Supporting Information

Construction of Covalent Organic Nanotubes by Light-induced Cross-linking of Diacetylene-based Helical Polymers

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1. General

Unless otherwise noted, all materials including dry solvents were obtained from commercial suppliers and used as received. All reactions were performed with dry solvents under an atmosphere of argon or nitrogen in glassware dried with a heat-gun by standard vacuum-line techniques. All work-up and purification procedures were carried out with reagent-grade solvents in air.

Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 precoated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm). LCMS analysis was conducted on Agilent Technologies 1200 series. Flash column chromatography was performed with silica gel 60N (Kanto Chemical Co., spherical, neutral, 40–100 mesh). Preparative recycling gel permeation chromatography (GPC) was performed with LC-9210II NEXT instrument (Japan Analytical Industry Ltd.) equipped with an in-line JAIGEL-3H and 5H columns using $CHCl_3$ as an eluent at the flow rate of 3.5 mL/min, UV and RI detectors. Molecular weight and its distribution of synthesized polymers were measured by gel permeation chromatography (GPC) on a Shimadzu Prominence 2000 instrument equipped with two in-line linear polystyrene gel columns (TOSOH TSKgel Multipore H_{XL}-M SEC columns 7.8 mm × 300 mm) at 40 °C, and tetrahydrofuran (THF) containing 0.1wt% tetra-*n*-butylammonium bromide (TBAB) was used as the eluent at the flow rate of 1.0 mL/min. The molecular weight calibration curve was obtained with standard polystyrenes (TOSOH TSKgel polystyrene standard). The absorption, CD and fluorescence spectra were obtained in a 1 cm quartz cell at 25 °C using a JASCO V570 spectrophotometer, a JASCO J720WN spectropolarimeter and JASCO FP-6600. Raman spectra were measured using in Via Reflex 48 (Renishaw) equipped with He-Ne lasers operated at 633 nm. Raman signal was detected by charge-coupled device (CCD). A 20x, 0.40 NA objective lens was used to focus the laser light onto the samples. Measurements were carried out at room temperature and atmospheric conditions. Fourier-transform infrared (FT-IR) spectra were recorded using a JASCO FT/IR-6100 spectrometer. The AFM measurements were performed using a Dimension FastScan (BrukerNano) at room temperature and atmospheric conditions with silicon tip on silicon nitride cantilevers (Fastscan-C, Bruker) in the tapping mode. The X-ray measurements were performed on a Rigaku R-AXIS IV detector system equipped with a Rigaku FR-E rotating-anode generator and confocal mirror monochromated CuKα radiation (0.15418 nm) focused through a 0.3 mm pinhole collimator, which was supplied at 45 kV voltage and 45 mA current, equipped with a flat imaging plate having a specimen-to-plate distance of 165.0 mm. The X-ray photographs were taken at room temperature. High-resolution mass spectra (HRMS) were obtained from Thermo Fisher Scientific Exactive and a Bruker Daltonics Ultraflex III TOF/TOF (MALDI TOF-MS) with *trans*-2-{3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene}malononitrile (DCTB) as matrix. Nuclear magnetic resonance (NMR) spectra were recorded on JEOL JMN-A-400 (^{1}H 400 MHz, ^{13}C 100 MHz) and a JEOL JMN-ECA-600II with Ultra COOLTM probe (^{1}H 600 MHz, ^{13}C 150 MHz). Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to Me_4Si (δ 0.00 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, dt = doublet of triplets, t = triplet, td = triplet of doublets, q = quintet, m = multiplet, brs = broad signal), coupling constant (Hz), and integration.

1-1. Measurement of UV/vis absorption and CD spectra

Measurements UV/vis absorption and CD spectra were performed with spectroscopic-grade solvents using 1 cm quartz cell. Unless otherwise stated, all experiments were carried out at 25 °C. Solutions of poly-PDE **1** or di-PDE **5** in solvent, which were filtered through a 0.45 μm membrane filter, were used for measurement. In the measurements in Fig. S7, 0.33 μg mL^{-1} solution of **1** was measured using 10 cm quartz cell.

1-2. Measurement of Raman spectra

Measurements of Raman spectra were performed on silicon substrate (SUMTEC) at room temperature. The silicon substrate was cleaned using ultrasonic cleaning in EtOH. The sample solution for Raman measurement was casted on the prepared silicon substrate, and the solvent was dried on a silicon substrate.

1-3. Measurement of fluorescence spectra

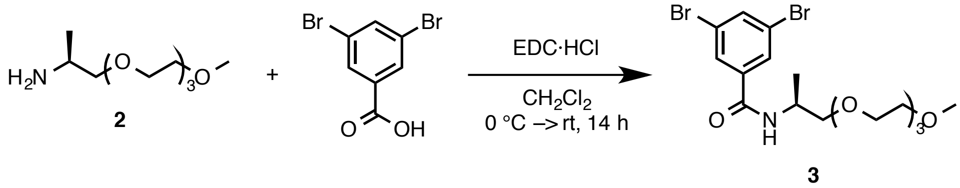
Measurements of fluorescence spectra were performed with degassed sample solution in chloroform (spectroscopic grade) using 1 cm quartz cell with a cap. Unless otherwise stated, all experiments were carried out at 25 °C. Sample solutions were filtered through a 0.45 μm membrane filter before measurements.

1-4. Measurement of transmission electron microscopy (TEM)

Transmission electron microscopy (TEM) observation was performed using a JEOL JEM-2100F at acceleration voltage of 80 keV at room temperature under high vacuum (10^{-5} Pa). The samples were dissolved in chloroform, and the solution was dropped onto a carbon-coated copper grid. Prior to the observations, TEM samples were heated at 80 °C under a vacuum of 10^{-5} Pa for 30 min to remove the residual solvent and impurities. TEM images were recorded on a Gatan MSC 794 1 k×1 k CCD camera with an exposure time of 0.3 s.

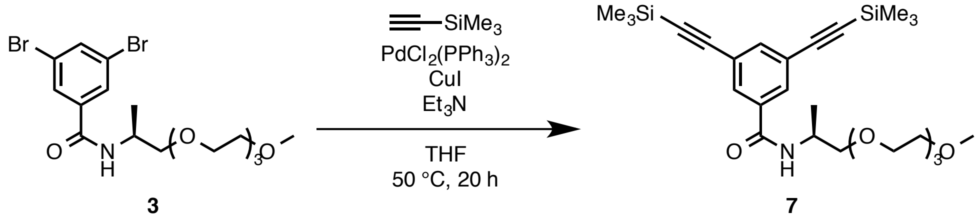
2. Synthesis and Characterization of New Compounds

(*S*)-3,5-Dibromo-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)benzamide (3)



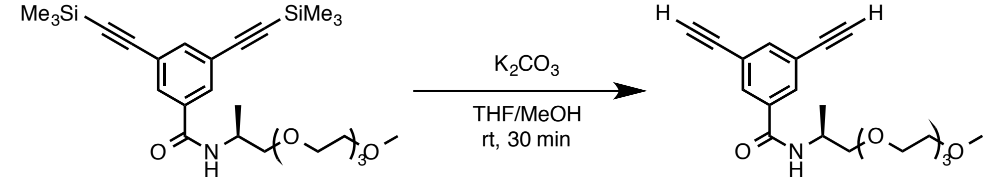
(*S*)-2,5,8,11-Tetraoxa-13-tetradecanamine (**2**) was prepared according to our previous report[S2]. To a 500-mL round-bottomed flask containing a magnetic stirring bar were added 3,5-dibromobenzoic acid (8.63 g, 30.8 mmol) and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC·HCl) (5.92 g, 30.9 mmol) in CH_2Cl_2 (350 mL) under N_2. Then, **2** (6.21 g, 28.0 mmol) was added at 0 °C. After stirring at room temperature for 14 h, the reaction mixture was treated with 2M HCl aqueous solution and saturated NH_4Cl aqueous solution, and the organic layer was separated. The aqueous layer was extracted with CH_2Cl_2. Then, the combined organic layers were dried over Na_2SO_4, filtered and concentrated *in vacuo*. The purification with flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:1) afforded amide **3** as a brown oil (12.2 g, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (d, *J* = 6.8 Hz, 3H), 3.33 (s, 3H), 3.49–3.52 (m, 2H), 3.55–3.70 (m, 12H), 4.28–4.36 (m, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 7.76 (t, *J* = 1.8 Hz, 1H), 7.91 (d, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.4, 46.1, 58.9, 70.4, 70.4, 70.6, 70.7, 71.8, 73.8, 123.0, 129.2, 136.5, 138.2, 164.1. One methylene carbon signal was overlapped. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}Br_2NNaO_5^+$ $[M+Na]^+$: 503.9992, found 503.9982.

(*S*)-*N*-(2,5,8,11-Tetraoxa-13-tetradecanyl)-3,5-bis{(trimethylsilyl)ethynyl}benzamide (7)



To a 200-mL round-bottomed flask containing a magnetic stirring bar were added **3** (11.3 g, 23.3 mmol) and triethylamine (9.7 mL, 69.5 mmol) in THF (40 mL) under N_2. The mixture was degassed by three freeze-pump-thaw cycles. Then, bis(triphenylphosphine)palladium dichloride (1.31 g, 1.88 mmol), copper(I) iodide (0.22 g, 1.16 mmol) and trimethylsilylacetylene (7.1 mL, 51.3 mmol) were added. The reaction mixture was stirred at 50 °C for 20 h. After cooling down to room temperature, the reaction mixture was filtered and the solvents were removed by evaporation. H_2O was added to the residue, and the organic layer was extracted with $CHCl_3$, dried over Na_2SO_4, filtered and concentrated *in vacuo*. The purification by flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:1) afforded **7** as a yellow oil (7.39 g, 61%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 0.24 (s, 18H), 1.28 (d, *J* = 7.2 Hz, 3H), 3.33 (s, 3H), 3.48–3.51 (m, 2H), 3.55–3.69 (m, 12H), 4.31–4.36 (m, 1H), 6.69 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 1.5 Hz, 1H), 7.81 (d, *J* = 1.8 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ –0.20, 17.5, 45.8, 58.9, 70.4, 70.5, 70.6, 70.6, 70.7, 71.8, 73.9, 96.0, 103.2, 123.8, 130.3, 135.3, 137.5, 165.3. HRMS (ESI) *m/z* calcd for $C_{27}H_{43}NNaO_5Si_2^+$ $[M+Na]^+$: 540.2572, found 540.2569.

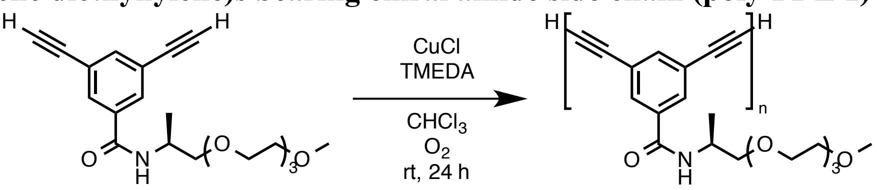
(*S*)-3,5-Diethynyl-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)benzamide (mono-PDE 4)



7 mono-PDE **4**

To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **7** (1.22 g, 2.35 mmol) and potassium carbonate (0.32 g, 2.34 mmol) in 24 mL of a THF/MeOH mixture (1:1). After stirring the mixture at room temperature for 30 min, the solvent was removed *in vacuo*. Crude product was purified by flash column chromatography on silica gel (eluent: EtOAc) afforded mono-PDE **4** as a colorless oil (0.61 g, 70%). This product was stable enough under ambient conditions, but seems to be gradually decomposed within few days. Therefore it should be stored under N_2 atmosphere and dark in a freezer or stored as TMS-protected precursor **7**. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.30 (d, *J* = 6.8 Hz, 3H), 3.13 (s, 2H), 3.33 (s, 3H), 3.48–3.52 (m, 2H), 3.54–3.69 (m, 12H), 4.29–4.39 (m, 1H), 6.96 (d, *J* = 7.2 Hz, 1H), 7.69 (t, *J* = 1.6 Hz, 1H), 7.91 (d, *J* = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.1, 45.5, 58.5, 70.0, 70.1, 70.2, 70.3, 71.4, 73.5, 77.2, 78.8, 81.5, 122.4, 130.6, 135.1, 137.3, 164.9. HRMS (ESI) *m/z* calcd for $C_{21}H_{27}NNaO_5^+$ $[M+Na]^+$: 396.1781, found 396.1790.

Poly(*m*-phenylene diethynylene)s bearing chiral amide side chain (poly-PDE 1)



mono-PDE **4** poly-PDE **1**

To a 100-mL round-bottomed flask containing a magnetic stirring bar were added mono-PDE **4** (0.61 g, 1.65 mmol), copper(I) chloride (48.8 mg, 0.49 mmol) and tetramethylethylenediamine (0.57 g, 4.89 mmol) in $CHCl_3$ (17 mL) under O_2. After stirring at room temperature for 24 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution. The mixture was extracted with $CHCl_3$, and the organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by gel permeation chromatography (GPC) afforded poly-PDE **1** as a colorless solid (0.24 g, 39% by weight). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20–1.50 (brs, –CH*CH₃*), 3.20–3.40 (m, –O*CH₃*), 3.40–3.74 (m, –*CH₂*O–) 4.25–4.39 (brs, –C*H*CH₃), 6.93 (brs, *N-H*), 7.50–8.0 (m, *Ar-H*). ^{1}H NMR (600 MHz, $CDCl_3$ containing 5 vol% TFE) δ 1.29 (d, *J* = 6.0 Hz, 3H, –CH*CH₃*), 3.33 (s, 3H, –O*CH₃*), 3.47–3.71 (m, 14H, –*CH₂*O–), 4.26–4.34 (m, 1H, –C*H*CH₃), 7.27 (m, *N-H*), 7.77–7.79 (m, 1H、 *Ar-H*), 7.94–7.97 (m, 2H, *Ar-H*). ^{13}C NMR (150 MHz, $CDCl_3$ containing 5 vol% TFE) δ 17.0, 46.3, 58.7, 70.2, 70.3, 70.3, 70.4, 71.7, 73.6, 75.1, 80.1, 122.6, 131.9, 135.5, 138.4, 165.8. IR ($CHCl_3$, cm^{-1}); 1635 (ν_{CO}), 3301 (ν_{NH}). IR ($CHCl_3$ containing 5 vol% TFE, cm^{-1}); 1644 (ν_{CO}), 3303 (ν_{NH}), 3428 (ν_{NH}). The average molecular number (M_n) and the average molecular weight (M_w) and polymer dispersion index (PDI = M_w/M_n) were estimated by HPLC (see Fig. S1 for details). The mass spectrum of poly-PDE **1** was obtained by MALDI TOF-MS with DCTB (*trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile) as the matrix.

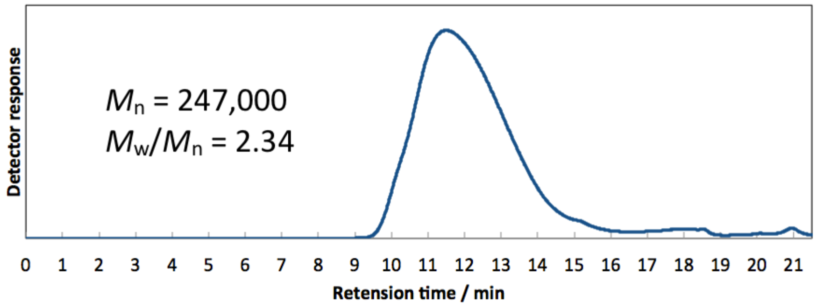


Figure S1. HPLC chart of purified poly-PDE **1** for the analysis of M_n and M_w/M_n. M_n and M_w/M_n were determined by HPLC analysis equipped with a polystyrene column eluted with THF containing TBAB (0.1 wt%) and polystyrenes standards (see General section for details) at the 1.0 mL/min of flow rate.

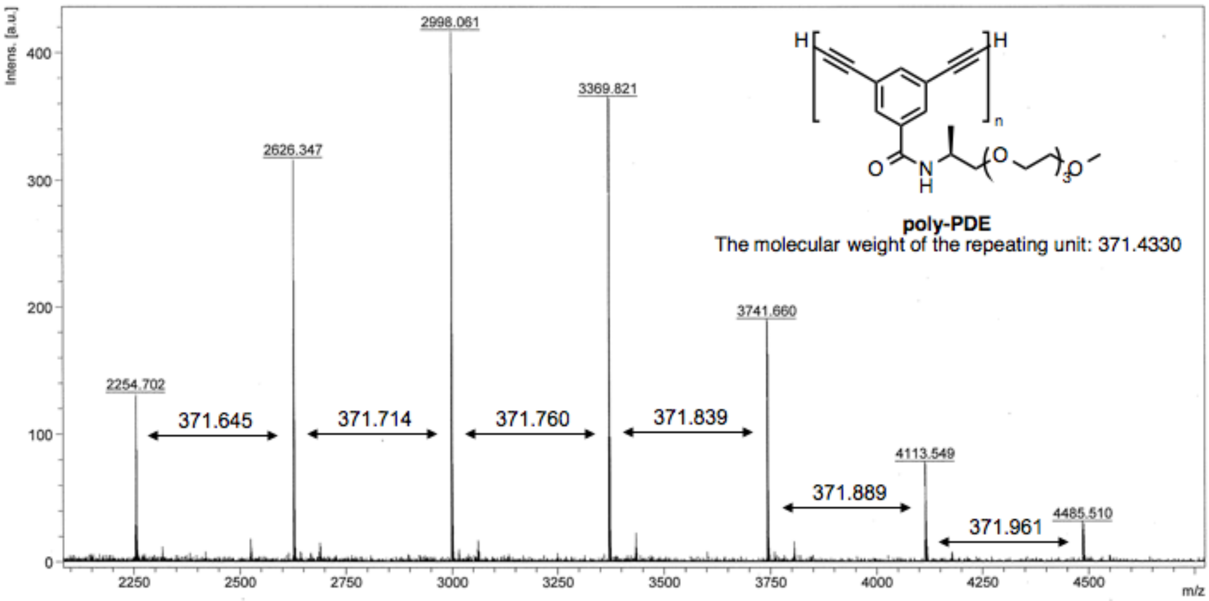
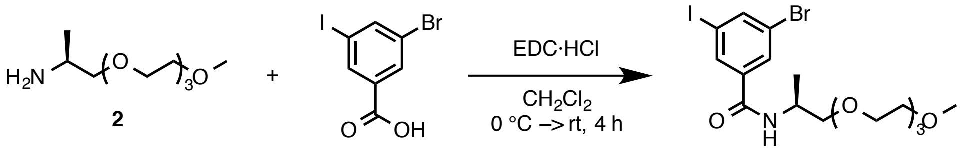


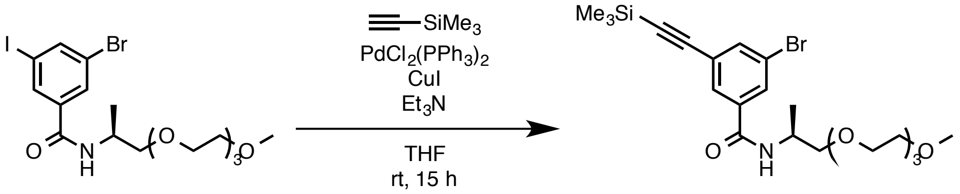
Figure S2. The mass spectrum of poly-PDE **1** by MALDI TOF-MS with DCTB as the matrix.

(*S*)-3-Bromo-5-iodo-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)benzamide (8)



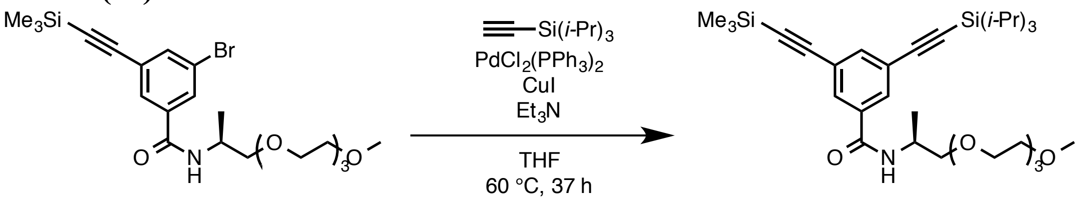
To a 300-mL round-bottomed flask containing a magnetic stirring bar were added 3-iodo-5-bromobenzoic acid (3.09 g, 9.45 mmol) and EDC·HCl (1.81 g, 9.44 mmol) in CH_2Cl_2 (100 mL) under N_2. Then, **2**[S2] (1.81 g, 8.19 mmol) was added at 0 °C. After stirring at room temperature for 4 h, the reaction mixture was treated with 2M HCl aqueous solution and saturated NH_4Cl aqueous solution, and the organic layer was separated. The aqueous layer was extracted with CH_2Cl_2. Then, the combined organic layers were dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:2) afforded **8** as an orange oil (2.33 g, 54%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.28 (d, *J* = 6.6 Hz, 3H), 3.33 (s, 3H), 3.50–3.52 (m, 2H), 3.55–3.69 (m, 12H), 4.29–4.35 (m, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 1.8 Hz, 2H), 8.09 (t, *J* = 1.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 17.3, 46.0, 58.8, 70.3, 70.4, 70.5, 70.6, 71.8, 73.8, 94.2, 122.9, 129.8, 134.9, 138.2, 141.9, 164.0. One methylene carbon signal was overlapped. HRMS (ESI) *m/z* calcd for $C_{17}H_{26}BrINO_5^+$ $[M+H]^+$: 530.0034, found 530.0024.

(*S*)-3-Bromo-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)-5-{(trimethylsilyl)ethynyl}benzamide (9)



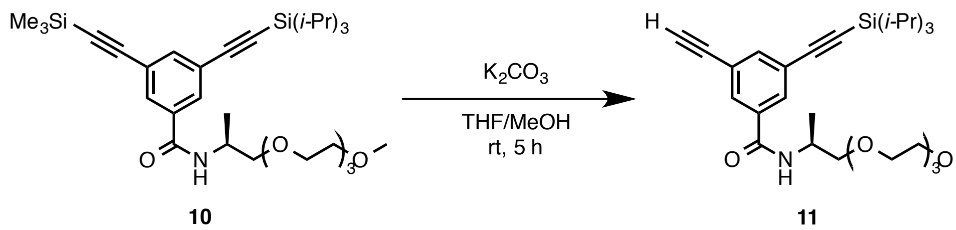
To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **8** (1.98 g, 3.73 mmol) and triethylamine (2.08 mL, 14.9 mmol) in THF (20 mL) under N_2. The mixture was degassed by three freeze-pump-thaw cycles. Then, bis(triphenylphosphine)palladium dichloride (0.21 g, 0.30 mmol) and copper(I) iodide (35.6 mg, 0.19 mmol) were added. After stirring, trimethylsilylacetylene (0.57 mL, 4.10 mmol) was added. After stirring at room temperature for 15 h, the reaction mixture was filtered and the solvents were removed by evaporation. $CHCl_3$ was added to the residue, and the residue was washed with saturated NH_4Cl aqueous solution. The organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:1) afforded **9** as a brown oil (1.68 g, 90%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 0.25 (s, 9H), 1.28 (d, J = 6.6 Hz, 3H), 3.33 (s, 3H), 3.49–3.51 (m, 2H), 3.55–3.69 (m, 12H), 4.29–4.36 (m, 1H), 6.87 (d, J = 7.2 Hz, 1H), 7.69 (t, J = 1.8 H, 1H), 7.80 (t, J = 1.5 H, 1H), 7.92 (t, J = 1.5 H, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ –0.28, 17.4, 45.9, 58.8, 70.4, 70.4, 70.5, 70.5, 70.7, 71.8, 73.8, 96.8, 102.5, 122.2, 125.2, 129.0, 130.4, 136.7, 136.8, 164.7. HRMS (ESI) *m/z* calcd for $C_{22}H_{34}BrNNaO_5Si^+$ $[M+Na]^+$: 522.1282, found 522.1275.

(*S*)-*N*-(2,5,8,11-Tetraoxa-13-tetradecanyl)-3-{(triisopropylsilyl)ethynyl}-5-{(trimethylsilyl)ethynyl}benzamide (10)



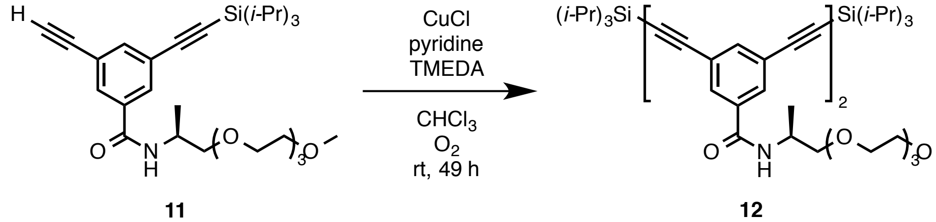
To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **9** (1.46 g, 2.91 mmol) and triethylamine (1.63 mL, 11.7 mmol) in THF (15 mL) under N_2. The mixture was degassed by three freeze-pump-thaw cycles. Then, bis(triphenylphosphine)palladium dichloride (0.17 g, 0.24 mmol) and copper(I) iodide (28.3 mg, 0.15 mmol) were added. After stirring, triisopropylsilylacetylene (0.72 mL, 3.21 mmol) was added. After stirring at 60 °C for 37 h, the reaction mixture was filtered and the solvents were removed by evaporation. $CHCl_3$ was added to the residue, and the residue was washed with saturated NH_4Cl aqueous solution, and the organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:1) afforded **10** as a brown oil (1.38 g, 79%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 0.25 (s, 9H), 1.13 (m, 21H), 1.29 (d, J = 6.6 Hz, 3H), 3.33 (s, 3H), 3.47–3.49 (m, 2H), 3.56–3.70 (m, 12H), 4.31–4.37 (m, 1H), 6.74 (d, J = 7.8 Hz, 1H), 7.65 (t, J = 1.2 Hz, 1H), 7.79 (t, J = 1.8 Hz, 1H), 7.85 (t, J = 1.5 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ –0.19, 11.2, 17.5, 18.6, 45.9, 58.9, 70.4, 70.5, 70.6, 70.7, 71.8, 73.9, 92.5, 95.9, 103.3, 105.2, 123.6, 124.1, 129.9, 130.6, 135.3, 137.5, 165.5. One methylene carbon signal was overlapped. HRMS (ESI) *m/z* calcd for $C_{33}H_{55}NNaO_5Si_2^+$ $[M+Na]^+$: 624.3511, found 624.3506.

(*S*)-3-Ethynyl-*N*-(2,5,8,11-tetraoxa-13-tetradecanyl)-5-{(triisopropylsilyl)ethynyl}benzamide (11)



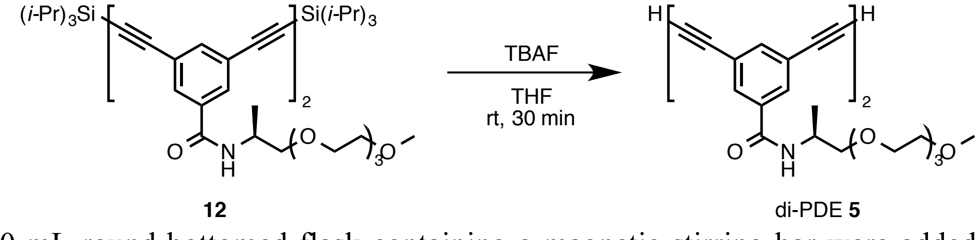
To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **10** (3.18 g, 5.29 mmol) and potassium carbonate (0.73 g, 5.30 mmol) in 50 mL of a THF/MeOH mixture (1:1). After stirring at room temperature for 5 h, the reaction mixture was filtered and the solvent was removed under reduced pressure. The residual mixture was extracted with $CHCl_3$ and washed with H_2O, and the organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash column chromatography on silica gel (eluent: hexane/EtOAc = 1:1) afforded **11** as an orange oil (1.63 g, 58%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.13 (m, 21H), 1.29 (d, *J* = 7.2 Hz, 3H), 3.13 (s, 1H), 3.33 (s, 3H), 3.47–3.50 (m, 2H), 3.55–3.71 (m, 12H), 4.31–4.37 (m, 1H), 6.80 (d, *J* = 7.2 Hz, 1H), 7.67 (t, *J* = 1.2 Hz, 1H), 7.83 (t, *J* = 1.8 Hz, 1H), 7.88 (t, *J* = 1.5 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 11.2, 17.5, 18.6, 45.9, 58.9, 70.4, 70.5, 70.6, 70.7, 71.8, 73.9, 78.6, 82.1, 92.8, 105.0, 122.6, 124.3, 130.2, 130.9, 135.5, 137.8, 165.4. One methylene carbon signal was overlapped. HRMS (ESI) *m/z* calcd for $C_{30}H_{48}NO_5Si^+$ $[M+H]^+$: 530.3296, found 530.3293.

