Supplementary Information

# Chiroptical Response Inversion upon Sample Flipping in Thin Films of a Chiral Benzo[1,2-*b*:4,5-*b'*]dithiophene-based Oligothiophene

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## General

All chemicals were purchased from Sigma Aldrich or Alfa Aesar and used as received without further purification. Commercial grade solvents were purified by conventional methods[1], distilled and stored over activated molecular sieves under nitrogen atmosphere. All the operations under inert atmosphere were carried out using standard Schlenk techniques and employing dried nitrogen. All reactions conversion was monitored by thin-layer chromatography (TLC) analysis on pre-coated silica gel plates ALUGRAM® Xtra SIL G/$UV_{254}$ (0.2 mm) purchased from VWR Macherey-Nagel. Column chromatography was performed with Fluka silica gel, pore size 60 Å, 70-230 mesh, 63-200 μm.

$^{1}$H-NMR and $^{13}$C-NMR spectra were recorded at room temperature in $CDCl_3$ or DMSO-$d_6$ solution with a Bruker Avance DRX 400 spectrometer, operating at a frequency of 400 MHz for $^{1}$H and 100 MHz for $^{13}$C, using the residual solvent peak as internal reference; chemical shifts (δ) values are given in parts per million (ppm) and coupling constants (J) in Hertz.

Mass spectra were obtained with a Perkin–Elmer Q-Mass 910 connected to a Perkin–Elmer 8500 gas chromatograph or with an Applied Biosystems- MDS Sciex API 4000 triple quadrupole mass spectrometer (Concord, Ont., Canada), equipped with a Turbo-V ion-spray (TIS) source. In the second case, the operative parameters were as follows: ion-spray voltage (IS), 5.0 kV; gas source 1(GS1), 25; gas source 2(GS2), 25; turbo temperature (TEM), 0°C; entrance potential (EP), 10 V; declustering potential (DP), 20 V; scan range, 300–1500 m/z. MS–MS spectra were produced by collision-induced dissociation (CID) of selected precursor ions in a LINAC collision cell (Q2) and mass-analyzed in the second mass filter (Q3).

UV-Vis absorption spectra were recorded at room temperature using a Jasco V-650 spectrophotometer. Fluorescence spectra were measured at room temperature on a Horiba Jobin-Yvon Fluorolog®-3 spectrofluorometer and equipped with a 450 W xenon arc lamp, double-grating excitation and single-grating emission monochromators. Electronic circular dichroism spectra were recorded at room temperature using a Jasco J-710 spectropolarimeter.

Optical microscopy images of thin films were obtained at room temperature using a ZEISS SteREO Discovery.V8 microscope provided with cross-polarized filters and equipped with a camera Canon PowerShot A640.

The fluorescence quantum yield ($\Phi_X$) of **1** in chloroform was determined at room temperature relative to fluorescein ($\Phi_{ST}$ = 0.79 in NaOH 0.1 M) using the following relation[2]:

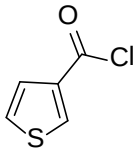
$$\Phi_X = \Phi_{ST}\left(\frac{Grad_X}{Grad_{ST}}\right)\left(\frac{\eta_X^2}{\eta_{ST}^2}\right)$$

where the subscripts *ST* and *X* are standard and dye respectively, *Grad* is the gradient from the plot of integrated fluorescence intensity vs absorbance for different solutions of standard and dyes, and $\eta$ is the refractive index of the solvent (*i.e.* water for standard and chloroform for dye). Refractive indexes were assumed 1.33 for water and 1.45 for chloroform.

## Synthesis

### Synthesis of thiophene-3-carbonyl chloride (4)[3]

Thiophene-3-carboxylic acid (**3**) (7.01 g, 54.9 mmol) and $CH_2Cl_2$ (50 mL) were mixed together, then oxalyl chloride (9.8 mL, 112.6 mmol) was added to the solution at 0 °C. The mixture was left under stirring for 24 h at room temperature, then it was evaporated under vacuum to give **4** (7.72 g, yield 96%) as a yellowish oil which was used without further purification.



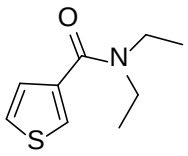

**4**

**$^1$H-NMR (400 MHz, $CDCl_3$), δ (ppm):** 7.41 (1H, dd, *J* = 5.2, 2.9 Hz), 7.59 (1H, dd, *J* = 5.2, 1.2 Hz), 8.39 (1H, dd, *J* = 2.9, 1.2 Hz).

**$^{13}$C-NMR (100 MHz, $CDCl_3$), δ (ppm):** 127.22, 128.14, 137.04, 138.24, 161.07.

### Synthesis of *N*,*N*-diethylthiophene-3-carboxamide (5)[3]

Diethylamine (13.6 mL, 132 mmol) and dry $CH_2Cl_2$ (40 mL) were mixed together, then a solution of thiophene-3-carbonyl chloride (**4**) (7.72 g, 52.7 mmol) in dry $CH_2Cl_2$ (40 mL) was added dropwise to the solution at 0 °C. The mixture was left under stirring for 4 h at room temperature, then it was hydrolyzed with water (80 mL) and extracted with $CH_2Cl_2$. The combined organic phases were washed with brine, dried over anhydrous $Na_2SO_4$ and the solvent was removed under vacuum. The crude product was purified through column chromatography ($SiO_2$, *n*-hexane/AcOEt 60:40) yielding **5** as a yellowish oil (9.02 g, yield 93%).



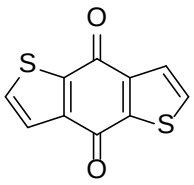

**5**

**$^1$H-NMR (400 MHz, $CDCl_3$), δ (ppm):** 1.17 (6H, s), 3.41 (4H, bs), 7.15 (1H, dd, *J* = 5.2, 1.2 Hz), 7.29 (1H, dd, *J* = 5.2, 2.8 Hz), 7.44 (1H, dd, *J* = 2.8, 1.2 Hz).

**$^{13}$C-NMR (100 MHz, $CDCl_3$), δ (ppm):** 13.07, 14.21, 40.06, 42.88, 124.83, 125.56, 126.67, 137.33, 166.46.

### Synthesis of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-dione (2)[3]

*N*,*N*-diethylthiophene-3-carboxamide (**5**) (3.54 g, 19.1 mmol) and dry THF (40 mL) were mixed together, then 1.6 M in hexane *n*-BuLi (13.6 mL, 21.7 mmol) was added dropwise to the solution at 0 °C. The mixture was left under stirring for 24 h at room temperature, then it was hydrolyzed with HCl 1 M and filtered to give **2** (1.63 g, yield 77%) as a yellow solid which was used without further purification.

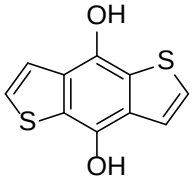


**2**

**$^{1}$H-NMR (400 MHz, DMSO-$d_6$), δ (ppm):** 7.62 (2H, d, *J* = 4.8 Hz), 8.14 (2H, d, *J* = 4.8 Hz).
**$^{13}$C-NMR (100 MHz, DMSO-$d_6$), δ (ppm):** 126.23, 135.79, 142.41, 144.28, 174.18.

### Synthesis of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-diol (6)[4]

Benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-dione (**2**) (0.66 g, 3.1 mmol) and ethanol (20 mL) were mixed together, then $NaBH_4$ (0.24 g, 6.3 mmol) was added portion-wise to the solution. The mixture was left under stirring for 5 h at room temperature, then it was hydrolyzed with HCl 1 M until pH ~ 2, diluted with cold $H_2O$ and filtered to give **6** (0.47 g, yield 71%) as a dark green solid which was used without further purification.

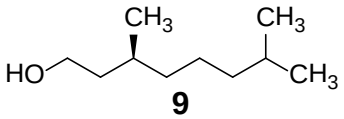


**6**

**$^{1}$H-NMR (400 MHz, DMSO-$d_6$), δ (ppm):** 7.55 (2H, d, *J* = 5.6 Hz), 7.62 (2H, d, *J* = 5.6 Hz), 9.78 (2H, s).
**$^{13}$C-NMR (100 MHz, DMSO-$d_6$), δ (ppm):** 112.82, 124.24, 125.88, 126.48, 138.27.

### Synthesis of (*S*)-3,7-dimethyloctan-1-ol (9)[5]

In a 95 mL stainless steel autoclave fitted with a Teflon inner crucible and a stirring bar, (*S*)-3,7-dimethyl-6-octen-1-ol (**8**) (10.0 g, 64 mmol), AcOEt (30 mL) and Pd/C 1 wt.% (1.0 g, 0.15 mol%) were mixed together. The reactor was pressurized with $H_2$ (40 atm) and the mixture was stirred for 24 h at room temperature. After removal of excess $H_2$ (fume hood), the reaction mixture was filtered through Celite and the solvent was removed under vacuum to give **9** (8.30 g, yield 82%) as a colourless oil which was used without further purification.



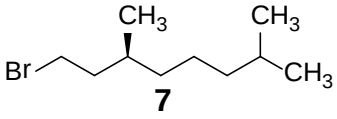
**9**

**$^{1}$H-NMR ($CDCl_3$), δ (ppm):** 0.83-0.87 (9H, m), 1.06-1.16 (3H, m), 1.18-1.30 (3H, m), 1.32-1.39 (1H, m), 1.43-1.62 (4H, m), 3.59-3.70 (2H, m).
**$^{13}$C-NMR ($CDCl_3$), δ (ppm):** 19.60, 22.55, 22.66, 24.65, 27.93, 29.49, 37.35, 39.23, 39.96, 61.19.

### Synthesis of (*S*)-1-bromo-3,7-dimethyloctane (7)[5]

(*S*)-3,7-Dimethyloctan-1-ol (**9**) (2.80 g, 18.2 mmol), triphenylphosphine (5.60 g, 21.5 mmol) and $CH_2Cl_2$ (50 mL) were mixed together, then *N*-bromosuccinimide (3.85 g, 21.6 mmol) was added portion-wise to the so-

lution at 0 °C. After stirring of the mixture for 2 h at 0 °C, the solvent was removed under vacuum and the solid residue was suspended in *n*-hexane. The mixture was stirred for 10 min at room temperature, then it was filtered through Celite and the solvent was removed under vacuum. The crude product was purified through column chromatography ($SiO_2$, *n*-hexane) yielding **7** (3.43 g, yield 86%) as a colourless liquid.



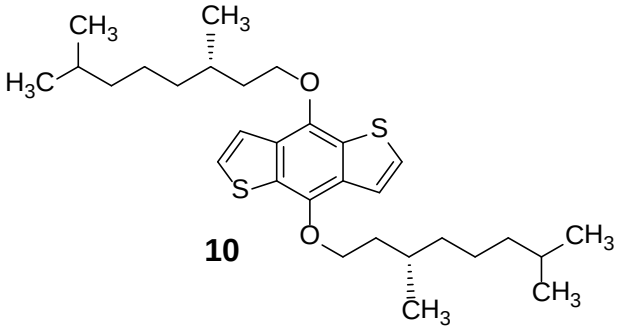

**7**

**$^1$H-NMR ($CDCl_3$), δ (ppm):** 0.84-0.88 (9H, m), 1.05-1.17 (3H, m), 1.19-1.34 (3H, m), 1.44-1.56 (1H, m), 1.57-1.69 (2H, m), 1.81-1.90 (1H, m), 3.35-3.47 (2H, m).

**$^{13}$C-NMR ($CDCl_3$), δ (ppm):** 18.94, 22.56, 22.66, 24.53, 27.93, 31.66, 32.09, 36.71, 39.16, 40.08.

### Synthesis of 4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (10)

Benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-diol (**6**) (0.31 g, 1.4 mmol), (*S*)-1-bromo-3,7-dimethyloctane (**7**) (0.66 g, 3.0 mmol), $K_2CO_3$ (1.93 g, 14.0 mmol) and $CH_3CN$ (30 mL) were mixed together. The mixture was refluxed under stirring for 30 h, then it was cooled to room temperature, filtered and the solvent was removed under vacuum. The residue was dissolved in $CH_2Cl_2$ (30 mL) and washed with $H_2O$ (3x30 mL), then the organic phase was dried over anhydrous $Na_2SO_4$ and the solvent was removed under vacuum. The crude product was purified through column chromatography ($SiO_2$, *n*-hexane/$CH_2Cl_2$ 50:50) to give **10** (0.89 g, yield 88%) as a colourless oil.




**10**

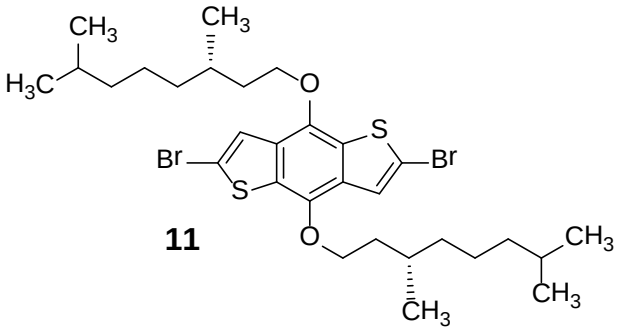
**$^1$H-NMR ($CDCl_3$), δ (ppm):** 0.91 (12H, d, *J* = 6.4 Hz), 1.01 (6H, d, *J* = 6.8 Hz), 1.16-1.25 (6H, m), 1.29-1.45 (6H, m), 1.52-1.62 (2H, m), 1.66-1.75 (2H, m), 1.78-1.90 (2H, m), 1.93-2.01 (2H, m), 4.29-4.39 (4H, m), 7.36 (2H, d, *J* = 5.6 Hz), 7.49 (2H, d, *J* = 5.6 Hz).

**$^{13}$C-NMR ($CDCl_3$), δ (ppm):** 19.70, 22.60, 22.70, 24.68, 27.94, 29.74, 37.32, 37.60, 39.25, 72.15, 120.28, 125.88, 130.04, 131.58, 144.54.

### Synthesis of 2,6-dibromo-4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (11)

4,8-Bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (**10**) (0.42 g, 0.8 mmol) and dry THF (20 mL) were mixed together, then 1.6 M in hexane *n*-BuLi (1.15 mL, 1.8 mmol) was added dropwise to the solution at -78 °C. The mixture was left under stirring for 15 min at -78 °C and for 30 min at room temperature, then the suspension was cooled to - 78 °C and carbon tetrabromide (0.66 g, 2.1 mmol) was added. The mixture was left under stirring for 4 h at room temperature, then it was hydrolyzed with water (30 mL) and ex-

tracted with $CH_2Cl_2$. The combined organic phases were washed with brine, dried over anhydrous $Na_2SO_4$ and the solvent was removed under vacuum. The crude product was purified through column chromatography ($SiO_2$, *n*-hexane → *n*-hexane/$CH_2Cl_2$ 9:1) to give **11** (0.19 g, yield 38%) as a yellowish oil.



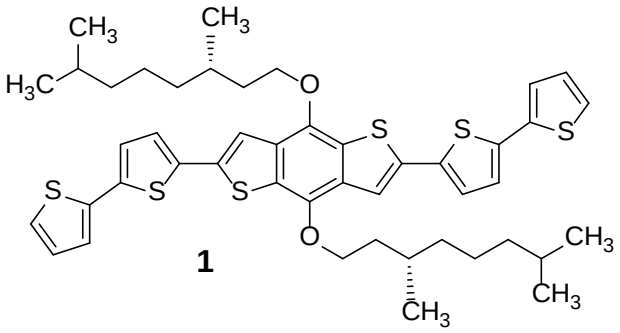

**11**

**$^1$H-NMR ($CDCl_3$), δ (ppm):** 0.87 (12H, d, *J* = 6.4 Hz), 0.96 (6H, d, *J* = 6.4 Hz), 1.11-1.20 (6H, m), 1.22-1.39 (6H, m), 1.49-1.59 (2H, m), 1.61-1.67 (2H, m), 1.69-1.79 (2H, m), 1.83-1.91 (2H, m), 4.17-4.26 (4H, m), 7.40 (2H, s).

