Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Synthesis of 3,7-diiodo-2,6-di(thiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difurans: functional building blocks for the design of new conjugated polymers.

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General Methods

All reactions were carried out at ambient atmosphere and temperature (18-25 °C) unless otherwise noted. Tetrahydrofuran and toluene were dried using an Innovative Technologies solvent purification system. Solvents used for Pd-catalyzed reactions were deoxygentated prior to use by bubbling a stream of argon through the stirred solvent for 30-60 minutes. Trimethylsilyl acetylene was purchased from GFS chemicals. Bis(triphenylphosphine)palladium(II) dichloride was purchased from Oakwood Products, Inc. All other chemicals were purchased from Sigma-Aldrich and used without further purification. 3-Decylthiophene[1], 2,5-diido-1,4-dimethoxybenzene[2] and 6,6'-dibromo-*N*,*N*'-(2-octyldodecanyl)isoindigo **6**[3, 4] were synthesized according to literature procedures. Nuclear magnetic resonance (NMR) spectra were carried out in $CDCl_3$ and recorded at either 400 MHz or 300 MHz (^{1}H NMR) and 150 MHz, 100 MHz or 75 MHz (^{13}C NMR) as noted. ^{1}H NMR spectra were internally referenced to the residual protonated solvent peak, and the ^{13}C NMR are referenced to the central carbon peak of the solvent. In all spectra, chemical shifts are given in δ relative to the solvent and coupling constants are reported in hertz (Hz). High-resolution mass spectra (HRMS) were recorded on a double-focusing magnetic sector mass spectrometer using ESI or APCI, as noted, at 70 eV. Melting points were obtained using a MELTEMP melting point apparatus with an upper temperature limit of 260 °C. Gel permeation chromatography (GPC) measurements were performed on a separation module equipped with three 5 μm I-gel columns connected in series (guard, HMW, MMW and LMW) with a UV-vis detector. Analyses were performed at 35 °C using THF as the eluent with the flow rate at 1.0 mL/min. Calibration was based on polystyrene standards. Thermogravimetric analysis measurements were performed over an interval of 50-850 °C at a heating rate of 20 °C/min under a N_2 atmosphere. Differential scanning calorimetry was performed with a first scan heating rate of 15 °C/min to erase thermal history and a second scan to measure transitions between 0-330 °C under nitrogen. Transitions were also measured with cooling at 15 °C/min. Cyclic voltammetry was performed using a potentiostat with a scanning rate of 100 mV/s. The polymer solutions (1-2 mg/mL) were drop-cast on a platinum electrode and Ag/Ag^{+} was used as the reference electrode. The reported values are referenced to Fc/Fc^{+} (-5.1 versus vacuum). All electrochemistry experiments were performed in dry, degassed CH_3CN under an argon atmosphere using 0.1 M tetrabutylammonium

hexafluorophosphate as the electrolyte. UV-visible spectroscopy was obtained on a Varian Cary Bio 50 using polymer solutions in THF and thin films spun from $CHCl_3$/*o*-dichlorobenzene solutions. The films were made by spin-coating 25 x 25 x 1 mm glass slides using 10 mg/mL polymer solutions at a spin rate of 1800 rpm on a spin-coater. X-ray crystal structure data for compound **2a** (CCDC 885622 was deposited with the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK.

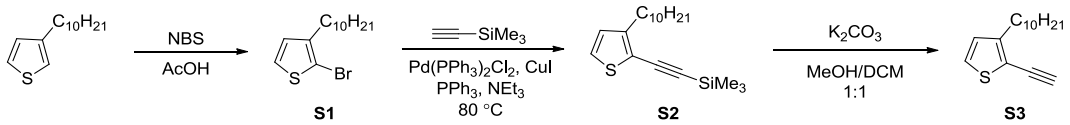
Device Fabrication and Characterization

All these devices were produced via a solution-based spin-casting fabrication process. All polymers were mixed with $PC_{60}BM$ (Sigma-Aldrich) (mixed 1:4 at 14 mg/mL for polymer and 56 mg/mL for $PC_{60}BM$) then dissolved in *o*-dichlorobenzene and magnetically stirred at 60 °C for 48 hours. ITO coated glass slides (Delta Technologies) were cleaned by consecutive 5 minute sonications in (i) isopropanol and acetone, (ii) precision cleaner detergent (dissolved in deionized water), (iii) ethanol and methanol, and then (iv) deionized water. The slides were then dried with nitrogen and cleaned with air plasma (Harrick Scientific plasma cleaner) for 10 minutes. Filtered (0.45μm) PEDOT:PSS (Clevios P^{TM}) was spin-coated onto the prepared substrates (9000 rpm/65 sec) after first being heated and stirred for one hour (80 °C, 1200 rpm). The casted PEDOT:PSS films were then annealed at 140 °C for 20 minutes. After cooling, the substrates were transferred to an argon-filled glovebox. After 48 hours of mixing, the Polymer:PCBM solutions were filtered (0.2 μm pore, VWR Scientific) and then stirred for an additional 5 hours at 60 °C . The solutions were heated up to 90 °C approximately 5 minutes prior to spin coating, after which the solutions were dropped onto the PEDOT:PSS-coated substrates by micropipette and spin-cast at 2000 rpm for 45 seconds. The active layer of the films was covered with a petri dish and annealed at 70 °C for 10 minutes. LiF (2 nm) and Al (120 nm) were successively thermally evaporated through a shadow mask under vacuum to complete the devices. J-V data was generated by illuminating the devices using an ETH quartzline lamp at 1 sun (calibrated using a crystalline silicon photodiode with a KG-5 filter).

Computation Methods

Electrostatic potential maps and frontier orbitals were generated using B3LYP/SVP density functional theory. All computations were performed using Gaussian09 through the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) on the San Diego Supercomputer Center's Gordon cluster. All side chains were truncated to methyl groups and only dimer-sized oligomers were examined.

Experimental Section

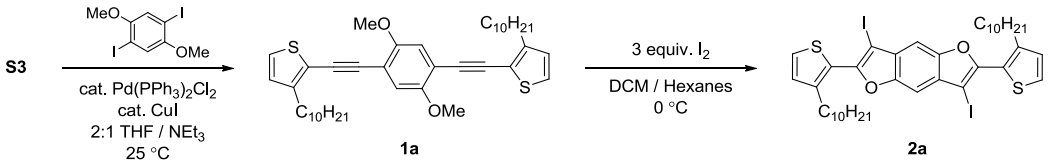


2-Bromo-3-decylthiophene (S1). To a stirred solution of 3-decylthiophene (21.10 g, 94 mmol) in 200 mL of glacial acetic acid was added *N*-bromosuccinimide (16.73 g, 94 mmol) in one portion. The

reaction mixture was stirred for 5 hours and diluted with 300 mL of H_2O. The organic layer was extracted with hexane (x3) and the combined organic layers were washed subsequently with 1N NaOH, H_2O and brine, and then dried over $MgSO_4$. The solvents were removed *in vacuo* and the resulting crude product was purified by vacuum distillation to afford a pale yellow oil (27.0 g, 95 %). ^{1}H NMR (300 MHz; $CDCl_3$) δ 0.88 (3H, t, *J* = 6.6 Hz), 1.24-1.34 (14H, m), 1.57 (2H, p), 2.56 (2H, t, *J* =7.7 Hz), 6.79 (1H, d, *J* = 5.7 Hz), 7.18 (1H, d, *J* = 5.6 Hz).

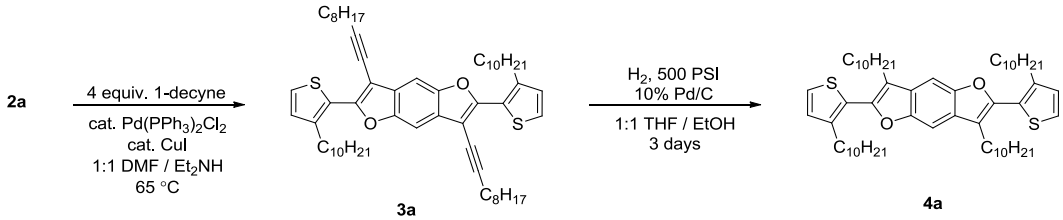
3-Decyl-2-(trimethylsilylethynyl)thiophene (S2). To a stirred, deoxygenated solution of 2-bromo-3-decylthiophene (15.17 g, 50 mmol) dissolved in 75 mL of triethylamine was added 351 mg of $Pd(PPh_3)_2Cl_2$ (1 mol %), 191 mg of CuI (2 mol %) and 262 mg of PPh_3 (2 mol %). Finally, trimethylsilyl acetylene (6.38 g, 65 mmol) was added and the reaction mixture was heated to 80 °C, under argon, for 16 hours. The reaction mixture was then cooled to room temperature and most of the solvent was removed *in vacuo*. Water was added to the resulting slurry and the organic layer was extracted with CH_2Cl_2 (x3). The combined organic layers were washed with brine and dried over $MgSO_4$. The solvents were removed *in vacuo* and the crude mixture was purified by flash chromatography on silica gel with hexanes as the eluent to afford the product as a yellow oil (12.99 g, 81 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.26 (9H, s), 0.89 (3H, t, *J* = 6.8 Hz), 1.25-1.35 (14H, m), 1.62 (2H, m), 2.69 (2H, t, *J* = 7.8 Hz), 6.83 (1H, d, *J* = 5.1 Hz), 7.12 (1H, d, *J* = 5.1 Hz); ^{13}C NMR (100 MHz; $CDCl_3$) δ 0.21, 14.36, 22.92, 29.48, 29.58, 29.61, 29.67, 29.85, 29.94, 30.35, 32.15, 97.76, 100.85, 118.41, 126.06, 128.25, 149.03. HRMS (APCI) *m/z*: M^+ calcd for $C_{19}H_{32}SSi$, 321.2067; found, 321.2073, deviation 1.9 ppm.

3-Decyl-2-ethynylthiophene (S3). To a stirred solution of **S2** (10.69 g, 33.3 mmol) in 200 mL of CH_2Cl_2/MeOH (1:1) was added K_2CO_3 (5.07 g, 36.7 mmol) in one portion. The suspension was stirred at room temperature overnight (16 hours) and poured into H_2O. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (x3). The combined organic layers were rinsed with brine and dried over $MgSO_4$. The solvent was removed *in vacuo* and the crude product was purified on a silica plug with hexanes as the eluent to afford a yellow oil (7.20 g, 87 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.89 (3H, t, *J* = 6.7 Hz), 1.25-1.35 (14H, m), 1.62 (2H, p), 2.71 (2H, t, *J* = 7.7 Hz), 3.43 (1H, s), 6.85 (1H, d, *J* = 5.0 Hz), 7.15 (1H, d, *J* = 5.0 Hz); ^{13}C NMR (100 MHz; $CDCl_3$) δ 14.35, 22.92, 29.47, 29.57, 29.63, 29.80, 29.81, 29.85, 30.43, 32.14, 76.97, 83.33, 117.19, 126.36, 128.24, 149.27. HRMS (ESI) *m/z*: M^+ calcd for $C_{16}H_{24}S$, 249.1671; found, 249.1670, deviation 0.6 ppm.



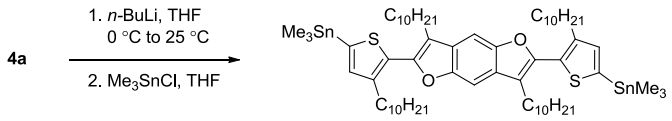
2,2'-((2,5-Dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (1a). To a stirred, deoxygenated solution of **S3** (5.302 g, 21.34 mmol) in 120 mL of THF/Et_3N (2:1) was added 1,4-dimethoxy-2,5-diidobenzene (4.04 g, 10.36 mmol). The solution was stirred at room temperature for 10 min (the 1,4-dimethoxy-2,5-diidobenzene does not dissolve completely at this point). Then $Pd(PPh_3)_2Cl_2$ (365 mg, 5 mol %) and CuI (198 mg, 10 mol %) were added to the reaction mixture and the flask was flushed with Ar for 10 min. The reaction mixture was stirred at room temperature for 2 days, until TLC indicated the disappearance of the dimethoxybenzene. Most of the solvent was then removed *in vacuo* and the resulting slurry was poured into water and extracted with CH_2Cl_2 (x3). The combined organic layers were dried over $MgSO_4$ and the solvent was removed *in vacuo*. The product was purified using column chromatography on silica using a gradient of hexane to hexane/ethyl acetate (99:1) to hexane/ethyl acetate (9:1) as the eluent. The resulting yellow solid was then purified further by recrystalization from hexane/ethanol. The product was collected by filtration and rinsed with cold ethanol to afford bright yellow crystals (5.81 g, 89 %), mp 84 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.87 (6H, t, *J* = 6.8 Hz), 1.22-1.40 (28H, m), 1.68 (4H, p, *J* = 7.3 Hz), 2.80 (4H, t, *J* = 7.6 Hz), 3.89 (6H, s), 6.89 (2H, d, *J* = 5.1 Hz), 6.97 (2H, s), 7.19 (2H, d, *J* = 5.1 Hz); ^{13}C NMR (150 MHz; $CDCl_3$) δ 14.33, 22.88, 29.55, 29.59, 29.66, 29.77, 29.85, 29.87, 30.47, 32.10, 56.56, 88.44, 91.84, 113.53, 115.07, 118.43, 126.42, 128.45, 148.45, 153.89. HRMS (APCI) *m/z*: M^+ calcd for $C_{40}H_{54}O_2S_2$, 631.3638; found, 631.3653, deviation 2.4 ppm.

2,6-Bis(3-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (2a). Compound **1a** (8.28 g, 13.1 mmol) was dissolved in 150 mL of CH_2Cl_2 and cooled to 0 °C. While stirring, a solution of 3 equiv of iodine (9.99 g, 39.3 mmol) in 200 mL of CH_2Cl_2/hexanes (3:1) was added dropwise over 10 minutes. Upon completion of the addition, the reaction mixture was stirred at 0 °C for 4 hours and was quenched by the addition of 50 mL of saturated aqueous sodium thiosulfate solution. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (x2). The organic layers were combined, dried over $MgSO_4$ and the solvents were removed *in vacuo*. The crude product was purified by recrystalization from hexanes/ethanol and collected by filtration, followed by rinsing with cold ethanol to afford fine, yellow crystals (7.89 g, 70 %), mp 104 °C. ^{1}H NMR (300 MHz; $CDCl_3$) δ 0.88 (6H, t, *J* = 6.6 Hz), 1.22-1.40 (28H, m), 1.68 (4H, p, *J* = 7.2 Hz), 2.90 (4H, t, *J* =7.7 Hz), 7.05 (2H, d, *J* = 5.1 Hz), 7.42 (2H, d, *J* = 5.1 Hz), 7.47 (2H, s); ^{13}C NMR (75 MHz; $CDCl_3$) δ 14.38, 22.92, 29.59, 29.64, 29.72, 29.87, 29.94, 30.24, 31.03, 32.15, 64.63, 103.03, 124.67, 127.09, 129.92, 131.39, 145.42, 151.54, 152.43. HRMS (ESI) *m/z*: M^+ calcd for $C_{38}H_{48}I_2O_2S_2$, 855.1258; found, 855.1252, deviation 0.7 ppm. UV-Vis (THF) λ_{max} = 259 nm, 360 nm.



3,7-Di(dec-1-yn-1-yl)-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (3a).[5] To a stirred, deoxygenated solution of **2a** (2.185 g, 2.6 mmol) and 1-decyne (1.41 g, 10.2 mmol) in 60 mL of DMF/Et_2NH (1:1) was added $Pd(PPh_3)_2Cl_2$ (107 mg, 6 mol %) and CuI (29 mg, 6 mol %). The solution was stirred under argon, heated to 65 °C and stirred for 8 hours. The reaction mixture was cooled to room temperature, poured into H_2O and extracted with CH_2Cl_2 (x3). The combined organic layers were washed with H_2O (x2), followed by brine (x1), dried over $MgSO_4$ and the solvent was removed *in vacuo*. The crude product was purified by chromatography on silica gel using a gradient of hexane to hexane/CH_2Cl_2 (98:2) to hexane/CH_2Cl_2 (95:5) as the eluent to afford light yellow crystals (2.14 g, 96 %), mp 56 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.89 (12H, m), 1.22-1.45 (48H, m), 1.55 (4H, m), 1.72 (8H, m), 2.60 (4H, t, *J* = 7.1 Hz), 3.07 (4H, t, *J* = 7.8 Hz), 6.89 (2H, d, *J* = 5.1 Hz), 7.34 (2H, d, *J* = 5.1 Hz), 7.62 (2H, s); ^{13}C NMR (75 MHz; $CDCl_3$) δ 14.35, 20.34, 22.92, 28.93, 29.26, 29.32, 29.42, 29.52, 29.60, 29.76, 29.82, 29.88, 29.89, 30.35, 31.22, 32.12, 32.13, 78.14, 99.79, 100.64, 101.10, 126.13, 126.18, 128.47, 130.22, 143.73, 151.04, 154.14. HRMS (ESI) *m/z*: M^+ calcd for $C_{58}H_{82}O_2S_2$, 875.5829; found, 875.5814, deviation 1.7 ppm. UV-Vis (THF) λ_{max} = 235 nm, 386 nm.

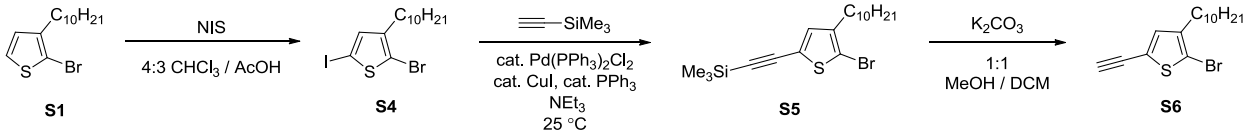
3,7-Didecyl-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (4a.) Dialkyne **3a** (3.40 g, 4.0 mmol) was dissolved in 20 mL of THF/ethanol (1:1) and Pd/C (10 %, 426 mg, 0.4 mmol) was added to the solution. The resulting mixture was placed in a Parr bomb apparatus, flushed twice with H_2 and stirred under pressurized H_2 (500 PSI) for 72 hours at room temperature. The reaction mixture was filtered through a pad of Celite to remove the Pd/C and rinsed with THF (x2). The solvent was removed *in vacuo* and the resulting solid was purified on a silica gel plug with hexane as the eluent to afford a pale yellow solid (3.35 g, 95 %), mp 57 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.86 (12H, m), 1.20-1.42 (56H, m), 1.63 (4H, p, *J* = 7.2 Hz), 1.72 (4H, p, *J* =7.5 Hz), 2.80 (8H, m), 7.02 (2H, d, *J* = 5.1 Hz), 7.36 (2H, d, *J* = 5.1 Hz), 7.53 (2H, s); ^{13}C NMR (150 MHz; $CDCl_3$) δ 14.34, 22.92, 24.69, 29.58, 29.65, 29.66, 29.70, 29.78, 29.85, 29.86, 29.93, 31.01, 32.13, 32.14, 100.48, 118.92, 126.00, 126.02, 127.94, 129.63, 143.62, 146.73, 151.39. HRMS (ESI) *m/z*: M^+ calcd for $C_{58}H_{90}O_2S_2$, 883.6455; found, 883.6450, deviation 0.6 ppm. UV-Vis (THF) λ_{max} = 248 nm, 346 nm.



5a

(5,5'-(3,7-Didecylbenzo[1,2-*b*:4,5-*b*']difuran-2,6-diyl)bis(4-decylthiophene-5,2-diyl))bis(trimethylstannane) (5a). To a stirred solution of **4a** (884 mg, 1.0 mmol) in 20 mL of anhydrous THF, under argon, at 0 °C was added *n*-BuLi in hexanes (2.5 M, 1.0 mL, 2.5 mmol) dropwise. The reaction mixture was warmed to room temperature and stirred for 2 hours. A solution of trimethylstannyl chloride in THF (1.0 M, 2.75 mL, 2.75 mmol) was then added to the reaction at 0 °C and the reaction was warmed to room temperature, stirred overnight and poured into H_2O. The layers were separated and the aqueous layer was extracted with ether (x3). The combined organic layers were dried

over $MgSO_4$ and the solvent was removed *in vacuo*. The resulting reddish oil was heated at 50 °C under vacuum to remove residual Me_3SnCl (1.14 g, 94 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.41 (81H, s), 0.87 (12H, m), 1.20-1.42 (56H, m), 1.64 (4H, p, *J* = 7.3 Hz), 1.73 (4H, p, *J* = 7.6 Hz), 2.82 (8H, m), 7.07 (2H, s), 7.51 (2H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ -7.98, 14.36, 22.93, 24.73, 29.56, 29.60, 29.67, 29.70, 29.79, 29.83, 29.88, 29.90, 29.92, 31.23, 32.15, 32.17, 100.32, 118.50, 127.97, 131.85, 137.89, 138.83, 144.58, 147.12, 151.37. HRMS (APCI) *m/z*: M^+ calcd for $C_{64}H_{106}O_2S_2Sn_2$, 1209.5765; found, 1209.5747, deviation 1.5 ppm.

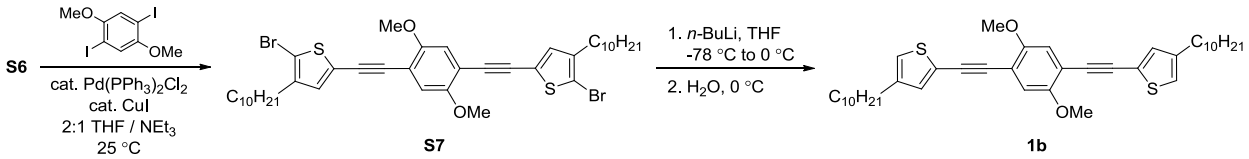


2-Bromo-3-decyl-5-iodothiophene (S4).[6] To a stirred solution of 2-bromo-3-decylthiophene (5.70 g, 18.8 mmol) in 35 mL of $CHCl_3$/AcOH (4:3) was added *N*-iodosuccinimide (5.92 g, 26.3 mmol) in one portion. The reaction was stirred in the absence of light for 16 hours and poured into H_2O. The layers were separated and the aqueous layer was extracted with hexanes (x3). The combined organic layers were then neutralized with 1 M KOH, washed subsequently with H_2O and brine, and dried over $MgSO_4$. The solvent was removed *in vacuo* and the crude oil was purified by column chromatography on silica with hexanes as the eluent to afford a pale pink oil (7.80 g, 97 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (3H, t, *J* = 6.6 Hz), 1.24-1.34 (14H, m), 1.53 (2H, m), 2.52 (2H, t, *J* = 7.7 Hz), 6.96 (1H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ 14.38, 22.93, 29.36, 29.41, 29.56, 29.60, 29.77, 29.83, 29.87, 32.13, 71.27, 111.90, 138.16, 144.43. HRMS (APCI) *m/z*: M^+ calcd for $C_{14}H_{22}BrIS_2$, 428.9743; found, 428.9751, deviation 1.9 ppm.

((5-Bromo-4-decylthiophen-2-yl)ethynyl)trimethylsilane (S5). To a stirred deoxygenated solution of 2-bromo-3-decyl-5-iodothiophene (7.80 g, 18.2 mmol) in 50 mL of THF/NEt_3 (1:1) was added $Pd(PPh_3)_2Cl_2$ (319 mg, 2.5 mol %) and CuI (173 mg, 5 mol %). The resulting suspension was stirred for 10 minutes under argon before trimethylsilyl acetylene (1.88 g, 19.1 mmol) was added dropwise and the reaction mixture was stirred at room temperature under argon. After 18 hours, TLC analysis indicated complete consumption of the starting material and most of the solvent was removed *in vacuo*. The resulting dark slurry was then filtered and rinsed with hexanes. The solvent was removed *in vacuo* and the crude oil was purified on a silica gel plug with hexanes as the eluent to afford a yellow oil (7.04 g, 97 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.23 (9H, s), 0.88 (3H, t, *J* = 6.8 Hz), 1.24-1.34 (14H, m), 1.53 (2H, p, *J* = 7.2 Hz), 2.49 (2H, t, *J* = 7.6 Hz), 6.92 (1H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ 0.02, 14.34, 22.92, 29.31, 29.55, 29.58, 29.61, 29.76, 29.77, 29.82, 32.13, 97.16, 99.93, 110.22, 123.15, 133.77, 142.36. HRMS (APCI) *m/z*: M^+ calcd for $C_{19}H_{31}BrSSi$, 399.1172; found, 399.1171, deviation 0.2 ppm.

2-Bromo-3-decyl-5-ethynylthiophene (S6). To a stirred solution of **S5** (7.04 g, 17.6 mmol) in 100 mL of CH_2Cl_2/MeOH (1:1) was added K_2CO_3 (2.68 g, 19.4 mmol) in one portion. The suspension was stirred at

room temperature for 8 hours and poured into H_2O. The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (x3). The combined organic layers were rinsed with brine and dried over $MgSO_4$. The solvent was removed *in vacuo* and the crude product was purified on a silica gel plug with hexanes as the eluent to afford an orange oil (5.52 g, 96 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (3H, t, *J* = 6.7 Hz), 1.24-1.34 (14H, m), 1.55 (2H, p, *J* = 7.0 Hz), 2.51 (2H, t, *J* =7.6 Hz), 3.35 (1H, s), 6.96 (1H, s); ^{13}C NMR (75 MHz; $CDCl_3$) δ 14.35, 22.92, 29.34, 29.56, 29.56, 29.60, 29.77, 29.82, 29.94, 32.12, 76.69, 82.19, 110.50, 121.94, 134.21, 142.39. HRMS (APCI) *m/z*: M^+ calcd for $C_{16}H_{23}BrS$, 327.0777; found, 327.0768, deviation 2.9 ppm.

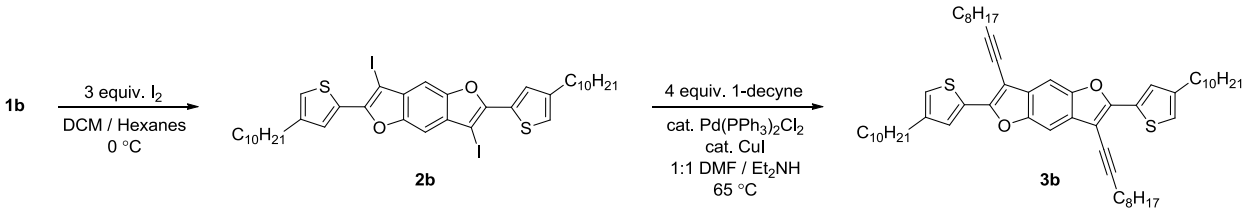


Note: the iodocyclization reaction was performed on compound **S7** and the resulting benzodifuran was insoluble in organic solvents at room temperature. Attempts were made to attach 1-decyne through Sonogashira chemistry; however, the elevated temperatures required lead to a loss of selectivity of the aryl iodide over the aryl bromide in the cross-coupling reaction. Consequently, the product was obtained in low yields along with multiple side-products. The bromines on compound **S7** were thus removed to facilitate alkynylation at the appropriate site on the molecule.