5,5'-(1,3-Butadiyne-1,4-diyl)bis[*N*-{(*S*)-2,5,8,11-tetraoxa-13-tetradecanyl}-3-{(triisopropylsilyl)ethynyl}benzamide] (12)



To a 100-mL round-bottomed flask containing a magnetic stirring bar were added **11** (1.59 g, 3.00 mmol), copper(I) chloride (88.9 mg, 0.90 mmol) and tetramethylethylenediamine (1.10 g, 9.49 mmol) in $CHCl_3$ (30 mL) under O_2. After stirring at room temperature for 49 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution. The mixture was extracted with $CHCl_3$, and the organic layer was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Purification by flash column chromatography on silica gel (eluent: $CHCl_3$/MeOH = 96:4) afforded **12** as a yellow solid (1.44 g, 91%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 1.13–1.14 (m, 42H), 1.30 (d, *J* = 6.6 Hz, 6H), 3.32 (s, 6H), 3.48–3.50 (m, 4H), 3.56–3.71 (m, 24H), 4.32–4.37 (m, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 7.71 (t, *J* = 1.5 Hz, 2H), 7.88 (t, *J* = 1.2 Hz, 2H), 7.92 (t, *J* = 1.8 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 11.2, 17.4, 18.6, 46.0, 58.8, 70.4, 70.5, 70.6, 70.7, 71.8, 73.9, 74.7, 80.5, 93.1, 104.8, 122.0, 124.4, 130.5, 131.4, 135.7, 138.0, 165.1. One methylene carbon signal was overlapped. HRMS (ESI) *m/z* calcd for $C_{60}H_{93}N_2O_{10}Si_2^+$ $[M+H]^+$: 1057.6363, found 1057.6361.

5,5'-(1,3-Butadiyne-1,4-diyl)bis[3-ethynyl-*N*-{(*S*)-2,5,8,11-tetraoxa-13-tetradecanyl}benzamide] (di-PDE 5)



To a 200-mL round-bottomed flask containing a magnetic stirring bar were added **12** (0.50 g, 0.47 mmol) and THF (20 mL). Then, to the flask was added a solution of tetra-*n*-butylammonium fluoride in THF (1.0 M, 0.47 mL, 0.47 mmol). After the mixture was stirred at room temperature for 30 min, the solvents were removed by evaporation. Purification by flash column chromatography on silica gel (eluent: $CHCl_3$/MeOH = 96:4) afforded di-PDE **5** as a white solid (0.33 g, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.30 (d, J = 6.8 Hz, 6H), 3.16 (s, 2H), 3.33 (s, 6H), 3.49–3.52 (m, 4H), 3.55–3.70 (m, 24H), 4.30–4.39 (m, 2H), 6.99 (d, J = 7.2 Hz, 2H), 7.72 (t, J = 1.4 Hz, 2H), 7.94 (t, J = 1.4 Hz, 2H), 7.96 (t, J = 1.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.5, 46.0, 58.9, 70.5, 70.5, 70.6, 70.6, 70.8, 71.9, 73.8, 74.9, 79.1, 80.3, 81.6, 122.3, 123.1, 131.3, 131.5, 135.7, 138.0, 164.9. HRMS (ESI) *m/z* calcd for $C_{42}H_{52}N_2NaO_{10}^+$ $[M+Na]^+$: 767.3514, found 767.3494.

3. Additional Spectroscopic Analyses for Helical Folding Behavior of poly-PDE 1 and Spectroscopic Analyses of di-PDE 5

3-1. Helical folding behavior of poly-PDE in various solvents (Fig. 3a)

Judging from UV/vis absorption and CD spectra (Fig. S3 and S4), poly-PDE **1** was found to form chiral helix structure (*helix*-**1**) in $CHCl_3$, CH_2Cl_2, THF and MeOH, and achiral random coil structure (*coil*-**1**) in 2,2,2-trifluoroethanol (TFE) and *N*,*N*'-dimethylformamide (DMF). In addition, poly-PDE **1** can take the both conformers (*coil*-**1** and *helix*-**1**) in MeOH.

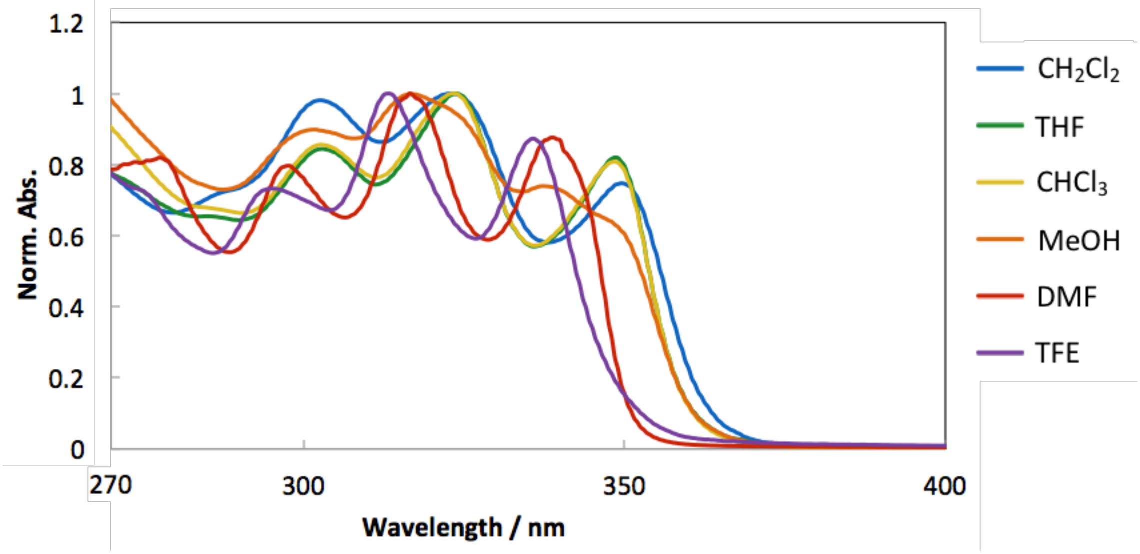


Figure S3. UV/vis absorption and CD spectra of poly-PDE **1** in various solvents

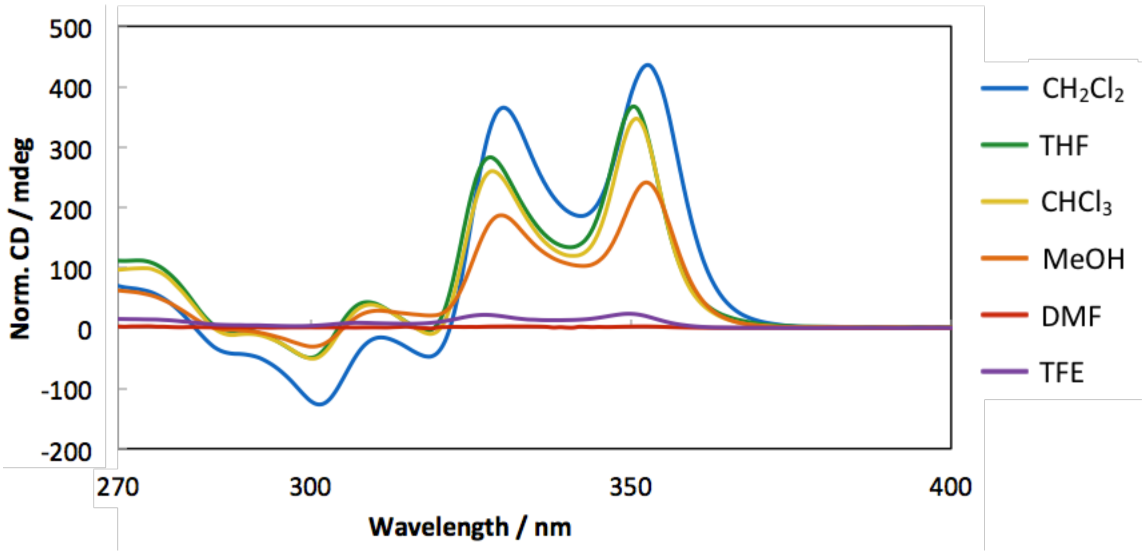


Figure S4. CD spectra of poly-PDE **1** in various solvents

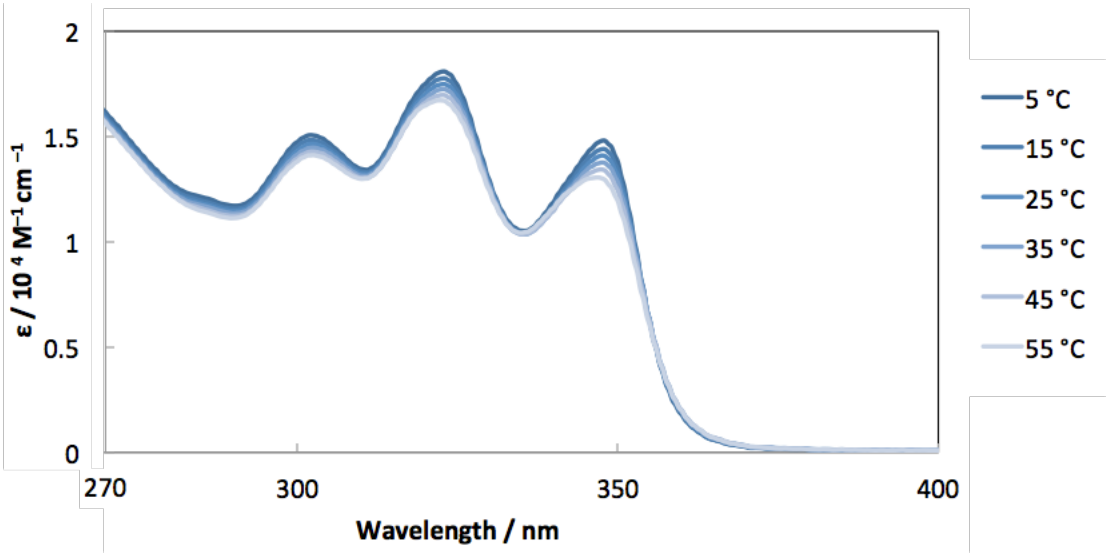


Figure S5. Temperature-dependent UV/vis absorption spectra of poly-PDE **1**

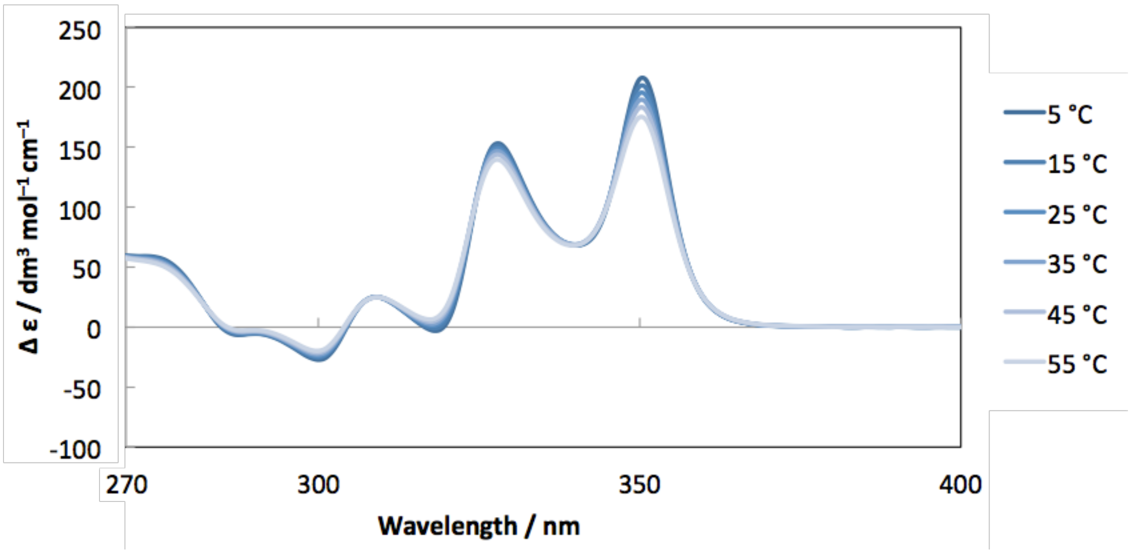


Figure S6. Temperature-dependent CD spectra of poly-PDE **1**

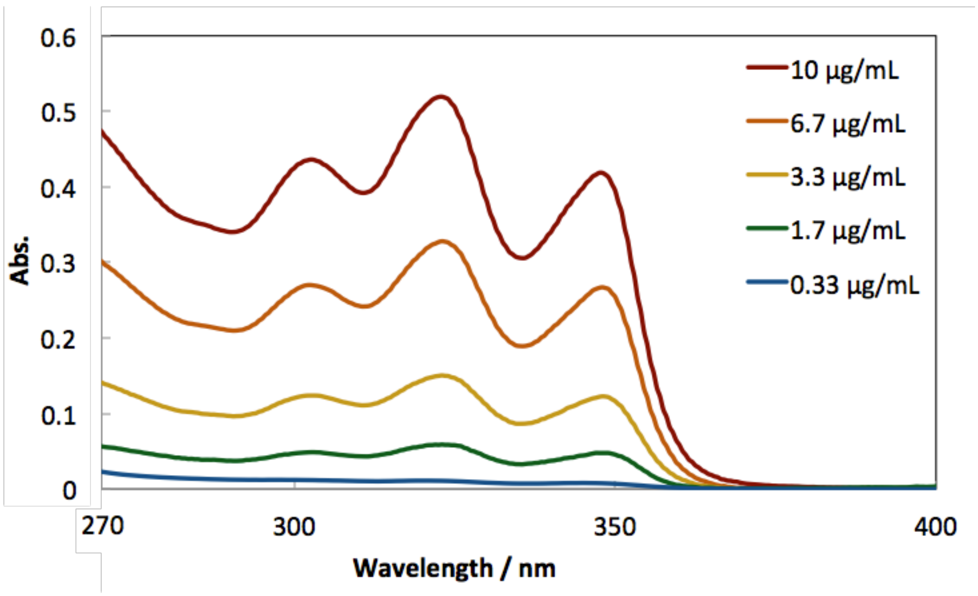


Figure S7. Concentration-dependent UV/vis absorption spectra of poly-PDE **1**

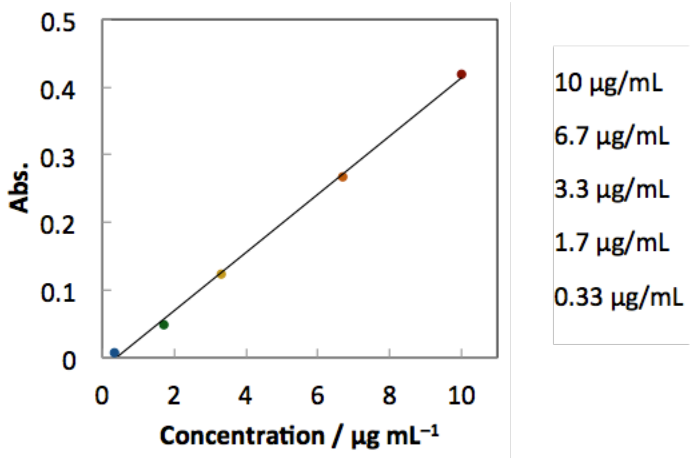


Figure S8. Plot of absorbance at 348 nm in concentration-dependent CD spectra of poly-PDE **1**

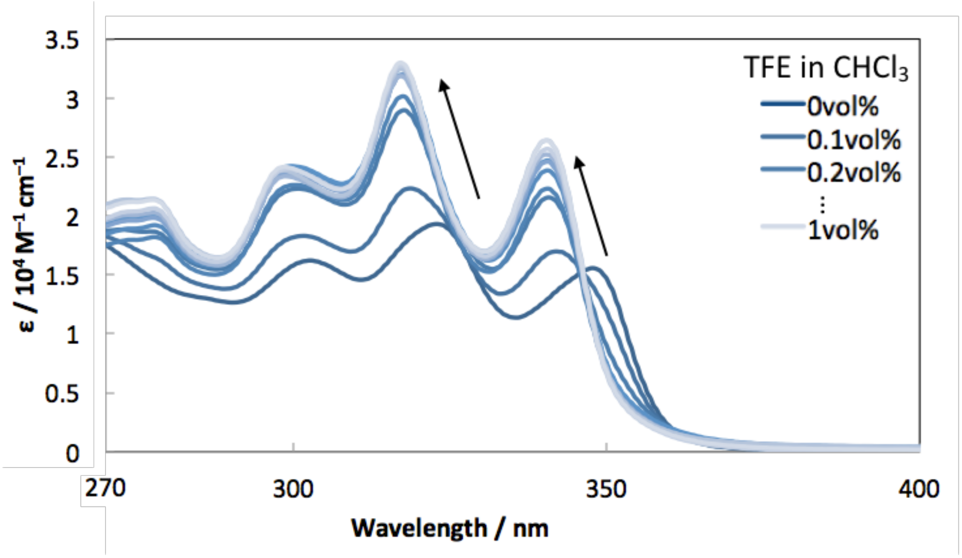


Figure S9. Spectral changes of poly-PDE **1** in UV/vis absorption spectra with increasing volume% of TFE in $CHCl_3$

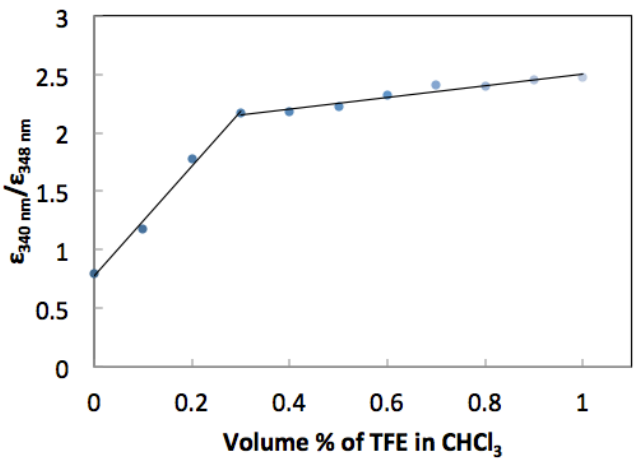


Figure S10. The ratio of molar absorbance coefficient of poly-PDE **1** at 340 nm to at 348 nm as a function of volume% of TFE in $CHCl_3$

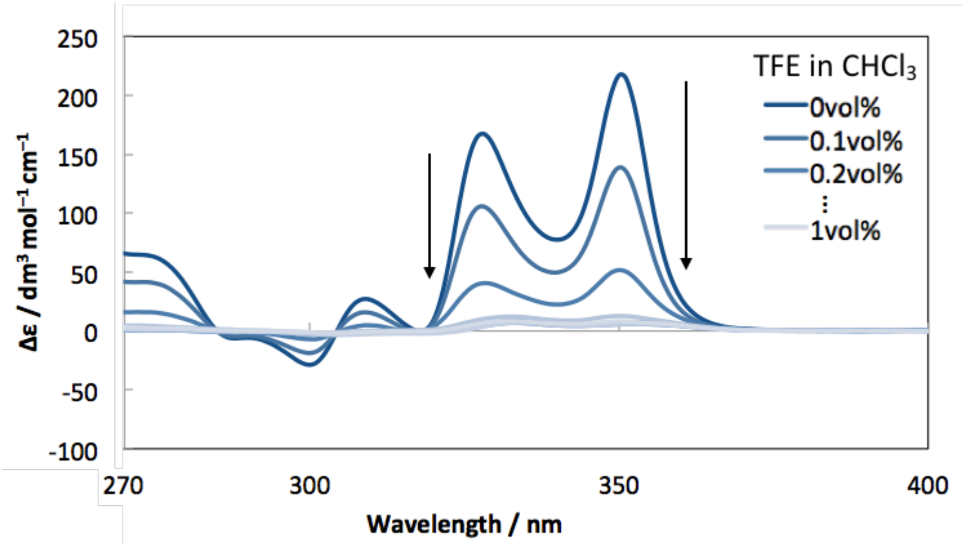


Figure S11. Spectral changes of poly-PDE **1** in CD spectra with increasing volume% of TFE in $CHCl_3$

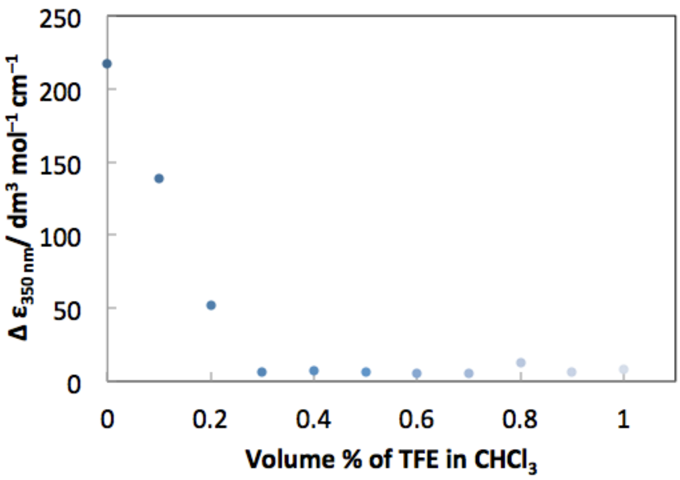


Figure S12. The ratio of molar circular dichroism of poly-PDE **1** at 340 nm to at 348 nm as a function of volume% of TFE in $CHCl_3$

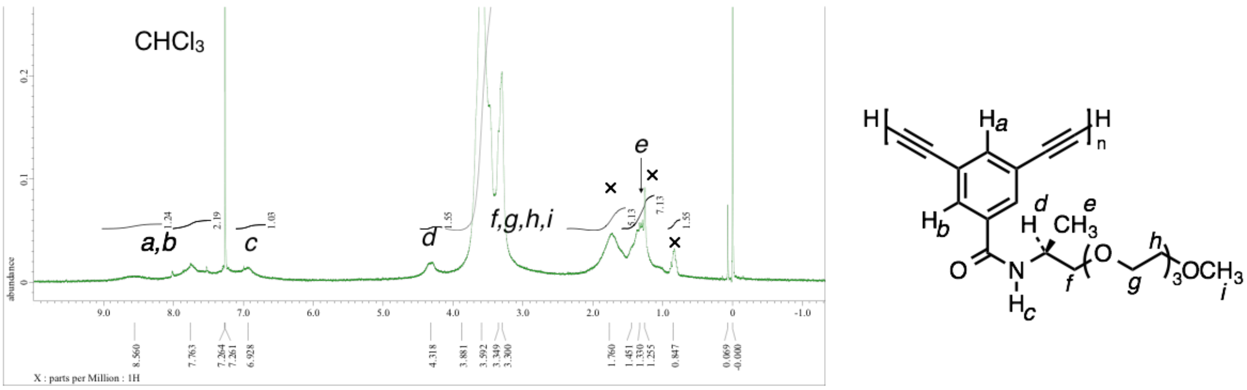


Figure S13. ^{1}H NMR spectrum of poly-PDE **1** in $CHCl_3$

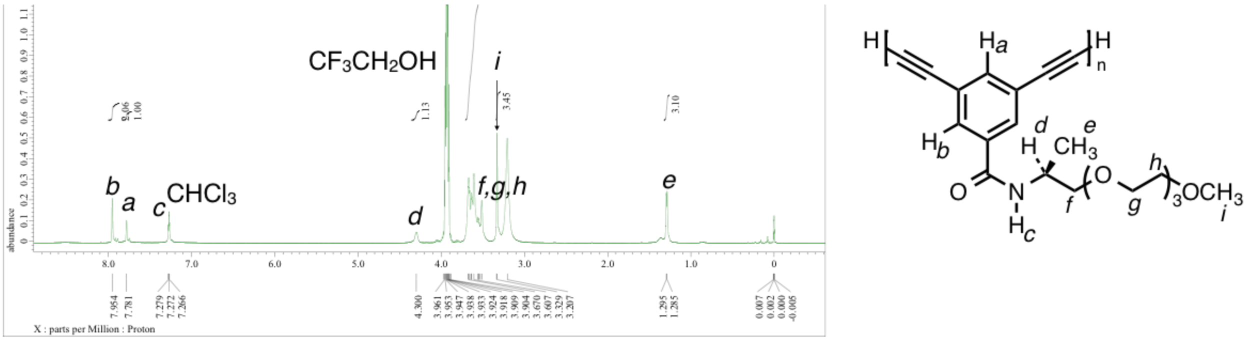


Figure S14. ^{1}H NMR spectrum of poly-PDE **1** in 5 vol% TFE/$CHCl_3$

3-2. UV/vis absorption and CD spectra of di-PDE 5

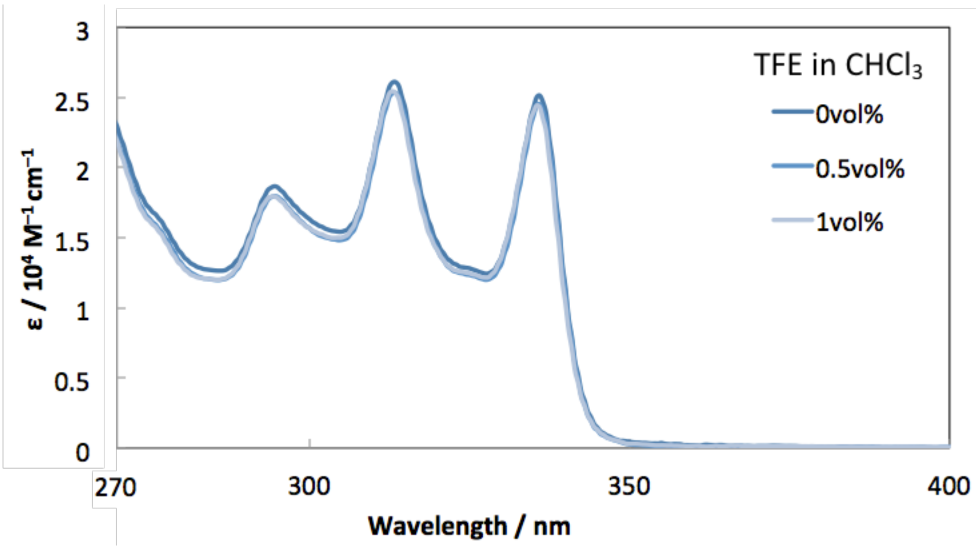


Figure S15. Spectral changes of di-PDE **5** in UV/vis absorption spectra with increasing volume% of TFE in $CHCl_3$

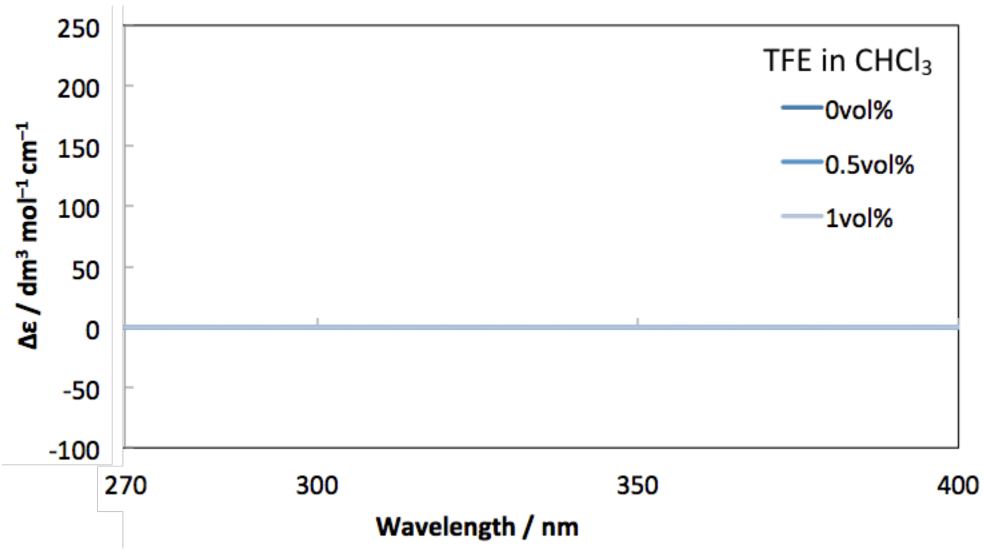


Figure S16. Spectral changes of di-PDE **5** in CD spectra with increasing volume% of TFE in $CHCl_3$

4. Wide-angle X-ray Diffraction (WAXD) Analysis

4-1. Preparation of magnetically oriented poly-PDE film for WAXD (Fig 4a in main manuscript)

The magnetically oriented films of *helix*-**1** for the X-ray diffraction measurements were prepared according to the reported procedure[S1,S2]. Poly-PDE **1** (1.2 mg) was put into a borosilicate glass capillary tube (length = 80 mm, diameter = 2.0 mm, wall thickness = 0.01 mm), and $CHCl_3$ (10 μL) was added. The prepared sample solution in a capillary tube was settled in a NMR tube upside down. Then the NMR tube was settled in a high magnetic field (14.1 T) inside a NMR apparatus (JEOL JMN-ECA-600II), and the sample solution was concentrated by the gradual solvent evaporation inside a NMR tube at room temperature for 16.5 h (spin off for 13 h and spin on for 3.5 h) to give magnetically oriented helical poly-PDE film on the inside wall of the capillary tube. Wide-angle X-ray photographs were taken at ambient temperatures from the edge-view position with a beam parallel to the film surface.