**$^{13}$C-NMR ($CDCl_3$), δ (ppm):** 19.71, 22.61, 22.71, 24.70, 27.97, 29.72, 37.25, 37.50, 39.24, 72.45, 114.96, 123.14, 130.89, 131.07, 142.57.

### Synthesis of 2,6-di([2,2'-bithiophen]-5-yl)-4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (1)

2,6-Dibromo-4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (**11**) (140 mg, 0.2 mmol), 2,2'-bithiophene-5-boronic acid pinacol ester (**12**) (190 mg, 0.7 mmol) and 1,4-dioxane (5 mL) were mixed together, then $K_2CO_3$ (90 mg, 0.6 mmol), $Ag_2O$ (100 mg, 0.4 mmol) and $Pd(PPh_3)_4$ (10 mg, 0.01 mmol) were added to the solution. The mixture was left under stirring for 90 h at 70 °C, then it was hydrolyzed with saturated ammonium chloride solution (10 mL) and extracted with $CHCl_3$ (3x15 mL). The combined organic phases were washed with brine, dried over anhydrous $Na_2SO_4$ and the solvent was removed under vacuum. The crude product was purified through column chromatography ($SiO_2$, petroleum ether → petroleum ether/$CH_2Cl_2$ 7:3) to give **1** (50 mg, yield 30%) as an orange solid.




**1**

**$^1$H-NMR ($CDCl_3$), δ (ppm):** 0.88 (12H, d, *J* = 7.2 Hz), 1.01 (6H, d, *J* = 6.8 Hz), 1.15-1.25 (6H, m), 1.29-1.46 (6H, m), 1.54-1.59 (2H, m), 1.69-1.76 (2H, m), 1.81-1.85 (2H, m), 1.91-2.00 (2H, m), 4.27-4.36 (4H, m), 7.03 (2H, dd, *J* = 4.4, 3.6 Hz), 7.11 (2H, d, *J* = 3.6 Hz), 7.20 (4H, d, *J* = 4.4 Hz), 7.21 (2H, d, *J* = 3.6 Hz), 7.46 (2H, s).

**$^{13}$C-NMR ($CDCl_3$), δ (ppm):** 19.81, 22.68, 22.76, 24.81, 28.05, 29.83, 37.36, 37.67, 39.34, 72.32, 116.04, 124.05, 124.44, 124.87, 125.99, 127.98, 129.34, 132.54, 136.10, 136.35, 136.95, 137.63, 143.98.

**LC-MS APCI (+) $[M+H]^+$:** 832.6.

## Computational details

DFT and TDDFT calculations were run with Gaussian'09 (Rev. D.01, Gaussian, Inc., Wallingford CT, 2013), with default grids and convergence criteria[6]. A truncated model of **1** was employed where the O-alkyl chains were placed by O-methyl groups. A starting structure of the model, with the thiophene rings put in the most stable all-trans conformation, was optimized with DFT method using ωB97X-D functional and 6-31G(d) basis set in vacuo. TDDFT calculations were run on the DFT-optimized structure using the CAM-B3LYP functional and the TZVP basis set, including 36 excited states and the IEF-PCM continuum solvent model for chloroform. UV spectra were generated by applying a Gaussian band shape with 0.3 eV exponential half-width, and a 40 nm wavelength shift.

## Supplementary Figures

### UV-Vis absorption and ECD spectra

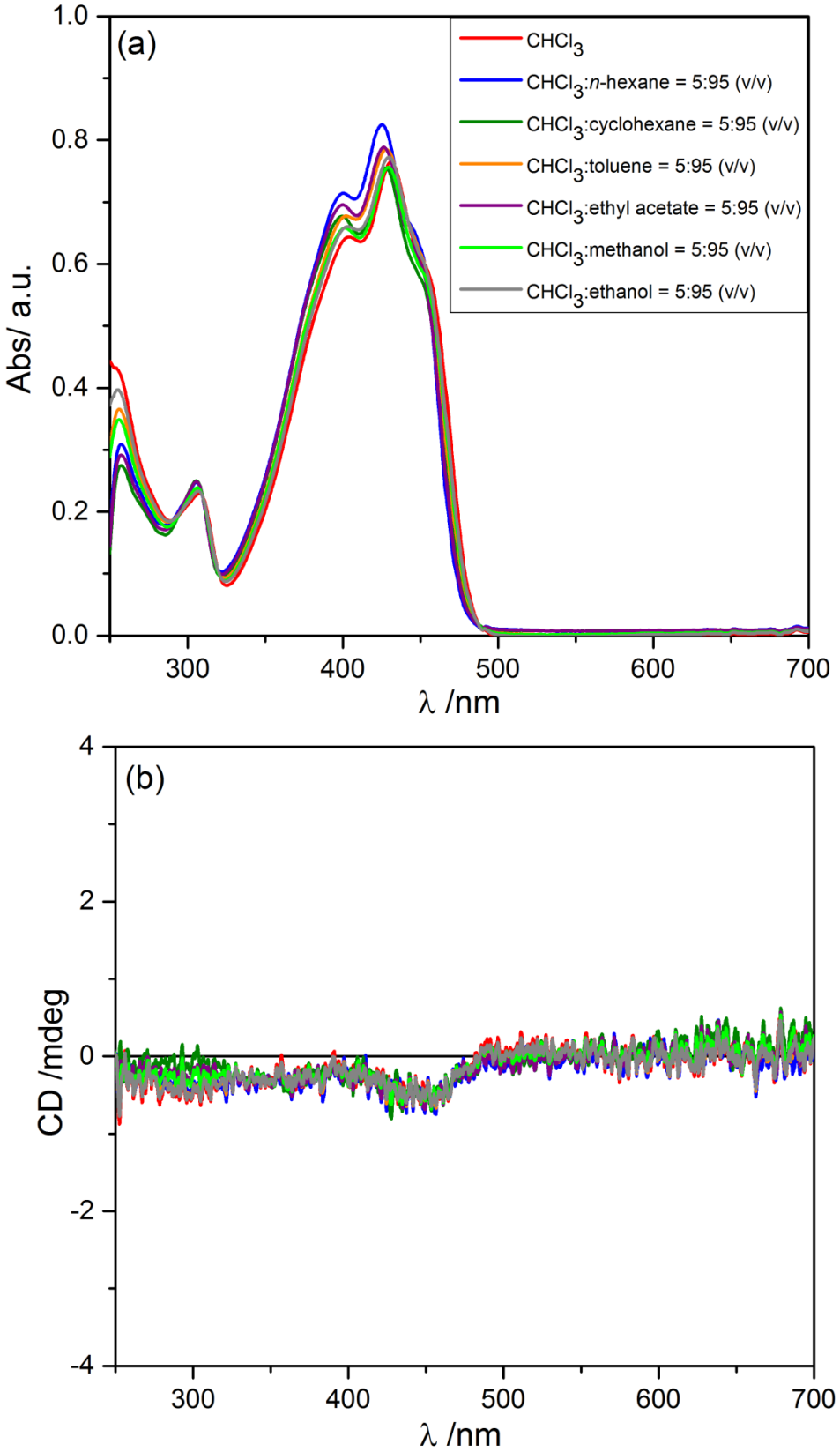



**Figure S1** – UV-Vis absorption (a) and ECD (b) spectra of **1** in $CHCl_3$ (blue line), $CHCl_3$:*n*-hexane 5:95 (red line), $CHCl_3$:cyclohexane 5:95 (dark green line), $CHCl_3$:toluene 5:95 (orange line), $CHCl_3$:ethyl acetate (violet line), $CHCl_3$:MeOH 5:95 (light green line) and $CHCl_3$:EtOH 5:95 (gray line) solution. Sample concentration: $1.0 \cdot 10^{-5}$ M; cell length: 1 cm.

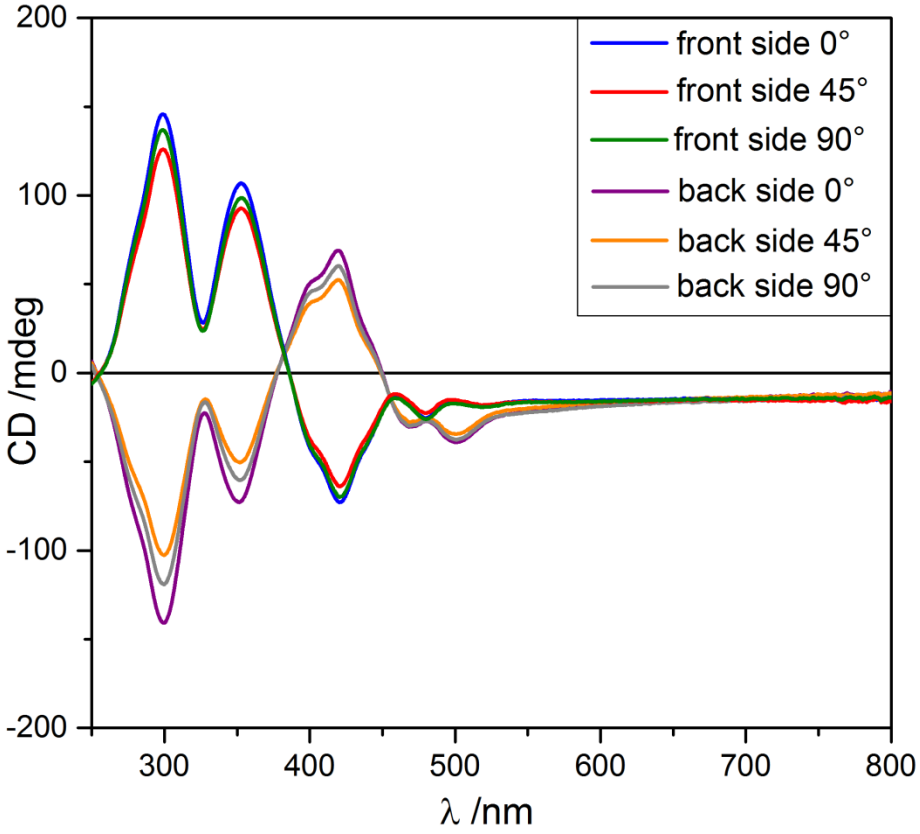



**Figure S2** – ECD spectra of **1** as thin film, prepared by drop casting technique of a $10^{-2}$ M $CHCl_3$ solution, recorded for the front and the back side at different rotation angle in the plane perpendicular to the light axis.

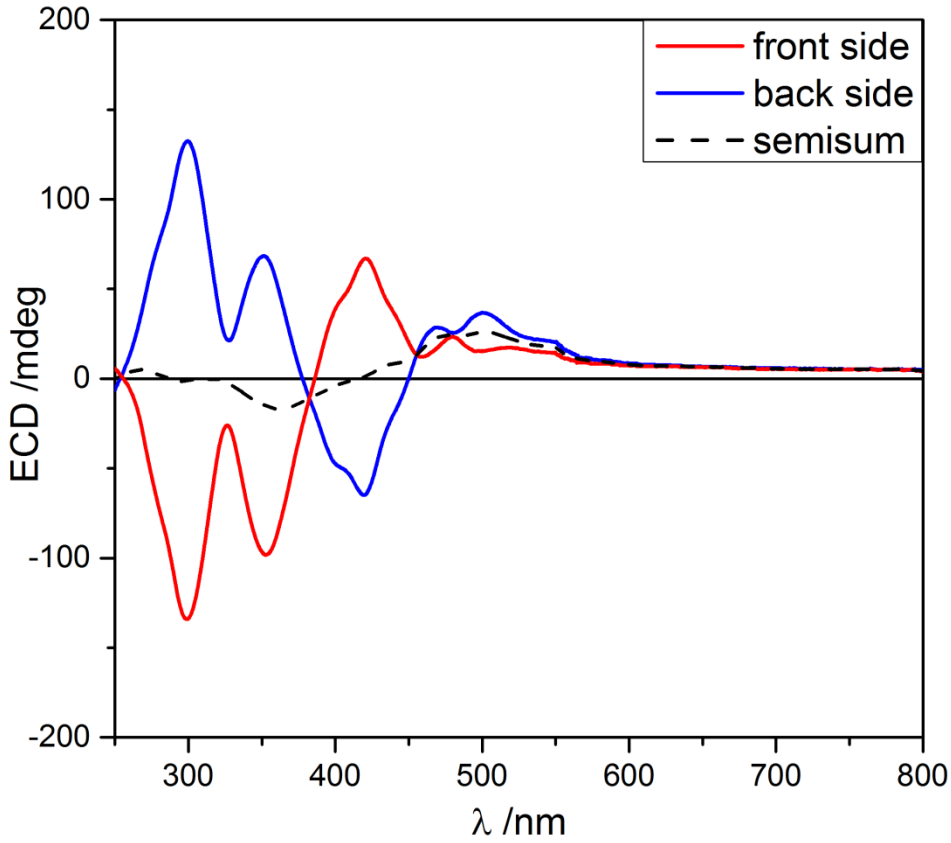



**Figure S3** – ECD spectra of *ent*-**1** as thin film, prepared by drop casting technique of a $10^{-2}$ M $CHCl_3$ solution, recorded for the front side (red line) and the back side (blue line); the black dashed line is the semi-sum of the two ECD spectra.

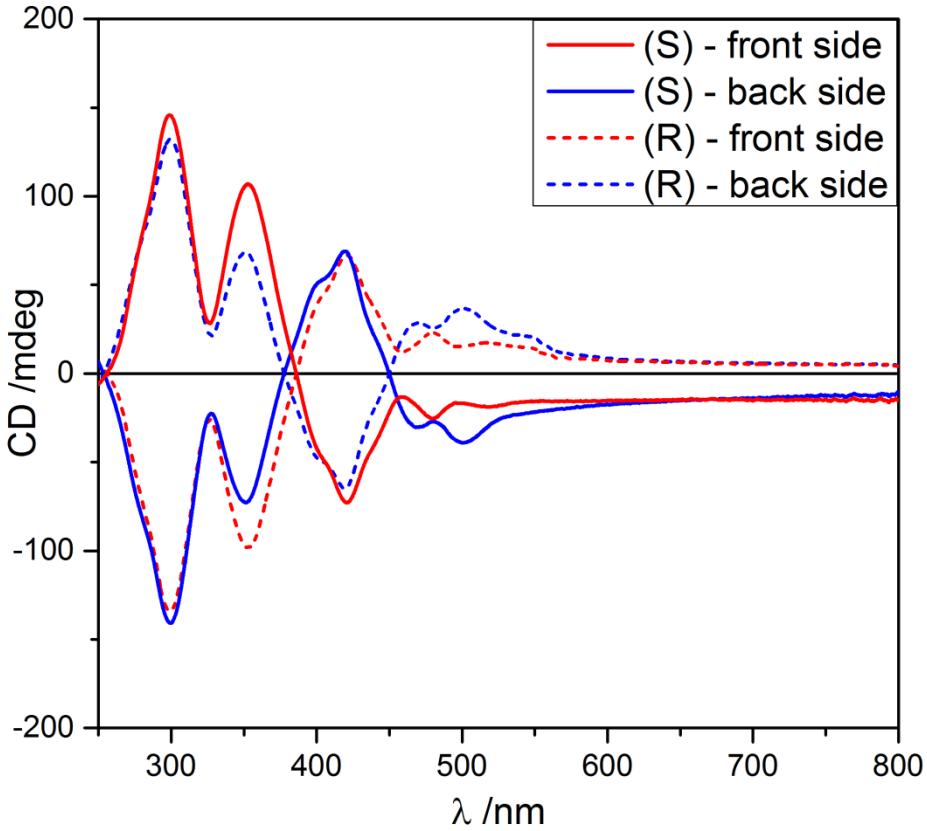



**Figure S4** – Confront of the ECD spectra of **1** (solid line) and *ent*-**1** (dashed line) as thin film, prepared by drop casting technique of a $10^{-2}$ M $CHCl_3$ solution, recorded with equal absorbance for the front side (red line) and the back side (blue line).

