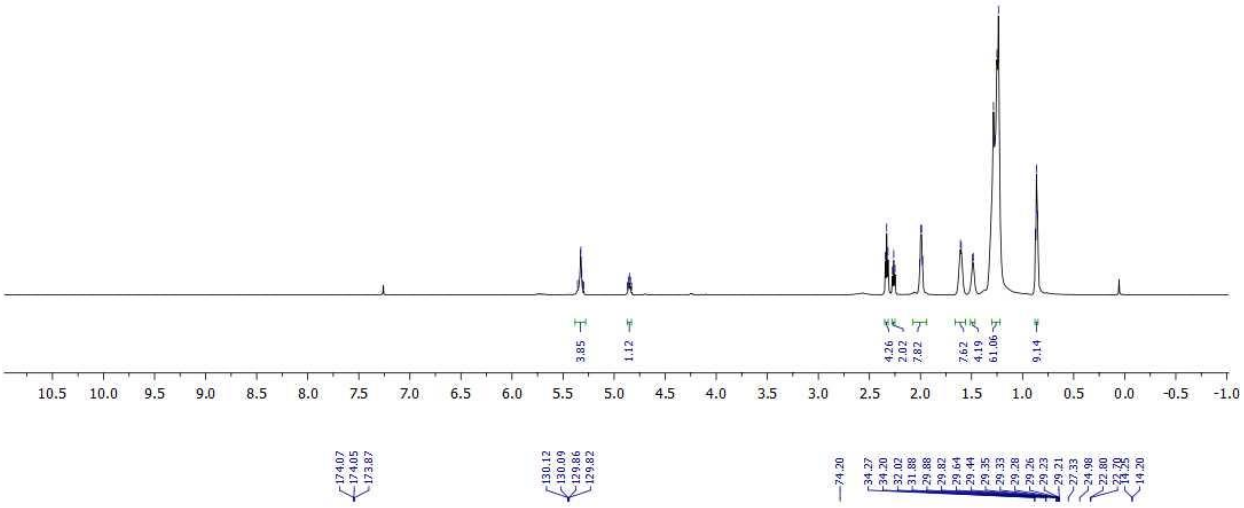


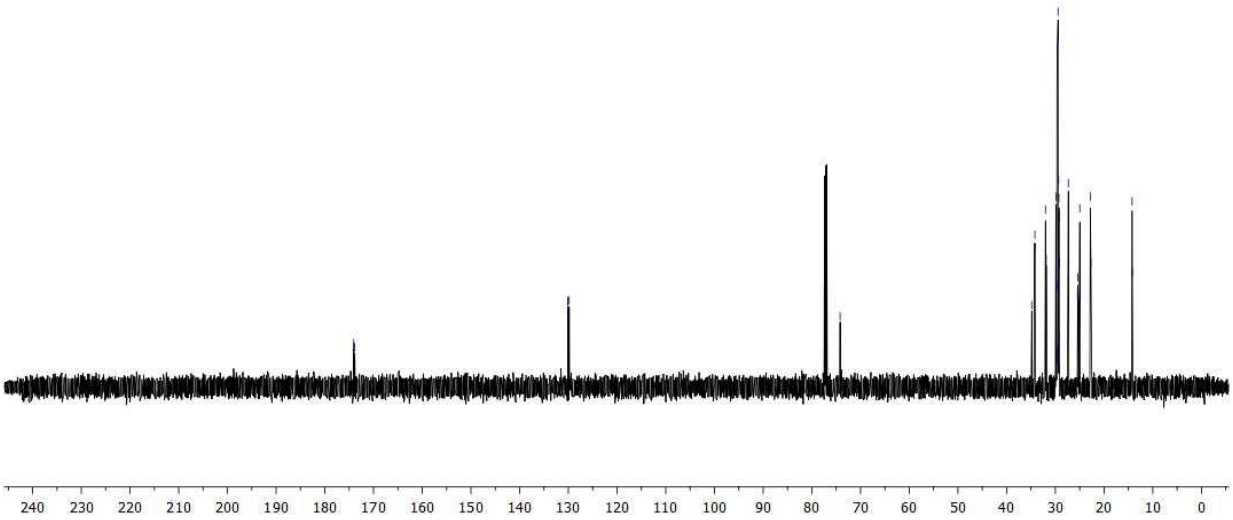


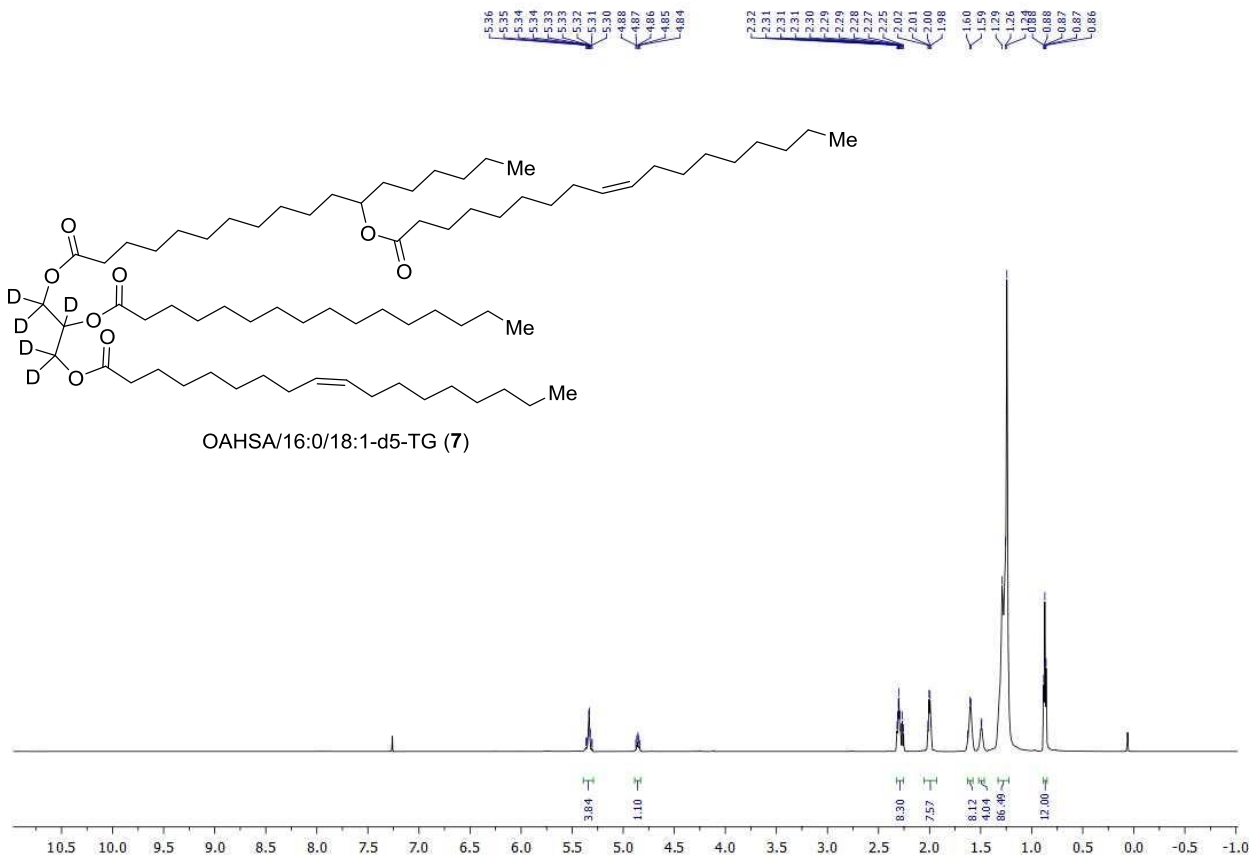
6

2-hydroxy-3-((12-(oleoyloxy) octadecanoyl)oxy)propyl-1,1,2,3,3-d5 oleate



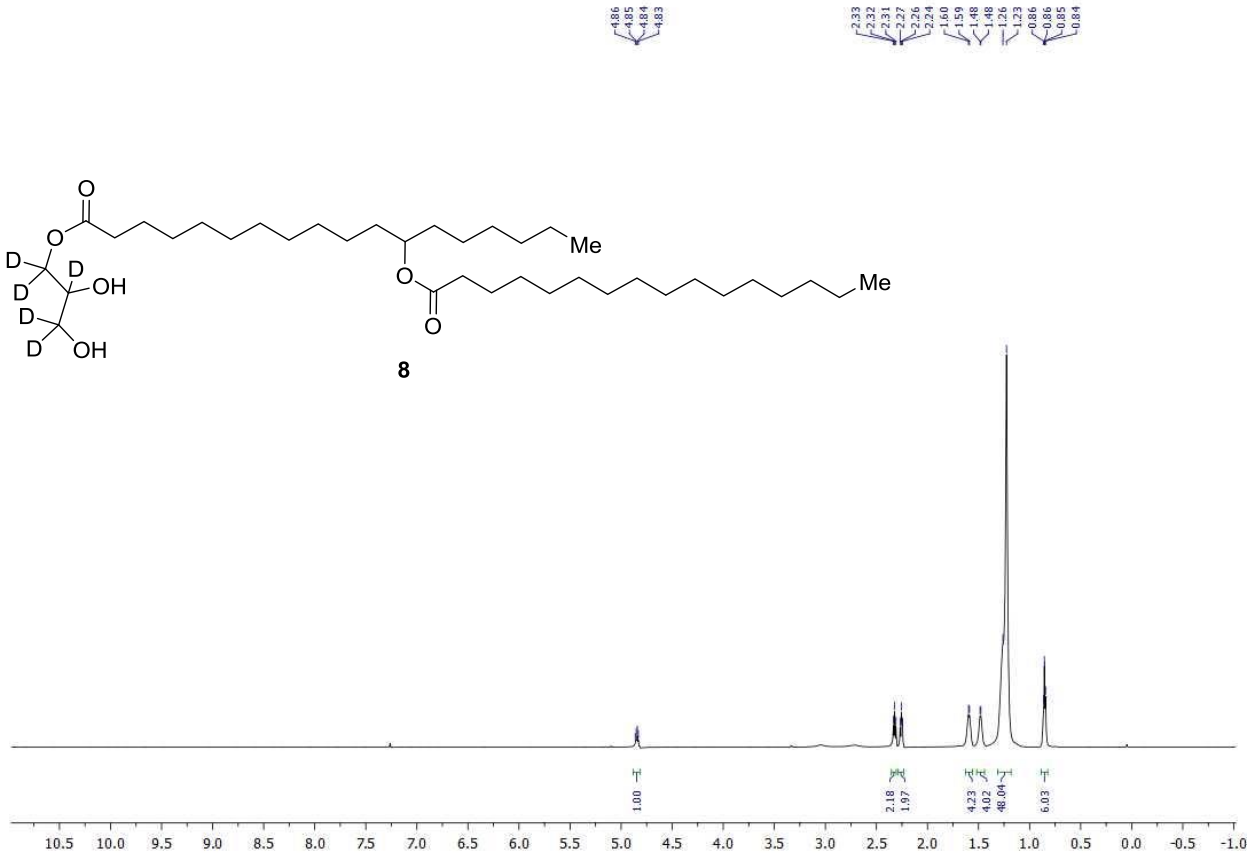
2-hydroxy-3-((12-(oleoyloxy) octadecanoyl)oxy)propyl-1,1,2,3,3-d5 oleate





OAHSA/16:0/18:1-d5-TG (**7**)

OAHSA/16:0/18:1-d5-TG (**7**)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2.31
2.27
2.26
2.24
1.60
1.59
1.48
1.48
1.26
1.23
0.86
0.86
0.85
0.84
O
O
D
D
D
OH
D
D
OH
Me
O
O
Me
1.00
2.18
1.97
4.23
4.02