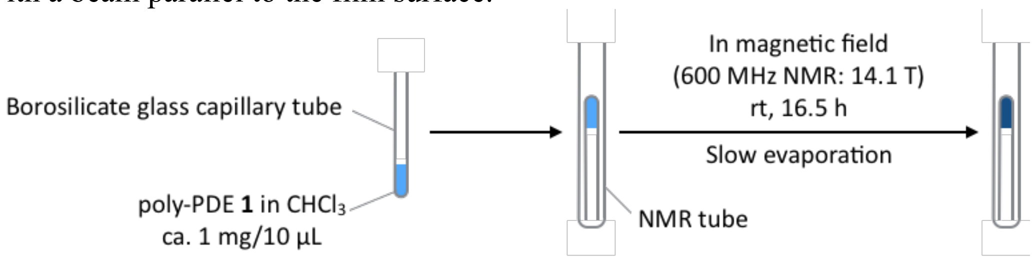


Figure S17. Preparation of magnetically oriented poly-PDE film

5. Molecular Modeling and Calculations of Helical Structures of poly-PDE 1 (Fig 4d in main manuscript)[S2]

The MM calculations were conducted using the Compass II forcefield[S3] as implemented in Materials Studio FORCITE of Dassault Systems BIOVIA operated using a PC running under Windows® 7. The polymer model (40 repeating monomer units) of poly-PDE **1** was constructed using the Polymer Builder tool in the Materials Studio Visualizer module so as to maintain the intramolecular hydrogen bonding networks between the amide residues (NH and CO) of the neighboring pendants (n and $n + 6$) and to satisfy the helical parameters (3.57 Å for the π-π stacking and ~6 monomer units per turn) obtained by the X-ray diffractions. The triethyleneglycol side groups were replaced with the terminal methyl groups for clarity. The geometrical parameters for the poly-PDE backbone were fixed during the following force field optimization. The dielectric constant was set to 1.0. The geometry optimizations were carried out without any cutoff by the smart minimizer in three steps. First, the starting conformations were subject to the steepest decent optimization in order to eliminate the worse steric conflicts. Second, subsequent optimization until the convergence using a conjugate gradient algorithm was performed. The fully optimized helical models of poly-PDE **1** were obtained by the further energy minimization using the Newton method with the 0.1 kcal/mol/Å convergence criterion.

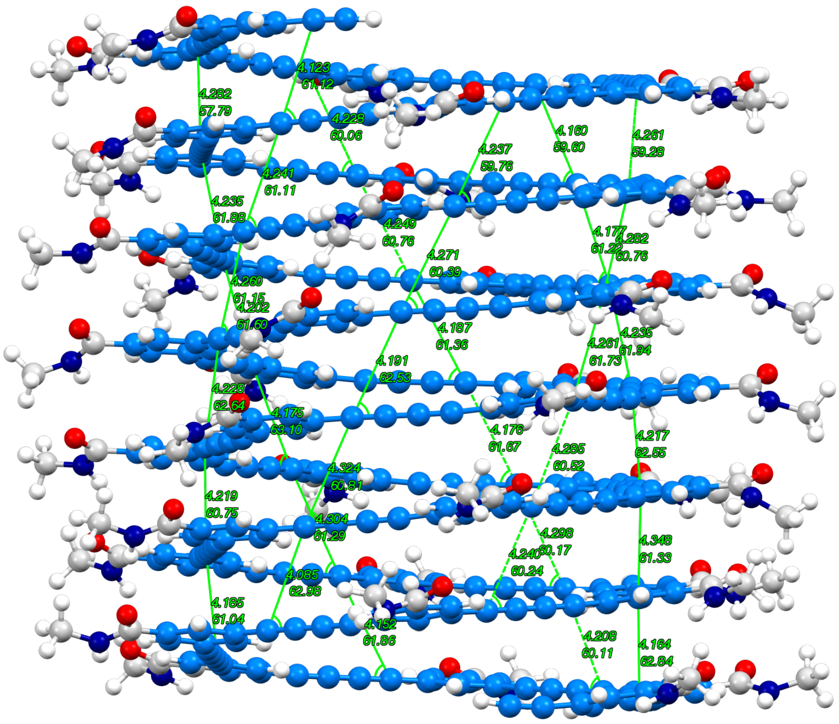


Figure S18. Optimized ball and stick model of helical poly-PDE **1**. Distance (d, Å) and angle (θ, °) between longitudinally aligned diacetylenes are highlighted with green lines.

Entry	*d* (Å)	*θ* (°)
1	4.123	61.12
2	4.282	57.79
3	4.228	60.06
4	4.160	59.60
5	4.261	59.28
6	4.237	59.76
7	4.241	61.11
8	4.235	61.88
9	4.249	60.76
10	4.177	61.22
11	4.282	60.76
12	4.271	60.39
13	4.260	61.15
14	4.202	61.60
15	4.187	61.36
16	4.235	61.94
17	4.261	61.73
18	4.191	62.53
19	4.228	62.64
20	4.175	63.10
21	4.176	61.67
22	4.217	62.55
23	4.285	60.52
24	4.324	60.81
25	4.219	60.75
26	4.304	61.29
27	4.298	60.17
28	4.348	61.33
29	4.240	60.24
30	4.085	62.98
31	4.185	61.04
32	4.152	61.86
33	4.208	60.11
34	4.164	62.84
average	4.226	61.12
standard deviation	0.05760	1.146
standar error (σ)	0.009879	0.1966

Table S1. Summary of *d* (Å) and *θ* (°) in optimized model of *helix*-**1**

Cartesian coordinates of optimized helical poly-PDE **1** (*helix*-**1**) are shown as follows;

C	-10.76000000	-6.64200000	4.50100000
C	-11.45500000	-6.47300000	3.53300000
C	-12.29000000	-6.20700000	2.38600000
C	-12.65700000	-7.23100000	1.51300000
H	-12.32000000	-8.25600000	1.71900000
C	-13.45100000	-6.96300000	0.39700000
C	-13.82200000	-8.02600000	-0.50600000
C	-13.88900000	-5.65700000	0.16600000
C	-13.56400000	-4.62700000	1.05400000
C	-14.09600000	-3.24400000	0.82300000
N	-13.48700000	-2.26600000	1.57800000
C	-13.72700000	-0.81200001	1.56900000
H	-14.32400000	-0.55300001	0.67400000
H	-14.31500000	-0.46300001	2.43800000
H	-12.71600000	-2.47000000	2.18900000
H	-12.78500000	-0.23000000	1.51100000
C	-14.13700000	-8.90700000	-1.26500000
C	-14.45100000	-9.78700000	-2.02400000
C	-14.76000000	-10.67000000	-2.78100000
O	-14.95200000	-2.98100000	-0.00600000
H	-14.49400000	-5.46200000	-0.74000000
C	-12.74900000	-4.91000000	2.15200000
H	-12.45000000	-4.12800001	2.86900000
C	-15.09300000	-11.74500000	-3.68600000
C	-15.78600000	-11.48700000	-4.87100000
H	-16.07800000	-10.44400000	-5.07700000
C	-16.10100000	-12.52400000	-5.75300000
C	-16.85300000	-12.27400000	-7.02800000
C	-15.70400000	-13.82400000	-5.43800000
H	-15.92300000	-14.66299999	-6.12100000
C	-14.71100000	-13.05200000	-3.38500000
H	-14.16900000	-13.25400000	-2.45100000
C	-15.00400000	-14.09600000	-4.26200000
C	-14.57800000	-15.44500000	-3.97500000
O	-17.37000000	-13.15300000	-7.69600000
N	-16.87100000	-10.95700000	-7.42700000
H	-16.30000000	-10.26400000	-6.97700000
C	-17.48000000	-10.37400000	-8.63700000
H	-17.68600000	-11.17800000	-9.37000000
H	-18.45400000	-9.89400000	-8.43200000
H	-16.80100000	-9.64900000	-9.12500000
C	-14.19300000	-16.57200000	-3.80400000
H	-13.83200000	-17.56000001	-3.68200000
C	-5.12700000	-18.87200000	6.67500000
C	-4.91300000	-18.06900000	7.54700000
C	-4.64000000	-17.11100000	8.59000000
C	-5.10300000	-15.80000001	8.48600000
H	-5.69000000	-15.50600001	7.60600000
C	-4.82500000	-14.86600001	9.48200000
C	-5.30900000	-13.51300000	9.35500000
C	-4.08300000	-15.25400001	10.60000000
C	-3.64100000	-16.57300000	10.73700000
C	-2.88600000	-16.98200000	11.96600000
N	-2.22500000	-18.18500000	11.84000000
C	-1.33500000	-18.85900000	12.80100000
H	-1.06500000	-18.14900000	13.60400000
H	-1.81300000	-19.72100000	13.30400000
H	-2.20600000	-18.68300000	10.96700000
H	-0.39000000	-19.19400000	12.32700000
C	-5.74700000	-12.40000000	9.23100000
C	-6.19400000	-11.29000000	9.10300000
C	-6.64500000	-10.18200000	8.97300000
O	-2.79400000	-16.29100000	12.96700000
H	-3.84900000	-14.48800000	11.36300000
C	-3.91300000	-17.49000000	9.71900000
H	-3.56800000	-18.53600001	9.77400000
C	-7.18500000	-8.85400000	8.81900000
C	-6.89100000	-7.86300001	9.75500000
H	-6.24200000	-8.14000001	10.60200000
C	-7.40900000	-6.57300001	9.61600000
C	-7.10200000	-5.50200001	10.62299999
C	-8.22200000	-6.28300001	8.51600000
H	-8.63000000	-5.26800001	8.36000000
C	-8.00700000	-8.55100000	7.73600000
H	-8.24800000	-9.33300000	7.00300000
C	-8.52800000	-7.26800000	7.57400000
C	-9.37200000	-6.98200000	6.43900000
O	-7.65800000	-4.41700001	10.64899999
N	-6.08200000	-5.81600001	11.49400000
H	-5.55300000	-6.66400001	11.39700000
C	-5.48100000	-4.99100001	12.55900000
H	-5.80900000	-3.94200001	12.43000000
H	-5.80800000	-5.28800001	13.57299999
H	-4.37300000	-4.99800001	12.51700000
C	-10.06600000	-6.80700000	5.47100000
C	-11.12400000	-15.21900000	-5.07300000
C	-10.90400000	-16.40100000	-5.05300000
C	-10.63000000	-17.81300000	-4.97100000
C	-9.99800000	-18.32700000	-3.84100001
H	-9.72400000	-17.64700000	-3.02300001
C	-9.71800000	-19.68700000	-3.73900001
C	-9.05800000	-20.19500000	-2.56300001
C	-10.08200000	-20.53900000	-4.78200000
C	-10.72600000	-20.04100000	-5.92000001
C	-11.12300000	-20.98500000	-7.01600001
N	-11.39600000	-20.38600000	-8.22300001
C	-11.93300000	-20.93400000	-9.48500001
H	-11.73300000	-22.02200000	-9.52800001
H	-13.02900001	-20.79100000	-9.56700001
H	-11.18200000	-19.41500000	-8.37300001
H	-11.44600000	-20.47000000	-10.36600001
C	-8.49600000	-20.57000000	-1.56700001
C	-7.93300000	-20.93600000	-0.56900001
C	-7.37200000	-21.30400000	0.42999999
O	-11.14800000	-22.19400000	-6.88300001
H	-9.83700000	-21.61299999	-4.68200000
C	-10.99800000	-18.67200000	-6.00700001
H	-11.51100000	-18.23500000	-6.88100001
C	-6.70500000	-21.77900000	1.61499999
C	-6.30300000	-23.11200000	1.69999999
H	-6.51700001	-23.76400000	0.83699999
C	-5.66300000	-23.59200000	2.84499999
C	-5.24400000	-25.02800000	2.95399999
C	-5.41400000	-22.71100000	3.90199999
H	-4.88400000	-23.04700000	4.81199999
C	-6.46000000	-20.91800000	2.68299999
H	-6.78700000	-19.87100000	2.61799999
C	-5.81100000	-21.37400000	3.82900000
C	-5.55300000	-20.46500000	4.92099999
O	-4.84500000	-25.53900000	3.98699999
N	-5.28300000	-25.72300000	1.76499999
H	-5.50700000	-25.27100000	0.89599999
C	-4.91700000	-27.12800000	1.50699999
H	-4.32300000	-27.50800000	2.35899999
H	-5.79400000	-27.79600000	1.42399999
H	-4.29200000	-27.23600000	0.59599999
C	-5.34000000	-19.67200000	5.80100000
C	-6.58600000	-6.11200000	4.20900000
C	-7.28800000	-5.58900000	3.38400000
C	-8.13999999	-5.01300000	2.37500000
C	-8.65199999	-5.81800000	1.35900000
H	-8.39600000	-6.88800000	1.33900000
C	-9.47900000	-5.27800000	0.37700000
C	-9.99200000	-6.11800000	-0.67600000
C	-9.80000000	-3.92100000	0.41900000
C	-9.28800000	-3.09900000	1.42700000
C	-9.65000000	-1.64300000	1.44800000
N	-8.78500000	-0.83800000	2.14000000
C	-8.86200000	0.58800000	2.50700000
H	-9.54300000	1.10700000	1.81000000
H	-9.25400000	0.73000000	3.53300000
H	-7.91700000	-1.20600000	2.48300000
H	-7.87100000	1.08200000	2.43100000
C	-10.39000000	-6.83700000	-1.55500000
C	-10.78200000	-7.56300001	-2.43000000
C	-11.17400000	-8.29700000	-3.29900000
O	-10.60400000	-1.17300000	0.86300000
H	-10.45400000	-3.51700000	-0.37700000
C	-8.45800000	-3.65400000	2.40500000
H	-8.03900000	-3.04800000	3.22900000
C	-11.65899999	-9.19900000	-4.31200000
C	-12.40599999	-8.71300000	-5.38900000
H	-12.60999999	-7.63100000	-5.43700000
C	-12.87899999	-9.58700000	-6.36600000
C	-13.66999999	-9.11900000	-7.55199999
C	-12.60599999	-10.95300000	-6.25500000
H	-12.95499999	-11.67000000	-7.02400000
C	-11.38199999	-10.56500001	-4.22100000
H	-10.77999999	-10.95700000	-3.38900000
C	-11.85799999	-11.44600001	-5.18800000
C	-11.57399999	-12.85600001	-5.10200000
O	-14.35499999	-9.88300000	-8.20599999
N	-13.51099999	-7.81500001	-7.95299999
H	-12.91399999	-7.16300001	-7.47499999
C	-13.82099999	-7.36200001	-9.32299999
H	-13.79699999	-8.22600001	-10.01699999
H	-14.82999999	-6.91900001	-9.40299999
H	-13.08099999	-6.63100001	-9.70699999
C	-11.34699999	-14.03700001	-5.08500000
C	-2.38000000	-19.30800000	3.47299999
C	-2.03700000	-18.73700000	4.47600000
C	-1.64000000	-18.03600000	5.67099999
C	-1.97700000	-16.69300001	5.83899999
H	-2.54100000	-16.17900001	5.04699999
C	-1.60300000	-16.00700001	6.99299999
C	-1.95300000	-14.61700001	7.15799999
C	-0.88400000	-16.67500001	7.98699999
C	-0.53600000	-18.02000001	7.82999999
C	0.22800000	-18.72200001	8.91099998
N	0.93400000	-19.82200001	8.50299998
C	1.67100000	-20.84800001	9.25999998
H	1.94500000	-20.44600002	10.25199998
H	1.07200000	-21.76500001	9.42399998
H	1.01900000	-20.03500001	7.52499998
H	2.61299999	-21.13100001	8.74699999
C	-2.23800000	-13.45600000	7.29199999
C	-2.52500000	-12.29500000	7.42299999
C	-2.81600000	-11.13400000	7.55099999
O	0.29800000	-18.32900001	10.05899998
H	-0.58800000	-16.10400000	8.88799999
C	-0.91700000	-18.69300000	6.66699999
H	-0.67100000	-19.75800000	6.50499999
C	-3.18900000	-9.74800000	7.69099999
C	-2.76800000	-9.01200000	8.79999999
H	-2.15800000	-9.53200000	9.55899999
C	-3.12900000	-7.66900000	8.93799999
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C	-3.93000000	-7.07200000	7.96099999
H	-4.23200000	-6.00900000	8.03299999
C	-3.98000000	-9.13600000	6.71900000
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C	-5.18900000	-7.17800000	5.85300000
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N	-1.55899999	-7.32300000	10.75600000
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H	-1.22799999	-7.48700000	12.87899999
H	0.19700000	-6.94100001	11.92099999
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C	-8.25799999	-13.79200001	-7.16600000
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H	-7.07899999	-15.49200000	-5.48300000
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H	-8.72500000	-18.80600000	-12.31800001
H	-10.31299999	-18.08000001	-12.62500001
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O	-9.43800000	-19.09500001	-9.82500001
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H	-3.32499999	-24.30400000	-3.40200000
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N	-4.20600000	-0.40000000	2.82399999
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H	-4.25400000	1.41499999	1.71399999
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H	-2.92400000	1.32800000	2.88999999
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H	-7.44800000	-8.89200000	-4.54600001
C	-8.67800000	-8.83100000	-6.33600001
C	-8.57700000	-10.24600001	-6.58300001
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H	-11.34899999	-3.80300001	-9.39899999
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H	-9.98099999	-2.68700001	-9.11499999
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C	0.66400001	-18.98100000	1.15000001
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C	0.95800001	-17.31100000	2.91400001
H	0.47100001	-16.57900000	2.25300001

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C	2.02700001	-17.88300000	4.99400001
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C	4.68800002	-21.93800000	5.47500001
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H	4.38800002	-22.75300000	6.15500001
H	3.42000001	-21.49700000	3.89400002
H	5.36600002	-22.37700000	4.71700001
C	1.11800001	-14.44600000	5.01500001
C	0.99900001	-13.31100000	5.39300001
C	0.87000001	-12.17500000	5.76900001
O	3.07800001	-19.98000001	6.61700001
H	2.38300001	-17.55500000	5.99100001
C	1.78800001	-19.55200001	3.26400001
H	1.93200001	-20.57200000	2.86700001
C	0.66200001	-10.81900000	6.20700001
C	1.19600001	-10.37400000	7.41800001
H	1.77800001	-11.09600000	8.01700001
C	0.98900001	-9.05900000	7.84100001
C	1.56000001	-8.55199999	9.12800001
C	0.22700001	-8.19399999	7.05000001
H	0.04900001	-7.13899999	7.34300001
C	-0.07999999	-9.94400000	5.41700001
H	-0.47899999	-10.29600000	4.45300001
C	-0.30099999	-8.63500000	5.83600001
C	-1.06099999	-7.73500000	5.01500000
O	1.17800001	-7.52900000	9.66400001
N	2.57700001	-9.28699999	9.66500001
H	2.93300002	-10.09900000	9.18700001
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H	3.17100002	-8.14299999	11.34300001
H	3.02500002	-9.89599999	11.68900001
H	4.41500002	-9.25999999	10.74700001
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C	-5.46999999	-12.40700000	-9.31000001
C	-4.90700000	-13.42900000	-8.54700001
H	-4.35899999	-13.17400000	-7.62700001
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H	-6.56299999	-11.86900000	-11.08600001
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C	-2.26999999	-20.82300000	-5.88700000
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C	-1.81199999	-19.16000000	-4.19200001
H	-1.82499999	-18.10800000	-3.86500000
C	-1.27699999	-20.14000000	-3.36200000
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O	-1.46499999	-24.13800000	-4.67400000
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C	-1.13599999	-24.79700000	-7.32100000
H	-0.29599999	-25.11900000	-6.67000000
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C	1.19900001	-5.70700000	2.43800000
C	0.42900001	-4.62900000	1.88200000
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N	0.63500001	-0.59600000	3.35299999
C	0.95100001	0.82700000	3.57799999
H	0.73700001	1.42900000	2.67199999
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H	2.01800001	0.97800000	3.82299999
C	-2.41599999	-4.19200000	-2.07200000
C	-3.00599999	-4.34700000	-3.10800000
C	-3.60499999	-4.51400000	-4.13700000
O	-1.28299999	-0.18700000	2.30899999
H	-1.75999999	-1.79200000	0.36000000
C	0.41500001	-3.37800000	2.49900000
H	1.02300002	-3.24200000	3.41500001
C	-4.38099999	-4.79000000	-5.31600000
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H	-6.60999999	-1.17900000	-9.75100001
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H	-5.65599999	0.02900000	-8.86900000
C	-5.28099999	-8.83300001	-7.92200001
C	2.66800001	-18.88400001	-3.40900001
C	3.20300001	-18.88000001	-2.33200001
C	3.75000001	-18.84500001	-1.00500001
C	3.73400001	-17.64800000	-0.29000001
H	3.33700001	-16.74100001	-0.77100001
C	4.22000001	-17.60000000	1.01299999
C	4.22400001	-16.35900000	1.73999999
C	4.72300002	-18.75900001	1.60000000
C	4.77900002	-19.95500001	0.87100000
C	5.39500002	-21.15200000	1.52099999
N	5.91100001	-22.12700000	0.72700000
C	6.92000002	-23.09100001	1.20100000
H	7.64400002	-22.60500000	1.88400000
H	6.46300002	-23.92900000	1.75300000
H	5.93000001	-22.04000000	-0.27600000
H	7.49800002	-23.52400001	0.36299999
C	4.27400001	-15.31800000	2.33899999
C	4.32400002	-14.27600001	2.93699999
C	4.36300002	-13.23400001	3.53599999
O	5.55300002	-21.22900001	2.72300000
H	5.11000002	-18.68400001	2.64000000
C	4.28600001	-19.99900001	-0.43400001
H	4.28600001	-20.92700000	-1.04000001
C	4.31600002	-11.99100001	4.25899999
C	4.92500002	-11.87700001	5.50899999
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C	4.83700002	-10.67600001	6.22099999
C	5.47200002	-10.52300001	7.56600000
C	4.13200002	-9.59500001	5.67799999
H	4.03800002	-8.62400001	6.21099999
C	3.64300001	-10.90100001	3.70899999
H	3.19300001	-11.00100001	2.70799999
C	3.55200002	-9.70400001	4.41499999
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H	6.94700002	-10.77700000	9.83400000
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H	8.24500002	-11.68700001	9.01099999
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H	-3.54900000	-9.97300001	-16.52200001
H	-5.26900000	-10.55400001	-16.45200000
H	-4.12400000	-8.93300001	-14.28900000
H	-4.87500000	-8.81800001	-16.47900001
C	-1.43999999	-14.38300000	-10.02800000
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O	-4.99500000	-11.94800001	-14.29300000
H	-3.41400000	-13.09300000	-12.55200000
C	-3.36300000	-9.69300000	-11.98000000
H	-3.71999999	-8.71800001	-12.36400000
C	-0.10399999	-17.71400001	-8.66800000
C	-0.28599999	-18.91800001	-9.34600000
H	-0.79199999	-18.88200001	-10.33200000
C	0.13700001	-20.11700001	-8.76400000
C	-0.05399999	-21.41800001	-9.47200000
C	0.72700001	-20.10900001	-7.49300000
H	1.07800001	-21.03500001	-6.98399999
C	0.51000001	-17.70800001	-7.41799999
H	0.65900001	-16.74400001	-6.90899999
C	0.92600001	-18.89900001	-6.82999999
C	1.56500001	-18.88300001	-5.54399999
O	0.02300001	-22.49300001	-8.91100000
N	-0.27999999	-21.35400001	-10.81300000
H	-0.07899999	-20.51200001	-11.32100000
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H	-0.07499999	-22.38400001	-12.66600000
C	2.11900001	-18.88400001	-4.47700001
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C	5.24100001	-6.30400001	1.58099999
C	4.57200001	-5.06100001	1.29299999
C	3.77900001	-4.95000001	0.15099999
H	3.70300001	-5.80800001	-0.53000001
C	3.10700001	-3.76600001	-0.13500001
C	2.31900001	-3.65000001	-1.33300001
C	3.21500001	-2.68500001	0.73699999
C	4.02600001	-2.78100001	1.87799999
C	4.16500001	-1.58200000	2.75799999
N	5.25100001	-1.48700000	3.57199999
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H	5.74000001	0.54800000	3.09399999
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H	5.91900001	-2.23100000	3.68699999
H	6.88300001	-0.23500000	4.20299999
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C	1.04900000	-3.38900001	-3.35800001
C	0.39900001	-3.26700001	-4.36200001
O	3.40000001	-0.63900000	2.68599999
H	2.67200001	-1.75200001	0.46599999
C	4.70400001	-3.96900001	2.15099999
H	5.34600001	-4.08300001	3.04399999
C	-0.44900000	-3.19200001	-5.52200001
C	-1.05600000	-1.98800001	-5.87800001
H	-0.85400000	-1.10100001	-5.24500001
C	-1.91000000	-1.93800001	-6.98400001
C	-2.56899999	-0.65900001	-7.38700001
C	-2.15900000	-3.10100001	-7.72300001
H	-2.82900000	-3.10700001	-8.61000001
C	-0.67600000	-4.33600001	-6.28400001
H	-0.16600000	-5.26800001	-6.00100001
C	-1.52600000	-4.29800001	-7.38600001
C	-1.74300000	-5.48200001	-8.17400001
O	-3.50299999	-0.60000002	-8.15900001
N	-2.01700000	0.48399998	-6.90400001
H	-1.08899999	0.47199998	-6.52000001
C	-2.50500000	1.86799999	-6.94300001
H	-3.30000000	1.95099999	-7.71000001
H	-2.92000000	2.22799998	-5.97900001
H	-1.69300000	2.55699998	-7.25200001
C	-1.91599999	-6.46800000	-8.84100000
C	4.95900001	-18.03300001	-6.84199999
C	5.50600001	-18.32500001	-5.80999999
C	6.09400001	-18.62400001	-4.52499999
C	6.27000001	-17.60200000	-3.59099999
H	5.98000001	-16.57700000	-3.85999999
C	6.81700001	-17.86400000	-2.33799999
C	7.01500001	-16.79800000	-1.38999999
C	7.18700001	-19.16700000	-2.00899999
C	7.03000001	-20.20100000	-2.94199999
C	7.48900001	-21.57500000	-2.56599999
N	7.75800001	-22.45800000	-3.56199999
C	8.89200002	-23.39400000	-3.49699999
H	9.86600002	-22.89000000	-3.69499999
H	8.92200002	-23.90200000	-2.51699999
H	7.56700001	-22.24300000	-4.52399999
H	8.81600002	-24.18100000	-4.26699999
C	7.21200001	-15.92100000	-0.58999999
C	7.40500002	-15.04700000	0.21300001
C	7.58100002	-14.17200000	1.02000001
O	7.73800001	-21.89100000	-1.41899999
H	7.63600001	-19.33300000	-1.00399999
C	6.48700001	-19.92500000	-4.19899999
H	6.34200001	-20.71500000	-4.95899999
C	7.68900002	-13.11300000	1.98900001
C	8.32500001	-13.33100000	3.21200001
H	8.74400001	-14.33799999	3.40300001
C	8.39400002	-12.30399999	4.15800001
C	9.07900002	-12.51699999	5.47000001
C	7.80900002	-11.06199999	3.87900001
H	7.83700002	-10.21700000	4.60200001
C	7.14100002	-11.86300000	1.70700001
H	6.66600001	-11.70600000	0.72600001
C	7.20100002	-10.83400000	2.64400001
C	6.64400002	-9.54200000	2.33700001
O	8.95700002	-11.76899999	6.42000001
N	9.93400002	-13.56999999	5.54800001
H	10.27700002	-14.00399999	4.71000001
C	10.60300002	-14.16099999	6.71400001
H	10.54400002	-13.45199999	7.56300001
H	10.16700002	-15.12699999	7.04300001
H	11.68100002	-14.31999999	6.50600001
C	6.18800001	-8.45799999	2.08300001
C	1.33600001	-5.17800001	-10.19700001
C	0.99000000	-5.97200001	-11.03300001
C	0.55100000	-6.97700001	-11.97000001
C	0.94000001	-8.30500001	-11.79000001
H	1.60400000	-8.55500001	-10.95000001
C	0.48200000	-9.30600002	-12.64600001
C	0.86300000	-10.68300001	-12.43800002
C	-0.36200000	-8.96300002	-13.70300002
C	-0.72500000	-7.62700002	-13.92200002
C	-1.64100000	-7.29600002	-15.06600002
N	-1.73600000	-6.00300002	-15.49400002
C	-2.85200000	-5.44300002	-16.27300002
H	-2.63500000	-5.36900002	-17.35700002
H	-3.73600000	-6.09300002	-16.12800002
H	-1.00400000	-5.32400002	-15.34400002
H	-3.15800000	-4.43800002	-15.92300002
C	1.17400001	-11.83400002	-12.27000001
C	1.48400000	-12.98400002	-12.09600002
C	1.79000001	-14.13400002	-11.90900001
O	-2.30700000	-8.15100001	-15.61900001
H	-0.72500000	-9.78500002	-14.35200002
C	-0.27999999	-6.63900001	-13.04000001
H	-0.59700000	-5.58500001	-13.13900001