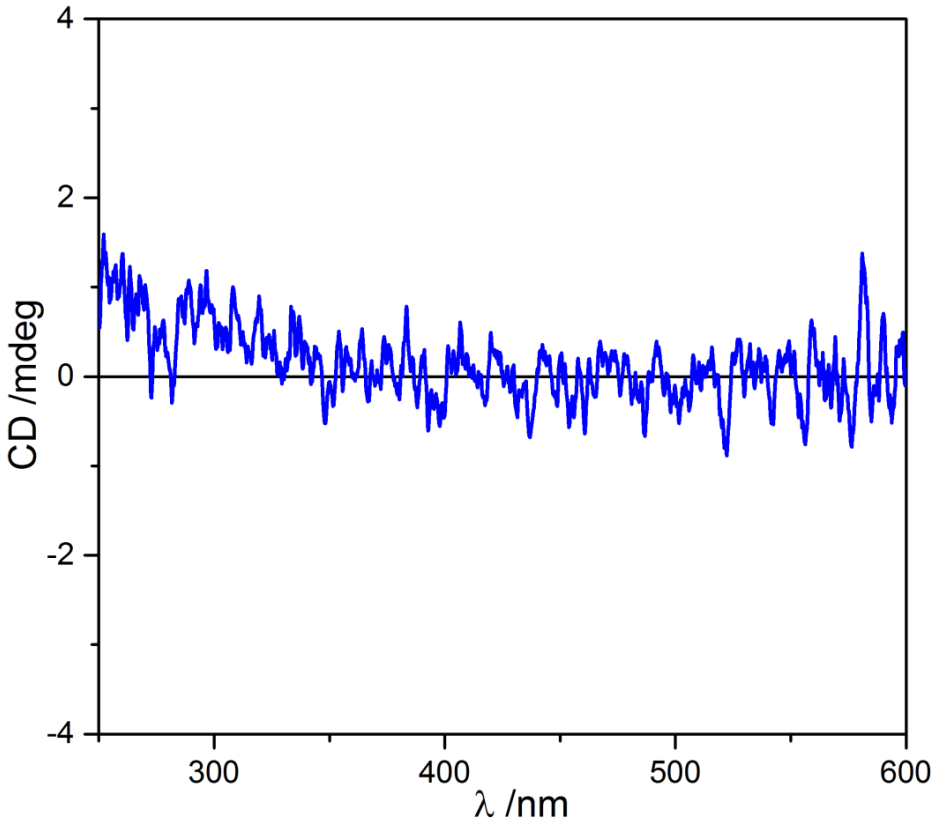



**Figure S5** – ECD spectrum of *racemic*-**1** as thin film, prepared by drop casting technique of a $10^{-2}$ M $CHCl_3$ solution obtained by mixing equal amounts of **1** and *ent*-**1**.

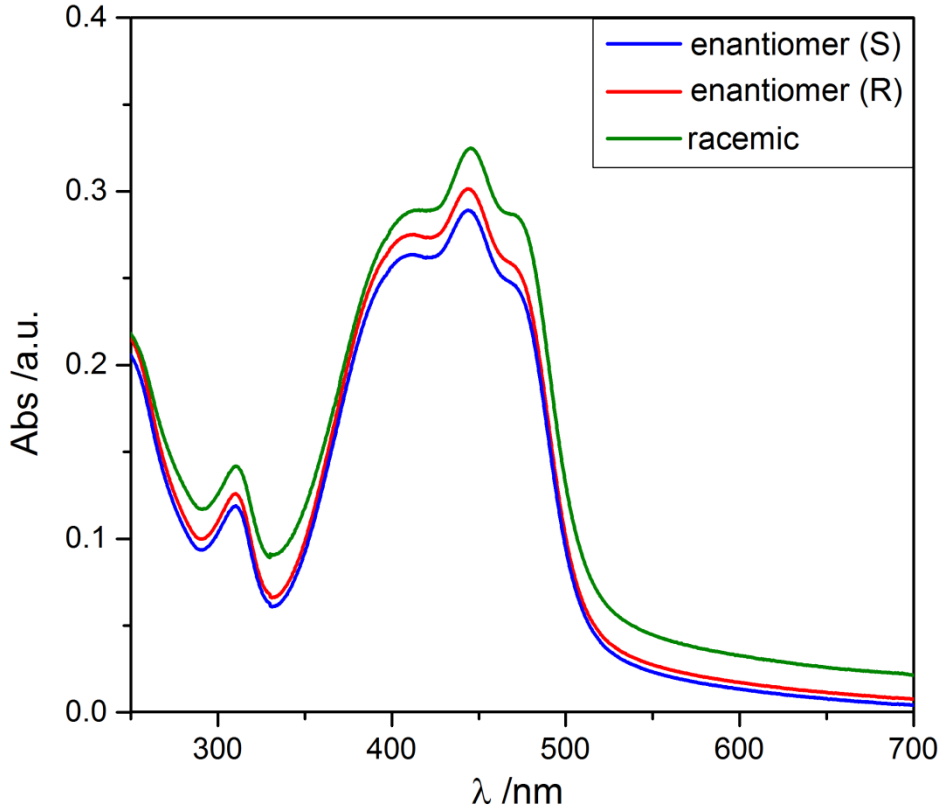



**Figure S6** – Confront of the UV-Vis absorption spectra of **1** (blue line), *ent*-**1** (red line) and *racemic* **1** (green line) as thin film, prepared by drop casting technique of a $10^{-2}$ M $CHCl_3$ solution.

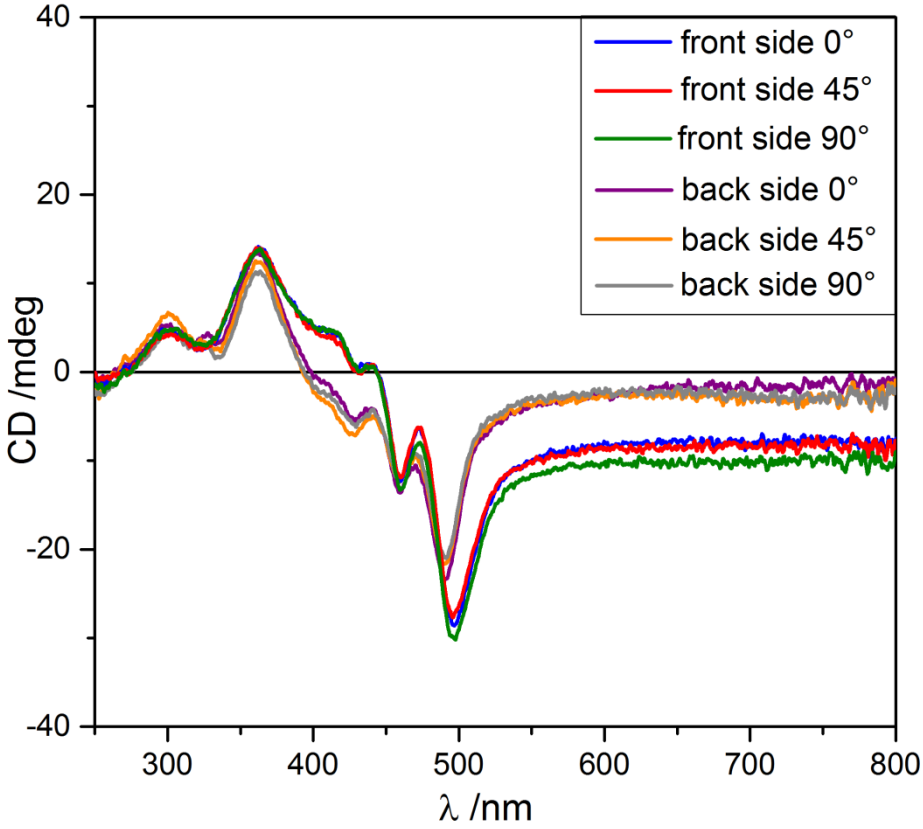



**Figure S7** – ECD spectra of **1** as thin film, after 10 minutes of annealing with $CHCl_3$ vapours, recorded for the front and the back side at different rotation angle in the plane perpendicular to the light axis.

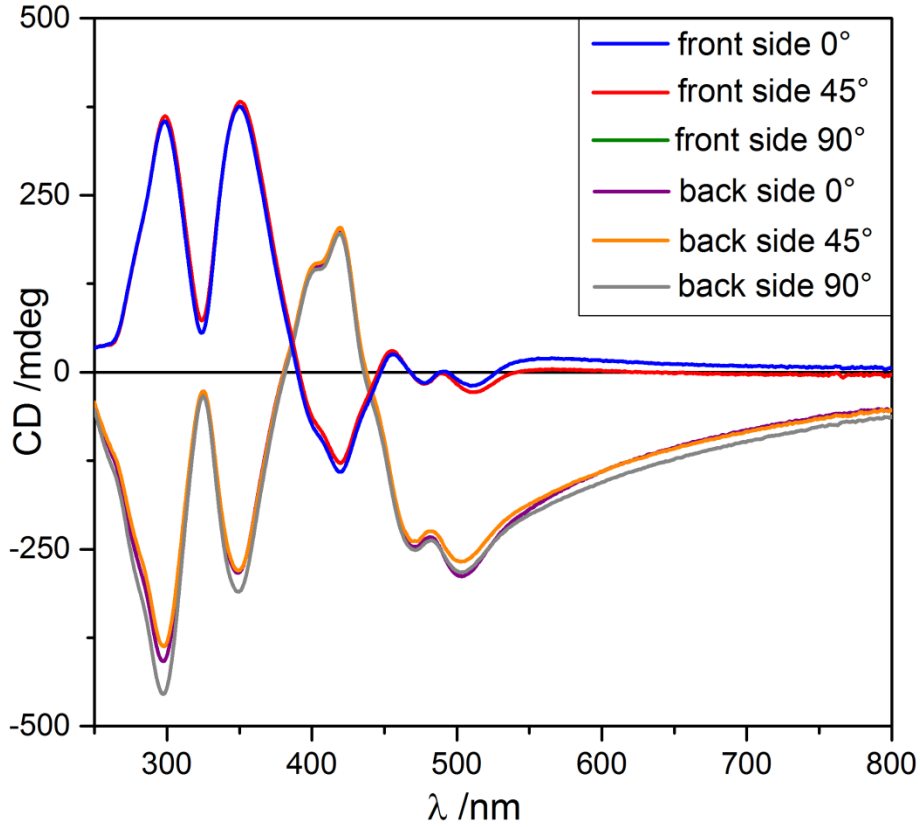



**Figure S8** – ECD spectra of **1** as thin film, after 60 minutes of annealing with $CHCl_3$ vapours, recorded for the front and the back side at different rotation angle in the plane perpendicular to the light axis.