5,5'-((2,5-Dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(2-bromo-3-decylthiophene) (S7). To a stirred, deoxygenated solution of **S6** (12.75 g, 39.0 mmol) in 200 mL of THF/Et_3N (2:1) was added 1,4-dimethoxy-2,5-diidobenzene (6.76 g, 17.3 mmol). The solution was stirred at room temperature for 10 minutes (the 1,4-dimethoxy-2,5-diidobenzene does not dissolve completely at this point). Then $Pd(PPh_3)_2Cl_2$ (364 mg, 3 mol %), CuI (198 mg, 6 mol %) and PPh_3 (273 mg, 6 mol %) were added to the reaction mixture and the flask was flushed with Ar for 10 minutes. The reaction mixture was stirred at room temperature, under argon, for 2 days. Most of the solvent was then removed *in vacuo* and the resulting slurry was poured into water and extracted with CH_2Cl_2 (x3). The combined organic layers were dried over $MgSO_4$ and the solvent was removed *in vacuo*. The product was purified using column chromatography on silica using hexane/CH_2Cl_2 (3:1) to afford a yellow, flaky solid (11.17 g, 82 %), mp 72 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (6H, t, *J* = 6.8 Hz), 1.23-1.35 (28H, m), 1.57 (4H, m), 2.53 (4H, t, *J* = 7.6 Hz), 3.88 (6H, s), 6.96 (2H, s), 7.01 (2H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ 14.35, 22.91, 29.33, 29.54, 29.62, 29.77, 29.79, 29.82, 29.86, 32.12. HRMS (APCI) *m/z*: M^+ calcd for $C_{40}H_{52}Br_2O_2S_2$, 787.1848; found, 787.1835, deviation 1.7 ppm.

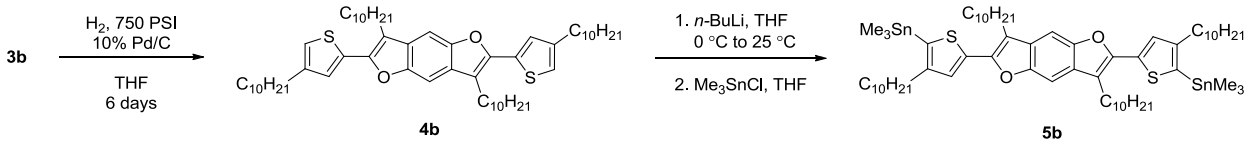
5,5'-((2,5-Dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (1b). To a stirred solution of **S7** (11.17 g, 14.2 mmol) in 125 ml of dry THF at -78 °C, under argon, was added *n*-BuLi in hexanes (2.5 M, 12.5 mL, 31.2 mmol) dropwise. The reaction mixture was stirred at -78 °C for 1 hour, warmed to room temperature and then quenched with 50 mL of H_2O. The layers were separated and the aqueous layer was extracted with diethyl ether. The combined organic layers were washed with brine and dried over $MgSO_4$. The solvent was removed *in vacuo* and the resulting yellow solid was passed through

a short pad of silica gel with hexane/CH_2Cl_2 (2:1) as the eluent to afford a flaky yellow solid (8.94 g, 99 %), mp 51 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (6H, t, *J* = 6.8), 1.23-1.35 (28H, m), 1.60 (4H, p, *J* = 7.4 Hz), 2.57 (4H, t, *J* =7.6 Hz), 3.88 (6H, s), 6.89 (2H, d), 6.98 (2H, s), 7.16 (2H, d); ^{13}C NMR (100 MHz; $CDCl_3$) δ 14.31, 22.87, 29.38, 29.52, 29.63, 29.77, 29.80, 30.45, 30.57, 32.08, 56.50, 88.90, 89.18, 113.32, 115.37, 122.65, 122.84, 133.60, 143.47, 153.85. HRMS (ESI) *m/z*: M^+ calcd for $C_{40}H_{54}O_2S_2$, 631.3638; found, 631.3623, deviation 2.4 ppm.



2,6-Bis(4-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (2b). Compound **1b** (8.94 g, 14.1 mmol) was dissolved in 150 mL of CH_2Cl_2 and cooled to 0 °C. While stirring, a solution of 3 equiv of iodine (10.74 g, 42.3 mmol) in 200 mL of CH_2Cl_2/hexanes (3:1) was added dropwise over 10 minutes. Upon completion of the addition, the reaction mixture was stirred at 0 °C for 4 hours and was quenched by the addition of 50 mL of saturated aqueous sodium thiosulfate solution. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (x2). The organic layers were combined, dried over $MgSO_4$ and the solvent was removed *in vacuo*. The resulting crude product was recrystalized from ethanol/$CHCl_3$ and collected by filtration, followed by rinsing with cold ethanol, to afford fine, yellow crystals (9.88 g, 82 %), mp 146 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (6H, t, *J* = 6.7 Hz), 1.23-1.40 (28H, m), 1.68 (4H, p, *J* = 7.4 Hz), 2.67 (4H, t, *J* = 7.7 Hz), 7.07 (2H, s), 7.42 (2H, s), 7.78 (2H, s); ^{13}C NMR (150 MHz; $CDCl_3$) δ 14.31, 22.92, 29.54, 29.57, 29.71, 29.85, 29.87, 30.65, 30.71, 32.16, 60.38, 102.73, 122.63, 128.85, 131.71, 132.09, 144.26, 151.27, 151.87. HRMS (APCI) *m/z*: M^+ calcd for $C_{38}H_{48}I_2O_2S_2$, 855.1258; found, 855.1254, deviation 0.5 ppm. UV-Vis (THF) λ_{max} = 256 nm, 360 nm, 379 nm, 401 nm.

3,7-Di(dec-1-yn-1-yl)-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (3b). To a stirred, deoxygenated solution of **2b** (4.27 g, 5.0 mmol) and 1-decyne (2.77 g, 20.0 mmol) in 110 mL of DMF/Et_2NH (1:1) was added $Pd(PPh_3)_2Cl_2$ (175 mg, 5 mol %) and CuI (48 mg, 5 mol %). The solution was stirred under argon, heated to 80 °C and stirred overnight. The reaction mixture was cooled to room temperature, poured into H_2O and extracted with CH_2Cl_2 (x3). The combined organic layers were washed with H_2O (x2), followed by brine (x1), dried over $MgSO_4$ and the solvent was removed *in vacuo*. The crude product was purified by chromatography on silica gel using a gradient of hexane to hexane/CH_2Cl_2 (95:5) as the eluent to afford bright yellow crystals (4.02 g, 92 %), mp 95 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.92 (12H, m), 1.26-1.45 (48H, m), 1.59 (4H, p, *J* = 7.0 Hz), 1.65-1.80 (8H, m), 2.65 (8H, m), 7.00 (2H, s), 7.57 (2H, s), 7.69 (2H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ 14.36, 20.34, 22.95, 29.04, 29.33, 29.47, 29.53, 29.59, 29.61, 29.76, 29.88, 29.89, 30.64, 30.67, 32.16, 71.74, 99.01, 100.03, 101.10, 121.74, 127.19, 128.84, 132.32, 144.00, 150.91, 153.59. HRMS (APCI) *m/z*: M^+ calcd for $C_{58}H_{82}O_2S_2$, 875.5829; found, 875.5814, deviation 1.7 ppm. UV-Vis (THF) λ_{max} = 231nm, 366 nm, 386 nm, 410 nm.



3,7-Didecyl-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (4b). Dialkyne **3b** (3.55 g, 4.2 mmol) was dissolved in 30 mL of THF and Pd/C (10 %, 4 47mg, 0.4 mmol) was added to the solution. The resulting mixture was placed in a Parr bomb apparatus, flushed twice with H_2 and stirred under pressurized H_2 (750 PSI) for 6 days at room temperature. The reaction mixture was filtered through a pad of Celite to remove the Pd/C and rinsed with THF (x2). The solvent was removed *in vacuo* and the resulting solid was purified on a silica gel plug with hexane as the eluent to afford a bright yellow solid (3.96 g, 95 %), mp 75 °C. ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88 (12H, m), 1.23-1.40 (56H, m), 1.48 (4H, m), 1.68 (4H, m), 1.75 (4H, m), 2.66 (4H, t, *J* = 7.6 Hz), 2.93 (4H, t, *J* = 7.7 Hz), 6.96 (2H, d, *J* = 1.3 Hz), 7.32 (2H, d, *J* = 1.4 Hz), 7.48 (2H, s); ^{13}C NMR (150 MHz; $CDCl_3$) δ 14.34, 22.93, 24.67, 29.45, 29.57, 29.59, 29.73, 29.79, 29.85, 29.86, 29.88, 30.08, 30.69, 32.14, 32.15, 100.08, 116.33, 120.45, 126.22, 128.93, 133.20, 147.47, 151.04. HRMS (APCI) *m/z*: M^+ calcd for $C_{58}H_{90}O_2S_2$, 883.6455; found, 883.6467, deviation 1.4 ppm. UV-Vis (THF) λ_{max} = 239 nm, 376 nm, 397 nm.

(5,5'-(3,7-Didecylbenzo[1,2-*b*:4,5-*b*']difuran-2,6-diyl)bis(3-decylthiophene-5,2-diyl))bis(trimethylstannane) (5b). To a stirred solution of **4b** (221 mg, 0.25 mmol) in 10 mL of anhydrous THF, under argon, at 0 °C was added *n*-BuLi in hexanes (2.5 M, 0.25 mL, 0.625 mmol) dropwise. The reaction mixture was warmed to room temperature and stirred for 2 hours. A solution of trimethylstannyl chloride in THF (1.0 M, 0.69 mL, 0.69 mmol) was then added to the reaction at 0 °C and the reaction was warmed to room temperature, stirred overnight and poured into H_2O. The layers were separated and the aqueous layer was extracted with ether (x3). The combined organic layers were dried over $MgSO_4$ and the solvent was removed *in vacuo*. The resulting yellow oil was heated at 50 °C under a vacuum to remove residual Me_3SnCl (284 mg, 94 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.43 (18H, s), 0.88 (12H, m), 1.23-1.40 (56H, m), 1.49 (4H, m), 1.65 (4H, p, *J* = 7.6 Hz), 1.76 (4H, p, *J* = 7.5 Hz), 2.64 (4H, t, *J* = 7.8 Hz), 2.94 (4H, t, *J* = 7.7 Hz), 7.45 (2H, s), 7.48 (2H, s); ^{13}C NMR (100 MHz; $CDCl_3$) δ -7.64, 14.37, 22.94, 24.70, 29.43, 29.61, 29.80, 29.85, 29.87, 29.90, 29.92, 30.07, 32.17, 32.31, 32.99, 99.97, 116.12, 127.16, 128.91, 132.91, 138.57, 147.62, 151.03, 151.50. HRMS (APCI) *m/z*: M^+ calcd for $C_{64}H_{106}O_2S_2Sn_2$, 1209.5765; found, 1209.5744, deviation 1.7 ppm.

General Polymerization Procedure ($PT_{in}BDFID$ and $PT_{out}BDFID$) with $Pd_2(dba)_3$. To a stirred, deoxygenated solution of bisstannane (**5a** or **5b)** and isoindigo **6** in 10 mL of toluene was added $Pd_2(dba)_3$ (2 mol %) and tri(*o*-tolyl)phosphine (8 mol %). The reaction mixture was heated to reflux, under argon, and stirred for 4 hours. A few drops of trimethyl(phenyl)tin was added and the mixture was stirred for 4 hours at reflux. A few drops of iodobenzene were added and the mixture was stirred overnight at reflux.

After cooling to room temperature, the polymer was precipitated in methanol. The precipitated polymer was filtered through a cellulose extraction thimble, placed into a Soxhlet extractor and washed with methanol, acetone, and $CHCl_3$. The polymer was recovered from the $CHCl_3$ extract by evaporation of the solvent.

Polymer $PT_{in}BDFID$: synthesized from bisstannane **5a** (479 mg, 94 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ. 0.88, 1.15-1.50, 1.73, 1.80, 2.02, 2.88, 2.93, 3.77, 7.04, 7.35, 7.58, 9.26. UV-Vis ($CHCl_3$) λ_{max} = 373 nm, 605 nm; UV-Vis (film) λ_{max} = 415 nm, 653 nm. GPC M_n = 32664, M_w = 76253, PDI = 2.33. TGA T_d = 397 °C. T_g = not observed.

Polymer $PT_{out}BDFID$: synthesized from bisstannane **5b** (365 mg, 86 %). ^{1}H NMR (400 MHz; $CDCl_3$) δ 0.88, 1.10-1.55, 1.76, 2.68, 2.83, 3.00, 3.76, 6.97, 7.23, 7.42, 7.53, 9.29. UV-Vis ($CHCl_3$) λ_{max} = 400 nm, 599 nm; UV-Vis (film) λ_{max} = 403 nm, 612 nm. GPC M_n = 17384, M_w = 33085, PDI = 1.90. TGA T_d = 407 °C. T_g = not observed.

General Polymerization Procedure ($PT_{in}BDFID$ and $PT_{out}BDFID$) with $Pd(PPh_3)_4$. To a stirred, deoxygenated solution of bisstannane (**5a** or **5b)** and isoindigo **6** in 10 mL of toluene was added $Pd(PPh_3)_4$ (5 mol %). The reaction mixture was heated to reflux, under argon, and stirred for 48 hours. A few drops of trimethyl(phenyl)tin was added and the mixture was stirred for 4 hours at reflux. A few drops of iodobenzene were added and the mixture was stirred overnight at reflux. After cooling to room temperature, the polymer was precipitated in methanol. The precipitated polymer was filtered through a cellulose extraction thimble, placed into a Soxhlet extractor and washed with methanol, acetone, and $CHCl_3$. The polymer was recovered from the $CHCl_3$ extract by evaporation of the solvent.

Polymer $PT_{in}BDFID$: synthesized from bisstannane **5a** (671 mg, 79 %). UV-Vis ($CHCl_3$) λ_{max} = 397 nm, 596 nm; UV-Vis (film) λ_{max} = 401 nm, 617 nm. GPC M_n = 35081, M_w = 18848, PDI = 1.86.

Polymer $PT_{out}BDFID$: synthesized from bisstannane **5b** (710 mg, 82 %). UV-Vis ($CHCl_3$) λ_{max} = 379 nm, 594 nm; UV-Vis (film) λ_{max} = 404 nm, 611 nm. GPC M_n = 20528, M_w = 15662, PDI = 1.31.

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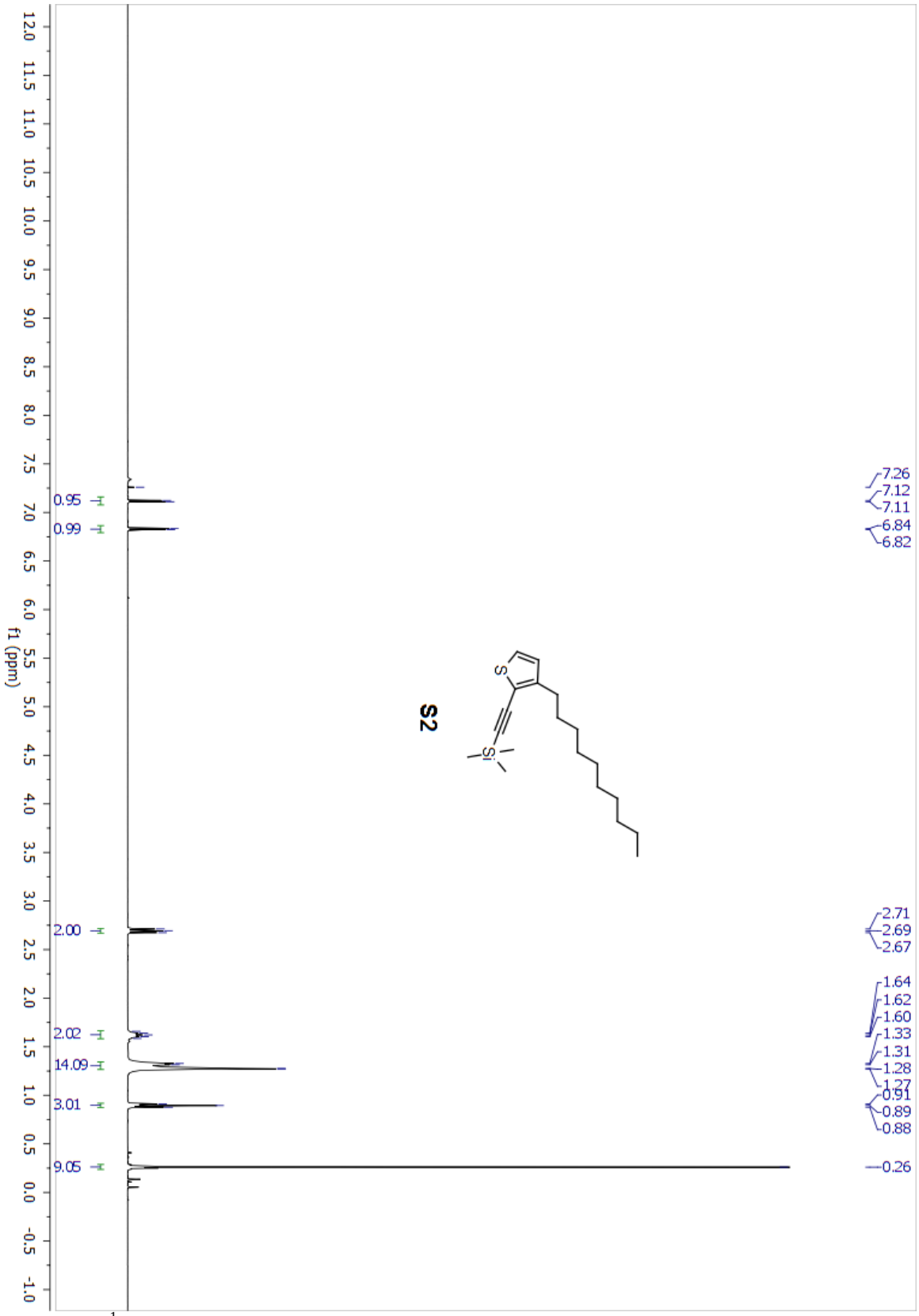

Figure S1. ^{1}H NMR of 3-decyl-2-(trimethylsilylethynyl)-thiophene (**S2**)

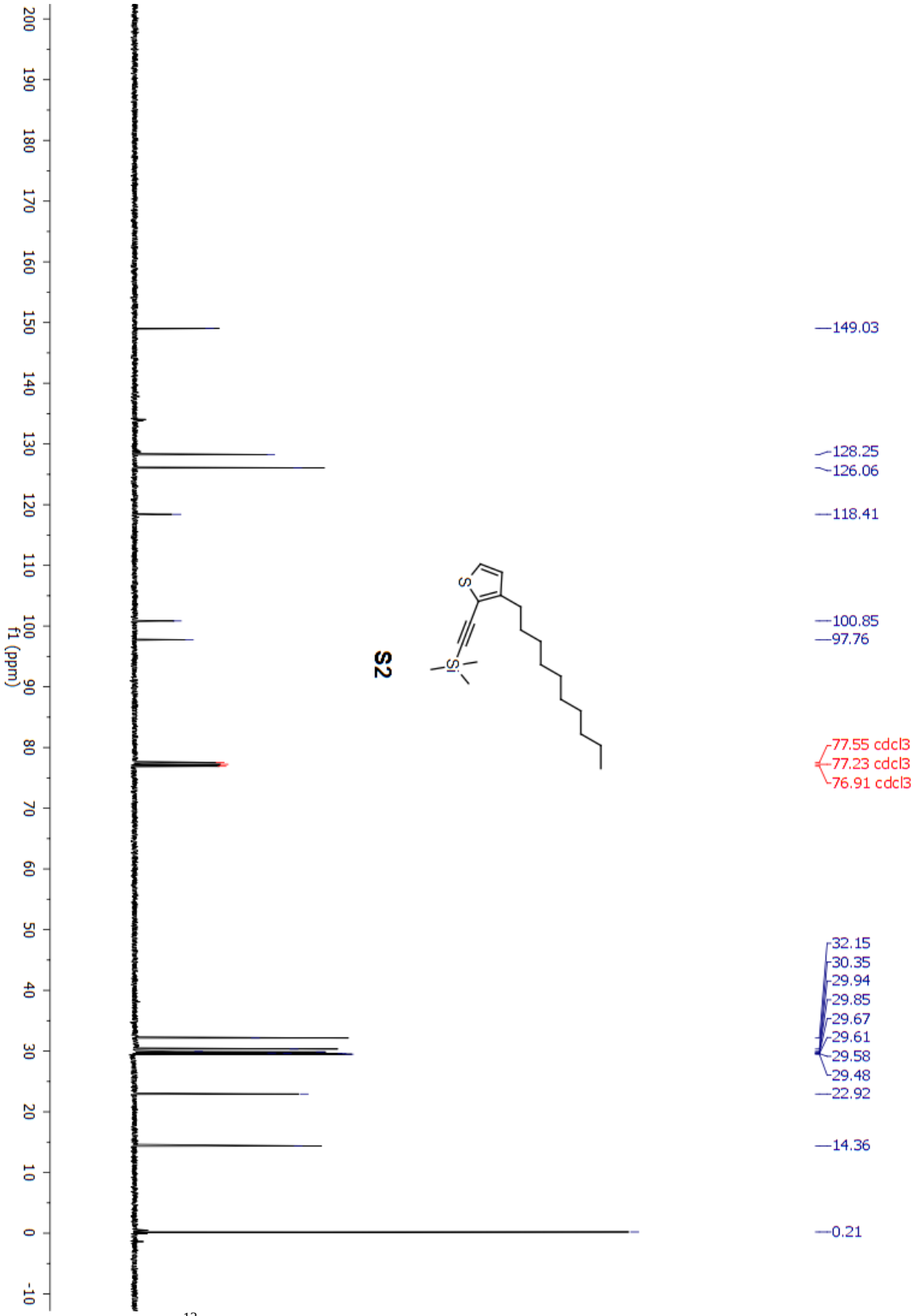

Figure S2. ^{13}C NMR of 3-decyl-2-(2-(trimethylsilyl)ethynyl)-thiophene (**S2**)

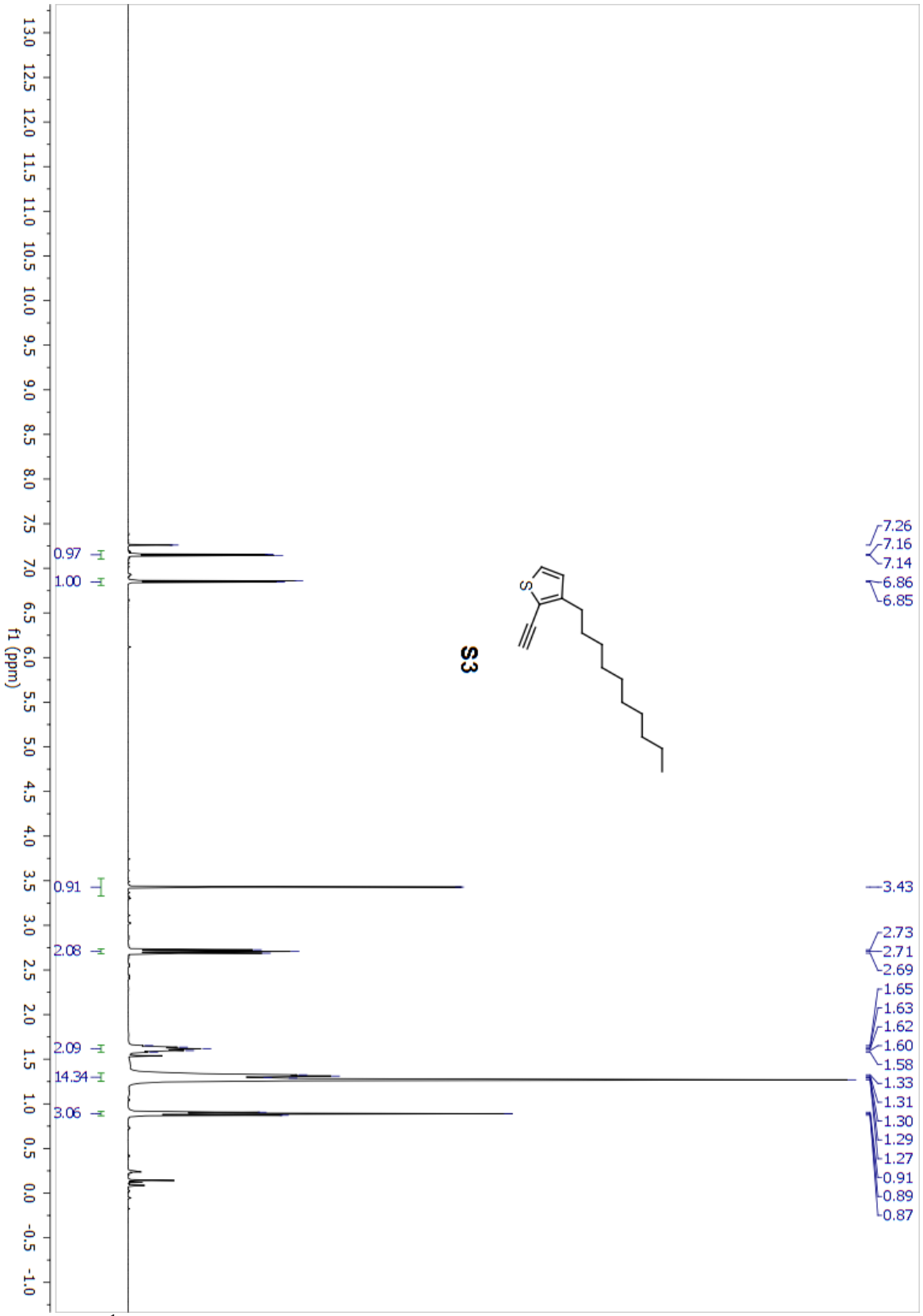

Figure S3. ^{1}H NMR of 3-decyl-2-ethynylthiophene (**S3**)

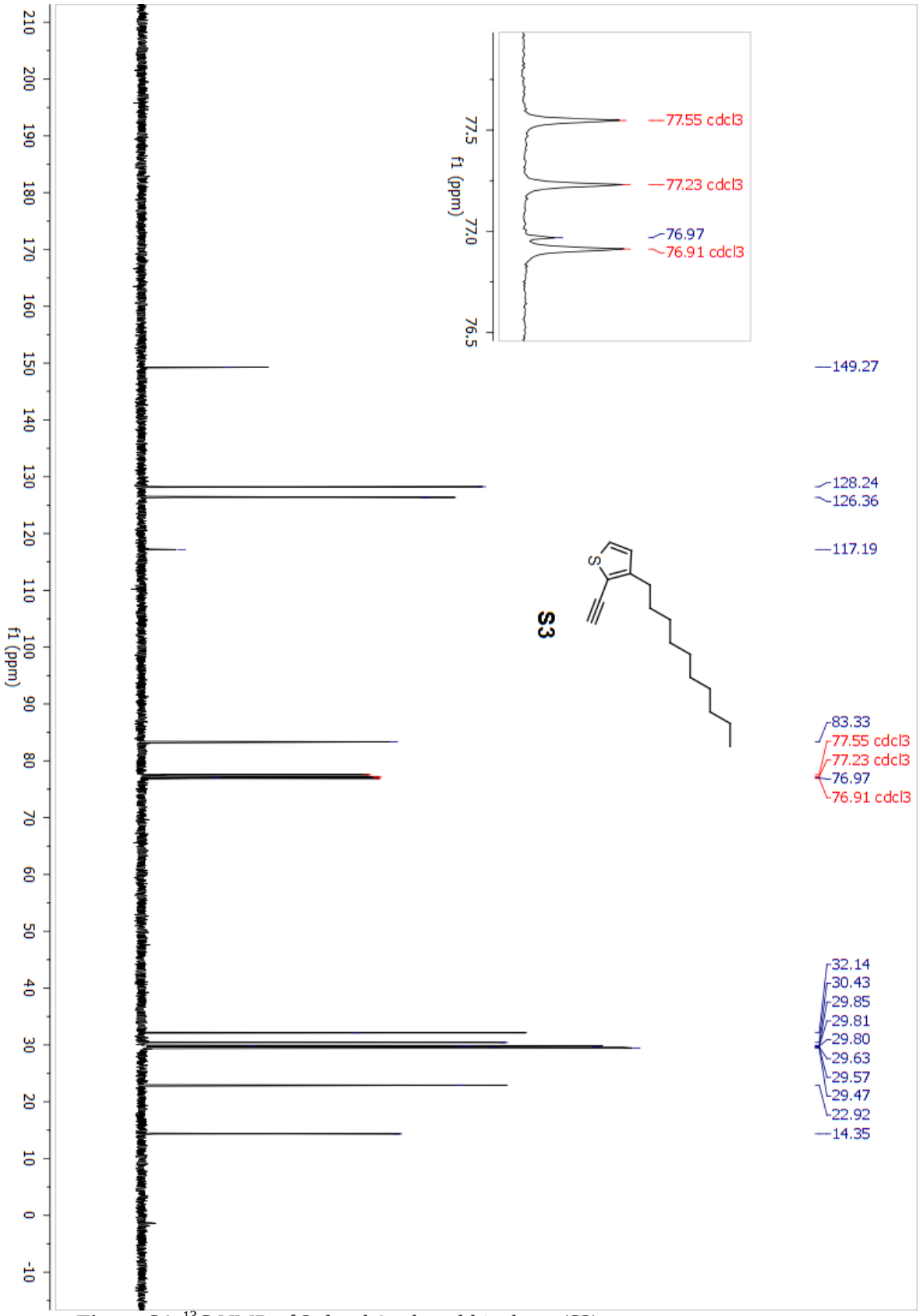

Figure S4. ^{13}C NMR of 3-decyl-2-ethynylthiophene (**S3**)