48.04
6.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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1.0
0.5
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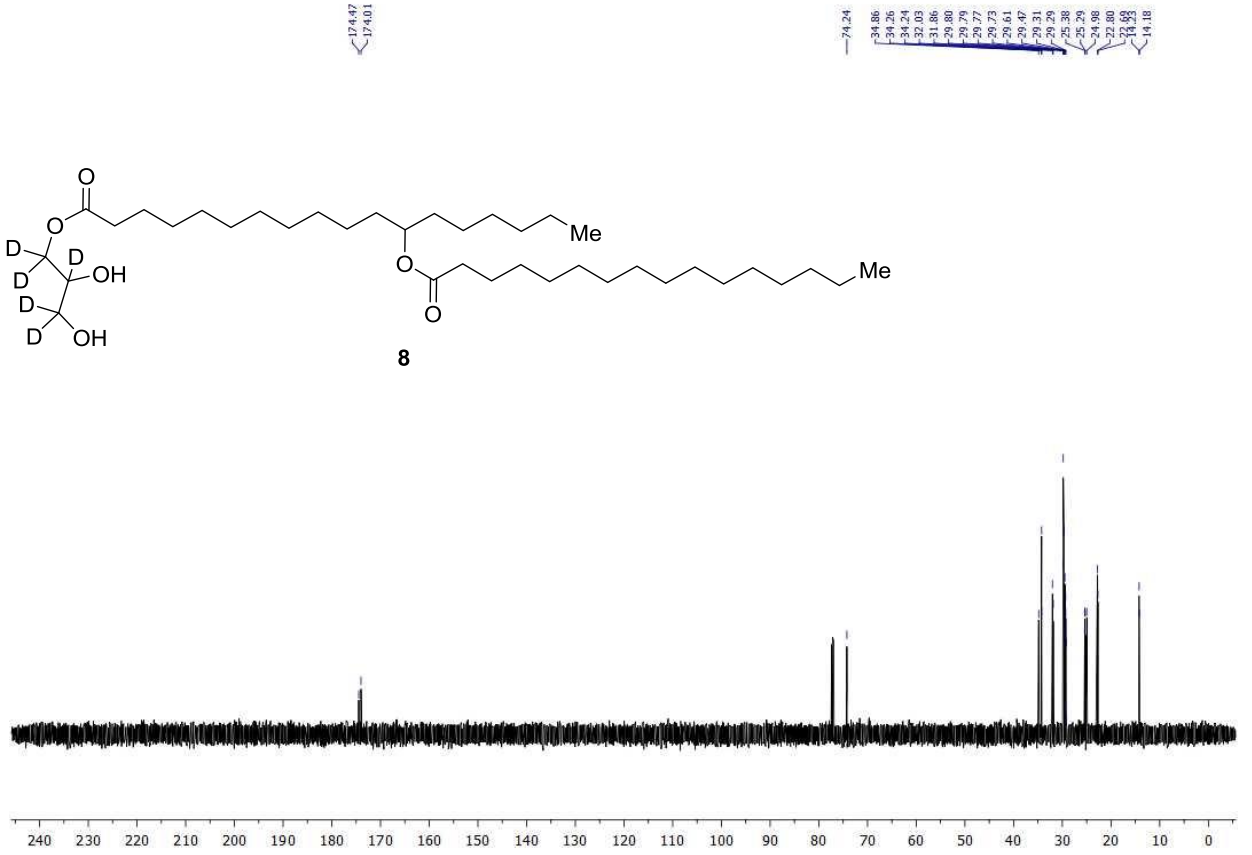
-0.5
-1.0

8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29.61
29.47
29.31
29.29
25.38
25.29
24.98
22.80
14.18
O
O
D
D
D
OH
D
D
OH
Me
O
O
Me
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220
210
200
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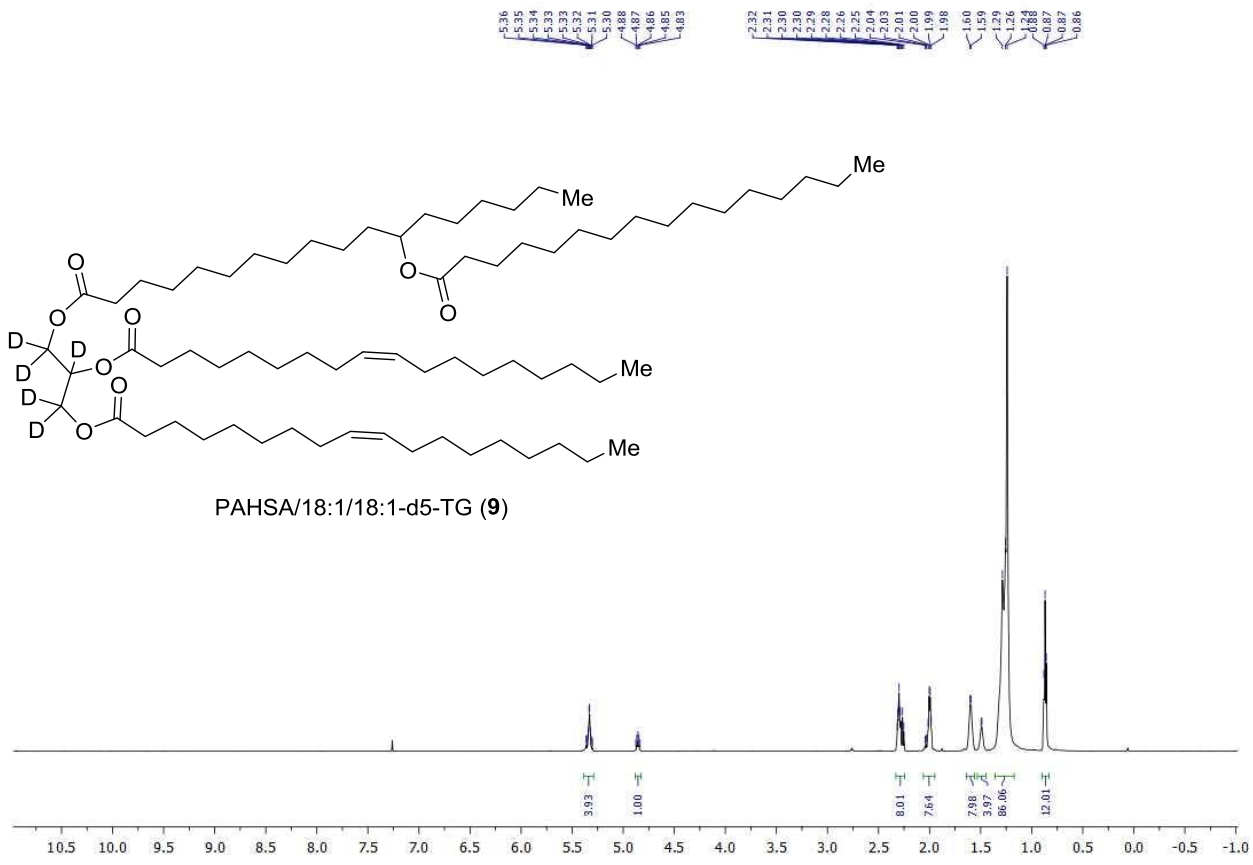
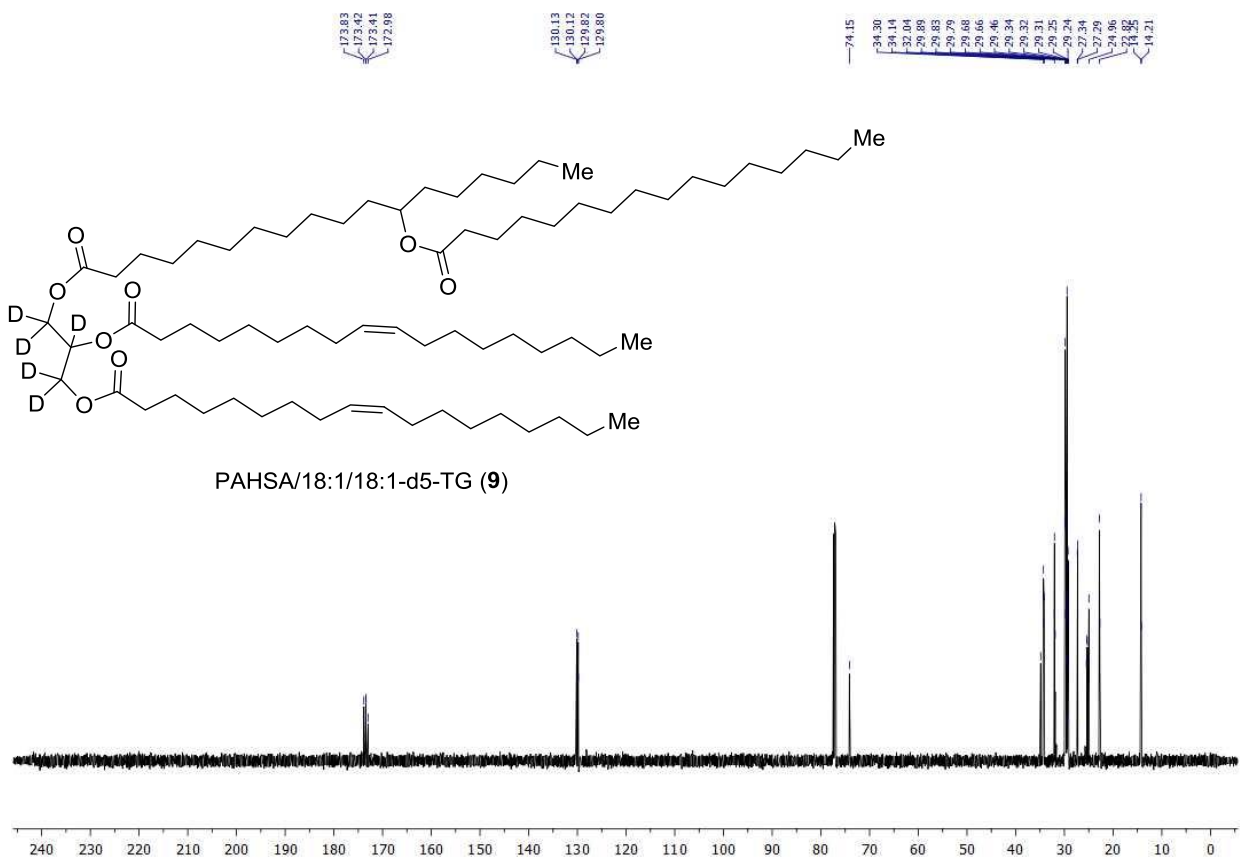
0

