Electronic Supplementary Information

Determination of the critical chain length for macromolecular crystallization using structurally flexible polyketones

Yuki Ide,[a] Yumehiro Manabe,[b] Yuya Inaba,[b] Yusuke Kinoshita,[a] Jenny Pirillo,[a] Yuh Hijikata,*[a] Tomoki Yoneda,[b] Kilingaru I. Shivakumar,[a] Saki Tanaka,[c] Hitoshi Asakawa,[c] and Yasuhide Inokuma*[a,b]

[a] Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Kita 21, Nishi 10, Kita-ku, Sapporo, Hokkaido 001-0021, Japan
[b] Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Kita 13, Nishi 8, Kita-ku, Sapporo, Hokkaido 060-8628, Japan
[c] Nanomaterials Research Institute (NanoMaRi), Graduate School of Natural Science and Technology, and Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa 920-1192, Japan

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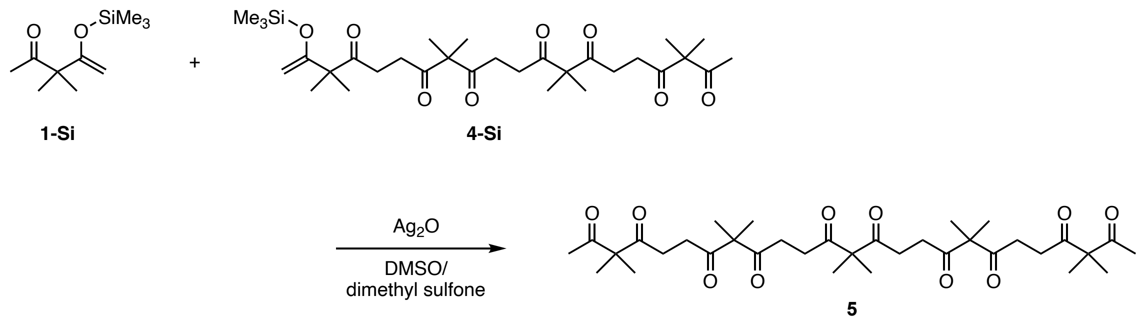
1. General Information

Solvents and reagents were purchased from WAKO Pure Chemical Industries Ltd., TCI Co., Ltd., Kanto Chemical Co., Inc., and Sigma-Aldrich Co., and used without further purification unless otherwise noted. Compounds **2**, **3**, **4**, **1-Si**, **2-Si**, **4-Si**, and **4-Si$_2$** were prepared according to the reported literatures.[1,2] All the ^{1}H, ^{13}C NMR spectra were recorded using a JEOL JMN-ECS400 spectrometer. Chemical shifts are reported in parts per million (ppm) relative to an internal standard tetramethylsilane (δ=0.00 ppm for ^{1}H) or a solvent residual peak (δ=77.16 ppm for ^{13}C in $CDCl_3$). Infrared spectra were measured using a JASCO Co. FT/IR-4700. ESI-TOF-MS spectra were recorded on a Thermo scientific Exactive spectrometer. Elemental analysis was performed using an Exceter Analytical, Inc. CE440 or MICRO CORDER JM10. MALDI-TOF mass spectra were recorded on a Bruker autoflex® maX spectrometer or Bruker Ultraflex III spectrometer. Thin layer chromatography (TLC) was performed on a silica gel sheet, MERCK silica gel 60 F_{254}. Preparative scale separations were performed using silica gel column chromatography (Wakosil® 60. 64 ~ 210 μm), a recycling HPLC LaboACE LC-5060 equipped with two JAIGEL-2HR columns in series for pentamer **5**, or a recycling HPLC LaboACE LC-7080 equipped with JAIGEL-2.5HR and 3 HR columns in series for heptamer **7**, nonamer **9**, dodecamer **11**, hexadecamer **12**, icosamer **13**, and polydisperse polymer ($N \geq 20$). Analytical HPLC chromatograms were recorded using a JASCO MD-2018 photodiode array detector quipped with a JASCO PU-2089 pump, JASCO AS-2059 sampler, JASCO CO-2060 column thermostat. Single crystal X-ray diffraction data were collected with Rigaku XtaLAB P200 diffractometer equipped with a HyPix-6000HE detector using multi-layer mirror (CuK_α radiation λ = 1.54184 Å). All structures were solved using a dual-space algorithm (SHELXT[3]) and refined using full-matrix least-squares method (SHELXL[4]). Powder X-ray diffraction (PXRD) and small angle X-ray scattering (SAXS) were measured using a Rigaku SmartLab X-ray diffractometer (CuK_α radiation λ = 1.54184 Å) equipped with a Hypix-3000 photon counting detector. Atomic force microscope (AFM) measurements were performed by frequency modulation mode using a laboratory-built AFM system combined with commercial AFM controllers. Differential Scanning Calorimetry (DSC) traces were recorded on a Hitachi DSC7000 instrument using an aluminum pan (sample amount: ca. 5 mg) under nitrogen atmosphere.

2. Synthetic Procedure

2-1 Synthesis of pentamer 5

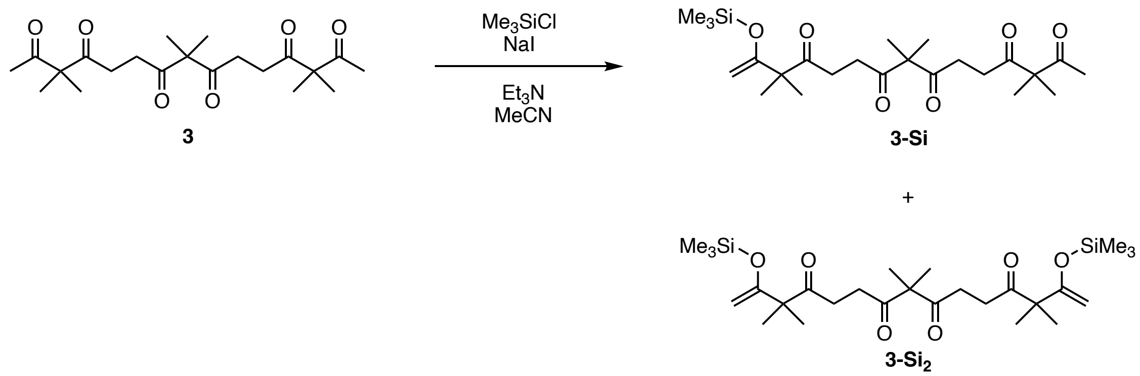


To a 50 mL round-bottom flask equipped with a reflux condenser, were added mono-silylated monomer **1-Si** (866 mg, 4.32 mmol), mono-silylated tetramer **4-Si** (500 mg, 0.864 mmol), dimethyl sulfoxide (73.9 µL, 1.04 mmol), dimethyl sulfone (1.47 g, 15.6 mmol), and silver(I) oxide (721 mg, 3.11 mmol). The reaction mixture was stirred at 100 ºC for 2 h. After cooled to room temperature, the reaction mixture was filtered through Celite pad with suction. The solid on funnel was washed with dichloromethane (100 mL), and the filtrate was evaporated under vacuum. The resulting solid was dissolved in ethyl acetate (15 mL) and washed with water (15 mL). The aqueous layer was extracted with ethyl acetate (3 × 15 mL) and the combined organic layer was washed with brine (5 × 15 mL). The organic layer was dried over anhydrous sodium sulfate, and solvents were evaporated *in vacuo*. The residue was purified by recycling preparative GPC using chloroform as a mobile phase. The separated product was dissolved in dichloromethane (0.5 mL) and recrystallized by adding diethyl ether (10 mL). The precipitated crystal was filtered on a funnel with suction using diethyl ether (20 mL) to give pentamer **5** (134 mg, 0.212 mmol, 25% yield) as a colorless solid.

3,3,8,8,13,13,18,18,23,23-Decamethylpentacosane-2,4,7,9,12,14,17,19,22,24-decaone (5) (pentamer)

R_f=0.30 (hexane:ethyl acetate:dichloromethane = 3:2:2), m.p. 96-97 ºC; ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.75-2.72 (m, 16H, ethylene), 2.16 (s, 6H, acetyl), 1.42-1.38 (18H, overlapping $C(CH_3)_2$), 1.37 ppm (s, 12H, $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.4 (2 × C=O), 208.2, 207.8, 62.2, 61.81, 61.76, 32.4-32.1 (4 × CH$_2$), 26.4, 21.83, 21.81, 21.6 ppm; IR(ATR, neat) 2991, 2981, 2936, 2921, 2871, 1692, 1462, 1441, 1389, 1374, 1363, 1237, 1209, 1197, 1174, 1164, 1127, 1088, 1070, 1036, 1011 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{35}H_{52}O_{10}Na^+$: 655.3453 [M+Na]$^+$; found: 655.3444; elemental analysis calcd (%) for $C_{35}H_{52}O_{10}$: C, 66.43; H, 8.28; N, 0.00; found: C, 66.40; H, 8.34; N, 0.04.

2-2 Silylation of trimer 3



To a 50 mL two-necked round-bottom flask, trimer **3** (5.00 g, 13.1 mmol) and sodium iodide (3.93 g, 26.2 mmol) were added. After the flask was purged with N_2 gas, acetonitrile (20 mL) and triethylamine (4.01 mL, 28.8 mmol) were added. The resulting suspension was cooled to 0 °C and trimethylchlorosilane (3.33 mL, 26.2 mmol) was added via syringe. The reaction mixture was stirred at 0 °C for 20 min and quenched by the addition of water (20 mL). From the reaction mixture, products were extracted with dichloromethane (20 mL). The aqueous layer was further extracted with dichloromethane (3 × 20 mL). The combined organic layer was washed with water (20 mL), dried over anhydrous sodium sulfate, and the solvent was evaporated. The residue was purified by silica-gel column chromatography (diameter: 4.0 cm, height: 18.0 cm, eluent: hexane/ethyl acetate = 4:1) to give mono-silylated product **3-Si** (2.06 g, 4.55 mmol, 35% yield) and bis-silylated product **3-Si₂** (844 mg, 1.60 mmol, 12% yield) as pale yellow oils.

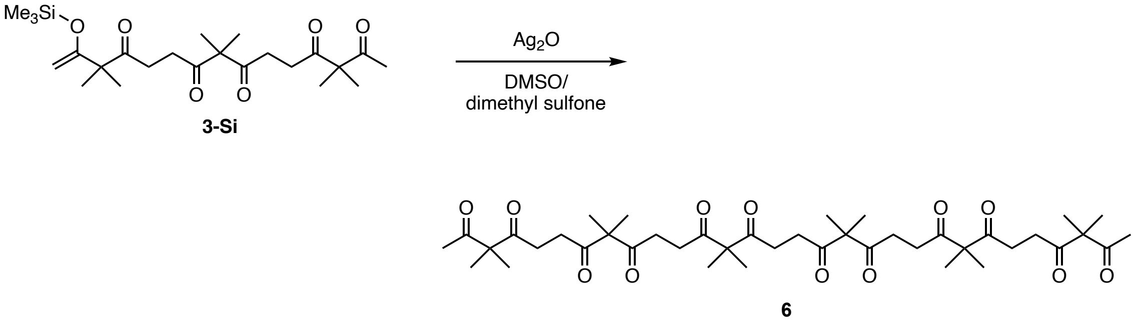
Mono-silylated product **3-Si**

R_f=0.30 (hexane:ethyl acetate = 4:1); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) : δ=4.31 (d, J = 2.1 Hz, 1H, vinyl), 4.18 (d, J = 2.1 Hz, 1H, vinyl), 2.85-2.79 (m, 2H, ethylene), 2.77-2.67 (m, 4H, ethylene), 2.67-2.60 (m, 2H, ethylene), 2.15 (s, 3H, acetyl), 1.40 (s, 6H, $C(CH_3)_2$), 1.37 (s, 6H, $C(CH_3)_2$), 1.22 (s, 12H, $C(CH_3)_2$), 0.20 (s, 9H, $Si(CH_3)_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=211.2, 208.6, 208.5, 208.4, 207.7, 162.1, 88.9, 62.2, 61.9, 53.5, 32.32, 32.27, 32.21, 31.0, 26.3, 23.1, 21.8, 21.6, 0.03; IR(ATR, neat) 2976, 2936, 2911, 2877, 1698, 1626, 1468, 1366, 1287, 1253, 1170, 1039, 1010, 847 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{24}H_{40}O_6SiNa^+$: 475.2486 $[M+Na]^+$; found: 475.2483.

Bis-silylated product **3-Si₂**

R_f=0.63 (hexane:ethyl acetate = 4:1); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=4.30 (d, J = 2.1 Hz, 2H, vinyl), 4.17 (d, J = 2.1 Hz, 2H, vinyl), 2.84-2.79 (m, 4H, ethylene), 2.69-2.62 (m, 4H, ethylene), 1.40 (s, 6H, $C(CH_3)_2$), 1.22 (s, 12H, $C(CH_3)_2$), 0.20 (s, 18H, $Si(CH_3)_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=211.2, 208.8, 162.1, 88.9, 61.9, 53.5, 32.4, 31.0, 23.1, 21.8, 0.04; IR(ATR, neat) 2975, 2936, 2911, 2878, 1670, 1625, 1286, 1253, 1169, 1038, 1009, 842 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{27}H_{48}O_6Si_2Na^+$, 547.2882 $[M+Na]^+$; found: 547.2878.

2-3 Synthesis of hexamer 6

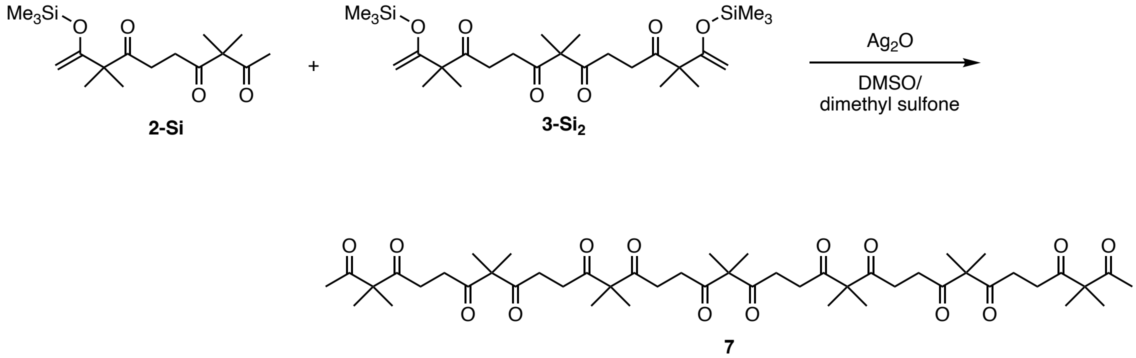


To a 30 mL round-bottom flask equipped with a reflux condenser, mono-silylated trimer **3-Si** (1.00 g, 2.21 mmol), dimethyl sulfoxide (31.4 µL, 0.442 mmol), dimethyl sulfone (624 mg, 6.63 mmol), and silver(I) oxide (308 mg, 1.33 mmol) were added. The reaction mixture was stirred at 100 °C for 2 h. After cooling to room temperature, the reaction mixture was filtered through a Celite pad with suction. The solid on funnel was washed with dichloromethane (100 mL). The filtrate was washed with water (3 × 100 mL), dried over anhydrous sodium sulfate, and solvents were removed *in vacuo*. The residue was chromatographed on a silica-gel column (diameter: 3.0 cm, height: 15.0 cm, eluent: hexane/ethyl acetate/dichloromethane = 4:3:4). The resulting crude product was washed with diethyl ether (5 mL) on a funnel with suction to give hexamer **6** (267 mg, 0.352 mmol, 32% yield) as a colorless solid.

3,3,8,8,13,13,18,18,23,23,28,28-Dodecamethyltriacontane-2,4,7,9,12,14,17,19,22,24,27,29-dodecaone (6) (hexamer)

R_f=0.23 (hexane:ethyl acetate:dichloromethane = 4:3:4); m.p. 119 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ=2.77-2.69 (m, 20H, ethylene), 2.15 (s, 6H, acetyl), 1.42-1.38 (24H, overlapping $C(CH_3)_2$), 1.37 ppm (s, 12H, $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ=208.6, 208.4 (3 × *C*=O), 208.2, 207.8, 62.2, 61.82, 61.76, 32.5-32.0 (5 × $\mathit{C}H_2$), 26.4, 21.84, 21.81, 21.6 ppm; IR(ATR, neat) 2992, 2981, 2936, 2921, 2870, 1692, 1461, 1441, 1389, 1375, 1363, 1239, 1209, 1198, 1175, 1162, 1126, 1087, 1072, 1054, 1035, 1012, 960, 951 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{42}H_{62}O_{12}Na^+$, 781.4134 $[M+Na]^+$; found: 781.4137; elemental analysis calcd (%) for $C_{42}H_{62}O_{12}$: C, 66.47; H, 8.23; N, 0.00; found: C, 66.45; H,8.30; N,0.02.

2-4 Synthesis of heptamer 7

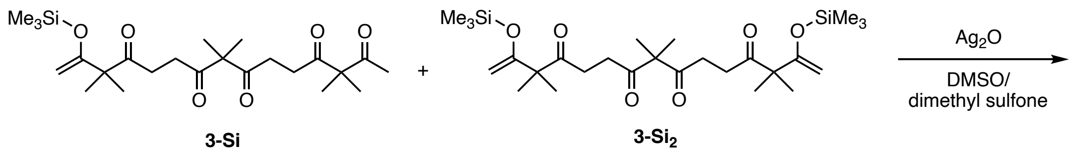


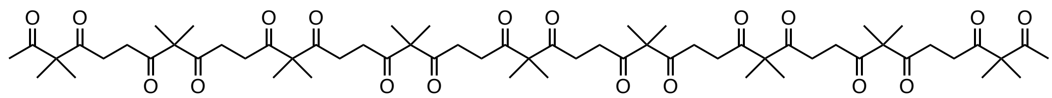
To a 50 mL round-bottom flask equipped with a reflux condenser, mono-silylated dimer **2-Si** (4.35 g, 13.3 mmol), bis-silylated trimer **3-Si₂** (1.40 g, 2.67 mmol), dimethyl sulfoxide (265 μL, 3.74 mmol), dimethyl sulfone (5.27 g, 56.0 mmol), and silver(I) oxide (2.60 g, 11.2 mmol) were added. The reaction mixture was stirred at 100 °C for 2 h, and filtered through Celite pad with suction. The solid on funnel was washed with dichloromethane (200 mL). The filtrate was washed with brine (3 × 200 mL), dried over anhydrous sodium sulfate, and solvents were removed *in vacuo*. The residue was dissolved in dichloromethane/methanol (40 mL, 1:1, v/v), and stirred with 3 M hydrochloric acid (1.1 mL) for 30 min at room temperature. The solution was neutralized with sat. aq. $NaHCO_3$ and the aqueous layer was extracted with dichloromethane (2 × 50 mL). The combined organic layer was washed with brine (50 mL), dried over anhydrous Na_2SO_4, and the solvents were evaporated under reduced pressure. The resulting mixture was separated by recycling preparative GPC using chloroform as a mobile phase. The separated product was passed through silica-gel column (diameter: 2.0 cm, height: 5.0 cm, eluent: hexane/ethyl acetate/dichloromethane = 1:1:1), and the resulting solid was washed with diethyl ether (5 mL) on a funnel to give heptamer **7** (100 mg, 0.113 mmol, 4% yield based on **3-Si₂**) as a colorless solid.

3,3,8,8,13,13,18,18,23,23,28,28,33,33-Tetradecamethylpentatriacontane-2,4,7,9,12,14,17,19,22,24,27,29,32,34-tetradecaone (7) (heptamer)

R_f=0.28 (hexane:ethyl acetate:dichloromethane = 1:1:1); m.p. 132-133 ºC; ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.78-2.68 (m, 24H, ethylene), 2.15 (s, 6H, acetyl), 1.43-1.38 (30H, overlapping $C(CH_3)_2$), 1.37 ppm (s, 12H, $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.4 (4 × C=O), 208.3, 207.8, 62.2, 61.85, 61.79 (2 × $C(CH_3)_2$), 32.4-32.2 (6 × CH_2), 26.4, 22.0-21.8 (3 × CH_3), 21.6 ppm; IR(ATR, neat) 2992, 2981, 2936, 2920, 2871, 1693, 1664, 1461, 1442, 1388, 1376, 1363, 1239, 1120, 1175, 1162, 1127, 1084, 1072, 1034, 1012, 959, 951 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{49}H_{72}O_{14}Na^+$, 907.4814 $[M+Na]^+$; found: 907.4825; elemental analysis calcd (%) for $C_{49}H_{72}O_{14}$: C, 66.49; H, 8.20; N, 0.00; found: C, 66.27; H, 8.25; N, 0.02.

2-5 Synthesis of nonamer 9





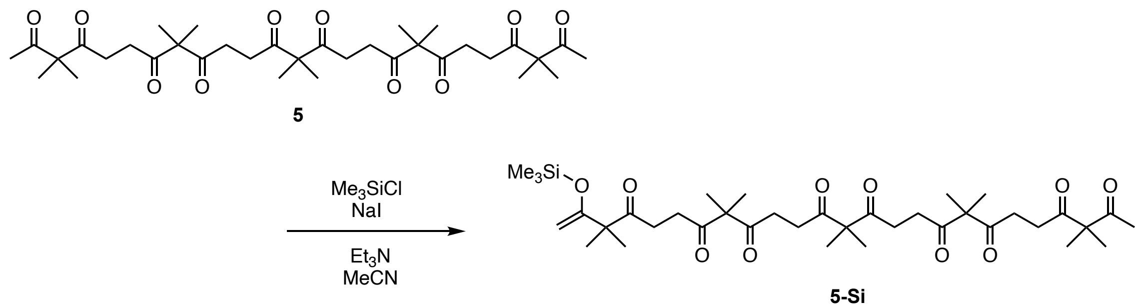
9

To a 50 mL round-bottom flask equipped with a reflux condenser, mono-silylated trimer **3-Si** (4.30 g, 9.50 mmol), bis-silylated trimer **3-Si₂** (997 mg, 1.90 mmol), dimethyl sulfoxide (189 µL, 2.66 mmol), dimethyl sulfone (3.76 g, 39.9 mmol), and silver(I) oxide (1.85 g, 7.98 mmol) were added. The reaction mixture was stirred at 100 °C for 2 h, and filtered through Celite pad with suction after cooled to room temperature. The solid on funnel was washed with dichloromethane (100 mL). The filtrate was washed with brine (3 × 100 mL), dried over anhydrous sodium sulfate, and solvents were removed *in vacuo*. The residue was dissolved in dichloromethane/methanol (28 mL, 1:1, v/v), and stirred with 3 M hydrochloric acid (0.80 mL) for 30 min at room temperature. The solution was neutralized with sat. aq. $NaHCO_3$ and the aqueous layer was extracted with dichloromethane (2 × 30 mL). The combined organic layer was washed with brine (60 mL), dried over anhydrous Na_2SO_4, and the solvents were evaporated under reduced pressure. The resulting mixture was separated by recycling preparative GPC using chloroform as a mobile phase. The separated product was passed through a silica gel column (diameter: 3.0 cm, height: 5.0 cm, eluent: hexane/ethyl acetate/dichloromethane = 1:1:1), and the resulting solids were washed with diethyl ether (5 mL) on a funnel to give nonamer **9** (149 mg, 0.131 mmol, 7% yield based on **3-Si₂**) as a colorless solid.

3,3,8,8,13,13,18,18,23,23,28,28,33,33,38,38,43,43-Octadecamethylpentatetracontan-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39,42,44-octadecaone (9) (nonamer)

R_f=0.18 (hexane:ethyl acetate:dichloromethane = 1:1:1); m.p. 140-142 ºC; ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.79-2.66 (m, 32H, ethylene), 2.15 (s, 6H, acetyl), 1.42-1.38 ppm (54H, overlapping $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.5 (6 × *C*=O), 208.3, 207.8, 62.2, 61.9-61.7 (4 × $C(CH_3)_2$), 32.5-32.1 (8 × CH_2), 26.4, 22.0-21.8 (4 × CH_3), 21.6 ppm; IR(ATR, neat) 2992, 2980, 2937, 2920, 2871, 1693, 1462, 1441, 1388, 1375, 1362, 1240, 1200, 1175, 1160, 1127, 1073, 1032, 1014, 959, 950 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{63}H_{92}O_{18}Na^+$, 1159.6176 $[M+Na]^+$; found: 1159.6161; elemental analysis calcd (%) for $C_{63}H_{92}O_{18}$: C, 66.53; H, 8.15; N, 0.00; found: C, 66.42; H, 8.21; N, 0.03.

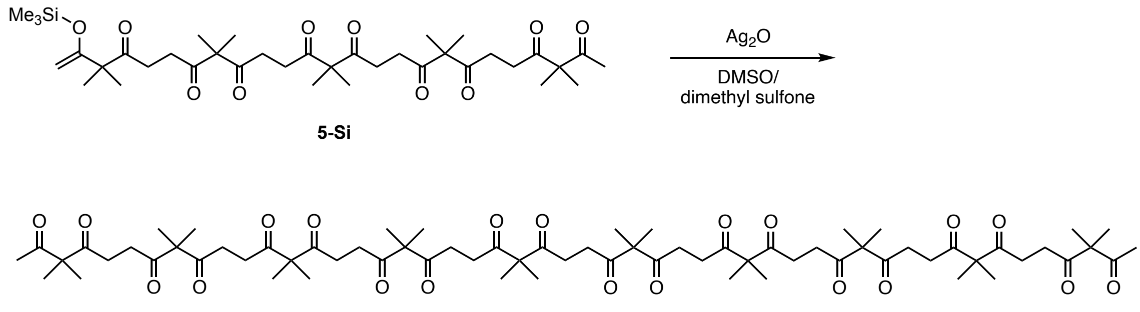
2-6 Silylation of pentamer 5



To a 20 mL two-necked round-bottom flask, pentamer **5** (1.00 g, 1.58 mmol) and sodium iodide (474 mg, 3.16 mmol) were added. After the flask was purged with N_2 gas, acetonitrile (3.0 mL) and triethylamine (485 µL, 3.50 mmol) were added. The resulting suspension was cooled to 0 °C and trimethylchlorosilane (401 µL, 3.17 mmol) was added via syringe. The reaction mixture was stirred at 0 °C for 2 h and quenched by the addition of water (10 mL). From the reaction mixture, products were extracted with dichloromethane (10 mL). The aqueous layer was further extracted with dichloromethane (3 × 10 mL). The combined organic layer was washed with water (10 mL), dried over anhydrous sodium sulfate, and the solvent was evaporated. The residue was purified by silica-gel column chromatography (diameter: 3.0 cm, height: 15.0 cm, eluent: hexane/ethyl acetate = 5:2) to give mono-silylated product **5-Si** (396 mg, 0.562 mmol, 36% yield).

Mono-silylated product **5-Si**
R_f=0.30 (hexane:ethyl acetate = 5:2); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=4.31 (d, J = 2.1 Hz, 1H, vinyl), 4.18 (d, J = 2.1 Hz, 1H, vniyl), 2.85-2.79 (m, 2H, ethylene), 2.77-2.67 (m, 12H, ethylene), 2.67-2.62 (m, 2H, ethylene), 2.15 (s, 3H, acetyl), 1.42-1.39 (18H, overlapping $C(CH_3)_2$), 1.37 (s, 6H, $C(CH_3)_2$), 1.22 (s, 6H, $C(CH_3)_2$), 0.20 ppm (s, 9H, $Si(CH_3)_3$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=211.3, 208.7-208.4 (6 × C=O), 208.3, 207.8, 162.1, 89.0, 62.3, 61.9-61.8 (3 × $C(CH_3)_2$), 53.6, 32.5-32.0 (7 × CH_2), 31.0, 26.4, 23.1, 22.1-21.8 (3 × CH_3), 21.7, 0.10 ppm; IR(ATR, neat) 2976, 2935, 2913, 2874, 1697, 1627, 1468, 1389, 1366, 1254, 1039, 1011, 850 cm^{-1}; HRMS(ESI): m/z calcd for $C_{38}H_{60}O_{10}SiNa^+$, 727.3848 $[M+Na]^+$; found: 727.3851; elemental analysis calcd (%) for $C_{38}H_{60}O_{10}Si$: C, 64.74; H, 8.58; N, 0.00; found: C, 64.39; H, 8.63; N, 0.00.