**$^{1}$H and $^{13}$C-NMR spectra**

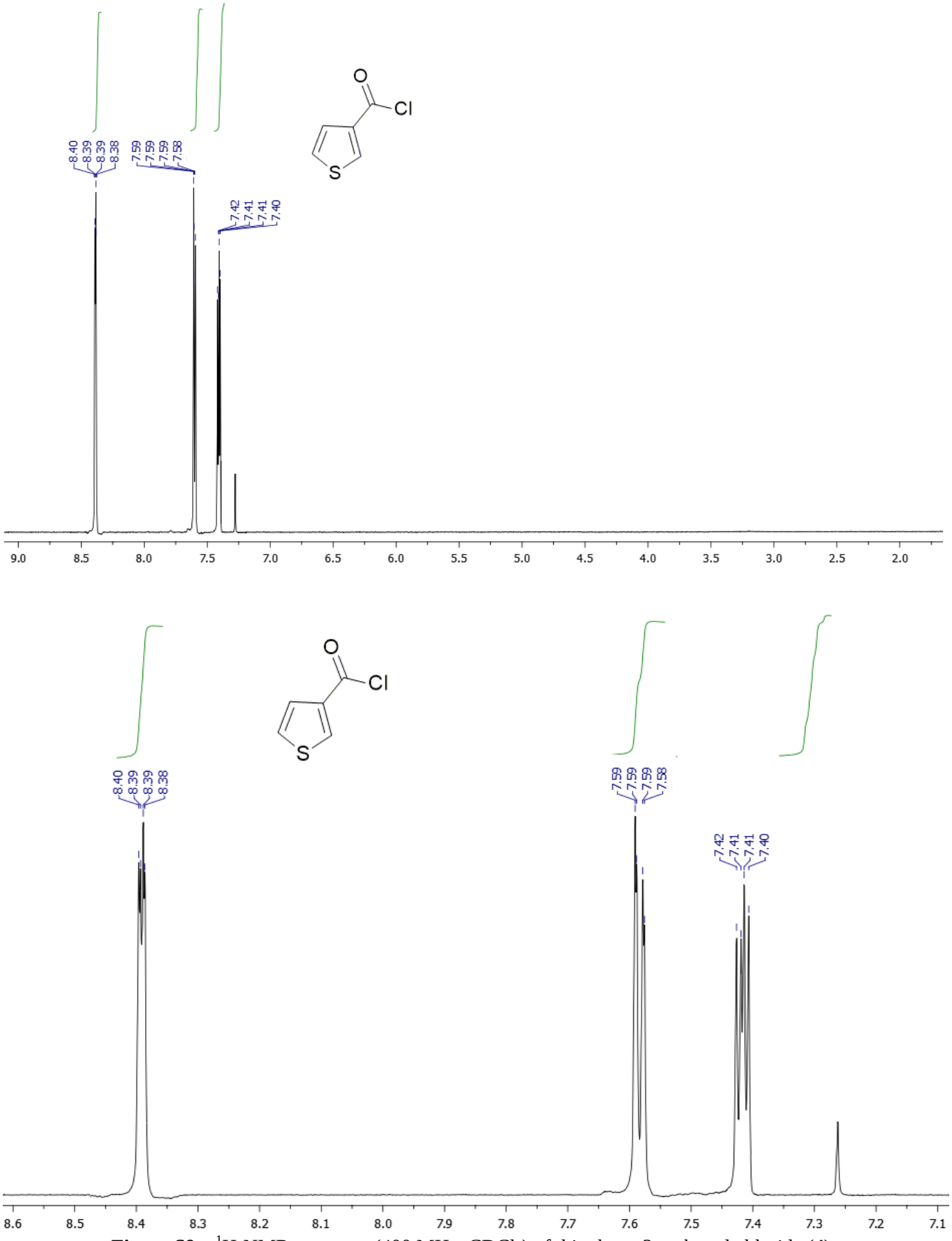



**Figure S9** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of thiophene-3-carbonyl chloride (**4**).

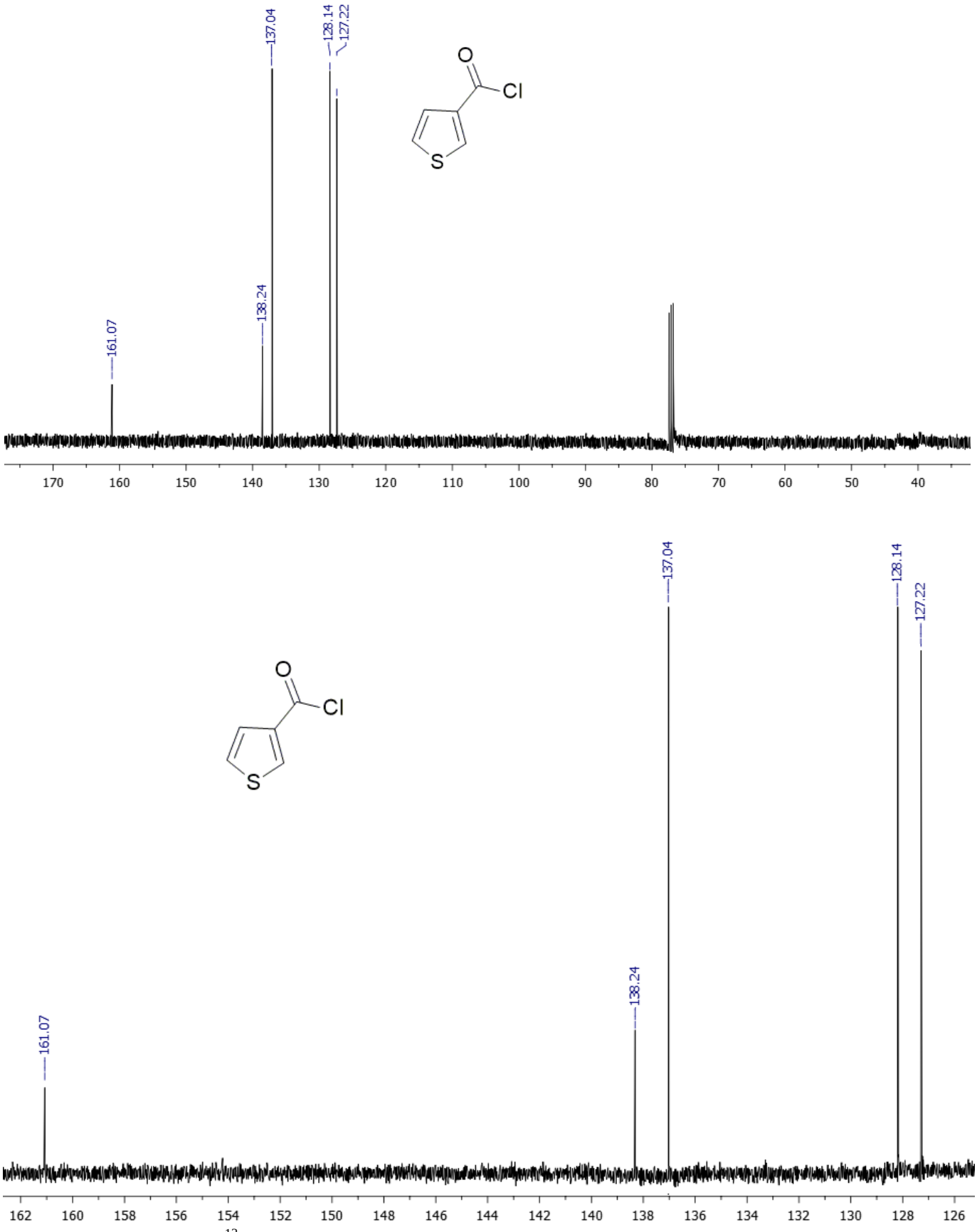



**Figure S10** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of thiophene-3-carbonyl chloride (**4**).

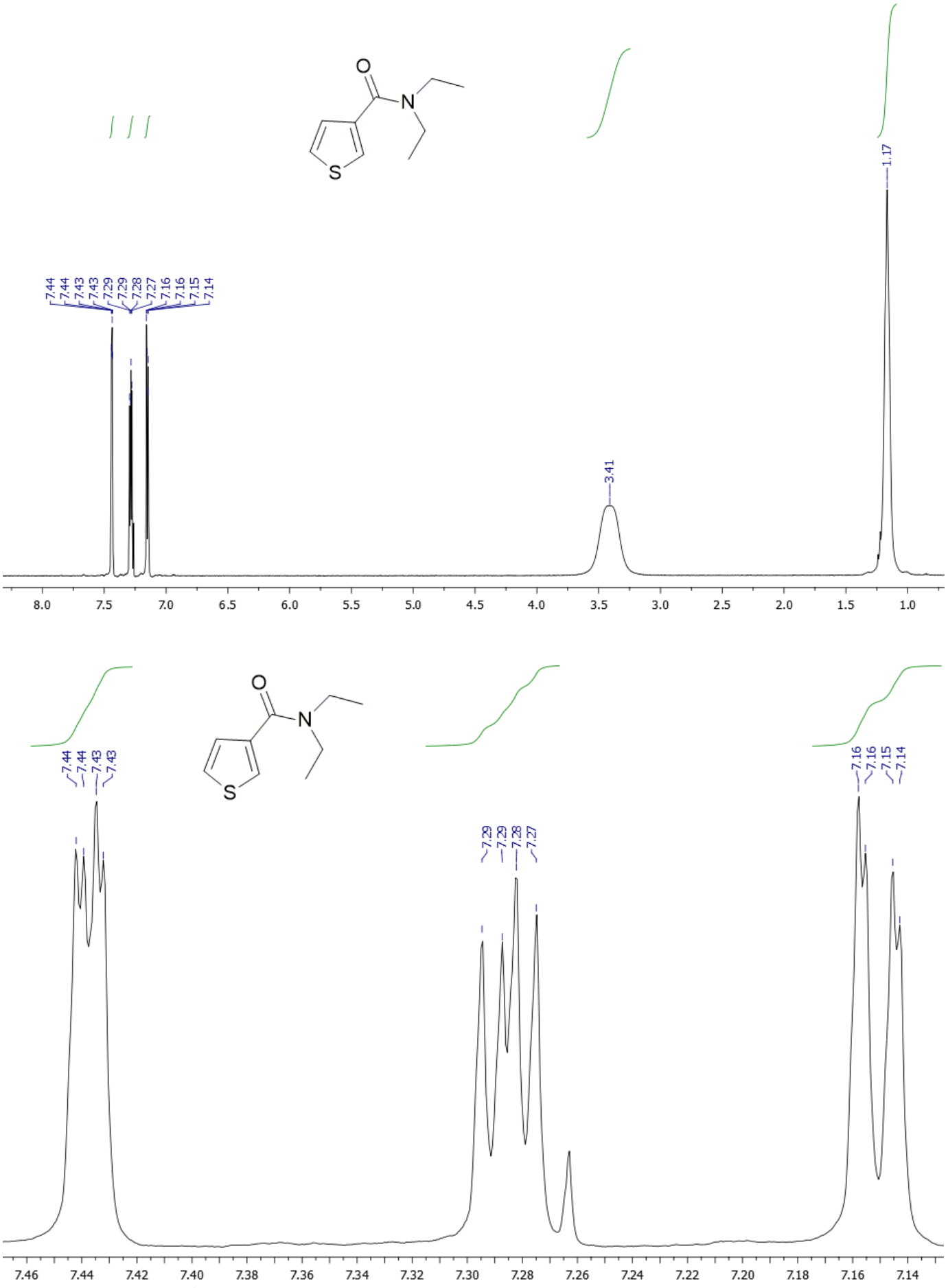
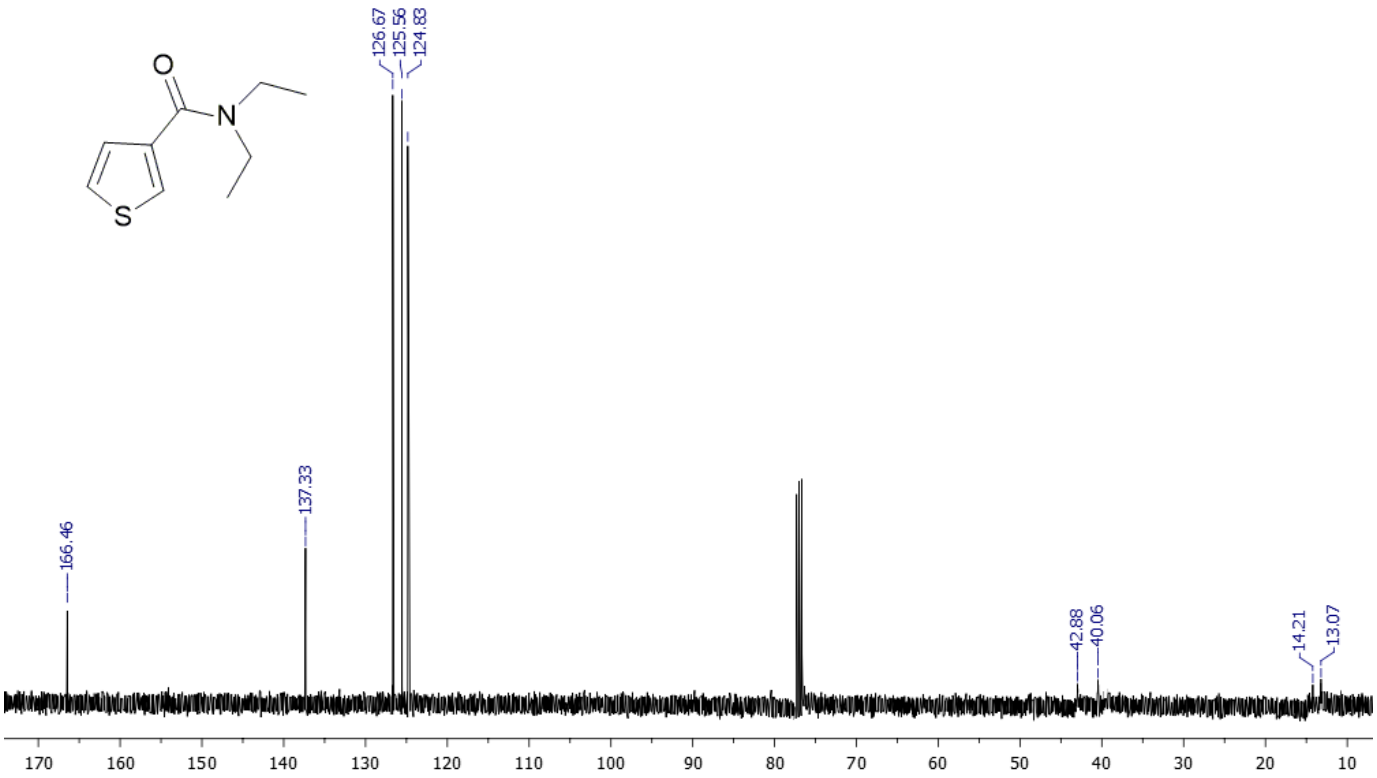