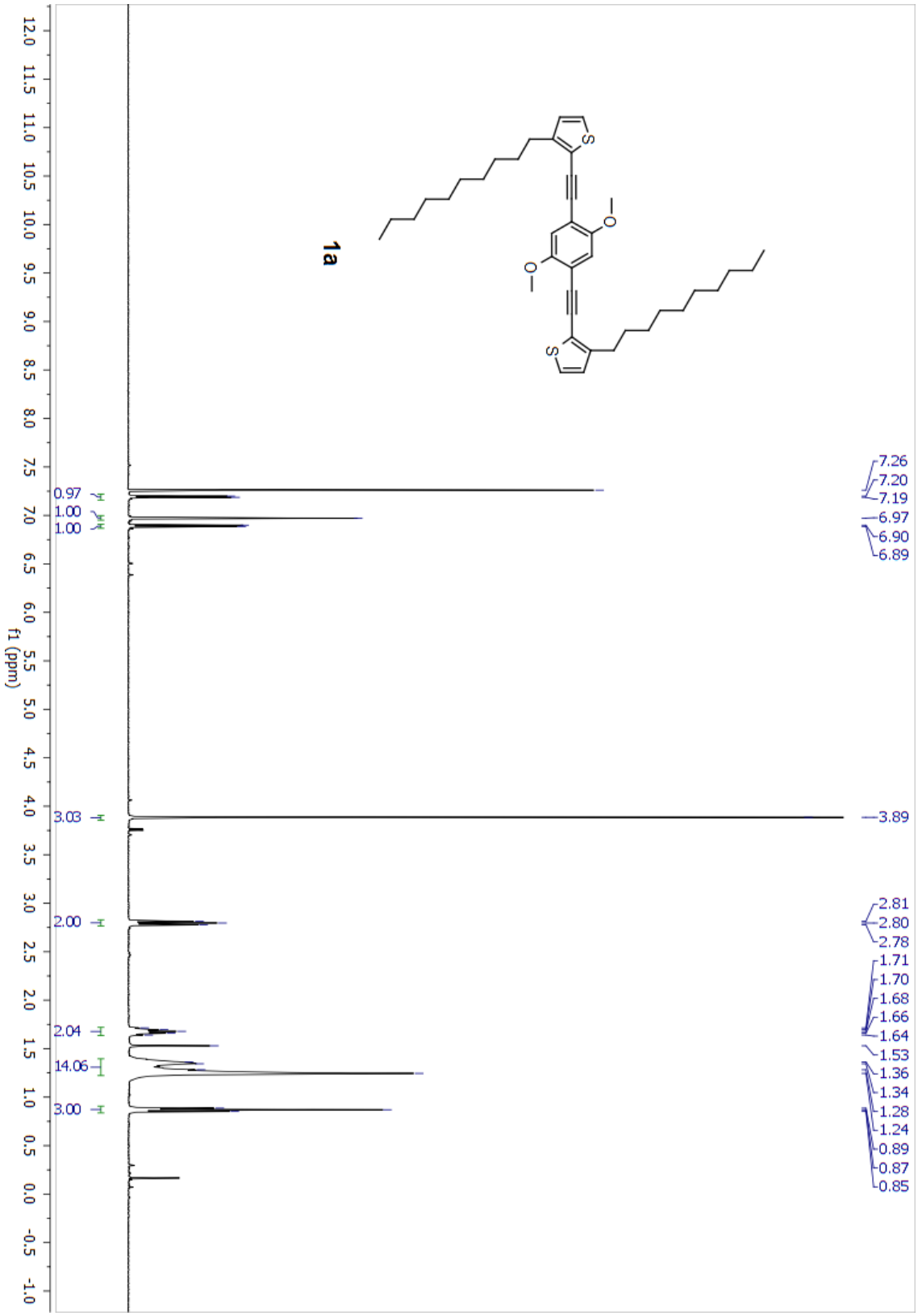

Figure S5. ^{1}H NMR of 2,2'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (**1a**)

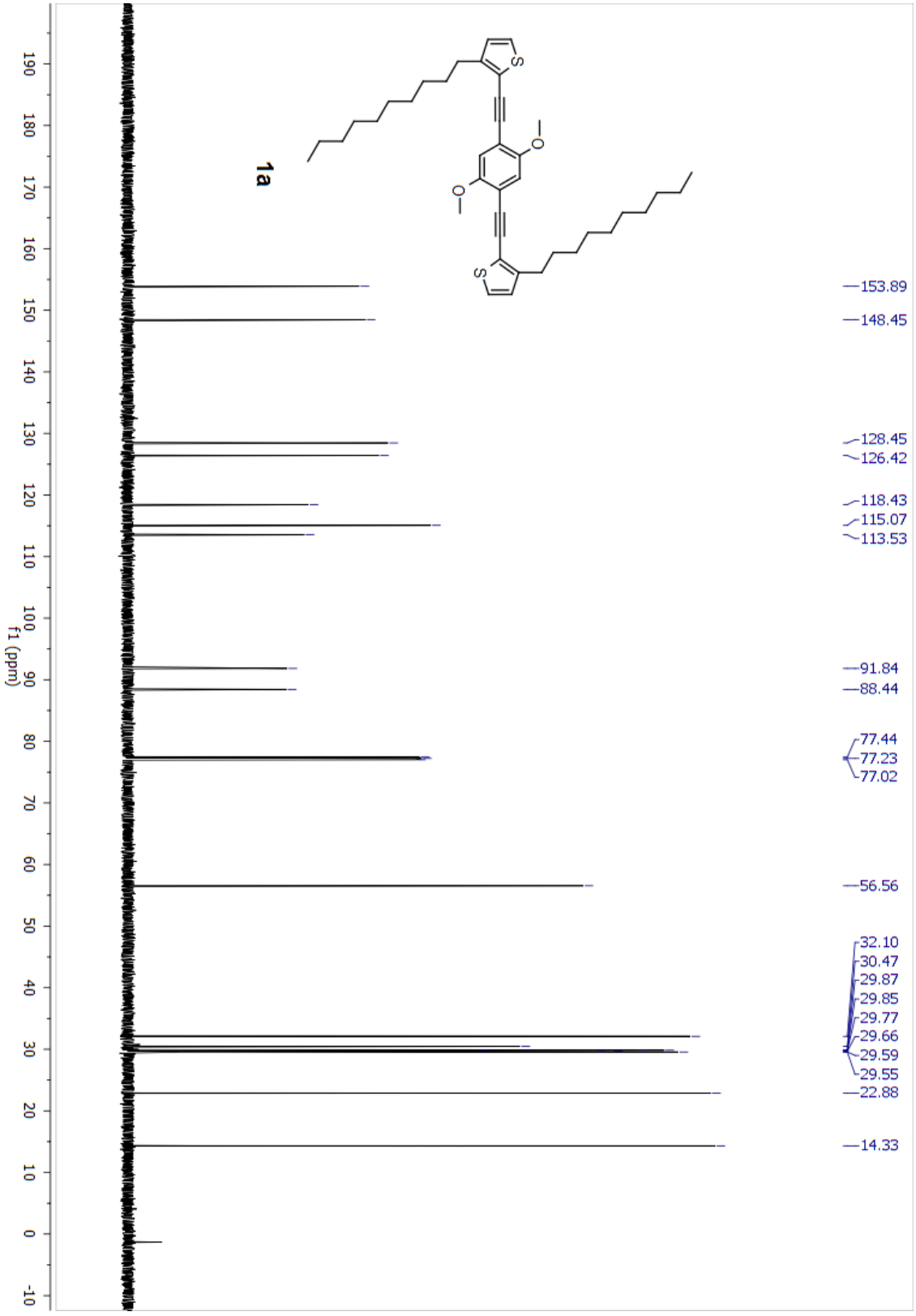

Figure S6. ^{13}C NMR of 2,2'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (**1a**)

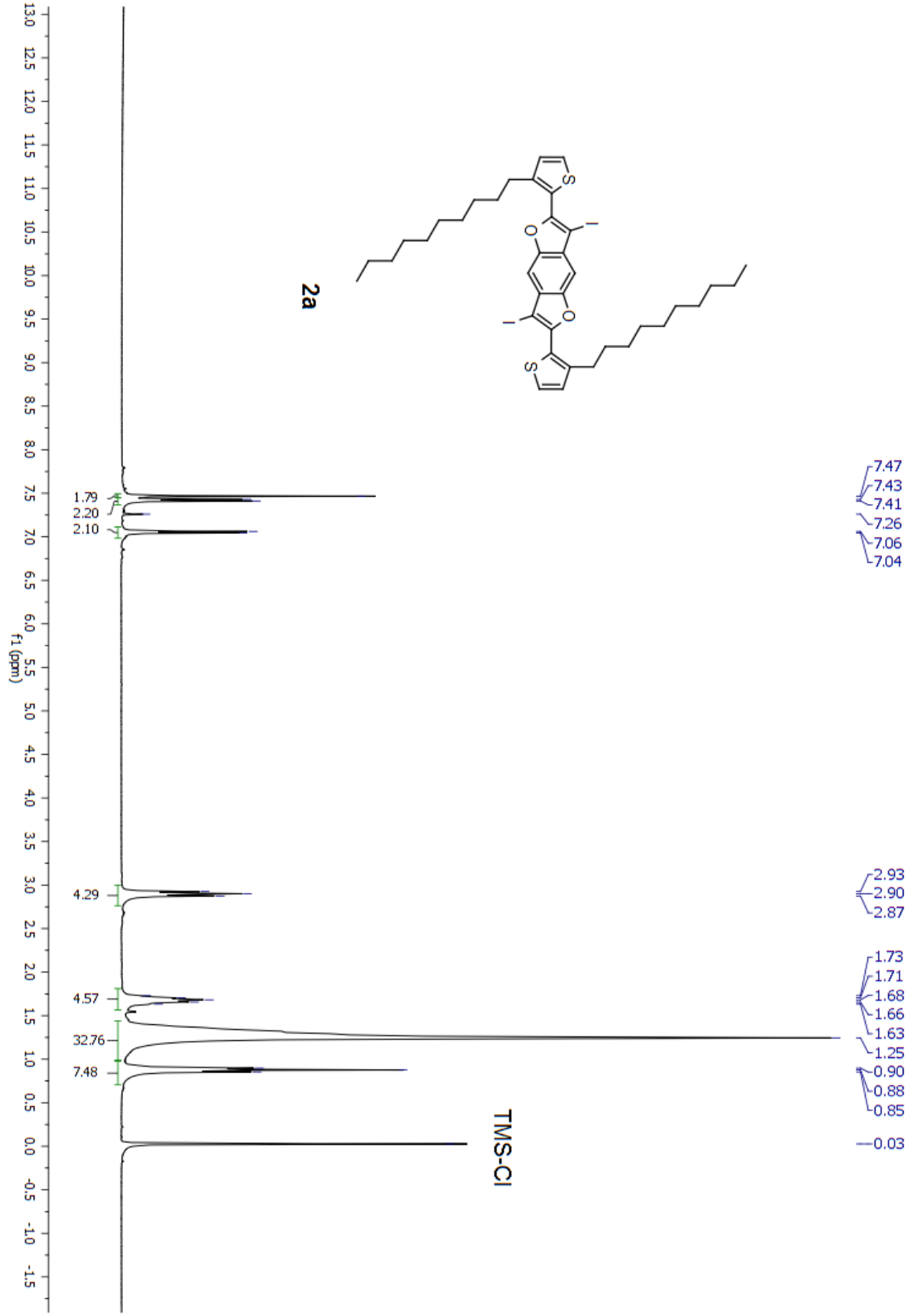

Figure S7. ^{1}H NMR of 2,6-bis(3-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (**2a**)

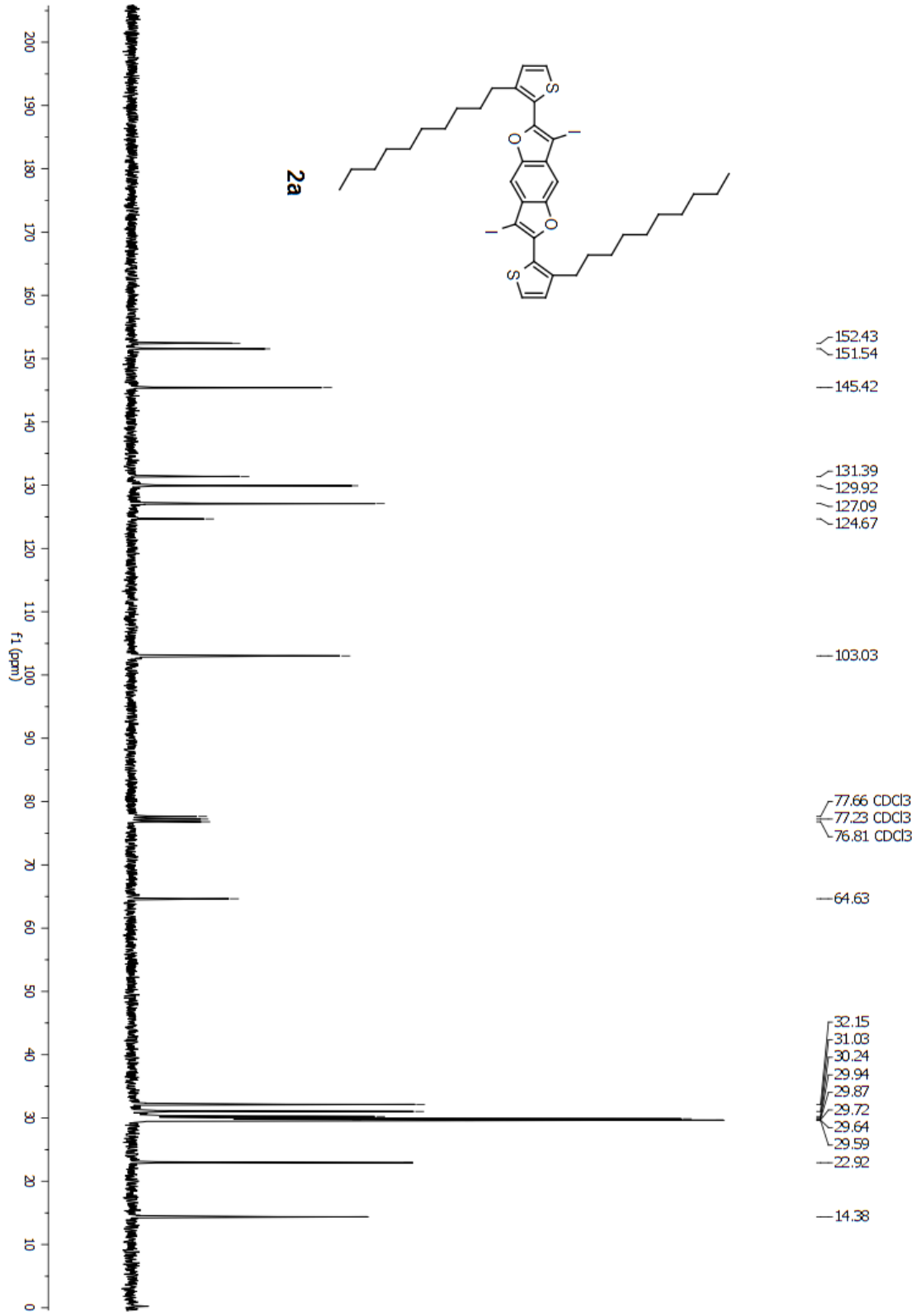

Figure S8. ^{13}C NMR of 2,6-bis(3-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (**2a**)

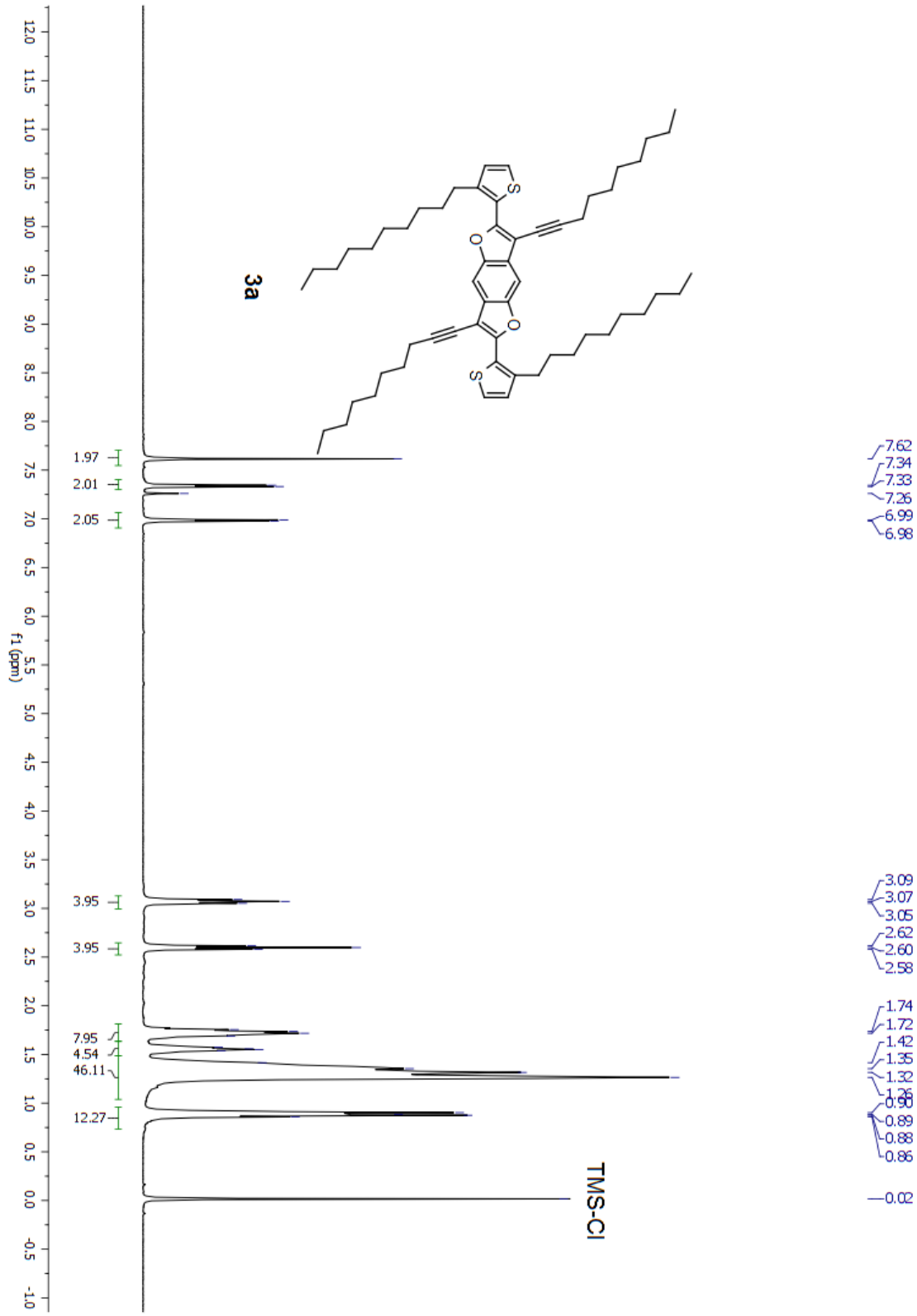

Figure S9. ^{1}H NMR of 3,7-di(dec-1-yn-1-yl)-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**3a**)

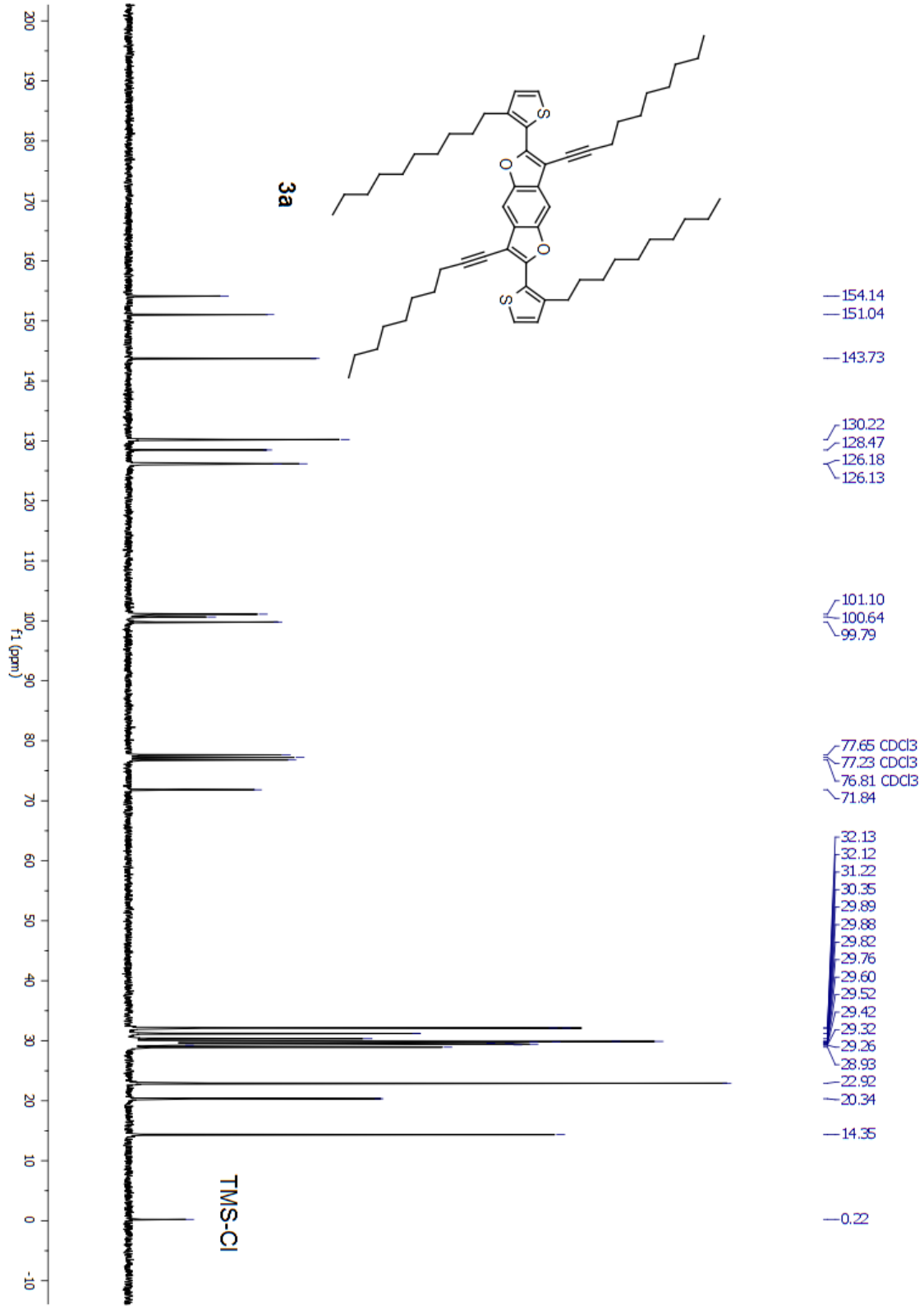

Figure S10. ^{13}C NMR of 3,7-di(dec-1-yn-1-yl)-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**3a**)

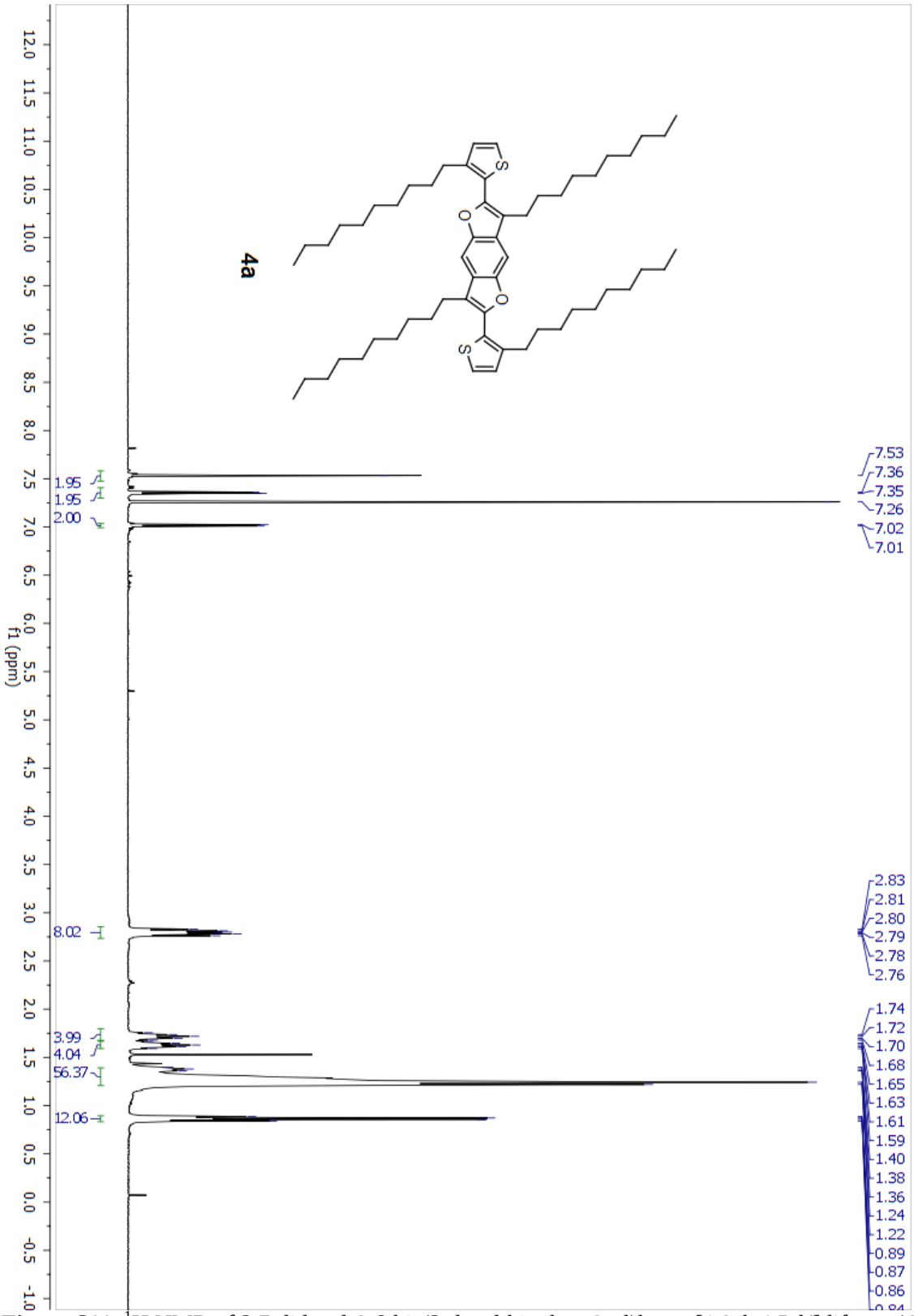

Figure S11. ^{1}H NMR of 3,7-didecyl-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**4a**)

