Effect of donor to acceptor ratio on electrochemical and spectroscopic properties of oligoalkylthiophene 1,3,4-oxadiazole derivatives

Aleksandra Kurowska[1], Pawel Zassowski[1], Anastasia S. Kostyuchenko[2,3], Tatyana Yu. Zheleznova[2], Kseniya V. Andryukhova[4], Alexander S. Fisyuk[2,4], Adam Pron[5], Wojciech Domagala[1,]*

[1] Department of Physical Chemistry and Technology of Polymers, Silesian University of Technology, Marcina Strzody 9, 44-100 Gliwice, Poland

[2] Laboratory of New Organic Materials, Omsk State Technical University, Mira ave. 11, Omsk 644050, Russian Federation

[3] RUDN University, 6 Miklukho-Maklaya st, Moscow 117198, Russian Federation

[4] Department of Organic Chemistry, Omsk F. M. Dostoevsky State University, Mira ave. 55A, Omsk 644077, Russian Federation

[5] Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland

Electronic Supplementary Information

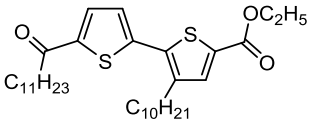
Synthetic procedures with instrumental and analytical product validation data

General Information

The IR spectra were recorded on an Infralum FT-801 spectrometer in KBr pellets for solids, or in thin films for liquid compounds. The ^{1}H and ^{13}C NMR spectra were obtained in $CDCl_3$ or DMSO with TMS as an internal standard, using a Bruker DRX 400 spectrometer (400 and 100 MHz, respectively). The elemental analyses were carried out on a Carlo Erba 1106 CHN analyzer. The melting points were determined on a Kofler bench. The reaction course and purity of the products were checked by thin-layer chromatography on Sorbfil UV-254 plates which were visualized with UV light. All chemicals were of analytical grade and purchased from Sigma-Aldrich Chemical Co. Compound **7a,**[1,2] **7b,**[2] **6,**[3] **4,**[4] terthiophene,[5,6] 1,4-di(2H-tetrazol-5-yl)benzene,[7] **7c,**[8] **3,**[9] were prepared according to known procedures.

Experimental and analytical data

Ethyl 3-decyl-5'-dodecanoyl-[2,2'-bithiophene]-5-carboxylate (8)



A mixture of lauric acid 1.74 g (8.7 mmol), 1.25 ml (17.4 mmol) thionyl chloride and one drop of DMF as a catalyst was stirred for 2.5 h at 45-50 ^{0}C. The excess of thionyl chloride was evaporated under reduced pressure. The obtained undecanoyl chloride and ethyl 3-decyl-[2,2'-bithiophene]-5-carboxylate **7a** (7.9 mmol) were dissolved in 15 ml anhydrous chlorobenzene. The solution was cooled in an ice bath and $SnCl_4$ (0.95 ml, 7.9 mmol) was then added with vigorous stirring. The reaction mixture was stirred for 1 h under cooling and for additional 4.5 h at room temperature. Then 5 ml 2M HCl was added slowly. The organic layer was washed with aqueous $NaHCO_3$ and water then dried over Na_2SO_4. The solvent was removed on a vacuum evaporator and the product purified by column chromatography (silica gel, hexane/EtOAc, 20/1).

Yield: 2.4 g (62%); yellow solid; Rf = 0.33 (silica gel, hexane/EtOAc, 20/1). M.p.=33-36^{0}C.

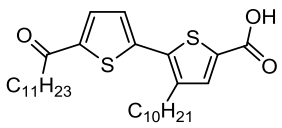
IR (KBr). ν cm^{-1}: 1664 (C=O), 1712 (CO_2Et).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.88 (6H, t., ^{3}J=6.8 Hz, $2CH_3$); 1.26-1.37 (30H, m., $15CH_2$); 1.38 (3H, t., ^{3}J=7.1 Hz, $OCH_2\underline{CH_3}$); 1.61-1.69 (2H, m., $ThCH_2\underline{CH_2}C_8H_{17}$); 1.72-1.79 (2H, m., $2\text{-}ThCOCH_2CH_2C_9H_{19}$); 2.78 (2H, t., ^{3}J=7.1 Hz, $Th\text{-}CH_2C_9H_{19}$); 2.88 (2H, t., ^{3}J=7.4 Hz, $Th\text{-}COCH_2C_{10}H_{21}$); 4.36 (2H, q., ^{3}J=7.2 Hz, OCH_2CH_3); 7.20 (1H, d., ^{3}J=3.9 Hz, Th-3'-H); 7.63(1H, s., Th-4-H); 7.64 (1H, d., ^{3}J=3.9 Hz, Th-4'-H).

^{13}C NMR (100 MHz, δ, ppm): 14.07 ($C_9H_{18}CH_3$, $COC_{10}H_{20}CH_3$), 14.40 ($COCH_2CH_3$), 22.70, 24.89, 29.33, 29.35, 29.39, 29.43, 29.45, 29.49, 29.51, 29.56, 29.60, 29.64, 30.30, 31.91, 31.93, 39.26 ($19CH_2$), 61.36 ($CO\text{-}CH_2CH_3$), 127.31 (3'-Th), 131.88 (4-Th), 132.67 (5-Th), 135.94 (4'-Th), 136.54 (2-Th), 141.70 (2'-Th), 143.00 (3-Th), 144.44 (5'-Th), 161.94 ($CO_2C_2H_5$), 193.31 (C=O).

Elemental analysis. Calculated for $C_{33}H_{52}O_3S_2$: C, 70.73%; H, 9.39%. found: C 70.66%, H 9.34%.

3-Decyl-5'-dodecanoyl-[2,2'-bithiophene]-5-carboxylic acid (9)



A solution of ethyl 3-decyl-5'-dodecanoyl-[2,2'-bithiophene]-5-carboxylate **8** 2.81 g (5.0 mmol) and potassium hydroxide 1.12 g, (20.0 mmol) in 6 mL ethanol was refluxed for 4 h. Ethanol was removed under reduced pressure, 8 ml of water was added to the residue and the mixture was acidified with dilute 2 N hydrochloric acid. The precipitate was separated and recrystallized from methanol.

Yield: 2.2 g (82%); yellow solid. M.p.=175-177^{0}C.

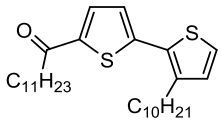
IR (KBr). ν cm^{-1}: 1668 (C=O), 2500-3460 (O-H).

^{1}H NMR (400 MHz, $CDCl_3$ δ, ppm): δ = 0.83-0.89 (6H, m., $2CH_3$); 1.18-1.33 (30H, m., $15CH_2$); 1.51 (2H, s., $ThCH_2CH_2C_8H_{17}$); 1.68-1.71 (2H, m., 2-$ThCOCH_2CH_2C_9H_{19}$); 2.59 (2H, s., Th-$CH_2C_9H_{19}$); 2.78-2.81 (2H, m., Th-$COCH_2C_{10}H_{21}$); 7.03 (1H, s., Th-3'-H); 7.46(1H, s., Th-4-H); 7.52 (1H, s., Th-4'-H).