**Figure S11** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of *N*,*N*-diethylthiophene-3-carboxamide (**5**).



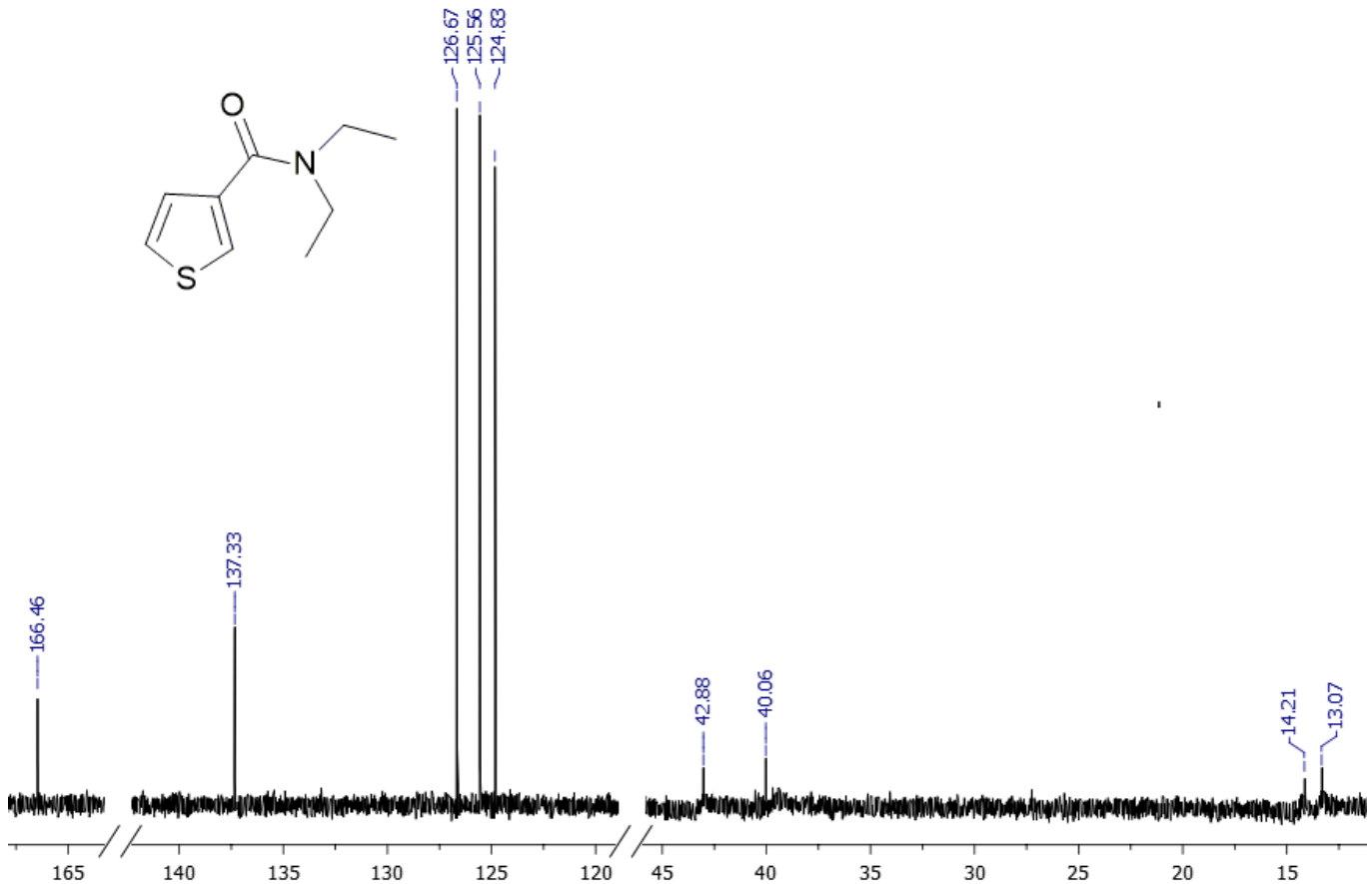




**Figure S12** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of *N*,*N*-diethylthiophene-3-carboxamide (**5**).

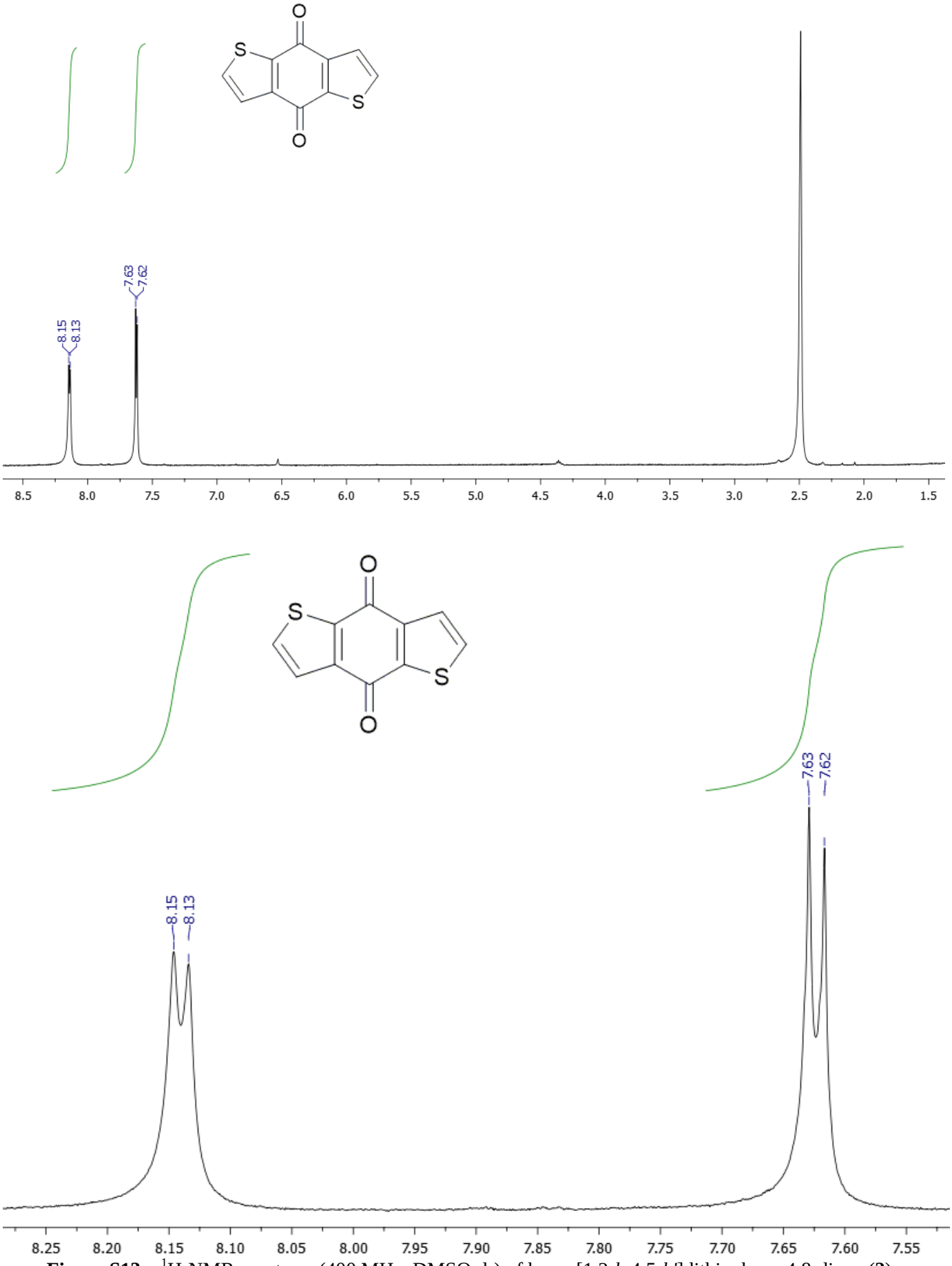



**Figure S13** – $^{1}$H-NMR spectrum (400 MHz, DMSO-$d_6$) of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-dione (**2**).

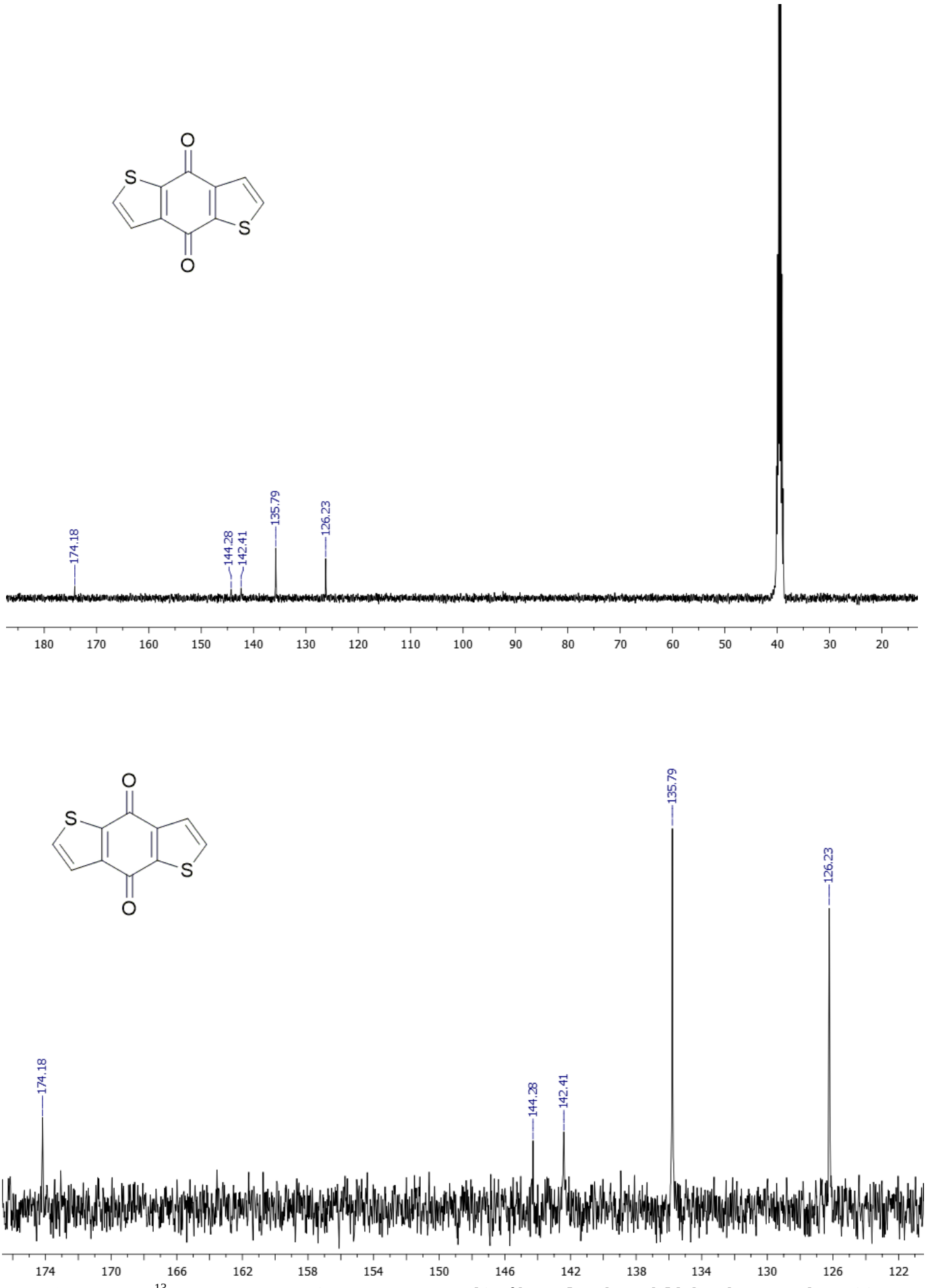



**Figure S14** – $^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$) of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-dione (**2**).

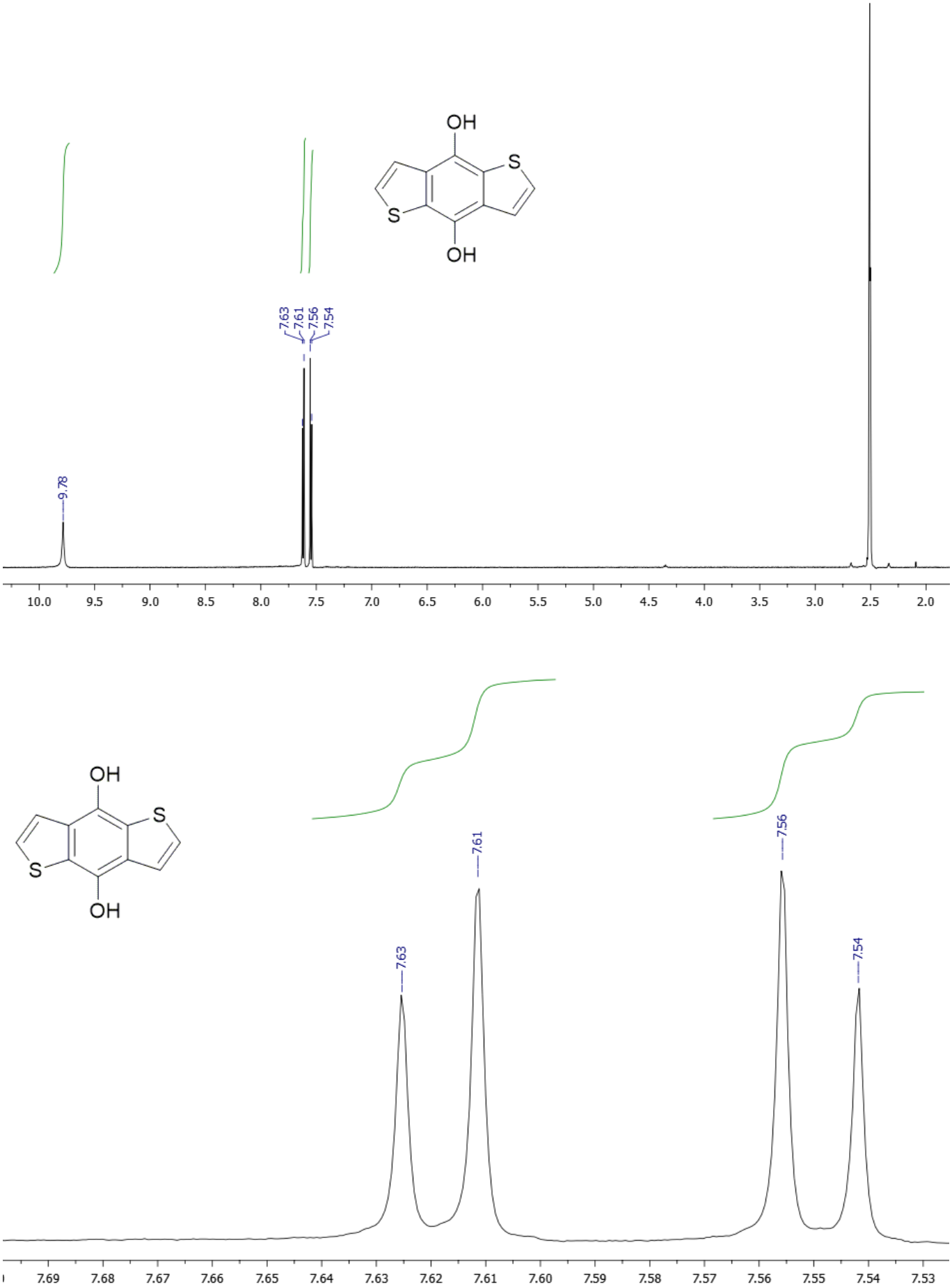
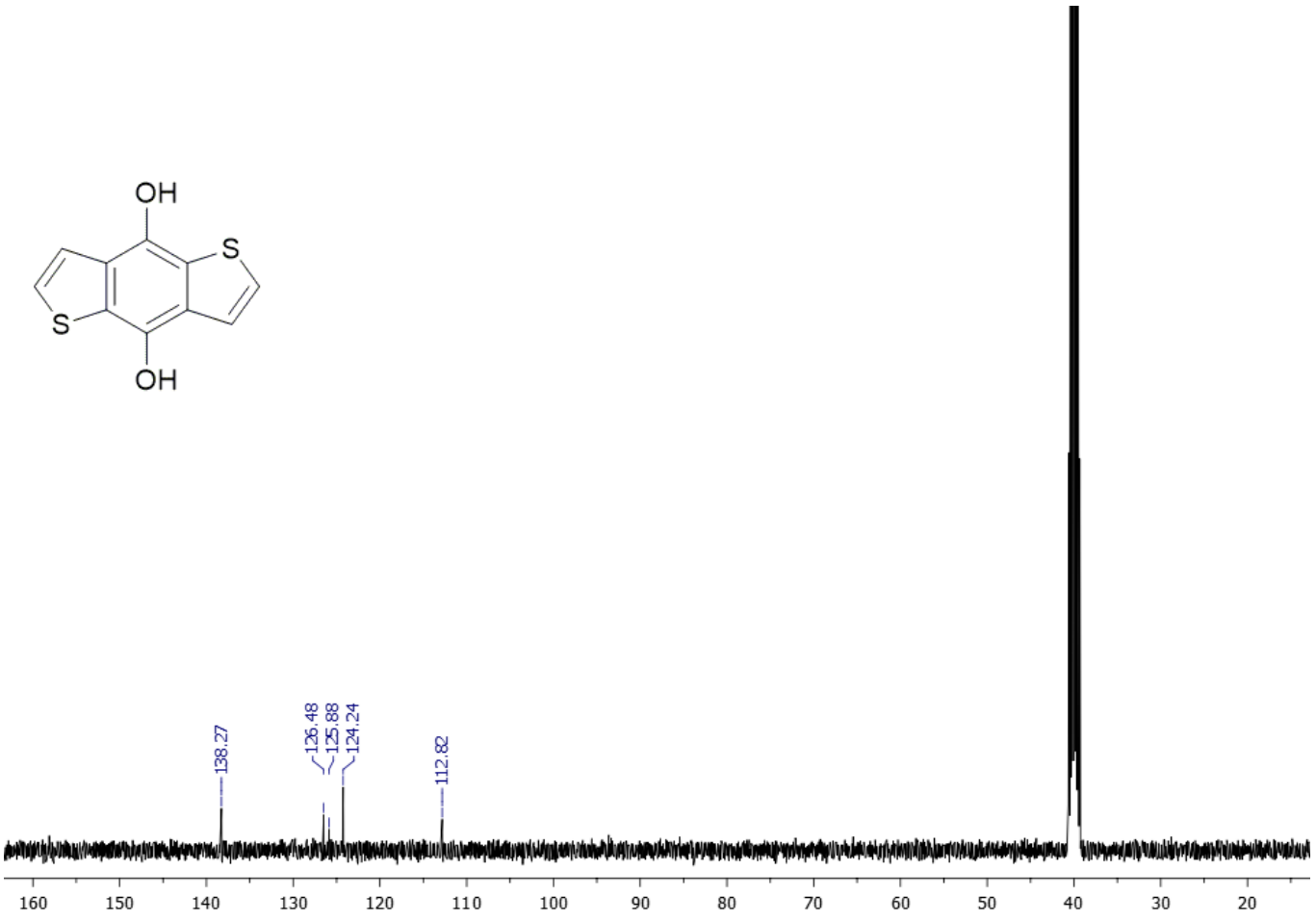



**Figure S15** – $^{1}$H-NMR spectrum (400 MHz, DMSO-$d_6$) of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-diol (**6**).