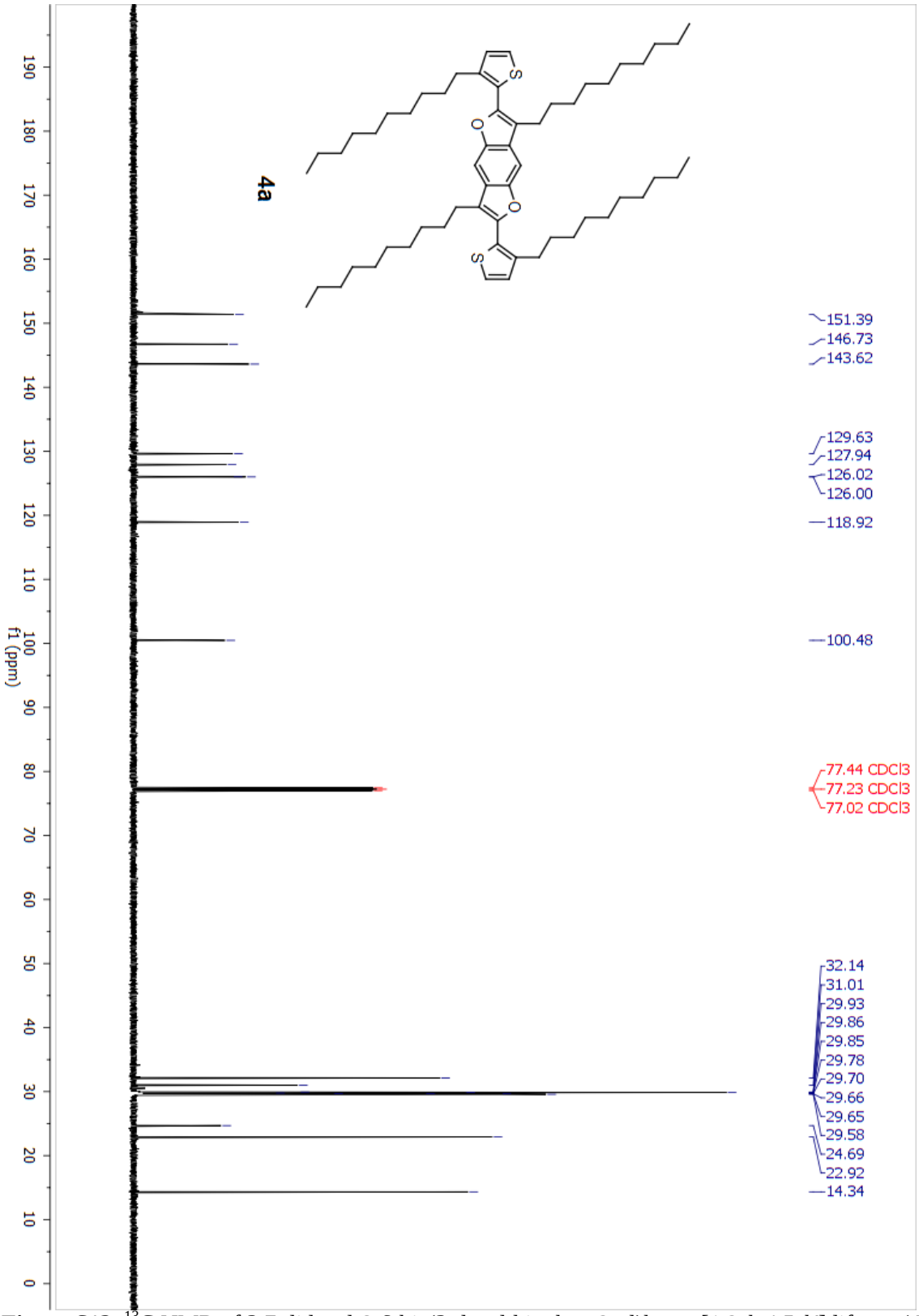

Figure S12. ^{13}C NMR of 3,7-didecyl-2,6-bis(3-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**4a**)

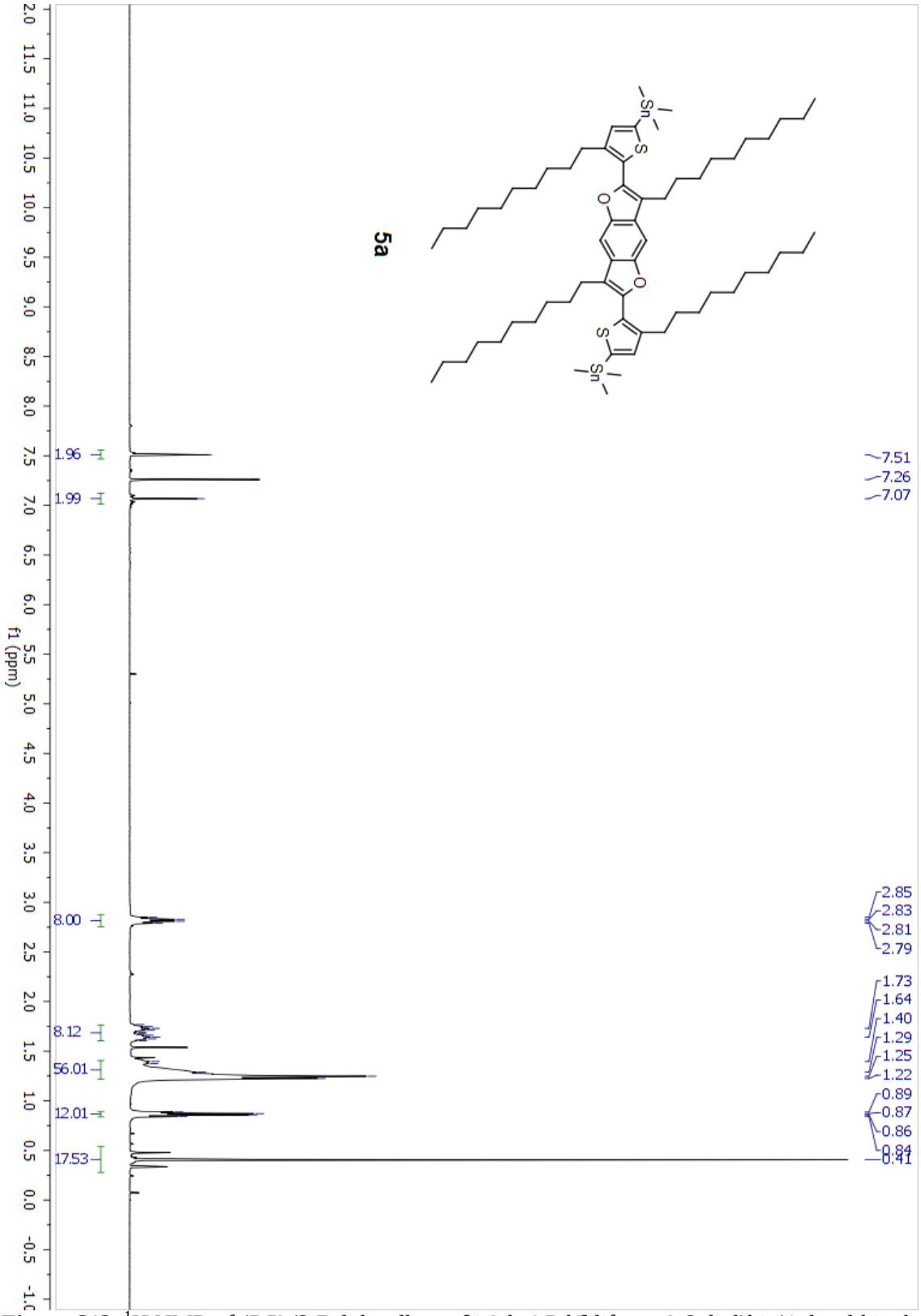

Figure S13. ^{1}H NMR of (5,5'-(3,7-didecylbenzo[1,2-b:4,5-*b*']difuran-2,6-diyl)bis(4-decylthiophene-5,2-diyl))bis(trimethylstannane) (**5a**)

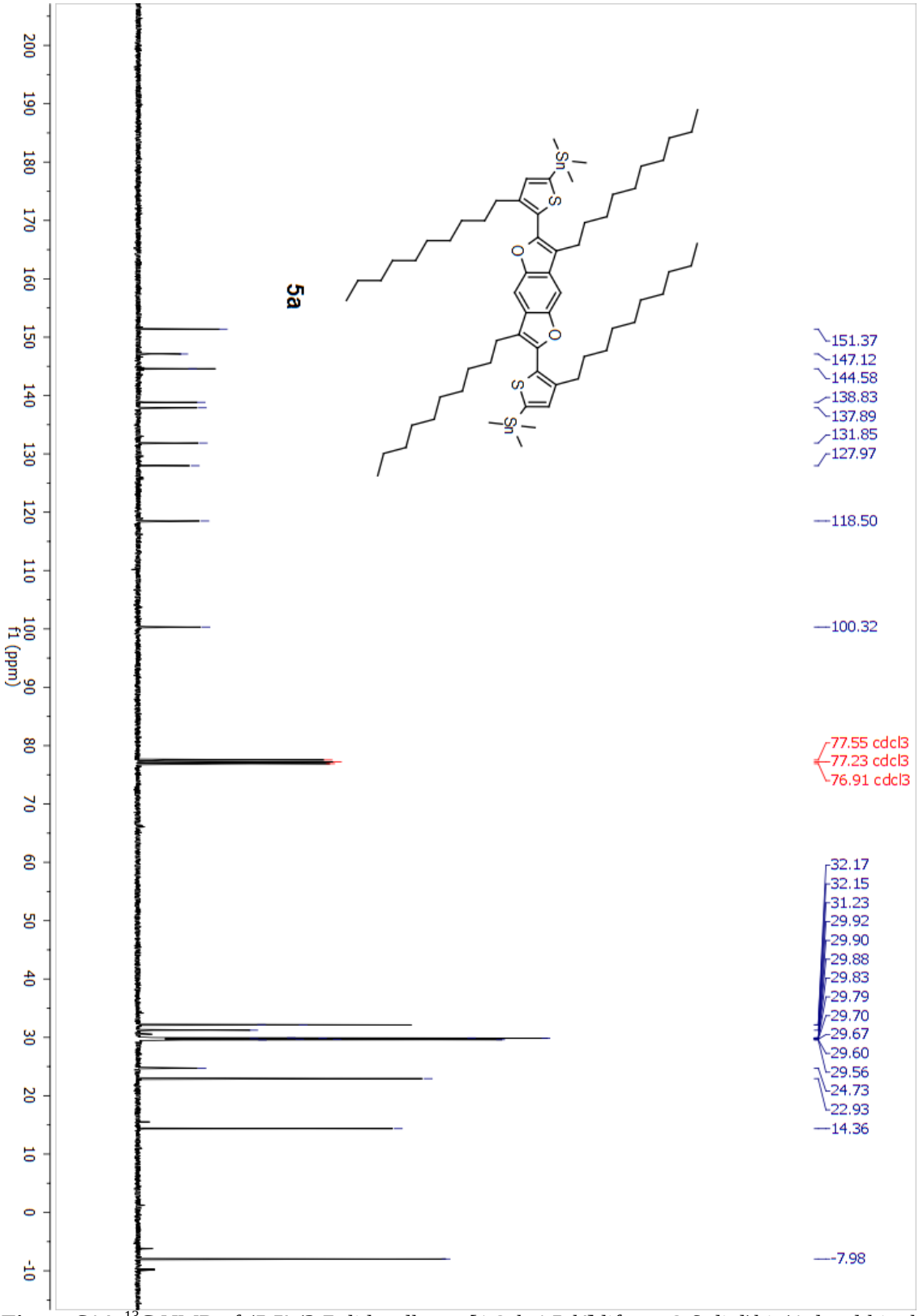

Figure S14. ^{13}C NMR of (5,5'-(3,7-didecylbenzo[1,2-*b*:4,5-*b*']difuran-2,6-diyl)bis(4-decylthiophene-5,2-diyl))bis(trimethylstannane) (**5a**)

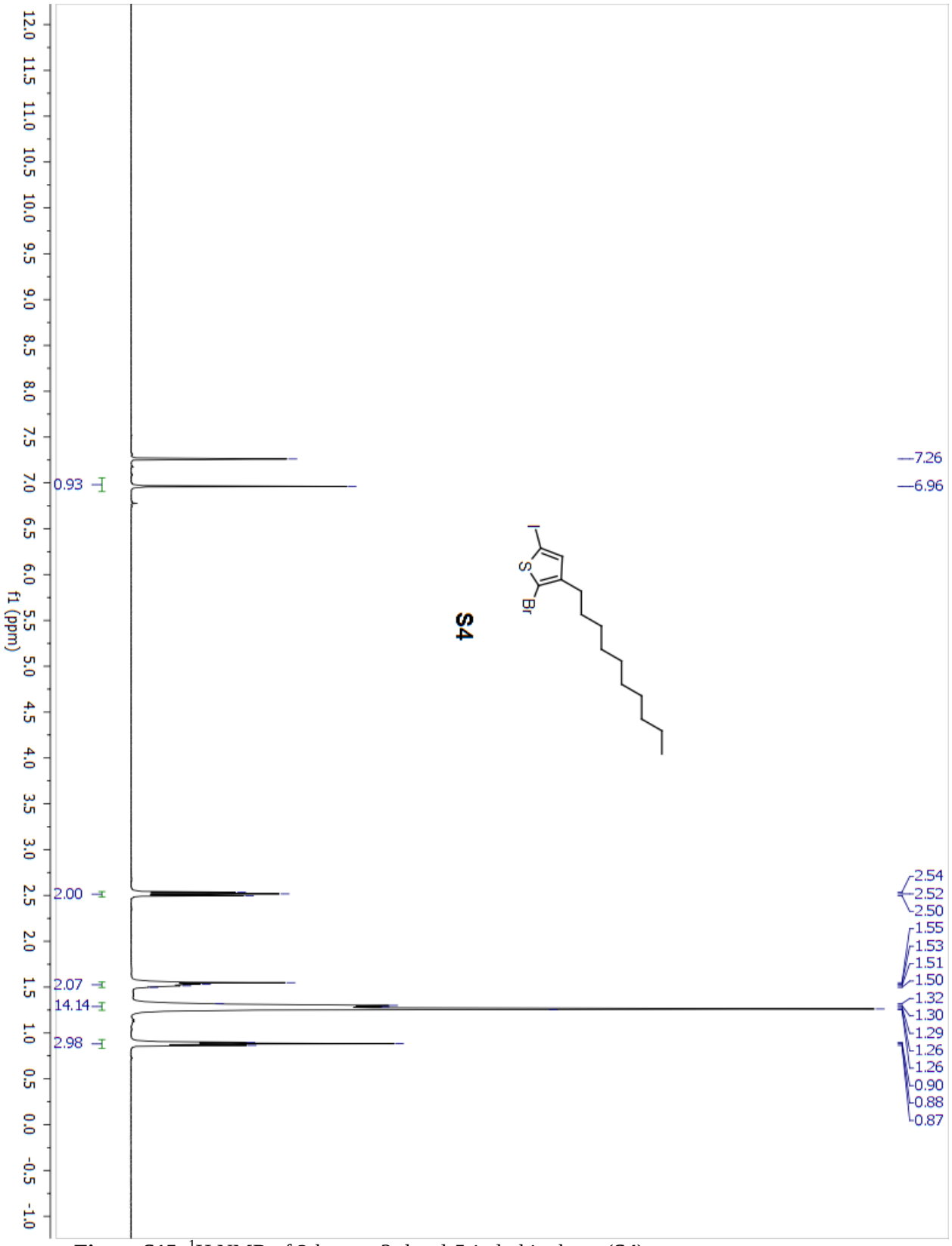

Figure S15. ^{1}H NMR of 2-bromo-3-decyl-5-iodothiophene (**S4**)

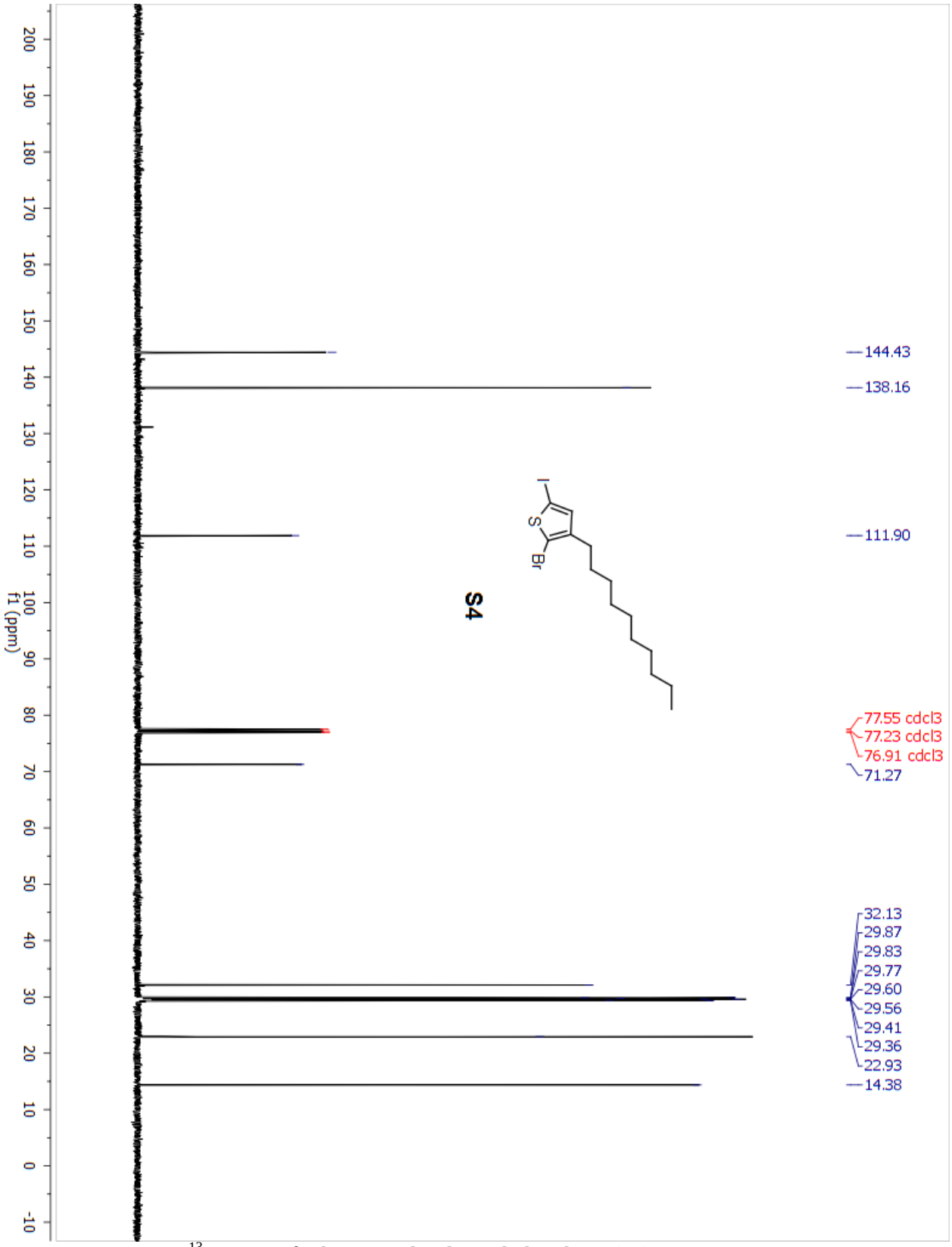

Figure S16. ^{13}C NMR of 2-bromo-3-decyl-5-iodothiophene (**S4**)

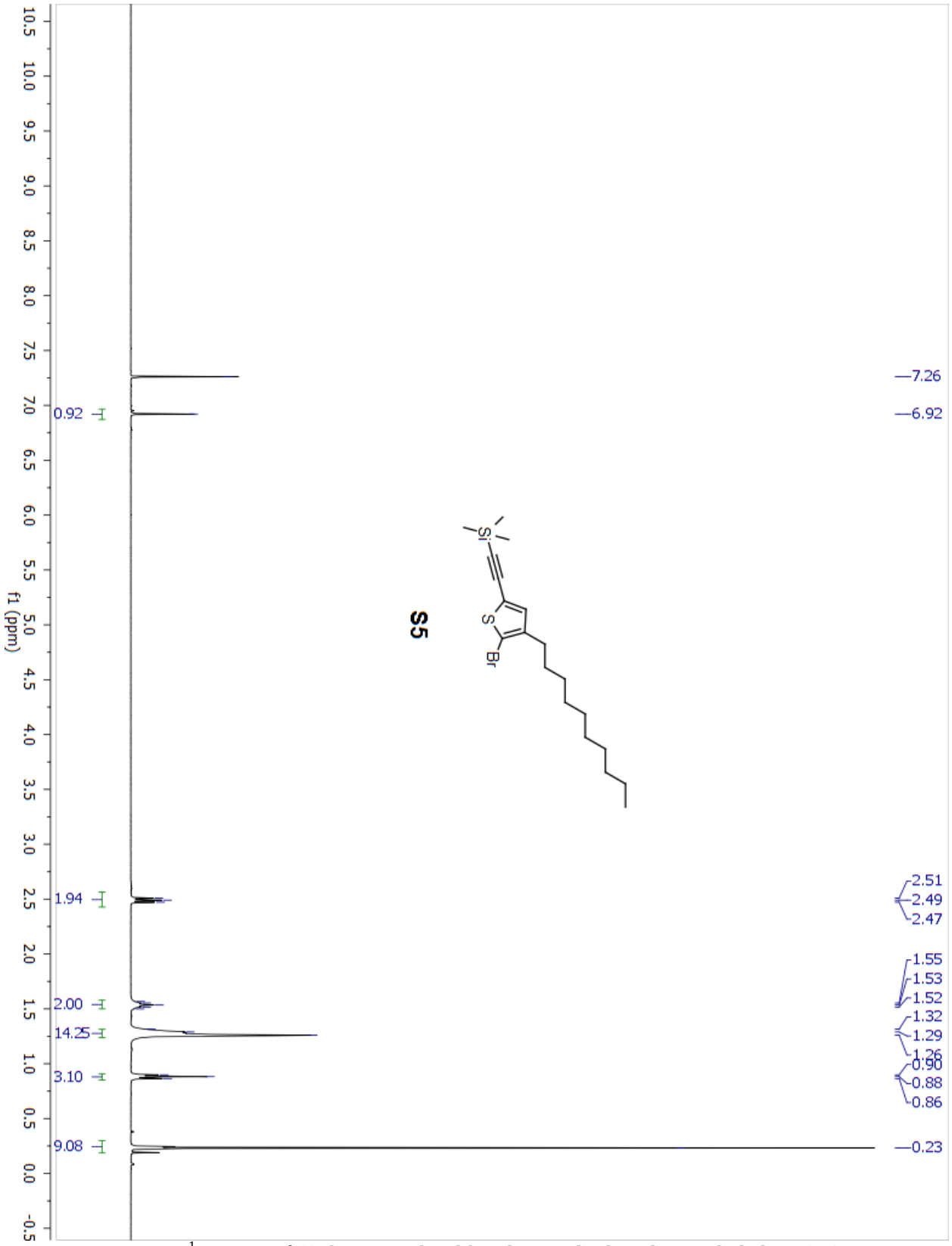

Figure S17. [1]H NMR of ((5-bromo-4-decylthiophen-2-yl)ethynyl)trimethylsilane (**S5**)

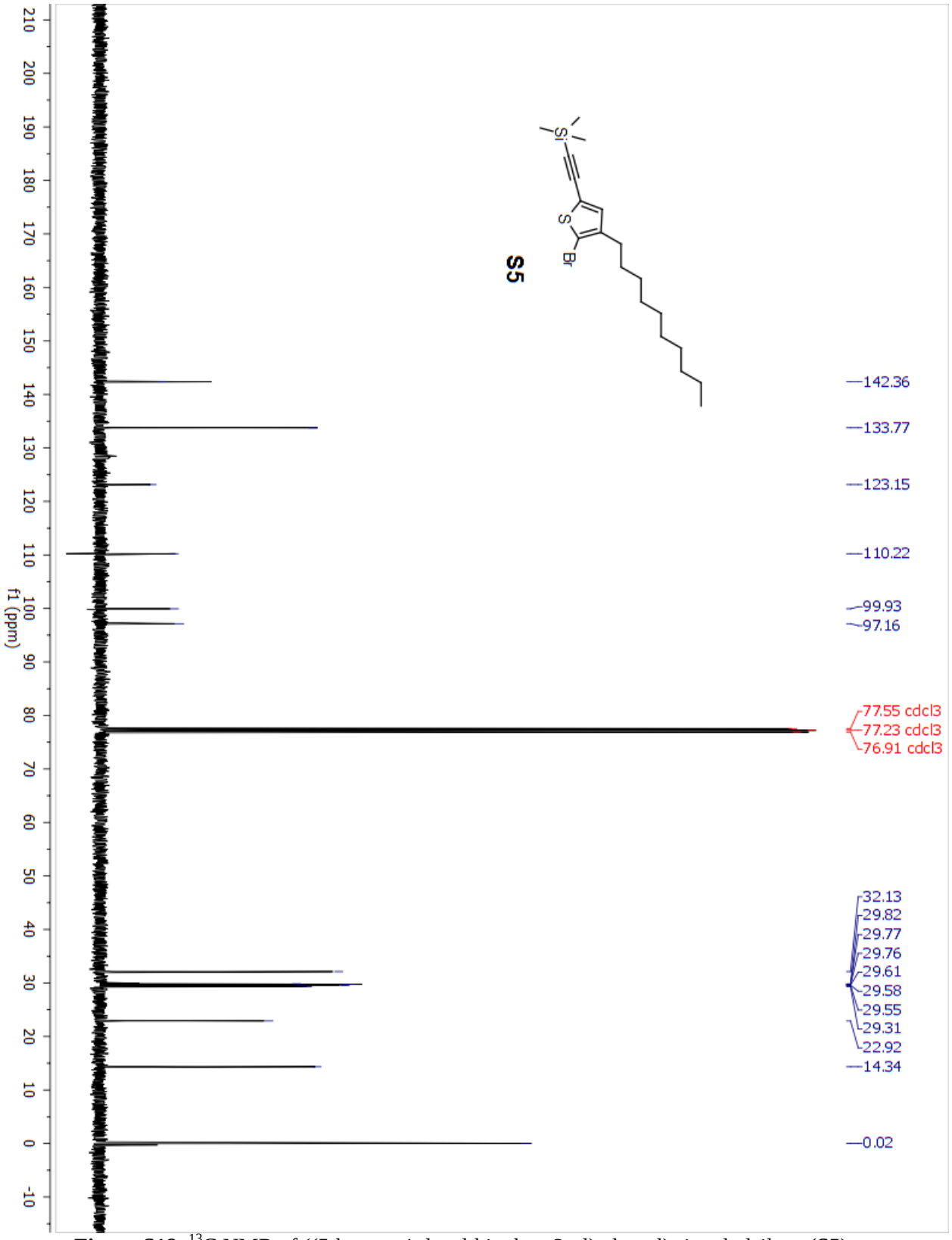

Figure S18. ^{13}C NMR of ((5-bromo-4-decylthiophen-2-yl)ethynyl)trimethylsilane (**S5**)