^{13}C NMR (100 MHz, δ, ppm): 14.13 ($C_9H_{18}CH_3$, $COC_{10}H_{20}CH_3$), 22.71, 24.73, 29.39, 29.45, 29.53, 29.59, 29.70, 30.16, 31.94, 39.12 ($19CH_2$); 126.89 (3'-Th); 131.75 (4'-Th); 133.90 (5-Th); 135.93 (2-Th); 136.54 (4-Th); 141.64 (2'-Th); 143.10 (5'-Th), 143.96 (3-Th), 166.95 (CO_2H), 193.09 (C=O).

Elemental analysis. Calculated for $C_{31}H_{48}O_3S_2$: C, 69.81%; H, 9.01 %. found: C, 69.88%; H, 9.08 %.

1-(3'-Decyl-[2,2'-bithiophen]-5-yl)dodecan-1-one (10)



A mixture of acid **9** (2.10 g, 3.9 mmol), 5.6 mL quinoline and (0.12 g, 2.0 mmol) copper was stirred for 1 h at 225 ^{0}C. 7 ml of 15% hydrochloric acid was added to the residue and the mixture was stirred for 30 min at room temperature. Then product was extracted with CH_2Cl_2 (10ml×3). The combined organic extract was washed with water (30 mL), dried (Na_2SO_4) and concentrated. The product purified by column chromatography (hexane/EtOAc, 20/1) and crystallized from ethanol.

Yield: 1.2 g (62%); yellow solid. M.p.=49-52 ^{0}C.

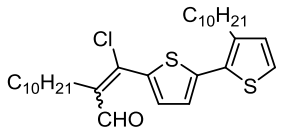
IR (KBr). ν cm^{-1}: 1649 (C=O).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.88 (6H, t., ^{3}J=6.8 Hz, $2CH_3$); 1.26-1.38 (30H, m., $15CH_2$); 1.59-1.68 (2H, m, $ThCH_2CH_2C_8H_{17}$); 1.72-1.79 (2H, m., 2-$ThCOCH_2CH_2C_9H_{19}$); 2.80 (2H, t., ^{3}J=7.8 Hz, Th-$CH_2C_9H_{19}$); 2.87 (2H, t., ^{3}J=7.4 Hz, Th-$COCH_2C_{10}H_{21}$); 6.95 (1H, d., ^{3}J=5.1 Hz, Th-4'-H); 7.12 (1H, d., ^{3}J=4.0 Hz, Th-3-H); 7.23 (1H, d., ^{3}J=5.1 Hz, Th-5'-H); 7.63 (1H, d., ^{3}J=4.0 Hz, Th-4-H).

^{13}C NMR (100 MHz, δ, ppm): 14.13 ($2CH_3$); 22.70, 24.99, 29.34, 29.35, 29.40, 29.45, 29.46, 29.48, 29.51, 29.52, 29.59, 29.61, 29.63, 29.64, 30.50, 31.91, 31.92, 39.15 ($19CH_2$); 125.13 (3-Th); 126.13 (5'-Th); 129.91(4'-Th); 130.48 (4-Th); 132.05 (2-Th); 141.39 (2'-Th); 143.06 (5-Th); 144.67(3'-Th); 193.42 (C=O).

Elemental analysis. Calculated for $C_{30}H_{48}OS_2$: C, 73.84%; H, 9.99%. found: C 73.71%, H 9.90%.

2-(Chloro(3'-decyl-[2,2'-bithiophen]-5-yl)methylene)dodecanal (11)



To DMF (8 ml) at 0^0C was added $POCl_3$ (0.75 ml, 8.2 mmol) and the mixture was stirred for 30 min at the same temperature. In the next step a solution of ketone **I9** (1.9 mmol) in DMF (2 ml) was added dropwise. The reaction mixture was heated at 60 - 65^0C for 5 h. Then the solution was poured on a crushed ice (20 g) in water (70 ml) and extracted with EtOAc (3 × 10 ml). The combined organic layers were washed with saturated solution of NaOAc and dried with anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel.

Yield: 0.61 g (60%); yellow oil. Rf=0.58, 0.60 (hexane/EtOAc, 20/1)

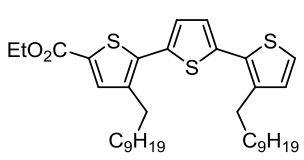
IR (KBr). ν cm^{-1}: 1671 (C=O). Z/E=19/81

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): **E-(11)**: 0.86-0.90 (6H, m., 2C$\underline{H}_3$); 1.25-1.68(32H, m., 16C$\underline{H}_2$); 2.55-2.59 (2H, m., =C-CH_2-); 2.75-2.79 (2H, m., -C$\underline{H}_2C_9H_{19}$); 6.96 (1H, d., ^{3}J=5.1 Hz, Th-4'-H); 7.04 (1H, d., ^{3}J=3.7 Hz, Th-3-H); 7.12 (1H, d., ^{3}J=3.7 Hz, Th-4-H); 7.23 (1H, d., ^{3}J=5.1 Hz, Th-5'-H); 9.75 (1 H, s., CHO); **Z-(11)**: 0.86-0.90 (6H, m., 2C$\underline{H}_3$); 1.25-1.68 (32H, m., 16C$\underline{H}_2$); 2.63-2.66 (2H, m., =C-CH_2-); 2.75-2.79 (2H, m., -C(O)CH_2C$\underline{H}_2C_9H_{19}$); 6.97 (1H, d., ^{3}J=5.1 Hz, Th-4'-H); 7.14 (1H, d., ^{3}J=3.8 Hz, Th-3-H); 7.26 (1H, d., ^{3}J=5.1 Hz, Th-5'-H); 7.57(1H, d., ^{3}J=3.8 Hz, Th-4-H); 10.36 (1 H, s., CHO).

^{13}C NMR (100 MHz, δ, ppm): **E-(11)**: 14.14 (CH_3); 22.70, 27.84, 28.72, 29.35, 29.38, 29.42, 29.44, 29.46, 29.49, 29.55; 29.58; 29.62; 29.68; 29.72; 29.76; 29.84; 30.57; 31.91 (18CH_2); 125.03 (3-Th); 125.33 (5'-Th); 129.32 (Cl-$\underline{C}$=); 130.36 (4'-Th); 131.98 (=$\underline{C}$-CHO); 132.93 (4-Th); 137.31(2'-Th); 141.03 (2-Th); 141.32 (3'-Th); 142.20 (5-Th); 189.73(CHO). **Z-(11)**: 28.55, 28.30 (2CH_2); 125.12 (3-Th); 125.75 (5'-Th); 130.47 (4'-Th); 135.05 (4-Th); 137.98 (2'-Th); 140.78(2-Th); 141.08 (3'-Th); 145.87 (5-Th); 192.02 (CHO).

Elemental analysis. Calculated for $C_{31}H_{47}ClOS_2$: C, 69.56%; H 8.85%. found: C, 69.61%; H, 8.91%.

Ethyl 3,3''-didecyl-[2,2':5',2''-terthiophene]-5-carboxylate (7d)



To a mixture of sodium ethoxide (90 mg, 1.3 mmol), ethyl mercaptoacetate (0.15 ml, 1.3 mmol) in 4 ml ethanol was added the solution of compound **11** (1.1 mmol) in 0.5 ml anhydrous THF. The reaction mixture was heated under reflux for 4 h. The solvent was evaporated under reduced pressure; the resulting solid residue was dissolved in 7 ml of water and 15 ml of EtOAc. The organic extract was washed with brine (30 mL), dried (Na_2SO_4) and concentrated. The product was purified by column chromatography on silica gel.