C	2.13200001	-15.50500002	-11.61400001
C	1.75100001	-16.53600002	-12.47500001
H	1.16900001	-16.27000002	-13.37500001
C	2.07200001	-17.86100002	-12.17100001
C	1.66600001	-18.99100002	-13.07000001
C	2.74800001	-18.15200002	-10.97800001
H	3.01300001	-19.19200002	-10.69100001
C	2.82500001	-15.80900002	-10.44200002
H	3.11700000	-14.98900002	-9.77100002
C	3.13100001	-17.12900002	-10.11100001
C	3.82800001	-17.44200002	-8.88500001
O	1.64900001	-20.14600002	-12.68300001
N	1.32500001	-18.72500002	-14.36200002
H	1.58400001	-17.86800002	-14.82000002
C	0.54800000	-19.59600002	-15.25600002
H	-0.04299999	-20.29100002	-14.63000002
H	-0.17700000	-19.03100002	-15.87200002
H	1.18000000	-20.18700002	-15.94800002
C	4.39800001	-17.73700002	-7.86600001
C	9.60100002	-8.35100000	0.38600000
C	9.24500002	-7.20099999	0.40000000
C	8.74700002	-5.84399999	0.39800000
C	7.96000002	-5.39599999	-0.66399999
H	7.75600002	-6.07999999	-1.49899999
C	7.42400002	-4.10799999	-0.66699999
C	6.60200002	-3.64900000	-1.76099999
C	7.68900002	-3.25899999	0.40700001
C	8.51000002	-3.67799999	1.46200001
C	8.76900002	-2.73099999	2.59900001
N	9.80800002	-2.97699999	3.44700001
C	9.94800002	-2.43099999	4.80600002
H	10.60800003	-1.54199999	4.85100001
H	8.94200003	-2.15999999	5.18100001
H	10.55500003	-3.61499999	3.22400001
H	10.34700002	-3.17499998	5.52000001
C	5.93000002	-3.22999999	-2.66800000
C	5.25800002	-2.81199999	-3.57500000
C	4.57600002	-2.40699999	-4.48100000
O	8.07400002	-1.74999998	2.78900001
H	7.23200002	-2.24799999	0.38500001
C	9.02300002	-4.97699999	1.45900001
H	9.62700002	-5.36499999	2.29900001
C	3.69700002	-2.01499999	-5.55700000
C	3.19500002	-0.71300000	-5.63800000
H	3.49000002	0.00200000	-4.84700000
C	2.31200002	-0.36200000	-6.66300000
C	1.73800002	1.02000000	-6.76600000
C	1.90800001	-1.33200000	-7.59000000
H	1.18000001	-1.10600000	-8.39700000
C	3.31900001	-2.95700000	-6.51400000
H	3.72700002	-3.97600000	-6.45000000
C	2.42300001	-2.62600000	-7.52900000
C	2.02100001	-3.60500000	-8.50900000
O	0.72400002	1.25400000	-7.40000000
N	2.37400001	2.04100000	-6.12500000
H	3.34800001	1.99400000	-5.86700000
C	1.77200002	3.33300000	-5.77100000
H	0.67200002	3.20700000	-5.77800000
H	2.04000002	3.66800000	-4.75100000
H	2.04200001	4.14899999	-6.47000000
C	1.67900001	-4.39200000	-9.35300001
C	7.20400001	-16.84100002	-10.25000001
C	7.76700001	-17.36300002	-9.32400001
C	8.39200001	-17.96100002	-8.17100001
C	8.76500001	-17.16200002	-7.09100002
H	8.59800001	-16.07600002	-7.15000002
C	9.32500001	-17.72700002	-5.94700002
C	9.69300001	-16.91300002	-4.81300002
C	9.52900001	-19.10500002	-5.90000002
C	9.19500001	-19.91500002	-6.99200002
C	9.43800001	-21.39300002	-6.90500002
N	9.45600001	-22.12000002	-8.05700002
C	9.28900001	-23.58000002	-8.15200002
H	10.25400001	-24.12100002	-8.23000002
H	8.74300001	-23.93100002	-7.25600002
H	9.54600001	-21.70100002	-8.96800003
H	8.67600001	-23.87300002	-9.02500002
C	10.02300001	-16.28300002	-3.84300002
C	10.34900001	-15.65400002	-2.86900002
C	10.65800001	-15.01800002	-1.89600002
O	9.62500001	-21.95700002	-5.84400002
H	9.96800001	-19.52500002	-4.97300002
C	8.60300001	-19.34000002	-8.11900002
H	8.26400001	-19.94800002	-8.97600002
C	10.92600001	-14.19100002	-0.74400002
C	11.55100001	-14.71600002	0.39099998
H	11.82400001	-15.78700002	0.37999998
C	11.77000001	-13.90700002	1.50899998
C	12.40700002	-14.44700002	2.75899998
C	11.33700001	-12.57500002	1.48999998
H	11.46800001	-11.90800001	2.36399998
C	10.52500002	-12.85500002	-0.75500002
H	10.03700001	-12.45600002	-1.65700002
C	10.72200002	-12.03800002	0.35799998
C	10.29000002	-10.65900002	0.35399998
O	12.28900002	-13.90000002	3.84099998
N	13.14400001	-15.59300002	2.67299998
H	13.53300001	-15.92700002	1.80399998
C	13.49200001	-16.46800002	3.80099998
H	12.79400002	-16.24900002	4.63099998
H	13.36700002	-17.54100002	3.56099998
H	14.52900001	-16.32400002	4.16199998
C	9.94600002	-9.50500002	0.36999998
C	4.94900001	-3.27600000	-10.70600000
C	4.45800001	-3.86900000	-11.63200000
C	3.85000001	-4.62200000	-12.70400000
C	4.08000001	-5.99300000	-12.80800000
H	4.74400001	-6.47900000	-12.07800000
C	3.47800001	-6.74500000	-13.81600000
C	3.71700001	-8.16299999	-13.91700000
C	2.64100001	-6.11000000	-14.73400000
C	2.43000001	-4.72899999	-14.66500000
C	1.54000001	-4.08299999	-15.68599999
N	1.60000001	-2.72499999	-15.83500000
C	0.54900001	-1.91399999	-16.47400000
H	0.75900001	-1.71699999	-17.54200000
H	-0.42099999	-2.43899999	-16.37700000
H	2.23900001	-2.15699999	-15.31200000
H	0.42800001	-0.93299999	-15.97499999
C	3.92300001	-9.34400000	-14.02200000
C	4.12700001	-10.52500000	-14.12300000
C	4.32200001	-11.71000000	-14.21100000
O	0.75500001	-4.71900000	-16.36300000
H	2.15700001	-6.72500000	-15.51700000
C	3.01700001	-3.99399999	-13.63400000
H	2.82700001	-2.91499999	-13.50800000
C	4.50800001	-13.14000000	-14.23000000
C	3.95400001	-13.91899999	-15.24899999
H	3.36700002	-13.40300000	-16.02799999
C	4.11100001	-15.30800000	-15.24199999
C	3.49900001	-16.17900000	-16.30500000
C	4.81400002	-15.91100000	-14.19199999
H	4.95100002	-17.00800000	-14.13999999
C	5.21300001	-13.75599999	-13.19600000
H	5.64000001	-13.13299999	-12.39500000
C	5.36300001	-15.13999999	-13.16700000
C	6.06200001	-15.77799999	-12.08100000
O	3.33600001	-17.37500000	-16.14600000
N	3.09100001	-15.57800000	-17.47300000
H	3.20500001	-14.59500000	-17.63300000
C	2.15000001	-16.16000000	-18.45199999
H	1.52300002	-16.92199999	-17.94700000
H	1.45800001	-15.39600000	-18.86099999
H	2.66300001	-16.63200000	-19.31199999
C	6.63400001	-16.31200002	-11.16700001
C	13.20100001	-9.34500002	-1.42600001
C	12.94600001	-8.19500002	-1.17600001
C	12.59600001	-6.82500002	-0.87900001
C	11.84300001	-6.08300002	-1.79000001
H	11.53800001	-6.54700002	-2.73900001
C	11.47100001	-4.76900002	-1.50700001
C	10.68100001	-4.01000002	-2.44700001
C	11.87000001	-4.19100002	-0.30200001
C	12.65200001	-4.91000002	0.60899999
C	13.06500001	-4.24500002	1.89199998
N	14.08300001	-4.80100002	2.61599999
C	14.33900002	-4.54700002	4.04599999
H	15.08200002	-3.74300002	4.20499999
H	13.38700001	-4.27400002	4.54199999
H	14.58600002	-5.60400003	2.29199999
H	14.71000002	-5.45100002	4.56699999
C	10.02900001	-3.36600002	-3.22700001
C	9.37300001	-2.72400002	-4.00700001
C	8.70800001	-2.09000002	-4.78500001
O	12.50500001	-3.25100002	2.31599999
H	11.55600001	-3.15100002	-0.08900001
C	12.99100001	-6.23500002	0.32499999
H	13.55300001	-6.85500002	1.04299999
C	7.85300001	-1.38600002	-5.71100001
C	7.51200001	-0.04900001	-5.49200001
H	7.90800001	0.44099999	-4.58500001
C	6.66400001	0.61999999	-6.37700001
C	6.25400000	2.04899999	-6.15300001
C	6.14000001	-0.07100001	-7.47500001
H	5.45200001	0.42399999	-8.18400000
C	7.33400001	-2.05400002	-6.82000001
H	7.60600001	-3.10600001	-6.98900001
C	6.47200000	-1.40600001	-7.70400001
C	5.91500000	-2.10800002	-8.83600002
O	5.27000000	2.53899999	-6.67300001
N	7.01300001	2.80599999	-5.29600000
H	7.83300001	2.44499999	-4.84800000
C	6.57100001	4.06499999	-4.67200000
H	5.46500001	4.07099999	-4.62400000
H	6.93500001	4.15699999	-3.63000000
H	6.91900001	4.95800000	-5.22700000
C	5.43400000	-2.69000001	-9.77300001
H	8.85200001	-14.61599999	-13.34100000
C	9.50700001	-15.29100002	-12.85400001
C	10.12900001	-16.12500002	-12.24700001
C	10.73300001	-17.09700002	-11.37000001
C	11.30700001	-16.66200002	-10.17800002
H	11.33700001	-15.58100002	-9.96400001
C	11.81200001	-17.57600002	-9.25600002
C	12.35300001	-17.09300002	-8.01100001
C	11.76200001	-18.94100002	-9.54900002
C	11.24000001	-19.39100002	-10.76900002
C	11.21700001	-20.86900001	-11.05500001
N	11.01400001	-21.30800001	-12.33600001
C	10.59900001	-22.68000002	-12.68600001
H	11.46000001	-23.34200002	-12.90700001
H	10.00500001	-23.11200002	-11.85500001
H	10.88100001	-20.67800001	-13.10300002
H	9.93900001	-22.68900002	-13.57400002
C	12.75000001	-16.58600002	-6.99400002
C	13.13000001	-16.05900002	-5.98000002
C	13.49300001	-15.53100002	-4.96200002
O	11.33700001	-21.69300001	-10.17000002
H	12.14200001	-19.65400002	-8.79500002
C	10.70200001	-18.46400002	-11.66200002
H	10.20600001	-18.78700002	-12.59200001
C	13.87200001	-14.94600003	-3.69800002
C	14.45300001	-15.74500003	-2.71200002
H	14.59300001	-16.81600002	-2.93400002
C	14.80400001	-15.20300003	-1.47500003
C	15.40000001	-16.05700003	-0.39300002
C	14.54700001	-13.85100003	-1.22500002
H	14.80100001	-13.39600003	-0.25100002
C	13.63200001	-13.59600003	-3.43700002
H	13.17200001	-12.97200003	-4.21600002
C	13.96200001	-13.04100003	-2.20000002
C	13.68800001	-11.65100003	-1.92200002
O	15.39900001	-15.72900003	0.77799998
N	15.91500001	-17.27600003	-0.76000002
H	15.90400001	-17.59400003	-1.71100003
C	16.19200002	-18.38900003	0.16499998
H	15.56200002	-18.26900003	1.06699998
H	15.93600002	-19.36900003	-0.28500002
H	17.25600002	-18.43000003	0.46699998
C	13.44700001	-10.49700003	-1.67500002

Table S2. Cartesian coordinates of optimized helical poly-PDE (*helix*-**1**)

6. AFM measurements (Fig. 5)

6-1. Helical polymer (*helix*-1) on HOPG

Highly oriented pyrolytic graphite (HOPG) substrates were cleaved before use by the Scotch tape inside a glovebox under an argon atmosphere. This HOPG substrate was settled inside a screw glass bottle equipped with a silicon rubber septum and taken out from the glovebox. This glass bottle was connected to a N_2/vacuum manifold through a needle and a tube. Stock solutions of poly-PDE in $CHCl_3$ (0.02 mg·mL^{-1}) degassed by three freeze-pump-thaw cycles were casted on a freshly cleaved surface on HOPG through a disposable syringe equipped with a needle, and dried *in vacuo* for 1.5 h. The AFM measurements were performed using a Dimension FastScan (BrukerNano) at room temperature and atmospheric conditions with a silicon tip on silicon nitride cantilevers (FastScan-C, Bruker, force constant: 0.8 N/m, resonant frequency: 300 kHz) in the tapping mode. The Nanoscope image processing software was used for the image analysis in which only Flatten and Plane Fit was performed.

6-2. Random-coiled polymer (*coil*-1) on HOPG

HOPG substrates were cleaved before use by the Scotch tape inside a glovebox under an argon atmosphere. This HOPG substrate was settled inside a screw glass bottle equipped with a silicon rubber septum and taken out from the glovebox. This glass bottle was connected to a N_2/vacuum manifold through a needle and a tube. Stock solutions of poly-PDE **1** in 9 vol% TFE/$CHCl_3$ (0.02 mg mL^{-1}) degassed by three freeze-pump-thaw cycles were casted (one or few drops) on a freshly cleaved surface on HOPG through a disposable syringe equipped with a needle. The HOPG substrate was exposed to the vapor atmosphere of 9 vol% TFE/$CHCl_3$ for 4 h. Then, the sample on HOPG was transferred into another screw glass bottle equipped with a silicon rubber septum, then dried *in vacuo* for 2 h. The AFM measurements were performed using a Dimension FastScan (BrukerNano) at room temperature and atmospheric conditions with a silicon tip on silicon nitride cantilevers (FastScan-C, Bruker, force constant: 0.8 N/m, resonant frequency: 300 kHz) in the tapping mode. The Nanoscope image processing software was used for the image analysis in which only Flatten and Plane Fit was performed.

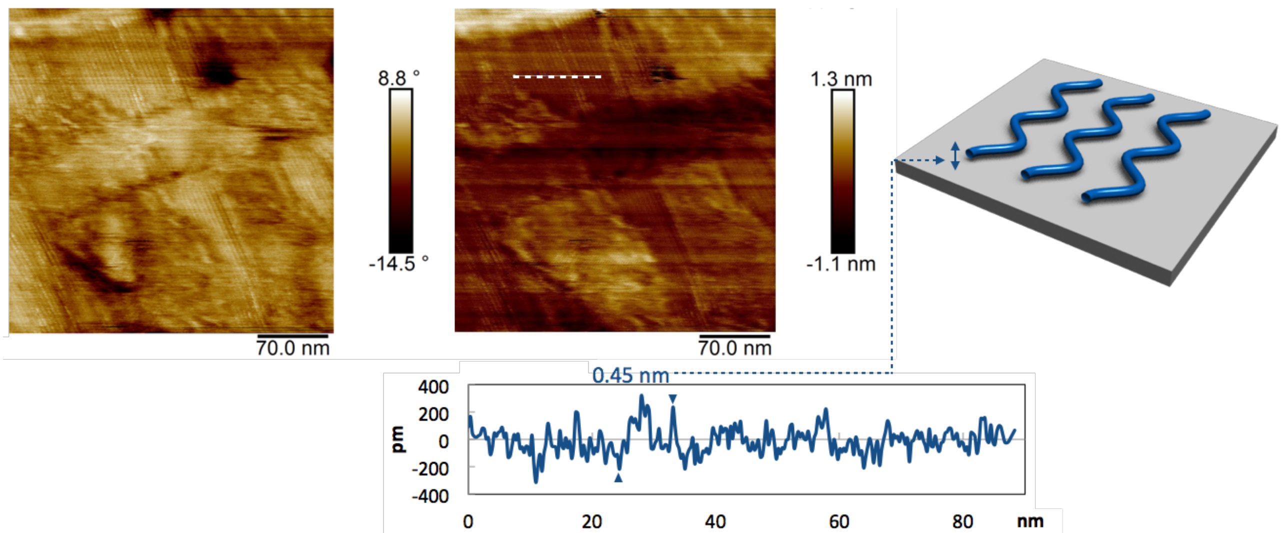

Figure S19. Phase image (left) and height image (right) of random-coiled poly-PDE (*coil*-**1**) on HOPG

7. General Procedures for Photochemical Cross-linking

7-1. Photochemical cross-linking of poly-PDE 1 by Hg lamp in $CHCl_3$ (Fig. 6a).

A solution of poly-PDE **1** (1 mg) in $CHCl_3$ (1 mL) was added into a test tube containing stirring bar equipped with a rubber septum. The solution was degassed by three freeze-pump-thaw cycles, and the tube was filled with N_2. The test tube was settled on a magnetic stirrer, and light irradiation by a 100-W high-pressure Hg lamp was conducted with stirring the solution for 1 h. The solvent was removed *in vacuo* to afford covalent ONT (**6**).

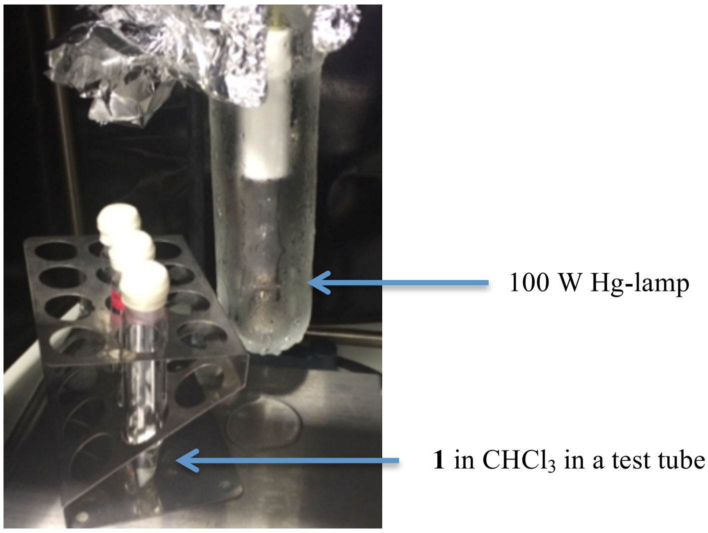

Figure S20. Solution-phase photochemical cross-linking of poly-PDE **1**

7-2. Photochemical cross-linking of poly-PDE 1 by Hg lamp on a silicon substrate (Fig. 8a).

A 0.1 mg·mL solution of poly-PDE (**1**) in $CHCl_3$ was prepared in a Schlenk tube. The solution was degassed by three freeze-pump-thaw cycles, and the tube was filled with N_2. A 5 mm × 5 mm silicon substrate was placed in a 30-mL flat-bottomed vial equipped with a silicon rubber septum and the air in the vial was replaced with N_2 by the usual Schlenk technique. Then, 1 drop of degassed solution of **1** was added on a silicon substrate under a N_2 atmosphere through a micro-syringe with a needle, and the solvent was evaporated. Light irradiation by a 100-W high-pressure Hg lamp was conducted for 10 minutes in a sealed vial under N_2. Emission and Raman spectra of the resulting sample on a silicon substrate were directly measured under air.

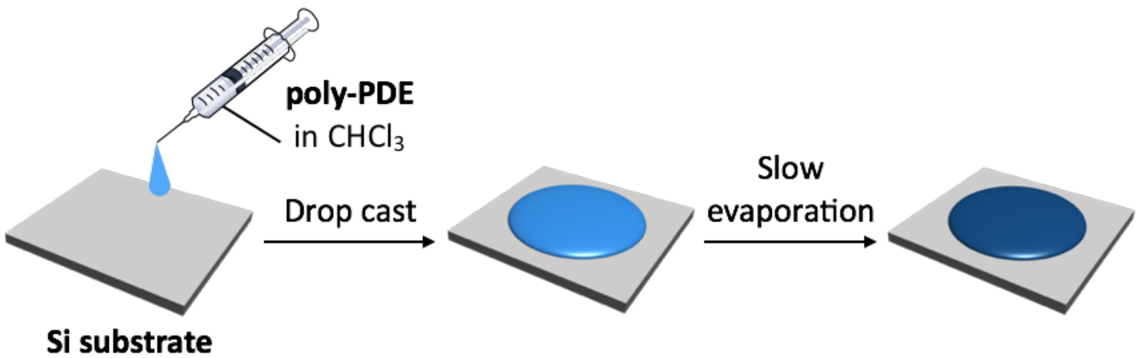

Figure S21. Schematic illustration of preparation method for helical poly-PDE (*helix*-**1**) on silicon substrate for photochemical cross-linking in the solid state

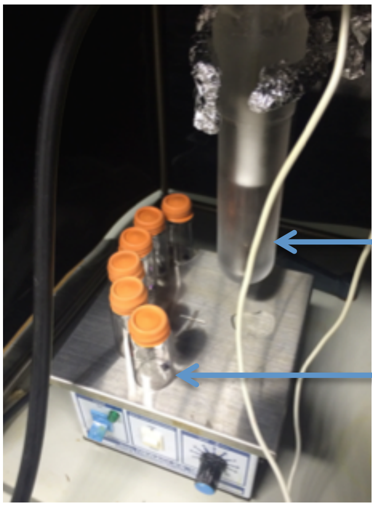

Figure S22. Solid-phase photochemical cross-linking of poly-PDE **1**

8. Additional Spectroscopic Analyses for Photochemical Reactions of poly-PDE 1 and di-PDE 5

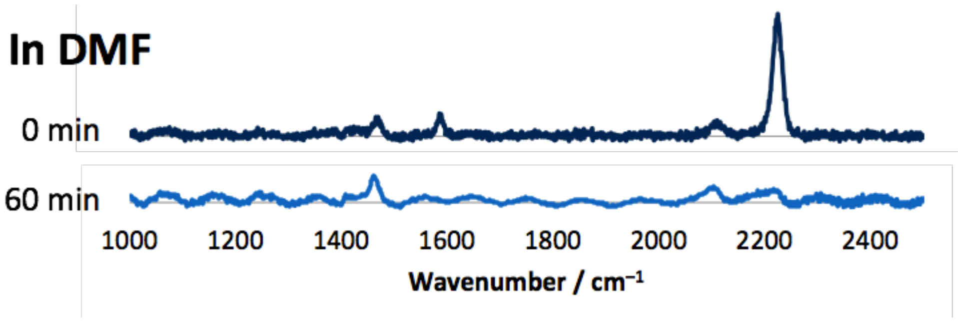

Figure S23. Raman spectra in photochemical cross-linking of poly-PDE **1** in DMF

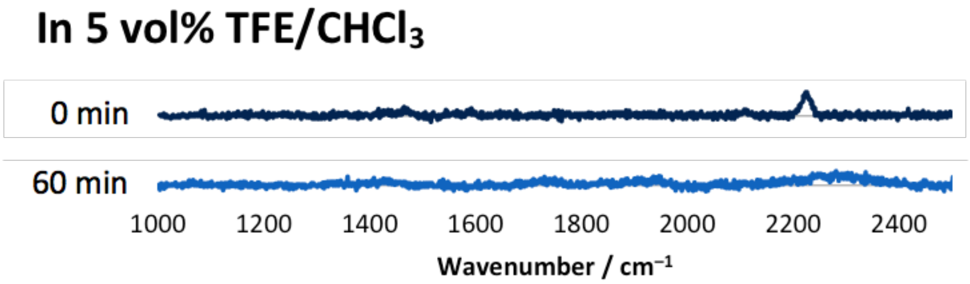

Figure S24. Raman spectra in photochemical reaction of poly-PDE **1** in 5 vol% TFE/$CHCl_3$

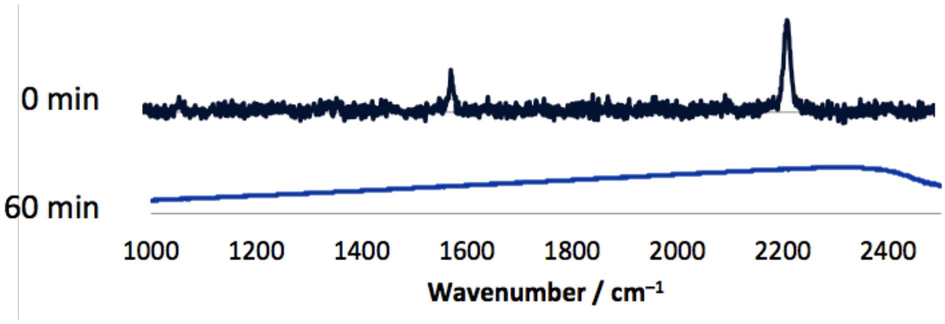

Figure S25. Raman spectra in photochemical reaction of di-PDE **5** in $CHCl_3$

After the photochemical cross-linking of poly-PDE **1** ($M_n = 3.29 \times 10^5$, $M_w/M_n = 2.63$) in $CHCl_3$, estimated M_n and M_w/M_n in terms of polystyrene standards were dramatically decrease to $M_n = 6.30 \times 10^4$ and $M_w/M_n = 2.38$, respectively (Fig. S26).