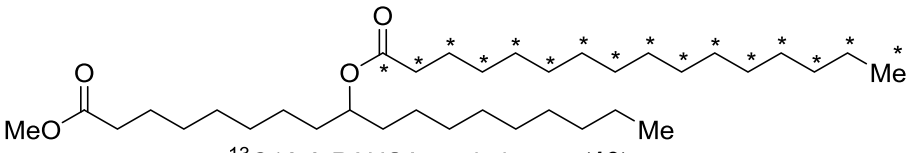
8



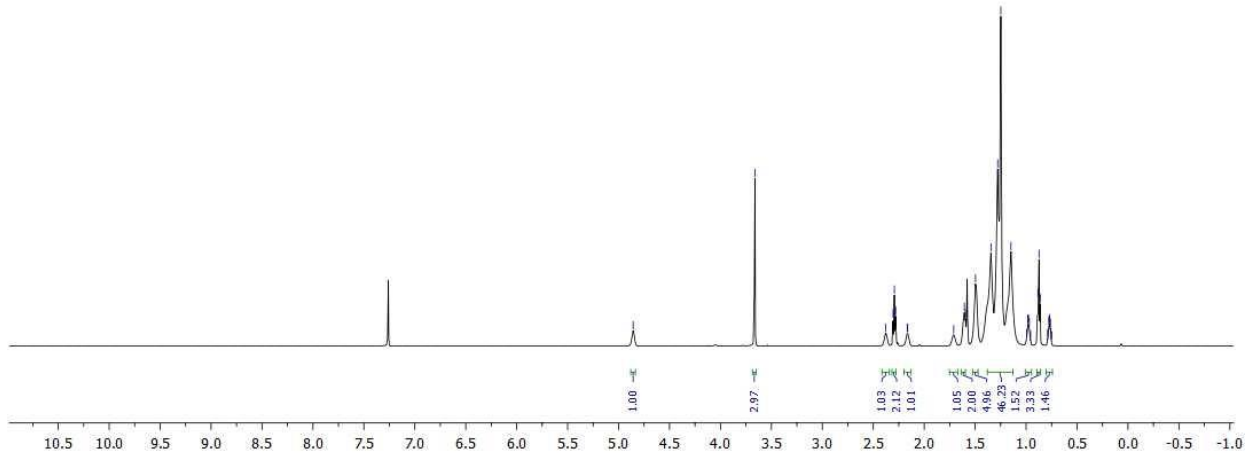
PAHSA/18:1/18:1-d5-TG (**9**)

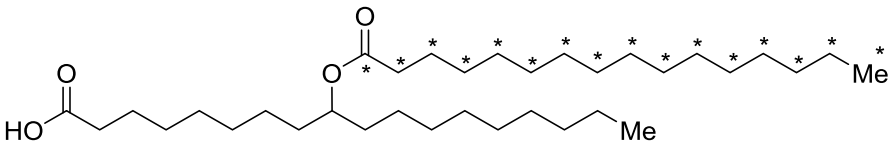


PAHSA/18:1/18:1-d5-TG (**9**)