Yield: 0.49 g (74%); yellow oil. Rf=0.51 (hexane/EtOAc, 20/1)

IR (KBr). ν cm^{-1}: 1710 (C=O).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.85-0.89 (6H, m, $2CH_3$), 1.25-1.33 (28H, m, $14CH_2$), 1.38 (3H, t, ^{3}J= 6.4 Hz, $OCH_2\underline{C}H_3$), 1.58-1.70 (4H, m, $2ThCH_2\underline{C}H_2C_8H_{17}$), 2.75-2.80 (4H, m, $2Th\underline{C}H_2C_9H_{19}$), 4.35 (2H, q, ^{3}J=7.2 Hz, $O\underline{C}H_2CH_3$), 6.94 (1H, d, ^{3}J=5.4 Hz, Th-4''-H), 7.07 (1H, d, ^{3}J=3.9 Hz, Th-4'-H), 7.15 (1H, d., ^{3}J=3.7 Hz, Th-3'-H), 7.18 (1H, d, ^{3}J=5.4 Hz, Th-5''-H), 7.25 (1H, s., Th-4-H). Z/E=19/81

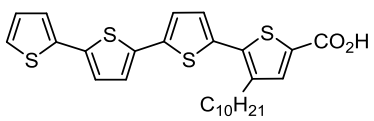
^{13}C NMR (100 MHz, δ, ppm): 14.13 ($2CH_3$), 14.39 ($OCH_2\underline{C}H_3$), 22.70, 29.33, 29.36, 29.37, 29.41, 29.46, 29.50, 29.57, 29.60, 29.64, 30.46, 30.73, 31.92 ($18CH_2$), 61.16 ($O\underline{C}H_2CH_3$), 124.14 (5''-Th), 126.19 (3'-Th), 127.06 (4'-Th), 129.99 (4''-Th), 130.18 (4-Th), 130.54 (2-Th), 134.83 (5-Th), 136.00 (2''-Th), 137.52 (2'-Th), 137.69 (5'-Th), 139.69 (3''-Th), 140.11 (3-Th), 162.21 (C=O).

Elemental analysis. Calculated for $C_{35}H_{52}O_2S_3$: C, 69.95%; H 8.72%. found: C, 70.02%; H 8.71%.

Substituted 2,2'-bithiophene-, 2,2':5',2''-terthiophene- and 3-decyl-[2,2':5',2'':5'',2'''-quaterthiophene] 5-carboxylic acids (12a-c);

Compound **12a, 12b** were prepared according to the known procedure [1] (see *Supporting Information*).

3-Decyl-[2,2':5',2'':5'',2'''-quaterthiophene]-5-carboxylic acid (12c)



To ether **7c** (1.5 mmol) in THF (10 mL) was added a solution of potassium hydroxide (0.40 g, 7.1 mmol) in 5 ml ethanol. The reaction mixture was stirred for night at room temperature. A solvent was removed under reduced pressure, 20 ml of water was added to the residue and the mixture was acidified with dilute 2 N hydrochloric acid. The precipitate was separated and crystallized.

Yield: 0.54 g (77%); M.p. = 145-147 ^{0}C (acetone); orange solid.

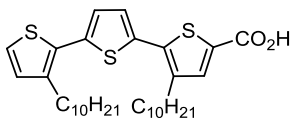
IR (KBr). ν cm^{-1}: 1661 (C=O), 2450-2600 (O-H).

^{1}H NMR (400 MHz, DMSO-d, δ, ppm 6): δ = 0.82 (t, ^{3}J=6.8 Hz, 3H, CH_3), 1.20-1.35 (m, 14H, $7CH_2$), 1.55-1.64 (m, 2H, $ThCH_2\underline{C}H_2C_8H_{17}$), 2.75 (t, ^{3}J=7.6 Hz, 2H, $Th\underline{C}H_2C_9H_{19}$), 7.09 (d.d, ^{3}J=3.5 Hz, ^{3}J=5.1 Hz, 1H, Th-4'''-H), 7.24 (d., ^{3}J=3.7 Hz, 2H, Th-3'-H, Th-4'-H), 7.28 (d., ^{3}J=3.7 Hz, 1H, Th-3''-H), 7.31-7.32 (m., 2H, Th-3''-H, Th-4''-H), 7.49 (d.d, ^{3}J=5.1 Hz, ^{4}J=1.0 Hz, 1H, Th-5'''-H), 7.58 (s., 1H, Th-4-H).

^{13}C NMR (100 MHz, δ, ppm): 13.36 (CH_3), 21.60, 28.21, 28.47, 28.52, 29.21, 30.86 ($9CH_2$), 124.05 (4''-Th), 124.46 (3''-Th), 124.59 (4'-Th), 125.12 (3'''-Th), 125.41 (5'''-Th), 127.88 (4'''-Th), 127.96 (3'-Th), 131.69 (2-Th), 133.02 (2''-Th), 134.02 (5''-Th), 135.29 (4-Th), 135.56 (5'-Th), 135.66 (2'-Th), 135.88 (2'''-Th), 135.80 (3-Th), 139.89 (5-Th), 162.02 (C=O).

Elemental analysis. Calculated for $C_{27}H_{30}O_2S_4$. C, 62.99%; H, 5.87%. found: C, 63.10%; H, 5.95%.

3,3''-didecyl-[2,2':5',2''-terthiophene]-5-carboxylic acid (12d)



A mixture of **7d** (1.5 mmol) and potassium hydroxide (0.40 g, 7.1 mmol) in ethanol (6 mL) was refluxed for 3 h. Ethanol was removed under reduced pressure, 8 ml of water was added to the residue and the mixture was acidified with dilute 2 N hydrochloric acid. The precipitate was separated and crystallized.

Yield: 0.58 g (68%); M.p. = 95-96 ^{0}C (ethanol); yellow solid.

IR (KBr). ν cm^{-1}: 1663 (C=O), 2400-3446 (O-H).

^{1}H NMR (400 MHz,$CDCl_3$, δ, ppm): δ = 0.86-0.89 (6H, m, $2CH_3$), 1.25-1.39 (28H, m, $14CH_2$), 1.61-1.71(4H, m, $ThCH_2C\underline{H}_2C_8H_{17}$), 2.76-2.81 (4H, m, $2ThC\underline{H}_2C_9H_{19}$), 6.94 (1H, d., ^{3}J=5.1 Hz, Th-4''-H), 7.08 (1H, d., ^{3}J=3.9 Hz, Th-4'-H), 7.18 (1H, d., ^{3}J=3.9 Hz, Th-3'-H), 7.20 (1H, d., ^{3}J=5.1 Hz, Th-5''-H), 7.71 (1H, s., Th-4-H).

^{13}C NMR (100 MHz, δ, ppm): 14.13 (CH_3), 22.70, 29.36, 29.42, 29.46, 29.51, 29.58, 29.60, 29.64, 30.41, 30.73, 31.92 ($18CH_2$), 124.23 (4'-Th), 126.23 (5''-Th), 127.40 (3'-Th), 129.26 (2-Th), 129.90 (5-Th), 130.20 (4''-Th), 134.54 (2''-Th), 137.61 (4-Th), 139.65 (2'-Th), 137.93 (5'-Th), 140.24 (3''-Th, 3-Th), 167.43 (C=O).