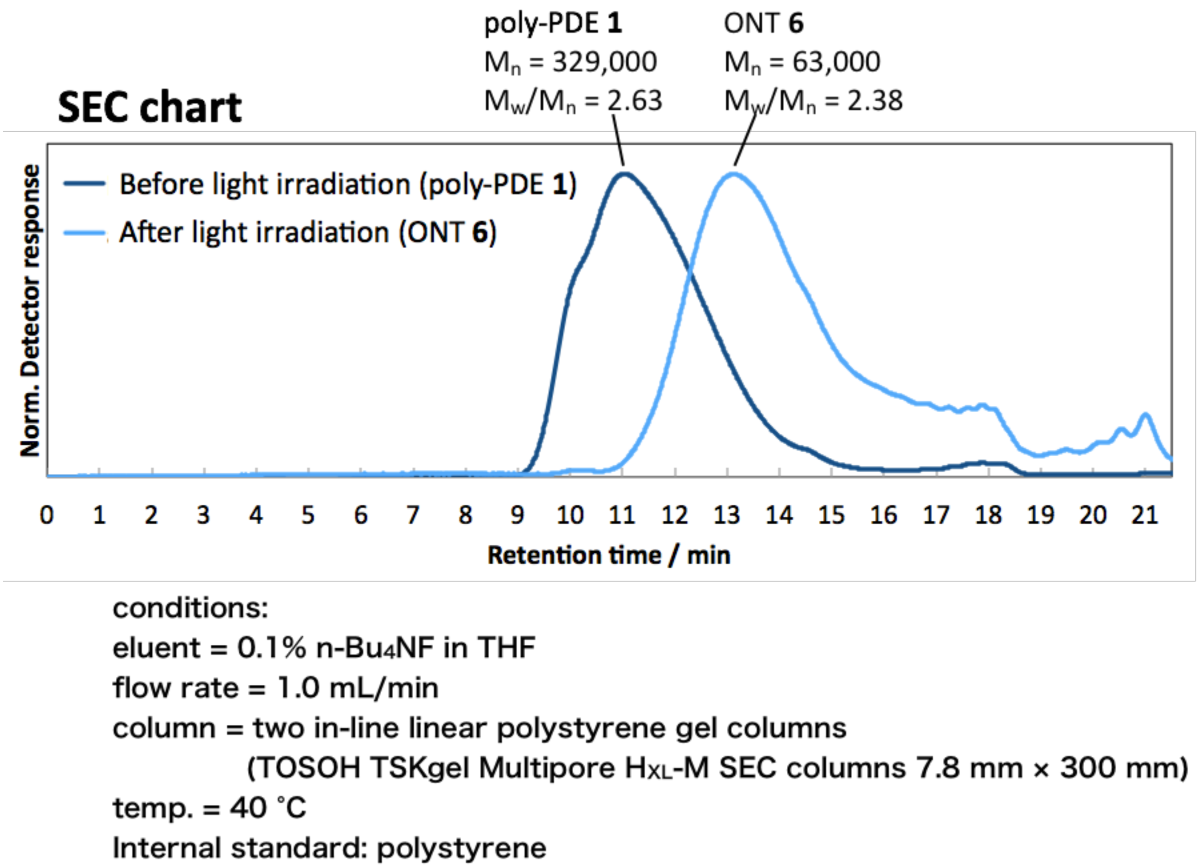

Figure S26. SEC analysis for ONT **6** prepared by photochemical cross-linking of poly-PDE **1** in $CHCl_3$

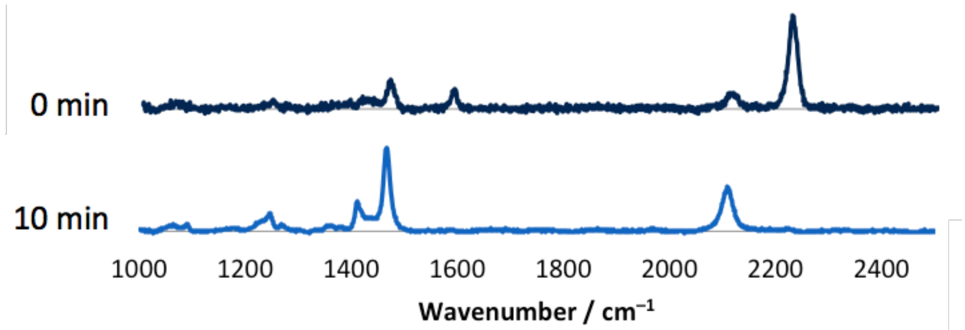

Figure S27. Raman spectra in photochemical cross-linking of poly-PDE **1** on silicon substrate

8-2. Experiments for observation of time-dependent changes of fluorescence spectra in photochemical cross-linking of poly-PDE (*helix*-1) in $CHCl_3$

A solution of poly-PDE **1** (10 μg·mL^{-1}) in $CHCl_3$ was added in a large-size Schlenk tube. The solution was degassed by three freeze-pump-thaw cycles, and then nitrogen was filled in a tube. The degassed solution was transferred by a syringe with being filtered by a membrane filter (0.45 μm hole diameter) to be added in a 1 cm quartz cell equipped with a hole-cap and a Teflon®-coated rubber seal under nitrogen atmosphere. Prepared solution in a quartz cell was settled in the fluorescence spectroscopic apparatus, and irradiated by 365 nm excitation light at 25 °C.

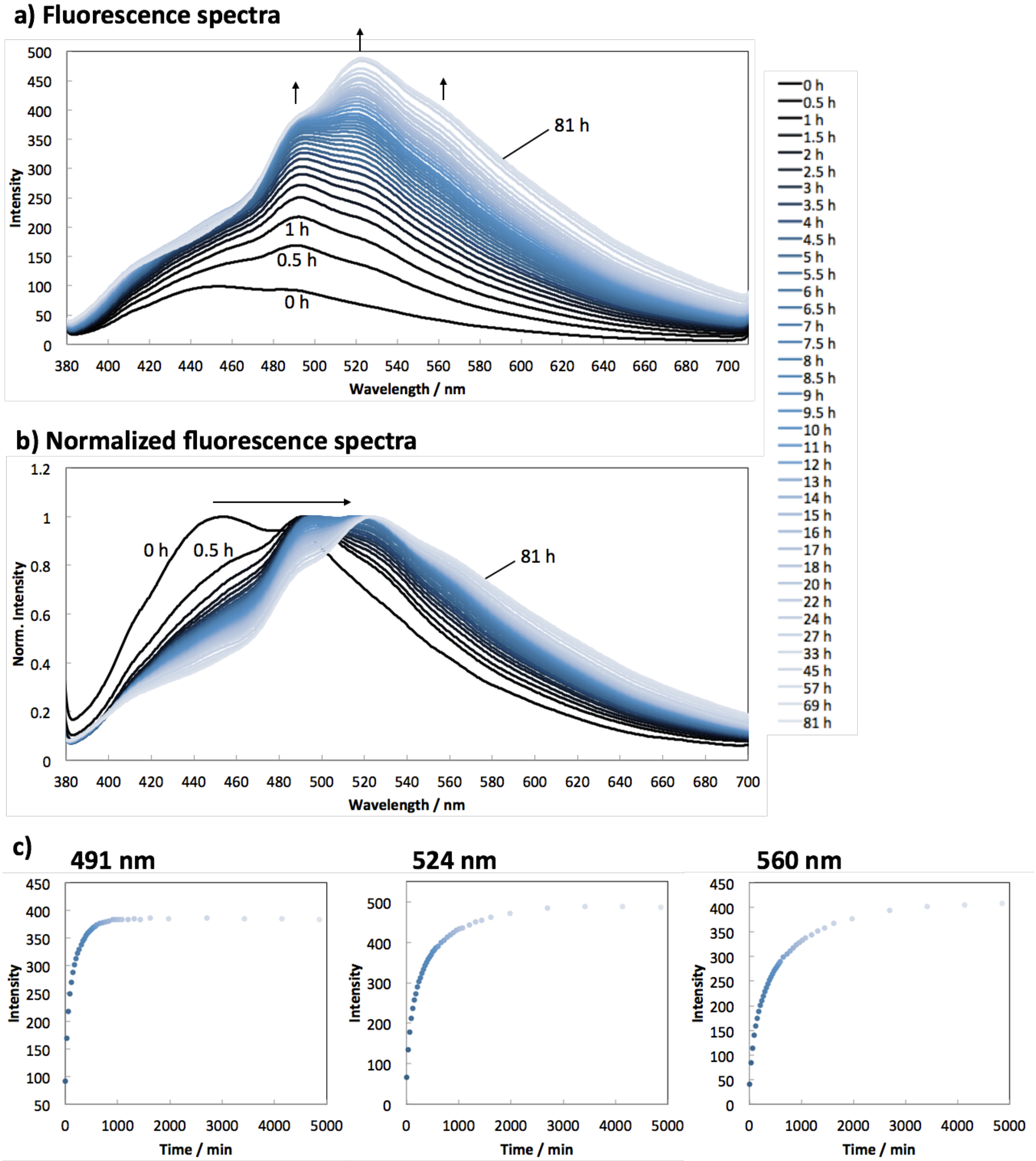

Figure S28. a) Time-dependent changes of fluorescence spectra (λ_{ex} = 365 nm) in photochemical cross-linking of poly-PDE **1** in $CHCl_3$ under irradiation of 365 nm excitation light in a fluorescence spectrophotometer at 25 °C. b) Normalized time-dependent changes of fluorescence spectra. c) Time-dependent changes of the fluorescence intensities at 491 nm, 524 nm and 560 nm.

After the photochemical cross-linking of *helix*-**1** in $CHCl_3$, ONT **6** showed blue-shift in the absorption spectrum and the very small Cotton effect in the CD spectrum in $CHCl_3$ (Fig. S29a and 29b). In the CD spectrum of ONT **6** in $CHCl_3$ (Fig. 29d, blue line), peaks appeared at 349, 327 and 307 nm were very similar to those of starting *helix*-**1** (348, 323 and 303 nm) rather than those of ONT **6** (340, 317 and 298 nm). Therefore, these peaks are considered to be those of unreacted *m*-phenylene diethynylene substructures. When 10 vol% TFE was added to ONT **6** in $CHCl_3$ solution, the absorption and CD spectra were almost unchanged. These results indicate that the unreacted *m*-phenylene diethynylene substructures still remain to some extent in ONT **6** but fixed due to the cross-linked network.

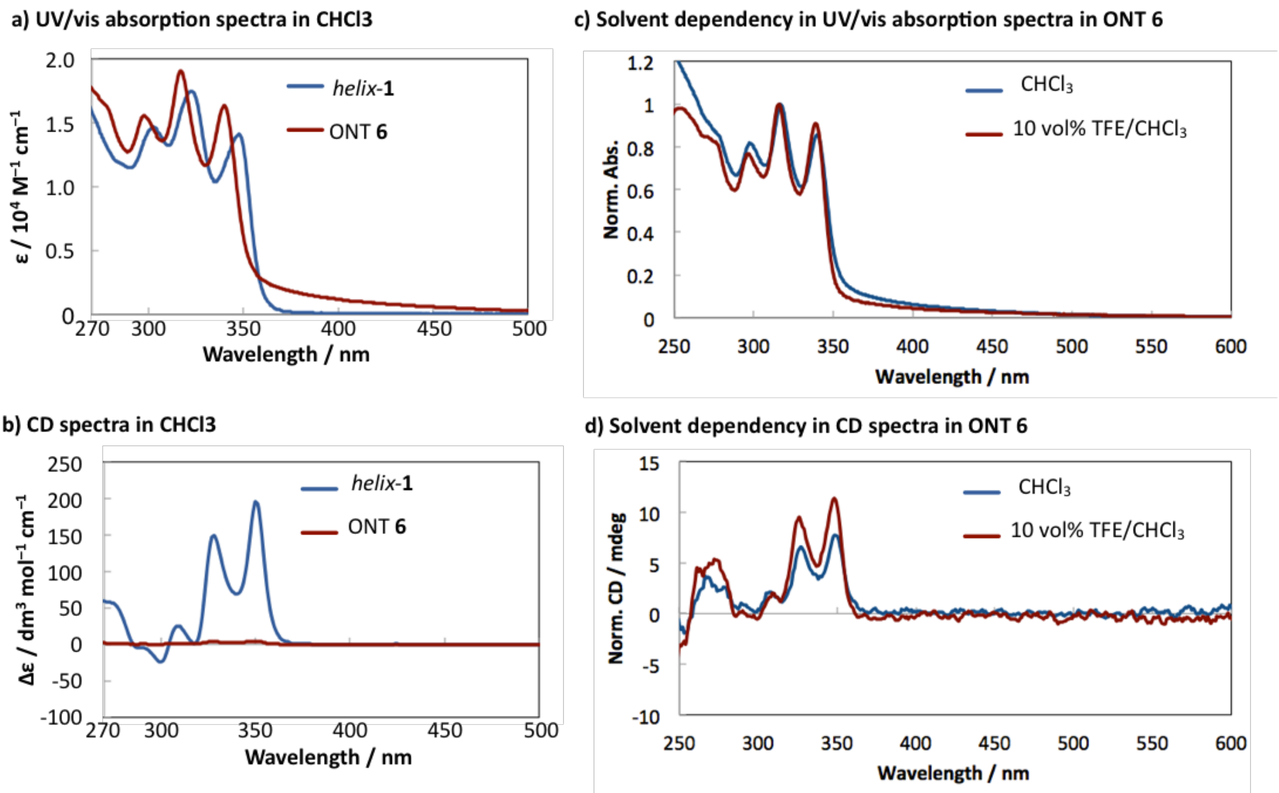

Figure S29. UV/vis/absorption and CD spectra of ONT **6** and their solvent dependency

9. Fluorescence and Raman Spectra in Photochemical Reaction of *coil*-1 on Silicon Substrate

Randum-coiled poly-PDE (*coil*-**1**) on a silicon substrate was prepared according to the procedure for photochemical cross-linking of *helix*-**1** on a silicon substrate (see, **7-2** and Fig. S21) by the drop-casting of 1 mg·mL^{-1} degassed solution of **1** in TFE/$CHCl_3$ (1:10). Photochemical reaction of *coil*-**1** on a silicon substrate was conducted in the same way as the reaction of *helix*-**1** on a silicon substrate.

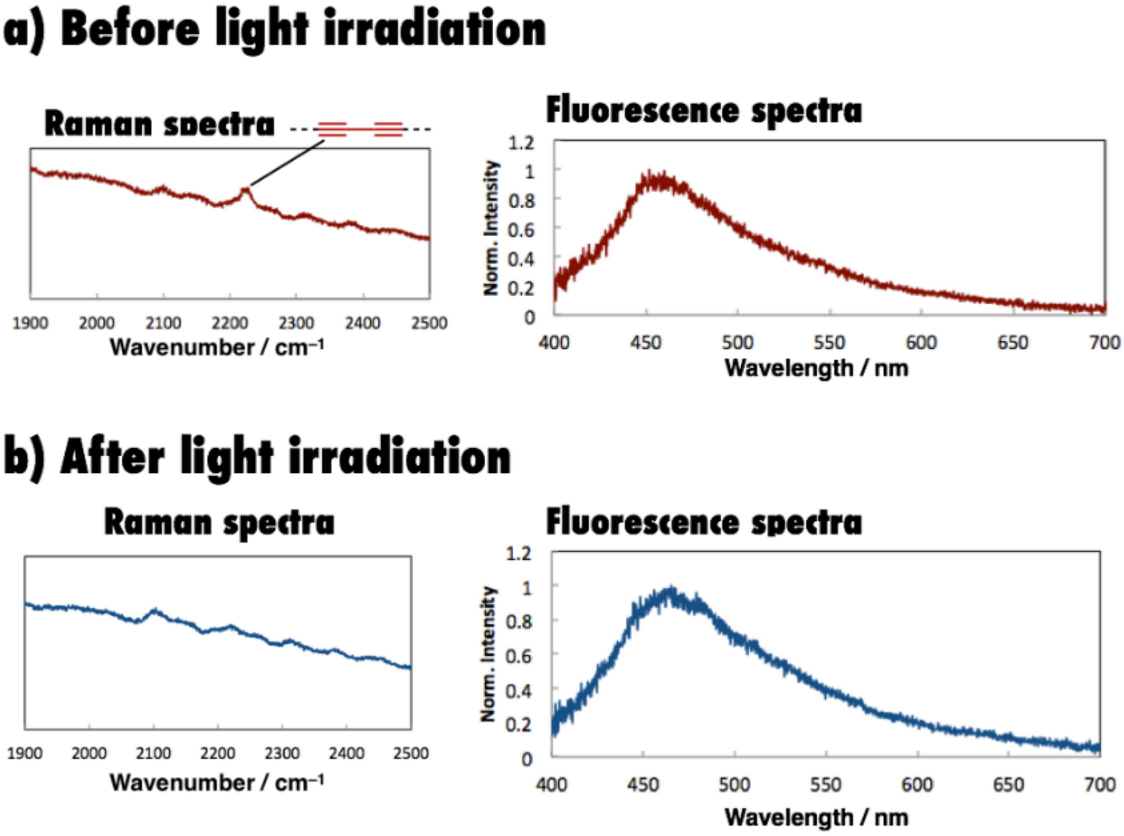

Figure S30. Raman spectra and fluorescence spectra (λ_{ex} = 370 nm) a) before and b) after photochemical reaction of *coil*-**1** on silicon substrate under irradiation of 100-W high-pressure Hg lamp.

10. Molecular Model for ONT 6 (Fig. 7b)

We conducted the molecular mechaniscs calculation by Gaussian 09 program[S4] for obtaining the molecular model for ONT **6** composed of 48 monomer units (Fig. 7b). Terminals of enyne structures in ONT **6** were replaced with methylene (CH_2), and side wall chiral amide chains were replaced with hydrogen atoms for optimization.

C	0.39700000	-0.08000000	-7.57200000
C	-0.32900000	-1.02500000	-7.50000000
C	-0.53100000	-3.34500000	-7.57800000
C	0.23500000	-3.85900000	-6.51400000
C	-0.77400000	-4.18600000	-8.68000000
C	0.38200000	-5.25200000	-6.35800000
C	-0.73200000	-5.57600000	-8.50100000
H	-0.95600000	-3.79500000	-9.60700000
C	1.03600000	-5.77700000	-5.21800000
C	-0.09000000	-6.10900000	-7.37200000
C	0.28300000	-6.17200000	-4.22800000
H	0.03000000	-7.12300000	-7.29700000
C	-0.40800000	-6.61500000	-3.36100000
C	-0.55500000	-8.02500000	-1.50700000
C	0.34100000	-7.51500000	-0.54900000
C	-0.90000000	-9.38600000	-1.42000000
C	0.52600000	-8.19000000	0.67400000
C	-0.82000000	-10.03300000	-0.17800000
H	-1.18200000	-9.91000000	-2.25300000
C	1.30000000	-7.60100000	1.70200000
C	-0.03300000	-9.47200000	0.84000000
C	0.65500000	-6.96500000	2.64100000
H	0.12800000	-10.00500000	1.69900000
C	0.06100000	-6.45800000	3.54500000
C	0.13400000	-5.70400000	5.75100000
C	-0.17300000	-6.35500000	6.96000000
C	1.11800000	-4.69700000	5.78200000
C	0.05700000	-5.68900000	8.17300000
H	-0.53700000	-7.31200000	6.96300000
C	1.44900000	-4.07000000	6.99900000
H	1.60600000	-4.43500000	4.92000000
C	0.94000000	-4.59900000	8.20200000
C	2.31100000	-2.94600000	7.01300000
H	1.21000000	-4.19700000	9.10500000
C	1.75200000	-1.76800000	7.06800000
C	1.25000000	-0.69300000	7.20300000
C	1.56000000	1.53900000	7.80200000
C	1.42100000	2.17500000	9.04900000
C	2.50500000	2.06400000	6.90000000
C	1.77200000	3.52800000	9.16800000
H	1.09200000	1.65800000	9.86800000
C	2.94300000	3.39600000	7.03600000
H	2.88600000	1.47000000	6.15700000
C	2.61000000	4.11000000	8.20400000
C	3.74200000	3.98900000	6.02900000
H	2.97500000	5.05300000	8.36200000
C	3.13700000	4.74300000	5.15300000
C	2.60200000	5.50200000	4.40300000
C	2.86100000	7.23500000	2.86600000
C	3.57100000	6.72600000	1.76300000
C	2.91500000	8.62000000	3.10600000
C	3.99300000	7.60500000	0.72300000
H	3.79000000	5.72700000	1.71100000
C	3.19200000	9.49100000	2.04100000
H	2.77800000	8.99300000	4.04800000
C	4.66900000	7.09200000	-0.40800000
C	3.76500000	8.98800000	0.86300000
C	3.94700000	6.83900000	-1.46600000
H	4.01000000	9.63600000	0.10900000
C	3.29900000	6.67400000	-2.45500000
C	3.30000000	6.39400000	-4.77300000
C	4.05100000	5.22900000	-5.02400000
C	3.18700000	7.33800000	-5.81100000
C	4.30700000	4.82500000	-6.34900000
H	4.42500000	4.68500000	-4.24000000
C	3.34300000	6.91700000	-7.14000000
H	3.01800000	8.32500000	-5.60500000
C	4.89900000	3.56500000	-6.60700000
C	3.99600000	5.70300000	-7.40600000
C	4.09400000	2.58100000	-6.90100000
H	4.24400000	5.46900000	-8.37100000
C	3.37300000	1.69400000	-7.24600000
C	2.59100000	0.75500000	-7.70500000
C	3.20800000	-0.39800000	-8.25400000
C	3.09300000	-0.68300000	-9.62700000
C	3.87300000	-1.33100000	-7.43400000
C	3.19700000	-2.01200000	-10.06500000
H	2.95800000	0.06800000	-10.30800000
C	4.10500000	-2.64200000	-7.89300000
H	4.19900000	-1.04900000	-6.50400000
C	3.74700000	-2.98200000	-9.21300000
C	4.73900000	-3.59200000	-7.05500000
H	3.88000000	-3.93500000	-9.56100000
C	3.95700000	-4.36600000	-6.35100000
C	3.23500000	-5.11400000	-5.76200000
C	2.43200000	-5.96700000	-5.18300000
C	3.01500000	-7.12100000	-4.60100000
C	2.71300000	-8.40300000	-5.09600000
C	3.83400000	-7.02900000	-3.45900000
C	2.79000000	-9.50700000	-4.23500000
H	2.46300000	-8.54000000	-6.07900000
C	4.02500000	-8.15200000	-2.63000000
H	4.30200000	-6.14400000	-3.23800000
C	3.52000000	-9.40200000	-3.04100000
C	4.74800000	-8.03100000	-1.41900000
H	3.68200000	-10.24100000	-2.47800000
C	4.05500000	-7.86400000	-0.32600000
C	3.41400000	-7.78300000	0.67900000
C	2.69600000	-7.76500000	1.77100000
C	3.36300000	-7.99900000	3.00100000
C	4.31800000	-7.09100000	3.50000000
C	3.02200000	-9.10200000	3.80500000
C	4.60300000	-7.04900000	4.87900000
H	4.81700000	-6.47100000	2.85400000
C	3.21100000	-9.02400000	5.19300000
H	2.66000000	-9.96300000	3.38800000
C	5.43900000	-6.03500000	5.40300000
C	4.07600000	-8.05100000	5.71800000
C	4.85100000	-4.98600000	5.91100000
H	4.32000000	-8.08200000	6.71200000
C	4.31100000	-4.05700000	6.43400000
C	3.71200000	-3.08100000	7.06400000
C	4.52000000	-2.22500000	7.85700000
C	5.47600000	-1.37200000	7.27100000
C	4.32800000	-2.14600000	9.24800000
C	5.94200000	-0.24100000	7.97000000
H	5.84400000	-1.58400000	6.33800000
C	4.69300000	-0.97500000	9.92800000
H	3.94600000	-2.93900000	9.77000000
C	6.79100000	0.69400000	7.33000000
C	5.57900000	-0.07200000	9.32000000
C	6.22300000	1.74800000	6.80900000
H	5.95800000	0.70300000	9.87000000
C	5.71000000	2.74400000	6.39700000
C	5.14500000	3.85800000	6.01700000
C	5.99600000	4.94200000	5.68000000
C	5.96800000	6.13400000	6.42600000
C	6.82000000	4.89600000	4.53800000
C	6.31100000	7.34100000	5.80100000
H	5.72400000	6.12500000	7.42000000
C	7.27400000	6.09000000	3.94500000
H	7.10000000	3.99100000	4.14800000
C	7.03100000	7.31600000	4.59600000
C	7.99800000	6.05200000	2.72800000
H	7.37500000	8.19500000	4.20100000
C	7.32200000	6.26300000	1.63300000
C	6.71600000	6.54000000	0.64200000
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C	7.06700000	-5.79000000	-8.02900000
C	7.81800000	-6.70500000	-5.47500000
H	6.67500000	-5.06500000	-4.78200000
C	7.83100000	-6.95900000	-7.89200000
H	6.73600000	-5.51400000	-8.95800000
C	8.40100000	-7.05700000	-4.23000000
C	8.03700000	-7.50100000	-6.61500000
C	7.60600000	-7.35800000	-3.23700000
H	8.32000000	-8.48000000	-6.52300000
C	6.90400000	-7.70800000	-2.33700000
C	6.14800000	-8.16500000	-1.37600000
C	6.79900000	-8.86700000	-0.33400000
C	6.93800000	-10.26700000	-0.38900000
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C	7.56900000	-10.95300000	0.66000000
H	6.58100000	-10.79500000	-1.19000000
C	7.97300000	-8.85800000	1.82600000
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C	7.93200000	-10.26500000	1.82600000
C	8.72700000	-8.16100000	2.80500000
H	8.14700000	-10.79300000	2.67600000
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C	7.87900000	-6.58000000	7.62800000
C	8.10700000	-4.40600000	6.57500000
C	8.79800000	-6.19000000	8.61300000
H	7.40400000	-7.48300000	7.71200000
C	9.05600000	-4.02400000	7.54500000
H	7.76600000	-3.71800000	5.89700000
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C	9.86500000	-2.86800000	7.37700000
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C	9.26500000	-1.70900000	7.28600000
C	8.74600000	-0.63300000	7.26700000
C	8.19200000	0.54700000	7.32300000
C	9.06300000	1.65600000	7.46400000
C	9.51200000	2.36300000	6.33100000
C	9.46600000	2.08500000	8.74400000
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H	9.07900000	1.65200000	9.58700000
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C	10.56100000	4.48300000	4.40000000
H	11.16200000	4.81100000	7.87000000
C	9.99800000	5.12600000	3.56500000
C	9.39700000	5.89700000	2.69600000
C	10.21700000	6.63900000	1.80300000
C	10.99200000	6.00500000	0.81100000
C	10.22500000	8.04600000	1.85300000
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H	11.21200000	5.00800000	0.89600000
C	10.60600000	8.77400000	0.71700000
H	9.97800000	8.54200000	2.71300000
C	12.09500000	6.08000000	-1.38400000
C	11.35500000	8.14100000	-0.28600000
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C	9.93200000	5.31000000	-4.40800000
C	10.62000000	5.04600000	-5.61700000
C	10.55200000	5.94400000	-6.69700000
C	11.27700000	3.81900000	-5.82600000
C	10.58200000	5.44000000	-8.00600000
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C	11.04700000	4.13500000	-8.23600000
C	12.07900000	2.08400000	-7.37100000
H	11.07800000	3.77500000	-9.19400000
C	11.33600000	1.01800000	-7.44300000
C	10.63600000	0.05700000	-7.55000000
C	9.85200000	-0.97500000	-7.72400000
C	10.48600000	-2.22800000	-7.90400000
C	11.00600000	-2.61200000	-9.15300000
C	10.64700000	-3.11100000	-6.82000000
C	12.01700000	-3.58400000	-9.20400000
H	10.64400000	-2.20600000	-10.02000000
C	11.70300000	-4.04200000	-6.83300000
H	9.98600000	-3.09500000	-6.03800000
C	12.24300000	-4.40100000	-8.08500000
C	12.24500000	-4.59200000	-5.56500000
H	12.77800000	-5.26600000	-8.19300000
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C	10.60900000	-6.27800000	-4.54200000
C	9.79200000	-7.17400000	-4.06100000
C	10.36800000	-8.27200000	-3.38000000
C	10.68500000	-8.16900000	-2.01200000
C	10.61500000	-9.50500000	-4.04800000
C	11.51600000	-9.13200000	-1.40700000
H	10.29000000	-7.41100000	-1.44800000
C	11.26500000	-10.54800000	-3.36900000
H	10.33200000	-9.63800000	-5.02300000
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C	11.57800000	-10.40300000	-2.00900000
C	11.56100000	-8.59300000	0.88700000
H	11.82300000	-11.22800000	-1.45600000
C	10.87600000	-8.43400000	1.85300000
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C	10.78400000	-8.28600000	4.16300000
C	11.23600000	-7.07400000	4.71800000
C	11.01300000	-9.47500000	4.88000000
C	12.27500000	-7.08700000	5.66800000
H	10.79300000	-6.18900000	4.45400000
C	11.97100000	-9.48800000	5.90600000
H	10.47900000	-10.32300000	4.67300000
C	13.17300000	-5.91500000	5.83200000
C	12.45800000	-8.27100000	6.40900000
C	12.50400000	-4.84500000	6.36000000
H	12.91900000	-8.24800000	7.32200000
C	11.91300000	-3.92100000	6.83300000
C	11.27200000	-2.92400000	7.38000000
C	12.06200000	-1.91500000	7.98100000
C	12.46000000	-1.99600000	9.32800000
C	12.48500000	-0.80400000	7.22700000
C	13.54400000	-1.22200000	9.77300000
H	11.95900000	-2.59700000	9.98700000
C	13.64200000	-0.10100000	7.61600000
H	11.94100000	-0.49100000	6.41900000
C	14.00700000	-0.16300000	8.97500000
C	14.46800000	0.61900000	6.61500000
H	14.58600000	0.56900000	9.39300000
C	13.81000000	1.70900000	6.11400000
C	13.23300000	2.66700000	5.69200000
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H	4.30900000	-0.77700000	10.85500000
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H	-6.16300000	-7.24100000	7.32800000
H	-15.72900000	-6.04200000	6.48100000