2-7 Synthesis of decamer 10

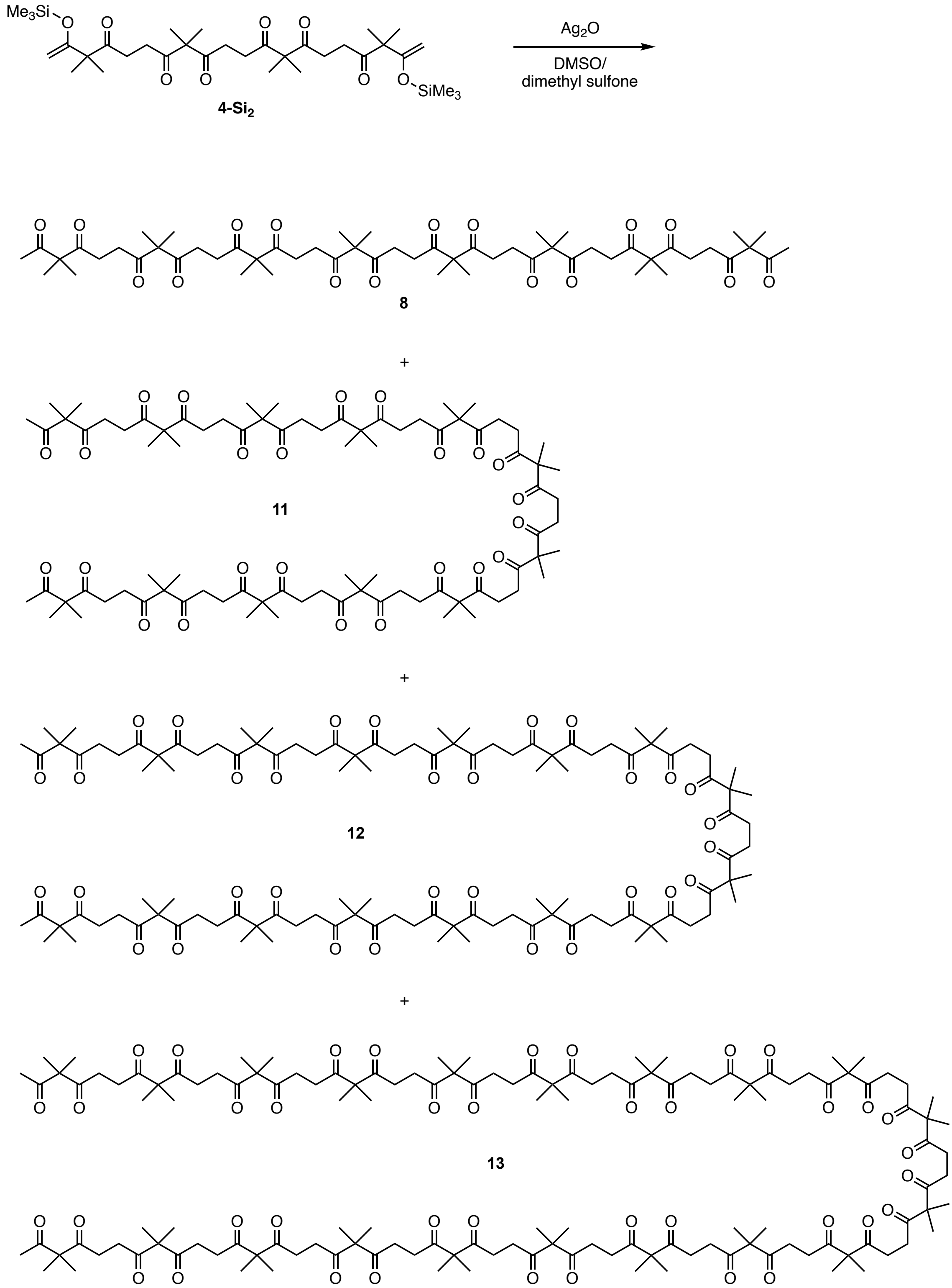


To a 10 mL round-bottom flask equipped with a reflux condenser, mono-silylated pentamer **5-Si** (300 mg, 0.426 mmol), dimethyl sulfoxide (6.04 µL, 85.1 µmol), dimethyl sulfone (120 mg, 1.27 mmol), and silver(I) oxide (59.1 mg, 0.255 mmol) were added. The reaction mixture was stirred at 100 °C for 2 h, and filtered through Celite pad with suction after cooled to room temperature. The solid on funnel was washed with dichloromethane (80 mL) and the filtrate was evaporated under vacuum. The residue was dissolved in dichloromethane (10 mL) and washed with brine (5 × 10 mL), dried over anhydrous sodium sulfate. After concentrated under reduced pressure, the mixture was chromatographed on a silica gel column (diameter: 2.0 cm, height: 17.0 cm, eluent: hexane/ethyl acetate/dichloromethane = 5:6:5). The resulting solid was suspended in methanol (0.5 mL) and sonicated for 3 min. The mixture was filtered with suction and washed with methanol (3.5 mL) to give decamer **10** (64.7 mg, 51.2 µmol, 24% yield) as a colorless solid.

3,3,8,8,13,13,18,18,23,23,28,28,33,33,38,38,43,43,48,48-Icosamethylpentacontan-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39,42,44,47,49-icosaone (10) (decamer)

R_f=0.23 (hexane:ethyl acetate:dichloromethane = 5:6:5); m.p. 142-143 ºC; ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.81-2.65 (m, 36H, ethylene), 2.15 (s, 6H, acetyl), 1.40 (48H, overlapping $C(CH_3)_2$), 1.37 ppm (12H, $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.5 (7 × C=O), 208.3, 207.8, 62.2, 61.9-61.7 (4 × $C(CH_3)_2$), 32.4-32.2 (9 × CH_2), 26.4, 22.8-22.0 (4 × CH_3), 21.6 ppm; IR(ATR, neat) 2992, 2980, 2937, 2920, 2871, 1693, 1462, 1441, 1388, 1375, 1363, 1240, 1201, 1175, 1160, 1128, 1074, 1015, 950 cm^{-1}; HRMS(ESI): m/z calcd for $C_{70}H_{102}O_{20}Na^+$, 1285.6857 $[M+Na]^+$; found: 1285.6804; elemental analysis calcd (%) for $C_{70}H_{102}O_{20}$: C, 66.54; H, 8.14; N, 0.00; found: C, 66.30; H, 8.17; N, 0.05.

2-8 Synthesis of octamer, dodecamer, hexadecamer, and icosamer (8, 11-13)



To a 50 mL round-bottom flask equipped with a reflux condenser, bis-silylated tetramer **4-Si$_2$** (2.00 g, 3.07 mmol), dimethyl sulfoxide (87.4 µL, 1.23 mmol), dimethyl sulfone (1.73 g, 18.4 mmol) and silver(I) oxide (855 mg, 3.69 mmol) were added. The reaction mixture was stirred at 100 °C for 3 h, and filtered through a Celite pad using dichloromethane (150 mL) after cooling to room temperature. The filtrate was washed with brine (3 × 150 mL), dried over anhydrous sodium sulfate, and the solvent was removed under vacuum. The residue was chromatographed on a silica gel column (diameter, 4.0 cm; height, 10.0 cm) using dichloromethane/methanol (10:1, v/v) as eluent. The residue was dissolved in dichloromethane/methanol (40 mL, 1:1, v/v), and stirred with 3 M hydrochloric acid (3.0 mL) at room temperature for 20 minutes. After neutralizing with saturated aqueous sodium bicarbonate solution (10 mL), the organic layer was separated. The aqueous layer was extracted with dichloromethane (2 × 50 mL). The combined organic layer was washed with brine (100 mL), and dried over anhydrous sodium sulfate, and the solvent was evaporated *in vacuo*. The resulting mixture of oligomers was separated by recycling preparative GPC using chloroform as a mobile phase. After the separation and evaporation, the separated oligomer fractions were passed through a silica-gel column (diameter, 1.5 cm; height, 5.0 cm) using dichloromethane/methanol (25:1, v/v) as an eluent. The resulting solids were suspended in methanol (0.5 mL) and sonicated for 3 min. The mixture was filtered on a funnel with suction and washed with methanol (3.5 mL) to give octamer **8** (137 mg, 135 µmol, 9% yield), dodecamer **11** (106 mg, 69.9 µmol, 7% yield), hexadecamer **12** (78.9 mg, 39.0 µmol, 5% yield), and icosamer **13** (49.8 mg, 19.7 µmol, 3% yield) as colorless solids.

NMR and mass spectroscopic data of octamer **8** matched with the reported literature.[S1]

3,3,8,8,13,13,18,18,23,23,28,28,33,33,38,38,43,43,48,48,53,53,58,58-Tetracosamethyl-hexacontane-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39,42,44,47,49,52,54,57,59-tetracosaone (11) (dodecamer)

m.p. 153-155 ºC; R_f=0.33 (dichloromethane/methanol = 25:1); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.80-2.64 (m, 44H, ethylene), 2.15 (s, 6H, acetyl), 1.43-1.35 ppm (72H, overlapping $C(CH_3)_2$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.5 (9 × *C*=O), 208.3, 207.8, 62.2, 61.8-61.7 (5 × *C*(CH_3)$_2$), 32.3-32.2 (11 × *C*H_2), 26.4, 22.0-21.7 (5 × *C*H_3), 21.6 ppm; IR(ATR, neat) 2992, 2980, 2937, 2920, 2873, 1692, 1463, 1441, 1388, 1377, 1364, 1240, 1203, 1174, 1161, 1128, 1074, 1014, 952 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{84}H_{122}O_{24}Na_2^{2+}$, 780.4055 [$M$+2Na]$^{2+}$; found: 780.4042; elemental analysis calcd (%) for $C_{84}H_{122}O_{24}$: C, 66.56; H, 8.11; N, 0.00; found: C, 66.32; H, 8.15; N, 0.01.

3,3,8,8,13,13,18,18,23,23,28,28,33,33,38,38,43,43,48,48,53,53,58,58,63,63,68,68,73,73,78,78-Dotriacontamethyloctacontane-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39,42,44,47,49,52,54,57,59,62,64,67,69,72,74,77,79-dotriacontaone (12) (hexadecamer)

m.p. 158-160 ºC; R_f=0.33 (dichloromethane/methanol = 25:1); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.82-2.64 (m, 60H, ethylene), 2.15 (s, 6H, acetyl), 1.43-1.35 ppm (96H, overlapping $C(CH_3)_2$); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6 208.5-208.4 (13 × *C*=O), 208.3, 207.8, 62.2, 62.0-61.6 (7 × *C*(CH_3)$_2$), 32.4-32.2 (15 × *C*H_2), 26.4, 22.2-21.7 (7 × *C*H_3), 21.6 ppm; IR(ATR, neat) 2991, 2980, 2937, 2921, 2874, 1695, 1463, 1442, 1388, 1364, 1240, 1074, 1015, 951 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{112}H_{162}O_{32}Na_2^{2+}$, 1032.5417 [$M$+2Na]$^{2+}$; found: 1032.5378. elemental analysis calcd (%) for $C_{112}H_{162}O_{32}$: C, 66.58; H, 8.08; N, 0.00; found: C, 66.27; H, 8.13; N, 0.01.

3,3,8,8,13,13,18,18,23,23,28,28,33,33,38,38,43,43,48,48,53,53,58,58,63,63,68,68,73,73,78,78,83,83,88,88,93,93,98,98-Tetracontamethylhectane-2,4,7,9,12,14,17,19,22,24,27,29,32,34,37,39,42,44,47,49,52,54,57,59,62,64,67,69,72,74,77,79,82,84,87,89,92,94,97,99-tetracontaone (13) (icosamer)

m.p. 164-167 ºC; R_f=0.33 (dichloromethane/methanol = 25:1); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.85-2.61 (m, 76H, ethylene), 2.15 (s, 6H, acetyl), 1.44-1.34 ppm (120H, overlapping $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.6, 208.5-208.3 (17 × *C*=O), 208.3, 207.8, 62.2, 62.0-61.6 (9 × $C(CH_3)_2$), 32.4-32.0 (19 × CH_2), 26.4, 22.0-21.7 (9 × CH_3), 21.6 ppm; IR(ATR, neat) 2980, 2937, 2920, 2875, 1692, 1464, 1388, 1364, 1240, 1074, 1014, 951 cm^{-1}; HRMS(ESI): *m/z* calcd for $C_{140}H_{202}O_{40}Na_2^{2+}$, 1284.6778 $[M+2Na]^{2+}$; found, 1284.6773; elemental analysis calcd (%) for $C_{140}H_{202}O_{40}$: C, 66.59; H, 8.06; N, 0.00; found: C, 66.30; H, 8.14; N, 0.01.

3. MALDI-TOF Mass Spectra

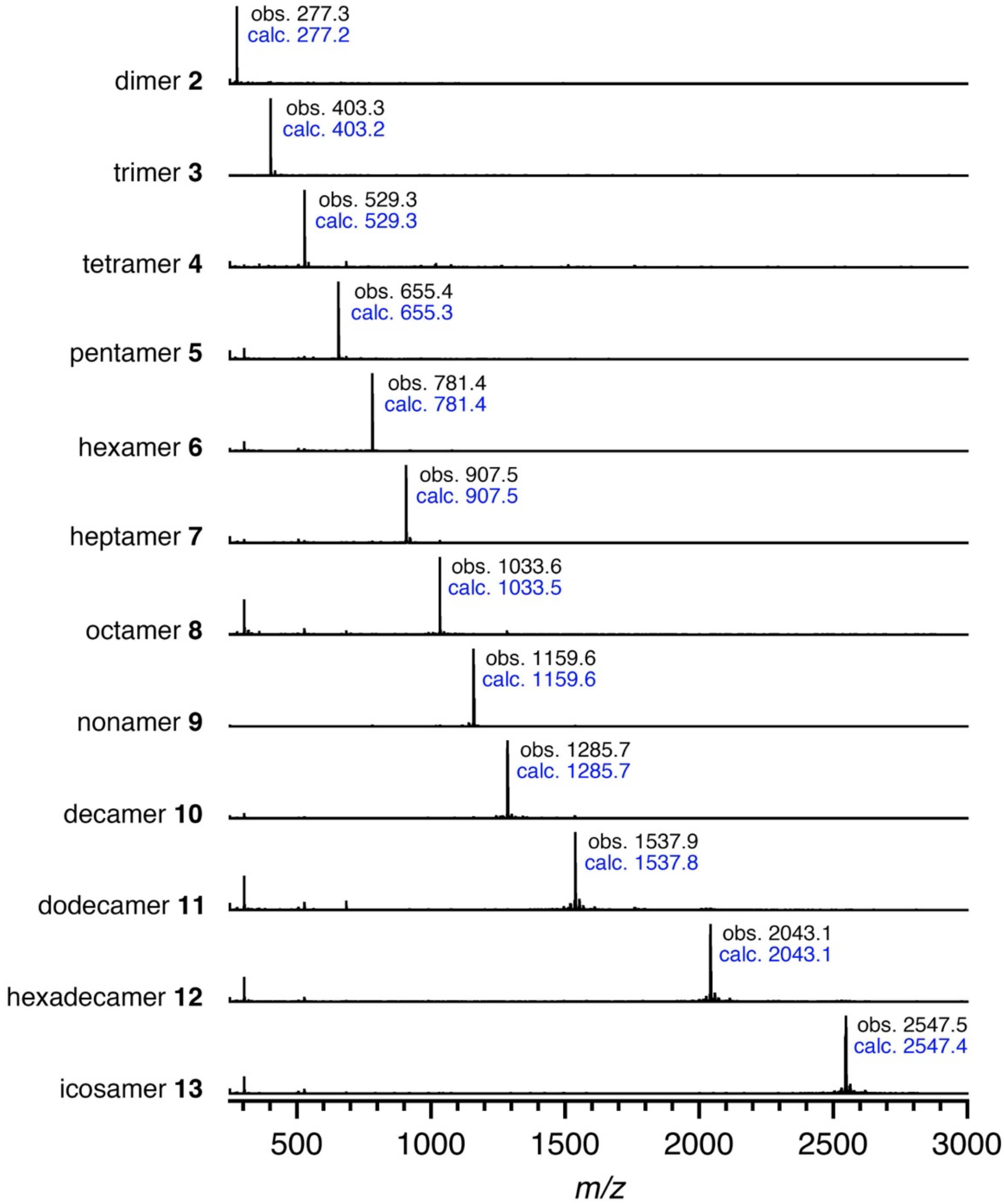


Fig. S1 MALDI-TOF mass spectra of discrete polyketone oligomers **2-13** using dithranol and $NaPF_6$ as matrixes (black values: observed *m/z*, blue values: calculated values for corresponding sodium mono-adduct ions $[M{+}Na]^+$).

4. Analytical HPLC Chromatograms

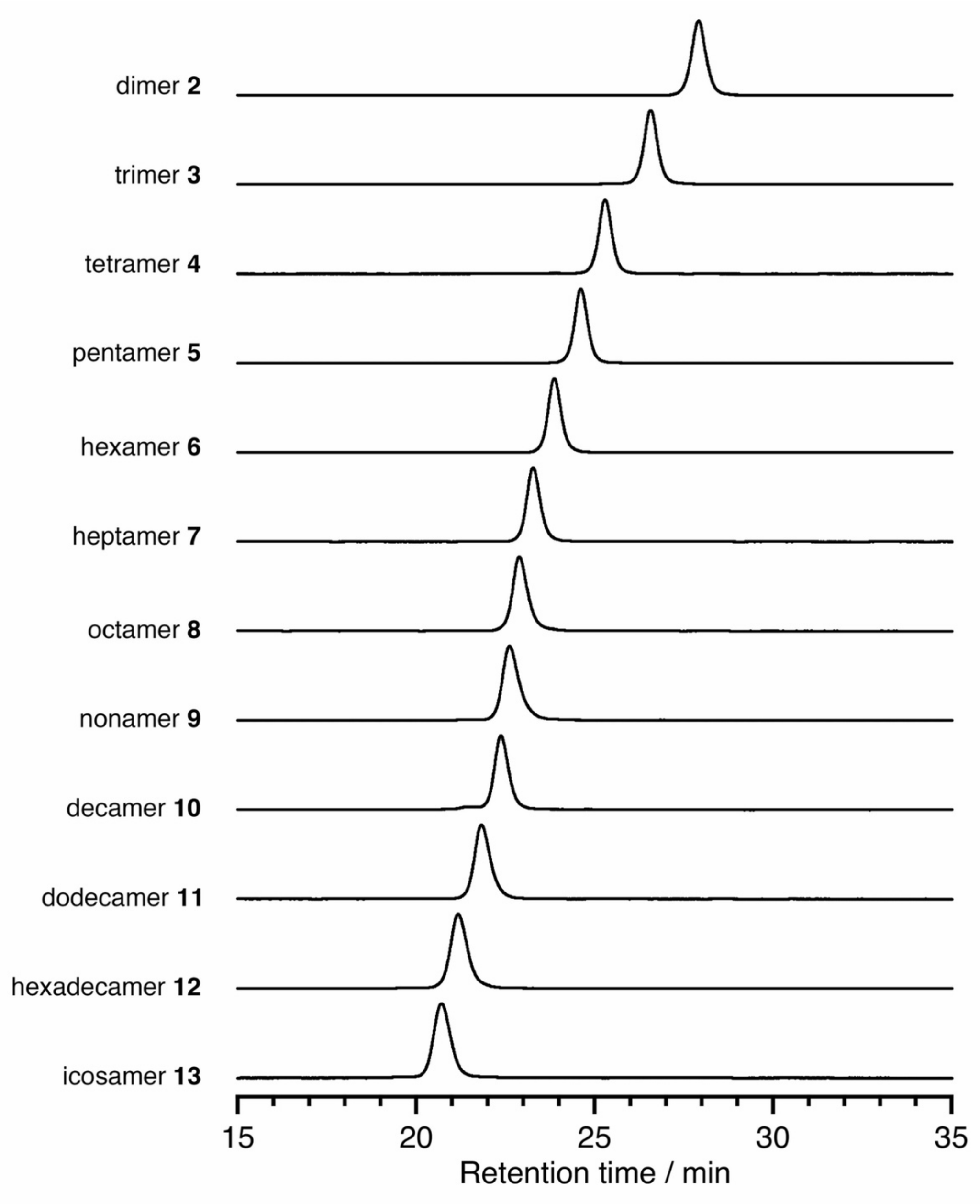


Fig. S2 HPLC chromatograms of discrete polyketone oligomers **2-13** (Column: TOSOH TSKgel G2000HXL×2, mobile phase: chloroform, column temperature: 55 °C, detection: UV absorption at 280 nm, flow rate: 0.5 mL/min).

5. Crystallographic Studies

5-1 Single crystal preparation details of pentamer 5 and hexamer 6

The single crystal of pentamer **5** was prepared by vapor diffusion of cyclohexene into a 1,2-dichloroethane solution overnight at room temperature. The grown single crystals in a vial were then thermally annealed at 50°C for 3.5 days and slowly cooled to room temperature. The diffraction data was recorded at -150°C. Similarly, the single crystal of hexamer **6** were prepared by vapor diffusion of cyclohexene into a 1,2-dichloroethane solution overnight at room temperatures. The grown single crystals in a vial were then thermally annealed at 50°C for 2 days. The diffraction data was recorded at -150 °C.

5-2 Crystallographic data for pentamer 5

$C_{35}H_{52}O_{10}$, M = 632.76, crystal size: 0.83 × 0.10 × 0.06 mm^3, Orthorhombic, space group $Pna2_1$, a = 10.4486(3) Å, b = 8.0259(2) Å, c = 41.6406(12) Å, $\alpha = \beta = \gamma$ = 90º, V = 3491.96(17) Å^3, Z = 4, T = 123(2) K, μ = 0.713 mm^{-1}, D_{calc} = 1.204 g/cm^3, 2.122º ≤ θ ≤ 67.494º, 5027 unique reflections out of 5956 with $I > 2\sigma(I)$, GOF = 1.083, R_1 = 0.1315 and wR_2 = 0.4120 for all data. CCDC deposit number: 2173799.

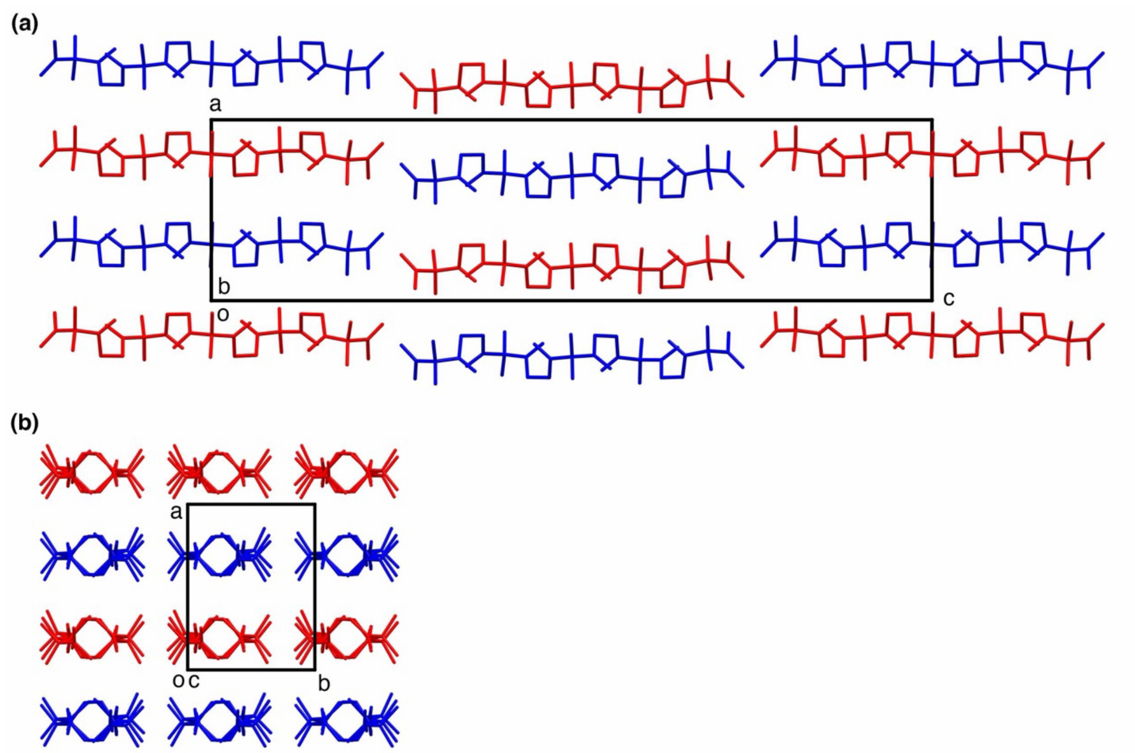


Fig. S3 Packing structure of pentamer **5** (a) viewed along b-axis and (b) c-axis. Left- and right-handed helices are indicated in blue and red, respectively. Hydrogen atoms are omitted for clarity.

5-3 Crystallographic data for hexamer 6

$C_{42}H_{62}O_{12}$, M = 758.91, crystal size: 0.38 × 0.06 × 0.01 mm^3, Orthorhombic, space group *Iba*2, a = 48.930(9) Å, b = 8.2077(17) Å, c = 10.3345(18) Å, $\alpha = \beta = \gamma$ = 90º, V = 4150.4(14) Å^3, Z = 4, T = 123(2) K, μ = 0.719 mm^{-1}, D_{calc} = 1.215 g/cm^3, 3.613º ≤ θ ≤ 51.377º, 1050 unique reflections out of 1893 with $I > 2\sigma(I)$, GOF = 1.619, R_1 = 0.1571 and wR_2 = 0.4353 for all data. CCDC deposit number: 2173800.

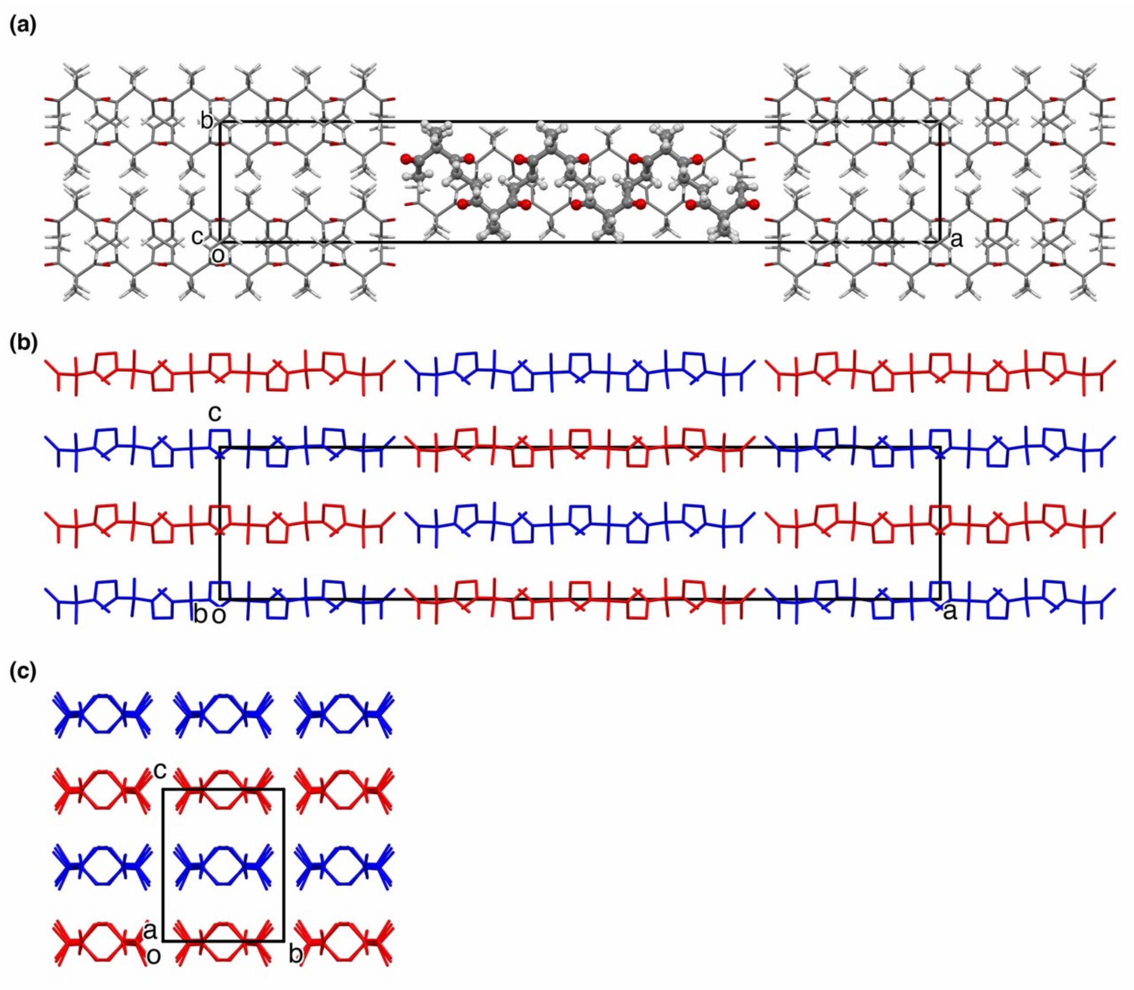


Fig. S4 Conformations and packing structures of hexamer **6** (a) viewed along *c*-axis, (b) *b*-axis, and (c) *a*-axis. In (b) and (c), left- and right-handed helices are indicated in blue and red, respectively, and hydrogen atoms are omitted for clarity.

5-4 Sample preparation details for PXRD studies

The samples of polyketone discrete oligomers **2**, **4-13** for the PXRD measurements were prepared by a slow evaporation of chloroform solution over 1 day at room temperature and further dried under vacuum overnight. The sample of trimer **3** was prepared via slow cooling from the melt and kept at –20 °C over 1 week. The obtained samples were ground and placed in the hollow of a silicon zero background sample holder for the diffraction measurements.