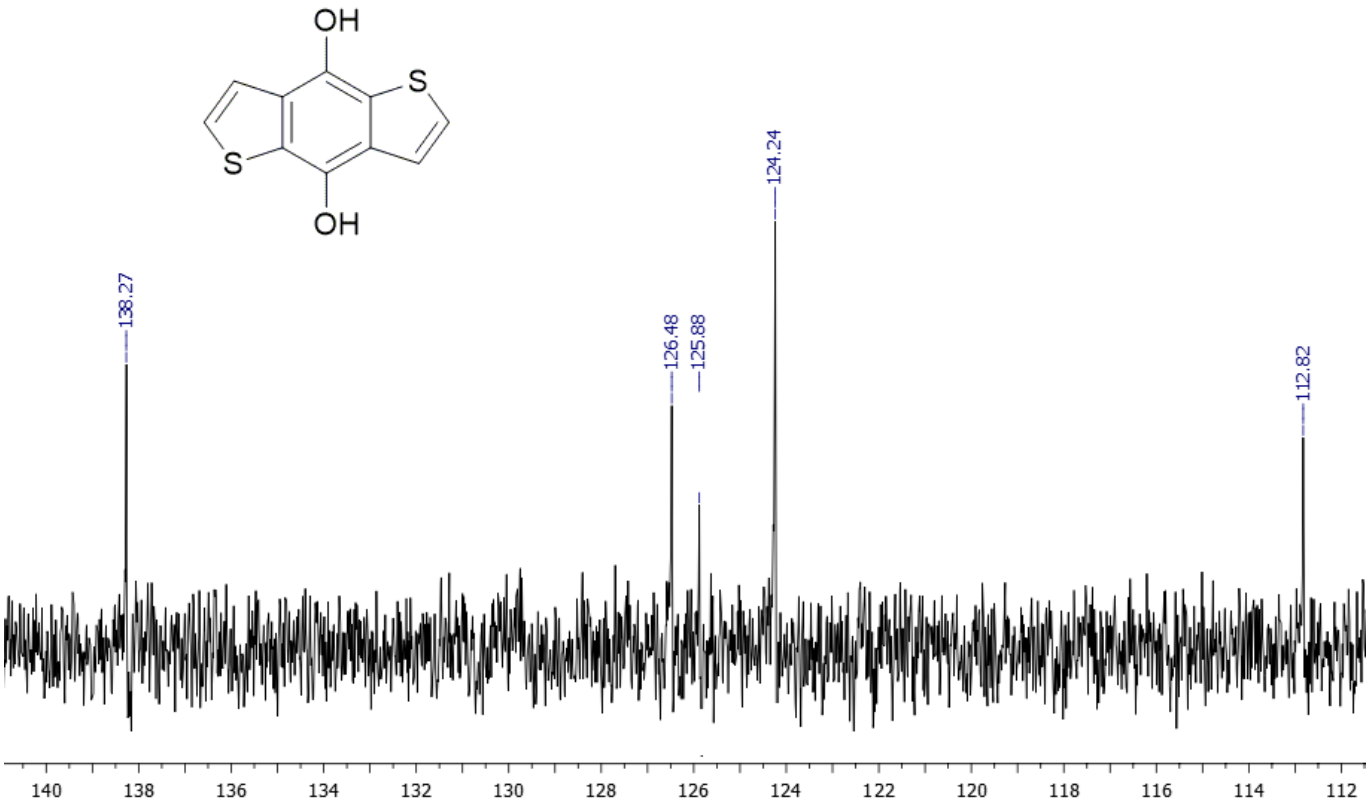




**Figure S16** – $^{13}$C-NMR spectrum (100 MHz, DMSO-$d_6$) of benzo[1,2-*b*:4,5-*b'*]dithiophene-4,8-diol (**6**).

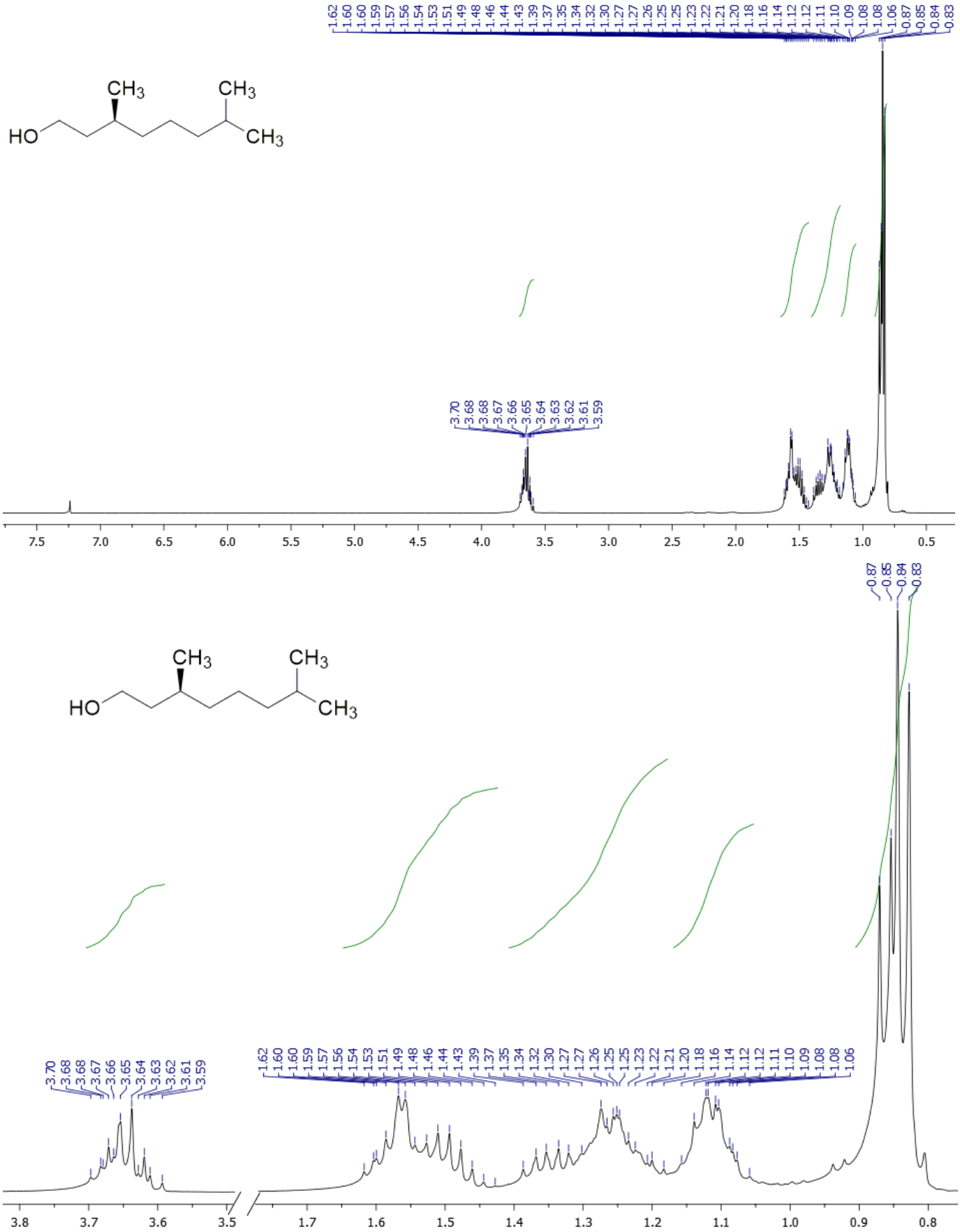
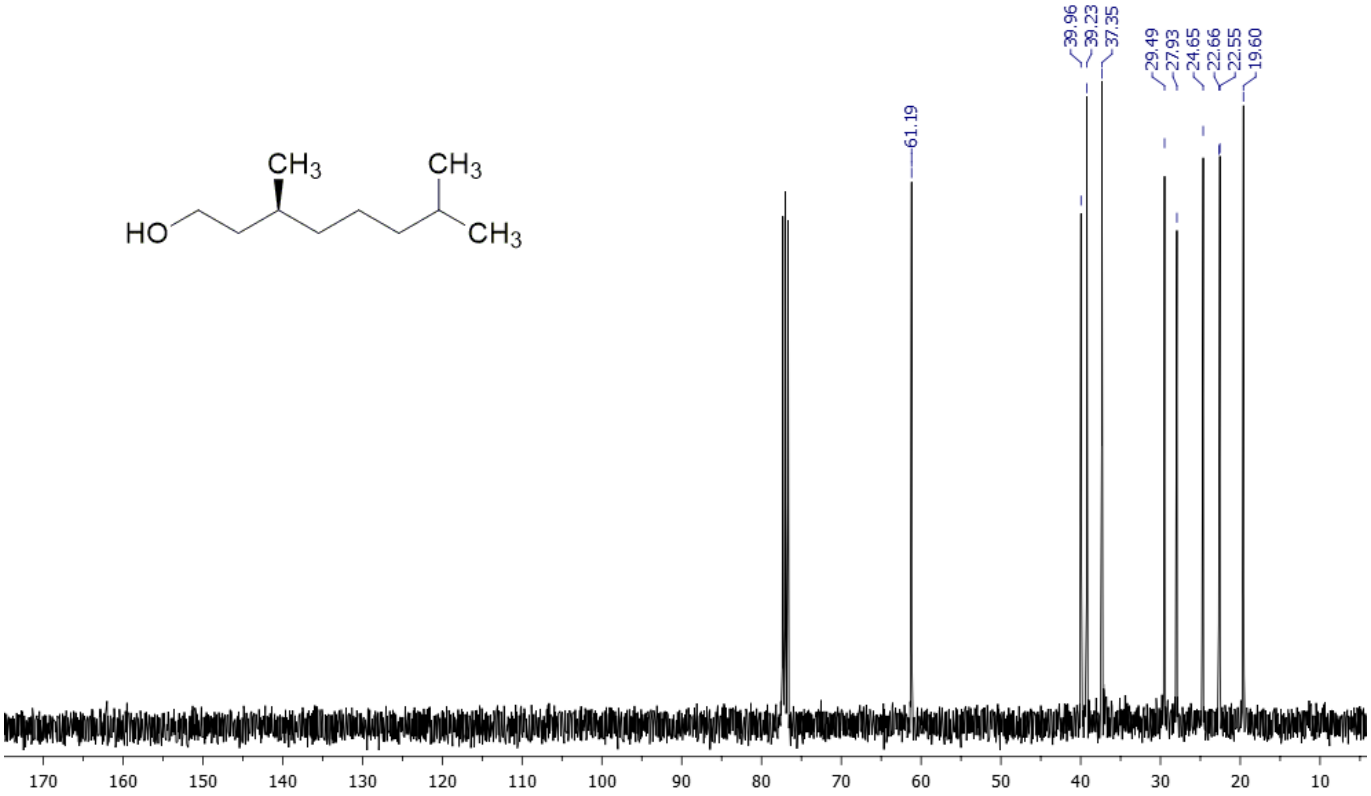