Table S3. Cartersian coordinates of molecular model for ONT (**6**)

11. Other TEM Images

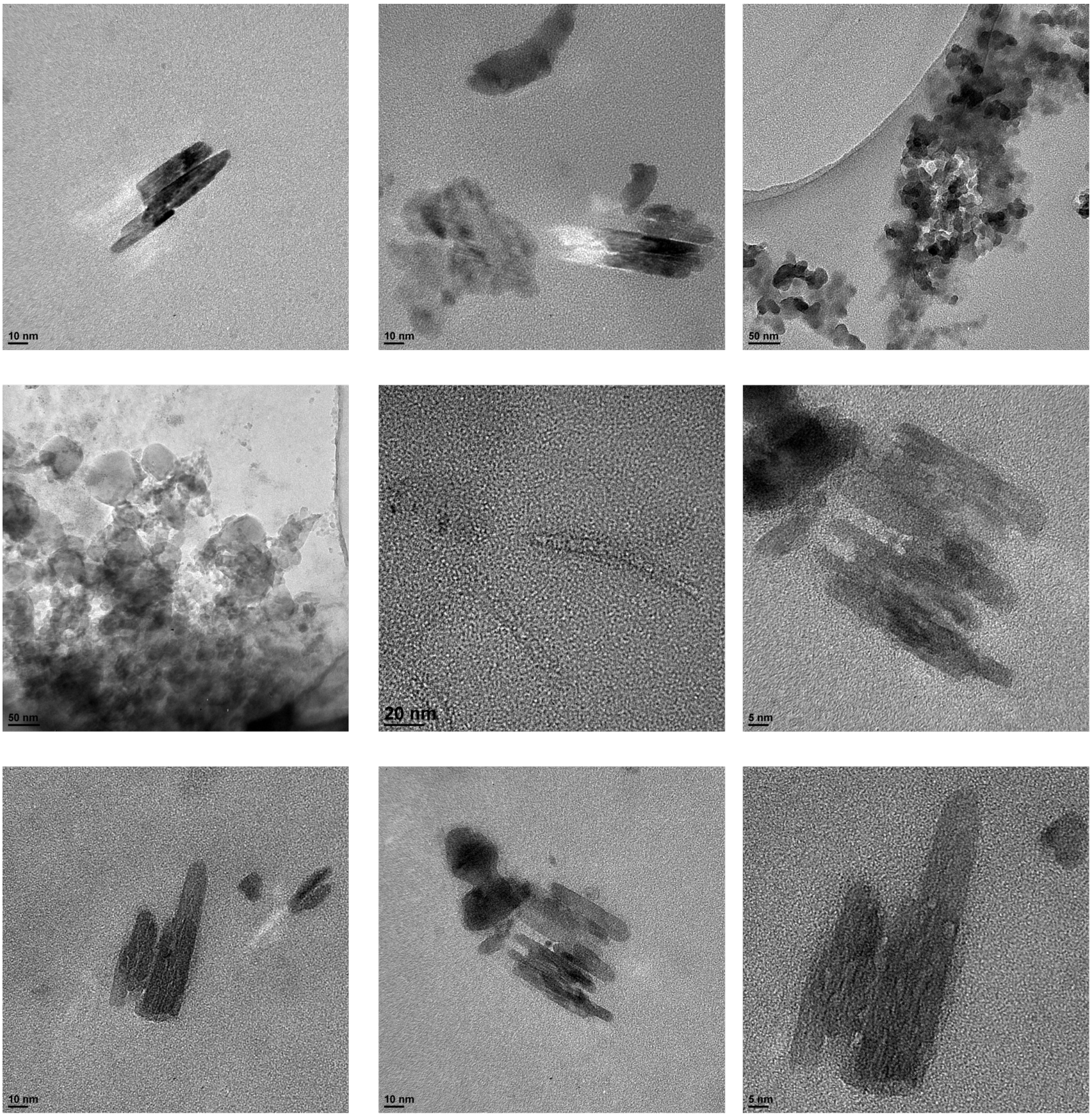

Figure S31.

12. References

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13. ^{1}H and ^{13}C NMR Spectra of Synthesized Compounds