The simulated PXRD patterns of oligomers **2-4** were generated using the previously reported single crystal X-ray structures.[1,2]

5-5 Observed and simulated PXRD patterns of oligomers 2-6

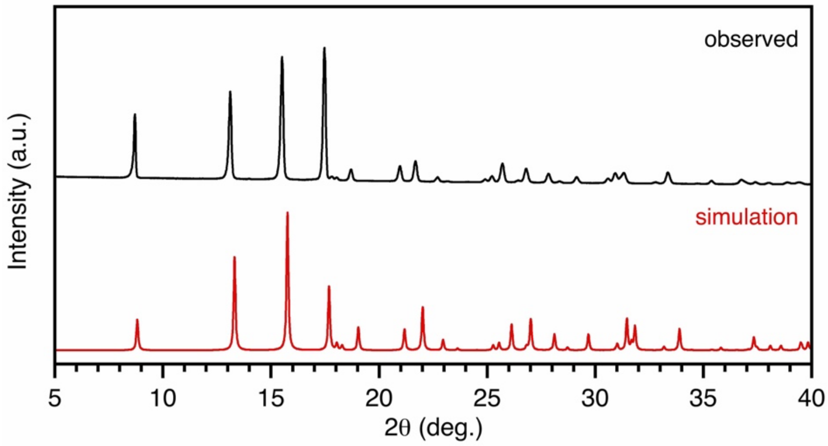


Fig. S5 Observed and simulated PXRD patterns of dimer **2**.

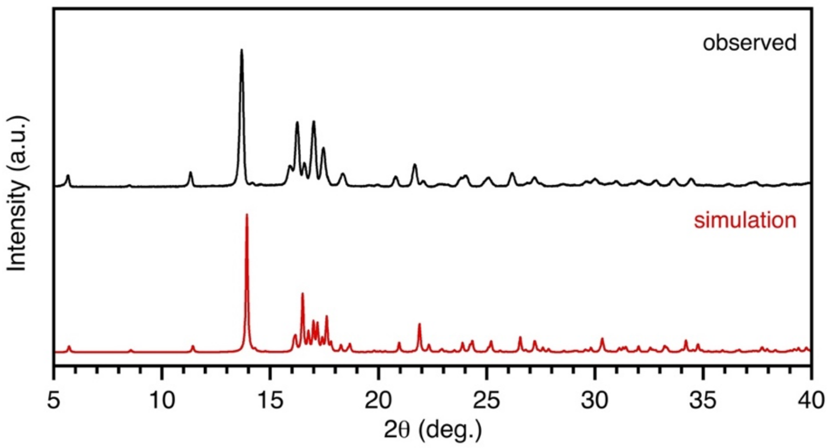


Fig. S6 Observed and simulated PXRD patterns of trimer **3**.

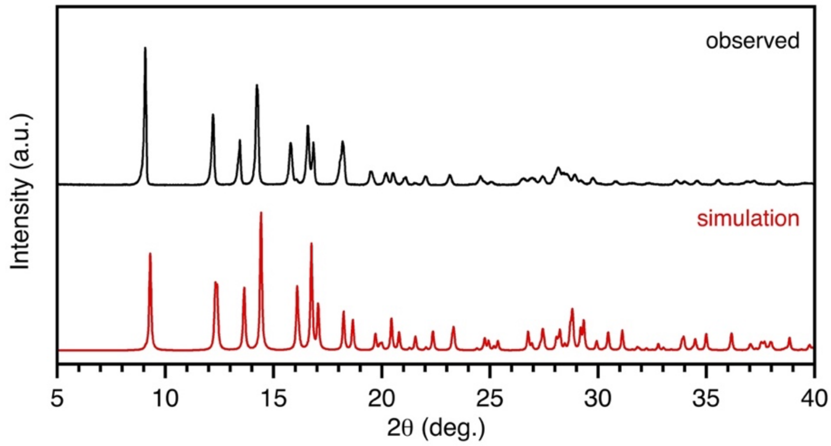


Fig. S7 Observed and simulated PXRD patterns of tetramer **4**.

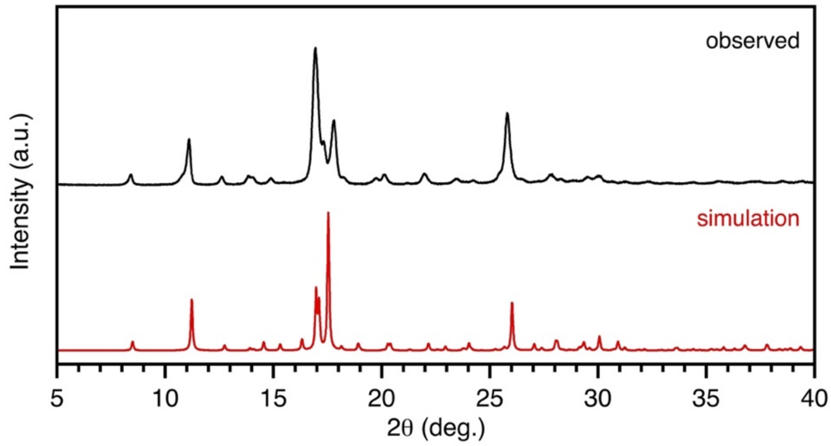


Fig. S8 Observed and simulated PXRD patterns of pentamer **5**.

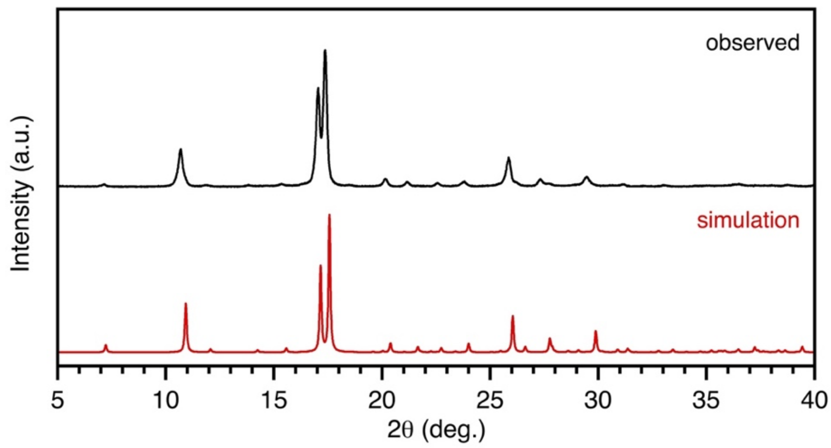


Fig. S9 Observed and simulated PXRD patterns of hexamer **6**.

5-6 SAXS measurement

The samples of tetramer **4**, octamer **8**, dodecamer **11**, hexadecamer **12**, and icosamer **13** for the SAXS diffraction were prepared by thermal annealing from the melt at specified temperatures over 1 day (40 °C for tetramer **4**, 100 °C for octamer **8**, dodecamer **11**, hexadecamer **12**, and icosamer **13**) then slowly cooled to room temperature. The annealed samples were ground and used for the diffraction measurements.

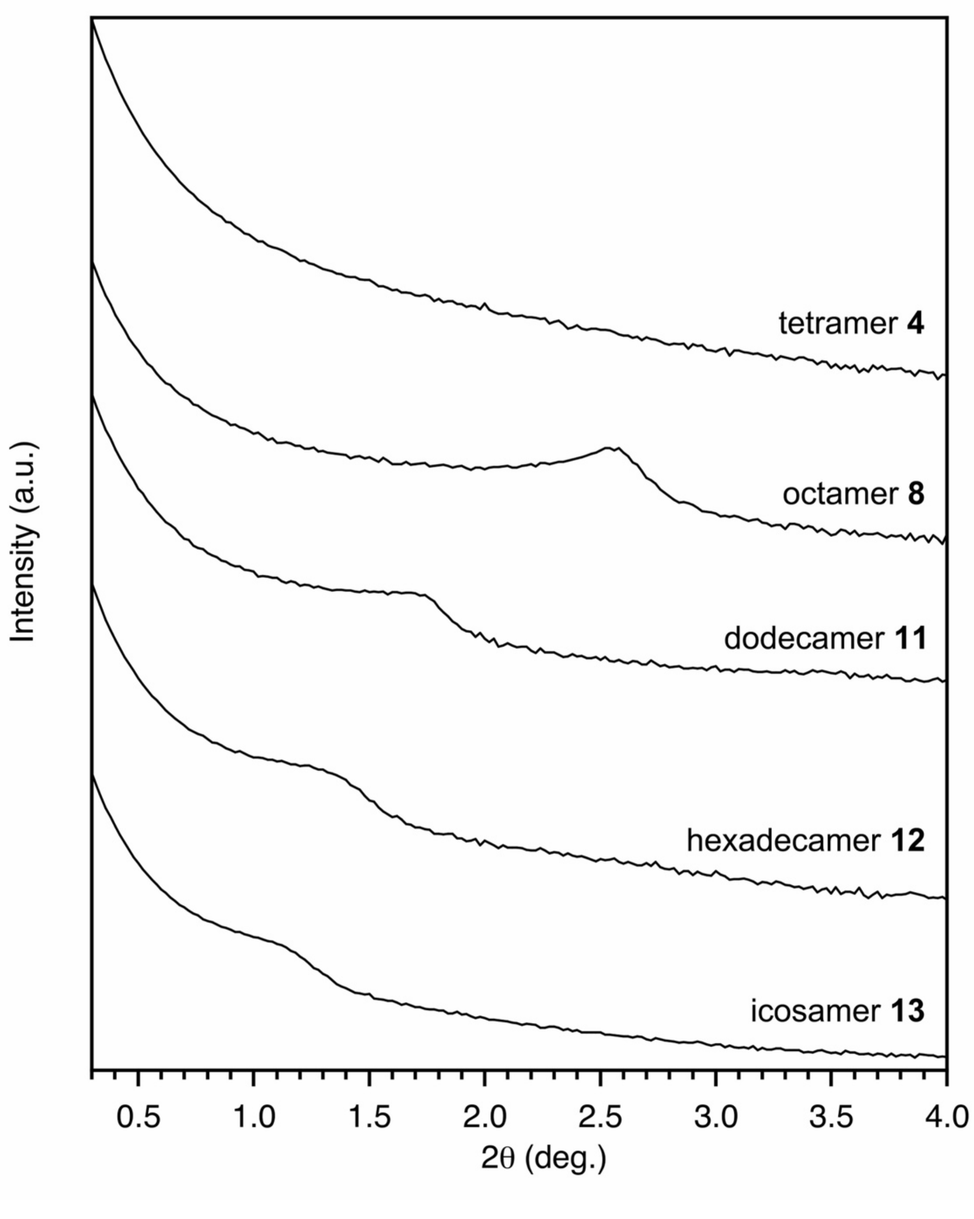
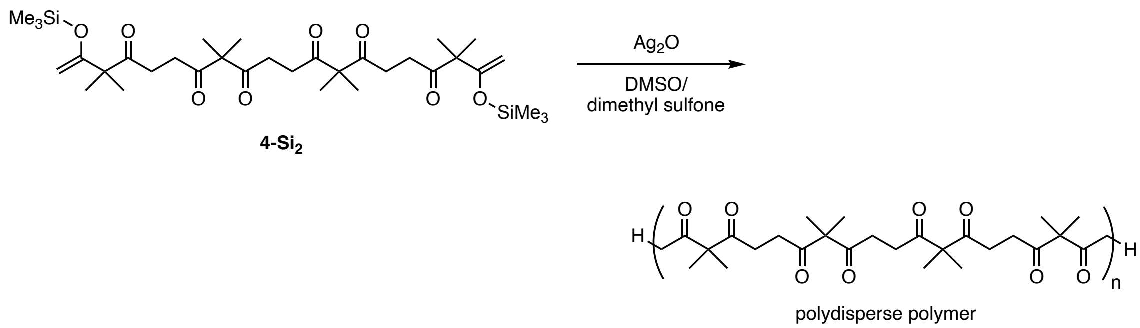


Fig. S10 SAXS profiles of discrete polyketone oligomers **4, 8, 11, 12, 13**.

6. Preparation and analysis of polydisperse polymer

6-1 Preparation of polydisperse polymer from 4-Si_2



The mixture of oligomers was prepared in the same manner as described in the section "**2-8 Synthesis of octamer 8, dodecamer 11, hexadecamer 12, and icosamer 13**" using bis-silylated tetramer **4-Si_2** (2.00 g, 3.07 mmol), dimethyl sulfone (1.73 g, 18.4 mmol), dimethyl sulfoxide (87.4 μL, 1.23 mmol) and silver(I) oxide (855 mg, 3.69 mmol). During GPC separation step, high-molecular weight component ($N \geq 20$) was collected. After evaporation of the solvent *in vacuo*, the mixture was passed through silica-gel column (diameter, 1.5 cm; height, 5.0 cm) using dichloromethane/methanol (25:1, v/v) as an eluent. The resulting solid was suspended in methanol (0.5 mL) and sonicated for 3 minutes, and then filtered with suction. The solid on funnel was washed using methanol (3.5 mL) to give polydisperse polymer (221 mg).

Polydisperse polymer ($N \geq 20$)

^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ=2.94-2.54 (m, 88H, ethylene), 2.15 (s, 6H, acetyl), 1.46-1.28 (138H, overlapping $C(CH_3)_2$); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$, 298 K): δ=208.9-208.1, 207.8, 62.2, 62.0-61.6, 32.5-32.0, 26.4, 22.2-21.7, 21.6 ppm; IR(ATR, neat) 2979, 2937, 2915, 2876, 1692, 1465, 1442, 1388, 1364, 1241, 1074, 1014, 950 cm^{-1}.

The degree of polymerization was expected as 23 from the integration ratio of ethylene and acetyl peaks.

6-2 MALDI-TOF Mass Spectrum

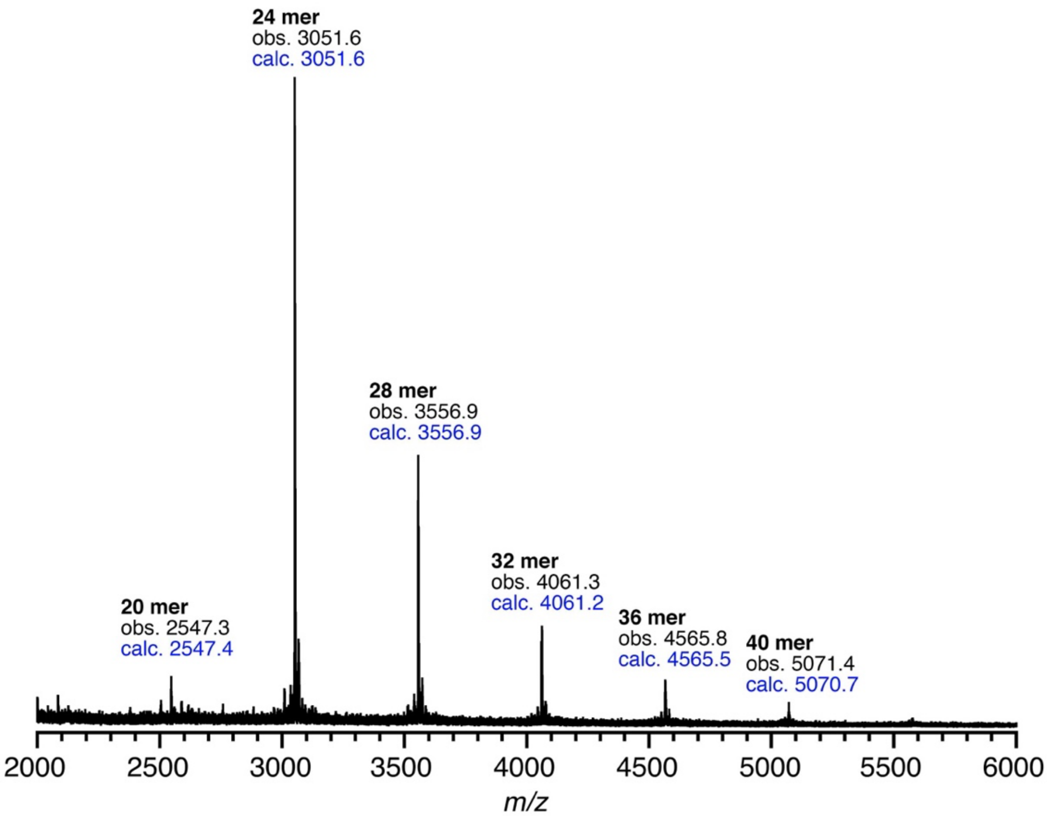


Fig. S11 MALDI-TOF mass spectrum of polydisperse polymer ($N \geq 20$) using dithranol and $NaPF_6$ as matrixes (black values: observed *m/z*, blue values: calculated values for corresponding sodium mono-adduct ions $[M\text{+Na}]^+$).

6-3 Analytical HPLC chromatograms

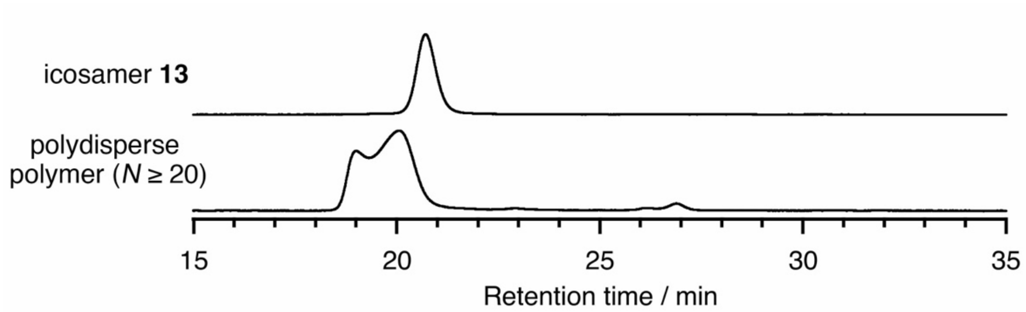


Fig. S12 HPLC chromatograms of icosamer **13** and polydisperse polymer ($N \geq 20$) (Column: TOSOH TSKgel G2000HXL×2, mobile phase: chloroform, column temperature: 55 °C, detection: UV absorption at 280 nm, flow rate: 0.5 mL/min).

6-4 PXRD pattern of polydisperse polymer ($N \geq 20$)

The sample of polydisperse polymer ($N \geq 20$) for the PXRD measurement was prepared by a slow evaporation of chloroform solution over 1 day at room temperature and further dried under vacuum overnight. The obtained sample was then ground and placed in the hollow of a silicon zero background sample holder for the diffraction measurement.

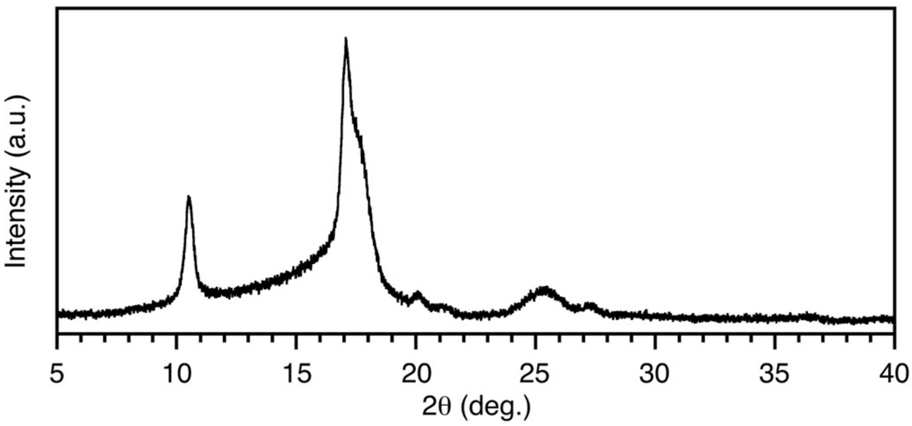


Fig. S13 PXRD pattern of polydisperse polymer ($N \geq 20$).

7. Atomic Force Microscope (AFM) Images

7-1 AFM system

AFM measurements were performed by frequency modulation (FM) mode using a laboratory-built AFM system combined with commercial AFM controllers. The laboratory-built AFM system was equipped with an ultra-low noise deflection sensor and a photothermal excitation module. The commercial AFM controllers of Asylum ARC2 (Oxford Instruments) and Nanonis OC4.5 (SPECS GmbH) were used as a general AFM controller and a cantilever oscillation controller, respectively.

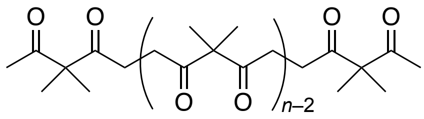
7-2 AFM cantilever and measurement condition

AFM cantilevers with a gold coating on the reflection side (160 AC-NG, MikroMasch) were used for the AFM measurements. The tip side of AFM cantilevers was coated with 30 nm thickness of Si using a magnetron sputter coater (QT150, Quorum Technologies) to improve the reproducibility of FM-AFM measurements in liquid, as reported in the previous studies[5,6]. The cantilever vibration was oscillated by a photothermal excitation method.

7-3 Sample preparation

A 0.05 mM solution of octamer **8** was prepared with chloroform (Wako, infinity pure grade). A highly oriented pyrolytic graphite (HOPG, 7 mm × 7 mm squares, NT-MDT, GRBS/0.6) was fixed with glue on an AFM sample holder. The solution (5 μL) was dropped onto a freshly cleaved HOPG surface and covered with a glass dish for slow evaporation. After the evaporation, the surface was rinsed three times with ultra-pure water (80 μL) and used for the AFM measurement.

8. Differential Scanning Calorimetry (DSC) Measurement



discrete polyketone oligomers

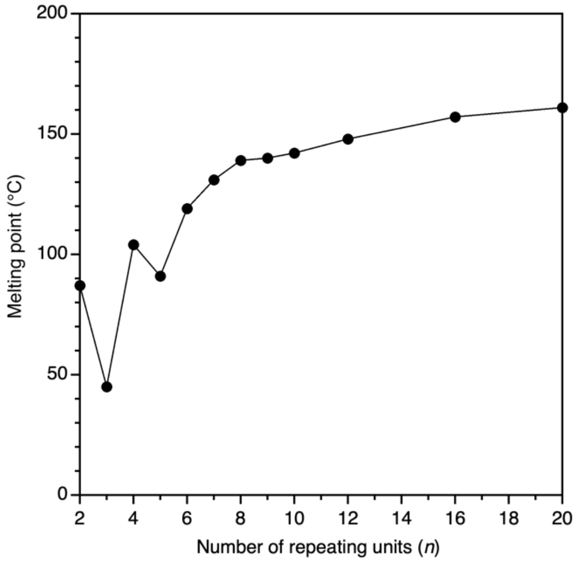


Fig. S14 Melting point plot of discrete polyketone oligomers **2-13** by DSC measurement (1st heated run, 10 °C/min.).

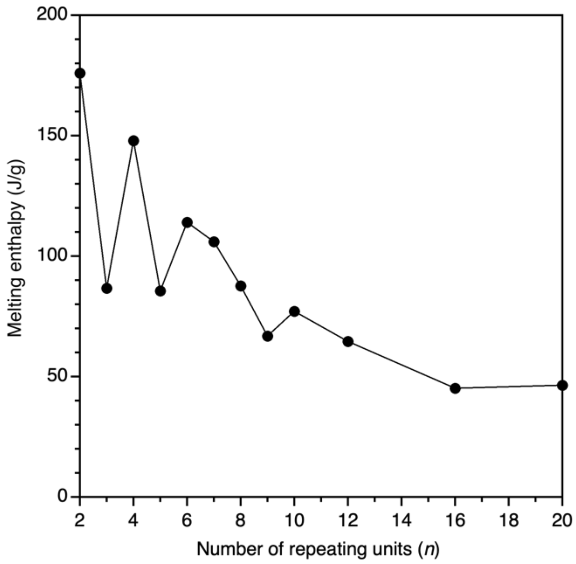


Fig. S15 Melting enthalpy plot of discrete polyketone oligomers **2-13** by DSC measurement (1st heated run, 10 °C/min.).

9. Theoretical Calculation

9-1 Computational Details

To obtain plausible packing structure of infinite polyketone chains, we referred to the crystal structure of hexamer **6**. The packing structure was optimized under periodic boundary condition without cell relaxation by the self-consistent-charge density-functional tight binding (DFTB) method with the third-order expansion as implemented in the DFTB+ package version 21.1.[7] The 3ob parameter set[8,9] with Hubbard parameters –0.1492 for C, –0.1857 for H, and –0.1575 for O were employed. Grimme's D3 type dispersion[10,11] was included. The optimization was followed by optimization with cell relaxation in the same calculation condition. After this optimization, the chain with the length of octamer **8**, dodecamer **11**, hexadecamer **12**, icosamer **13** were modeled from the optimized polymer with infinite length by termination of H atoms. The all models with finite length can have C_2 symmetry, and we optimized each model with C_2 symmetry at the B3LYP/6-31G(d,p) level of theory with Grimme's type dispersion correction[10,11] using Gaussian 16 Rev. C01.[12]

9-2 Optimized Structures

The chain lengths from the optimized polyketone structures were determined as the distances between the two oxygen atoms of the terminal carbonyl groups.

The helical chain of polyketones were moderately twisted after the optimizations in hexadecamer **12**, and icosamer **13**. These results are probably because the optimization was performed under vacuum condition without considering the packing structure. Still, the multiple intramolecular hydrogen bonds within the chains were maintained after the optimization, which were suggested in the optimized polymer model with infinite length.

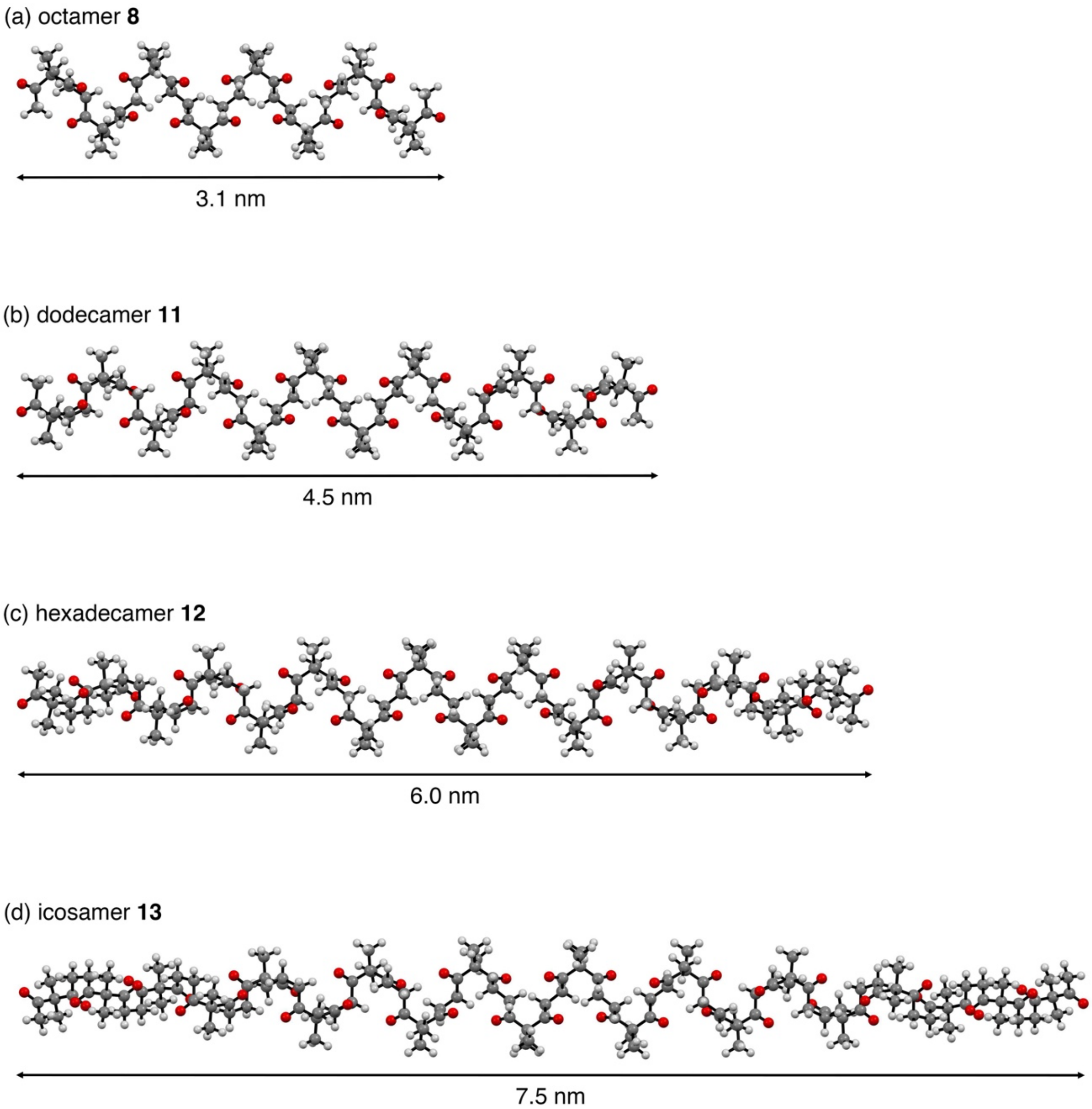


Fig. S16 Optimized structure of (a) octamer **10**, (b) dodecamer **11**, (c) hexadecamer **12**, and (d) icosamer **13**.