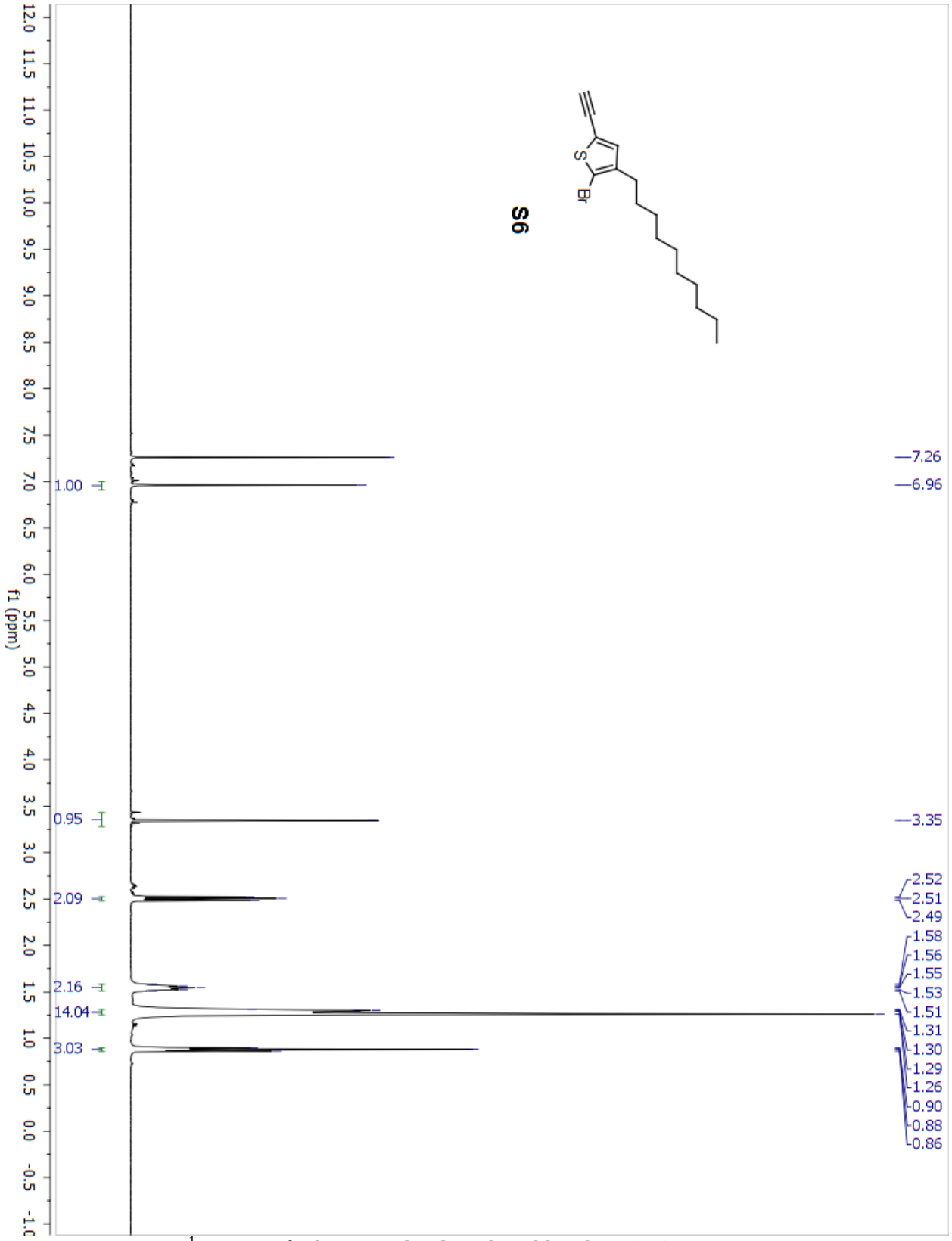

Figure S19. ^{1}H NMR of 2-bromo-3-decyl-5-ethynylthiophene (**S6**)

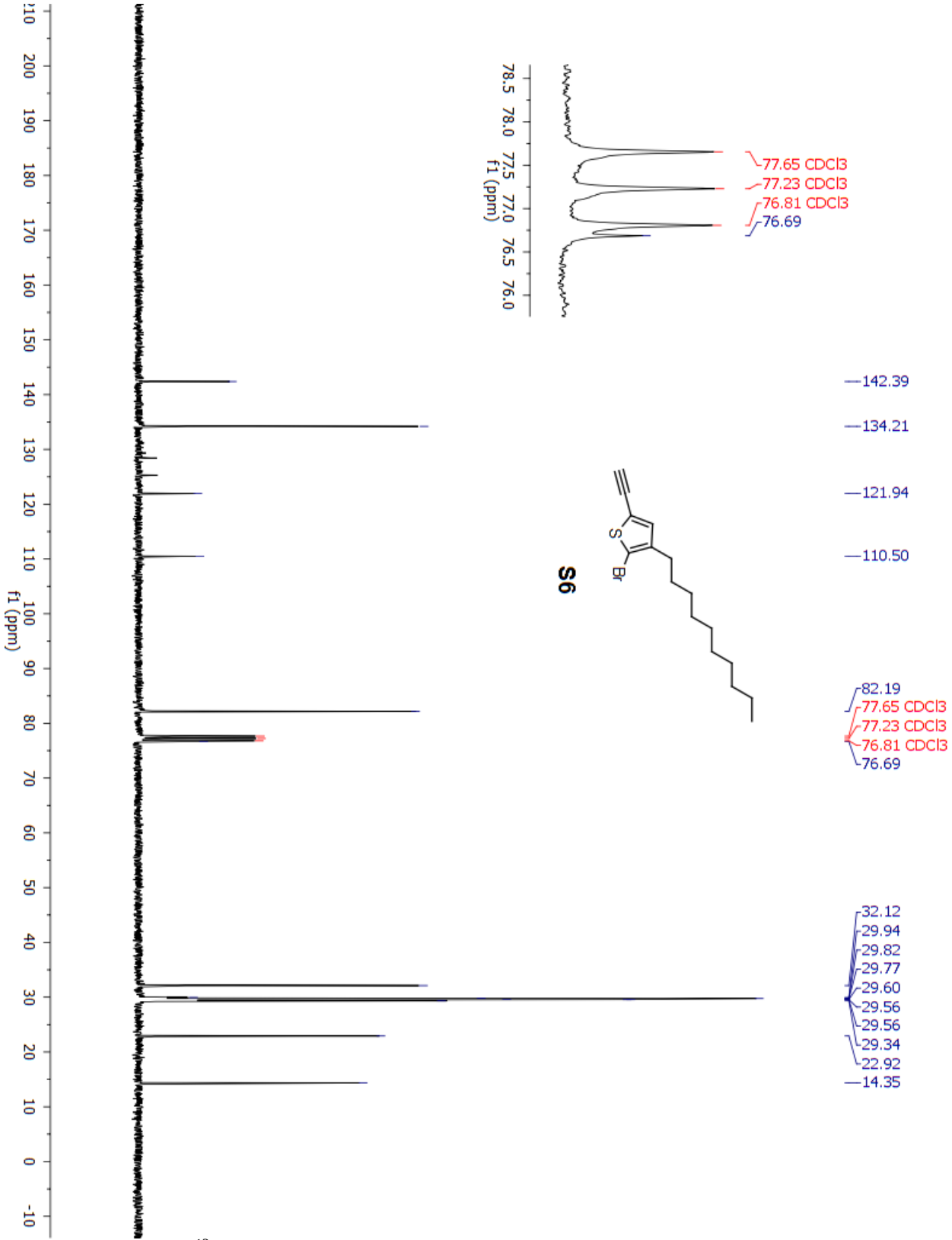

Figure S20. ^{13}C NRM of 2-bromo-3-decyl-5-ethynylthiophene (**S6**)

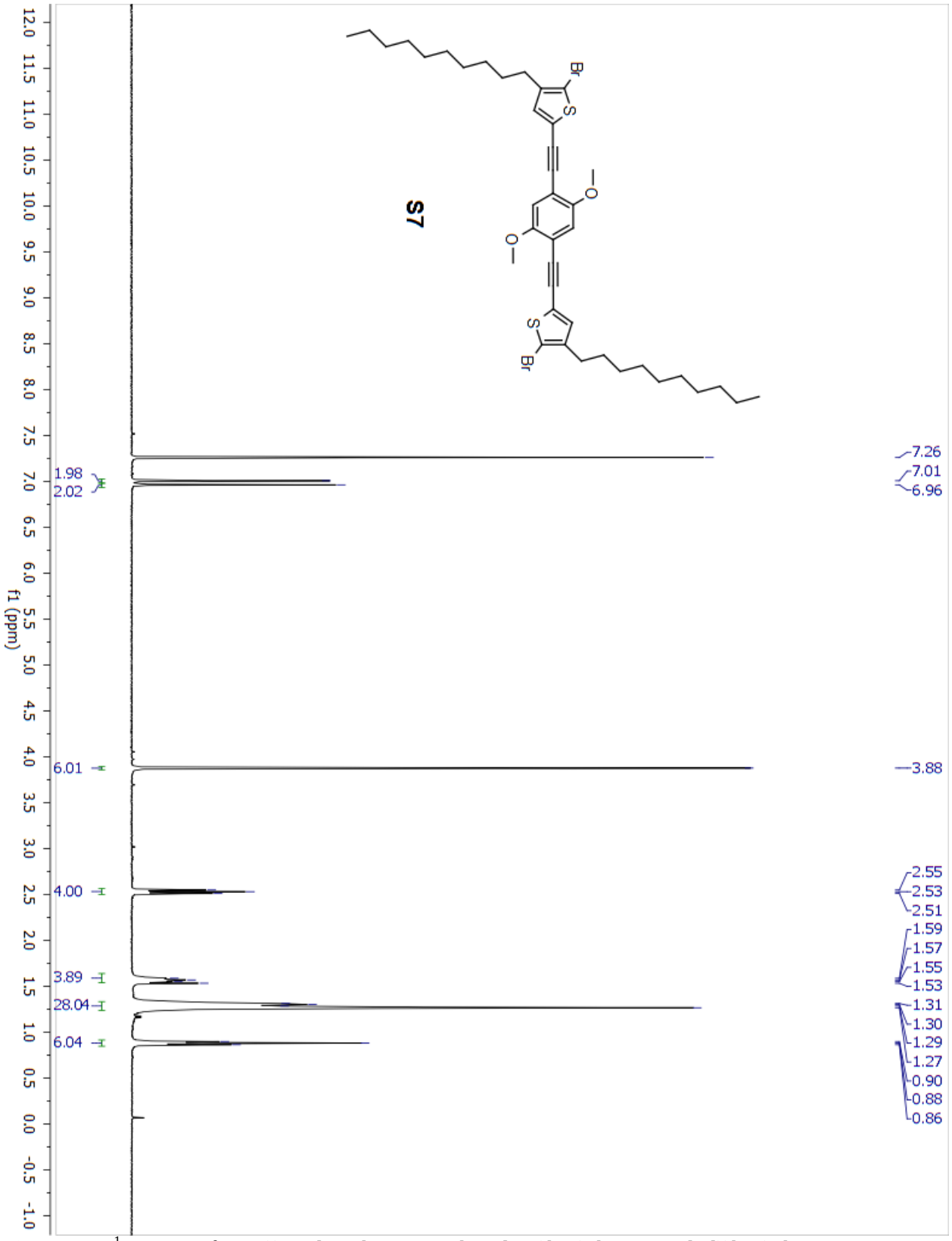

Figure S21. ^{1}H NMR of 5,5'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(2-bromo-3-decylthiophene) (**S7**)

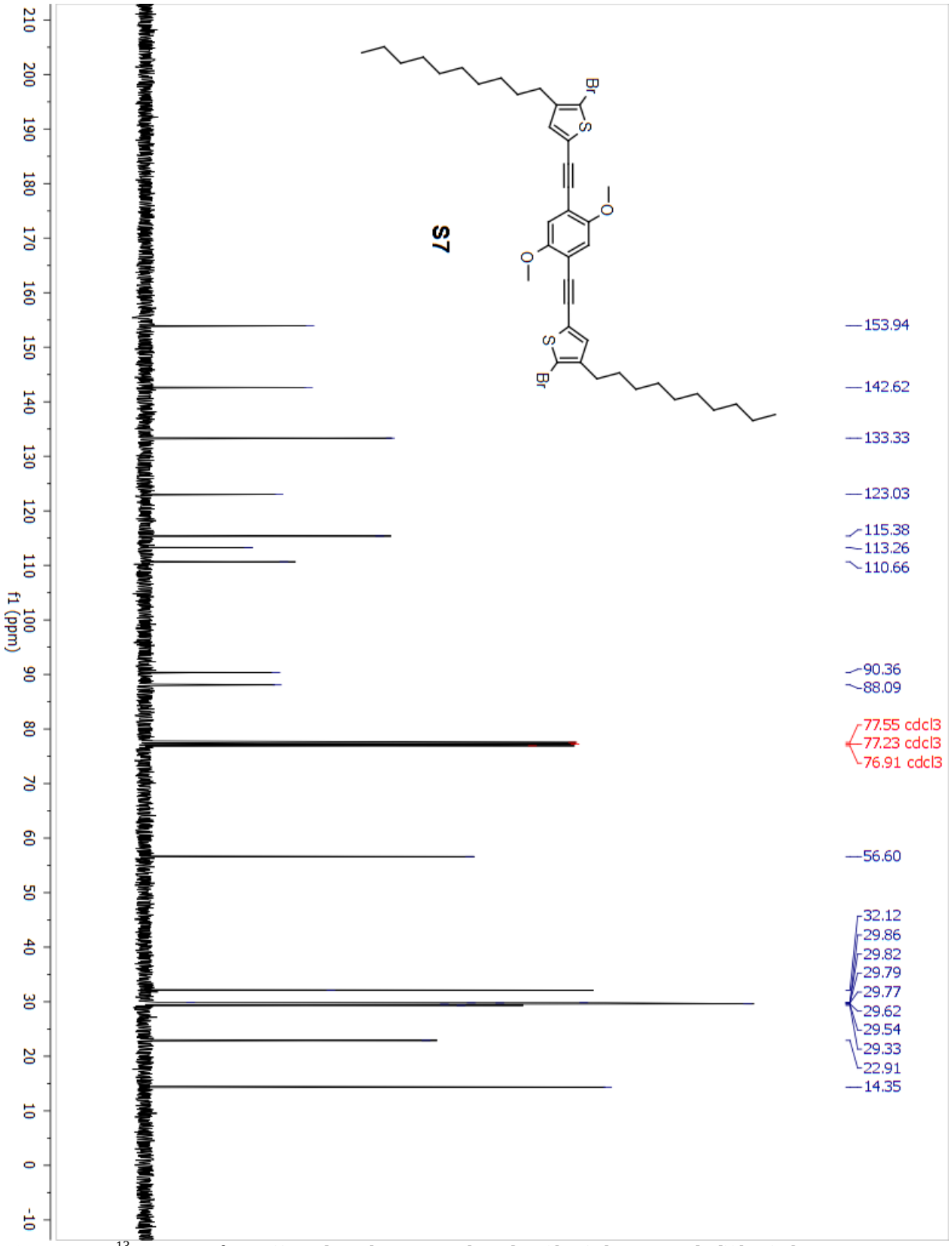

Figure S22. ^{13}C NMR of 5,5'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(2-bromo-3-decylthiophene) (**S7**)

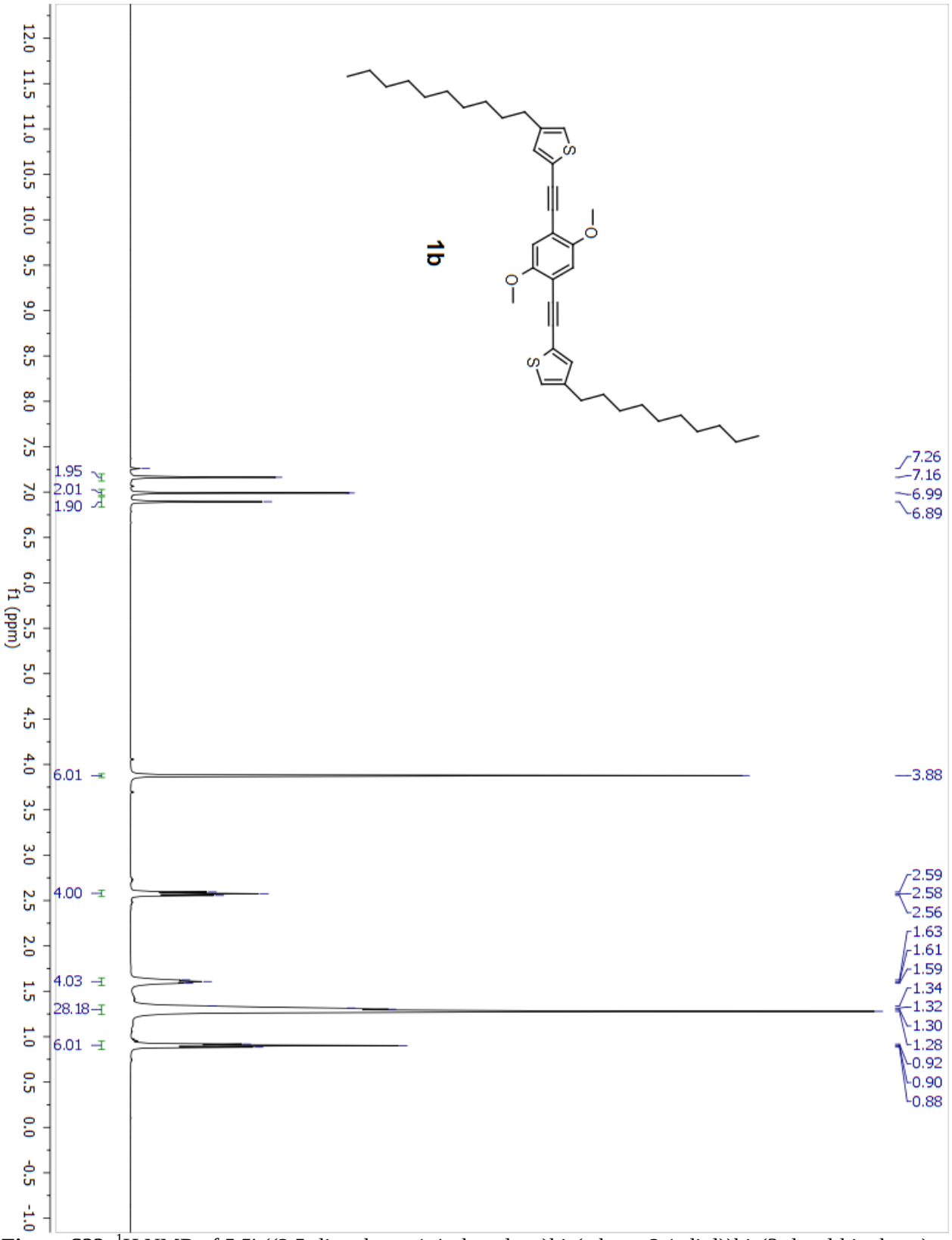

Figure S23. ^{1}H NMR of 5,5'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (**1b**)

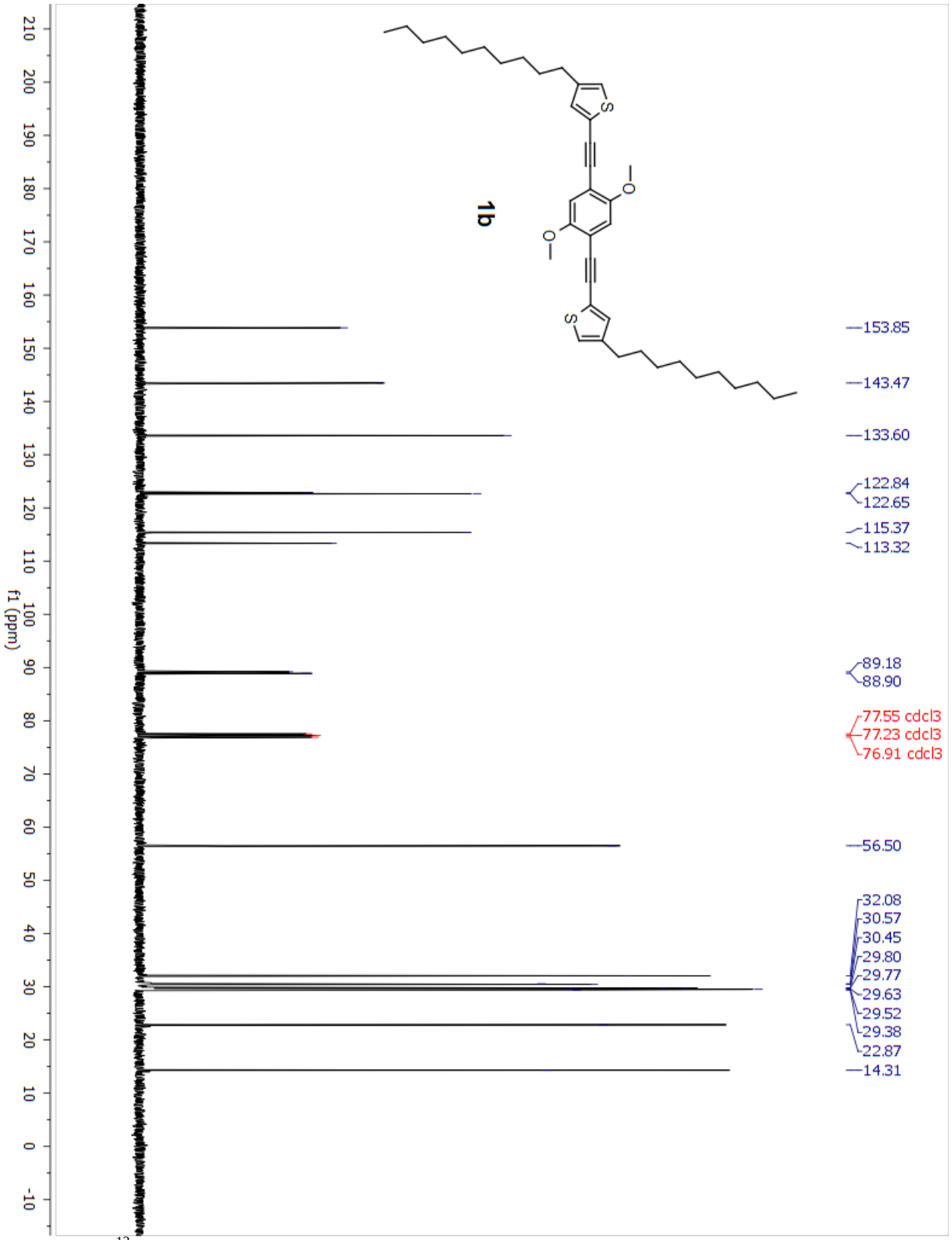

Figure S24. ^{13}C NMR of 5,5'-((2,5-dimethoxy-1,4-phenylene)bis(ethyne-2,1-diyl))bis(3-decylthiophene) (**1b**)

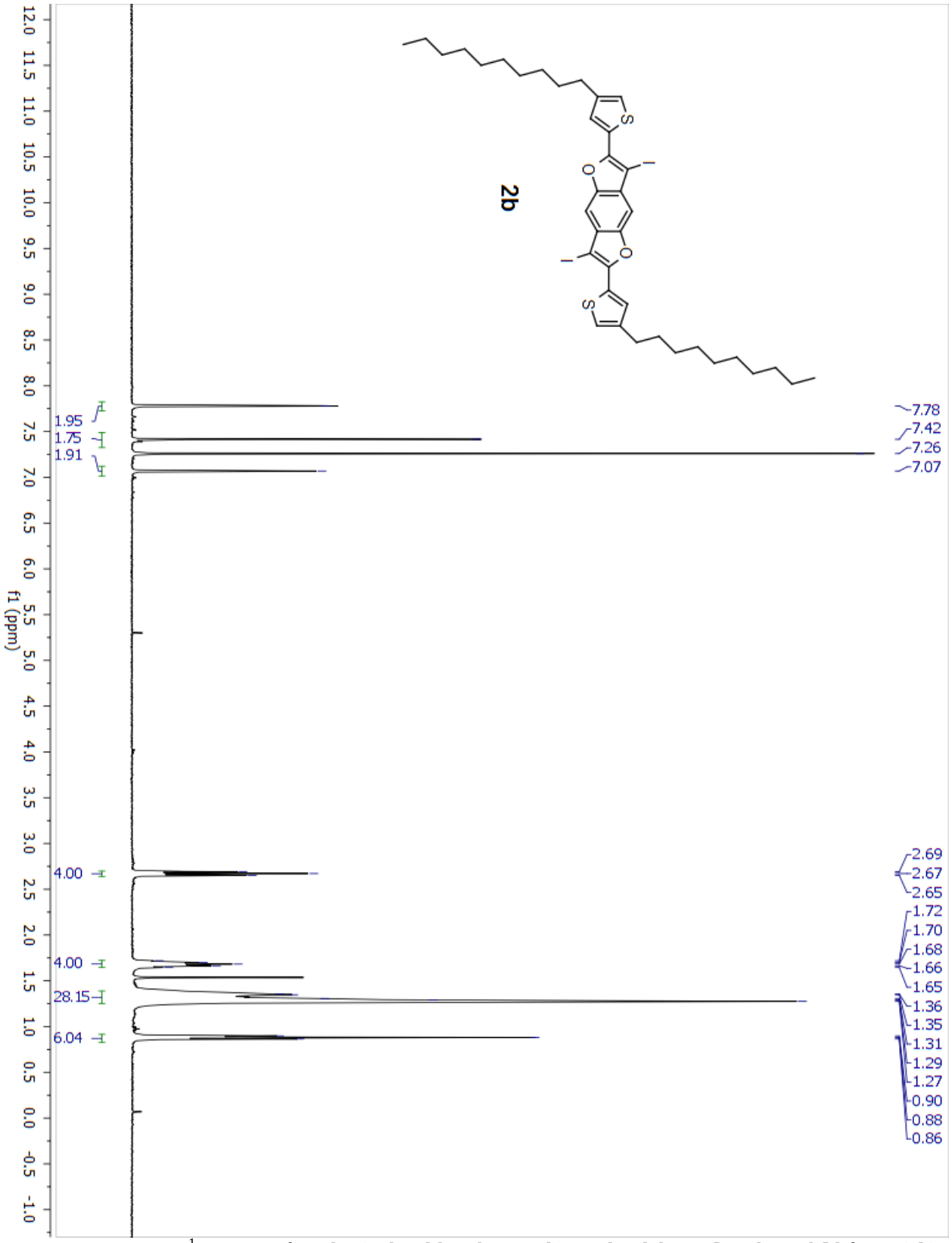

Figure S25. ^{1}H NMR of 2,6-bis(4-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (**2b**)