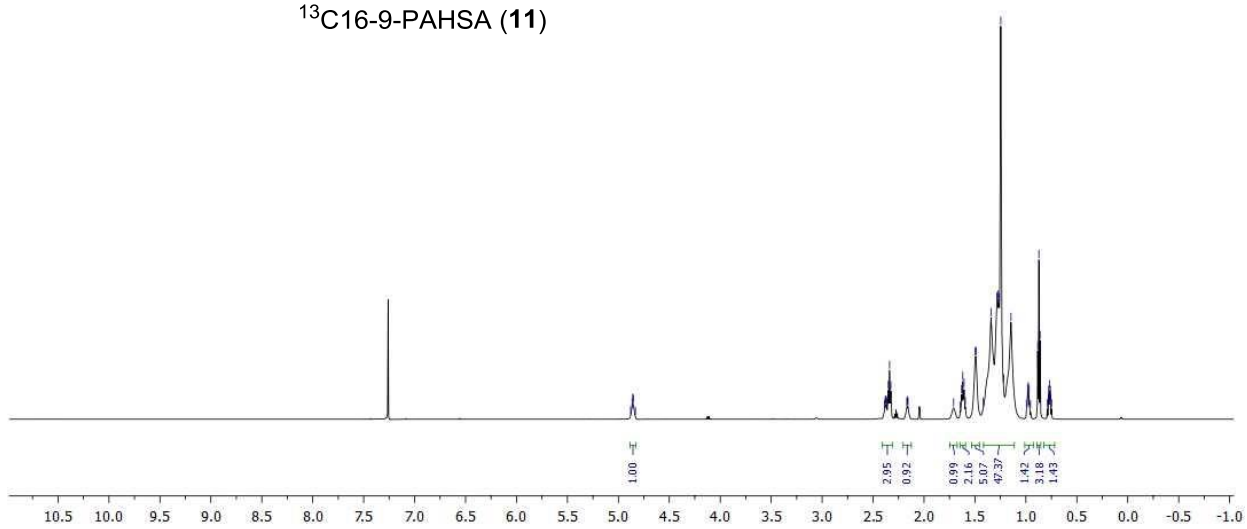


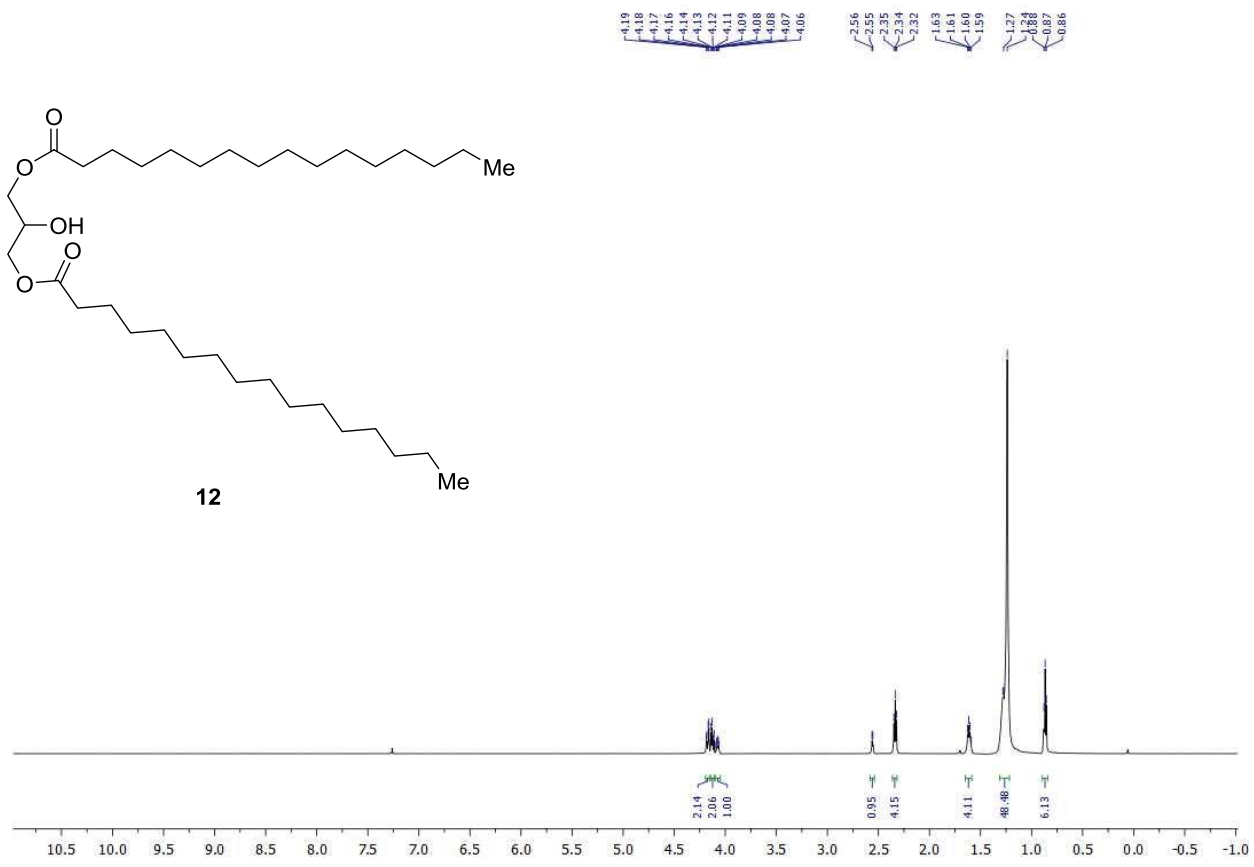
^{13}C16-9-PAHSA methyl ester (**10**)





^{13}C16-9-PAHSA (**11**)

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4.12
4.11
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4.08
4.08
4.07
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2.56
2.55
2.35
2.34
2.32
1.63
1.61
1.60
1.59
1.27
1.24
0.88
0.87
0.86
O
O
Me
OH
O
O
Me
12
2.14
2.06
1.00
0.95
4.15
4.11
48.48
6.13
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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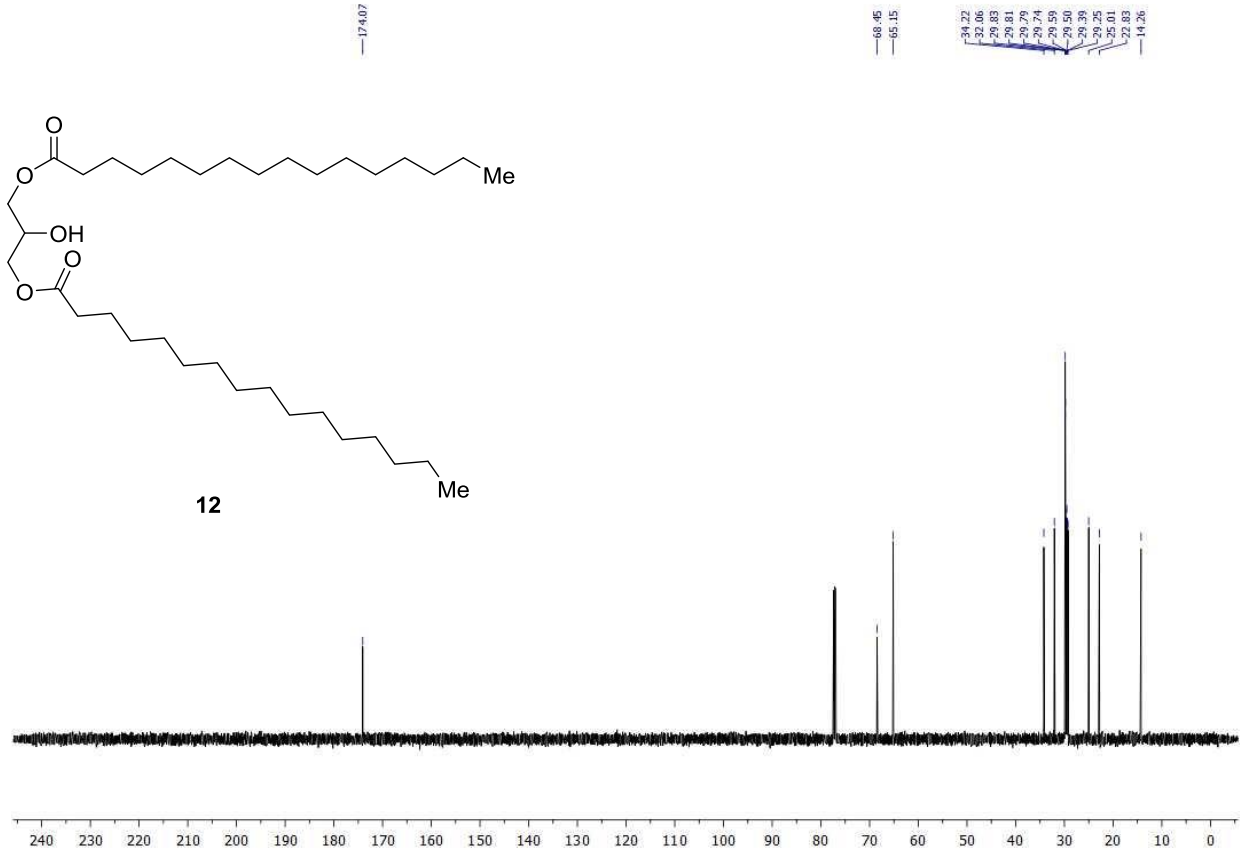
-1.0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29.39
29.25
25.01
22.83
14.26
O
O
Me
OH
O
O
Me
12
240
230
220
210
200
190
180
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150
140
130
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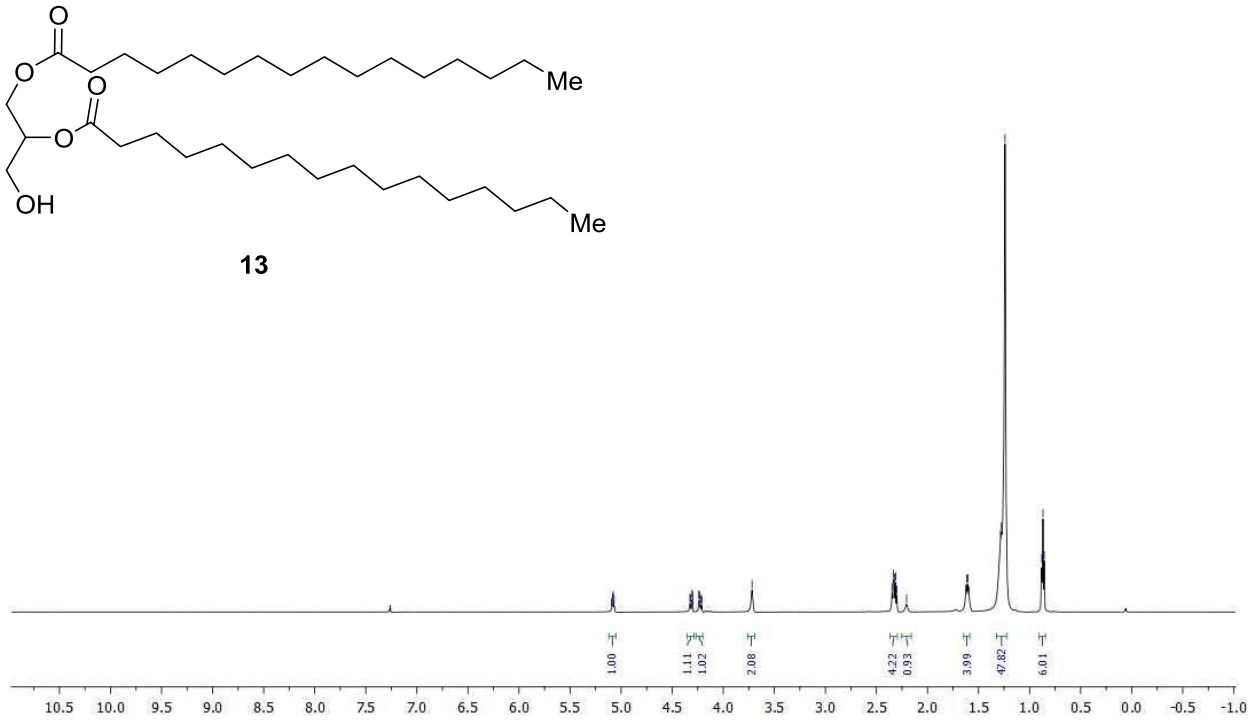
10
0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4.23
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2.33
2.32
2.31
2.30
2.20
1.63
1.62
1.60
1.28
1.24
0.88
0.87
0.86
O
O
O
O
OH
Me
Me
1.00
1.11
1.02
2.08
4.22
0.93
3.99
47.82
6.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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0.5
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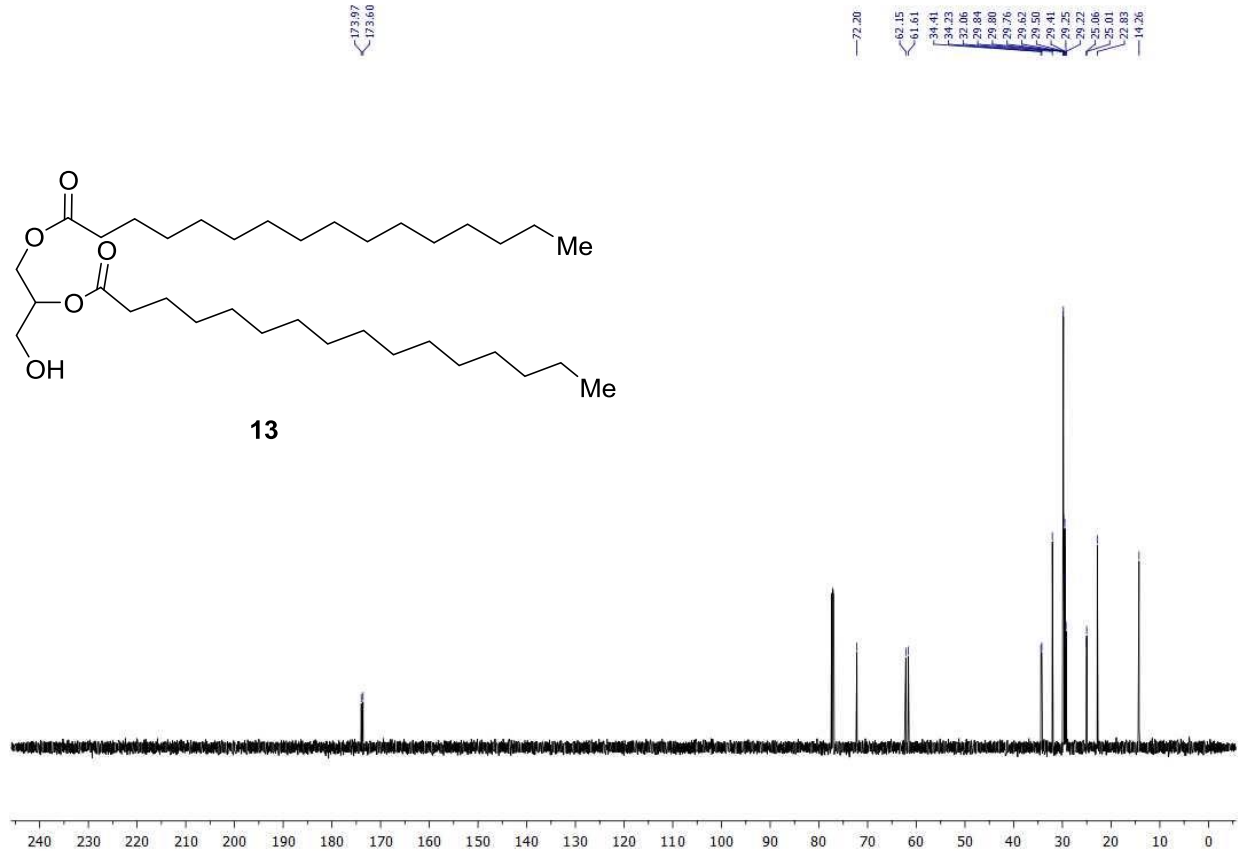
-1.0