10. NMR Spectra

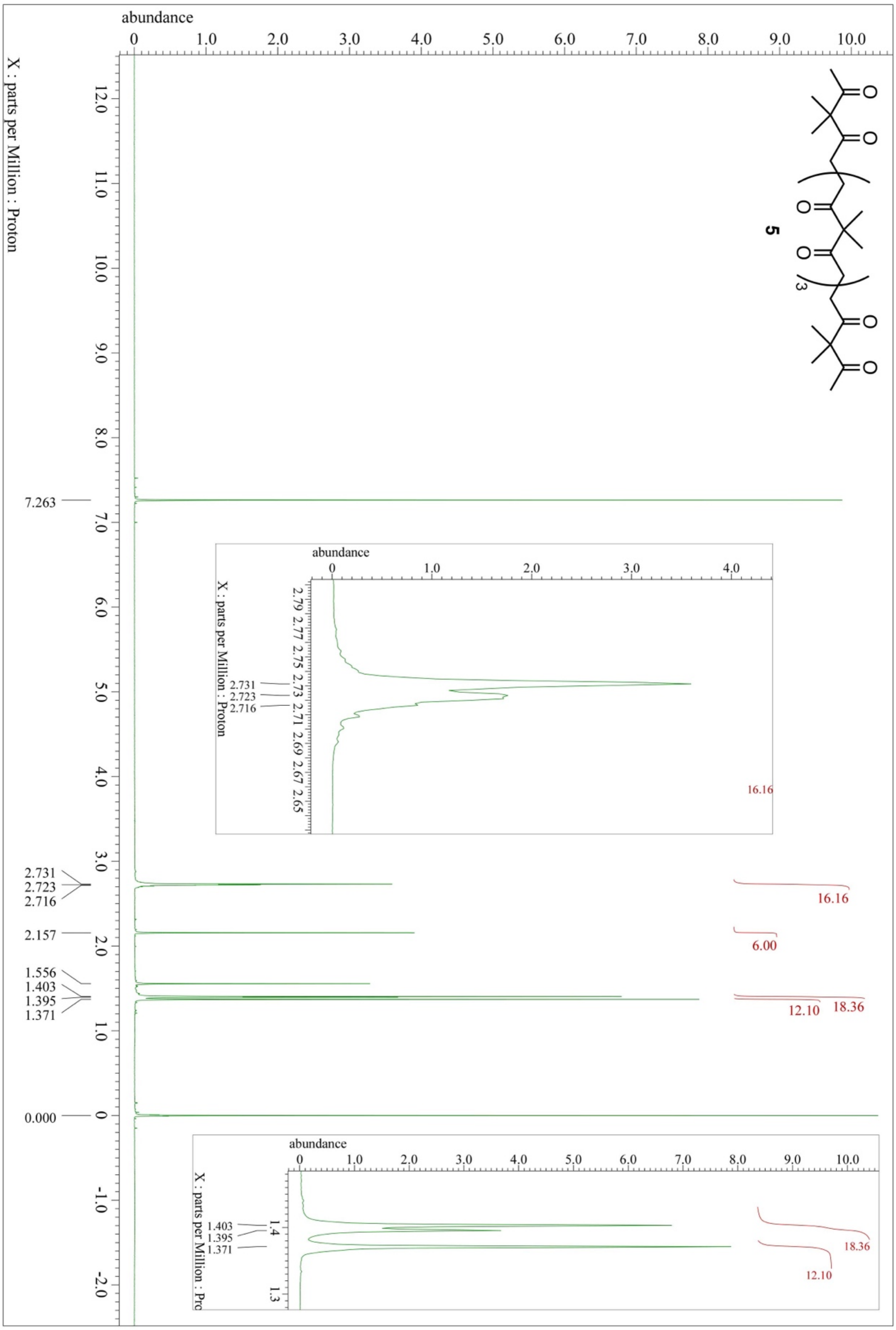


Fig. S17 ^{1}H NMR spectrum of pentamer **5** (400 MHz, $CDCl_3$, 298 K).

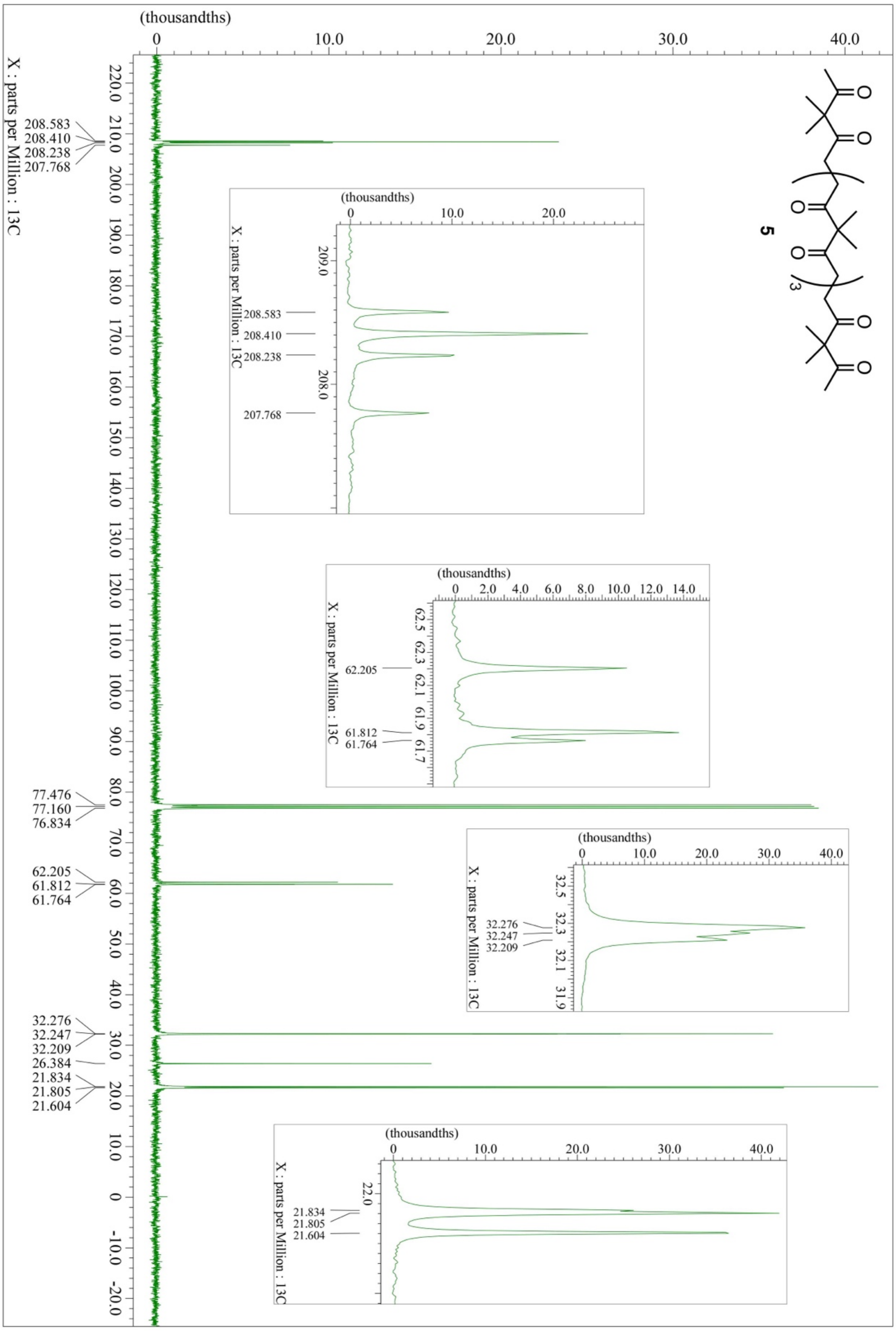


Fig. S18 $^{13}C\{^{1}H\}$ NMR spectrum of pentamer **5** (100 MHz, $CDCl_3$, 298 K).

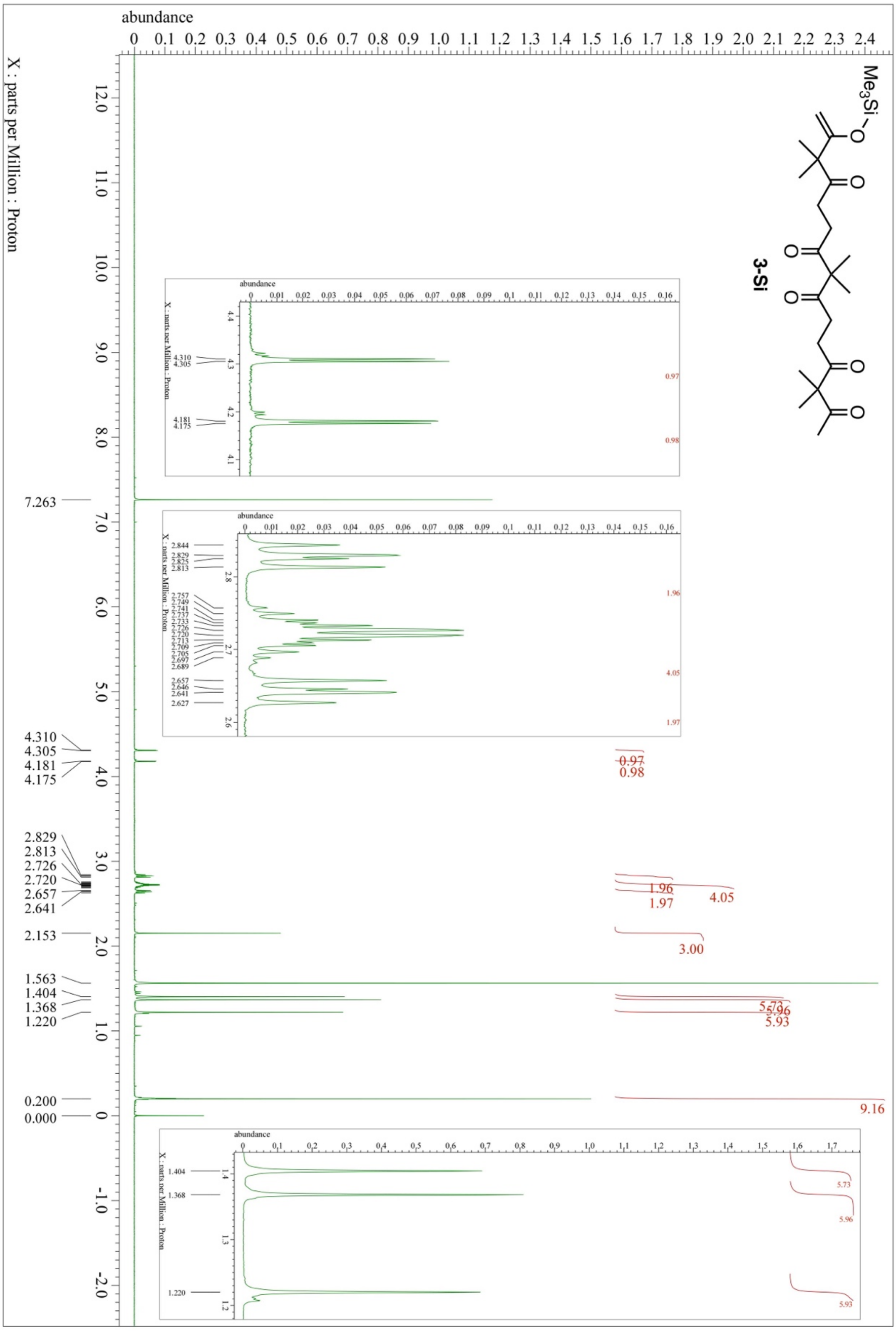


Fig. S19 ^{1}H NMR spectrum of mono-silylated trimer **3-Si** (400 MHz, $CDCl_3$, 298 K).

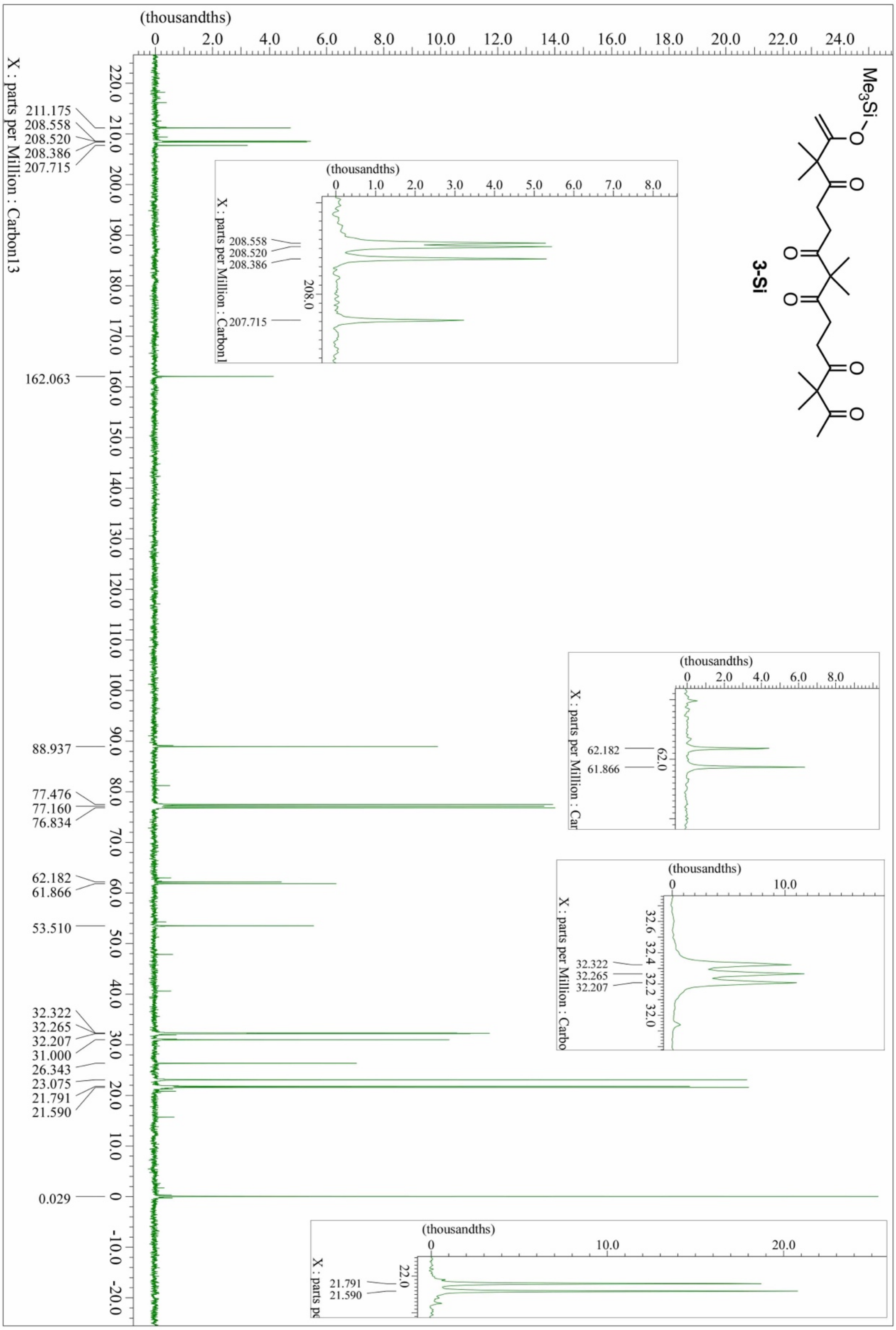


Fig. S20 $^{13}C\{^{1}H\}$ NMR spectrum of mono-silylated trimer **3-Si** (100 MHz, $CDCl_3$, 298 K).

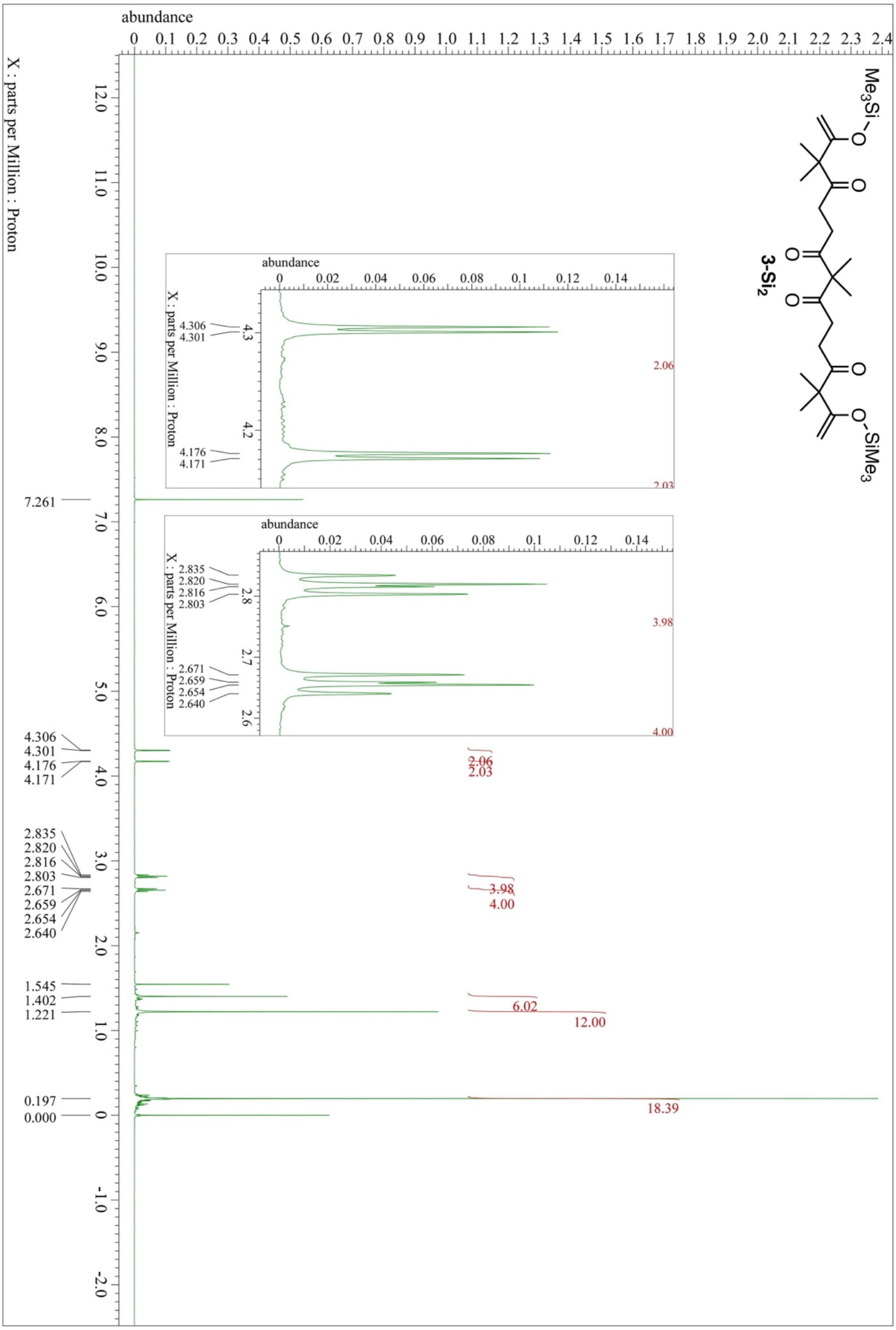


Fig. S21 [1]H NMR spectrum of bis-silylated trimer **3-Si₂** (400 MHz, $CDCl_3$, 298 K).

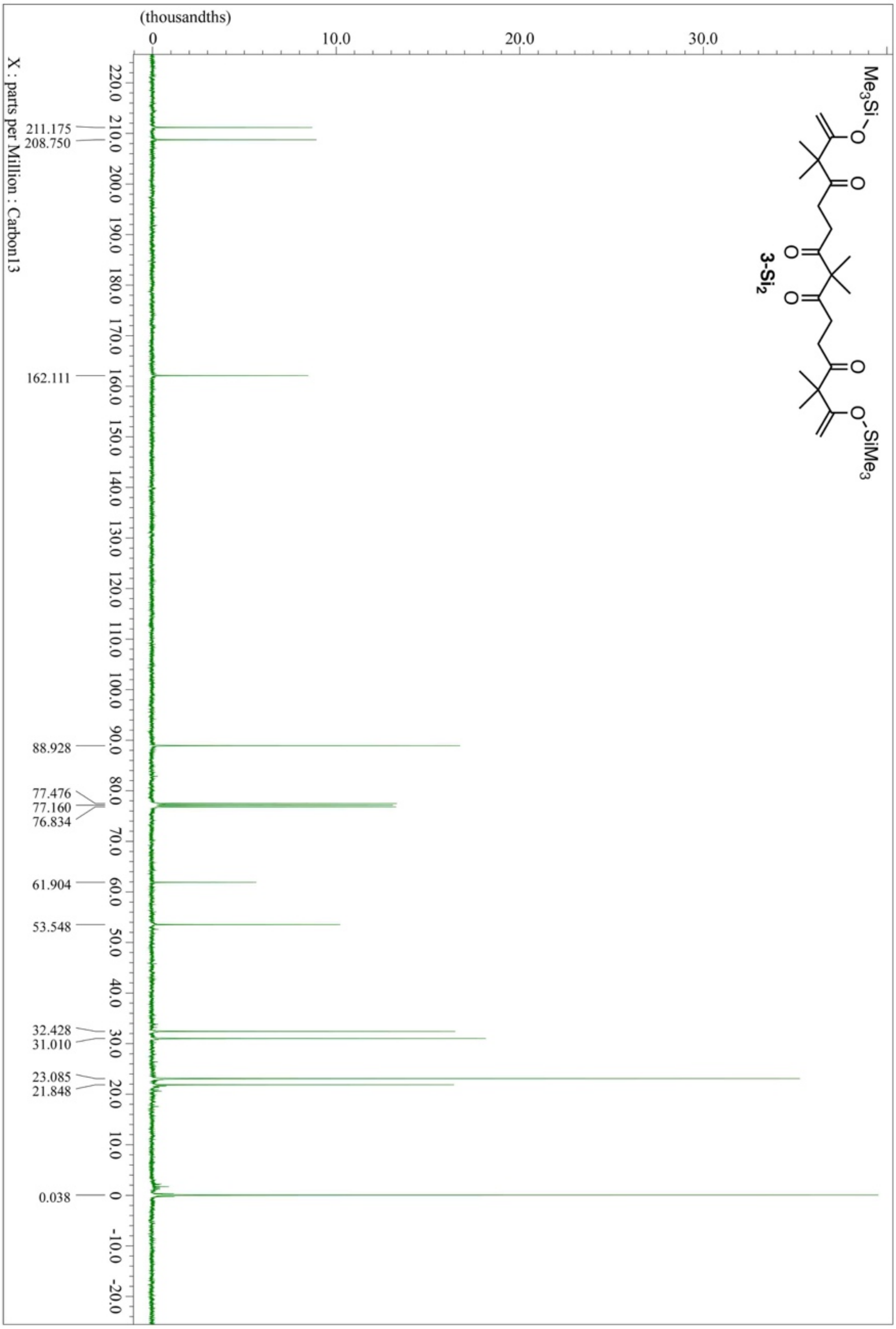


Fig. S22 $^{13}C\{^{1}H\}$ NMR spectrum of bis-silylated trimer **3-Si$_2$** (100 MHz, $CDCl_3$, 298 K).

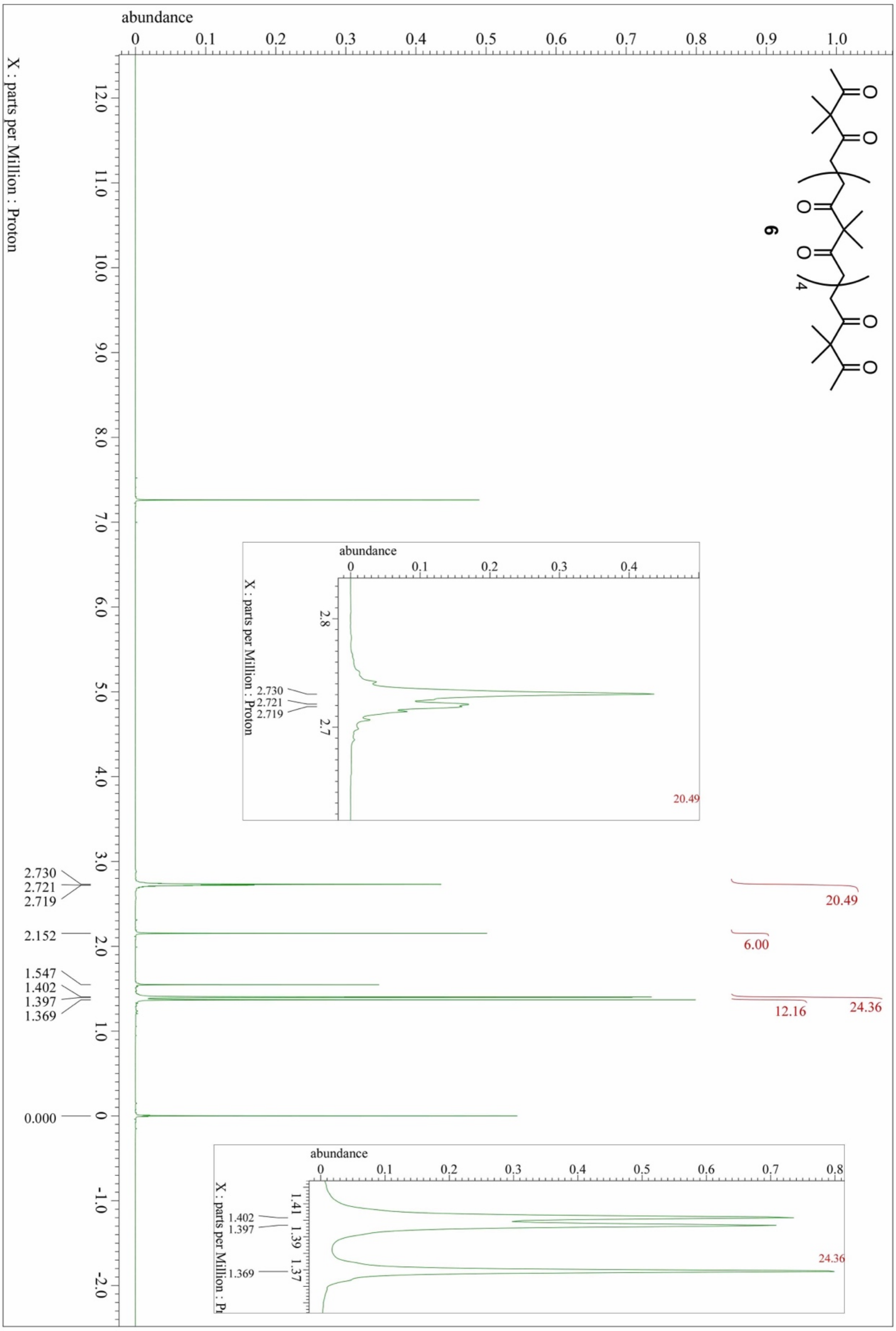


Fig. S23 [1]H NMR spectrum of hexamer **6** (400 MHz, $CDCl_3$, 298 K).