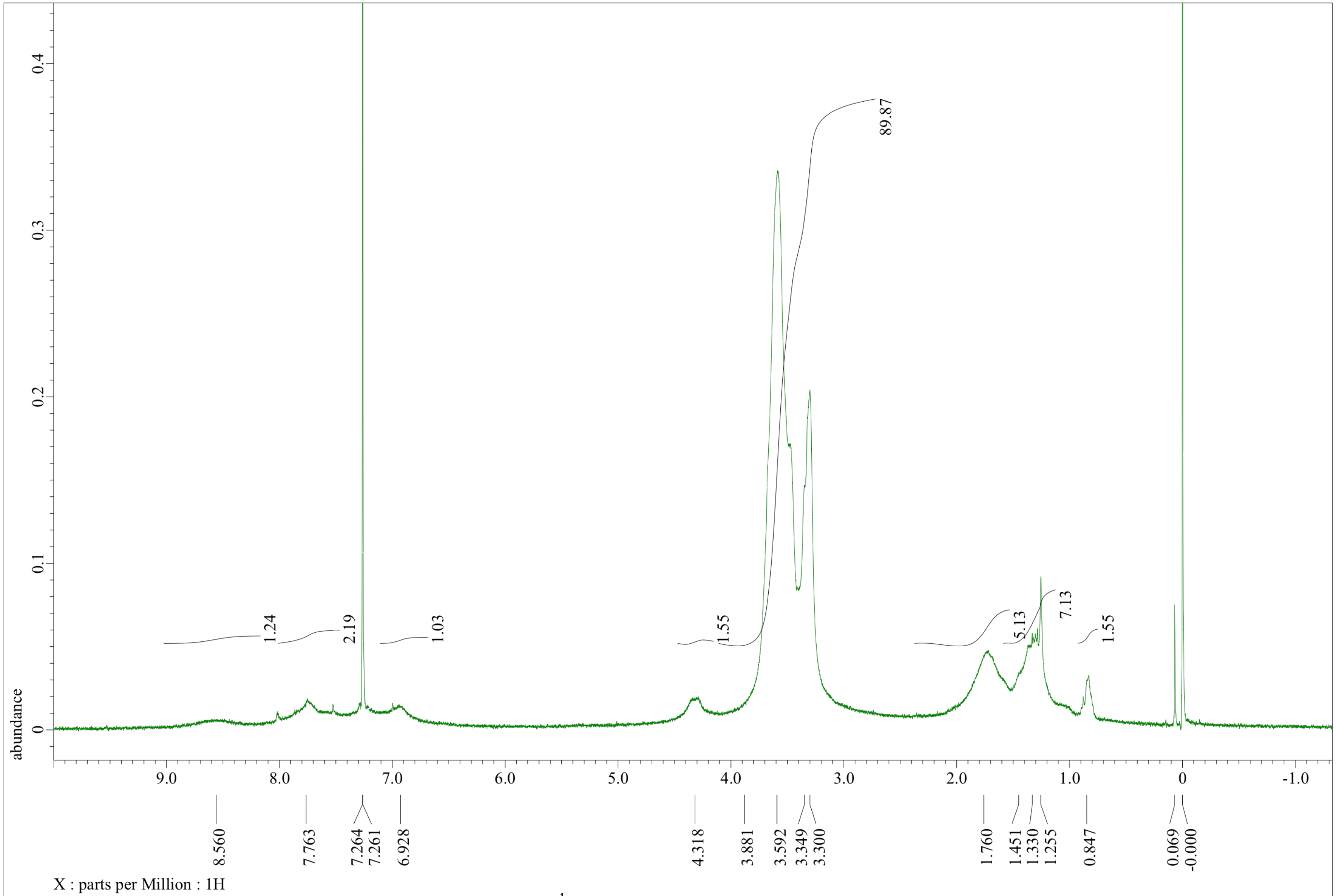

Figure S32. ^{1}H NMR of poly-PDE **1** in $CDCl_3$

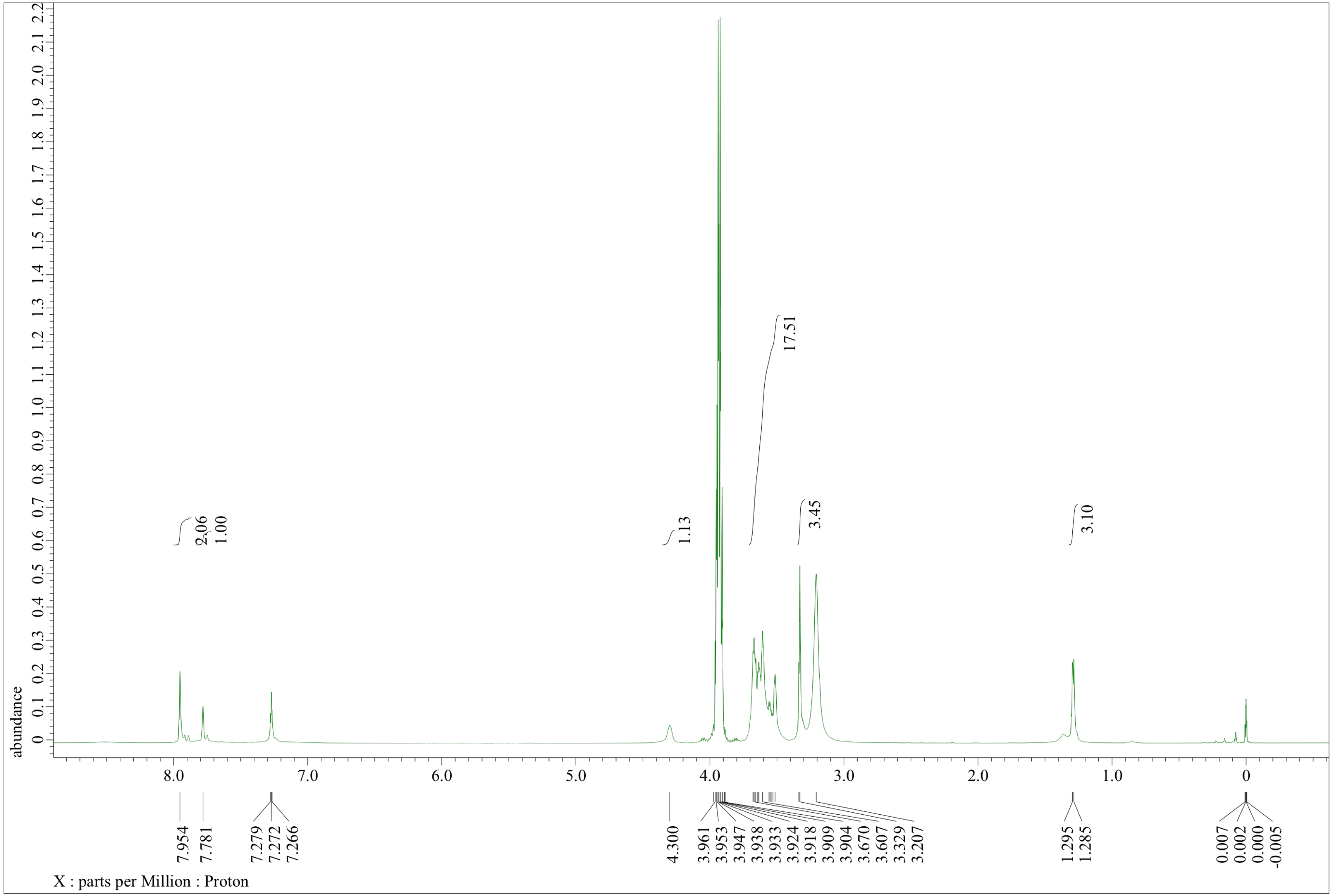

Figure S33. ^{1}H NMR of poly-PDE **1** in 5 vol% TFE/$CDCl_3$

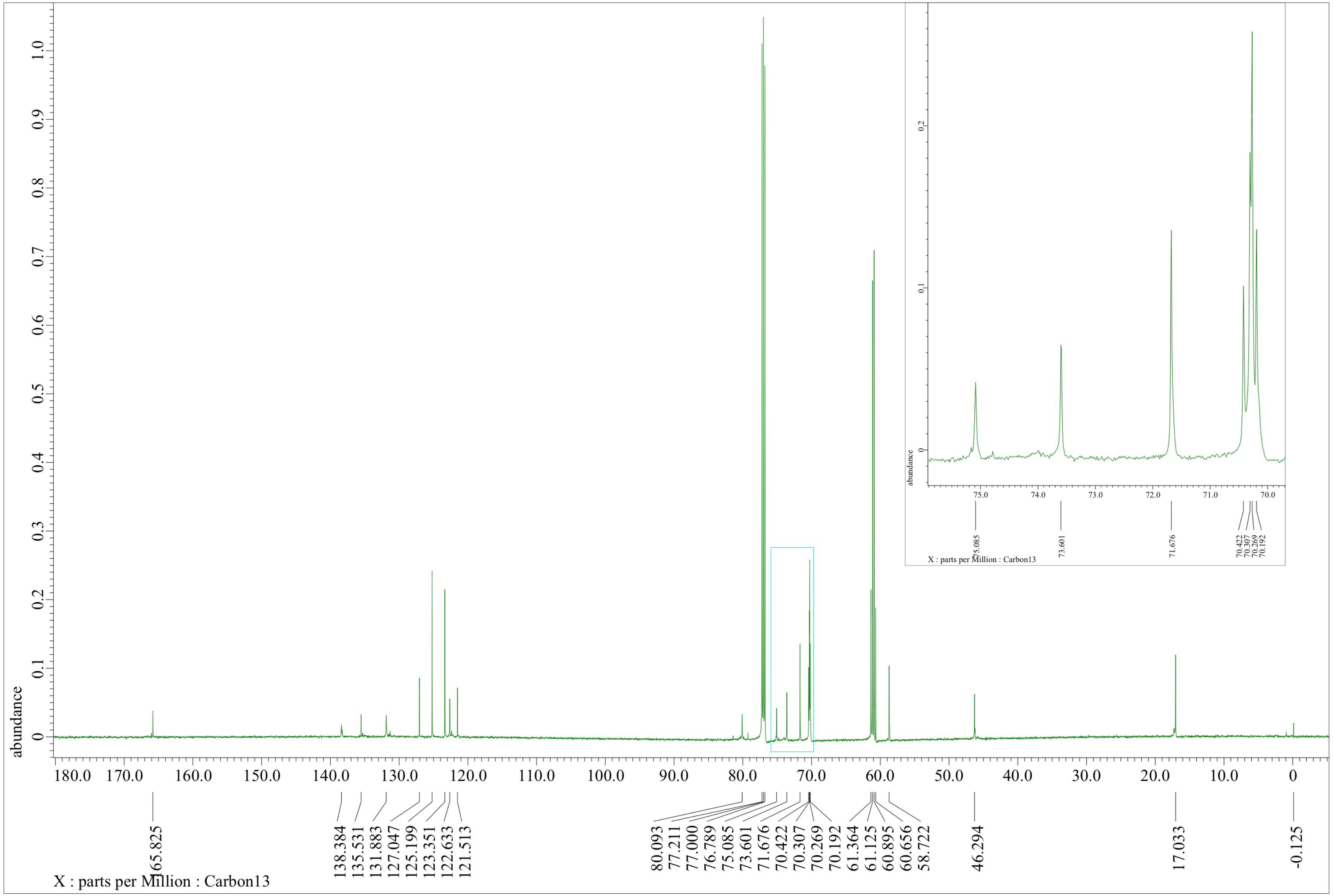

Figure S34. ^{13}C NMR of poly-PDE **1** in 5 vol% TFE/$CDCl_3$

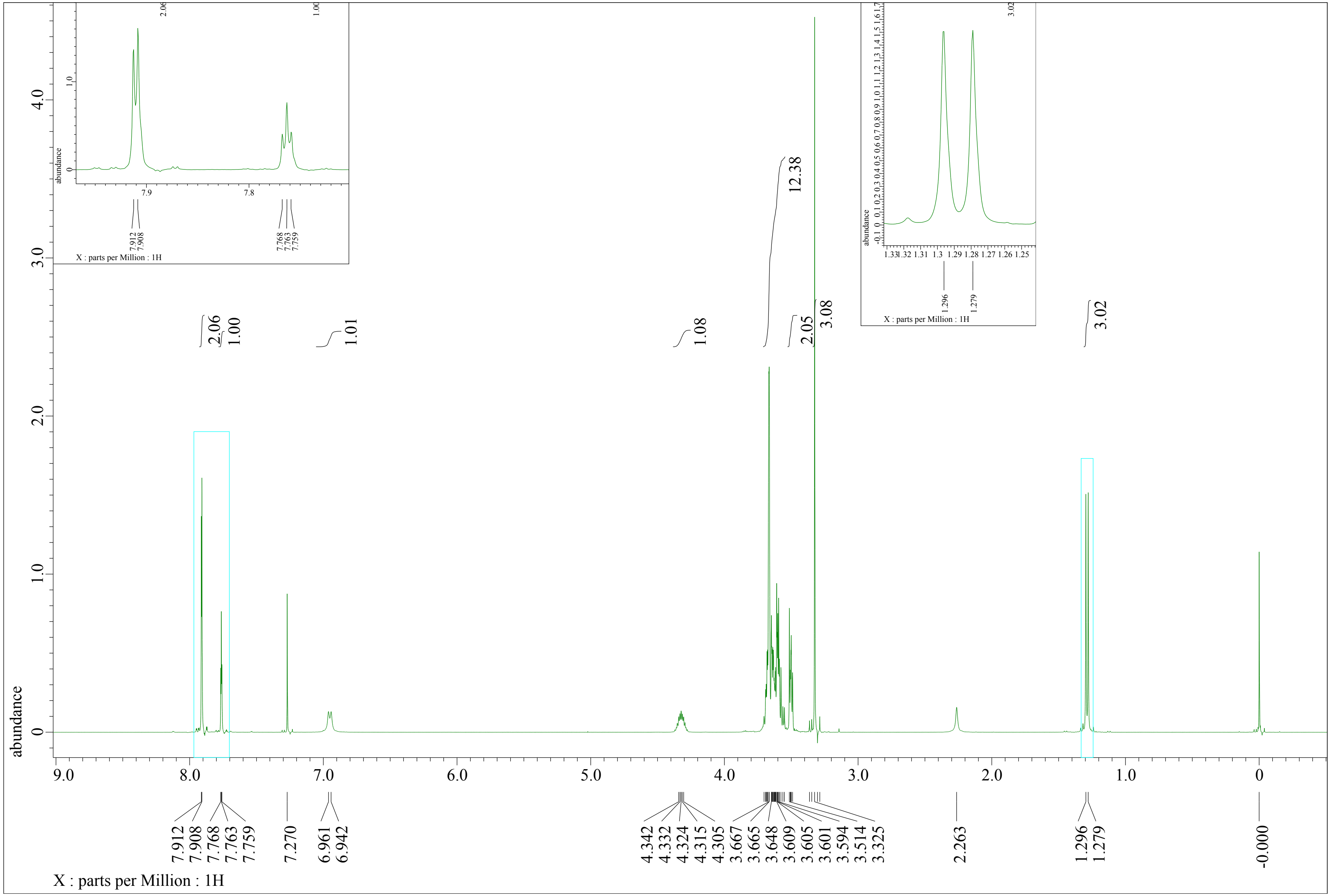

Figure S35. ^{1}H NMR of **3** in $CDCl_3$

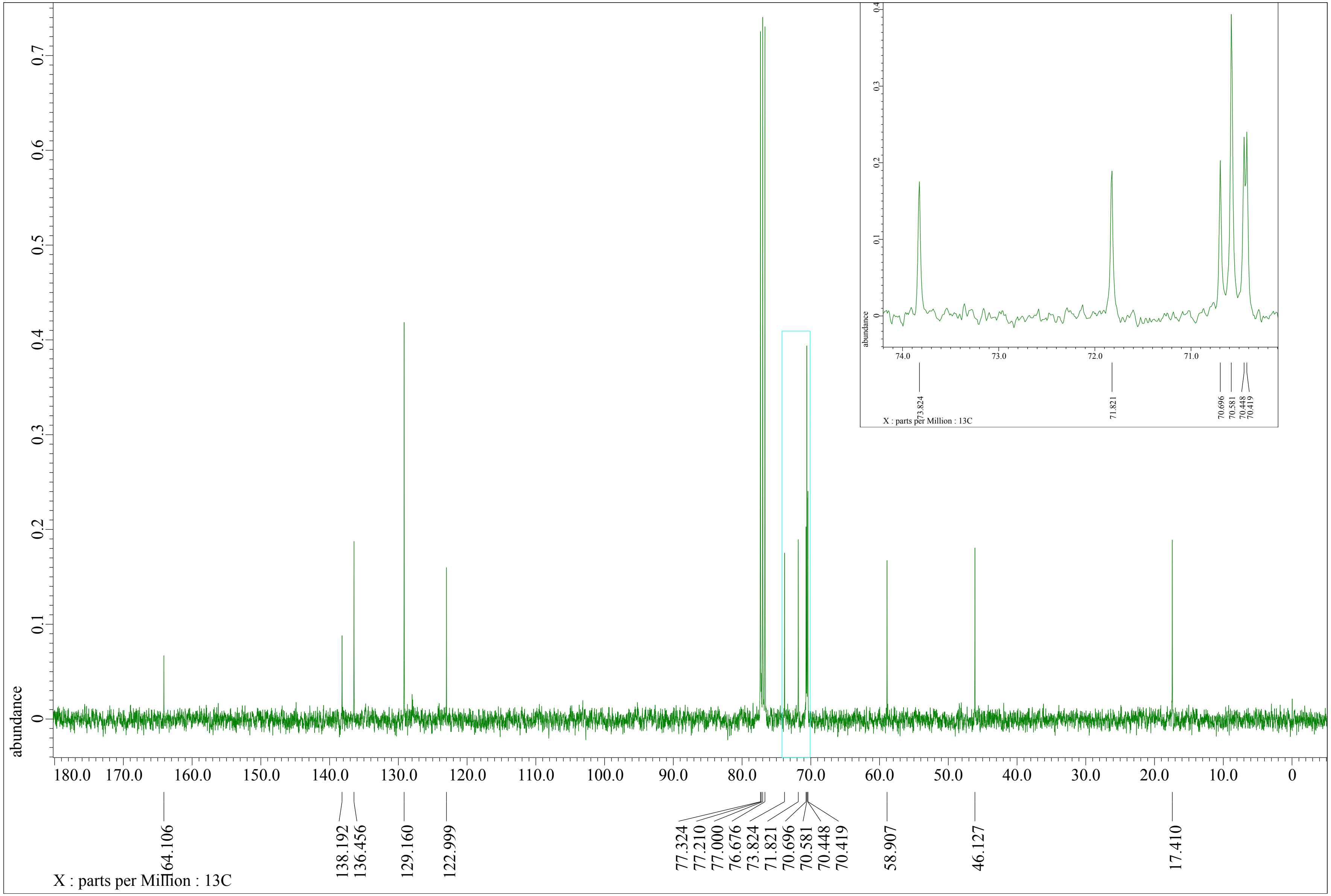

Figure S36. ^{13}C NMR of **3** in $CDCl_3$

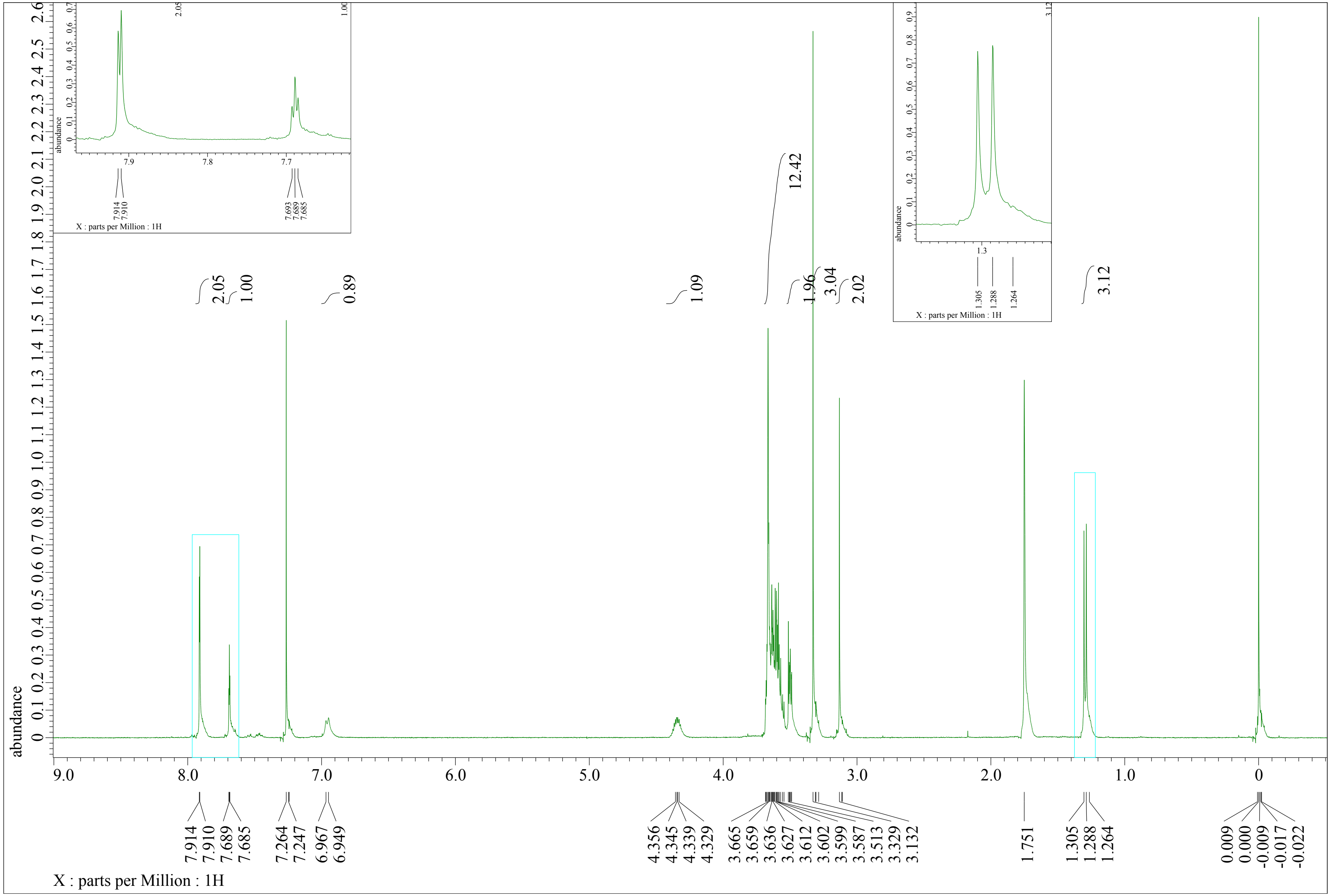

Figure S37. ^{1}H NMR of **4** in $CDCl_3$

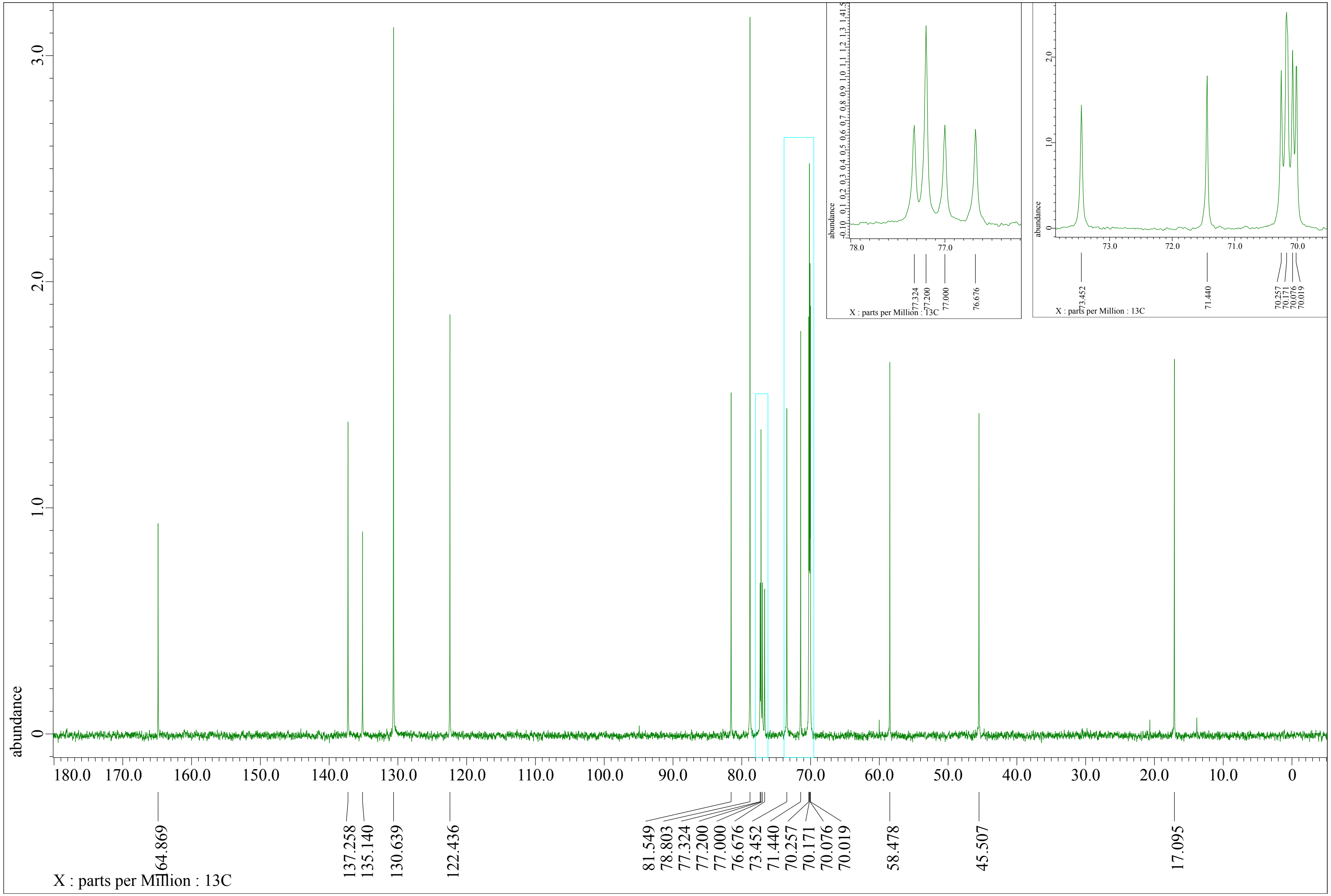

Figure S38. ^{13}C NMR of **4** in $CDCl_3$

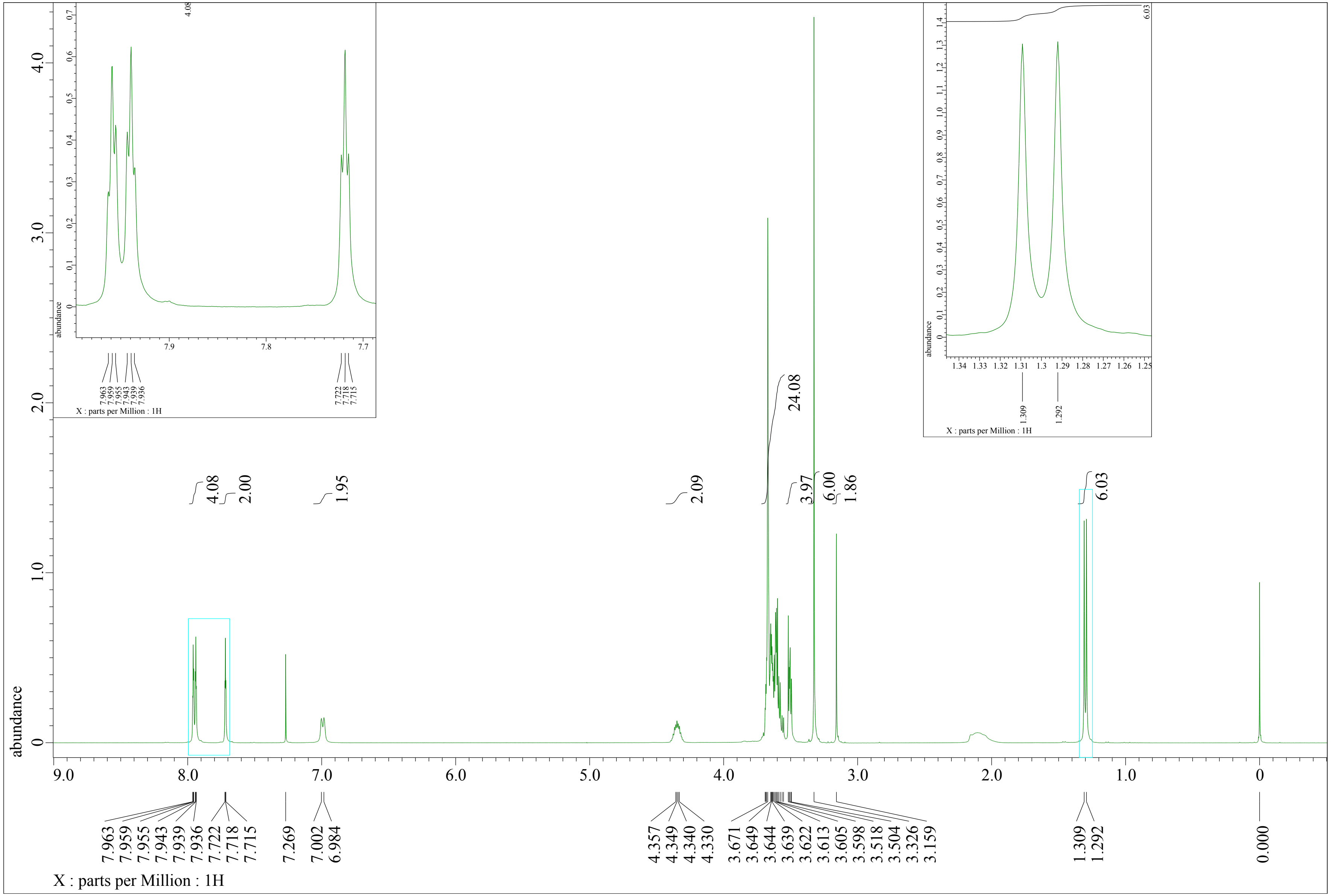

Figure S39. ^{1}H NMR of **5** in $CDCl_3$

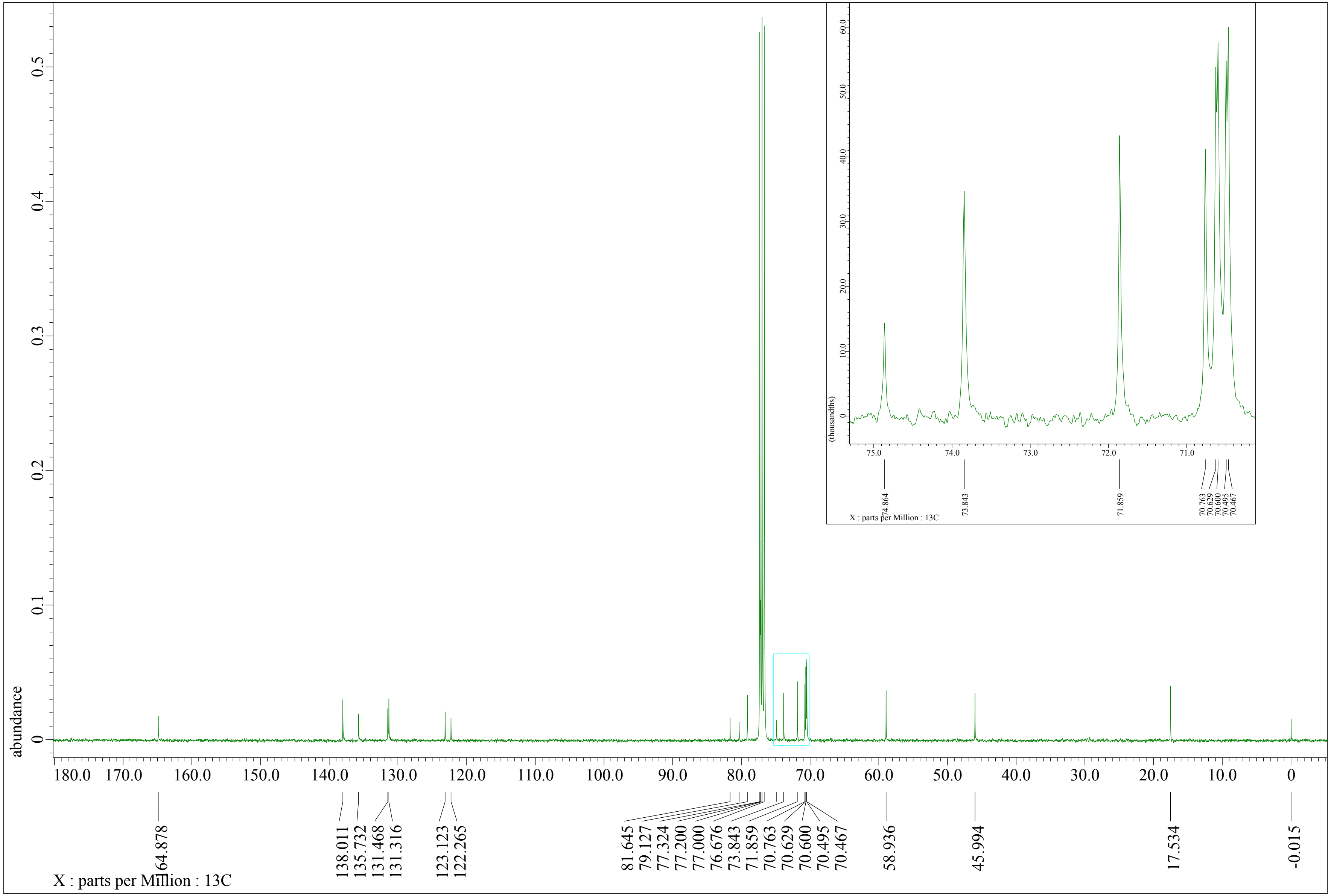

Figure S40. ^{13}C NMR of **5** in $CDCl_3$

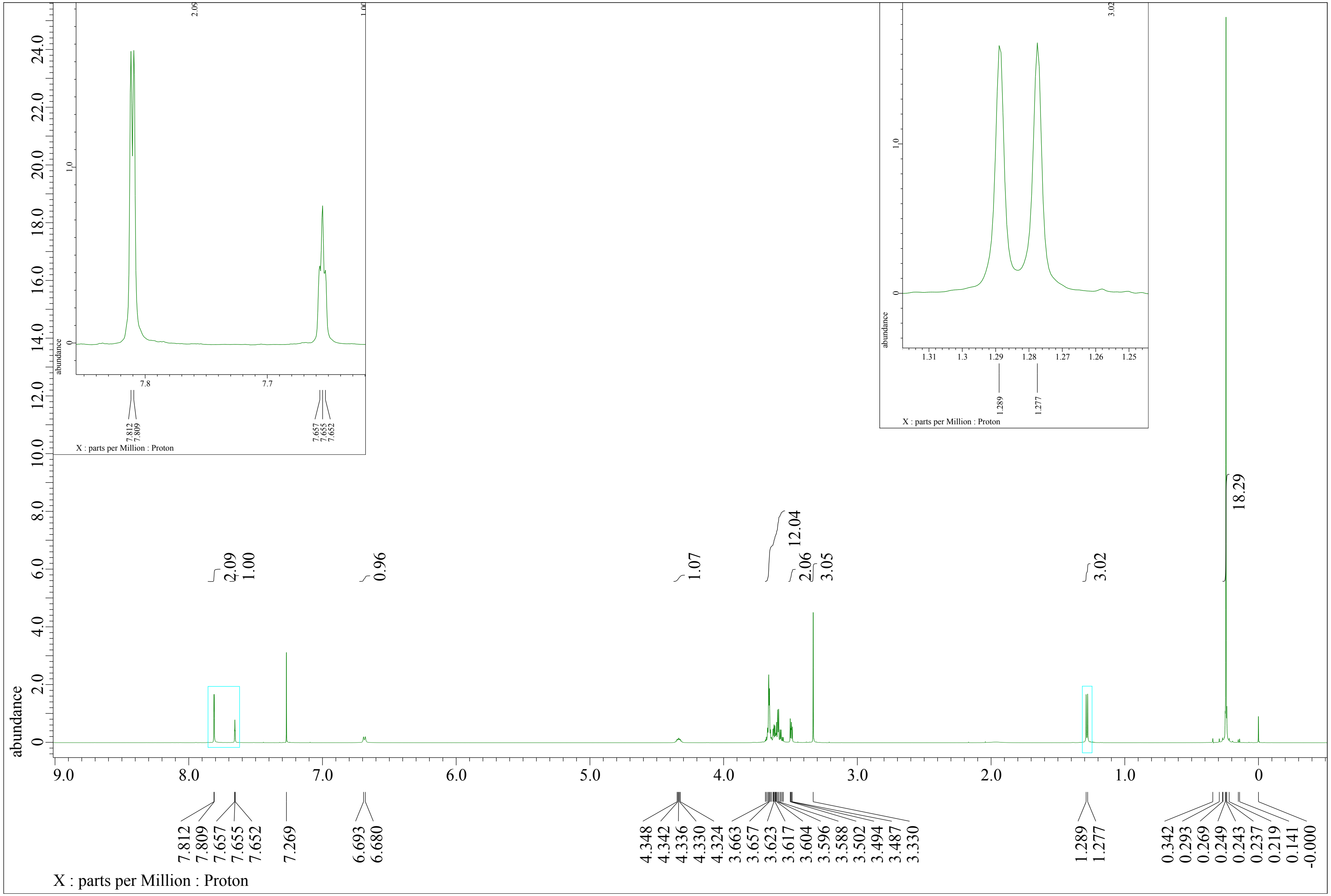

Figure S41. ^{13}C NMR of **7** in $CDCl_3$