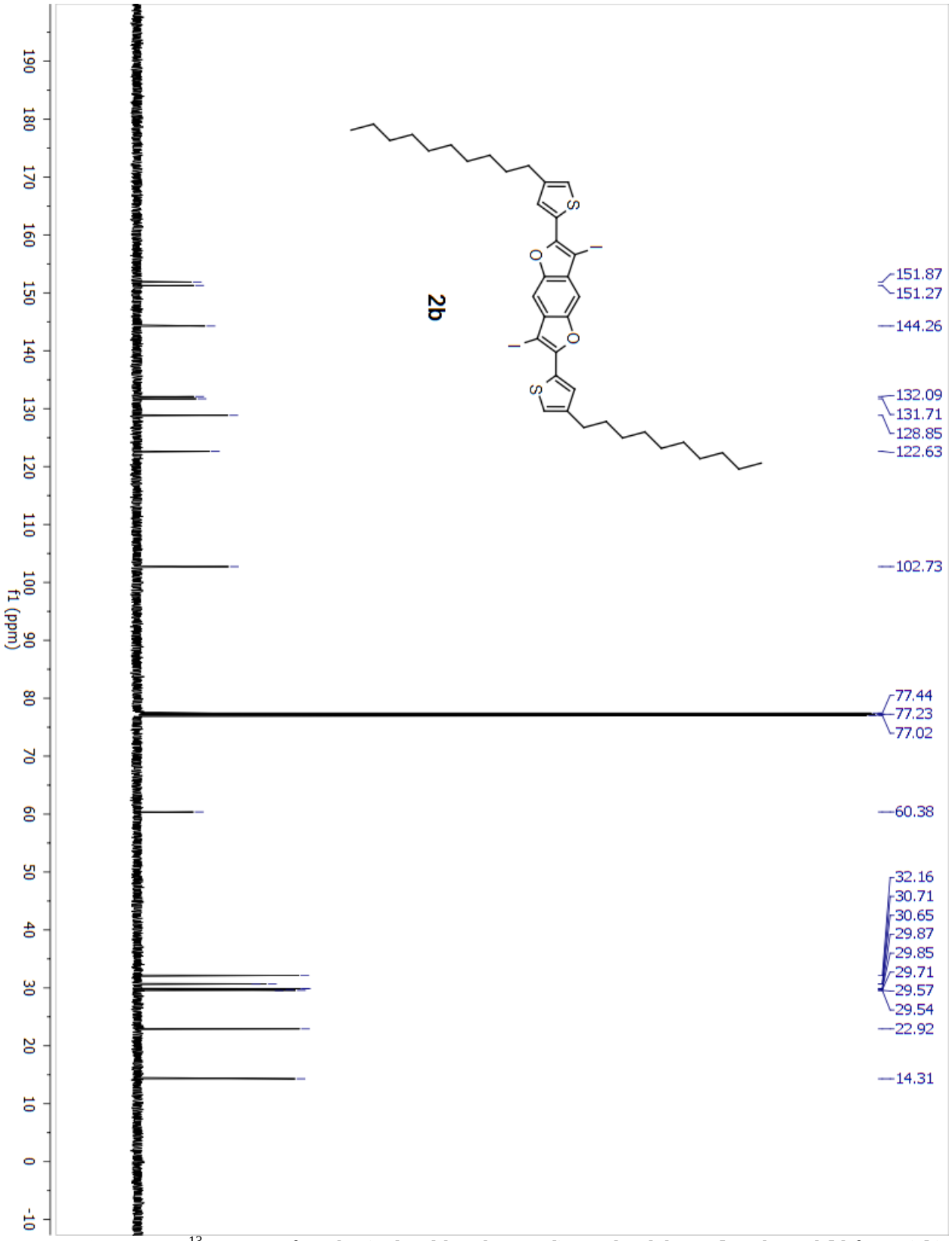

Figure S26. ^{13}C NMR of 2,6-bis(4-decylthiophen-2-yl)-3,7-diiodobenzo[1,2-*b*:4,5-*b*']difuran (**2b**)

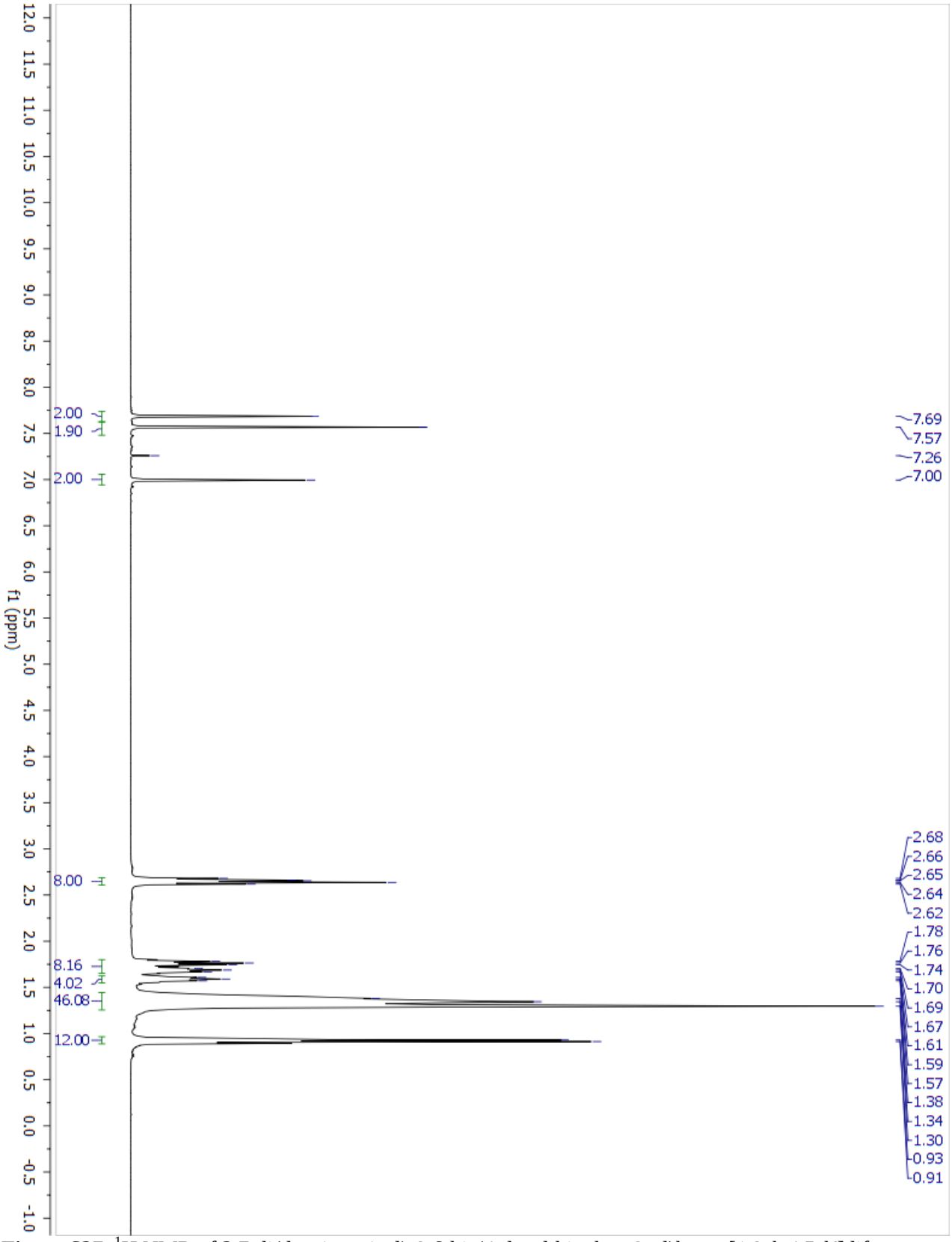

Figure S27. ^{1}H NMR of 3,7-di(dec-1-yn-1-yl)-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**3b**)

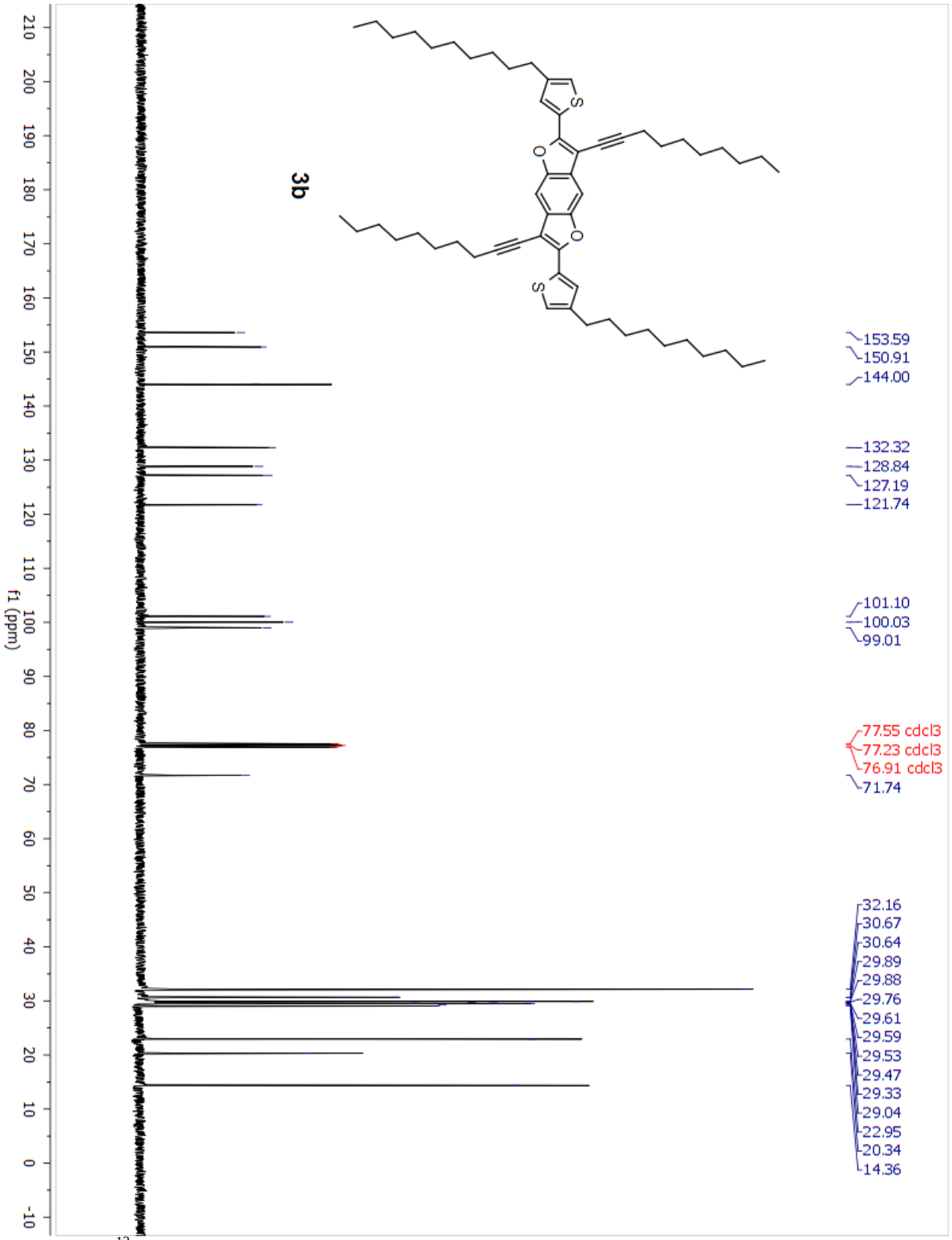

Figure S28. ^{13}C NMR of 3,7-di(dec-1-yn-1-yl)-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**3b**)

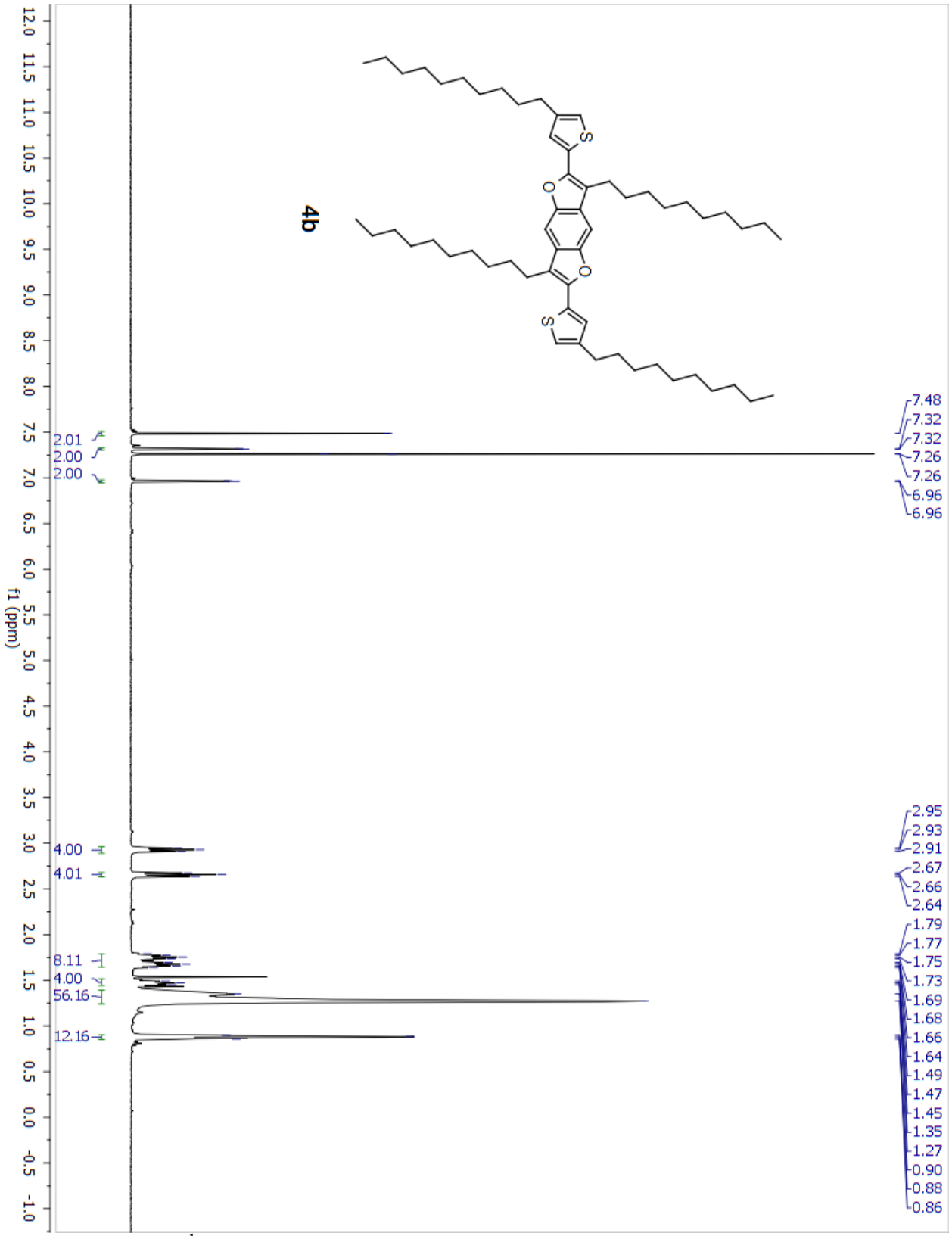

Figure S29. ^{1}H NMR of 3,7-didecyl-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**4b**)

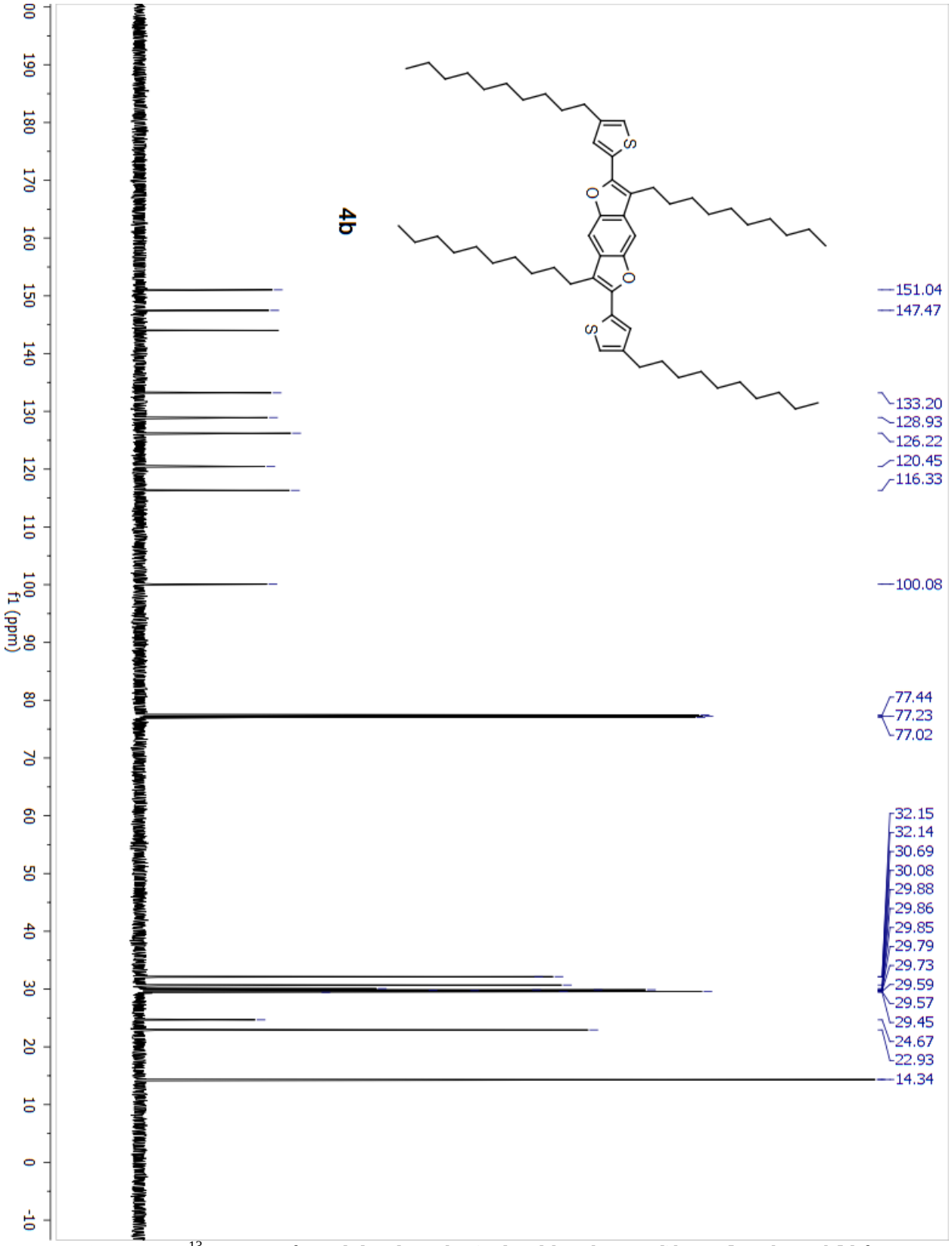

Figure S30. ^{13}C NMR of 3,7-didecyl-2,6-bis(4-decylthiophen-2-yl)benzo[1,2-*b*:4,5-*b*']difuran (**4b**)

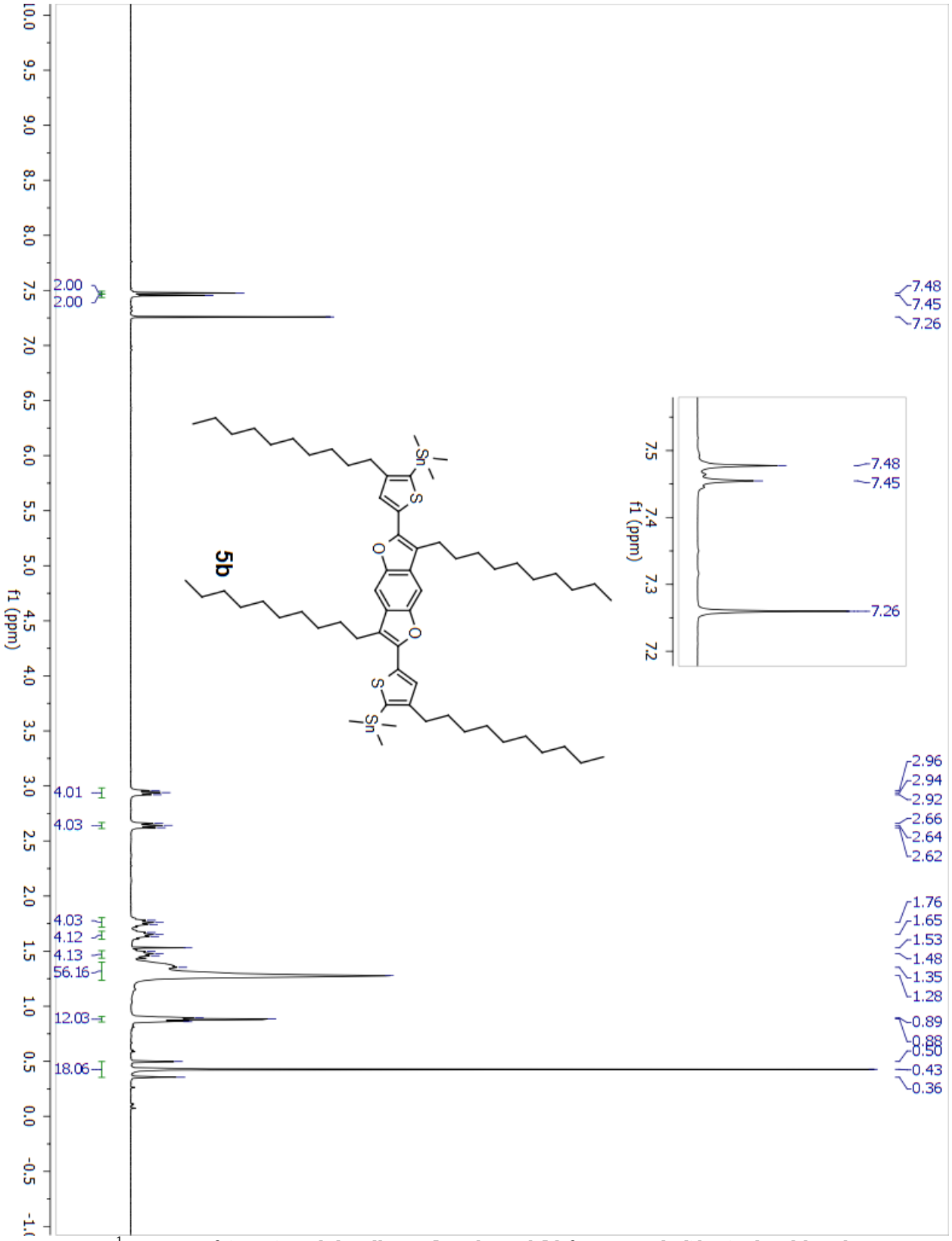

Figure S31. ^{1}H NMR of (5,5'-(3,7-didecylbenzo[1,2-*b*:4,5-*b*']difuran-2,6-diyl)bis(3-decylthiophene-5,2-diyl))bis(trimethylstannane) (**5b**)

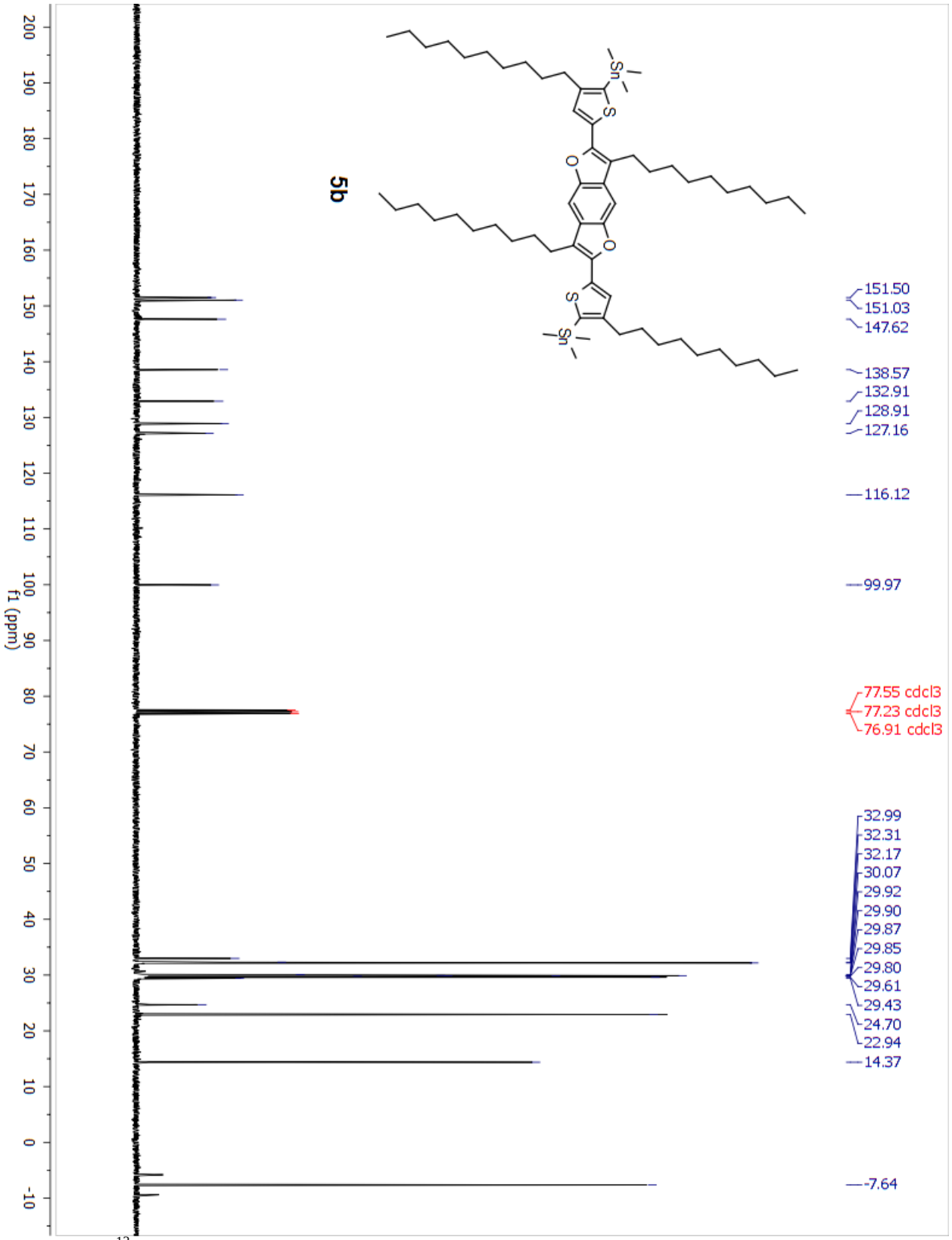

Figure S32. ^{13}C NMR of (5,5'-(3,7-didecylbenzo[1,2-*b*:4,5-*b*']difuran-2,6-diyl)bis(3-decylthiophene-5,2-diyl))bis(trimethylstannane) (**5b)**

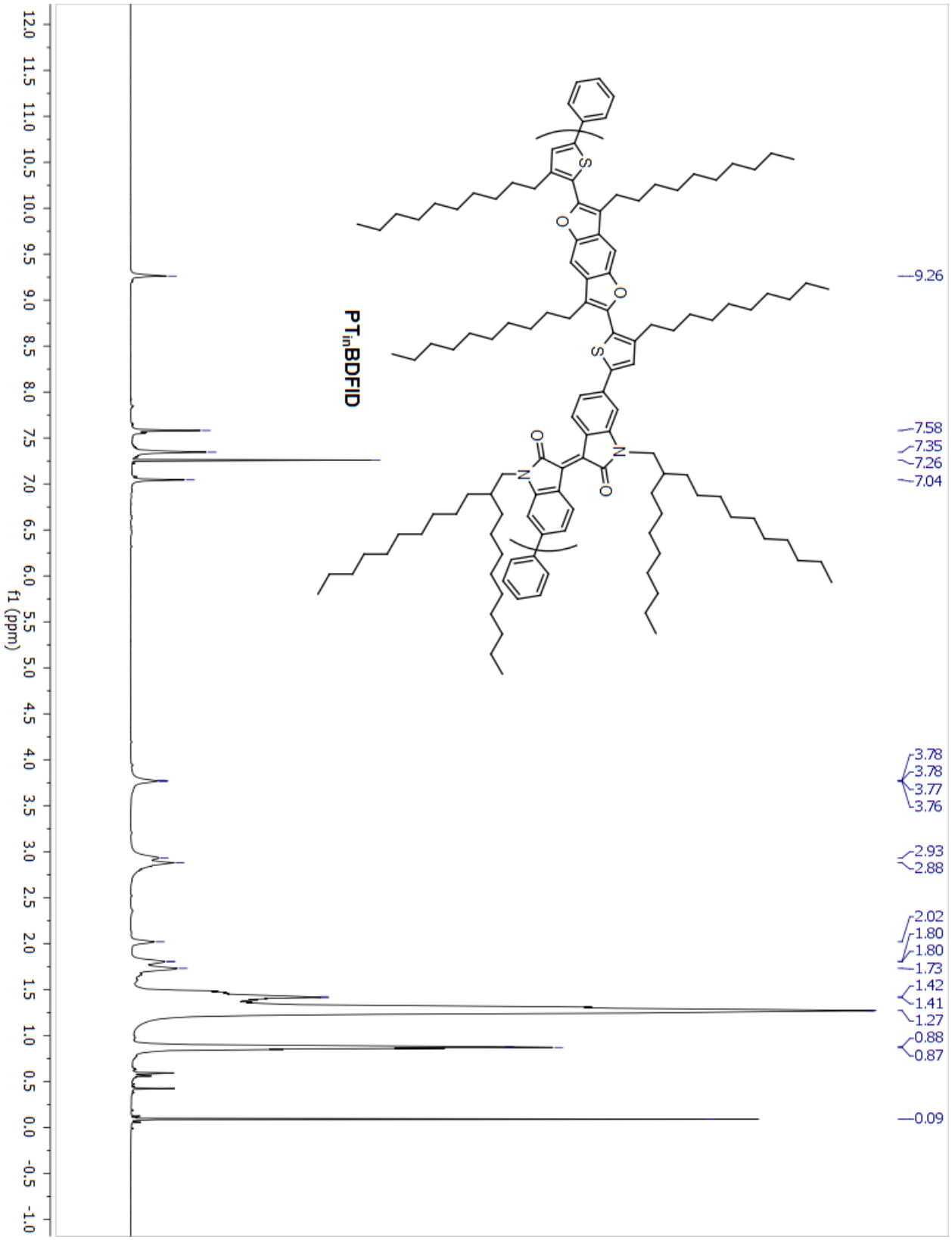

Figure S33. ^{1}H NMR of **PT_{out}BDFID**.