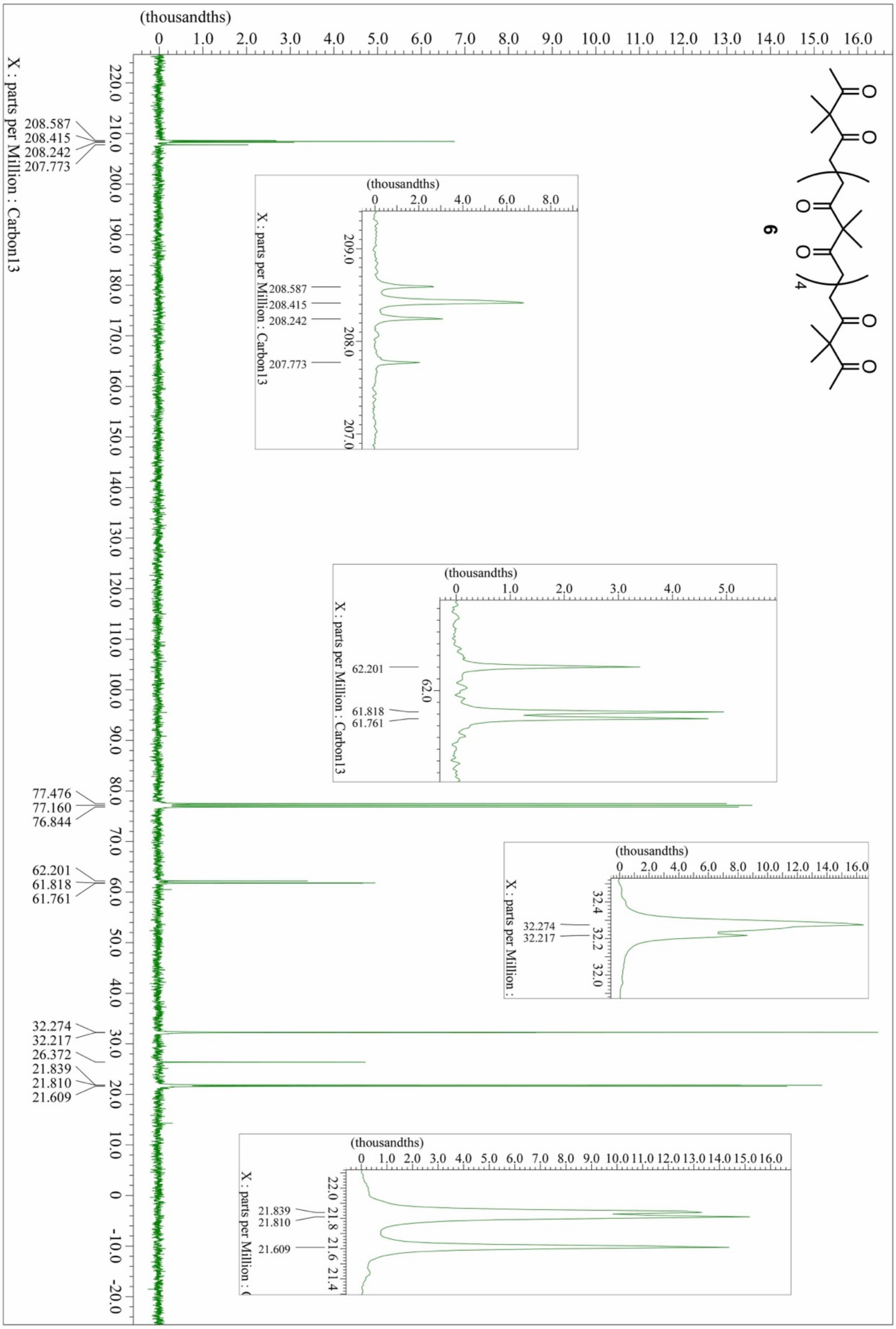


Fig. S24 $^{13}C\{^{1}H\}$ NMR spectrum of hexamer **6** (100 MHz, $CDCl_3$, 298 K).

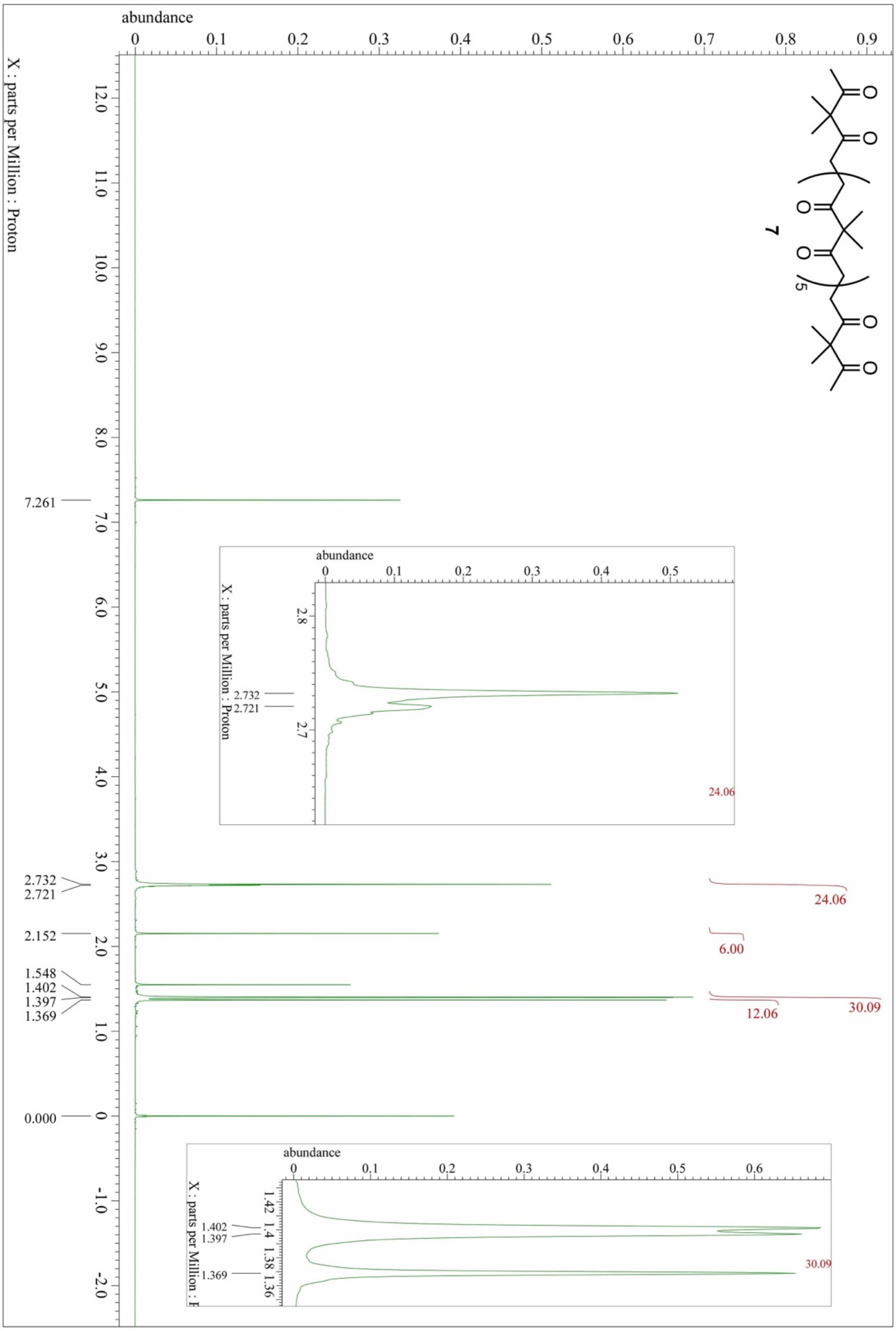


Fig. S25 ^{1}H NMR spectrum of heptamer **7** (400 MHz, $CDCl_3$, 298 K).

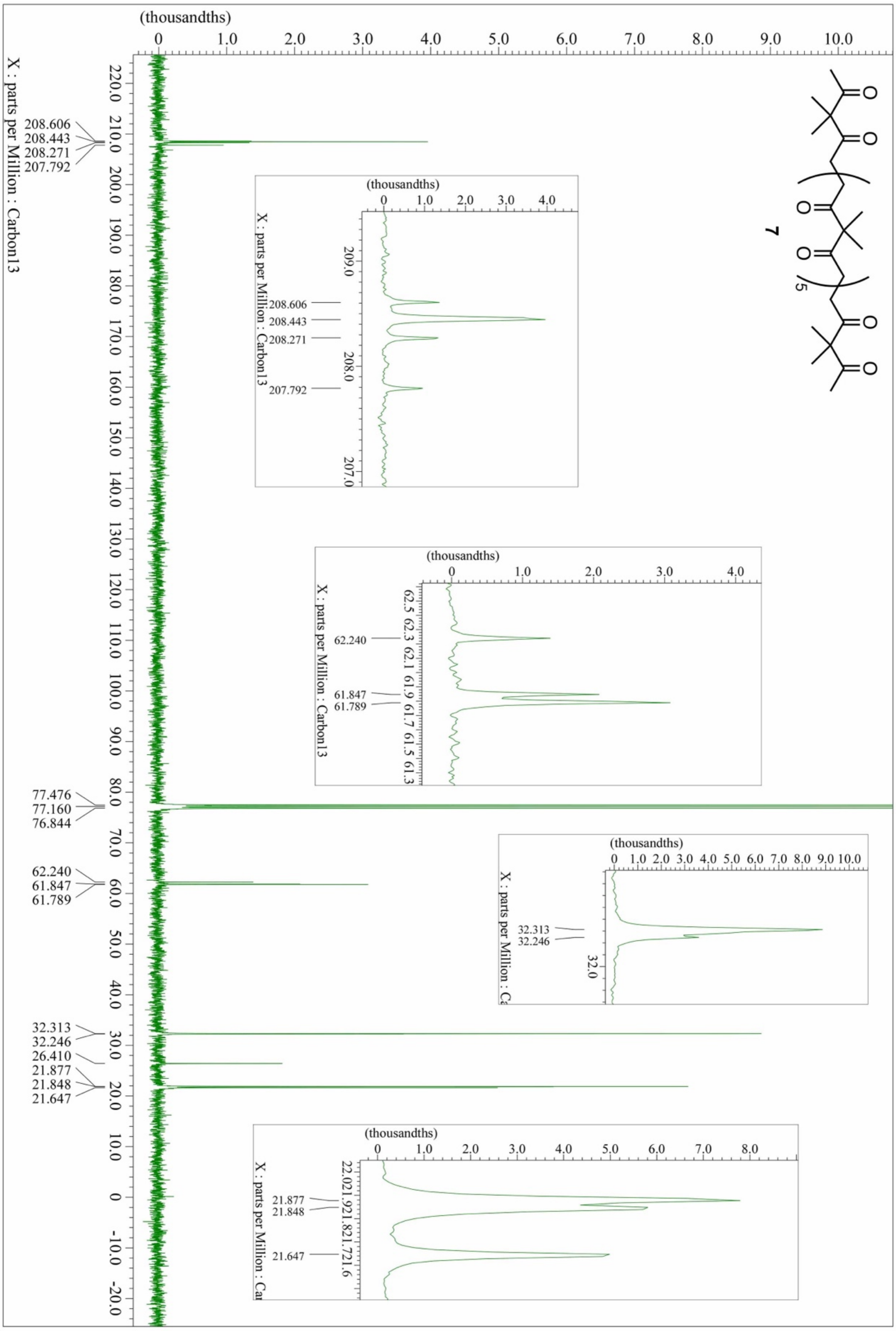


Fig. S26 $^{13}C\{^{1}H\}$ NMR spectrum of heptamer **7** (100 MHz, $CDCl_3$, 298 K).

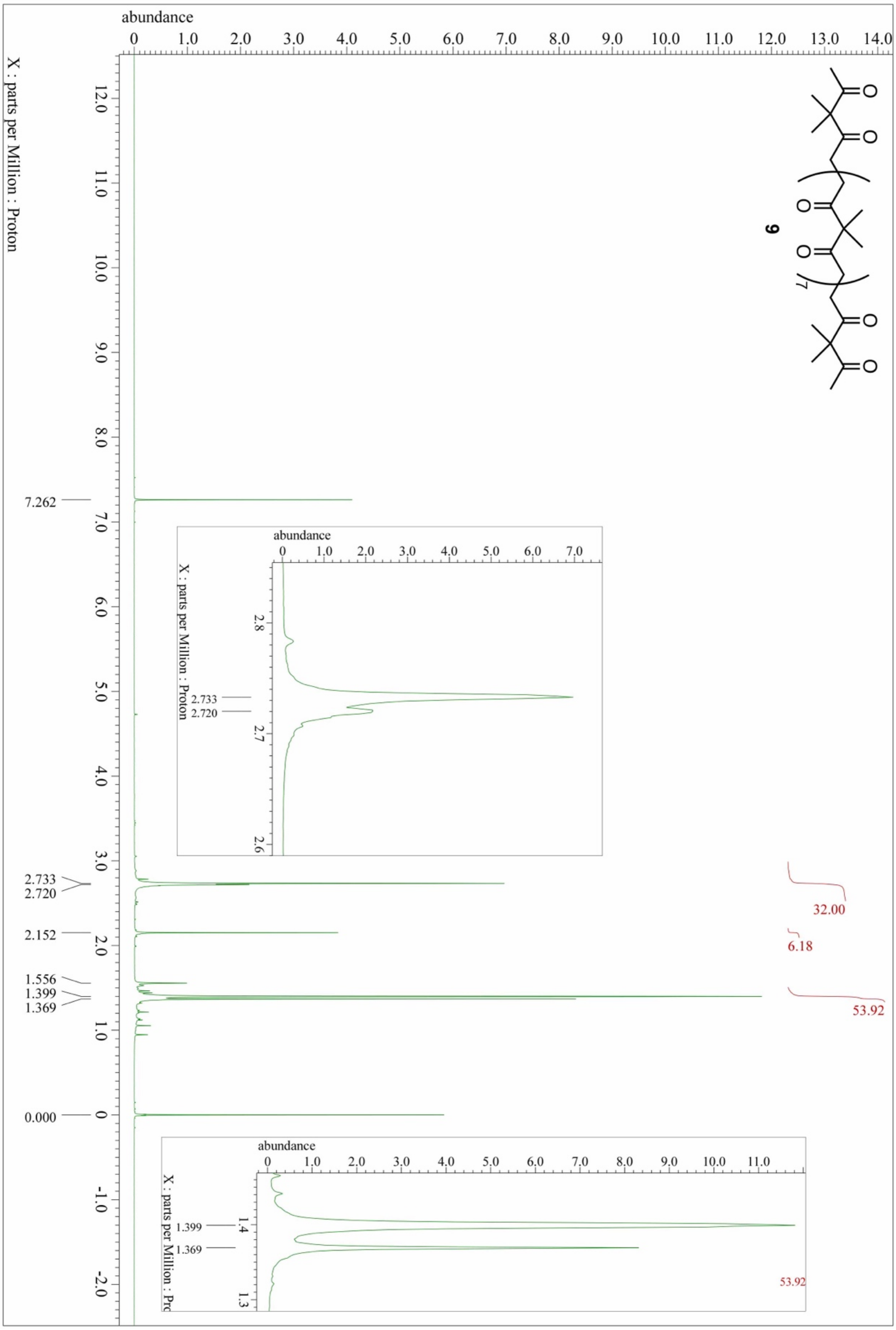


Fig. S27 [1]H NMR spectrum of nonamer **9** (400 MHz, $CDCl_3$, 298 K).

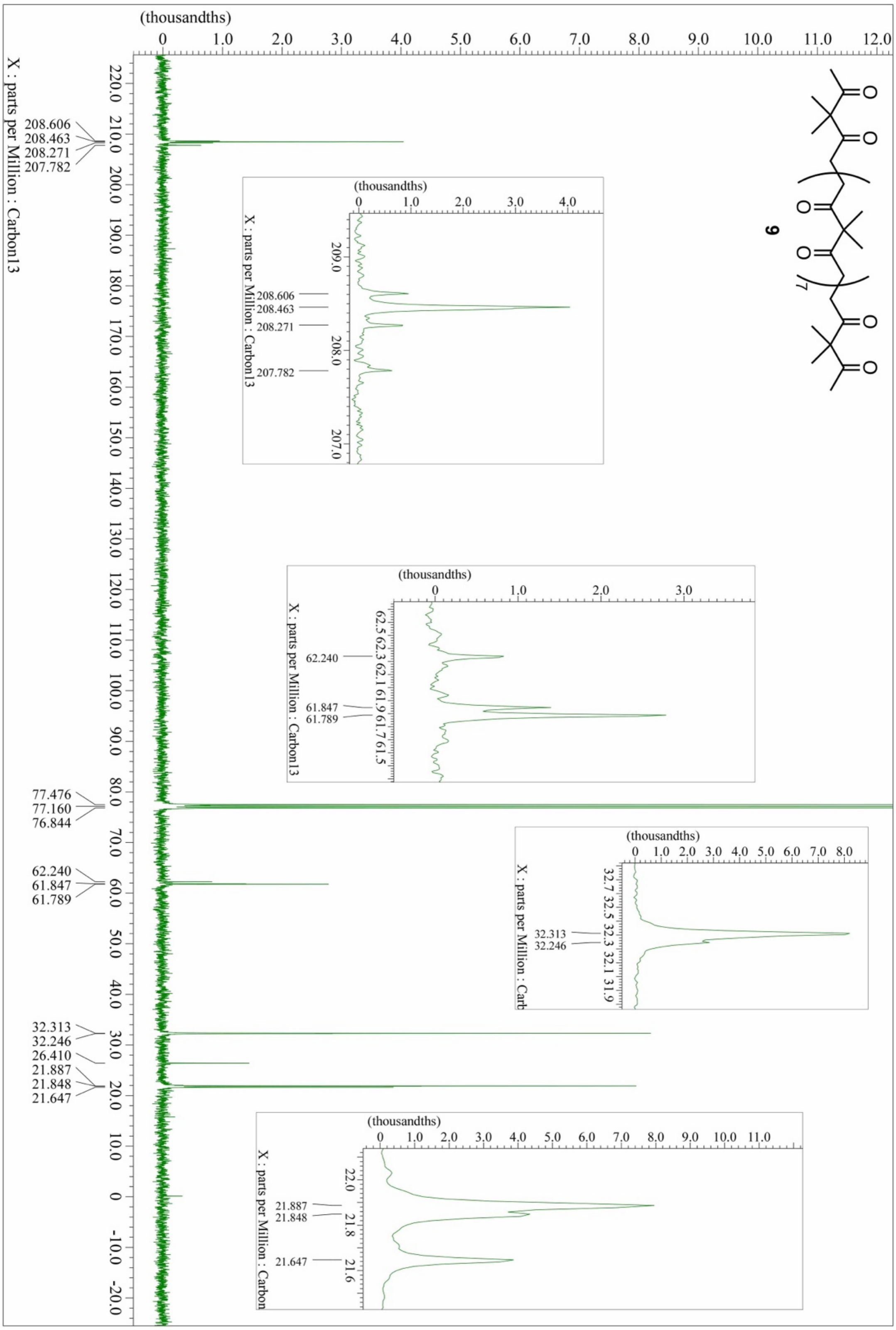


Fig. S28 $^{13}C\{^{1}H\}$ NMR spectrum of nonamer **9** (100 MHz, $CDCl_3$, 298 K).

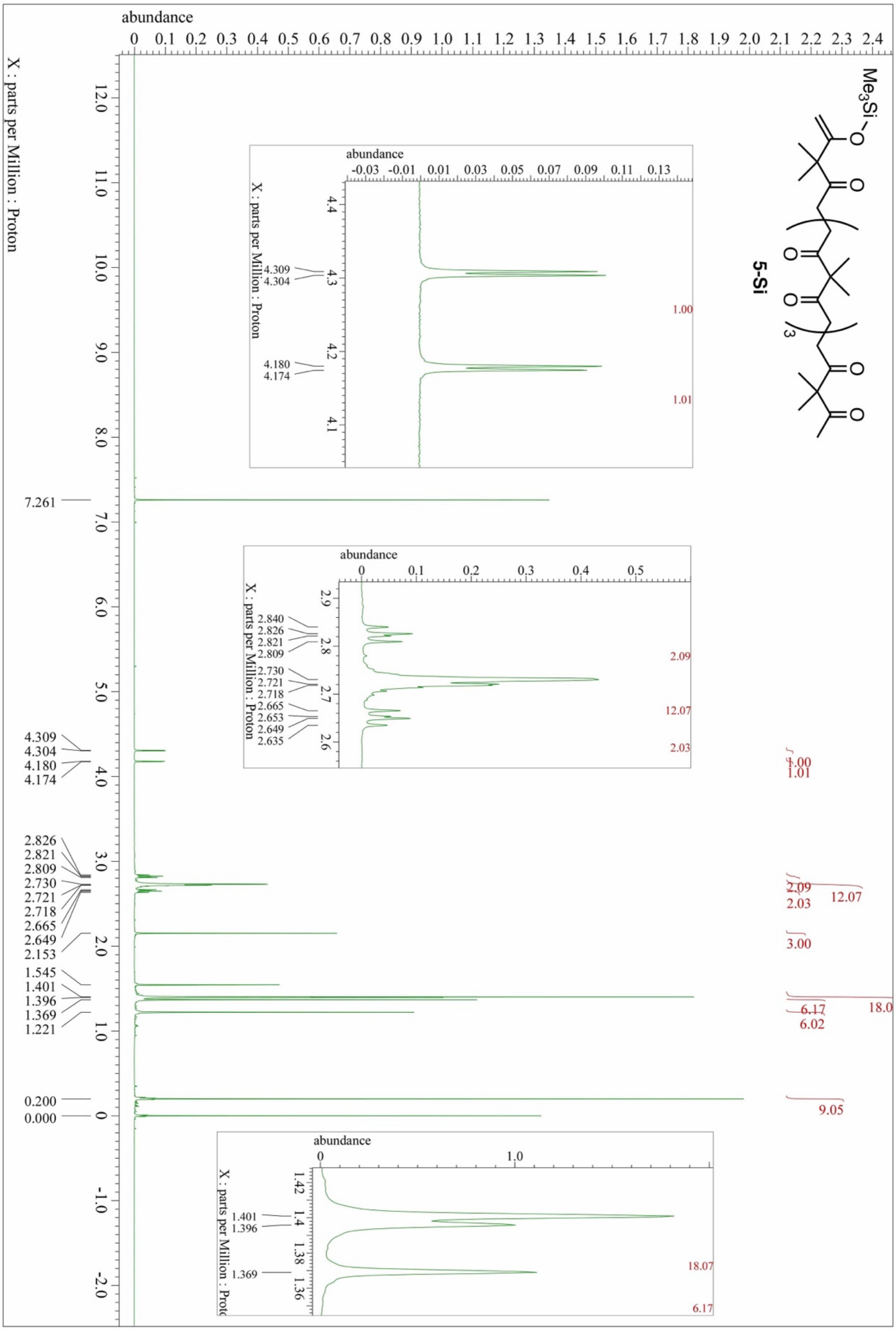


Fig. S29 ^{1}H NMR spectrum of mono-silylated pentamer **5-Si** (400 MHz, $CDCl_3$, 298 K).

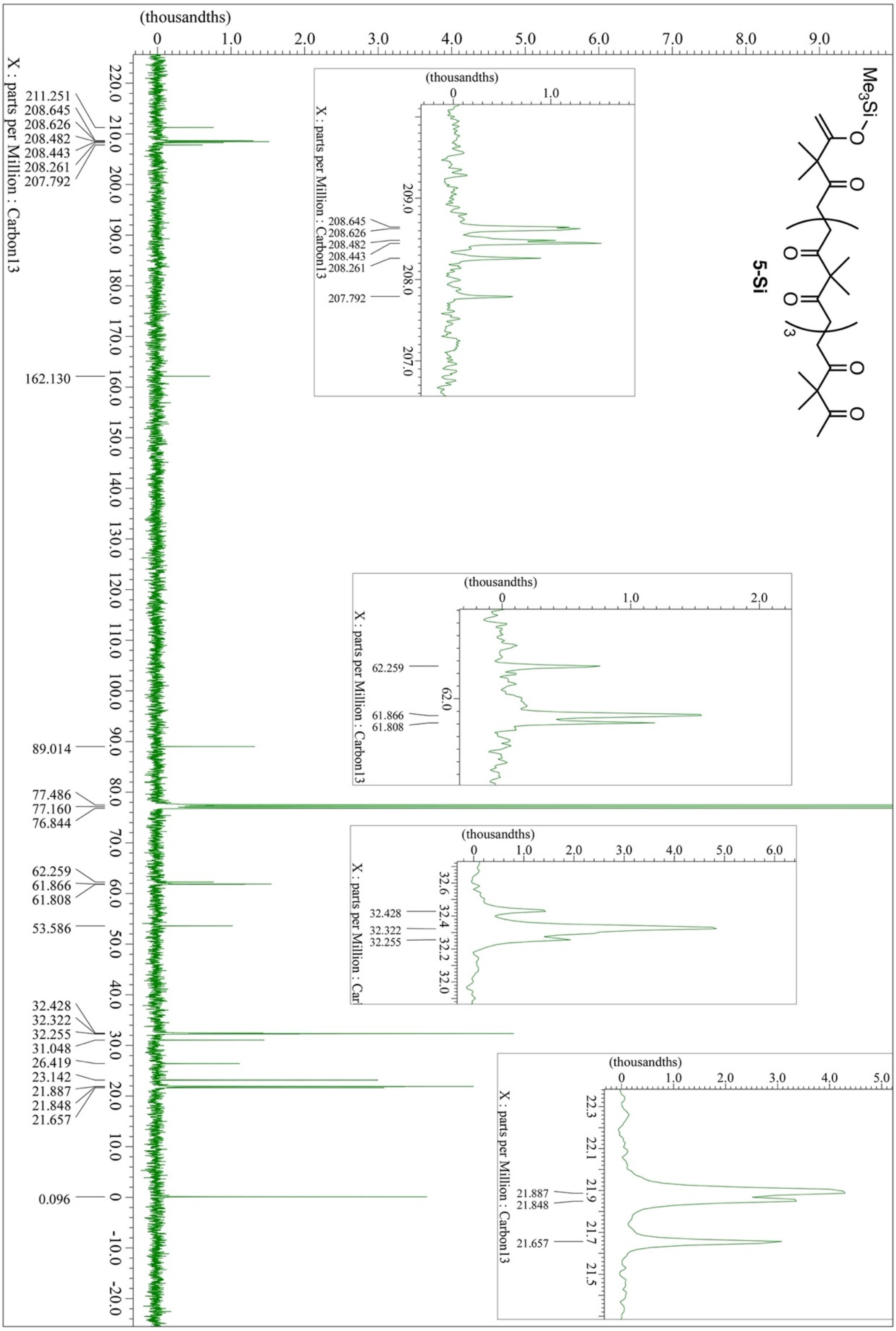


Fig. S30 $^{13}C\{^{1}H\}$ NMR spectrum of mono-silylated pentamer **5-Si** (100 MHz, $CDCl_3$, 298 K).

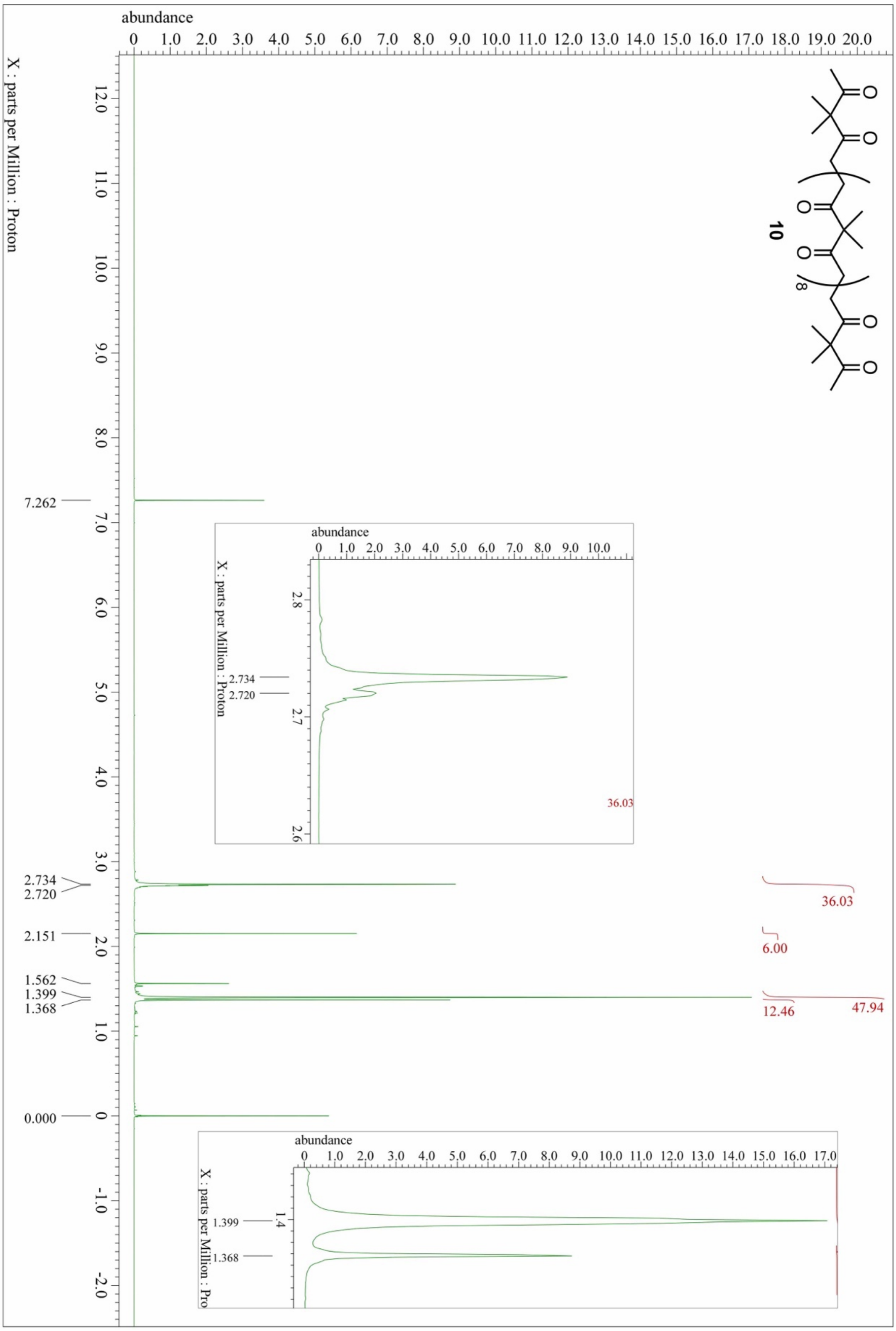


Fig. S31 ^{1}H NMR spectrum of decamer **10** (400 MHz, $CDCl_3$, 298 K).