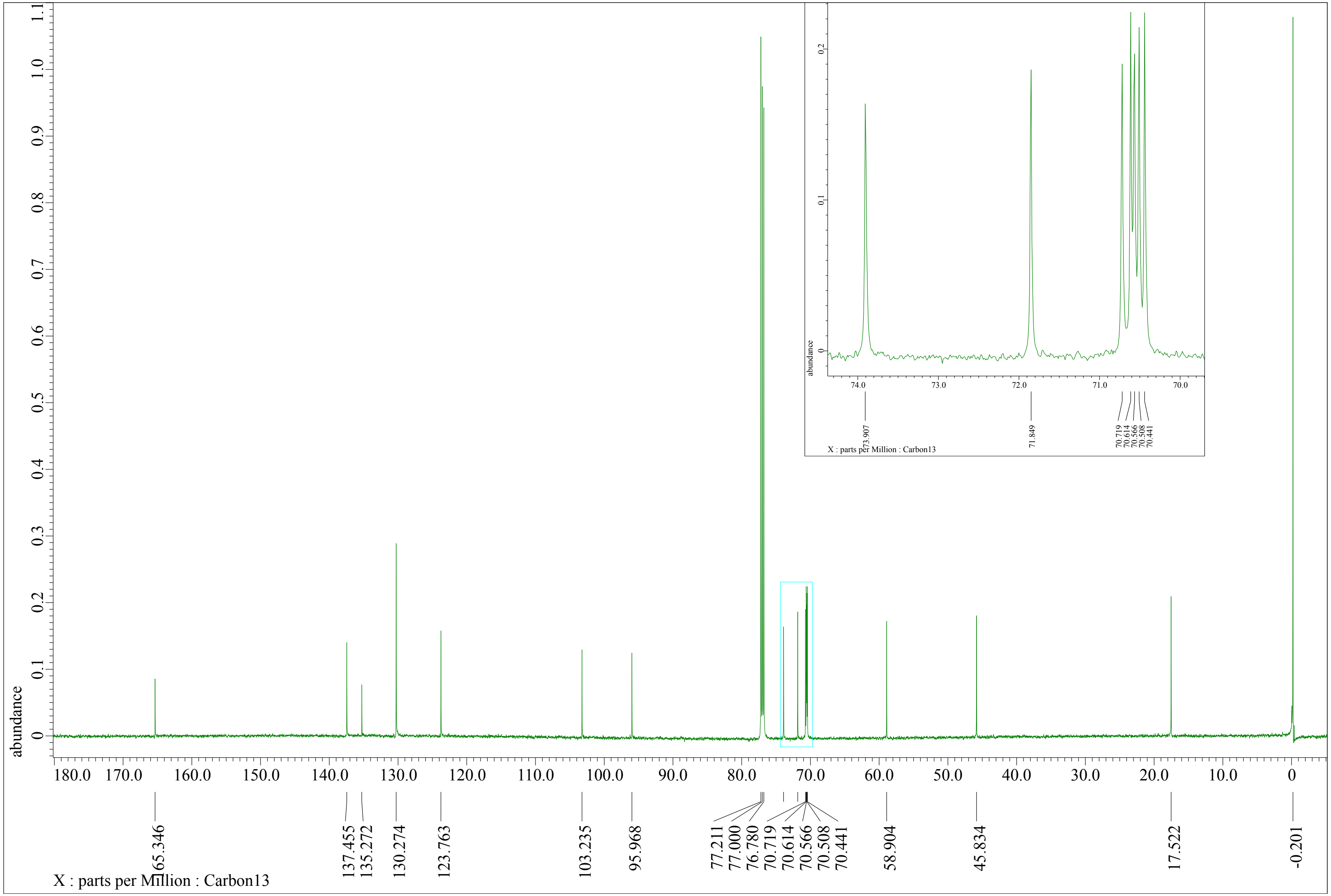

Figure S42. ^{13}C NMR of **7** in $CDCl_3$

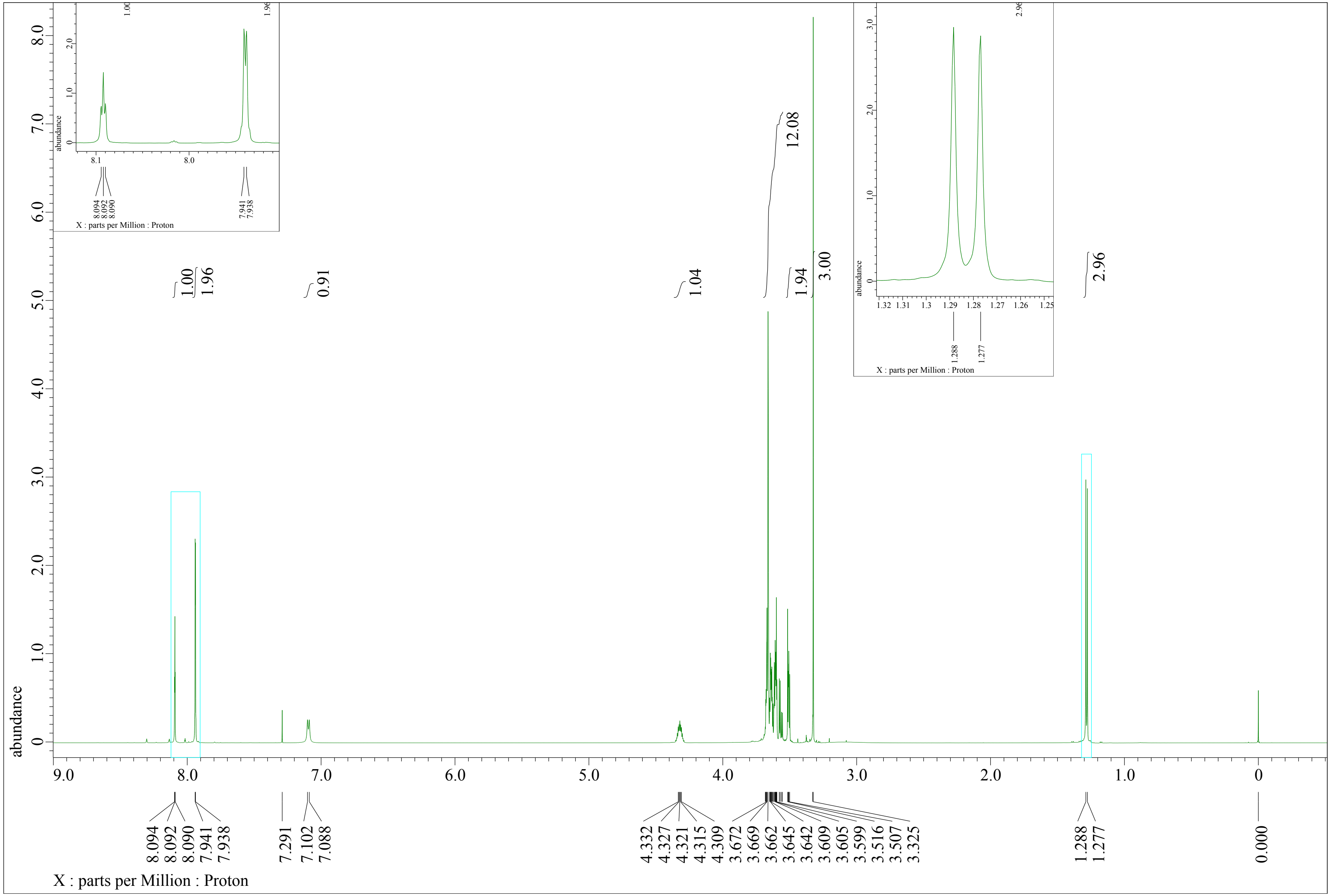

Figure S43. ^{1}H NMR of **8** in $CDCl_3$

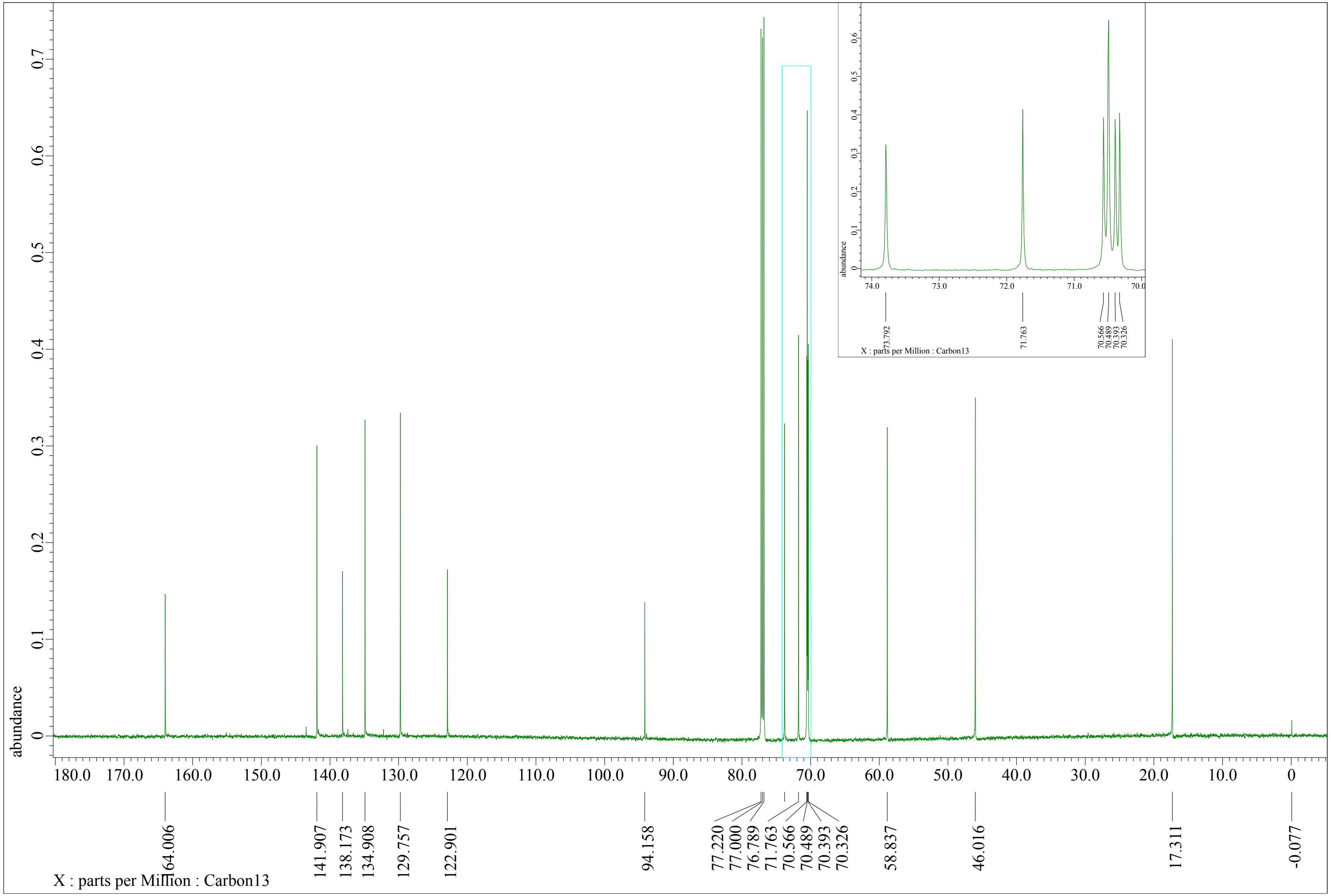

Figure S44. ^{13}C NMR of **8** in $CDCl_3$

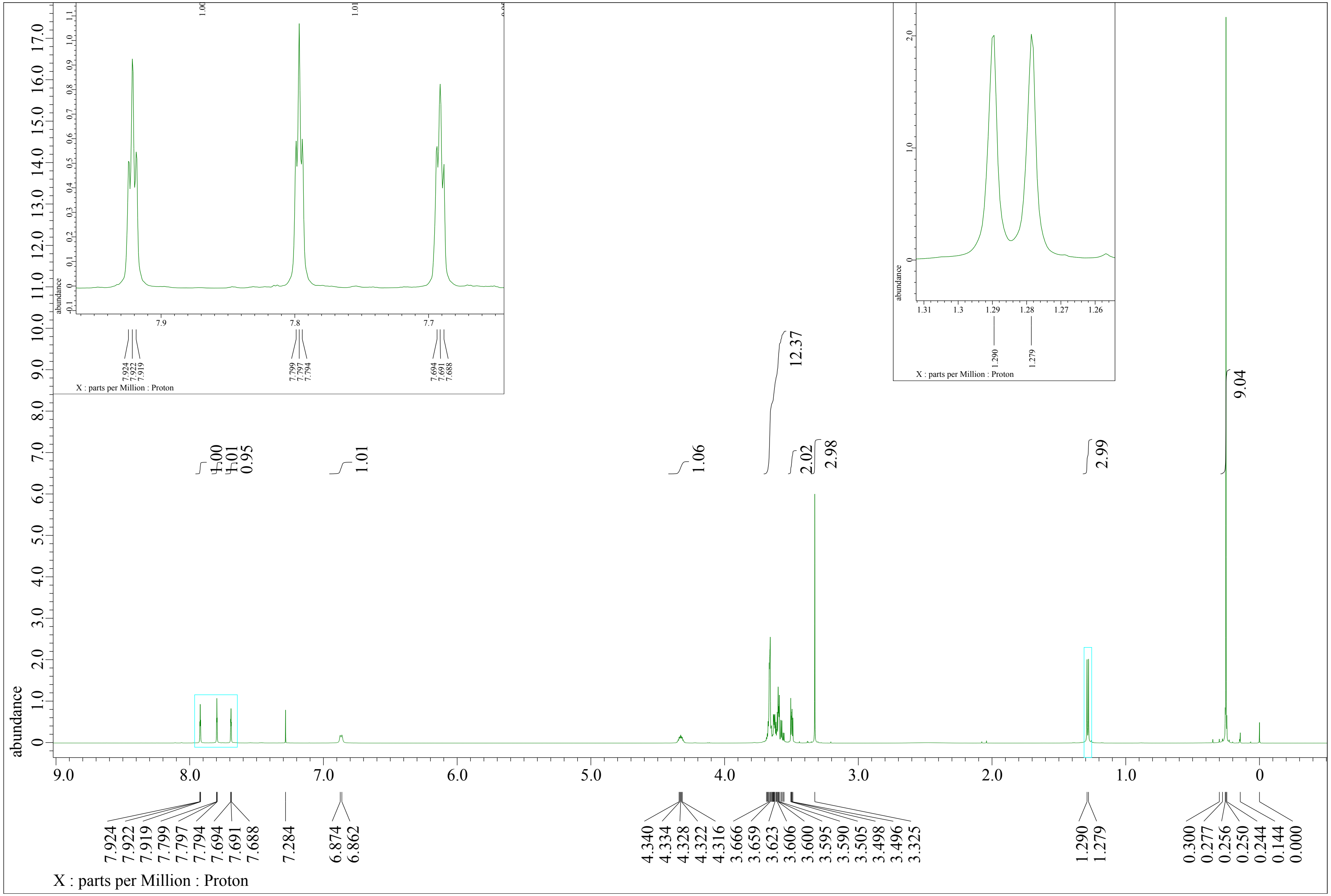

Figure S45. ^{1}H NMR of **9** in $CDCl_3$

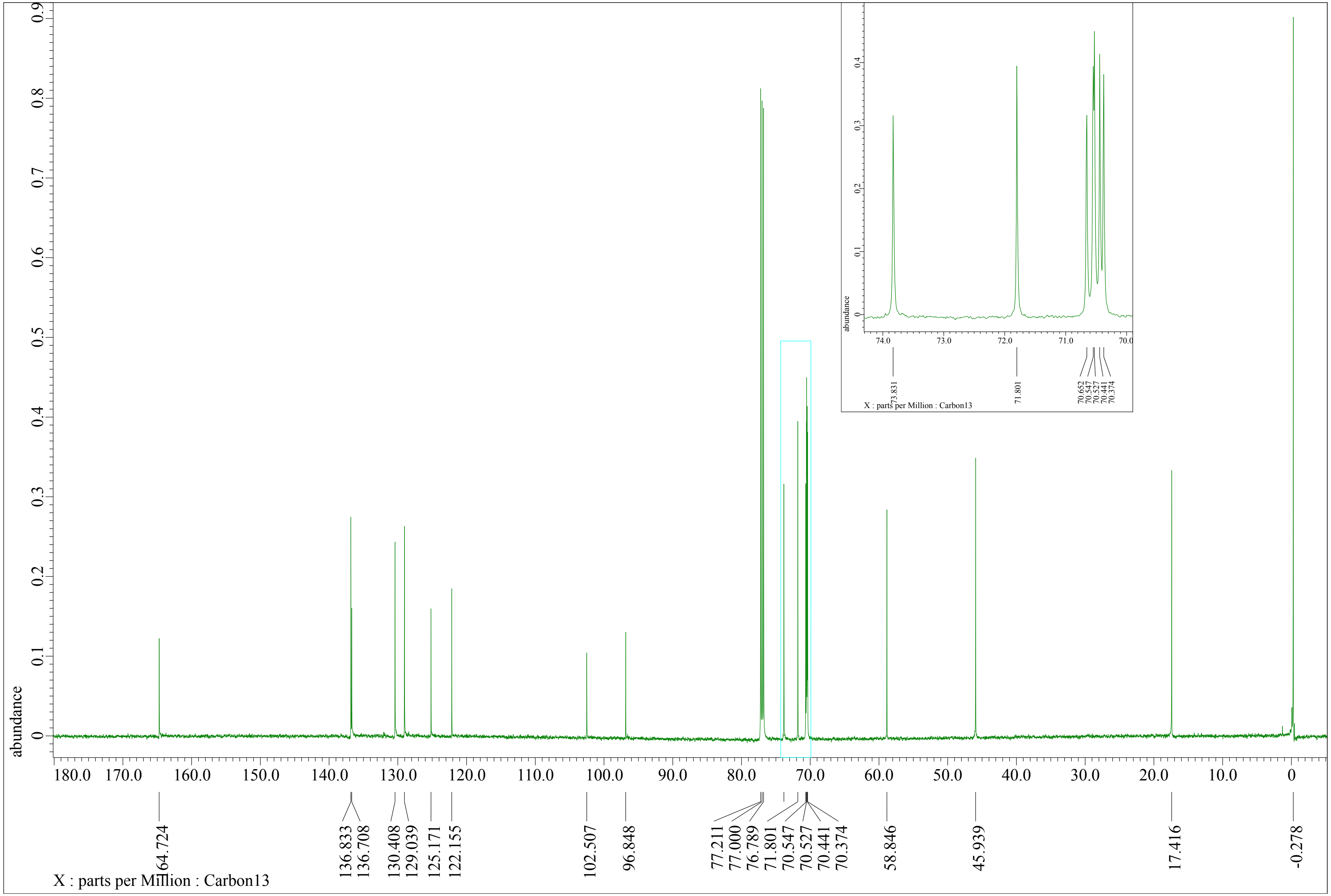

Figure S46. ^{13}C NMR of **9** in $CDCl_3$

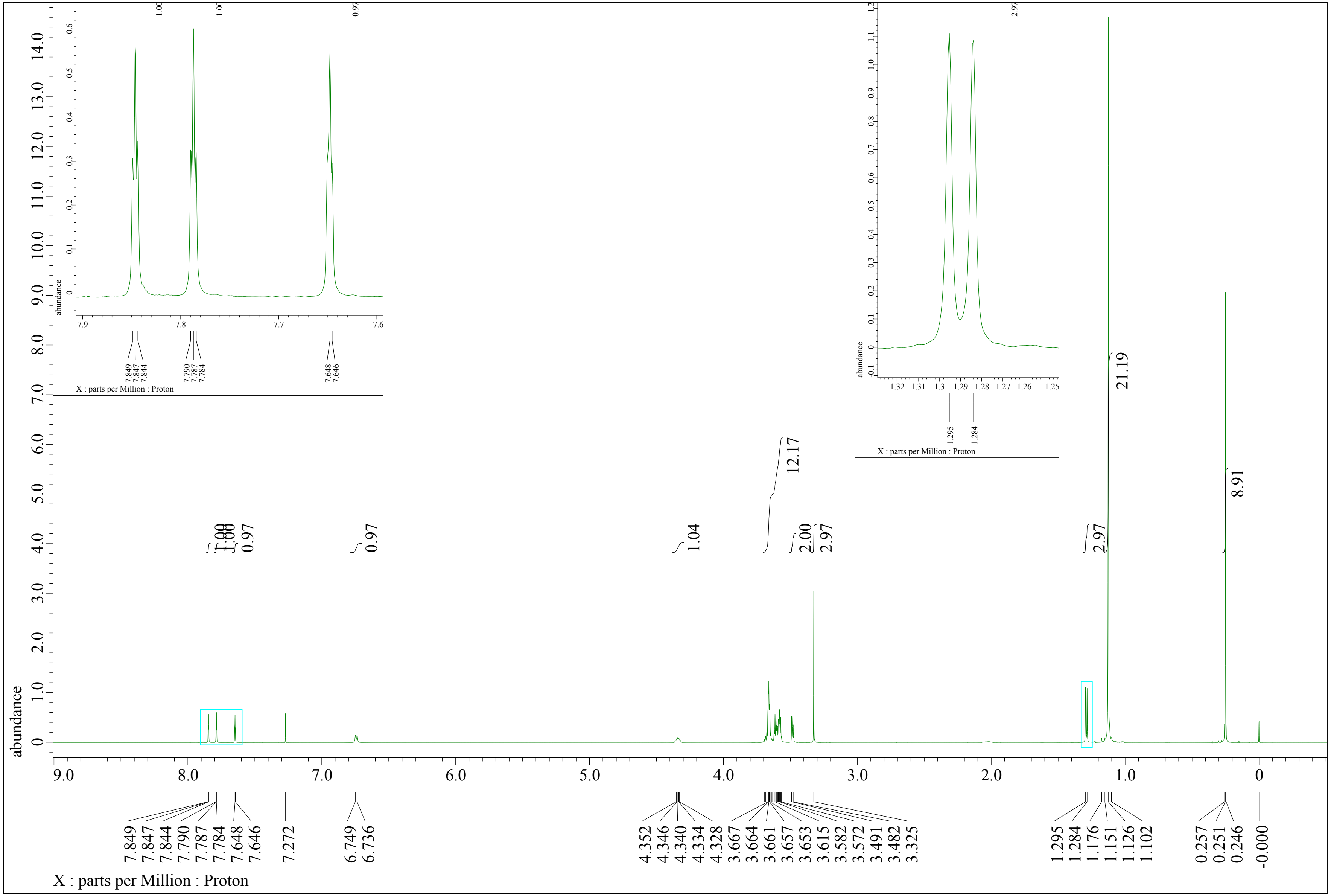

Figure S47. ^{1}H NMR of **10** in $CDCl_3$

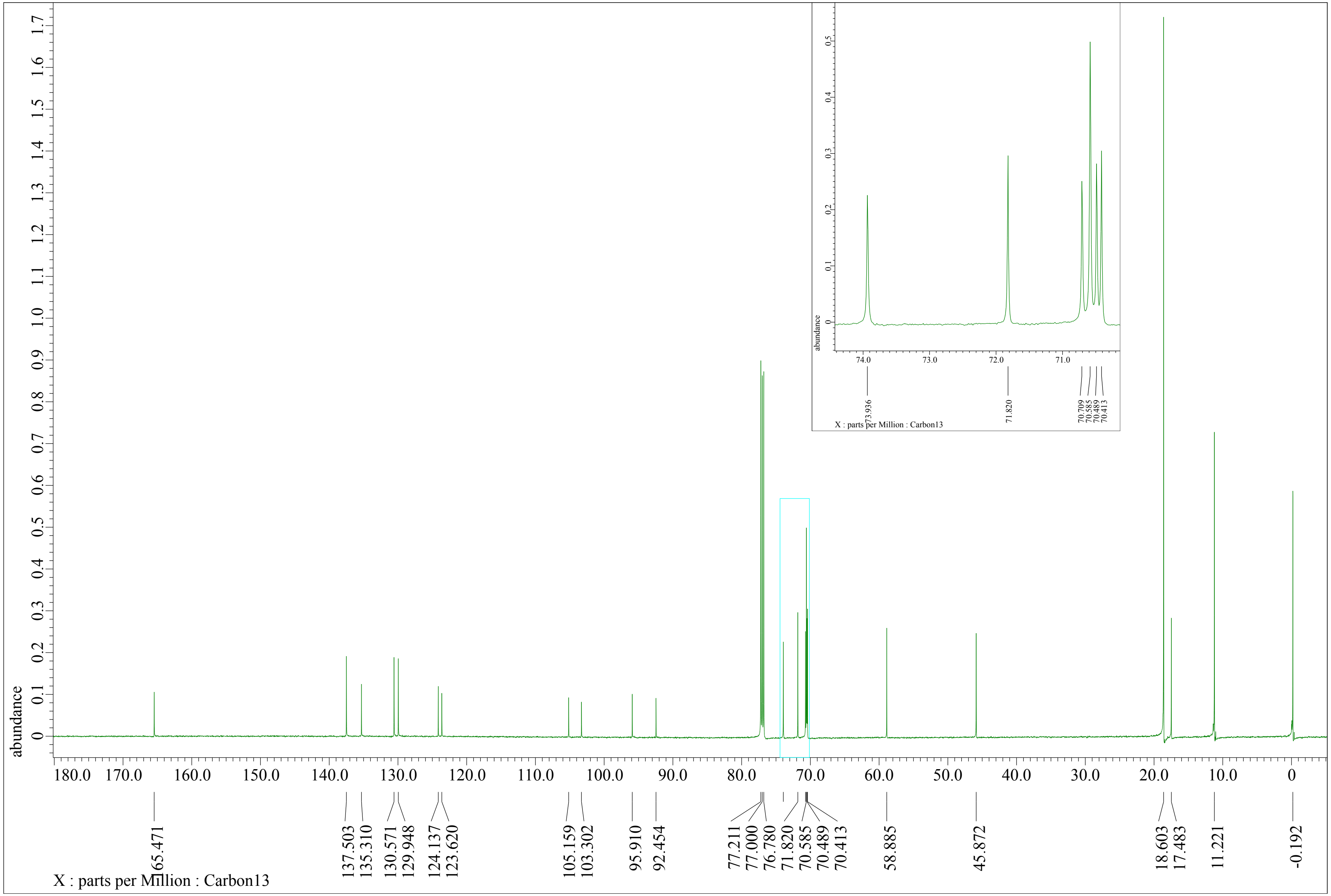

Figure S48. ^{13}C NMR of **10** in $CDCl_3$

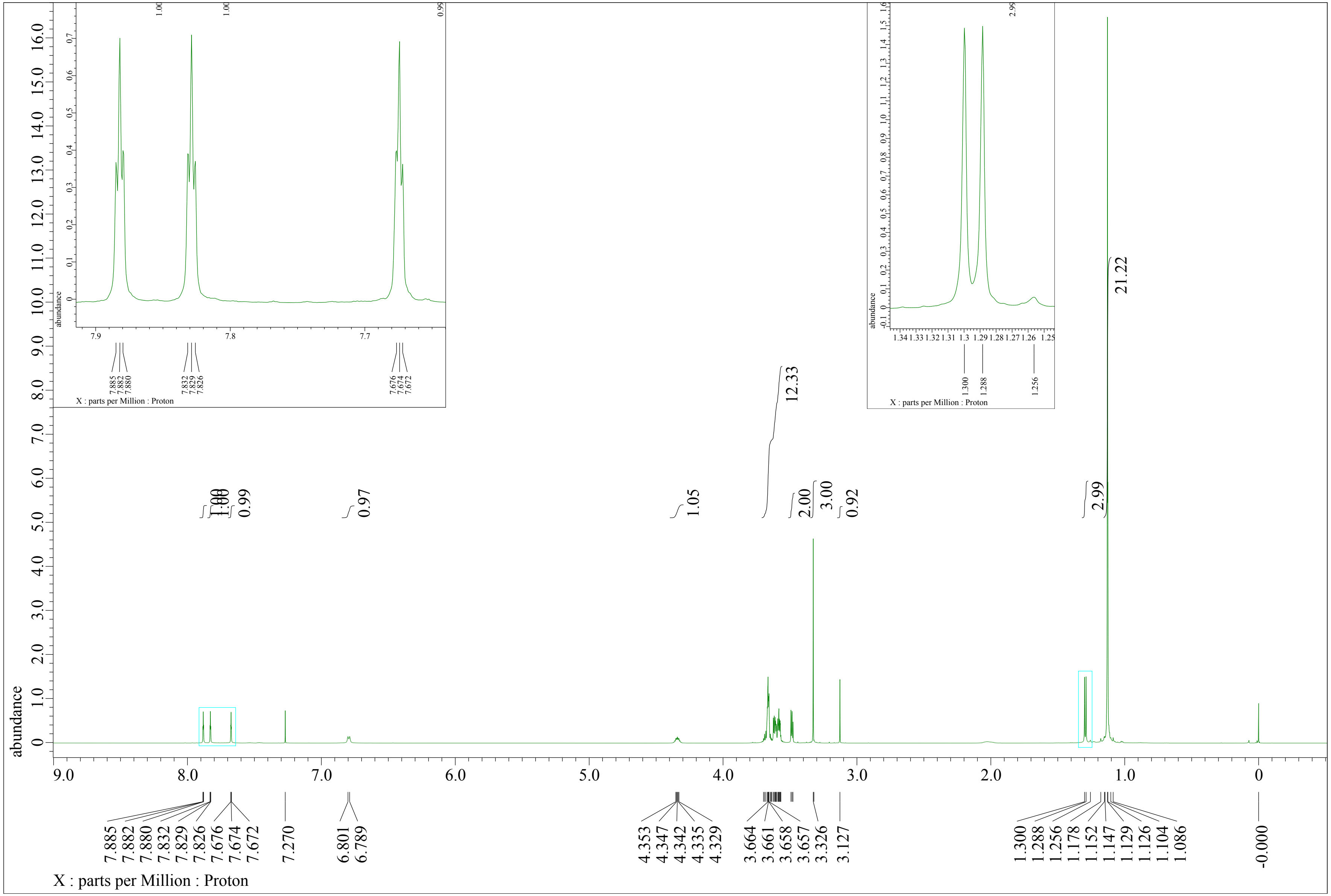

Figure S49. ^{1}H NMR of **11** in $CDCl_3$

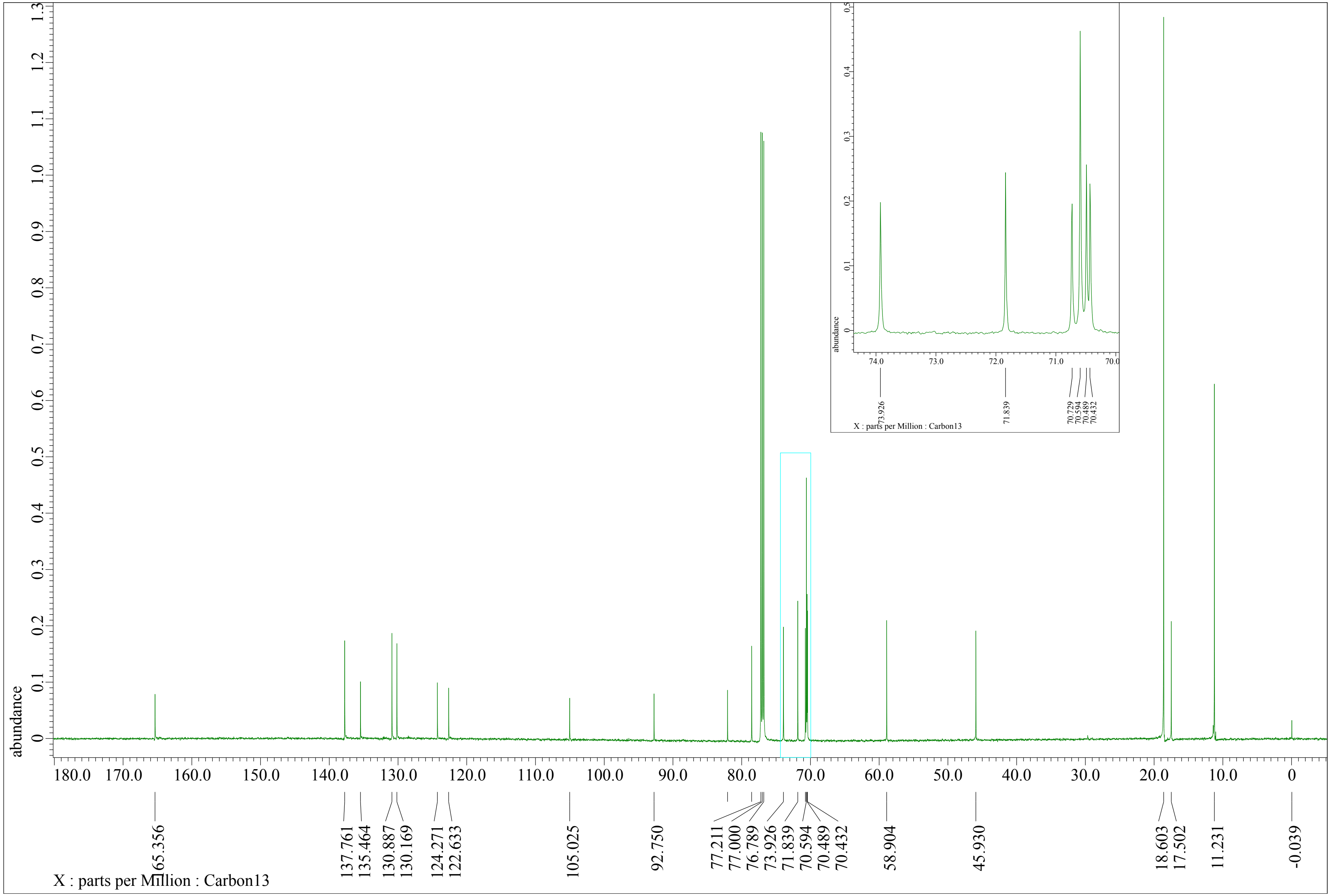

Figure S50. ^{13}C NMR of **11** in $CDCl_3$

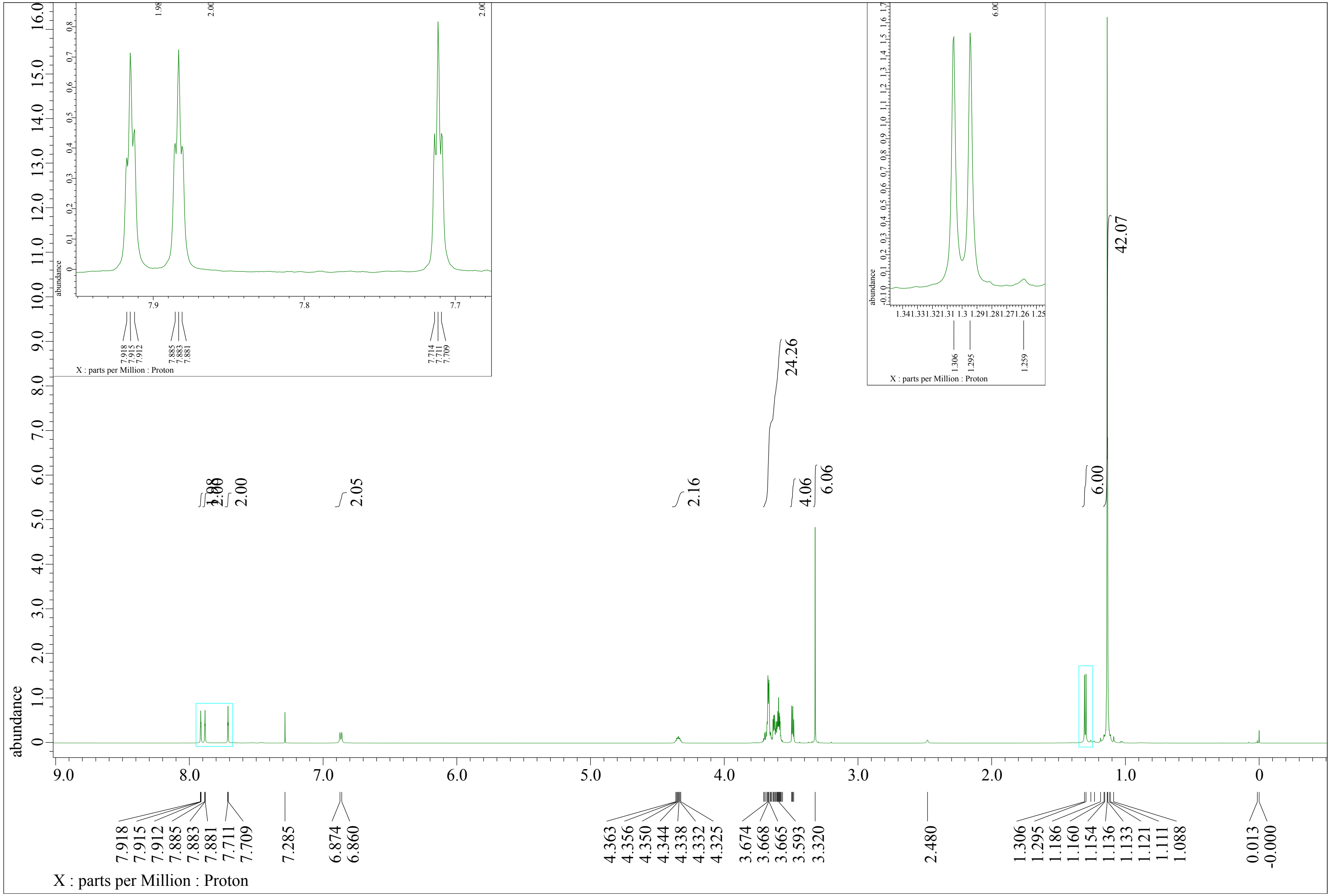

Figure S51. ^{1}H NMR of **12** in $CDCl_3$

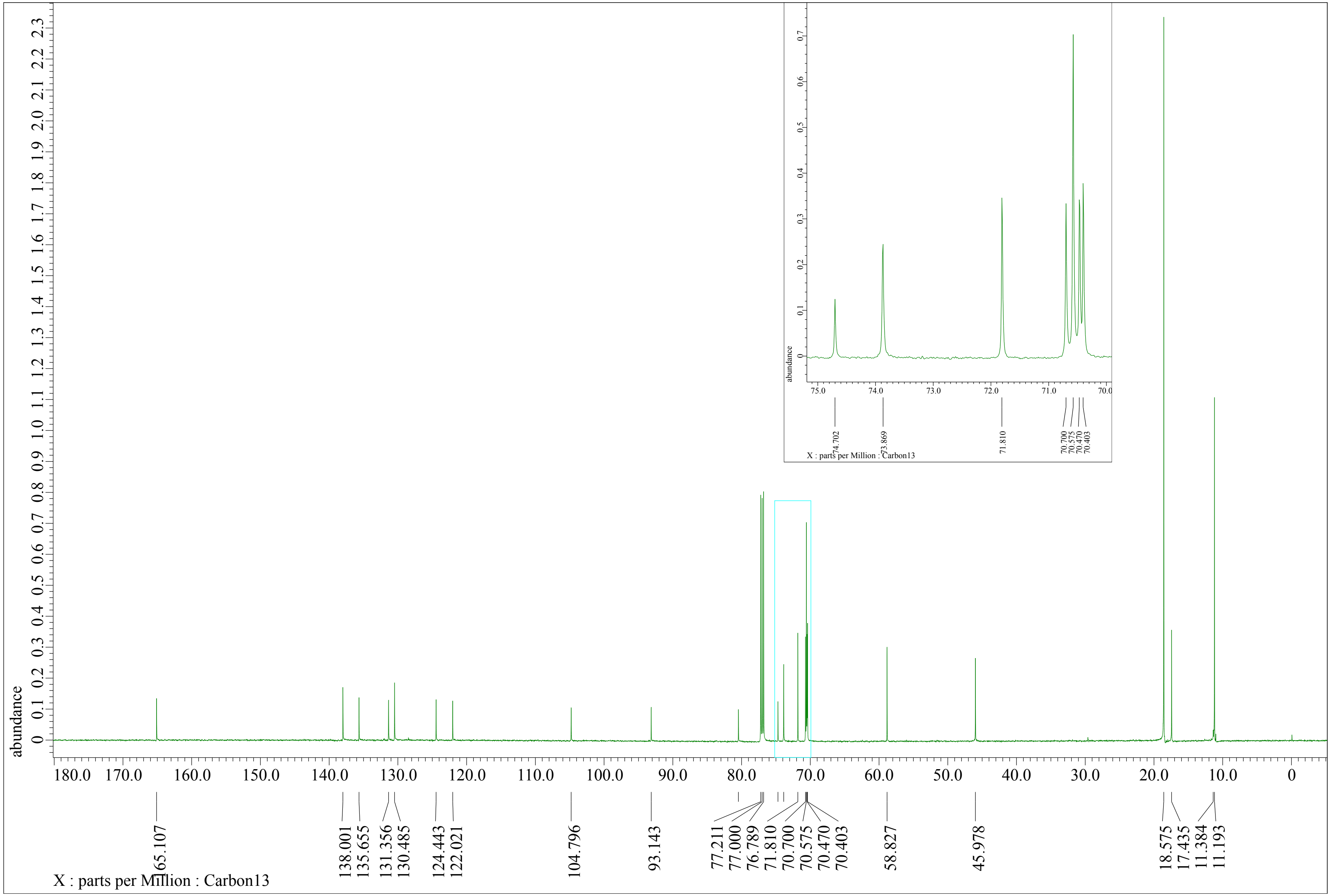

Figure S52. ^{13}C NMR of **12** in $CDCl_3$