Elemental analysis. Calculated for $C_{33}H_{48}O_2S_3$: C, 69.18%; H, 8.44%. found: C, 69.26%; H, 8.55%.

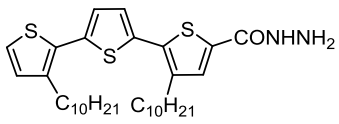
Substituted 2,2'-bithiophene-, 2,2':5',2''-terthiophene- and 3-decyl-[2,2':5',2'':5'',2'''-quaterthiophene] 5-carbohydrazides (13a, b, d);

Compound **13a, 13b** were prepared according to the known procedure [2,9] (see *Supporting Information*).

General Procedure

A solution of hydrazine hydrate 97 % (0.78 ml) and **7d** (1.6 mmol) in 1.5 ml of ethanol was heated under reflux for 15 h. The resulting solution was cooled to room temperature, then 5 mL of water was added. The precipitate was separated and crystallized from methanol.

3,3''-Didecyl-[2,2':5',2''-terthiophene]-5-carbohydrazide (13d)



Yield: 0.70 g (75%); M.p. = 84-86 ^{0}C (methanol); yellow solid. Rf=0.42 ($CHCl_3$/EtOAc/EtOH, 6/3/1).

IR (KBr). ν cm^{-1}: 1622 (C=O), 3065-3274 (NH).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.85-0.88 (6H, m, $2CH_3$), 1.25-1.39 (28H, m, $14CH_2$), 1.61-1.68 (4H, m, $ThCH_2C\underline{H}_2C_8H_{17}$), 2.77 (4H, t., ^{3}J=7.3 Hz, $2ThC\underline{H}_2C_9H_{19}$), 4.12 (2H, s., $CONHNH_2$), 6.94 (1H, d., ^{3}J=4.9 Hz, Th-4''-H), 7.06 (1H, d., ^{3}J=3.4 Hz, Th-4'-H), 7.12 (1H, d., ^{3}J=3.4 Hz, Th-3'-H), 7.19 (1H, d., ^{3}J=4.9 Hz, Th-5''-H), 7.40 (1H, s., Th-4-H), 7.44 (1H, s., $CONHNH_2$).

^{13}C NMR (100 MHz, δ, ppm): 14.13 ($2CH_3$), 22.69, 29.33, 29.36, 29.44, 29.46, 29.51, 29.58, 29.63, 30.51, 30.73, 31.91 ($18CH_2$), 124.13 (3'-Th), 126.15 (5''-Th), 127.08 (4'-Th), 129.93 (4''-Th), 130.16 (4-Th), 131.62 (2-Th), 132.57 (2''-Th), 134.54 (5'-Th), 135.67 (5-Th), 137.50 (3-Th), 140.01 (3''-Th), 140.10 (2'-Th), 163.23 (C=O).

Elemental analysis. Calculated for $C_{33}H_{50}N_2OS_3$: C, 67.53%; H, 8.59%; N, 4.77%. found: C, 67.66%; H, 8.57%; N, 4.82%.

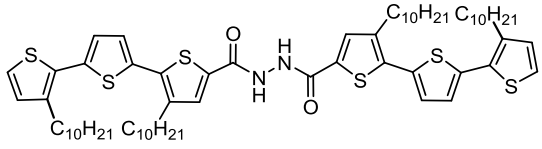
Synthesis of N,N'-bis(3-decyl-2,2'-bithiophene-5-oyl), N,N'-bis(3-decyl-2,2':5',2''-terthiophene-5-oyl), N,N'-bis (3,3''-decyl- 2,2':5',2''-terthiophene 5-oyl)hydrazines (14a-d) and N,N'-Bis(3-decyl-2,2':5',2'':5'',2'''-quaterthiophene -5-oyl)hydrazine (14c)

Compound **14a, b** were prepared according to the known procedure [2,9] (see *Supporting Information*).

General Procedure for the synthesis of compounds 14d:

A carbohydrazide **13 d** (0.9 mmol) was added to a solution of carboxylic acid **12 d** (0.9 mmol) and DCC (N N'-dicyclohexylcarbodiimide) (0.18 g, 0.9 mmol) in anhydrous THF (5 mL). The mixture was stirred at room temperature for 3-6 h. To mixture was added 100 μl acetic acid (10%). Then the precipitate of N,N'-dicyclohexylurea was filtered off and washed with THF (15 mL). The solvent was then removed under reduced pressure and the resulting crude product was purified by crystallization from methanol or ethyl acetate.

N,N'-Bis(3,3''-decyl-2,2':5',2''-terthiophene-5-oyl)hydrazine (14d)



Yield: 0.70 g (68%); M.p.=85-87^{0}C, yellow solid. Rf=0.7 ($CHCl_3$).

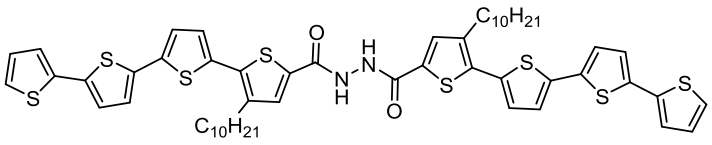
IR (KBr). ν cm^{-1}: 1627 (C=O), 3204-3300 (NH).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.76-0.80 (12H, m, $4CH_3$), 1.14-1.77 (56H, m, $28CH_2$), 1.50-1.59 (8H, m, $4ThCH_2C\underline{H}_2C_8H_{17}$), 2.62-2.68 (8H, m., $4ThC\underline{H}_2C_9H_{19}$), 6.84 (2H, d., ^{3}J=5.3 Hz, 2Th-4''-H), 6.92 (2H, d., ^{3}J=3.8 Hz, 2Th-3'-H), 6.99 (2H, d., ^{3}J=3.8 Hz, 2Th-4'-H), 7.08 (2H, d., ^{3}J=5.3 Hz, 2Th-5''-H), 7.52 (2H, s., 2Th-4-H), 9.66 (2H, s., 2NH).

^{13}C NMR (100 MHz, δ, ppm): 14.10 ($4CH_3$), 22.67, 29.34, 29.36, 29.45, 29.53, 29.58, 29.62, 29.64, 30.38, 30.68, 31.89, 31.91 ($18CH_2$), 123.97 (5''-Th), 126.00 (4'-Th), 127.09 (3'-Th), 130.04 (4''-Th), 130.08 (4-Th), 131.69 (2-Th), 132.60 (2''-Th), 134.55 (5'-Th), 137.10 (2'-Th), 137.49 (5-Th), 139.92 (3-Th), 140.14 (3''-Th), 161.02 (C=O).

Elemental analysis. Calculated for $C_{66}H_{96}N_2O_2S_6$: C, 69.42%; H, 8.47%; N, 2.45%. found: C,69.51 %; H, 8.52%; N, 2.43%.

N,N'-Bis(3-decyl-2,2':5',2'':5'',2'''-quaterthiophene -5-oyl)hydrazine (14c)



Oxalyl chloride (0.62 mL, 7.2 mmol) was added to a suspension of **12c** (0.59 g, 1.9 mmol) in 3 mL of dry dichloromethane under cooling (ice bath). After the addition of one drop of DMF to the resulting mixture, it was stirred for 30 min under cooling then at r.t. for additional 4 h. The solvent and the excess of oxalyl chloride were removed under reduced pressure and the final product (acid chloride) was used in subsequent reactions without further purification. Crude acid chloride was dissolved in 5 mL of dichloromethane, cooled in an ice bath. Then, a mixture of 90 mg (0.90 mmol) of hydrazine dihydrochloride and 0.72 mL (9 mmol) of dry pyridine were added. The reaction mixture was stirred for 30 min under cooling and left overnight at rt. After removal of the solvent in vacuum the residue was treated with 10 mL of ice water and stirred for 15 min. The precipitate was filtered out, washed with water and dried and recrystallized from ethyl acetate.