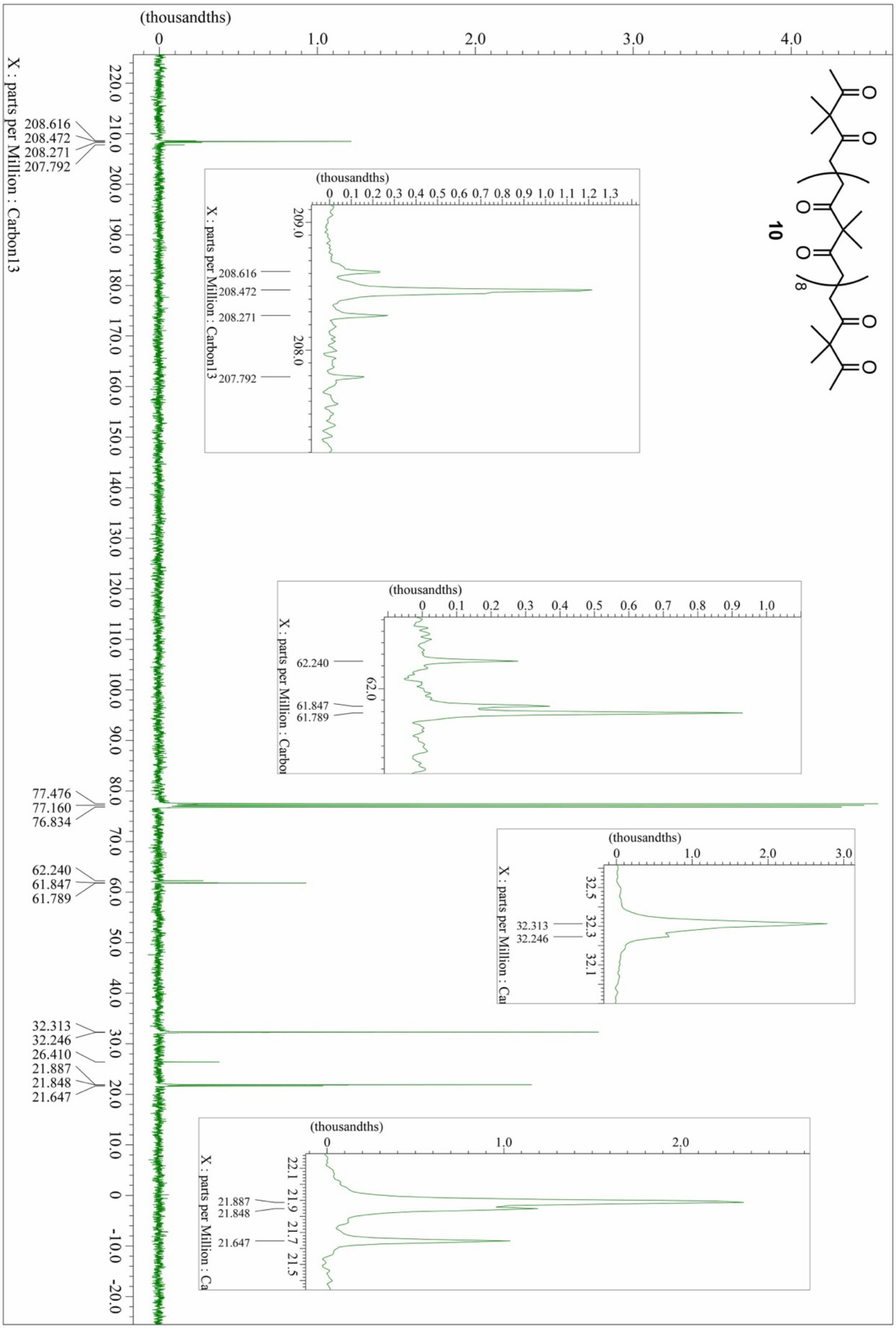


Fig. S32 $^{13}C\{^{1}H\}$ NMR spectrum of decamer **10** (100 MHz, $CDCl_3$, 298 K).

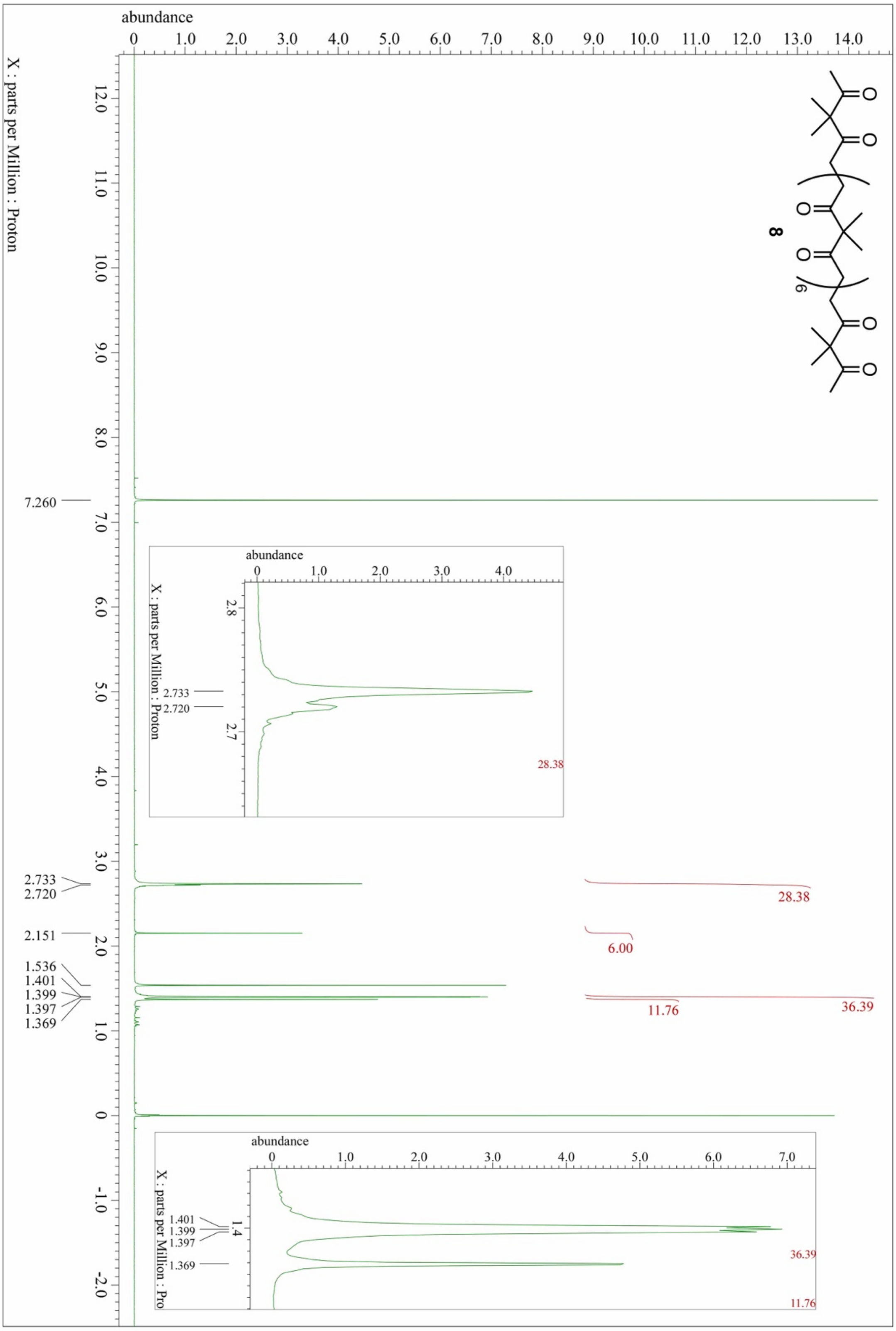


Fig. S33 ^{1}H NMR spectrum of ocatamer **8** (400 MHz, $CDCl_3$, 298 K).

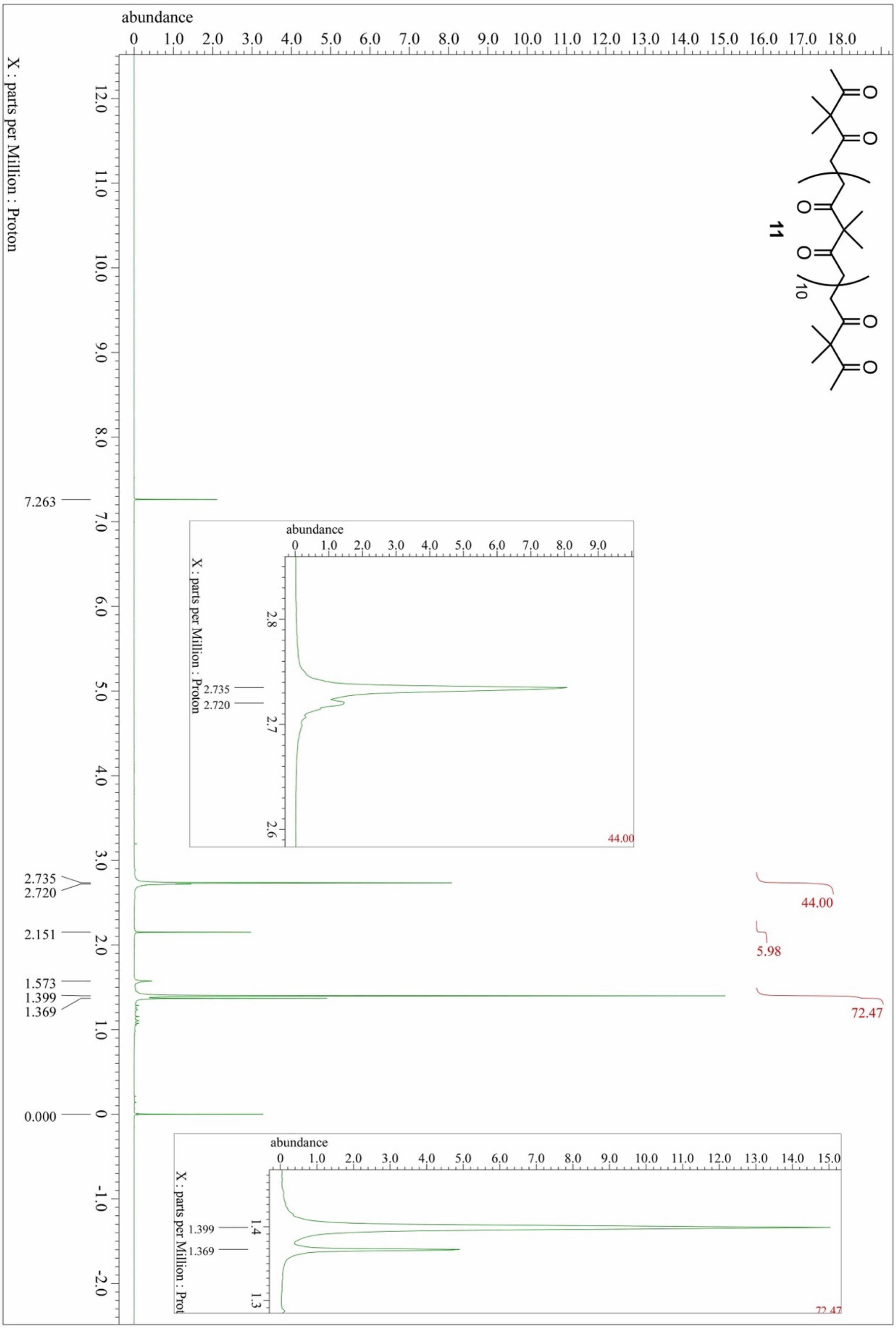


Fig. S34 ^{1}H NMR spectrum of dodecamer **11** (400 MHz, $CDCl_3$, 298 K).

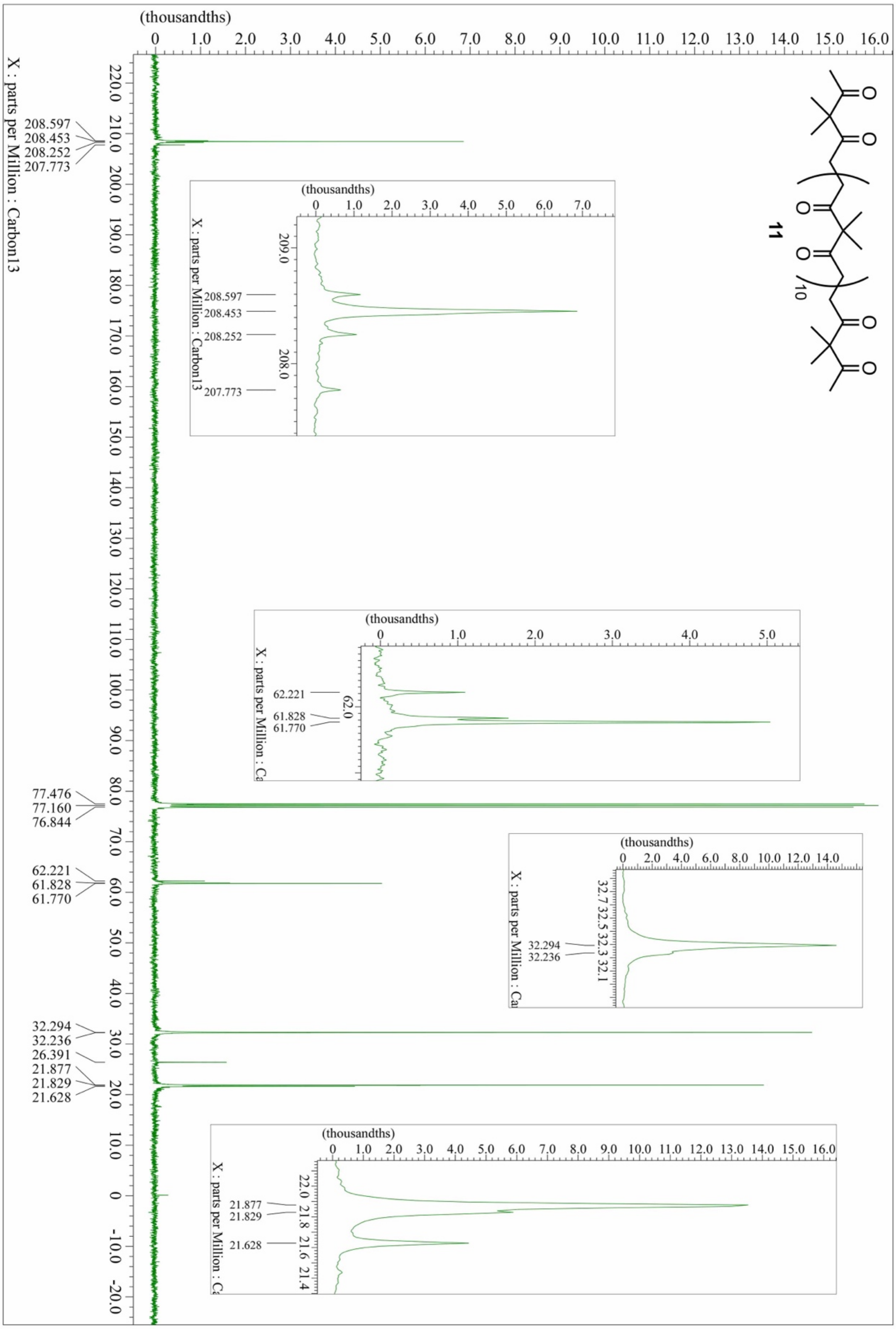


Fig. S35 $^{13}C\{^{1}H\}$ NMR spectrum of dodecamer **11** (100 MHz, $CDCl_3$, 298 K).

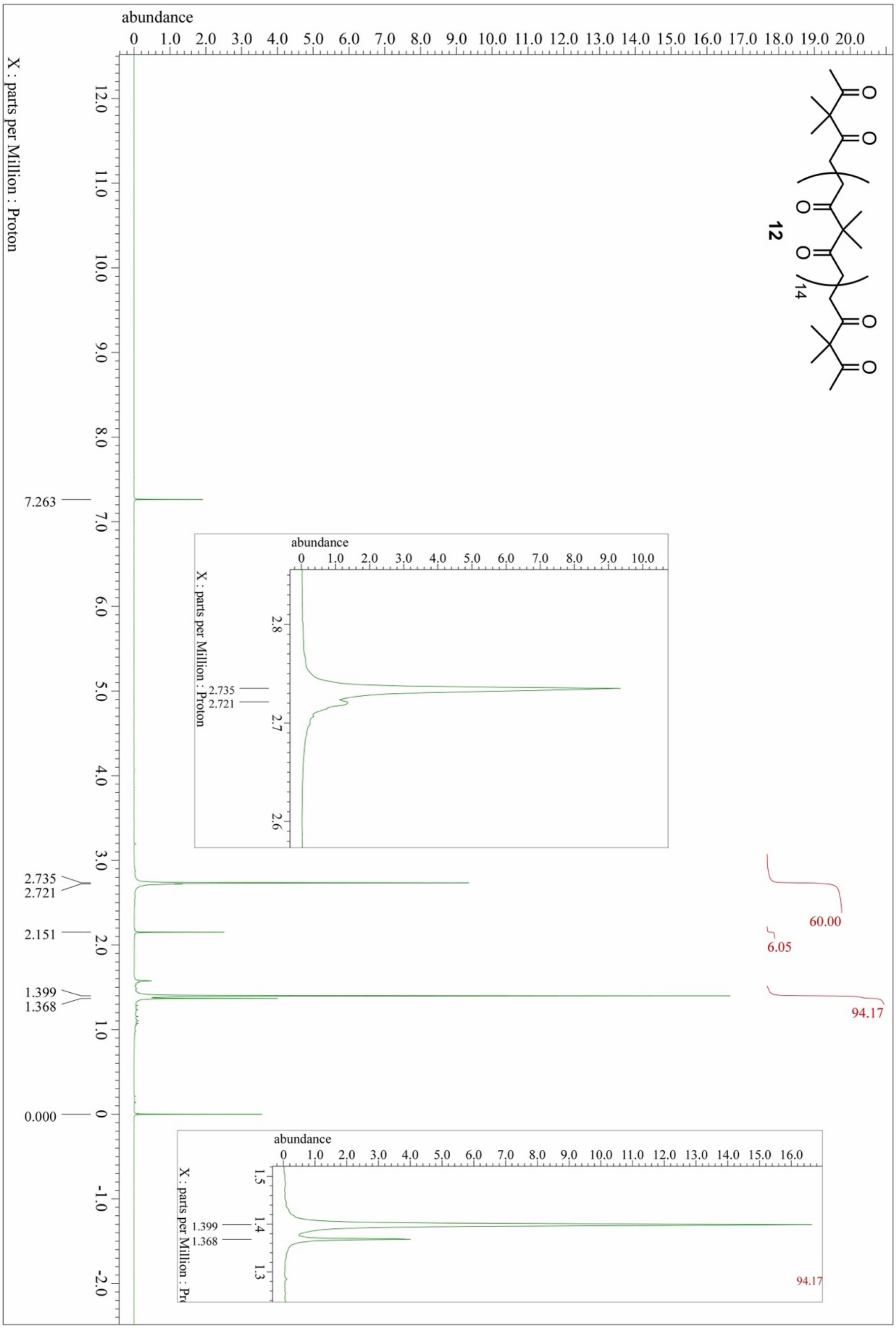


Fig. S36 ^{1}H NMR spectrum of hexadecamer **12** (400 MHz, $CDCl_3$, 298 K).

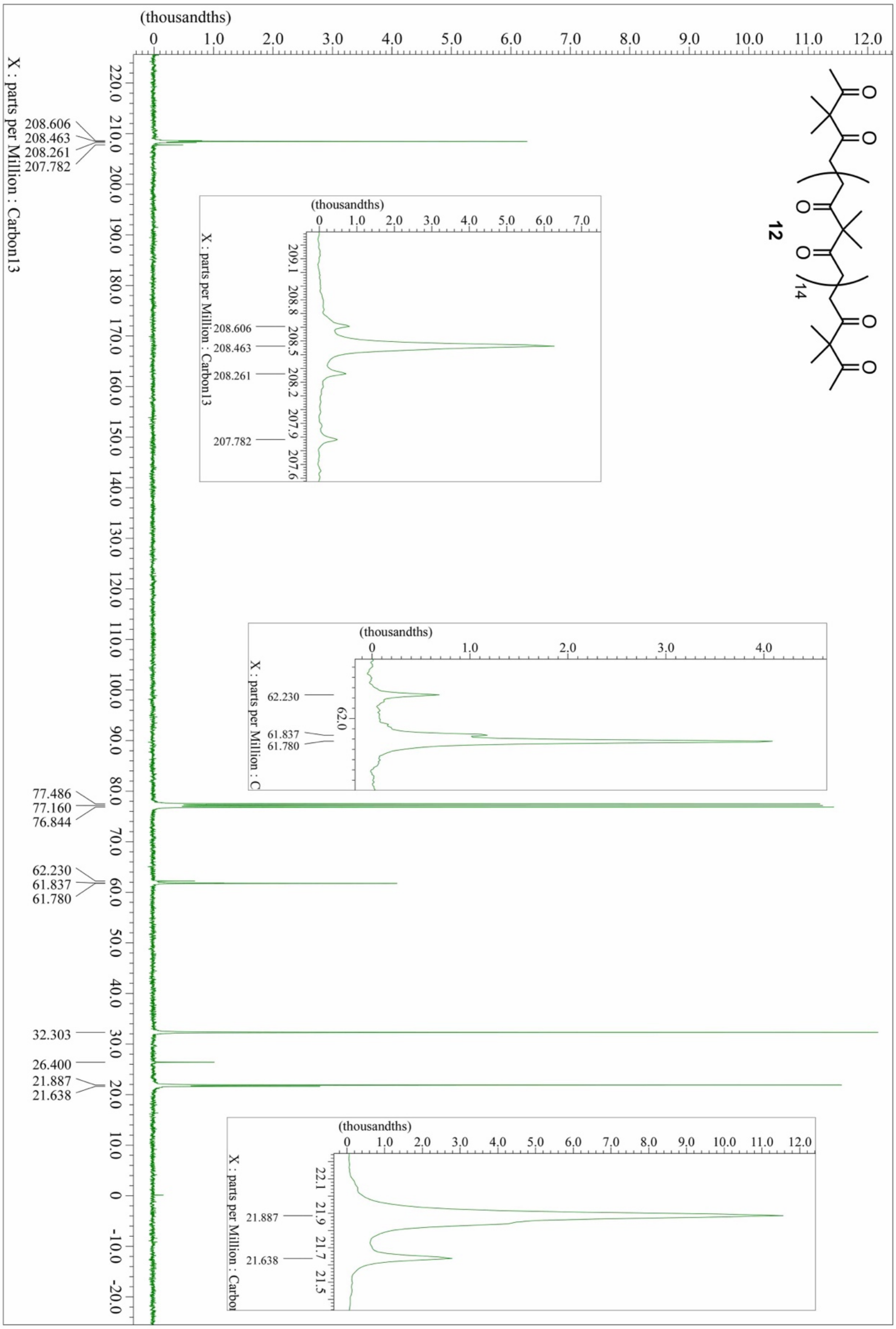


Fig. S37 $^{13}C\{^{1}H\}$ NMR spectrum of hexadecamer **12** (100 MHz, $CDCl_3$, 298 K).

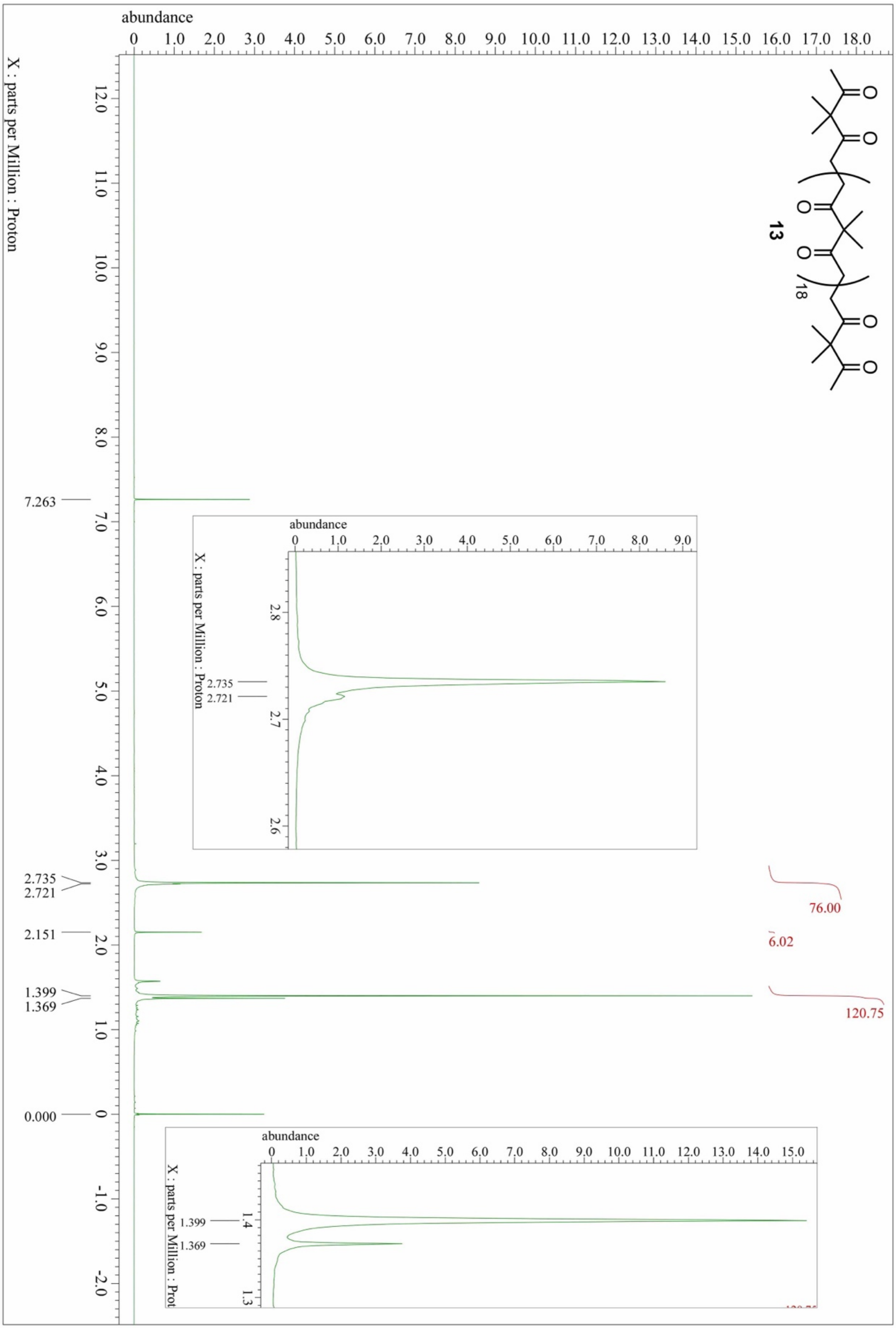


Fig. S38 ^{1}H NMR spectrum of icosamer **13** (400 MHz, $CDCl_3$, 298 K).