**Figure S17** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of (*S*)-3,7-dimethyloctan-1-ol (**9**).



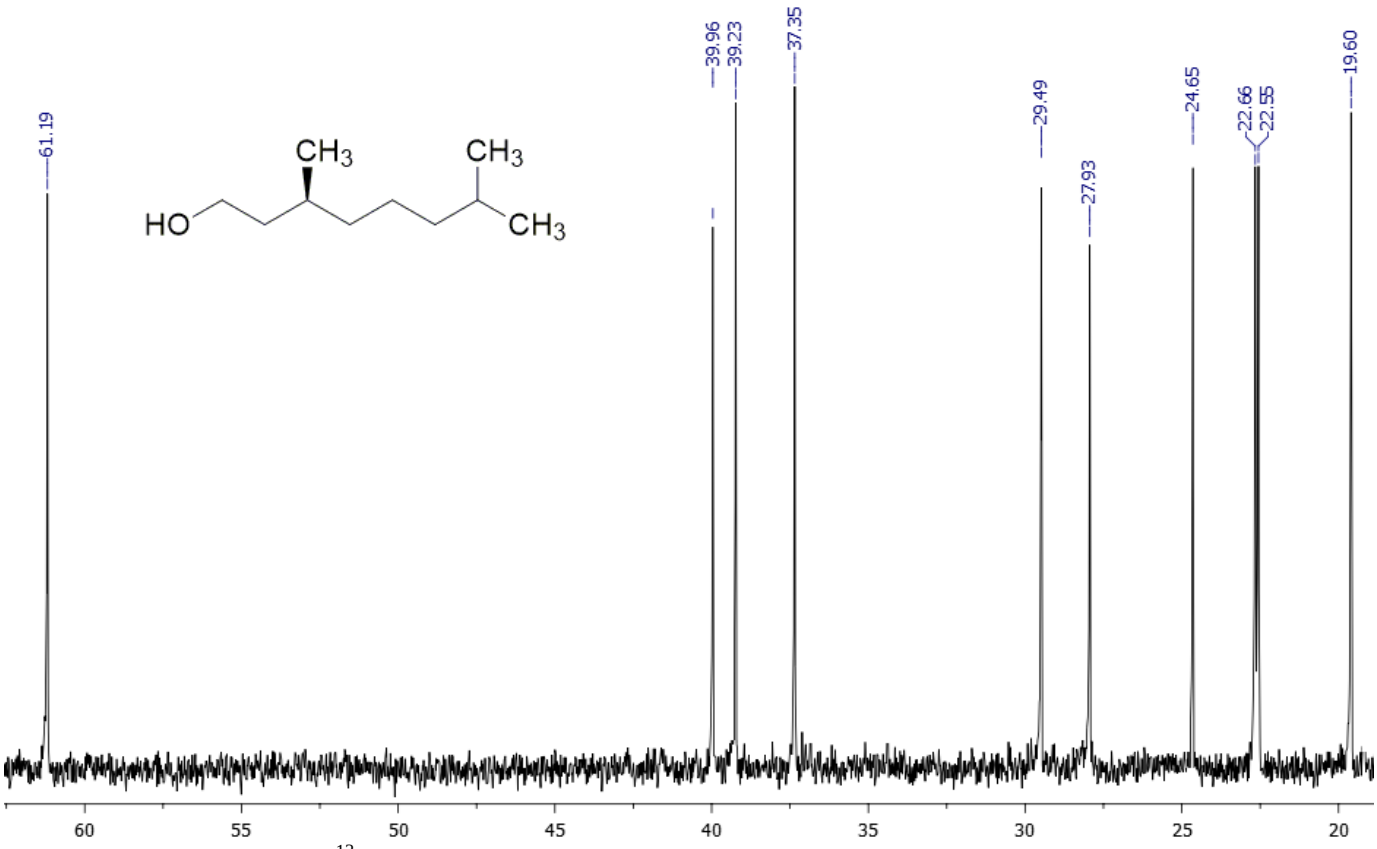




**Figure S18** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of (*S*)-3,7-dimethyloctan-1-ol (**9**).

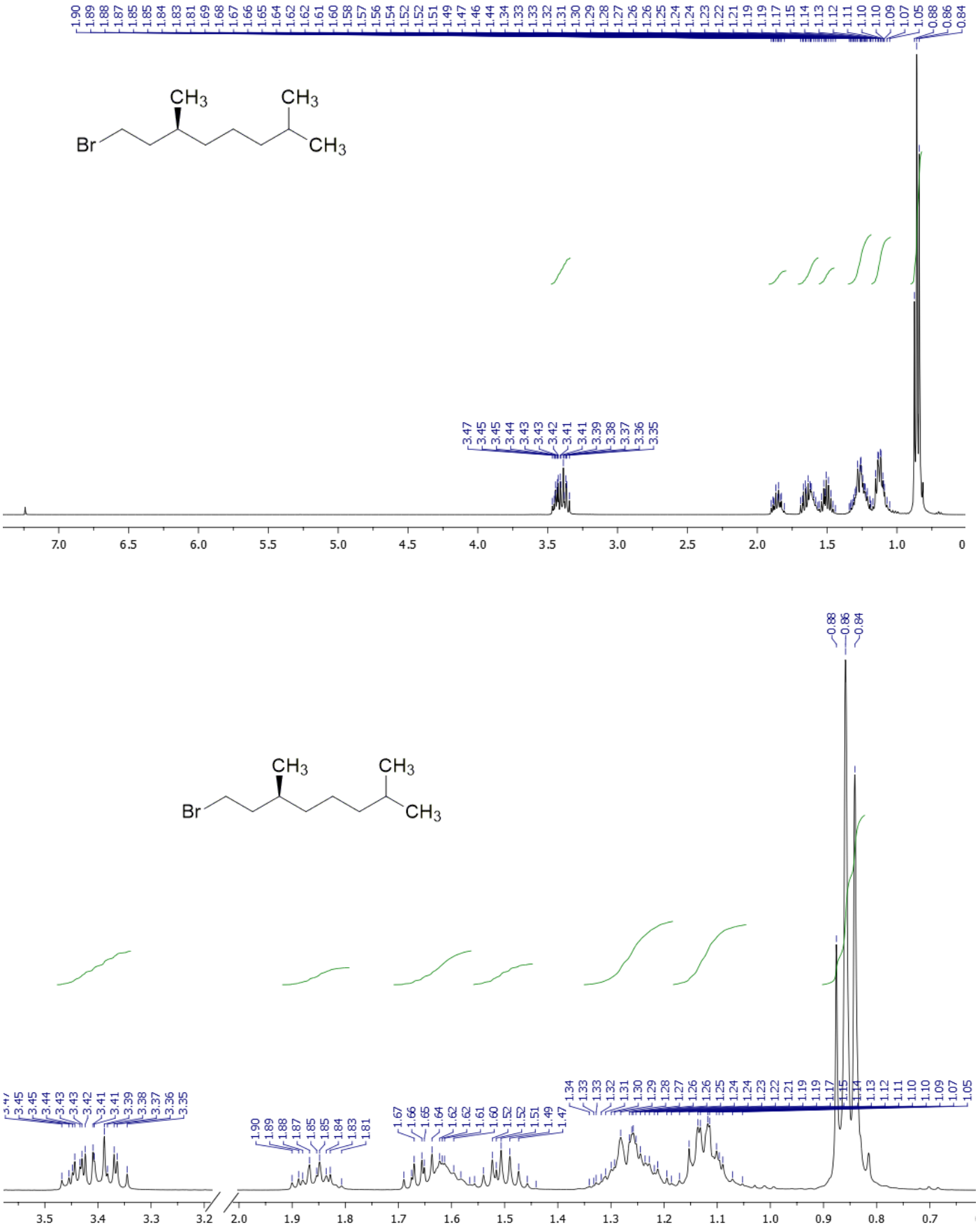



**Figure S19** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of (*S*)-1-bromo-3,7-dimethyloctane (**7**).

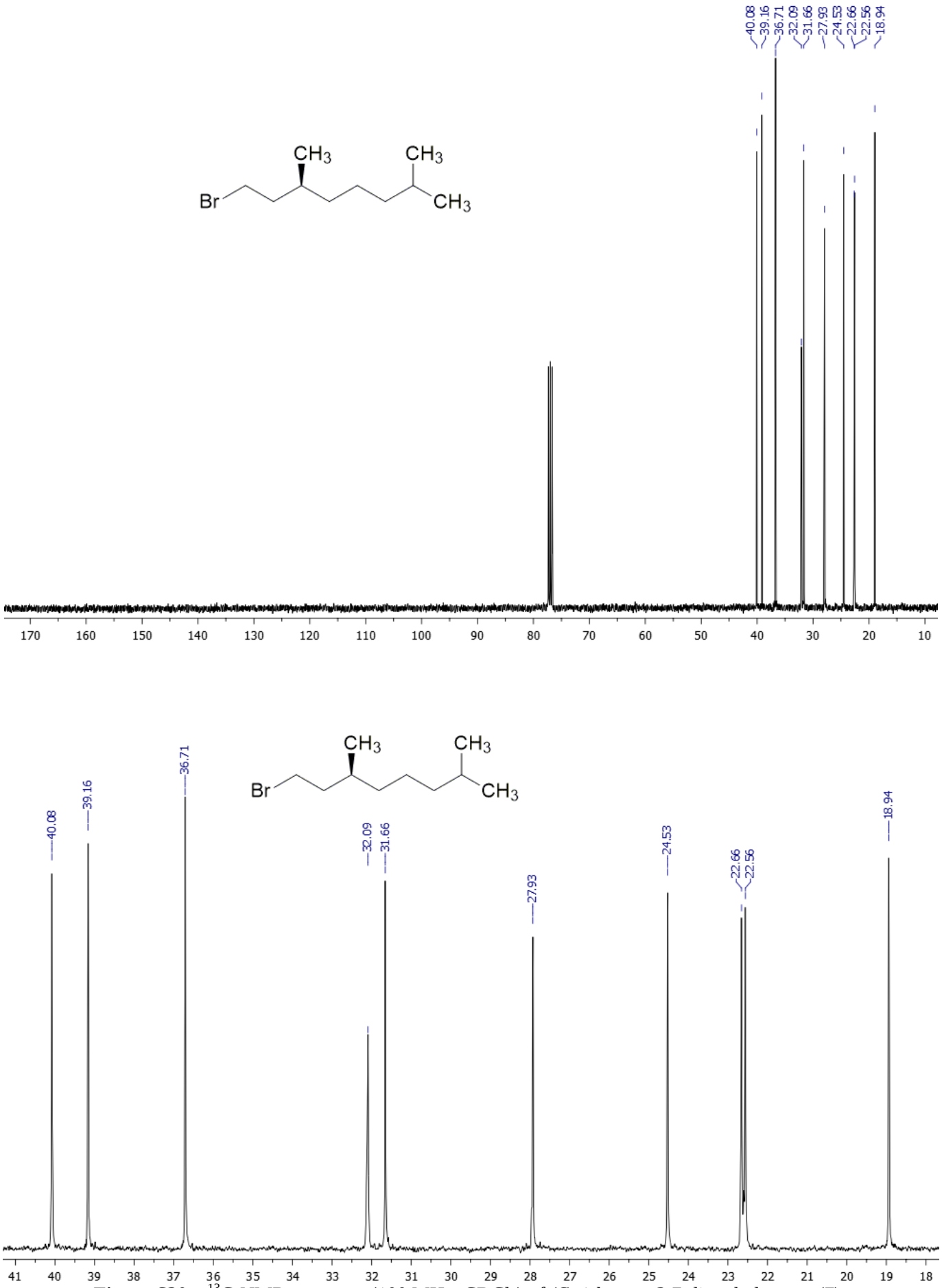



**Figure S20** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of (*S*)-1-bromo-3,7-dimethyloctane (**7**).

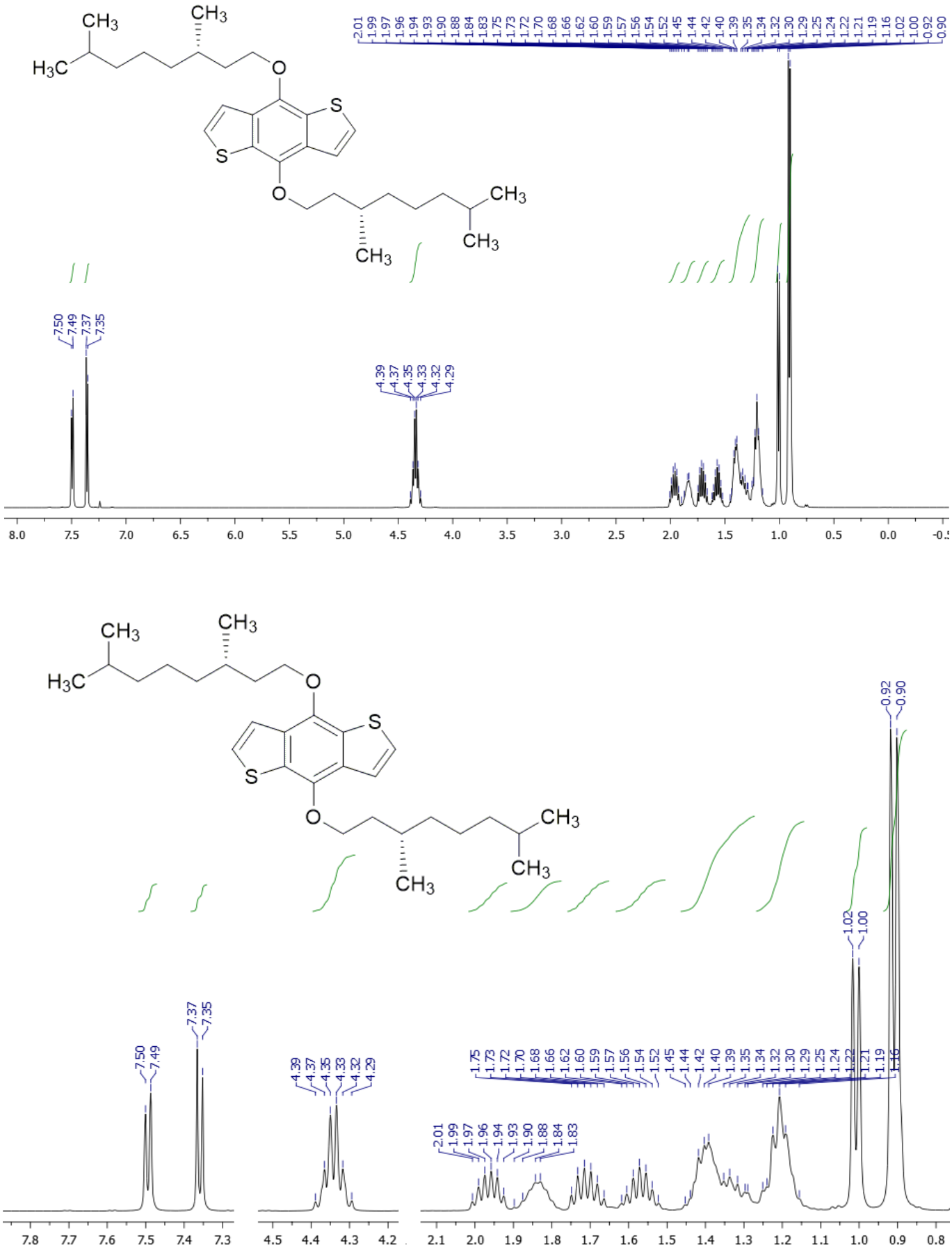


**Figure S21** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of 4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*] dithiophene (**10**).

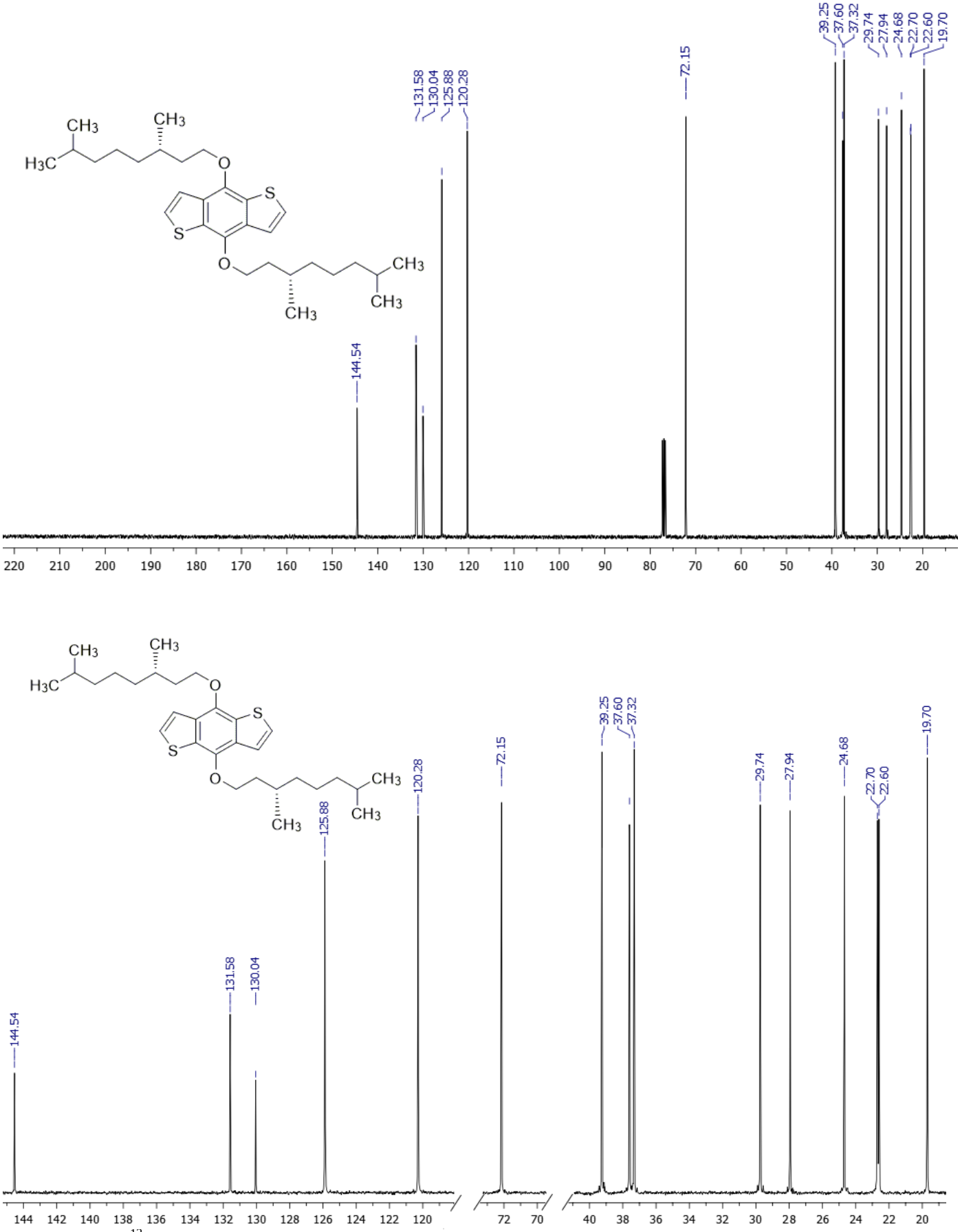



**Figure S22** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of 4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*] dithiophene (**10**).