13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29.41
29.25
29.22
25.06
25.01
22.83
14.26
O
O
O
O
OH
Me
Me
240
230
220
210
200
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140
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100
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60
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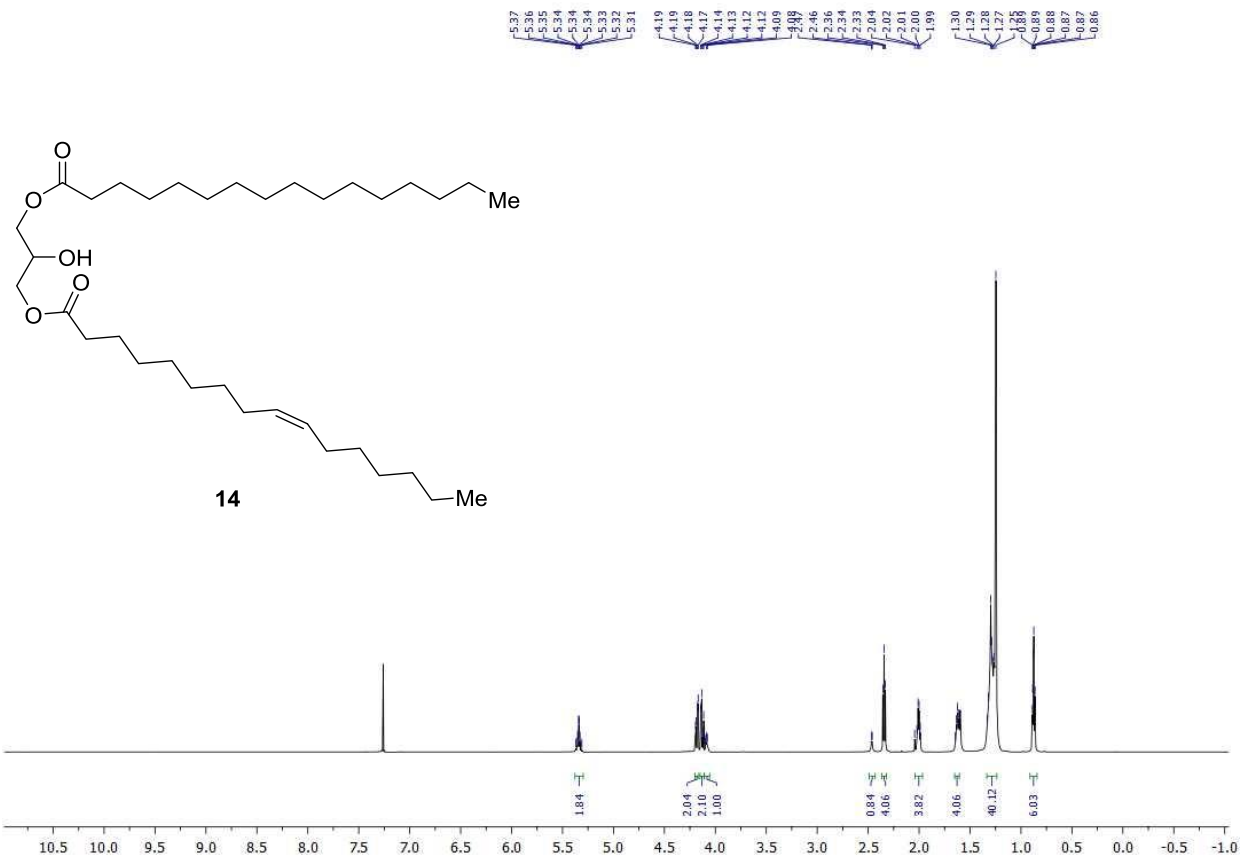
0