Yield: 0.74 g (76%); M.p.= 131-135 ^{0}C ($CHCl_3$), yellow solid. Rf=0.72 ($CHCl_3$).

IR (KBr). ν cm^{-1}: 1627 (C=O), 3200-3400 (NH).

^{1}H NMR (400 MHz, DMSO-d6, δ, ppm): δ = 0.81-0.84 (6H, m, $2CH_3$), 1.17-1.40 (28H, m, $14CH_2$), 1.55-1.68 (4H, m, $2ThCH_2C\underline{H}_2C_8H_{17}$), 2.76 (4H, t, ^{3}J=7.6 Hz, $2ThC\underline{H}_2C_9H_{19}$), 7.09 (2H, d.d, ^{3}J=3.7 Hz, ^{3}J=5.0 Hz, 2Th-4'''-H), 7.24 (4H, d., ^{3}J=3.7 Hz, 2Th-3'-H, 2Th-4'-H), 7.27-7.33 (6H, m., 2Th-3'''-H, 2Th-3''-H, 2Th-4''-H), 7.49 (2H, d., ^{3}J=5.0 Hz, 2Th-5'''-H), 7.79 (2H, s., 2Th-4-H), 10.39 (2H., s., 2NH).

^{13}C NMR (100 MHz, δ, ppm): 13.35 (CH_3), 21.59, 28.19, 28.22, 28.26, 28.29, 28.49, 28.55, 29.23, 30.85 ($9CH_2$), 124.01 (4''-Th), 124.04 (3''-Th), 124.47 (4'-Th), 124.58 (3'''-Th), 125.06 (5'''-Th), 125.38 (4'''-Th), 127.72 (3'-Th), 127.94 (4-Th), 133.12 (2-Th), 134.13 (2''-Th), 134.56 (5''-Th), 135.82 (5'-Th), 136.63 (2'-Th), 136.79 (2'''-Th), 139.76 (3-Th), 139.89 (5-Th), 161.99 (C=O).

Elemental analysis. Calculated for $C_{54}H_{60}N_2O_2S_8$. C, 63.24%; H, 5.90%; N, 2.73%. found: C, 63.35%; H, 6.05%; N, 2.80%.

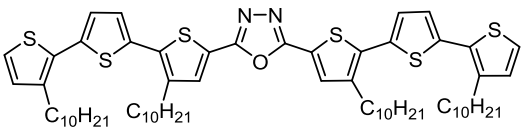
Synthesis of target 1,3,4-oxadiazole compounds: 1, 2 and 5

General Procedure for the synthesis of compounds 1, 2:

A mixture of **14 c**, or **14d** (0.5 mmol), 3 mL phosphoryl chloride (41.2 mmol) was heated to 80-90 ºC and stirred at this temperature under inert atmosphere for 3-5 h, then cooled to r.t. The excess of phosphoryl

chloride was removed under reduced pressure and 30 mL of ice water were added. The product: **1** or **2** was extracted with $CHCl_3$ (3 × 20 mL). The extract was washed with saturated solution of sodium chloride (30 mL) and aqueous solution of $NaHCO_3$ and dried with Na_2SO_4. Then the solvent was evaporated under reduced pressure. The crude product was purified by column chromatography.

2,5-Bis(3,3''-didecyl-[2,2':5',2''-terthiophen]-5-yl)-1,3,4-oxadiazole (2)



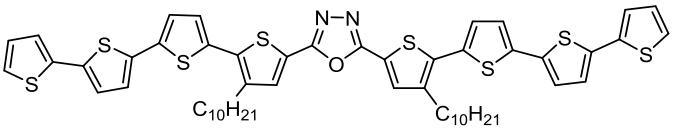
Yield: 0.48 g (85%); M.p.= 52-54^{0}C (hexane/EtOAc, 20/1), yellow solid. Rf=0.36 (hexane/EtOAc, 20/1).
IR (KBr). ν cm^{-1}: 1580 (C=N).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.85-0.89 (12H, m, $4CH_3$), 1.26-1.46 (56H, m, $28CH_2$), 1.61-1.77 (8H, m, $4ThCH_2C\underline{H}_2C_8H_{17}$), 2.77-2.86 (8H, m., $4ThC\underline{H}_2C_9H_{19}$), 6.96 (2H, d., ^{3}J=5.2 Hz, 2Th-4''-H), 7.10 (2H, d., ^{3}J=3.8 Hz, 2Th-3'-H), 7.19 (2H, d., ^{3}J=3.8 Hz, 2Th-4'-H), 7.21 (2H, d., ^{3}J=5.2 Hz, 2Th-5''-H), 7.65 (2H, s., 2Th-4-H).

^{13}C NMR (100 MHz, δ, ppm): 14.13 ($2CH_3$), 22.70, 29.36, 29.48, 29.52, 29.56, 29.59, 29.62, 29.64, 30.50, 30.74, 31.92 ($18CH_2$), 121.81 (5''-Th), 124.20 (4'-Th), 126.25 (3'-Th), 127.16 (2-Th), 129.93 (4''-Th), 130.20 (5-Th), 132.52 (2''-Th), 134.36 (4-Th), 135.85 (5'-Th), 137.66 (3-Th), 140.19 (3''-Th), 140.42 (2'-Th), 160.00 (2,5-Oxadiazole).

Elemental analysis. Calculated for $C_{66}H_{94}N_2OS_6$: C, 70.53%; H, 8.43%; N, 2.49%. found: C, 70.58%; H, 8.56%; N, 2.51%.

2,5-Bis(3-decyl-[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl)-1,3,4-oxadiazole (1)



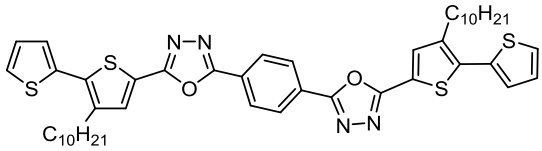
Yield: 0.05 g (10%); M.p.= 117-119 ^{0}C (benzene), orang solid. Rf= 0.53 (benzene),
IR (KBr). ν cm^{-1}: 1580 (C=N).

^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0.87 (6H, t, ^{3}J=6.7 Hz, $2CH_3$), 1.24-1.46 (28H, m, $14CH_2$), 1.67-1.75 (4H, m, $2ThCH_2C\underline{H}_2C_8H_{17}$), 2.81 (4H, t, ^{3}J=7.8 Hz, $2ThC\underline{H}_2C_9H_{19}$), 7.01 (2H, d.d, ^{3}J=3.7 Hz, ^{3}J=5.1 Hz, 2Th-4'''-H), 7.07 (2H, d., ^{3}J=3.7 Hz, 2Th-4''-H), 7.09 (2H, d., ^{3}J=3.7 Hz, 2Th-3''-H), 7.12 (4H, s., 2Th-3'-H, 2Th-4'-H), 7.17 (2H, d., ^{3}J=3.7 Hz, 2Th-3'''-H), 7.22 (2H, d., ^{3}J=5.1 Hz, ^{4}J=0.6 Hz, 2Th-5'''-H), 7.60 (2H, s., 2Th-4-H).