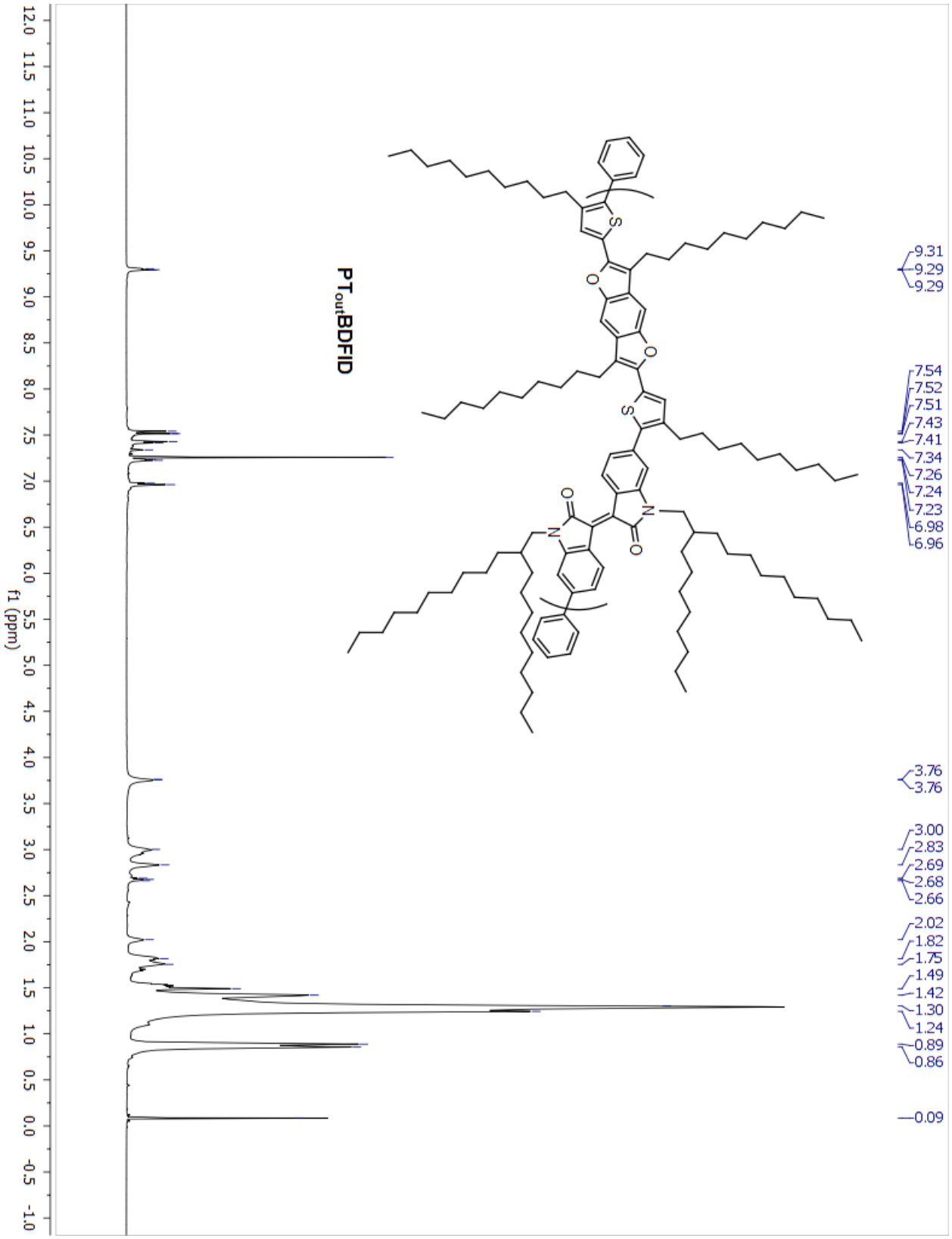

Figure S34. ^{1}H NMR of **PT$_{out}$BDFID**.

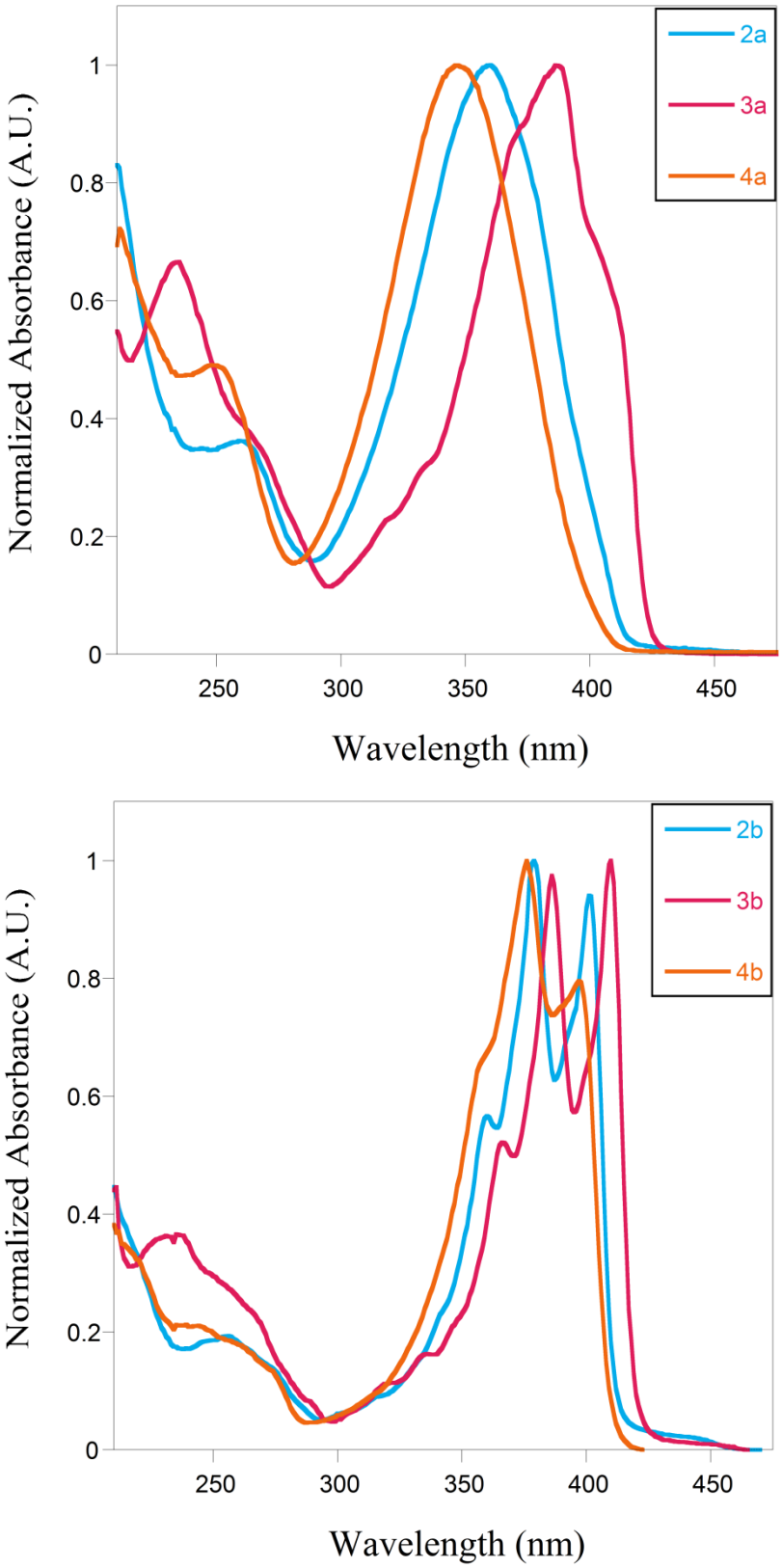

Figure S35. Normalized UV-vis absorption spectra of **2a**, **3a**, **4a**, **2b**, **3b**, and **4b** solutions in THF.

Table S1. Optical properties of Compounds **2a**, **3a**, **4a**, **2b**, **3b**, and **4b**.

Compound	**2a**	**3a**	**4a**	**2b**	**3b**	**4b**
λ_{max} (nm)	360	386	346	379, 401	386, 410	376, 397

Table S2. Electronic and optical properties of PTBDFID

Polymer	E_{onset}^{ox} (eV)	E_{onset}^{red} (eV)	HOMO[a] (eV)	LUMO[b] (eV)	E_g^{opt} (eV)[c]	E_g^{EC} (eV)[d]
PT_{out}BDFID	0.56	-1.35	-5.66	-3.75	1.67	1.91
PT_{in}BDFID	0.60	-1.32	-5.70	-3.78	1.58	1.88

[a] HOMO= -(E_{onset}^{ox} + 5.1) (eV). [b] LUMO = -(E_{onset}^{red} + 5.1) (eV).
[c] Estimated from the optical absorption edge. [d] Onset of potentials (vs Fc).

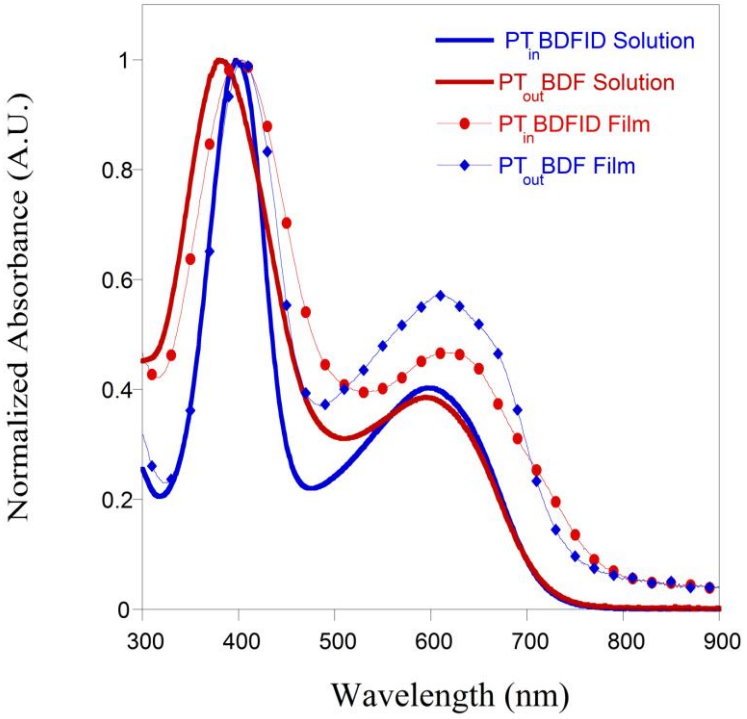

Figure S36. Normalized UV-vis absorption spectra of solutions ($CHCl_3$) and thin films of **PT_{in}BDFID** and **PT_{in}BDFID** polymerized using $Pd(PPh_3)_4$

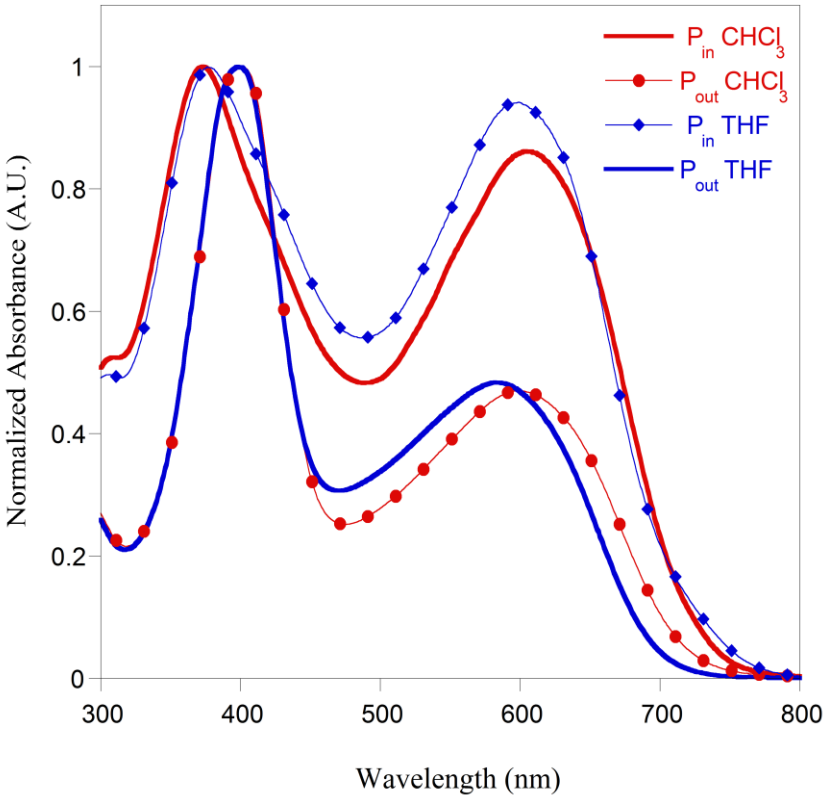

Figure S37. Normalized UV-vis absorption spectra of solutions of **PT_{in}BDFID** and **PT_{in}BDFID** polymers (polymerized using $Pd_2(dba)_3$/P(*o*-tol)$_3$) in THF and $CHCl_3$.

Table S3. Optical properties of PT_{out}BDFID and PT_{in}BDFID.

Polymer	Solvent	λ_{max} high-energy (nm)	λ_{max} low-energy (nm)
PT_{out}BDFID	THF	398	599
PT_{out}BDFID	$CHCl_3$	373	608
PT_{in}BDFID	THF	398	582
PT_{in}BDFID	$CHCl_3$	400	598

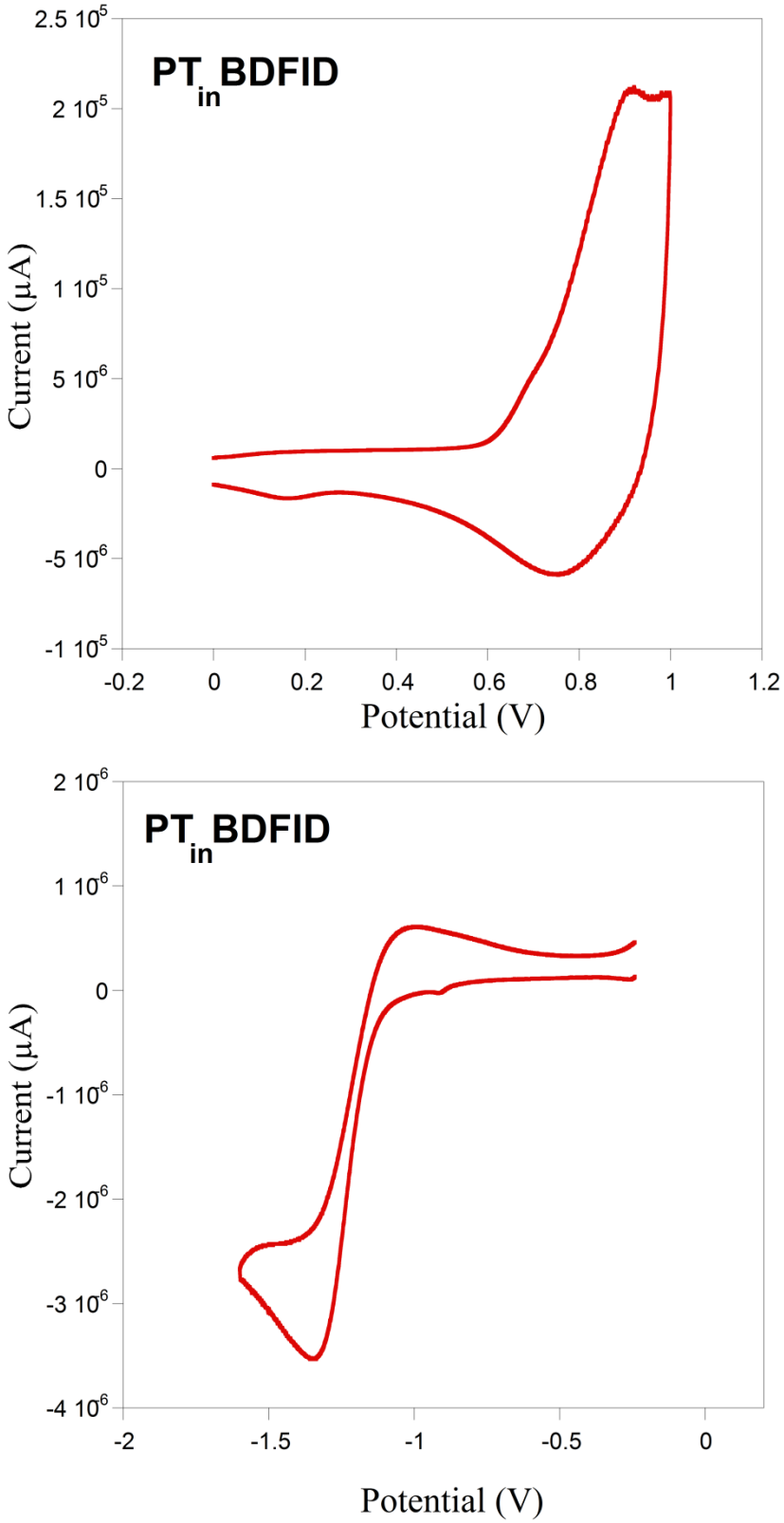

Figure S38. Cyclic voltammetry traces of **PT_{in}BDFID.**

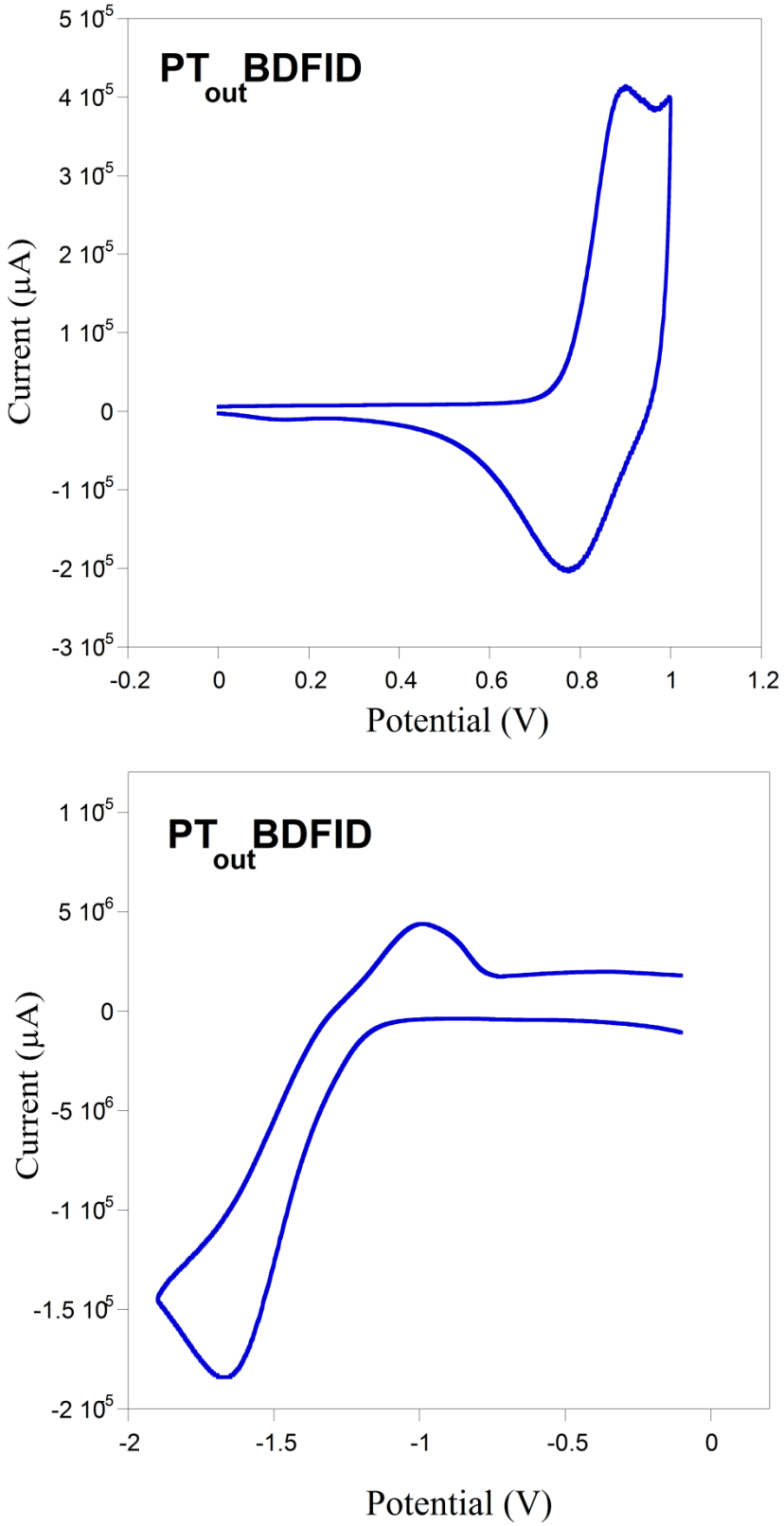

Figure S39. Cyclic voltammetry traces of **PT_{out}BDFID.**

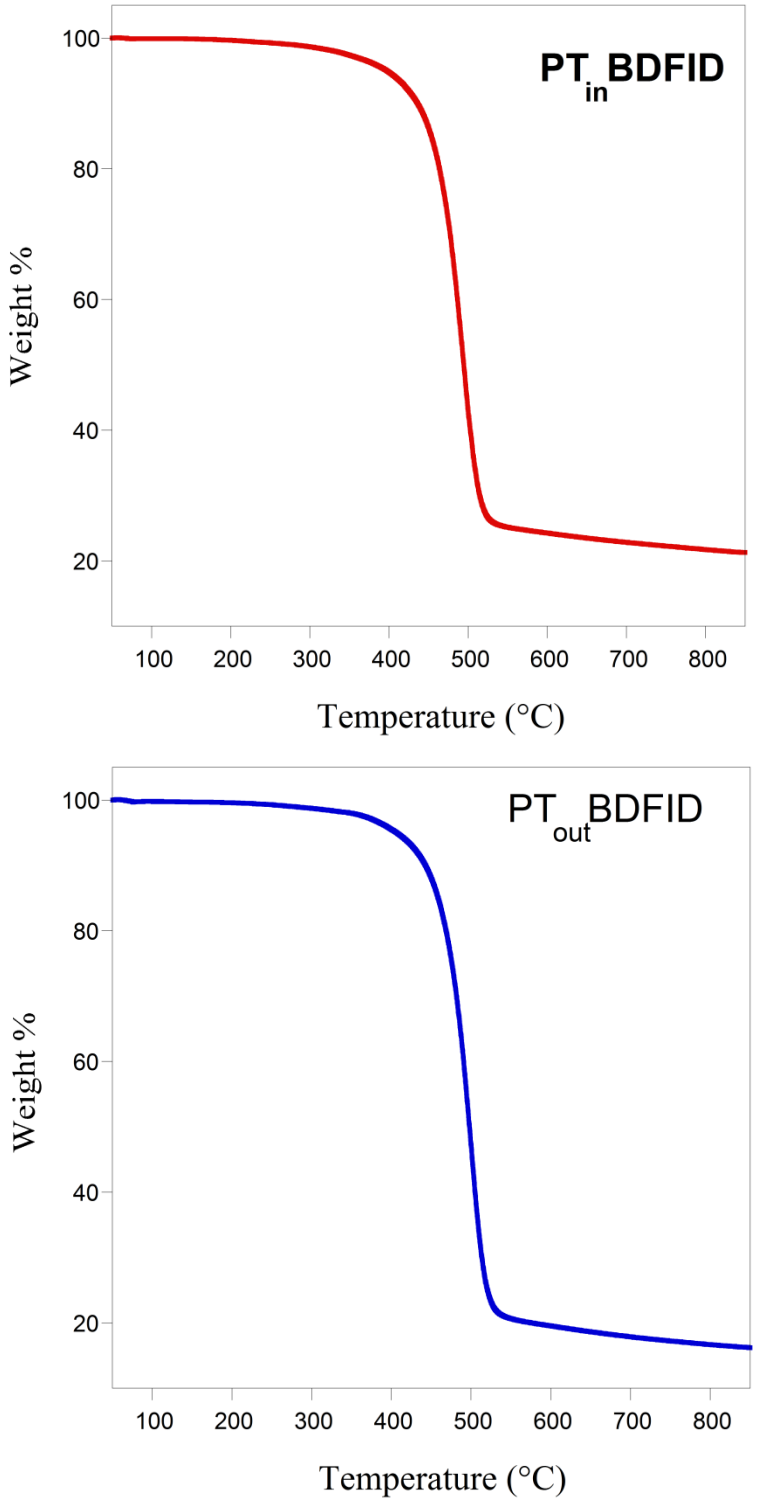

Figure S40. Thermal Gravometric Analysis of **PT$_{in}$BDFID** (top) and **PT$_{out}$BDFID** (bottom).