13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1.00
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4.06
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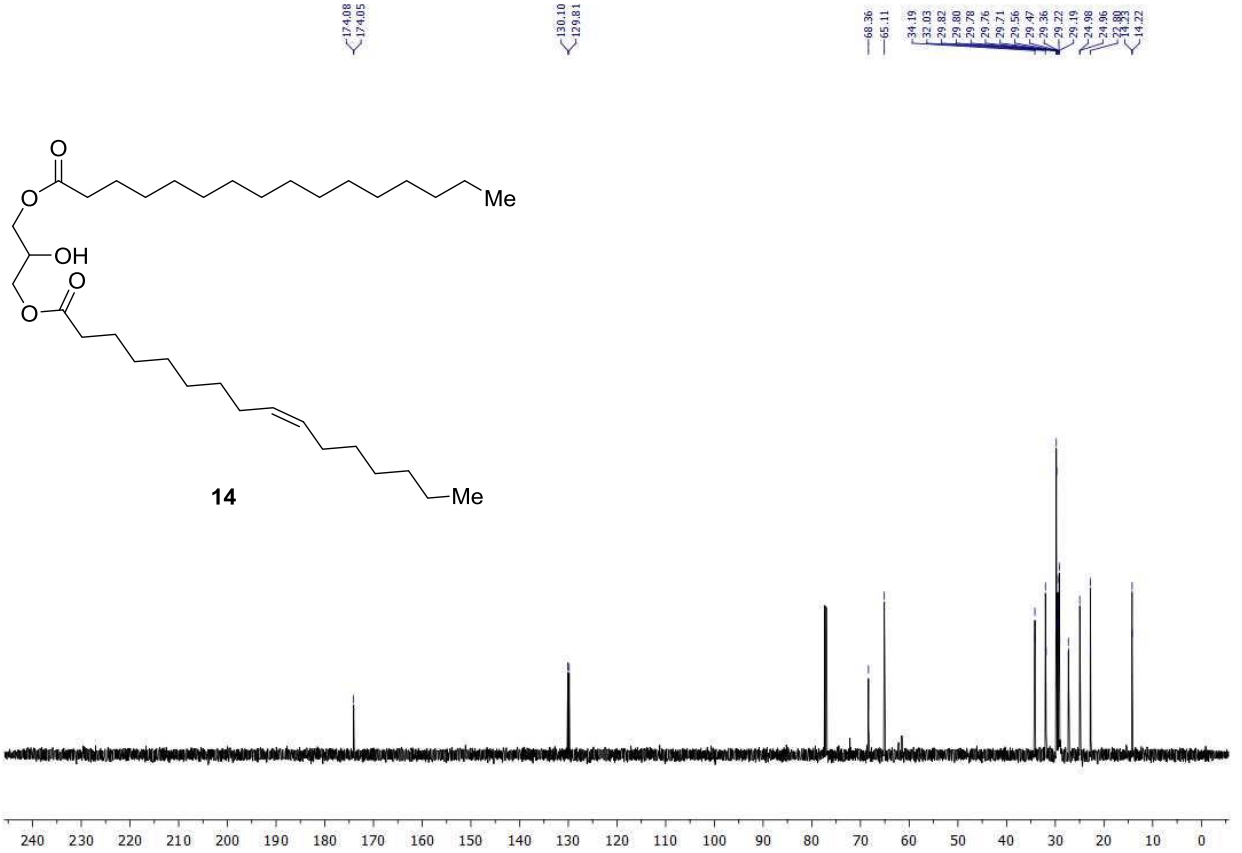
6.03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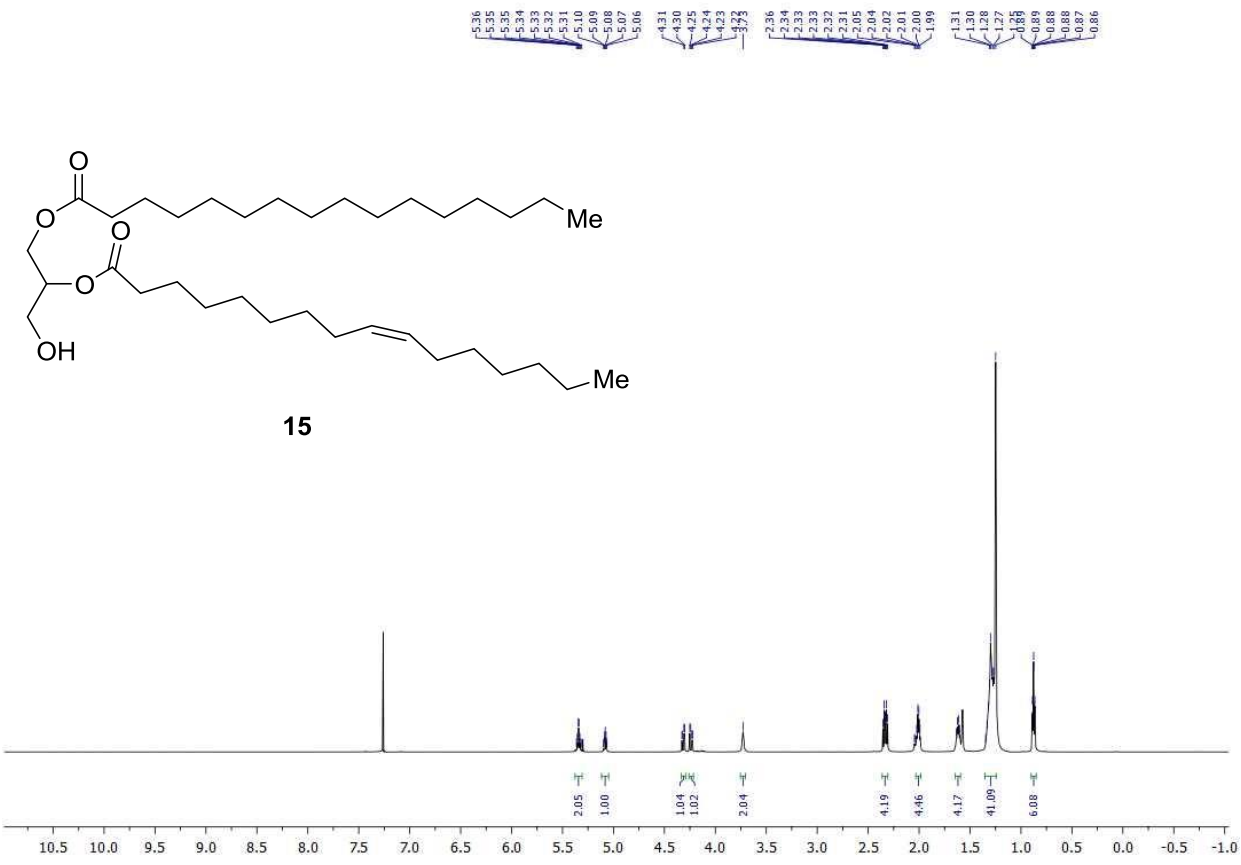
OH
O
Me



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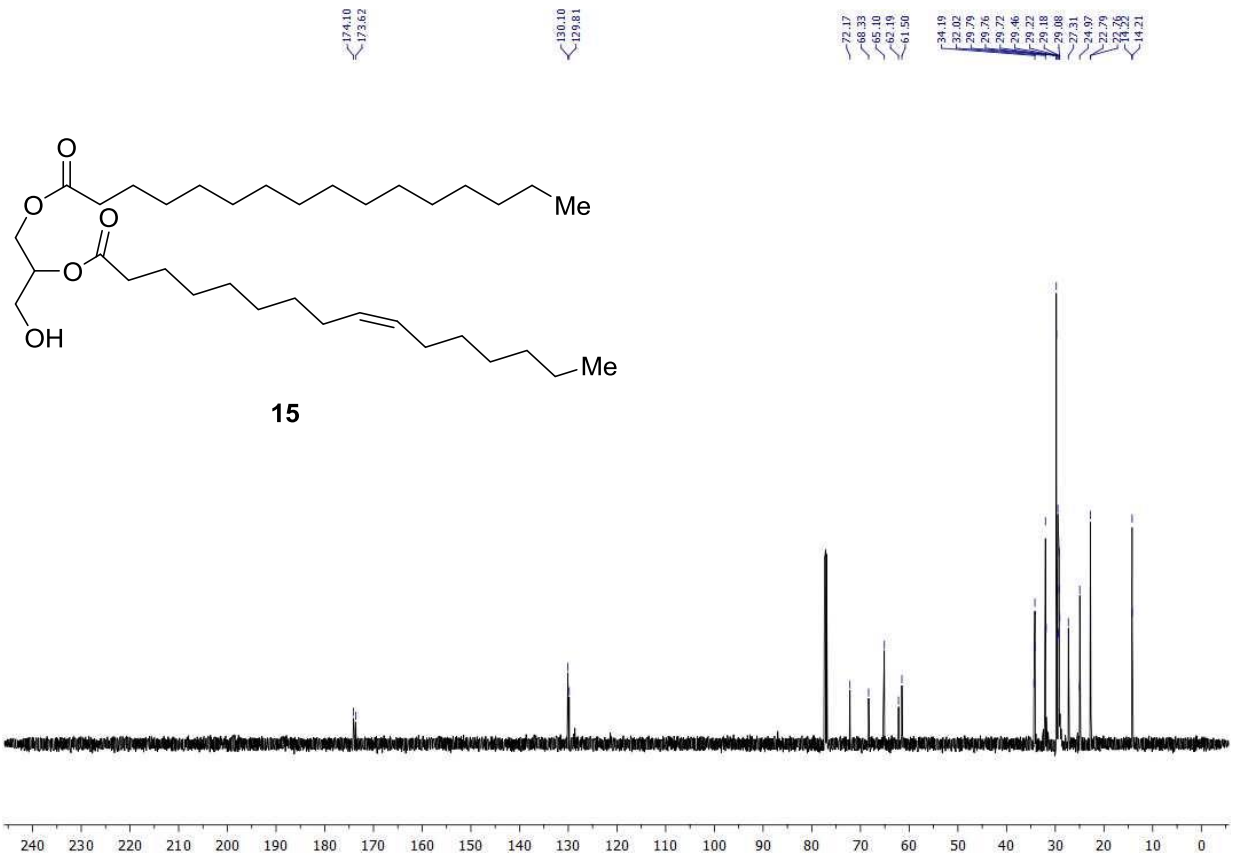