^{13}C NMR (100 MHz, δ, ppm): 14.09 (CH_3), 22.70, 29.37, 29.47, 29.50, 29.56, 29.63, 29.66, 30.40, 31.96 ($9CH_2$), 122.05 (2-Th), 123.96 (4''-Th), 124.07 (3''-Th), 124.47 (4'-Th), 124.65 (4'''-Th), 124.72 (3'''-Th), 124.74 (5'''-Th), 127.95 (3'-Th), 132.48 (4-Th), 133.76 (2''-Th), 135.74 (5'-Th), 135.48 (5''-Th), 137.00 (2'-Th), 137.04 (2'''-Th), 138.30 (3-Th), 140.65 (5-Th), 159.99 (2,5-Oxadiazole).

Elemental analysis. Calculated for $C_{54}H_{58}N_2OS_8$. C, 64.37%; H, 5.80%; N, 2.78%. found: C, 64.47%; H, 5.94%; N, 2.87%.

Synthesis of 1,4-bis(5-(3-decyl-[2,2'-bithiophen]-5-yl)-1,3,4-oxadiazol-2-yl)benzene (5)



To a mixture of 0.56 mmol DCC, 0.56 mmol of carboxylic acid **12a** in dry tetrahydrofuran was added 1,4-di(2H-tetrazol-5-yl)benzene (0.28 mmol). The reaction mixture was stirred for 60 min at rt. then under reflux for 15 h (TLC control: $CHCl_3$). The urea precipitated was filtered off and washed with THF. The solvent was removed under reduced pressure, using a rotary evaporator. The crude product was purified by column chromatography (eluent - benzene / ethyl acetate, 20/1).

Yield: 0.096 g (46%); yellow solid; Rf = 0.5 ($CHCl_3$); Mp. = 150-152^{0}C. IR (KBr). ν cm-1: 1569 (C=N).

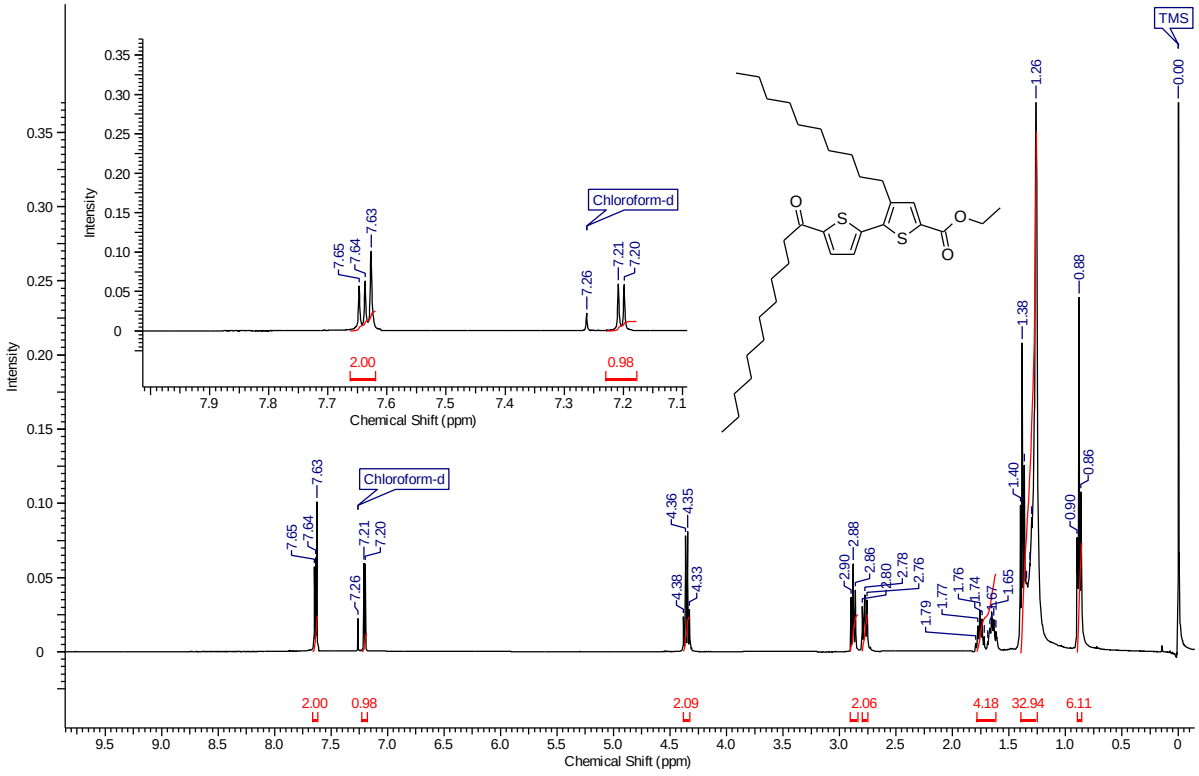
^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): δ = 0,87 (6H, t., ^{3}J=6.5 Hz, $2CH_3$), 1.20-1.42 (28H, m., $14CH_2$), 1.65-1.72 (4H, m., 2-Th$CH_2C\underline{H}_2C_8H_{17}$), 2.79 (4H, t., ^{3}J=7.8 Hz, 2Th$C\underline{H}_2C_9H_{19}$), 7.10 (2H, d.d., ^{3}J=3.5 Hz, ^{3}J=5.0 Hz, 2Th-4'-H), 7.22 (2H, d.d., ^{3}J=3.5 Hz, ^{4}J=1.0 Hz. 2Th-3'-H), 7.38 (2H, d.d.,^{3}J=5.0 Hz, ^{4}J=1.0 Hz, 2Th-5'-H), 7.66 (2H, s., Th-4-H), 8.23 (4H,s., C_6H_4).

^{13}C NMR (100 MHz, δ, ppm):14.09 (CH_3); 22.65, 29.23, 29.30, 29.39, 29.47, 29.55, 29.57, 30.40, 31.87(CH_2); 121.68 (2-Th); 126.26 (3'-Th); 127.06 (5'-Th); 126.71 (4'-Th); 127.06, 127.38, 127.69 (1,2,3,4,5,6-Ph); 132.67 (4-Th); 134.59 (5-Th); 136.38 (3-Th); 140.52 (2'-Th); 161.03(2,2'-oxadiazole); 162.96(2,2'-oxadiazole).