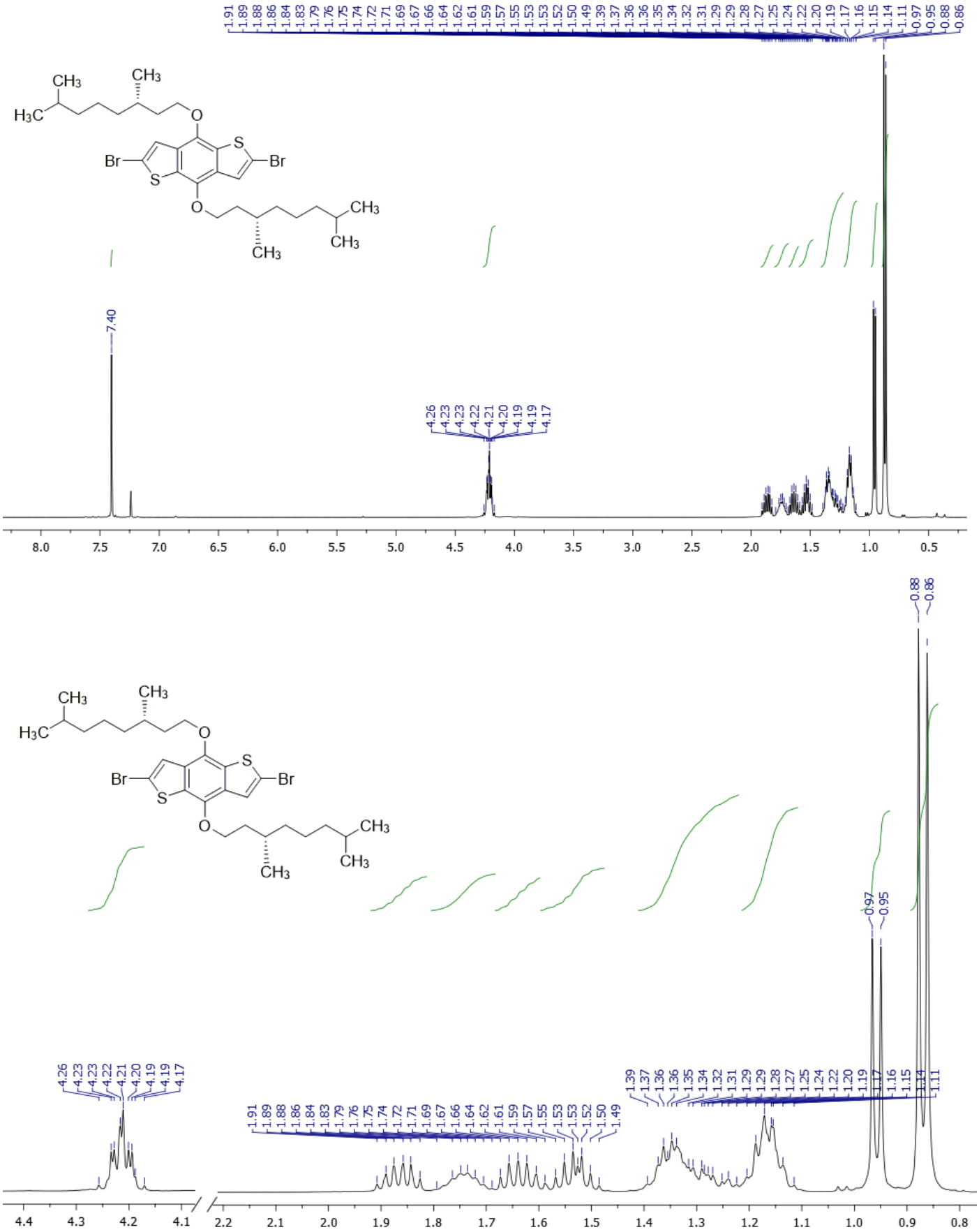



**Figure S23** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of 2,6-dibromo-4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b*′]dithiophene (**11**).

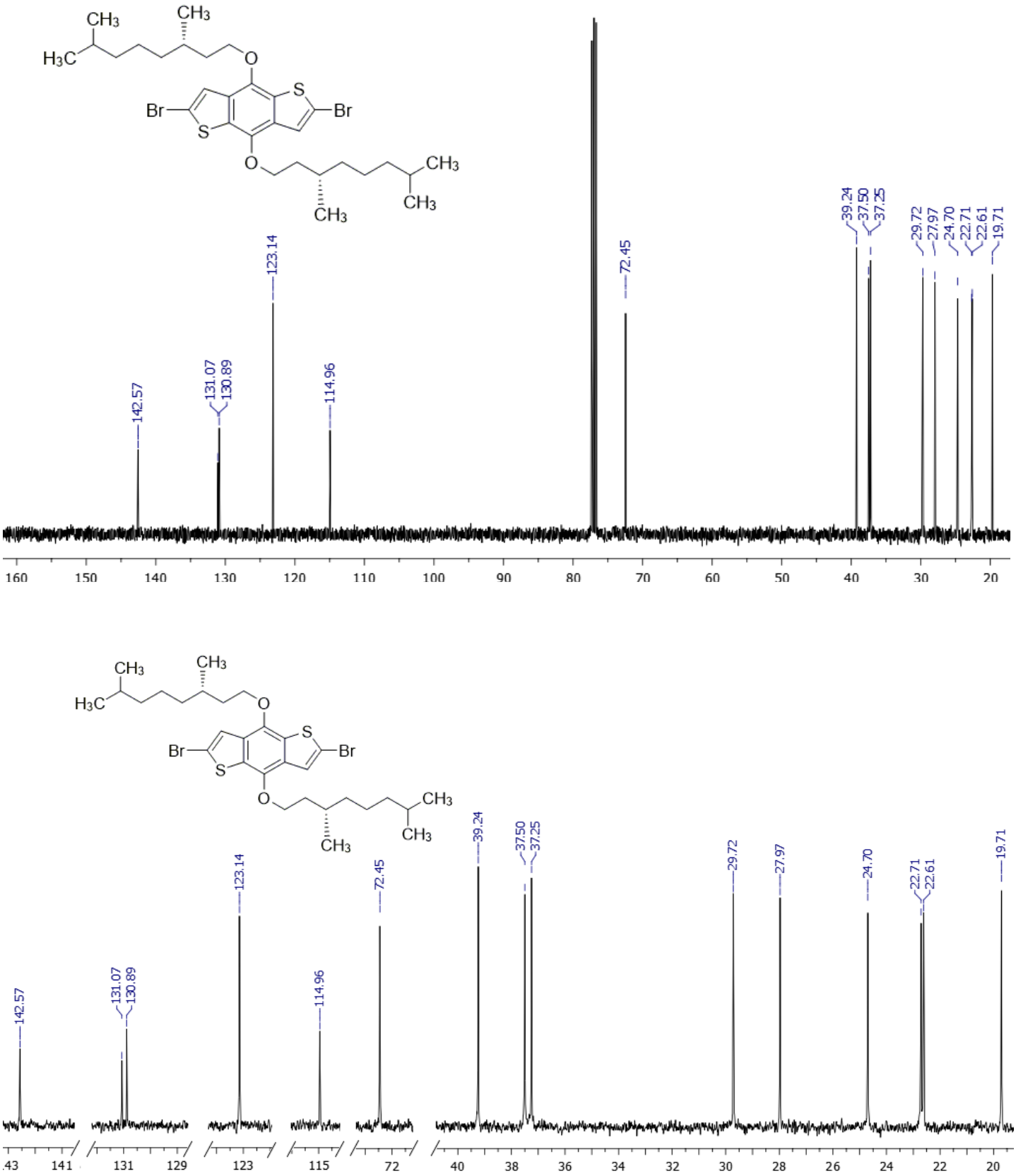






**Figure S24** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of 2,6-dibromo-4,8-bis(((*S*)-3,7-dimethyloctyl)oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (**11**).

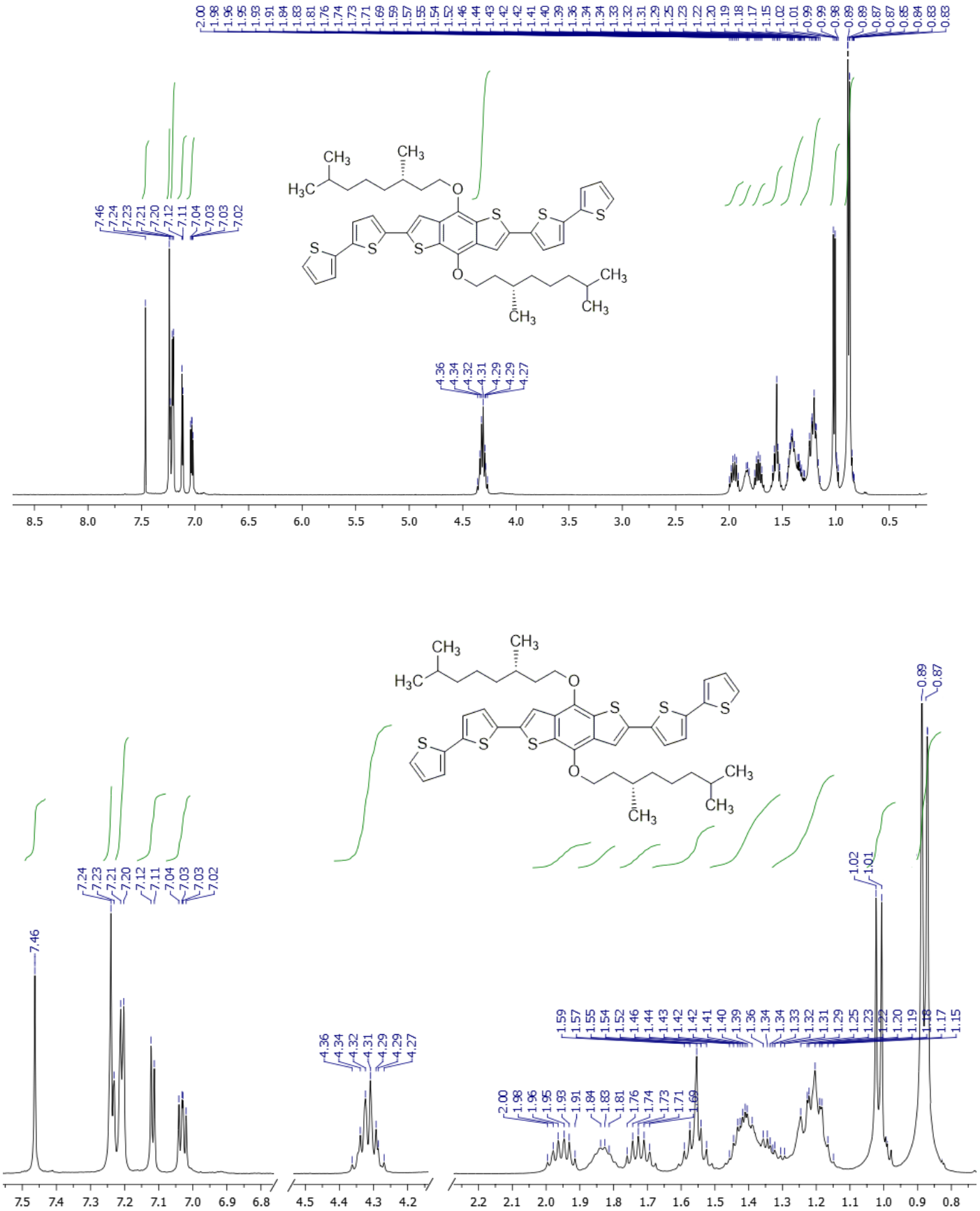


**Figure S25** – $^{1}$H-NMR spectrum (400 MHz, $CDCl_3$) of 2,6-di([2,2'-bithiophen]-5-yl)-4,8-bis(((*S*)-3,7-dimethyloctyl) oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (**1**).

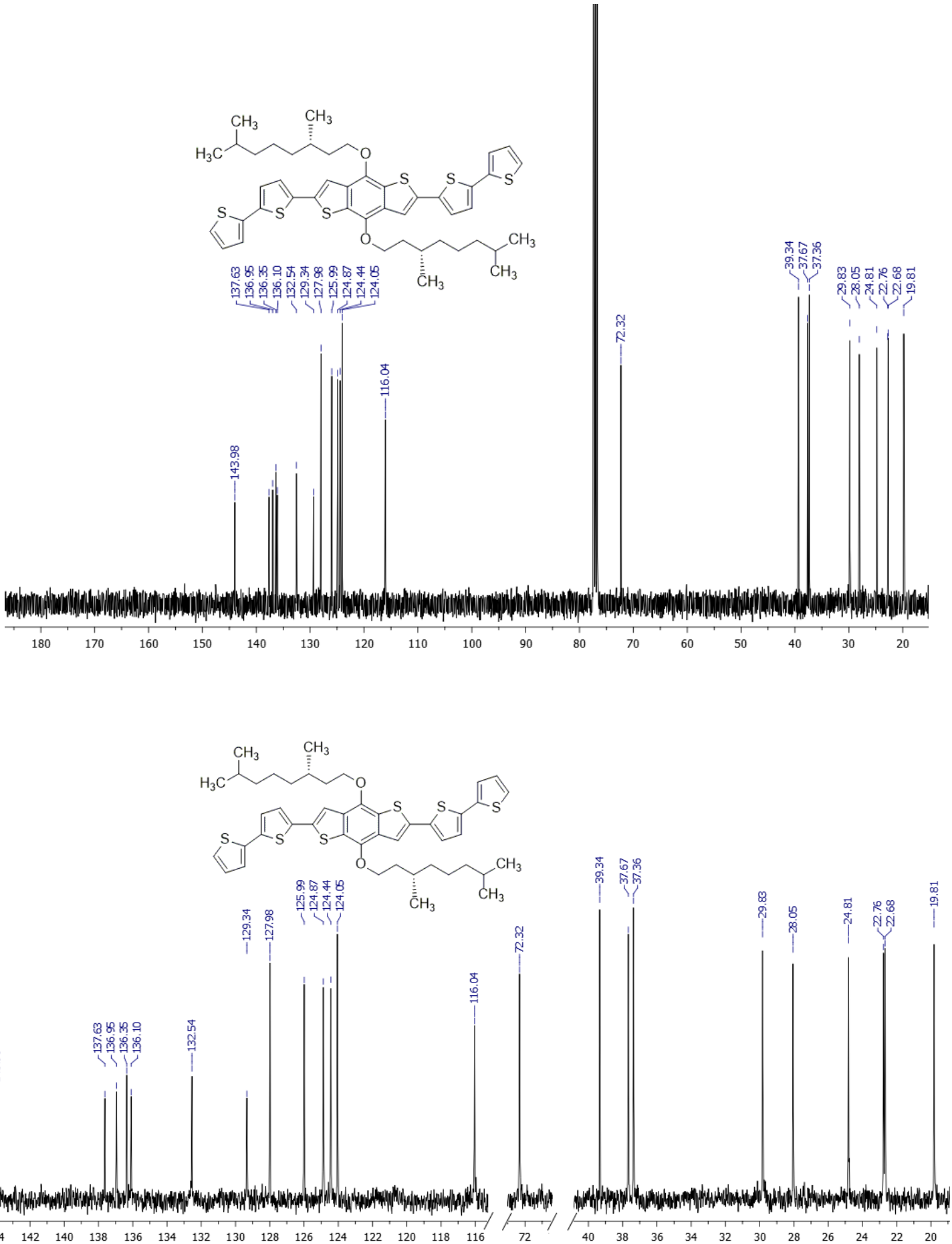



**Figure S26** – $^{13}$C-NMR spectrum (100 MHz, $CDCl_3$) of 2,6-di([2,2'-bithiophen]-5-yl)-4,8-bis(((*S*)-3,7-dimethyloctyl) oxy)benzo[1,2-*b*:4,5-*b'*]dithiophene (**1**).

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