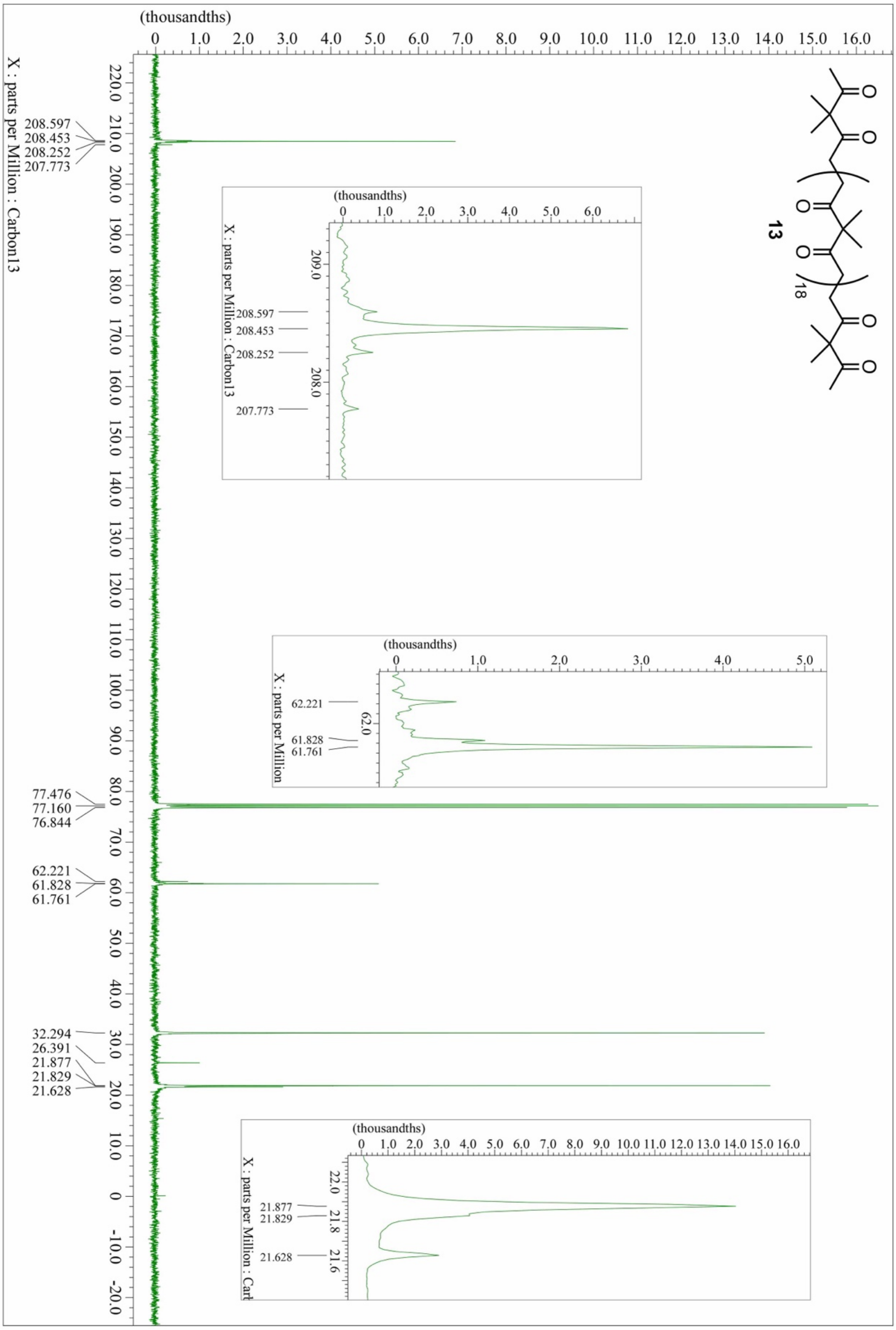


Fig. S39 $^{13}C\{^{1}H\}$ NMR spectrum of icosamer **13** (100 MHz, $CDCl_3$, 298 K).

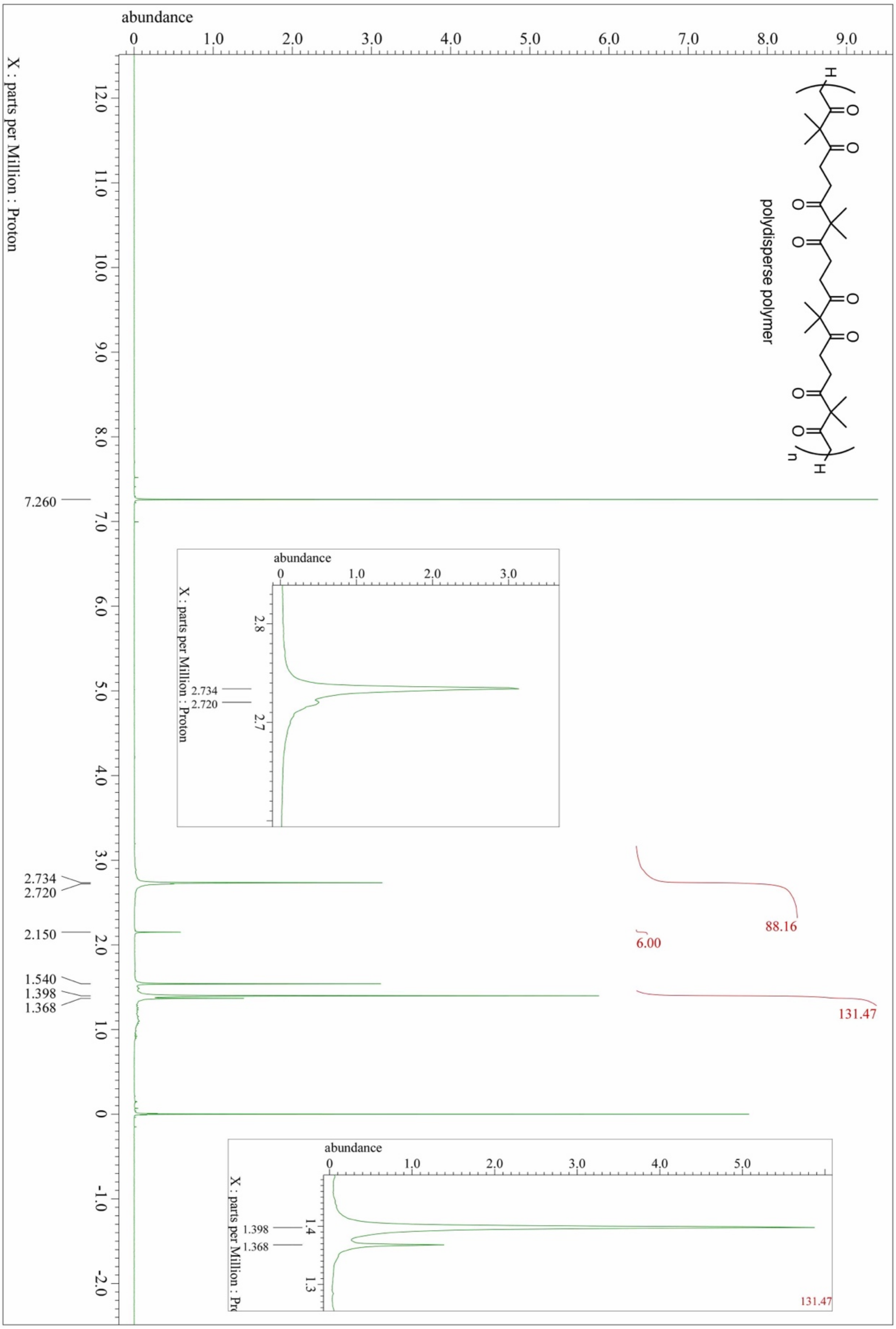


Fig. S40 ¹H NMR spectrum of polydisperse polymer ($N \geq 20$) (400 MHz, $CDCl_3$, 298 K).

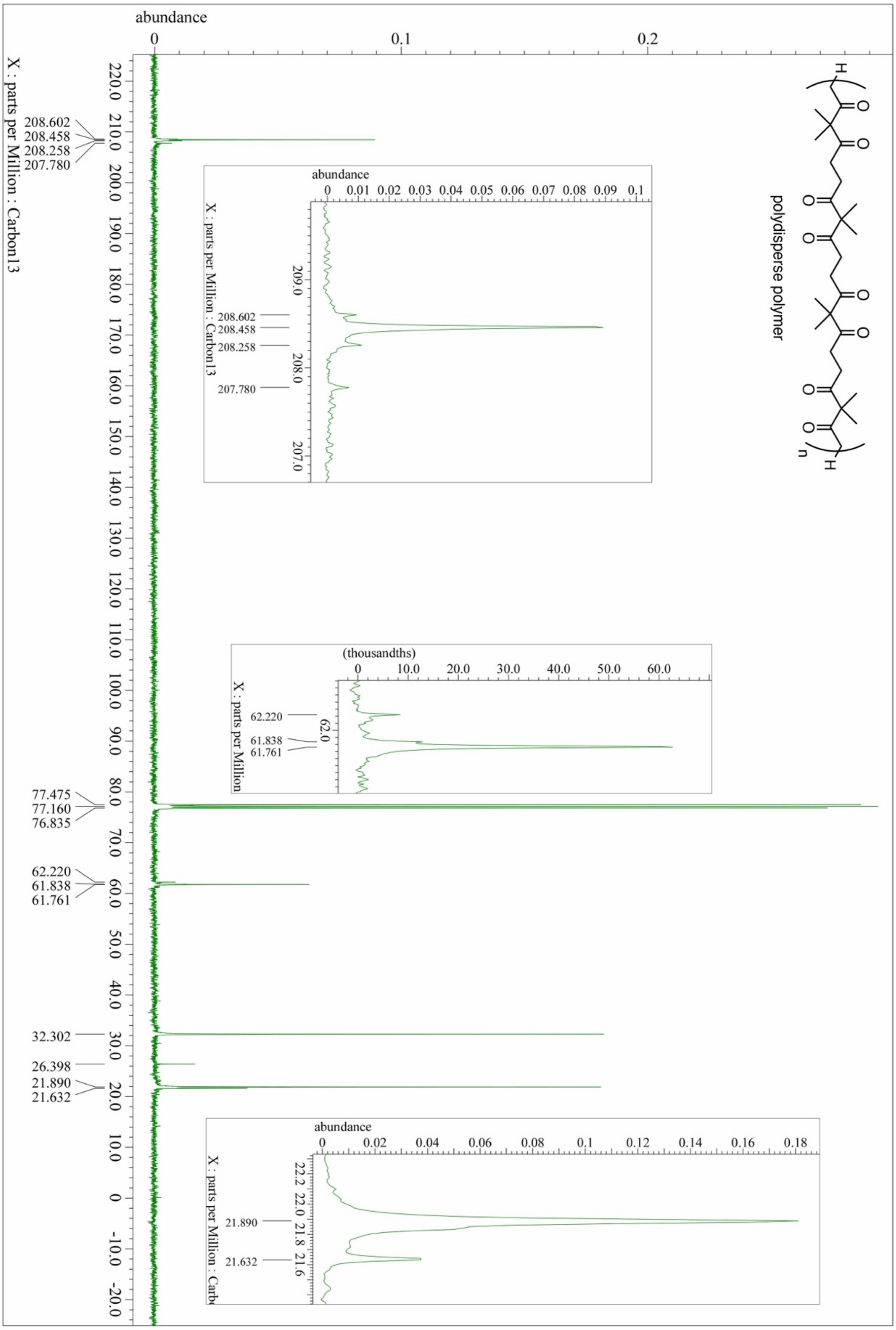


Fig. S41 $^{13}C\{^{1}H\}$ NMR spectrum of polydisperse polymer($N \geq 20$) (100 MHz, $CDCl_3$, 298 K).

11. Cartesian Coordinates of Optimized Structures

Octamer **8**

Total Energy (hartree) = -3387.44684762

C	-0.41640900	14.29564100	-0.87854600
C	0.95753600	14.12619200	-1.48441000
C	-2.76559600	13.51814400	-0.39804700
H	1.46056200	13.27816500	-1.00553500
H	0.90214800	13.91108700	-2.55482100
H	-1.98457400	13.92461500	-3.07200900
H	-3.21141300	14.39317900	-0.87652000
H	-2.60515400	13.77368400	0.64966100
O	-0.71050300	15.27174900	-0.21576200
C	1.44961200	-13.15718200	-1.10861300
C	0.86848500	-11.85850900	-0.51629300
C	0.41640900	-14.29564100	-0.87854600
C	-0.11976400	-10.59303000	1.44904700
C	0.66046400	-11.81683000	0.98995600
C	2.76559600	-13.51814400	-0.39804700
C	1.69168900	-12.97380200	-2.61687300
C	-1.54217700	-10.56810800	0.92112900
C	-0.95753600	-14.12619200	-1.48441000
C	-2.36555500	-9.28558100	1.16028900
C	-3.69608000	-9.37873500	0.39046400
H	-0.16924200	-10.57091400	2.54469300
H	0.39365100	-9.67388700	1.14796500
H	0.17132800	-12.74627600	1.30081000
H	1.64860100	-11.82257100	1.46419100
H	3.47457900	-12.68719200	-0.46425000
H	3.21141300	-14.39317900	-0.87652000
H	2.60515400	-13.77368400	0.64966100
H	2.49769400	-12.25283700	-2.77582500
H	0.80800100	-12.58773600	-3.12510600
H	1.98457400	-13.92461500	-3.07200900
H	-0.90214800	-13.91108700	-2.55482100

H	-1.46056200	-13.27816500	-1.00553500
H	-4.29369300	-10.20190200	0.78743700
H	-3.53584700	-9.57757400	-0.67051200
H	-3.13587400	-10.04572000	3.04749700
O	0.71050300	-15.27174900	-0.21576200
O	0.59382500	-10.91001800	-1.22914100
O	-2.03806100	-11.53120500	0.36322400
C	2.02856000	-5.68511200	-0.47887000
C	1.24547100	-4.39730400	-0.14178600
C	1.10456000	-6.91303200	-0.33572200
C	-0.35695700	-3.12596400	1.35533200
C	0.53008200	-4.35282500	1.19571300
C	3.21405400	-5.81669900	0.49544200
C	2.54103600	-5.60971500	-1.92913000
C	-1.49507200	-3.08238800	0.35276400
C	-0.19596100	-6.89477200	-1.11722400
C	-2.34772800	-1.79587000	0.31194200
C	-1.58134500	-8.05091500	0.66437300
C	-1.11248500	-8.06238700	-0.77857400
C	-3.33680300	-1.87199800	-0.86606600
C	-2.63561400	-9.14880000	2.67086400
H	-0.79801900	-3.11759400	2.35946800
H	0.22898900	-2.20460700	1.27035000
H	-0.04797300	-5.27435400	1.32270700
H	1.29508800	-4.35963300	1.98164200
H	3.83781000	-4.91904800	0.45340800
H	3.82238000	-6.68066500	0.21928400
H	2.87815000	-5.97231500	1.52188200
H	3.25714300	-4.79060100	-2.02300600
H	1.73158600	-5.41368500	-2.63411700
H	3.03783900	-6.54506300	-2.20307400

H	0.05672200	-6.92203300	-2.18404800
H	-0.70045400	-5.93756800	-0.94659500
H	-0.62246600	-9.01940300	-0.98688700
H	-2.00364800	-8.02781700	-1.41698000
H	-4.26091200	-8.44835000	0.49979800
H	-4.03973300	-2.69171100	-0.70284600
H	-2.82620600	-2.06718400	-1.81043000
H	-3.27949000	-8.28538800	2.85112200
H	-1.71439600	-8.98762000	3.23316400
H	-3.71413500	-2.56185700	1.82079100
O	1.43397600	-7.85827200	0.35887700
O	1.23836900	-3.45730300	-0.91624900
O	-1.75735700	-4.02242200	-0.37629500
O	-1.38211500	-7.10599600	1.40655700
C	2.34772800	1.79587000	0.31194200
C	1.49507200	3.08238800	0.35276400
C	1.43397600	0.56588100	0.12111100
C	-0.53008200	4.35282500	1.19571300
C	0.35695700	3.12596400	1.35533200
C	3.11556300	1.66414700	1.64043600
C	3.33680300	1.87199800	-0.86606600
C	-1.24547100	4.39730400	-0.14178600
C	0.48928000	0.58317500	-1.06627800
C	-2.02856000	5.68511200	-0.47887000
C	-1.43397600	-0.56588100	0.12111100
C	-0.48928000	-0.58317500	-1.06627800
C	-2.54103600	5.60971500	-1.92913000
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H	-0.22898900	2.20460700	1.27035000
H	0.79801900	3.11759400	2.35946800
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H	3.78227000	0.80034900	1.59499900
H	2.44060300	1.50755100	2.48334900
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O	-1.23836900	3.45730300	-0.91624900
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C	1.54217700	10.56810800	0.92112900
C	1.58134500	8.05091500	0.66437300
C	-0.66046400	11.81683000	0.98995600
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C	-3.21405400	5.81669900	0.49544200
H	-1.64860100	11.82257100	1.46419100
H	-0.17132800	12.74627600	1.30081000
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H	3.13587400	10.04572000	3.04749700
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H	1.71439600	8.98762000	3.23316400
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H	3.53584700	9.57757400	-0.67051200
H	4.26091200	8.44835000	0.49979800
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H	0.70045400	5.93756800	-0.94659500
H	-0.05672200	6.92203300	-2.18404800
H	-3.03783900	6.54506300	-2.20307400
H	-2.49769400	12.25283700	-2.77582500
H	-0.80800100	12.58773600	-3.12510600
H	-3.82238000	6.68066500	0.21928400
H	-2.87815000	5.97231500	1.52188200
H	-3.47457900	12.68719200	-0.46425000
O	1.38211500	7.10599600	1.40655700
O	2.03806100	11.53120500	0.36322400
O	-0.59382500	10.91001800	-1.22914100
O	-1.43397600	7.85827200	0.35887700
H	-1.53615600	-15.03512700	-1.31741600
H	1.53615600	15.03512700	-1.31741600

Dodecamer **11**

Total Energy (Hartree) = -5080.57582749

C	-2.70442200	9.19991500	1.14865800
C	-1.94419300	10.51217900	0.85966600
C	-1.87080100	7.99268300	0.66667000
C	0.19572300	11.87112800	0.90719400
C	-0.52812700	10.62315600	1.39343000
C	-2.94429900	9.08554000	2.66560300
C	-4.04954100	9.20939100	0.39885100
C	0.39445400	11.89376600	-0.59708500
C	-1.40639500	8.00543400	-0.77790100
C	0.95782500	13.19290800	-1.21338700
C	0.85368700	6.94906400	-0.32589700
C	-0.44600600	6.87033700	-1.10502900
C	0.94043200	13.08241100	-2.74940700
C	2.99877600	5.94105700	0.52544600
H	1.18672200	11.92777400	1.37373900
H	-0.33806700	12.77813200	1.21044100
H	0.02664000	9.71794100	1.12434000
H	-0.58577200	10.63329700	2.48863200
H	-3.47430100	9.96979100	3.03157600
H	-3.54921900	8.20094300	2.87592100
H	-2.00823200	8.97516100	3.21536900
H	-4.68052900	10.01205100	0.78654100
H	-3.91558700	9.39042000	-0.66882200
H	-4.56661200	8.25572300	0.53972500
H	-2.29694000	7.92967900	-1.41361400
H	-0.95414000	8.97817000	-0.99868400
H	-0.91276800	5.89643900	-0.92278600
H	-0.19541400	6.89532300	-2.17250000
H	2.80631000	6.63437200	-2.18056300
H	1.61467800	12.28438500	-3.06754400
H	-0.05349400	12.83478100	-3.12542000
H	3.57461200	6.82476300	0.24231200
H	2.65287700	6.09477500	1.54886600
H	3.00910100	12.52109100	-0.94787400
O	-1.63094300	7.06616600	1.42013800
O	-2.48417600	11.41954000	0.25201700
O	0.15253300	10.92955900	-1.30083300
O	1.14947800	7.91730200	0.35159500
C	-2.73662500	16.71043200	1.77048400
C	-2.11609900	18.00912400	1.21533400
C	-2.12179900	15.48331600	1.06224300
C	-0.09634300	19.33889500	0.46079200
C	-0.60206100	18.10911800	1.20181000
C	-2.44371600	16.63079700	3.28086200

C	-4.25695600	16.72212500	1.52538900
C	-0.43224100	19.31955100	-1.02266400
C	-2.19307900	15.45119600	-0.45302100
C	-0.16244500	20.61029200	-1.81976500
C	0.08813200	14.39522000	-0.78819300
C	-1.40121800	14.30263200	-1.06265800
C	-0.44600600	20.36501300	-3.31211000
C	2.39978200	13.39883500	-0.71344800
H	0.99370500	19.40320300	0.55578900
H	-0.49214800	20.26268600	0.89645000
H	-0.18372200	17.19669400	0.76399600
H	-0.25902900	18.13343000	2.24345700
H	-2.81918900	17.52553500	3.78590600
H	-2.93895200	15.75445300	3.70431100
H	-1.37599400	16.52617500	3.48050100
H	-4.71361000	17.54040000	2.08599700
H	-4.49514600	16.87907200	0.47206300
H	-4.69935300	15.77807300	1.85649800
H	-3.24943400	15.35938900	-0.73339400
H	-1.85341200	16.41495300	-0.84682600
H	-1.77075100	13.33676400	-0.70182600
H	-1.53898100	14.29644800	-2.15067400
H	1.27121900	14.02313500	-3.19921400
H	0.29465400	19.67168500	-3.71892000
H	-1.42772800	19.91830400	-3.46981500
H	2.83738400	14.27138000	-1.20323500
H	2.43239800	13.58114100	0.36189100
H	1.98329200	20.25668800	-1.90423600
O	-1.63094300	14.57689800	1.71090700
O	-2.82455000	18.92716700	0.84106800
O	-0.89186200	18.33019100	-1.56417400
O	0.59732900	15.37887700	-0.28068700
C	-1.11456200	21.71608200	-1.28298000
C	-2.60124400	21.45669300	-1.35967100
C	1.29547800	21.05962900	-1.62178900
H	-2.85556600	20.62206200	-0.69611300
H	-2.91007700	21.17587400	-2.37001000
H	-0.38184600	21.30431100	-3.86934000
H	1.49909300	21.92838800	-2.25192400
H	1.49274000	21.35855600	-0.59195700
O	-0.66436400	22.73904000	-0.80410700
C	0.16244500	-20.61029200	-1.81976500
C	0.43224100	-19.31955100	-1.02266400
C	1.11456200	-21.71608200	-1.28298000
C	0.60206100	-18.10911800	1.20181000
C	0.09634300	-19.33889500	0.46079200
C	-1.29547800	-21.05962900	-1.62178900
C	0.44600600	-20.36501300	-3.31211000
C	2.11609900	-18.00912400	1.21533400
C	2.60124400	-21.45669300	-1.35967100
C	2.73662500	-16.71043200	1.77048400
C	4.25695600	-16.72212500	1.52538900
H	0.25902900	-18.13343000	2.24345700
H	0.18372200	-17.19669400	0.76399600
H	0.49214800	-20.26268600	0.89645000
H	-0.99370500	-19.40320300	0.55578900
H	-1.98329200	-20.25668800	-1.90423600
H	-1.49909300	-21.92838800	-2.25192400
H	-1.49274000	-21.35855600	-0.59195700
H	-0.29465400	-19.67168500	-3.71892000
H	1.42772800	-19.91830400	-3.46981500
H	0.38184600	-21.30431100	-3.86934000
H	2.91007700	-21.17587400	-2.37001000
H	2.85556600	-20.62206200	-0.69611300
H	4.71361000	-17.54040000	2.08599700
H	4.49514600	-16.87907200	0.47206300
H	2.81918900	-17.52553500	3.78590600
O	0.66436400	-22.73904000	-0.80410700
O	0.89186200	-18.33019100	-1.56417400
O	2.82455000	-18.92716700	0.84106800
C	-0.95782500	-13.19290800	-1.21338700
C	-0.39445400	-11.89376600	-0.59708500

C	-0.08813200	-14.39522000	-0.78819300
C	0.52812700	-10.62315600	1.39343000
C	-0.19572300	-11.87112800	0.90719400
C	-2.39978200	-13.39883500	-0.71344800
C	-0.94043200	-13.08241100	-2.74940700
C	1.94419300	-10.51217900	0.85966600
C	1.40121800	-14.30263200	-1.06265800
C	2.70442200	-9.19991500	1.14865800
C	2.12179900	-15.48331600	1.06224300
C	2.19307900	-15.45119600	-0.45302100
C	4.04954100	-9.20939100	0.39885100
C	2.44371600	-16.63079700	3.28086200
H	0.58577200	-10.63329700	2.48863200
H	-0.02664000	-9.71794100	1.12434000
H	0.33806700	-12.77813200	1.21044100
H	-1.18672200	-11.92777400	1.37373900
H	-3.00910100	-12.52109100	-0.94787400
H	-2.83738400	-14.27138000	-1.20323500
H	-2.43239800	-13.58114100	0.36189100
H	-1.61467800	-12.28438500	-3.06754400
H	0.05349400	-12.83478100	-3.12542000
H	-1.27121900	-14.02313500	-3.19921400
H	1.53898100	-14.29644800	-2.15067400
H	1.77075100	-13.33676400	-0.70182600
H	1.85341200	-16.41495300	-0.84682600
H	3.24943400	-15.35938900	-0.73339400
H	4.69935300	-15.77807300	1.85649800
H	4.68052900	-10.01205100	0.78654100
H	3.91558700	-9.39042000	-0.66882200
H	2.93895200	-15.75445300	3.70431100
H	1.37599400	-16.52617500	3.48050100
H	3.47430100	-9.96979100	3.03157600
O	-0.59732900	-15.37887700	-0.28068700
O	-0.15253300	-10.92955900	-1.30083300
O	2.48417600	-11.41954000	0.25201700
O	1.63094300	-14.57689800	1.71090700
C	-1.82320700	-5.75405300	-0.45166400
C	-1.08767900	-4.44151600	-0.10452400
C	-0.85368700	-6.94906400	-0.32589700
C	0.46551000	-3.12290500	1.40446900
C	-0.37456900	-4.38104600	1.23354100
C	-2.99877600	-5.94105700	0.52544600
C	-2.34381800	-5.68371700	-1.89936000
C	1.60385700	-3.02890200	0.40551500
C	0.44600600	-6.87033700	-1.10502900
C	2.40879600	-1.71162900	0.37727100
C	1.87080100	-7.99268300	0.66667000
C	1.40639500	-8.00543400	-0.77790100
C	3.40695900	-1.74452000	-0.79504000
C	2.94429900	-9.08554000	2.66560300
H	0.90360600	-3.10585900	2.40979800
H	-0.15414900	-2.22327800	1.32517800
H	0.23771800	-5.28128300	1.35272100
H	-1.13876100	-4.42363800	2.01912900
H	-3.65665300	-5.06755300	0.49560900
H	-3.57461200	-6.82476300	0.24231200
H	-2.65287700	-6.09477500	1.54886600
H	-3.09046300	-4.89112300	-1.98296600
H	-1.54482700	-5.45088200	-2.60509100
H	-2.80631000	-6.63437200	-2.18056300
H	0.19541400	-6.89532300	-2.17250000
H	0.91276800	-5.89643900	-0.92278600
H	0.95414000	-8.97817000	-0.99868400
H	2.29694000	-7.92967900	-1.41361400
H	4.56661200	-8.25572300	0.53972500
H	4.13861800	-2.53880800	-0.63224000
H	2.90936400	-1.95279500	-1.74354300
H	3.54921900	-8.20094300	2.87592100
H	2.00823200	-8.97516100	3.21536900
H	3.79303300	-2.43445500	1.89094000
O	-1.14947800	-7.91730200	0.35159500
O	-1.11388600	-3.49603100	-0.87208500

O	1.90256400	-3.95250500	-0.33045900
O	1.63094300	-7.06616600	1.42013800
C	-2.40879600	1.71162900	0.37727100
C	-1.60385700	3.02890200	0.40551500
C	-1.45202300	0.51481400	0.18638300
C	0.37456900	4.38104600	1.23354100
C	-0.46551000	3.12290500	1.40446900
C	-3.16320400	1.55848100	1.71109700
C	-3.40695900	1.74452000	-0.79504000
C	1.08767900	4.44151600	-0.10452400
C	-0.50992600	0.56517800	-1.00206800
C	1.82320700	5.75405300	-0.45166400
C	1.45202300	-0.51481400	0.18638300
C	0.50992600	-0.56517800	-1.00206800
C	2.34381800	5.68371700	-1.89936000
C	3.16320400	-1.55848100	1.71109700
H	1.13876100	4.42363800	2.01912900
H	-0.23771800	5.28128300	1.35272100
H	0.15414900	2.22327800	1.32517800
H	-0.90360600	3.10585900	2.40979800
H	-3.79303300	2.43445500	1.89094000
H	-3.79800400	0.67059100	1.67408300
H	-2.47780700	1.43107100	2.55053200
H	-4.13861800	2.53880800	-0.63224000
H	-2.90936400	1.95279500	-1.74354300
H	-3.93469100	0.78906700	-0.86800800
H	-1.12001700	0.51131700	-1.91191500
H	-0.01397200	1.54145400	-1.02325200
H	0.01397200	-1.54145400	-1.02325200
H	1.12001700	-0.51131700	-1.91191500
H	3.93469100	-0.78906700	-0.86800800
H	3.09046300	4.89112300	-1.98296600
H	1.54482700	5.45088200	-2.60509100
H	3.79800400	-0.67059100	1.67408300
H	2.47780700	-1.43107100	2.55053200
H	3.65665300	5.06755300	0.49560900
O	-1.48655700	-0.43295700	0.95081800
O	-1.90256400	3.95250500	-0.33045900
O	1.11388600	3.49603100	-0.87208500
O	1.48655700	0.43295700	0.95081800
H	3.13712900	-22.35152500	-1.04186900
H	-3.13712900	22.35152500	-1.04186900