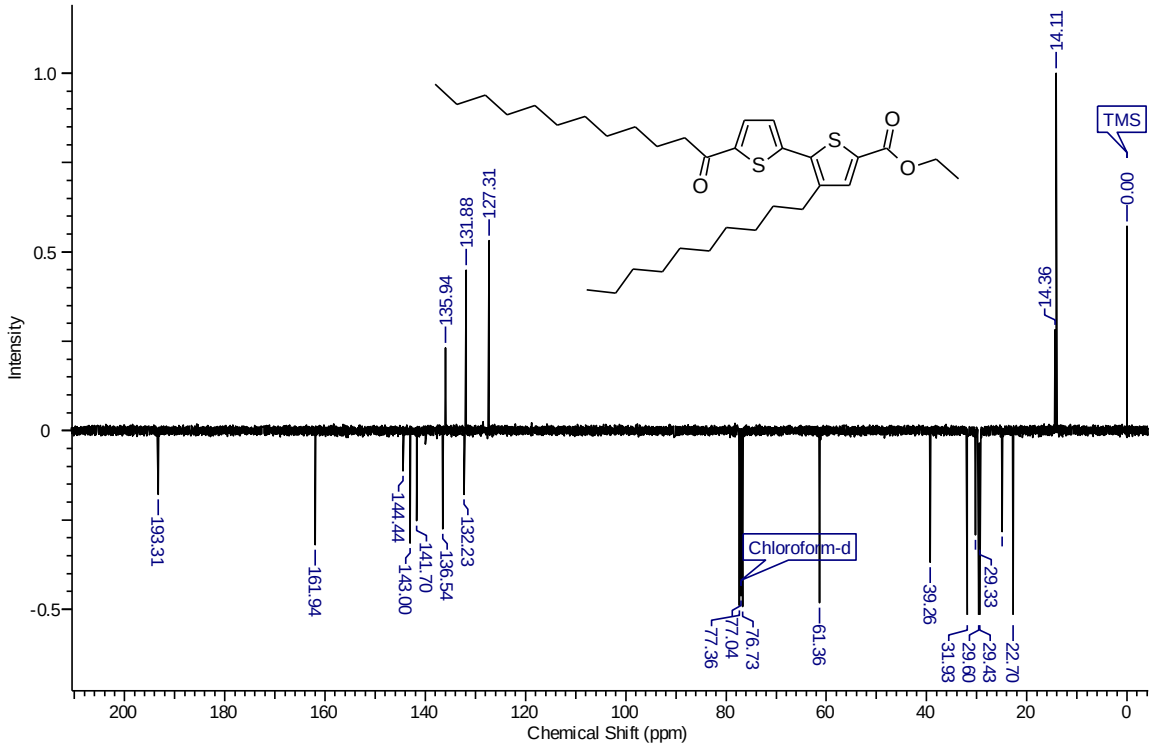
NMR Spectra

Ethyl 3-decyl-5'-dodecanoyl-[2,2'-bithiophene]-5-carboxylate (8)

^{1}H NMR (400 MHz, $CDCl_3$)