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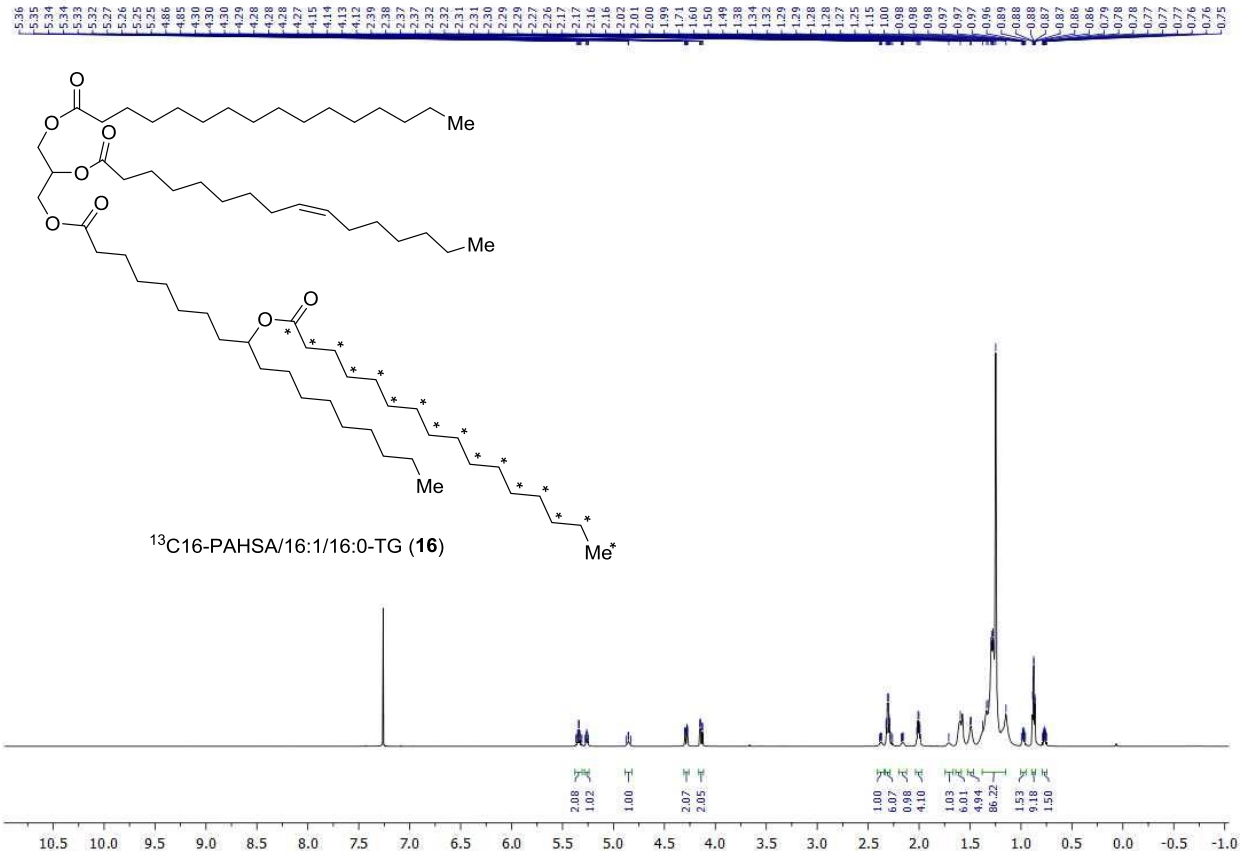
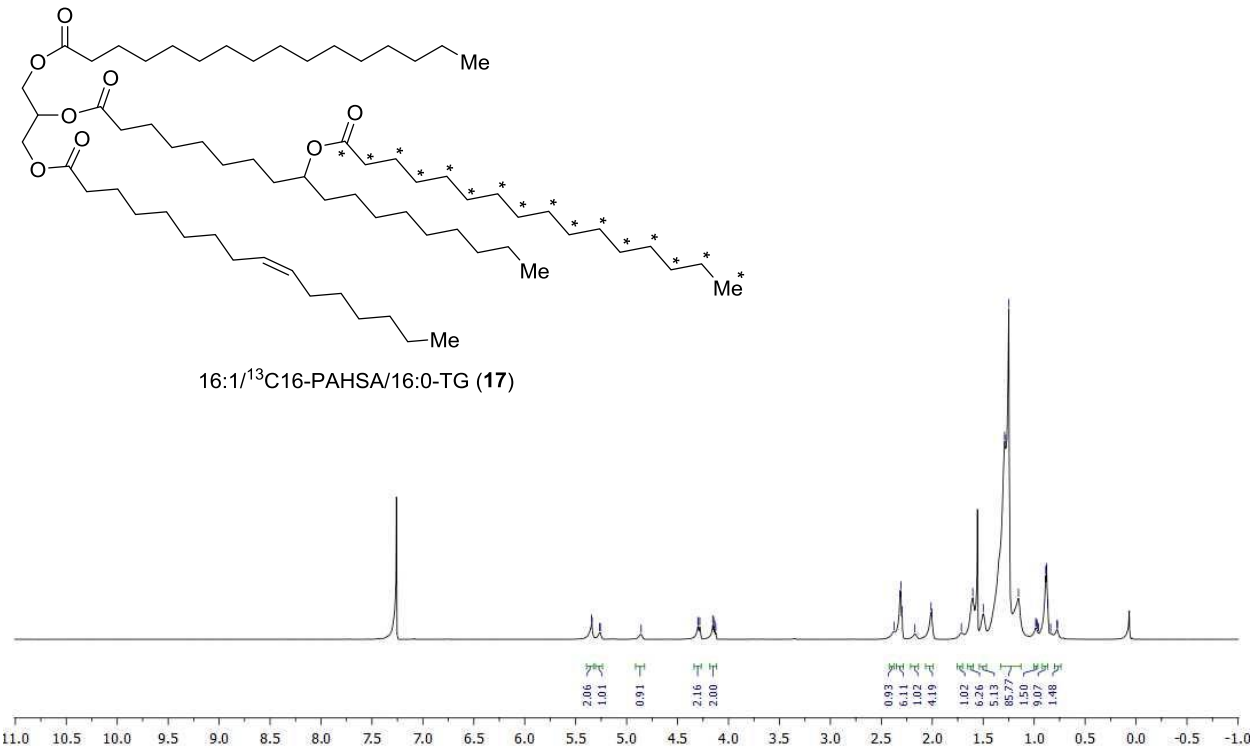
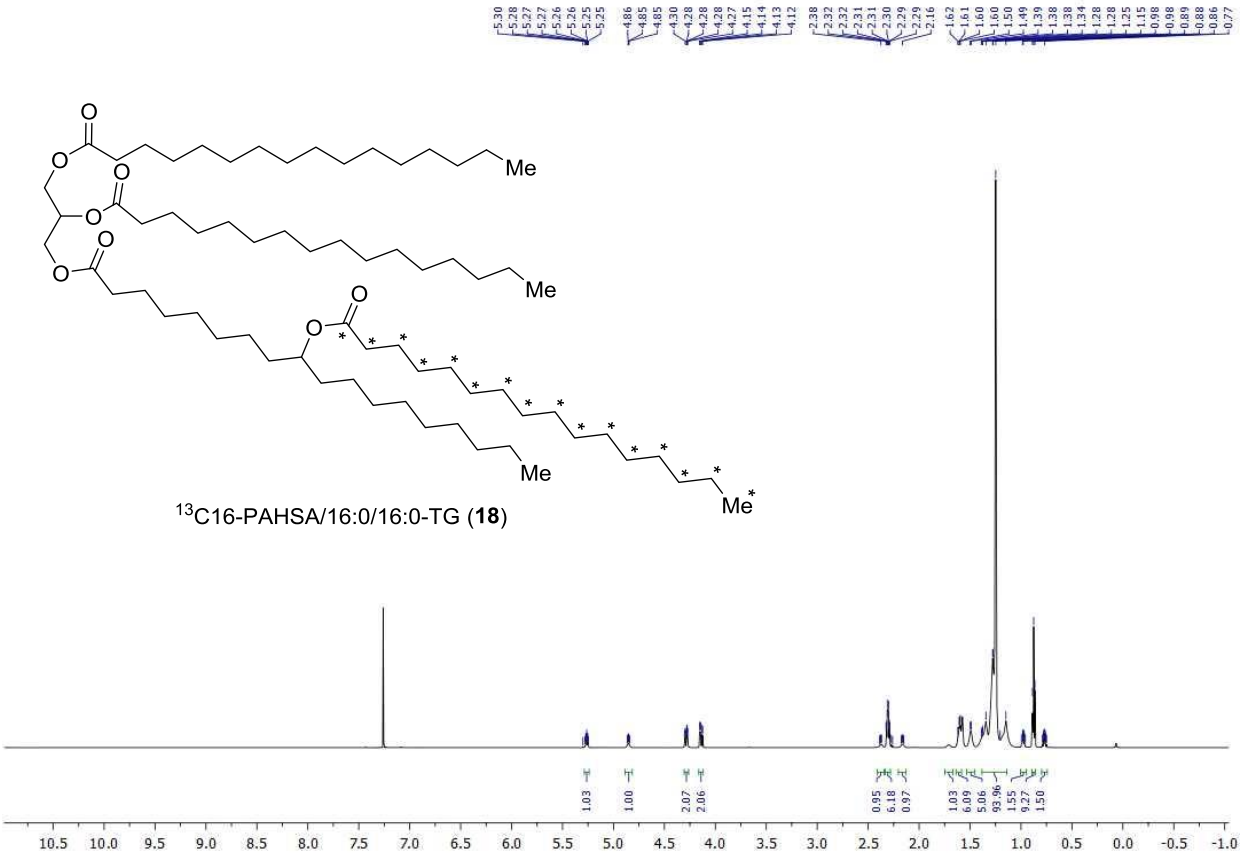