Hexadecamer **12**

Total energy (Hartree) = -6773.70480655

C	-2.18151300	1.99238000	0.28981800
C	-1.22260400	3.20217000	0.31875100
C	-1.37823900	0.68779300	0.09774100
C	0.90814300	4.30147900	1.14322300
C	-0.07897100	3.15513500	1.31497200
C	-2.94838500	1.93166200	1.62395300
C	-3.16872500	2.14729200	-0.88198800
C	1.61753500	4.27826900	-0.19797100
C	-0.43750100	0.62296900	-1.09111100
C	2.50504100	5.49284900	-0.54614800
C	1.37823900	-0.68779300	0.09774100
C	0.43750100	-0.62296900	-1.09111100
C	3.00154800	5.36665200	-1.99847000
C	2.94838500	-1.93166200	1.62395300
H	1.67531900	4.24754200	1.92523400
H	0.41135700	5.26953300	1.26799100
H	0.42586700	2.18659500	1.23375100
H	-0.51374300	3.19081100	2.32128700
H	-3.46702900	2.87780500	1.80435100
H	-3.68634500	1.12746600	1.58705600
H	-2.28303600	1.72169400	2.46294600
H	-3.79749900	3.02518300	-0.71880500

H	-2.64974800	2.29315700	-1.83070600
H	-3.80941800	1.26358600	-0.95474300
H	-1.05025200	0.64297100	-2.00057800
H	0.17315400	1.53186800	-1.11338800
H	-0.17315400	-1.53186800	-1.11338800
H	1.05025200	-0.64297100	-2.00057800
H	3.80941800	-1.26358600	-0.95474300
H	3.64428100	4.48867900	-2.09182200
H	2.17433800	5.23760100	-2.69829800
H	3.68634500	-1.12746600	1.58705600
H	2.28303600	-1.72169400	2.46294600
H	4.24823600	4.58151300	0.38170900
O	-1.52851200	-0.24929900	0.86139400
O	-1.40933300	4.15720100	-0.41404000
O	1.52657700	3.33795500	-0.96698500
O	1.52851200	0.24929900	0.86139400
C	-1.54987900	9.46156300	1.10789000
C	-0.63697500	10.67238700	0.81716600
C	-0.87636400	8.16333400	0.61274000
C	1.65385600	11.75824400	0.84867400
C	0.78696600	10.60596100	1.33712700
C	-1.78846000	9.36941100	2.62654100
C	-2.89037700	9.64043500	0.37109200
C	1.83754400	11.76597300	-0.65756500
C	-0.42488200	8.12702100	-0.83548100
C	2.55004300	12.98959400	-1.27364000
C	1.69093300	6.79733100	-0.40675800
C	0.38584600	6.88412700	-1.17594500
C	2.49896900	12.89397400	-2.80986200
C	3.70254700	5.52879000	0.42161000
H	2.64930400	11.68937800	1.30399000
H	1.23944000	12.72212000	1.16284400
H	1.22363900	9.64077100	1.05919400
H	0.74125000	10.61772900	2.43288400
H	-2.20230300	10.31021000	3.00119400
H	-2.49566000	8.56477900	2.83893500
H	-0.86814900	9.14195000	3.16685800
H	-3.41403800	10.51274900	0.76801000
H	-2.74469000	9.80915200	-0.69707600
H	-3.51970900	8.75697700	0.51308700
H	-1.32297500	8.16472800	-1.46397500
H	0.14161400	9.03803400	-1.05596400
H	-0.19597800	5.97390100	-0.99548700
H	0.62999400	6.88490900	-2.24520000
H	3.57514900	6.25473200	-2.27960100
H	3.06287500	12.01978800	-3.14224700
H	1.47687600	12.77672500	-3.17353700
H	4.37985100	6.33715600	0.13787700
H	3.38622100	5.71753800	1.44873900
H	4.50476000	12.06478700	-1.04139900
O	-0.74823100	7.20930400	1.35923600
O	-1.06760400	11.64252300	0.21936700
O	1.47168900	10.84301800	-1.36330800
O	2.10860600	7.71757700	0.27342200
C	-0.64025700	16.91001500	1.78971500
C	0.11610900	18.12960300	1.22054200
C	-0.18987400	15.62481400	1.06172000
C	2.27452100	19.22208700	0.46186700
C	1.63161800	18.05635900	1.20056200
C	-0.32699700	16.78556500	3.29246600
C	-2.15387100	17.09940100	1.57822200
C	1.91218600	19.26360800	-1.01116000
C	-0.28109500	15.61951100	-0.45295200
C	2.36358400	20.50408500	-1.81285500
C	1.84375200	14.28858200	-0.82927700
C	0.35097700	14.38625600	-1.08333000
C	1.77061200	20.44150500	-3.23284400
C	4.01287900	13.00969500	-0.79260100
H	3.36639500	19.14635700	0.53293300
H	2.00293600	20.17736200	0.92355000
H	1.93716500	17.09913300	0.76478500
H	1.97723600	18.04358600	2.24136000

H	-0.57793000	17.71688600	3.80861000
H	-0.91670300	15.97420300	3.72444800
H	0.72393500	16.55011500	3.46786200
H	-2.49993100	17.96143600	2.15253000
H	-2.39467100	17.29056300	0.53125600
H	-2.69587300	16.21099400	1.91534800
H	-1.34341800	15.66741900	-0.72159700
H	0.17467700	16.53655600	-0.84131100
H	-0.13260400	13.47095100	-0.72566700
H	0.19972600	14.40861700	-2.16939800
H	2.93982300	13.78903400	-3.25847100
H	2.17839600	19.57822900	-3.76302000
H	0.68580300	20.32562300	-3.21292900
H	4.54941900	13.82512400	-1.28240600
H	4.08189100	13.17753800	0.28337400
H	4.27049000	19.58393200	-2.30926000
O	0.19188000	14.65675400	1.69482200
O	-0.49355500	19.11150600	0.83543900
O	1.31714600	18.35455000	-1.56162200
O	2.47927300	15.19685200	-0.32409700
C	0.48102200	24.34657900	2.26252000
C	1.00956600	25.57793200	1.49828900
C	0.63697500	23.07691800	1.39713900
C	2.75890500	26.67914900	0.03422600
C	2.41294400	25.49582600	0.92716300
C	1.29502000	24.18558300	3.56056700
C	-1.00947700	24.54815600	2.59340200
C	1.90127300	26.74854000	-1.22020600
C	0.01291500	23.10065300	0.01429700
C	2.01439700	28.02386900	-2.07748000
C	1.86453800	21.78878400	-1.11793100
C	0.37879700	21.88457400	-0.82557900
C	1.17673300	27.86196800	-3.35799600
C	3.90198700	20.52092200	-1.88159700
H	3.80636400	26.60830500	-0.28074100
H	2.66909400	27.62929800	0.57177700

H	2.52543100	24.55423400	0.37946800
H	3.11449900	25.44535700	1.76893900
H	1.24385400	25.10285400	4.15437100
H	0.88582000	23.36226900	4.14983400
H	2.34006300	23.94756100	3.35540200
H	-1.12448300	25.39785800	3.26954100
H	-1.59623900	24.76457000	1.69910300
H	-1.41190000	23.65434200	3.07892400
H	-1.07545300	23.14512900	0.14254900
H	0.30055900	24.02840200	-0.49153900
H	0.05075600	20.95940600	-0.33968600
H	-0.14696800	21.92894600	-1.78703300
H	2.02535100	21.34870000	-3.78856700
H	1.62756400	27.10041100	-3.99953500
H	0.15928500	27.53840400	-3.13823000
H	4.23255600	21.34909900	-2.51213100
H	4.34879000	20.66572000	-0.89669100
H	3.92037200	27.42424200	-2.93999900
O	1.21408300	22.09777800	1.83481500
O	0.33213000	26.58569800	1.39700800
O	1.15772200	25.83880100	-1.54091600
O	2.64094200	22.68810500	-0.84791000
C	1.46622800	29.21564600	-1.24268800
C	0.03440400	29.13626600	-0.76643100
C	3.48642900	28.29251200	-2.43463700
H	-0.05955800	28.31629300	-0.04507800
H	-0.65369300	28.92711200	-1.58970900
H	1.14519200	28.80490700	-3.91186900
H	3.54881100	29.15171500	-3.10632300
H	4.08167900	28.53209600	-1.55310900
O	2.18151300	30.16145500	-0.97385700
C	-2.01439700	-28.02386900	-2.07748000
C	-1.90127300	-26.74854000	-1.22020600
C	-1.46622800	-29.21564600	-1.24268800
C	-2.41294400	-25.49582600	0.92716300
C	-2.75890500	-26.67914900	0.03422600

C	-3.48642900	-28.29251200	-2.43463700
C	-1.17673300	-27.86196800	-3.35799600
C	-1.00956600	-25.57793200	1.49828900
C	-0.03440400	-29.13626600	-0.76643100
C	-0.48102200	-24.34657900	2.26252000
C	1.00947700	-24.54815600	2.59340200
H	-3.11449900	-25.44535700	1.76893900
H	-2.52543100	-24.55423400	0.37946800
H	-2.66909400	-27.62929800	0.57177700
H	-3.80636400	-26.60830500	-0.28074100
H	-3.92037200	-27.42424200	-2.93999900
H	-3.54881100	-29.15171500	-3.10632300
H	-4.08167900	-28.53209600	-1.55310900
H	-1.62756400	-27.10041100	-3.99953500
H	-0.15928500	-27.53840400	-3.13823000
H	-1.14519200	-28.80490700	-3.91186900
H	0.65369300	-28.92711200	-1.58970900
H	0.05955800	-28.31629300	-0.04507800
H	1.12448300	-25.39785800	3.26954100
H	1.59623900	-24.76457000	1.69910300
H	-1.24385400	-25.10285400	4.15437100
O	-2.18151300	-30.16145500	-0.97385700
O	-1.15772200	-25.83880100	-1.54091600
O	-0.33213000	-26.58569800	1.39700800
C	-2.36358400	-20.50408500	-1.81285500
C	-1.91218600	-19.26360800	-1.01116000
C	-1.86453800	-21.78878400	-1.11793100
C	-1.63161800	-18.05635900	1.20056200
C	-2.27452100	-19.22208700	0.46186700
C	-3.90198700	-20.52092200	-1.88159700
C	-1.77061200	-20.44150500	-3.23284400
C	-0.11610900	-18.12960300	1.22054200
C	-0.37879700	-21.88457400	-0.82557900
C	0.64025700	-16.91001500	1.78971500
C	-0.63697500	-23.07691800	1.39713900
C	-0.01291500	-23.10065300	0.01429700

C	2.15387100	-17.09940100	1.57822200
C	-1.29502000	-24.18558300	3.56056700
H	-1.97723600	-18.04358600	2.24136000
H	-1.93716500	-17.09913300	0.76478500
H	-2.00293600	-20.17736200	0.92355000
H	-3.36639500	-19.14635700	0.53293300
H	-4.27049000	-19.58393200	-2.30926000
H	-4.23255600	-21.34909900	-2.51213100
H	-4.34879000	-20.66572000	-0.89669100
H	-2.17839600	-19.57822900	-3.76302000
H	-0.68580300	-20.32562300	-3.21292900
H	-2.02535100	-21.34870000	-3.78856700
H	0.14696800	-21.92894600	-1.78703300
H	-0.05075600	-20.95940600	-0.33968600
H	-0.30055900	-24.02840200	-0.49153900
H	1.07545300	-23.14512900	0.14254900
H	1.41190000	-23.65434200	3.07892400
H	2.49993100	-17.96143600	2.15253000
H	2.39467100	-17.29056300	0.53125600
H	-0.88582000	-23.36226900	4.14983400
H	-2.34006300	-23.94756100	3.35540200
H	0.57793000	-17.71688600	3.80861000
O	-2.64094200	-22.68810500	-0.84791000
O	-1.31714600	-18.35455000	-1.56162200
O	0.49355500	-19.11150600	0.83543900
O	-1.21408300	-22.09777800	1.83481500
C	-2.55004300	-12.98959400	-1.27364000
C	-1.83754400	-11.76597300	-0.65756500
C	-1.84375200	-14.28858200	-0.82927700
C	-0.78696600	-10.60596100	1.33712700
C	-1.65385600	-11.75824400	0.84867400
C	-4.01287900	-13.00969500	-0.79260100
C	-2.49896900	-12.89397400	-2.80986200
C	0.63697500	-10.67238700	0.81716600
C	-0.35097700	-14.38625600	-1.08333000
C	1.54987900	-9.46156300	1.10789000

C 0.18987400 -15.62481400 1.06172000
C 0.28109500 -15.61951100 -0.45295200
C 2.89037700 -9.64043500 0.37109200
C 0.32699700 -16.78556500 3.29246600
H -0.74125000 -10.61772900 2.43288400
H -1.22363900 -9.64077100 1.05919400
H -1.23944000 -12.72212000 1.16284400
H -2.64930400 -11.68937800 1.30399000
H -4.50476000 -12.06478700 -1.04139900
H -4.54941900 -13.82512400 -1.28240600
H -4.08189100 -13.17753800 0.28337400
H -3.06287500 -12.01978800 -3.14224700
H -1.47687600 -12.77672500 -3.17353700
H -2.93982300 -13.78903400 -3.25847100
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H 0.13260400 -13.47095100 -0.72566700
H -0.17467700 -16.53655600 -0.84131100
H 1.34341800 -15.66741900 -0.72159700
H 2.69587300 -16.21099400 1.91534800
H 3.41403800 -10.51274900 0.76801000
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H 0.91670300 -15.97420300 3.72444800
H -0.72393500 -16.55011500 3.46786200
H 2.20230300 -10.31021000 3.00119400
O -2.47927300 -15.19685200 -0.32409700
O -1.47168900 -10.84301800 -1.36330800
O 1.06760400 -11.64252300 0.21936700
O -0.19188000 -14.65675400 1.69482200
C -2.50504100 -5.49284900 -0.54614800
C -1.61753500 -4.27826900 -0.19797100
C -1.69093300 -6.79733100 -0.40675800
C 0.07897100 -3.15513500 1.31497200
C -0.90814300 -4.30147900 1.14322300
C -3.70254700 -5.52879000 0.42161000
C -3.00154800 -5.36665200 -1.99847000
C 1.22260400 -3.20217000 0.31875100
C -0.38584600 -6.88412700 -1.17594500
C 2.18151300 -1.99238000 0.28981800
C 0.87636400 -8.16333400 0.61274000
C 0.42488200 -8.12702100 -0.83548100
C 3.16872500 -2.14729200 -0.88198800
C 1.78846000 -9.36941100 2.62654100
H 0.51374300 -3.19081100 2.32128700
H -0.42586700 -2.18659500 1.23375100
H -0.41135700 -5.26953300 1.26799100
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H -4.24823600 -4.58151300 0.38170900
H -4.37985100 -6.33715600 0.13787700
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H -3.64428100 -4.48867900 -2.09182200
H -2.17433800 -5.23760100 -2.69829800
H -3.57514900 -6.25473200 -2.27960100
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H 0.19597800 -5.97390100 -0.99548700
H -0.14161400 -9.03803400 -1.05596400
H 1.32297500 -8.16472800 -1.46397500
H 3.51970900 -8.75697700 0.51308700
H 3.79749900 -3.02518300 -0.71880500
H 2.64974800 -2.29315700 -1.83070600
H 2.49566000 -8.56477900 2.83893500
H 0.86814900 -9.14195000 3.16685800
H 3.46702900 -2.87780500 1.80435100
O -2.10860600 -7.71757700 0.27342200
O -1.52657700 -3.33795500 -0.96698500
O 1.40933300 -4.15720100 -0.41404000
O 0.74823100 -7.20930400 1.35923600
H -0.23510600 30.07718700 -0.28588700
H 0.23510600 -30.07718700 -0.28588700

Icosamer **13**

Total Energy (Hartree) = -8466.83377003

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C	0.99227500	8.15240200	-0.71684700
C	-1.48724200	11.78521500	-0.92051900
C	-0.63807300	10.62487100	-1.42093200
C	1.91273400	9.35877300	-2.72664400
C	3.02787900	9.59902900	-0.47415400
C	-1.66831300	11.78170400	0.58611000
C	0.54392900	8.11416000	0.73225800
C	-2.36197200	13.00949300	1.21467200
C	-1.59175700	6.81840000	0.29996200
C	-0.28406700	6.88125000	1.06716400
C	-2.30898900	12.89947800	2.74989600
C	-3.62188600	5.58374200	-0.53433100
H	-2.48426700	11.73519400	-1.37481500
H	-1.05949000	12.74595100	-1.22659900
H	-1.08803900	9.66375700	-1.15028100
H	-0.59459900	10.64549400	-2.51667200
H	2.33866500	10.29593000	-3.09686000
H	2.60717100	8.54535400	-2.94750800
H	0.98686200	9.14842500	-3.26442300
H	3.56252300	10.46618500	-0.86773700
H	2.88899700	9.76311400	0.59564100
H	3.64375400	8.70745700	-0.62425300
H	1.44393200	8.13524300	1.35875700
H	-0.00885800	9.03196700	0.95928200
H	0.28396200	5.96367400	0.88023200
H	-0.52611100	6.87906200	2.13691400
H	-3.48431700	6.29605700	2.16953300
H	-2.88433800	12.03035000	3.07593600
H	-1.28781100	12.76482500	3.11011500
H	-4.28673400	6.40119700	-0.24728500
H	-3.30269800	5.77187300	-1.56071700
H	-4.33024300	12.11496900	0.97822800
O	0.84800200	7.20485000	-1.46864200
O	1.23496000	11.62617900	-0.30184200
O	-1.31358200	10.84755300	1.28278300
O	-1.99789000	7.74933600	-0.37259100
C	0.87100800	16.91672500	-1.81848800
C	0.13663000	18.14102200	-1.23050400
C	0.40668700	15.62994100	-1.10242900
C	-2.00095300	19.25457300	-0.44335200
C	-1.37955600	18.09053600	-1.20291700
C	0.54630600	16.81418800	-3.32045800
C	2.38855700	17.08106600	-1.61453000
C	-1.63131900	19.26846400	1.02830900
C	0.50450700	15.60662600	0.41164700
C	-2.06642300	20.50002500	1.85154900
C	-1.63815700	14.30268100	0.78134600
C	-0.14317400	14.37579500	1.03090400
C	-1.46955900	20.40828000	3.26833500
C	-3.82539500	13.05508100	0.73729400
H	-3.09416000	19.19660600	-0.51057300
H	-1.71715100	20.21281600	-0.89156800
H	-1.69718300	17.13146500	-0.78008500
H	-1.73078200	18.09889300	-2.24193200
H	0.80819400	17.74741200	-3.82765500
H	1.12067700	15.99887900	-3.76548400
H	-0.50925800	16.59690800	-3.49159800
H	2.74376100	17.94491800	-2.18047300
H	2.63877200	17.25574500	-0.56687900
H	2.91507700	16.18890000	-1.96600300
H	1.56848200	15.63632700	0.67625500
H	0.06357100	16.52570300	0.81202800
H	0.32601900	13.45753900	0.66193100
H	0.01189800	14.38424000	2.11664100

H	-2.73630700	13.79665600	3.20727200
H	-1.88334600	19.53998000	3.78557500
H	-0.38585700	20.28332400	3.24289500
H	-4.34905000	13.87344200	1.23603400
H	-3.89444900	13.23416500	-0.33688100
H	-3.98217800	19.59336900	2.33953200
O	0.00919200	14.67404900	-1.74433500
O	0.76358600	19.10835200	-0.83663600
O	-1.04307800	18.34445900	1.56120500
O	-2.26236400	15.22531000	0.28843200
C	-0.16415100	24.38150400	-2.17672000
C	-0.64718200	25.61032600	-1.37639500
C	-0.33153800	23.10190500	-1.32867100
C	-2.36835400	26.73022700	0.11013200
C	-2.05282600	25.55710500	-0.80752200
C	-1.00575200	24.26030600	-3.46082600
C	1.32423800	24.55289900	-2.53301100
C	-1.49647300	26.76374500	1.35171600
C	0.30265300	23.09741300	0.04980400
C	-1.61006300	28.00863500	2.25847400
C	-1.55553800	21.79134600	1.17692500
C	-0.07108500	21.87247900	0.87305000
C	-0.54630600	27.93376000	3.36965900
C	-3.60426600	20.53304900	1.92612100
H	-3.41268700	26.66968100	0.43977500
H	-2.26960700	27.68263500	-0.42158800
H	-2.19174200	24.60338700	-0.28730600
H	-2.75283100	25.55077500	-1.65185300
H	-0.94951900	25.18804000	-4.03779200
H	-0.62407700	23.44118900	-4.07403800
H	-2.05091100	24.03837600	-3.23932000
H	1.44642800	25.41085800	-3.19759900
H	1.93282900	24.74094900	-1.64703700
H	1.69583800	23.65815700	-3.04098600
H	1.39052500	23.13282200	-0.08518400
H	0.02856400	24.02026200	0.57195500
H	0.24140100	20.95118000	0.36992100
H	0.46300800	21.89494100	1.83073100
H	-1.71443700	21.30843000	3.83973600
H	-0.74845500	27.07555800	4.01406100
H	0.45657000	27.80157000	2.96053200
H	-3.92311200	21.35455200	2.57121200
H	-4.05269700	20.69934800	0.94533700
H	-3.22403600	27.11625600	3.41092300
O	-0.92551500	22.13694600	-1.77561900
O	0.07249600	26.58423400	-1.24331300
O	-0.75434500	25.84581400	1.65184600
O	-2.32187200	22.70592200	0.93146900
C	-1.27003400	31.83579000	-2.22830000
C	-1.46613700	33.07163400	-1.32598400
C	-1.12155500	30.56456100	-1.36385900
C	-2.54928600	34.19229700	0.67108800
C	-2.56904000	33.00860700	-0.28581900
C	-2.50173700	31.69298800	-3.14258200
C	0.00209100	32.01643400	-3.07726200
C	-1.29622800	34.24070200	1.53214800
C	-0.03748700	30.57212600	-0.30248200
C	-1.07351100	35.51071200	2.37574200
C	-1.37527600	29.28724500	1.42648100
C	-0.09478400	29.35926100	0.61582700
C	0.17423900	35.33273400	3.25839200
C	-3.02000400	28.04876000	2.87663700
H	-3.41396900	34.13727700	1.34239400
H	-2.64278500	35.14375500	0.13645700
H	-2.49172700	32.06592000	0.26607900
H	-3.52815300	32.97407000	-0.81706500
H	-2.65473600	32.61184600	-3.71610500
H	-2.34727200	30.86594900	-3.83876900
H	-3.40491900	31.47033300	-2.57200200
H	-0.12228600	32.86779900	-3.74963400
H	0.87655000	32.21930800	-2.45673700
H	0.18679800	31.11916400	-3.67506900

H	0.93060600	30.59840400	-0.81733000
H	-0.10572200	31.50248800	0.27111600
H	0.01939300	28.43051900	0.04653700
H	0.74418300	29.39127600	1.32146100
H	-0.57010500	28.84345300	3.97679800
H	-0.01604900	34.56793100	4.01574000
H	1.03748100	35.00558800	2.67867000
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O	-1.83359600	29.59631600	-1.56099600
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O	-0.50158000	33.31827200	1.56205300
O	-2.18100200	30.20072900	1.45465300
C	-0.85847300	36.70495600	1.40397900
C	0.29272200	36.61440700	0.42926800
C	-2.30885900	35.78691500	3.25013000
H	0.10291000	35.79858500	-0.27796100
H	1.23469100	36.39231100	0.93768000
H	0.41469900	36.27057800	3.76783600
H	-2.11142300	36.64044600	3.90264100
H	-3.18373700	36.03891000	2.65017200
O	-1.60835400	37.66185200	1.42621300
C	2.06642300	-20.50002500	1.85154900
C	1.63131900	-19.26846400	1.02830900
C	1.55553800	-21.79134600	1.17692500
C	1.37955600	-18.09053600	-1.20291700
C	2.00095300	-19.25457300	-0.44335200
C	3.60426600	-20.53304900	1.92612100
C	1.46955900	-20.40828000	3.26833500
C	-0.13663000	-18.14102200	-1.23050400
C	0.07108500	-21.87247900	0.87305000
C	-0.87100800	-16.91672500	-1.81848800
C	0.33153800	-23.10190500	-1.32867100
C	-0.30265300	-23.09741300	0.04980400
C	-2.38855700	-17.08106600	-1.61453000
C	1.00575200	-24.26030600	-3.46082600
H	1.73078200	-18.09889300	-2.24193200
H	1.69718300	-17.13146500	-0.78008500
H	1.71715100	-20.21281600	-0.89156800
H	3.09416000	-19.19660600	-0.51057300
H	3.98217800	-19.59336900	2.33953200
H	3.92311200	-21.35455200	2.57121200
H	4.05269700	-20.69934800	0.94533700
H	1.88334600	-19.53998000	3.78557500
H	0.38585700	-20.28332400	3.24289500
H	1.71443700	-21.30843000	3.83973600
H	-0.46300800	-21.89494100	1.83073100
H	-0.24140100	-20.95118000	0.36992100
H	-0.02856400	-24.02026200	0.57195500
H	-1.39052500	-23.13282200	-0.08518400
H	-1.69583800	-23.65815700	-3.04098600
H	-2.74376100	-17.94491800	-2.18047300
H	-2.63877200	-17.25574500	-0.56687900
H	0.62407700	-23.44118900	-4.07403800
H	2.05091100	-24.03837600	-3.23932000
H	-0.80819400	-17.74741200	-3.82765500
O	2.32187200	-22.70592200	0.93146900
O	1.04307800	-18.34445900	1.56120500
O	-0.76358600	-19.10835200	-0.83663600
O	0.92551500	-22.13694600	-1.77561900
C	2.36197200	-13.00949300	1.21467200
C	1.66831300	-11.78170400	0.58611000
C	1.63815700	-14.30268100	0.78134600
C	0.63807300	-10.62487100	-1.42093200
C	1.48724200	-11.78521500	-0.92051900
C	3.82539500	-13.05508100	0.73729400
C	2.30898900	-12.89947800	2.74989600
C	-0.78784500	-10.66621000	-0.90391600
C	0.14317400	-14.37579500	1.03090400
C	-1.68194300	-9.44426100	-1.20644000
C	-0.40668700	-15.62994100	-1.10242900

C	-0.50450700	-15.60662600	0.41164700
C	-3.02787900	-9.59902900	-0.47415400
C	-0.54630600	-16.81418800	-3.32045800
H	0.59459900	-10.64549400	-2.51667200
H	1.08803900	-9.66375700	-1.15028100
H	1.05949000	-12.74595100	-1.22659900
H	2.48426700	-11.73519400	-1.37481500
H	4.33024300	-12.11496900	0.97822800
H	4.34905000	-13.87344200	1.23603400
H	3.89444900	-13.23416500	-0.33688100
H	2.88433800	-12.03035000	3.07593600
H	1.28781100	-12.76482500	3.11011500
H	2.73630700	-13.79665600	3.20727200
H	-0.01189800	-14.38424000	2.11664100
H	-0.32601900	-13.45753900	0.66193100
H	-0.06357100	-16.52570300	0.81202800
H	-1.56848200	-15.63632700	0.67625500
H	-2.91507700	-16.18890000	-1.96600300
H	-3.56252300	-10.46618500	-0.86773700
H	-2.88899700	-9.76311400	0.59564100
H	-1.12067700	-15.99887900	-3.76548400
H	0.50925800	-16.59690800	-3.49159800
H	-2.33866500	-10.29593000	-3.09686000
O	2.26236400	-15.22531000	0.28843200
O	1.31358200	-10.84755300	1.28278300
O	-1.23496000	-11.62617900	-0.30184200
O	-0.00919200	-14.67404900	-1.74433500
C	2.42518600	-5.52545900	0.43320900
C	1.55554000	-4.29970300	0.07991900
C	1.59175700	-6.81840000	0.29996200
C	-0.12236400	-3.15707200	-1.43916900
C	0.84653500	-4.31792300	-1.26156500
C	3.62188600	-5.58374200	-0.53433100
C	2.92348100	-5.40085900	1.88512400
C	-1.26881900	-3.18336100	-0.44537500
C	0.28406700	-6.88125000	1.06716400
C	-2.20917000	-1.95910700	-0.42277600
C	-0.99227500	-8.15240200	-0.71684700
C	-0.54392900	-8.11416000	0.73225800
C	-3.20328500	-2.09637000	0.74544800
C	-1.91273400	-9.35877300	-2.72664400
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H	0.39721200	-2.19615200	-1.35982000
H	0.33466700	-5.27874000	-1.38180500
H	1.61456700	-4.28015900	-2.04365400
H	4.18206200	-4.64473300	-0.49842100
H	4.28673400	-6.40119700	-0.24728500
H	3.30269800	-5.77187300	-1.56071700
H	3.57873500	-4.53183700	1.97528800
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H	-0.28396200	-5.96367400	0.88023200
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H	-3.84503400	-2.96472400	0.58153600
H	-2.69033700	-2.24831700	1.69649100
H	-2.60717100	-8.54535400	-2.94750800
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H	-3.50227700	-2.82655800	-1.94134500
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C	0.12236400	3.15707200	-1.43916900
C	2.96975900	1.88830900	-1.75994400
C	3.20328500	2.09637000	0.74544800

C	-1.55554000	4.29970300	0.07991900
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C	-2.96975900	-1.88830900	-1.75994400
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H	0.14880800	-1.53429300	0.98470500
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H	0.37626700	37.55614000	-0.11394600
H	-0.37626700	-37.55614000	-0.11394600

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