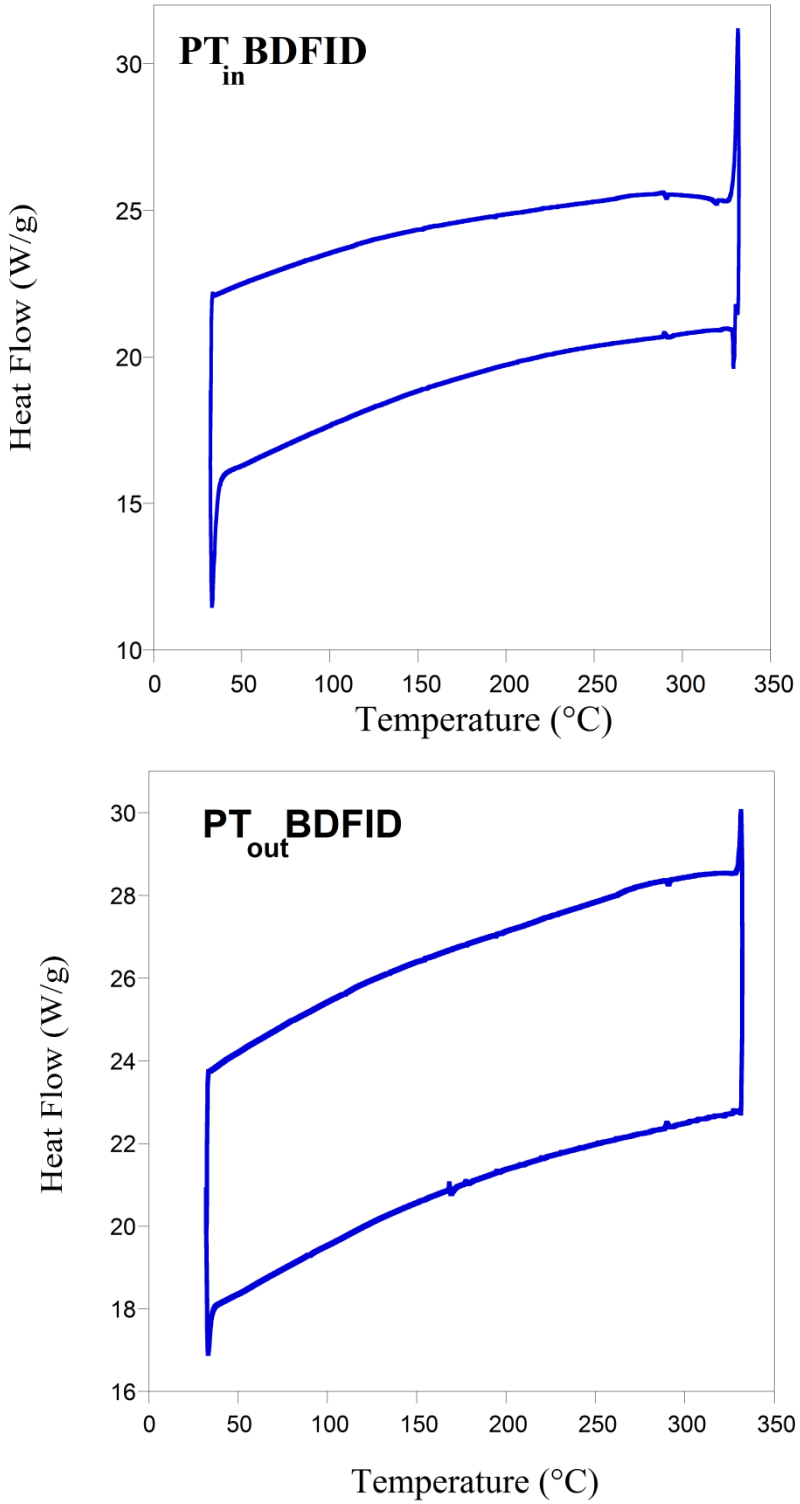

Figure S41. Differential Scanning Calorimetry of **PT_{in}BDFID** (top) and **PT_{out}BDFID** (bottom).

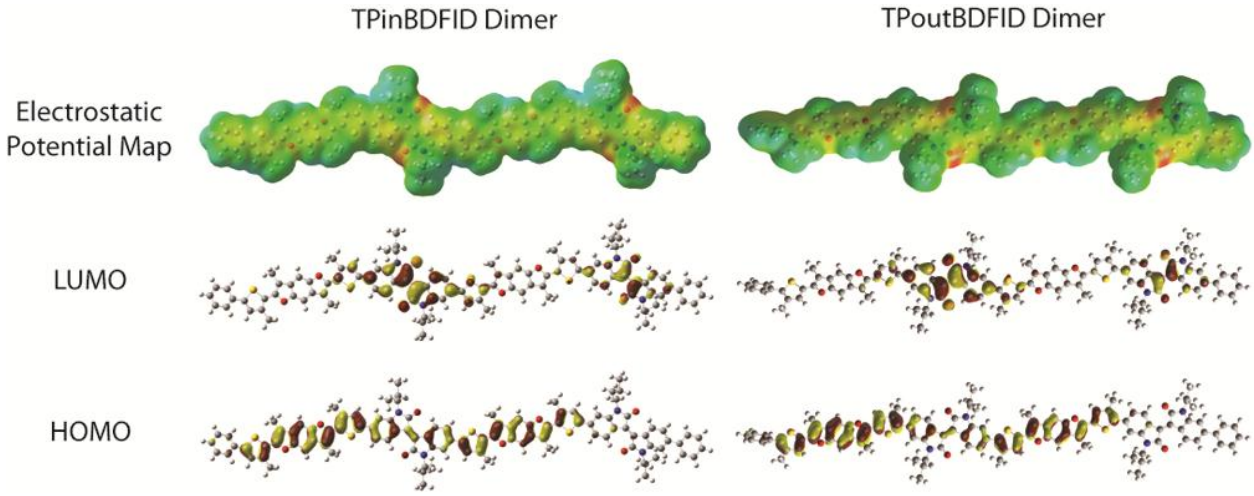

Figure S42. The electrostatic potential maps and frontier orbitals for TPinBDFID and TPoutBDFID dimers.

Table S4. Cartesian coordinates of optimized geometry for **TP_{in}BDFID** dimer.

C	-18.78532000	0.77393700	0.35373700
C	-18.49161200	-0.58254100	0.66071100
C	-20.05115200	1.33913000	0.39942600
C	-19.52782000	-1.45536900	1.04255700
C	-21.08683300	0.46628700	0.78099700
H	-20.21827600	2.38909600	0.15522700
C	-20.79306200	-0.89052100	1.08709200
H	-19.36092900	-2.50478800	1.28924800
O	-17.63898000	1.42321100	0.01166600
C	-16.60520500	0.51206200	0.09007700
O	-21.93970500	-1.54028600	1.42661700
C	-22.97398400	-0.63002400	1.34514400
C	-17.06997200	-0.73198100	0.48271200
C	-22.51088200	0.61233700	0.94927500
C	-23.29093600	1.87230200	0.72807300
H	-23.56523900	2.36431900	1.67746700
H	-22.70127000	2.59410000	0.14343100
H	-24.22701600	1.68598000	0.17856600
C	-16.28869500	-1.99372000	0.68923900
H	-15.54799000	-1.89483900	1.50058700
H	-16.95803100	-2.82496600	0.95385200
H	-15.73474400	-2.29013100	-0.21691500
C	-24.28527200	-1.13572700	1.67687600
C	-24.68900200	-2.45677900	1.88590500

S	-25.62905100	-0.03241900	1.89918100
C	-26.07216400	-2.53816700	2.20619200
C	-26.73907300	-1.32887400	2.25081600
H	-26.57294700	-3.49301000	2.37368800
C	-15.29354100	1.01137600	-0.24011700
C	-14.92237500	2.29047200	-0.67111100
S	-13.89413700	-0.03473700	-0.11731000
C	-13.52370300	2.38235000	-0.88982400
C	-12.80667300	1.22269200	-0.64572800
H	-13.05650300	3.30180800	-1.24499100
C	-15.85064200	3.45496300	-0.89750600
H	-16.63218600	3.21569200	-1.63428000
H	-16.37293300	3.74516900	0.02687700
H	-15.28671600	4.32577000	-1.26265700
C	-23.81467800	-3.67919200	1.78342500
H	-23.28147000	-3.72177800	0.82213300
H	-23.04317300	-3.69327400	2.56893300
H	-24.42180100	-4.59091400	1.88292100
C	-11.37195100	0.98269400	-0.77928800
C	-10.48722300	2.06425100	-1.00421100
C	-10.82759400	-0.31620900	-0.69401900
C	-9.13112500	1.81418400	-1.14034800
H	-10.86574600	3.08375300	-1.05817900
C	-9.46317200	-0.55897200	-0.83660800
H	-11.49032000	-1.16863800	-0.52930400
C	-8.57152500	0.50301600	-1.07318600
N	-8.11538700	2.74889500	-1.32917800
H	-9.08360000	-1.57391700	-0.78269000
C	-7.11807700	0.62989700	-1.22279600
C	-6.87931700	2.12580200	-1.35760500
C	-8.23622100	4.19597600	-1.40653000
C	-6.09931900	-0.30944700	-1.28428600
O	-5.83944500	2.74812000	-1.48964500
C	-8.18461500	4.77398400	-2.83483900
H	-7.40136500	4.61765400	-0.82599200
H	-9.17095100	4.49288000	-0.90442500
C	-4.63792100	-0.18311400	-1.31341200
C	-6.35334200	-1.80520100	-1.38481900
C	-8.15730800	6.30523800	-2.76598000
H	-7.22923100	4.43484800	-3.27158500
C	-9.32831700	4.27074600	-3.72144800
C	-4.09179500	-1.49551700	-1.44008900
C	-3.72354300	0.87893300	-1.19245100
N	-5.12317400	-2.42958200	-1.50201100
O	-7.40175200	-2.42715600	-1.39036600
H	-8.07537900	6.74471000	-3.77257200
H	-9.08013800	6.70109800	-2.30665600
H	-7.30412000	6.67016700	-2.17154900
H	-9.34973300	3.17174700	-3.78165200
H	-10.30825100	4.60655900	-3.33925400
H	-9.22583500	4.65743200	-4.74811200

C	-2.72939300	-1.74705400	-1.46160300
C	-2.35161000	0.63495500	-1.21129000
H	-4.09384100	1.89471000	-1.10118400
C	-5.01324400	-3.87684100	-1.59064800
C	-1.82343000	-0.66588500	-1.34921600
H	-2.35973600	-2.76765100	-1.54714000
H	-1.67259100	1.48710800	-1.13483500
C	-5.24087600	-4.45704800	-3.00073200
H	-5.77030100	-4.29741500	-0.91108600
H	-4.02384100	-4.17308200	-1.20690300
C	-5.25670900	-5.98831500	-2.92835200
H	-6.24393100	-4.12061300	-3.31583300
C	-4.21808000	-3.95257300	-4.02380200
H	-5.46957200	-6.42776800	-3.91560900
H	-4.28111600	-6.38334300	-2.59443900
H	-6.02420700	-6.35415600	-2.22719000
H	-4.20579500	-2.85355200	-4.08524400
H	-3.19752200	-4.28760300	-3.76826600
H	-4.44866500	-4.33865700	-5.02966100
C	-0.38358200	-0.91252100	-1.37839800
S	0.76363400	0.32442600	-0.93529700
C	0.29366400	-2.06874700	-1.72862900
C	2.13333000	-0.72356700	-1.24041800
C	1.70845500	-1.98931700	-1.65929300
H	-0.21665300	-2.97420600	-2.05967900
C	3.47839400	-0.24568900	-1.03264700
C	2.59858500	-3.15113700	-2.01525700
O	4.47293800	-1.20141500	-1.08649900
C	4.00902800	1.00821300	-0.78122900
H	3.34862700	-2.87466500	-2.77103400
H	3.15775500	-3.51691800	-1.14023700
H	1.99832600	-3.98313200	-2.41167100
C	5.65911000	-0.57242500	-0.86485100
C	5.43199800	0.81636900	-0.66217200
C	3.29067600	2.31666300	-0.65375300
C	6.90383300	-1.18242600	-0.83944100
C	6.51847800	1.67600000	-0.41398300
H	2.76843800	2.41220000	0.31406100
H	3.99903800	3.15498300	-0.72830500
H	2.53423100	2.45012300	-1.44311000
C	7.99042000	-0.32293900	-0.59111900
H	7.01877000	-2.25513500	-1.00081100
C	7.76351300	1.06601100	-0.38899900
H	6.40273700	2.74817200	-0.24953500
C	9.41398100	-0.51349300	-0.48246700
O	8.95016200	1.69484000	-0.16799100
C	9.94438100	0.73931600	-0.22346900
C	10.13633300	-1.81809300	-0.62756000
C	11.28994100	1.21168200	-0.01008900
H	10.58326200	-2.15355200	0.32383100
H	9.44745700	-2.60655300	-0.96365200

H	10.95456300	-1.75718800	-1.36345200
C	11.74412800	2.52448200	0.16176700
S	12.62033400	0.07592500	0.07652200
C	13.14935100	2.56982200	0.35159600
C	10.89350400	3.76746500	0.14876100
C	13.79157400	1.34278300	0.33217400
H	13.68107600	3.51285500	0.48465900
H	10.32331500	3.86230500	-0.78755400
H	10.15443900	3.76287800	0.96443500
H	11.52448700	4.66128400	0.26082800
C	15.21327400	1.04555700	0.49110300
C	16.11321200	2.06323800	0.88779100
C	15.73013400	-0.24597500	0.25622800
C	17.45904100	1.76305700	1.02490600
H	15.75125600	3.06919500	1.09396200
C	17.08566900	-0.53795300	0.39309300
H	15.05795900	-1.04695600	-0.05927000
C	17.99462600	0.46405500	0.77701600
N	18.47726400	2.62080700	1.43566100
H	17.44992900	-1.53909700	0.18741900
C	19.43345100	0.51178500	1.06309800
C	19.68286000	1.94485800	1.51192100
C	18.36588500	4.01595900	1.83069800
C	20.43782800	-0.43673800	0.96065000
O	20.71312600	2.48943400	1.86784600
C	18.78309800	5.03128300	0.74808900
H	19.01637600	4.15103300	2.70833100
H	17.32953800	4.20251100	2.15527100
C	21.85037100	-0.43292400	1.36951700
C	20.23837600	-1.79197900	0.29883100
C	18.78625700	6.44310600	1.34574500
H	19.82032500	4.77716400	0.46852200
C	17.90982500	4.95415900	-0.50835200
C	22.41829600	-1.67683600	0.96883300
C	22.68398600	0.45597900	2.06993000
N	21.45706500	-2.44677500	0.31647200
O	19.24039400	-2.28501100	-0.19889100
H	19.12424700	7.18473500	0.60493800
H	17.77476400	6.74086500	1.67358400
H	19.45546300	6.51335900	2.21849300
H	17.90829900	3.94486700	-0.94779100
H	16.86343500	5.22667100	-0.28496600
H	18.27337700	5.65136100	-1.28021000
C	23.73819500	-2.02008500	1.23066900
C	24.01065800	0.11486900	2.33892700
H	22.29082300	1.41272100	2.39713800
C	21.60376900	-3.78959600	-0.22253300
C	24.56322200	-1.11286800	1.92869600
H	24.14616300	-2.96611300	0.87531900
H	24.62484000	0.81614900	2.90682700
C	21.78909700	-3.85454100	-1.75158000

H	20.69074600	-4.34337100	0.04544700
H	22.44913900	-4.27673800	0.28911600
C	21.76819600	-5.31808200	-2.20780400
H	20.91255900	-3.34780400	-2.19141300
C	23.05490700	-3.13469000	-2.22766700
H	21.85149500	-5.39109700	-3.30365300
H	22.61149400	-5.88388300	-1.77420600
H	20.83581200	-5.82384600	-1.90869700
H	23.07346300	-2.08124800	-1.90856200
H	23.96430000	-3.62191200	-1.83487600
H	23.12219200	-3.14924600	-3.32736000
C	-28.15402200	-1.06714500	2.54128400
C	-28.77998600	0.13345700	2.14712500
C	-28.93282000	-2.02340700	3.22678100
C	-30.12666100	0.36784000	2.42599600
H	-28.20727700	0.88652700	1.59987500
C	-30.28086700	-1.79017000	3.49656700
H	-28.47062400	-2.95182900	3.56814700
C	-30.88654900	-0.59321700	3.09950600
H	-30.58742100	1.30637800	2.10725900
H	-30.86161000	-2.54640100	4.03114600
H	-31.94203000	-0.41062800	3.31553700
C	25.97818500	-1.45451600	2.22422400
C	26.98095900	-0.46504600	2.21138000
C	26.35921200	-2.77603200	2.52960000
C	28.31055500	-0.78444600	2.49204200
H	26.71786600	0.56307400	1.95332700
C	27.68830300	-3.09516700	2.81354700
H	25.59870300	-3.55904900	2.57355000
C	28.67111800	-2.10090300	2.79556500
H	29.07164100	-0.00019500	2.46646000
H	27.95655300	-4.12618800	3.05868400
H	29.71186400	-2.35051300	3.01699300

Table S5. Cartesian coordinates of optimized geometry for **TP_{out}BDFID** dimer.

C	18.79184300	-0.96006900	-0.73415000
C	18.64791900	0.21273600	0.05785700
C	20.00626500	-1.51401600	-1.11091600
C	19.78988900	0.89423000	0.51789800
C	21.14782300	-0.83198200	-0.65192400
H	20.05748800	-2.41725500	-1.72052600
C	21.00391400	0.34009600	0.14154000
H	19.73887900	1.79619700	1.12939900
O	17.56291700	-1.44672400	-1.06048900
C	16.62691800	-0.60837600	-0.49507900
O	22.23297900	0.82527400	0.46930900
C	23.16887900	-0.01156100	-0.09886000
C	17.22838800	0.42328600	0.19869400
C	22.56771200	-1.03955300	-0.79715700

C	23.23265700	-2.15088700	-1.55082700
H	23.78134100	-2.83445700	-0.88050300
H	22.49077100	-2.75055400	-2.09782700
H	23.95942600	-1.77098100	-2.28777300
C	16.56241900	1.53589200	0.94933900
H	15.99049300	1.16424200	1.81660000
H	17.30595100	2.25273400	1.32655200
H	15.85581700	2.09514100	0.31373800
C	24.54231100	0.34970000	0.14773200
C	24.99578900	1.45041500	0.85284700
S	25.89320900	-0.59653900	-0.42189000
C	26.41364100	1.55130700	0.94026500
C	27.05515400	0.50479400	0.28719700
C	15.25433600	-0.97085800	-0.73768100
C	14.80077200	-2.04501200	-1.48487600
S	13.90405800	-0.07859400	-0.08879300
C	13.38537300	-2.16543400	-1.54793300
C	12.73912500	-1.15736200	-0.83470300
H	24.31107400	2.17891700	1.28791500
C	27.09349600	2.70271400	1.63446700
H	26.47974700	3.61342100	1.55846500
H	27.24093900	2.50279400	2.71013300
H	28.08068000	2.91907100	1.20159600
H	15.48630000	-2.72684600	-1.98868100
C	12.71449500	-3.24999000	-2.34958000
H	13.36316400	-3.56924800	-3.17935800
H	12.51075000	-4.14469800	-1.73619400
H	11.75548400	-2.91723700	-2.77167400
C	11.30940100	-0.89150400	-0.64776200
C	10.83930000	0.43958600	-0.54573900
C	10.36999700	-1.93916400	-0.54407100
C	9.48603300	0.67173600	-0.35446000
H	11.53666000	1.27170200	-0.64282700
C	9.01006900	-1.69488500	-0.34830500
H	10.71098100	-2.97341800	-0.57459200
C	8.52734500	-0.37833200	-0.24515400
N	8.84592000	1.90608100	-0.27399600
H	8.31850600	-2.52541400	-0.25254600
C	7.20357300	0.24166300	-0.09391200
C	7.47854500	1.73799900	-0.14584900
C	9.44113500	3.22850300	-0.38697000
C	5.93724400	-0.29038100	0.09039200
O	6.71040800	2.68203000	-0.07889400
C	9.66815600	3.95389400	0.95421500
H	8.75865300	3.83375900	-1.00317100
H	10.38988200	3.13413300	-0.93903500
C	4.60191700	0.32166400	0.13303500
C	5.68354300	-1.76950000	0.34217700
C	10.15752800	5.38174900	0.68559600
H	8.68066900	4.01832500	1.44357000
C	10.62195000	3.19862700	1.88545200

C	3.66022000	-0.71433000	0.40432600
C	4.08692600	1.61316200	-0.07378300
N	4.32406900	-1.93041500	0.54605900
O	6.46362800	-2.70480900	0.38883000
H	10.27898900	5.94090000	1.62670000
H	11.13614200	5.37904700	0.17420300
H	9.45011200	5.94178400	0.05273100
H	10.26991000	2.17657000	2.09368700
H	11.63301200	3.12398300	1.44869100
H	10.71765100	3.71973500	2.85156700
C	2.29549200	-0.48648100	0.49582500
C	2.71420300	1.85074900	0.00471100
H	4.76623500	2.42901100	-0.29721500
C	3.74040900	-3.24381400	0.77001600
C	1.79427900	0.82250900	0.29942600
H	1.61319200	-1.29908300	0.74524800
H	2.35004000	2.85653700	-0.20110200
C	3.82092300	-3.74998300	2.22392000
H	4.28330400	-3.94872900	0.12171300
H	2.69328800	-3.21872800	0.42808800
C	3.31584400	-5.19600700	2.28932000
H	4.89142700	-3.75038100	2.49358700
C	3.07305800	-2.84754600	3.21059600
H	3.40772600	-5.60012400	3.30973200
H	2.25140700	-5.26101600	2.00295600
H	3.88529800	-5.85638400	1.61535800
H	3.44067800	-1.81033300	3.17879600
H	1.99047200	-2.82858600	2.99519400
H	3.19702800	-3.21171500	4.24308400
C	0.35399400	1.08412500	0.38289500
S	-0.76387300	-0.16084100	-0.14368500
C	-0.33534400	2.20669600	0.83873000
C	-2.15219900	0.81603300	0.25400300
C	-1.74514400	2.03901500	0.76019900
C	0.28547700	3.45671000	1.40565900
C	-3.50876300	0.37571500	0.05354800
H	-2.46037800	2.79697700	1.08051200
H	0.50209700	4.19948700	0.61845600
H	-0.40214000	3.93488800	2.11954200
H	1.23077100	3.24749900	1.92650100
O	-4.47776700	1.30391400	0.36682200
C	-4.06830900	-0.80461700	-0.39523200
C	-5.68581200	0.72757100	0.11883600
C	-5.49471600	-0.59689500	-0.36440900
C	-3.35912400	-2.05036500	-0.83085200
C	-6.92112900	1.32906300	0.30573000
C	-6.60775200	-1.39289300	-0.69203100
H	-2.63760800	-2.39792700	-0.07320000
H	-4.07493100	-2.86681400	-1.00468900
H	-2.79534000	-1.89922400	-1.76739200
C	-8.03406200	0.53291800	-0.02164700

H	-7.00894800	2.34931800	0.68178900
C	-7.84311800	-0.79102900	-0.50610300
H	-6.51997200	-2.41320600	-1.06795200
C	-9.46030400	0.74145000	0.00832700
O	-9.05132800	-1.36635900	-0.75607000
C	-10.02018500	-0.43798500	-0.44242200
C	-10.16747100	1.98801300	0.44460500
C	-11.37673500	-0.87581600	-0.64883000
H	-10.69715300	1.84947300	1.40289300
H	-9.45451300	2.81454000	0.57852000
H	-10.91771600	2.31386300	-0.29422300
C	-11.78393800	-2.08689000	-1.18288400
S	-12.76504500	0.08875100	-0.22286300
C	-13.19371000	-2.25381400	-1.26293100
H	-11.06880300	-2.83623000	-1.52310700
C	-13.88343400	-1.14343700	-0.77816100
C	-13.81367700	-3.49031300	-1.85956400
C	-15.32325200	-0.88307000	-0.68498200
H	-13.12280000	-3.95496800	-2.57913600
H	-14.03674400	-4.24887000	-1.08937600
H	-14.75528700	-3.26809400	-2.38179100
C	-15.82100200	0.43395000	-0.83006800
C	-16.24643900	-1.91864000	-0.42843600
C	-17.18406400	0.66363100	-0.72183100
H	-15.13657800	1.25357900	-1.04918600
C	-17.61663000	-1.67662300	-0.32084200
H	-15.88653700	-2.93382000	-0.26654000
C	-18.12658700	-0.37457400	-0.46295200
N	-17.84857900	1.87834700	-0.87185100
H	-18.29606000	-2.49403700	-0.10360000
C	-19.46673300	0.23032000	-0.46108500
C	-19.21606500	1.70360100	-0.75480000
C	-17.27296500	3.17707700	-1.18405300
C	-20.72844300	-0.29433300	-0.23582600
O	-20.00167600	2.62827300	-0.86645200
C	-17.11217400	4.12148200	0.02381800
H	-17.94070700	3.65427300	-1.91774500
H	-16.30160500	3.01402700	-1.67756900
C	-22.07806200	0.28308700	-0.34215200
C	-20.96431600	-1.71977800	0.24422800
C	-16.64757500	5.49897400	-0.46306300
H	-18.11818500	4.23684700	0.46341700
C	-16.17605300	3.55939500	1.09862900
C	-23.00850900	-0.72140700	0.05217300
C	-22.60820100	1.51525200	-0.76298200
N	-22.32708100	-1.88187000	0.41440700
O	-20.16838500	-2.61327900	0.47798200
H	-16.57125900	6.20833800	0.37598700
H	-15.65255600	5.44069400	-0.93809900
H	-17.34645200	5.92668600	-1.20001900
H	-16.50949400	2.57478600	1.46101000

H	-15.14702400	3.44637700	0.71532700
H	-16.13132700	4.23460200	1.96824200
C	-24.38229900	-0.51975300	0.04679300
C	-23.98881000	1.72236200	-0.77469400
H	-21.93670700	2.30735600	-1.07658900
C	-22.89144800	-3.15273000	0.84123400
C	-24.89689000	0.72546400	-0.37214400
H	-25.05795000	-1.30127100	0.39349000
H	-24.36906100	2.68129500	-1.13153600
C	-22.84278100	-3.40309000	2.36173800
H	-22.31671400	-3.94398900	0.33564700
H	-23.92863200	-3.21051600	0.47457600
C	-23.31284000	-4.83143200	2.66051300
H	-21.78128500	-3.32513000	2.65430600
C	-23.64316500	-2.36902100	3.16006800
H	-23.24383200	-5.05232600	3.73730800
H	-24.36550800	-4.97656000	2.36044900
H	-22.70542600	-5.57968500	2.12598200
H	-23.30875500	-1.34093400	2.95266500
H	-24.72010100	-2.42694400	2.92430200
H	-23.53337700	-2.54178600	4.24272400
C	-26.36198300	0.96928900	-0.38573900
C	-27.26830600	-0.05901500	-0.71118700
C	-26.88865000	2.23805000	-0.07286400
C	-28.64508500	0.17135700	-0.72413500
H	-26.88764600	-1.04550300	-0.98549800
C	-28.26542200	2.46799200	-0.08289600
H	-26.21041100	3.04722200	0.20655800
C	-29.15093200	1.43607600	-0.40881200
H	-29.32689800	-0.64062400	-0.99026100
H	-28.64960000	3.45886300	0.17311000
H	-30.22878800	1.61663700	-0.41753200
C	28.49216900	0.22857200	0.12016800
C	28.99686600	-0.27430900	-1.09786400
C	29.40394700	0.44175400	1.17487400
C	30.35622300	-0.54521200	-1.25589900
H	28.31268500	-0.43674800	-1.93422800
C	30.76511700	0.17759100	1.01094200
H	29.03787800	0.79108700	2.14138000
C	31.24897400	-0.31633900	-0.20397000
H	30.72215100	-0.92987800	-2.21142700
H	31.45101300	0.34758800	1.84501200
H	32.31430900	-0.52515800	-0.32936100