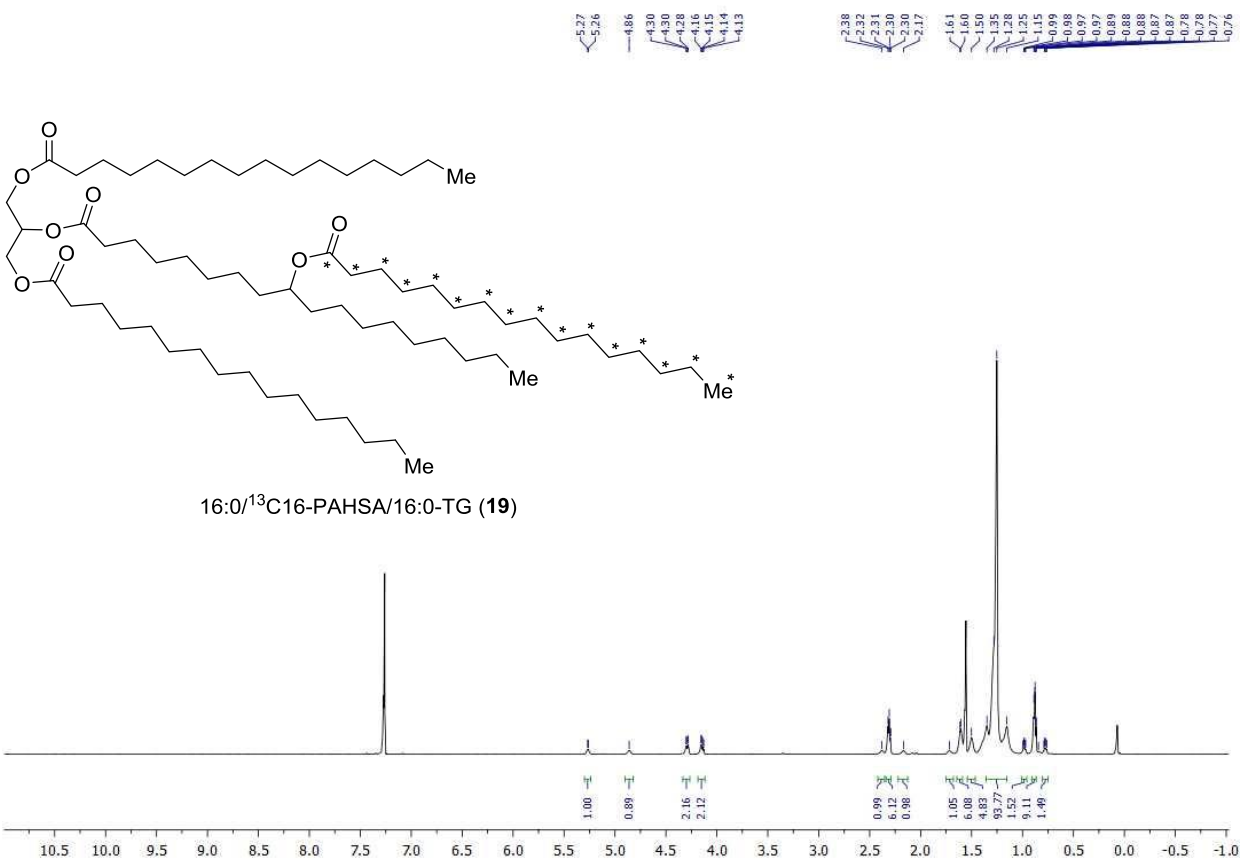
^{13}C16-PAHSA/16:1/16:0-TG (**16**)



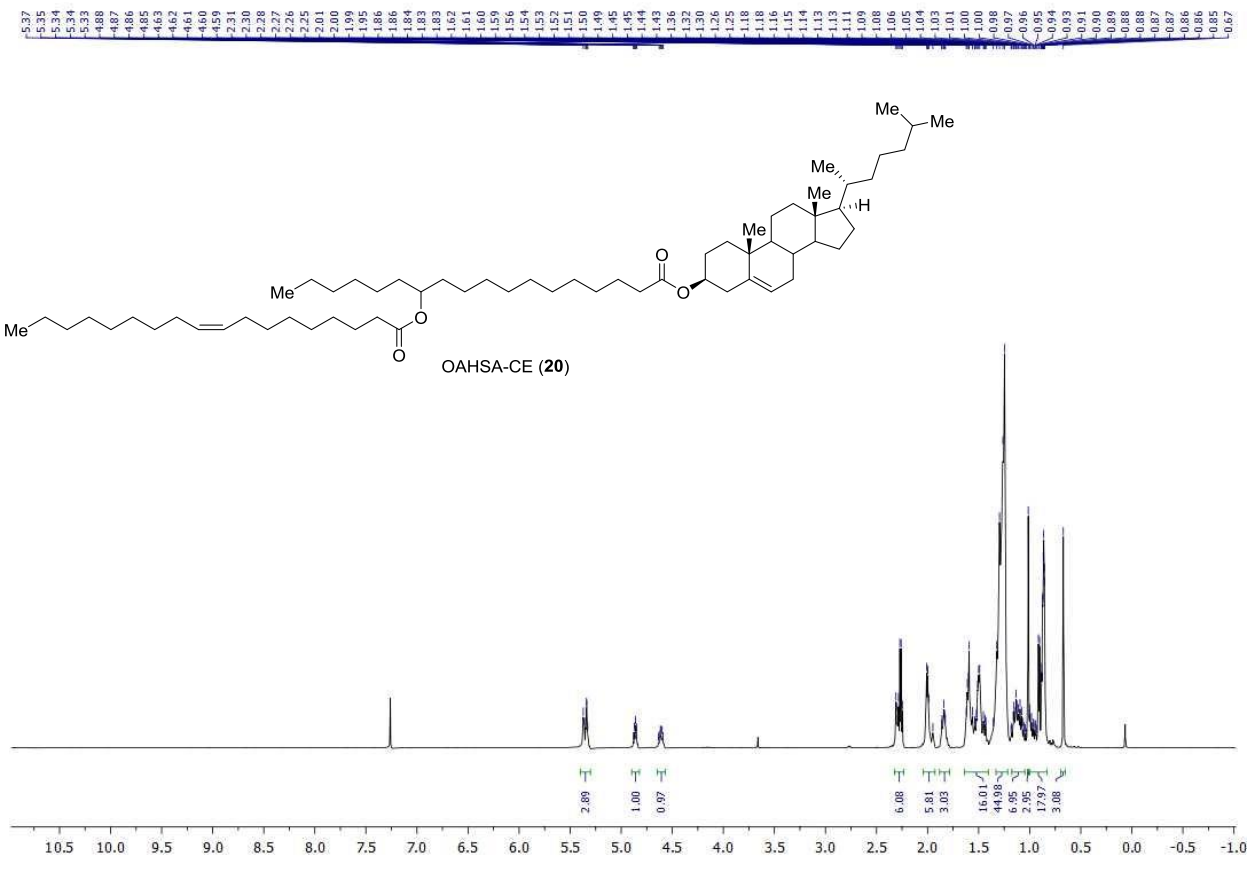
16:1/^{13}C16-PAHSA/16:0-TG (**17**)

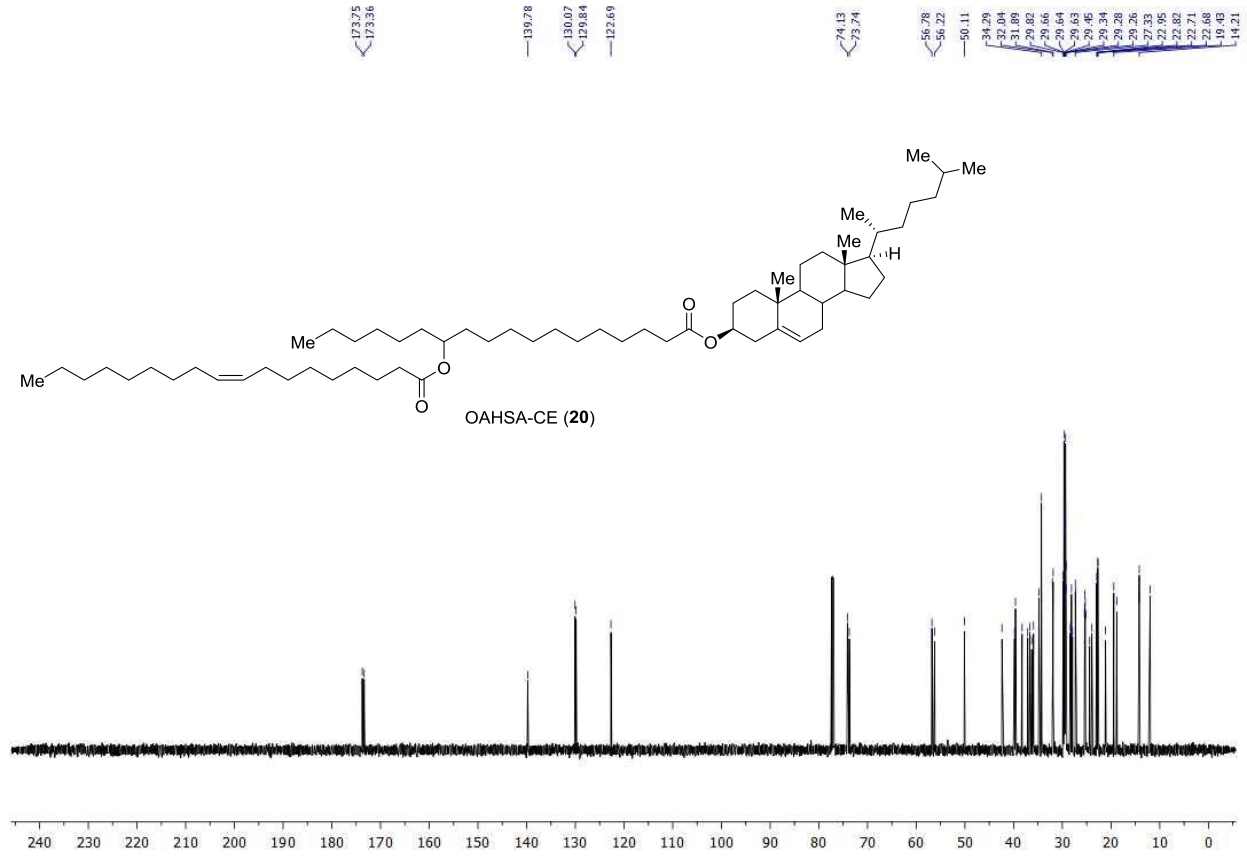


^{13}C16-PAHSA/16:0/16:0-TG (**18**)



16:0/^{13}C16-PAHSA/16:0-TG (**19**)


OAHSA-CE (20)


OAHSA-CE (20)