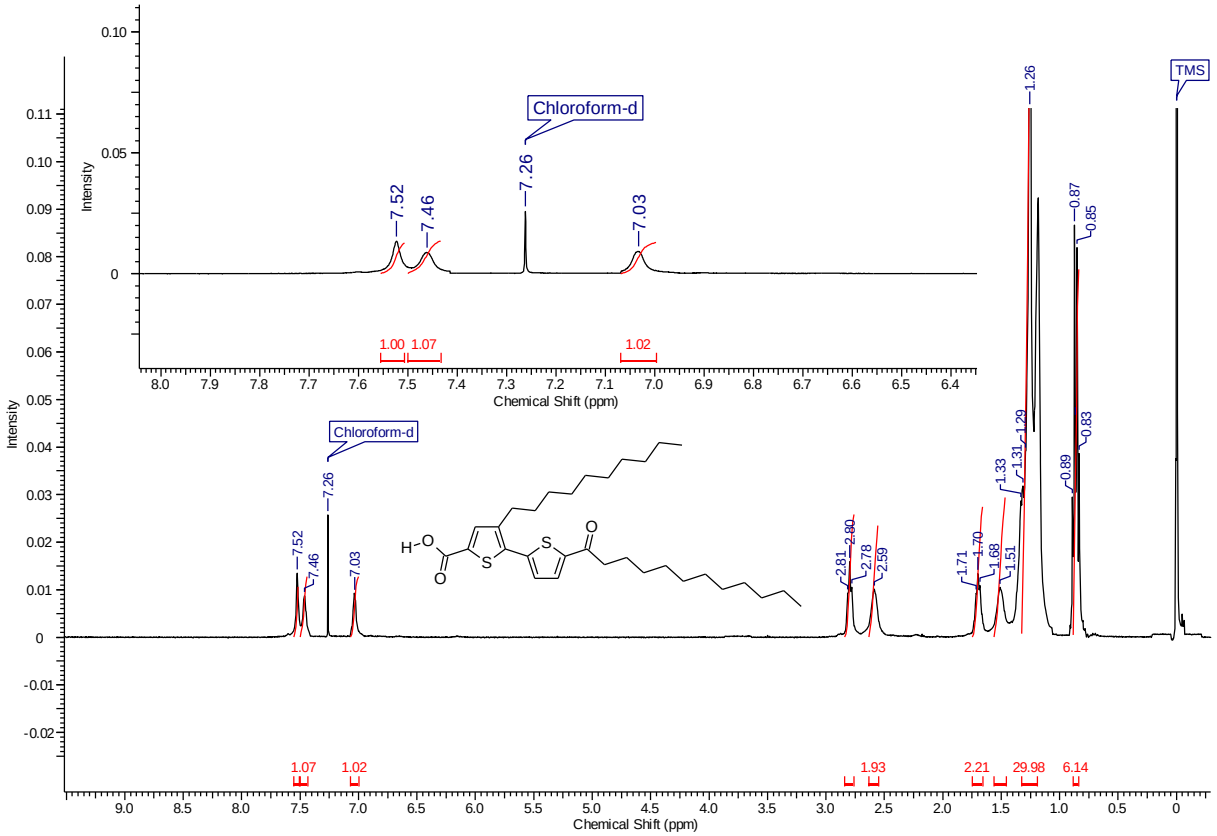


^{13}C NMR (100 MHz, δ, ppm) **(8)**

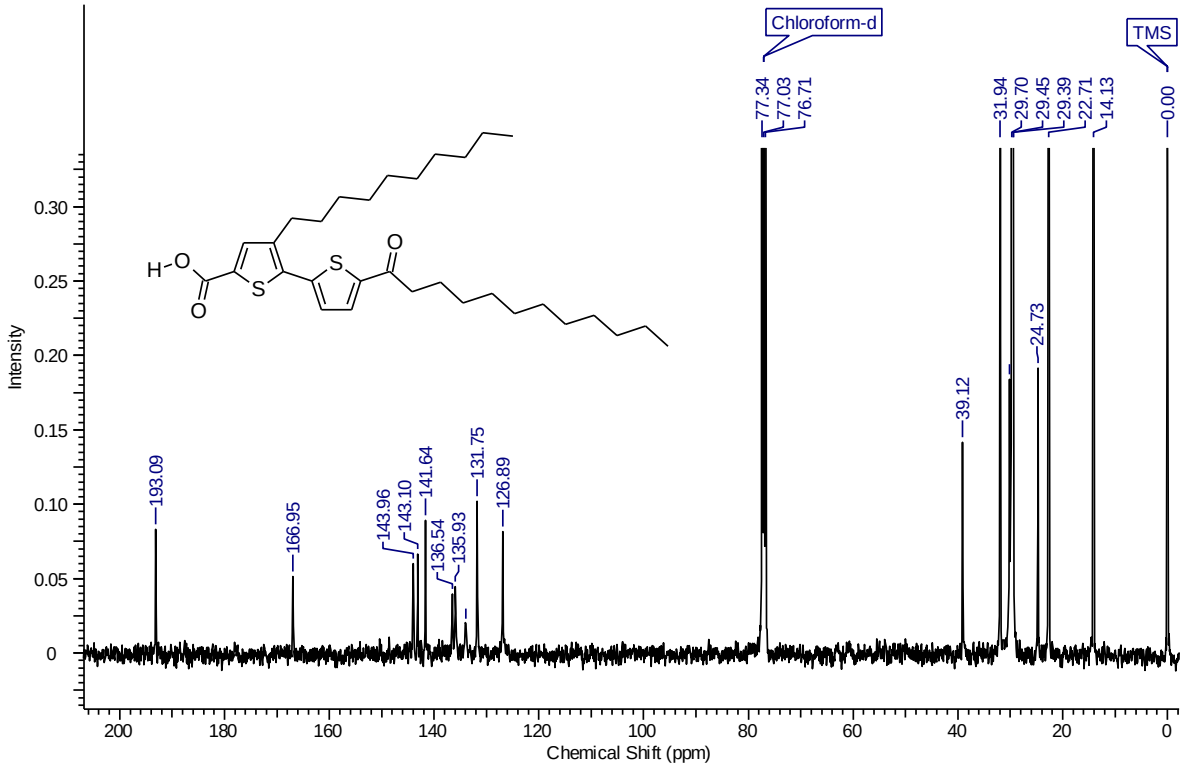


3-Decyl-5'-dodecanoyl-[2,2'-bithiophene]-5-carboxylic acid (9)

^{1}H NMR (400 MHz, $CDCl_3$)

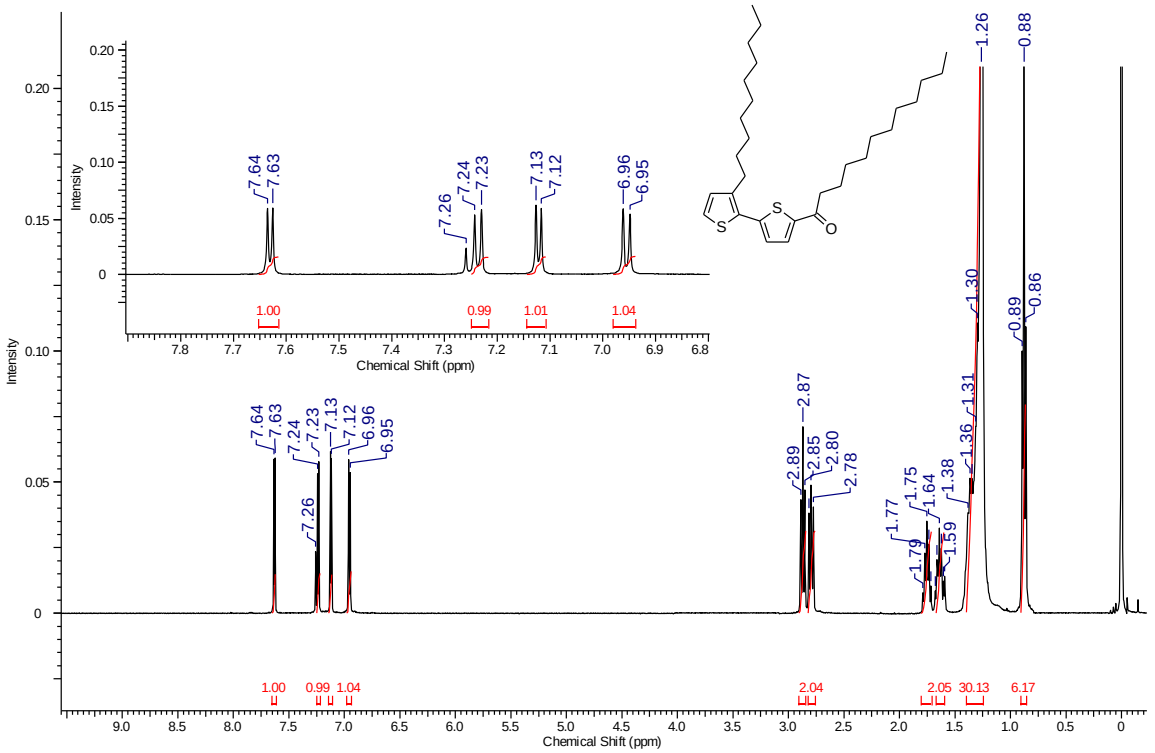


^{13}C NMR (100 MHz, δ, ppm) **(9)**

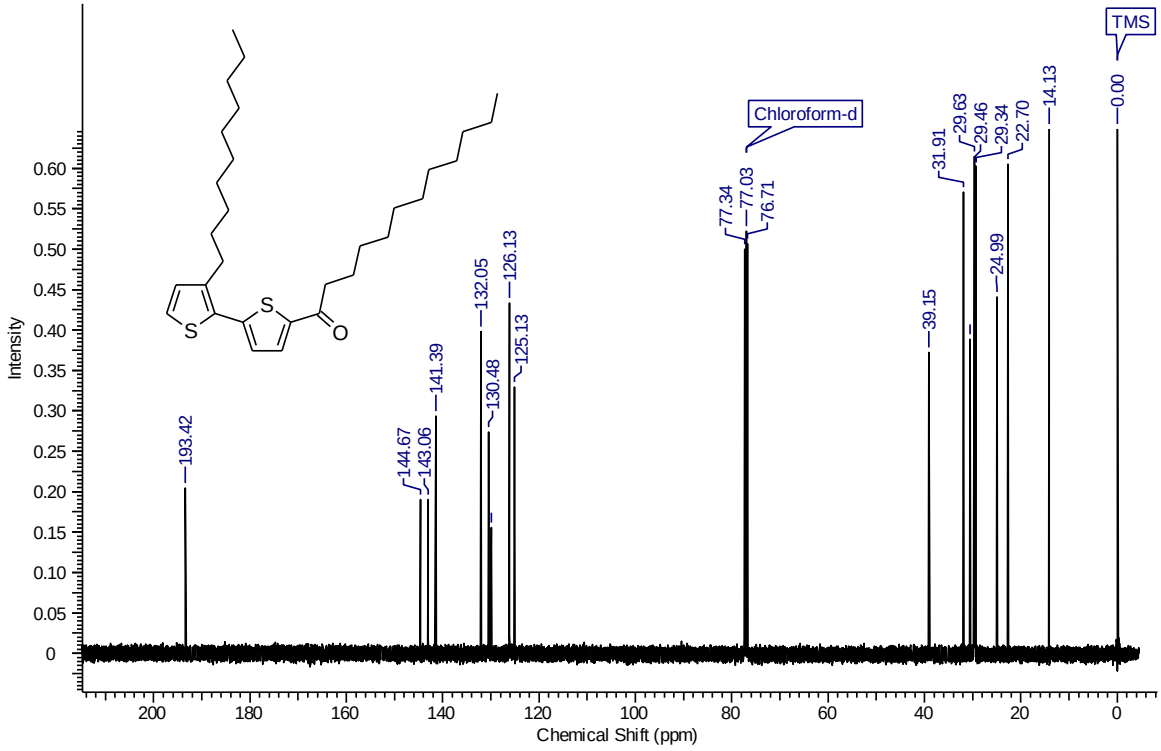


1-(3'-Decyl-[2,2'-bithiophen]-5-yl)dodecan-1-one (10)

^{1}H NMR (400 MHz, $CDCl_3$)

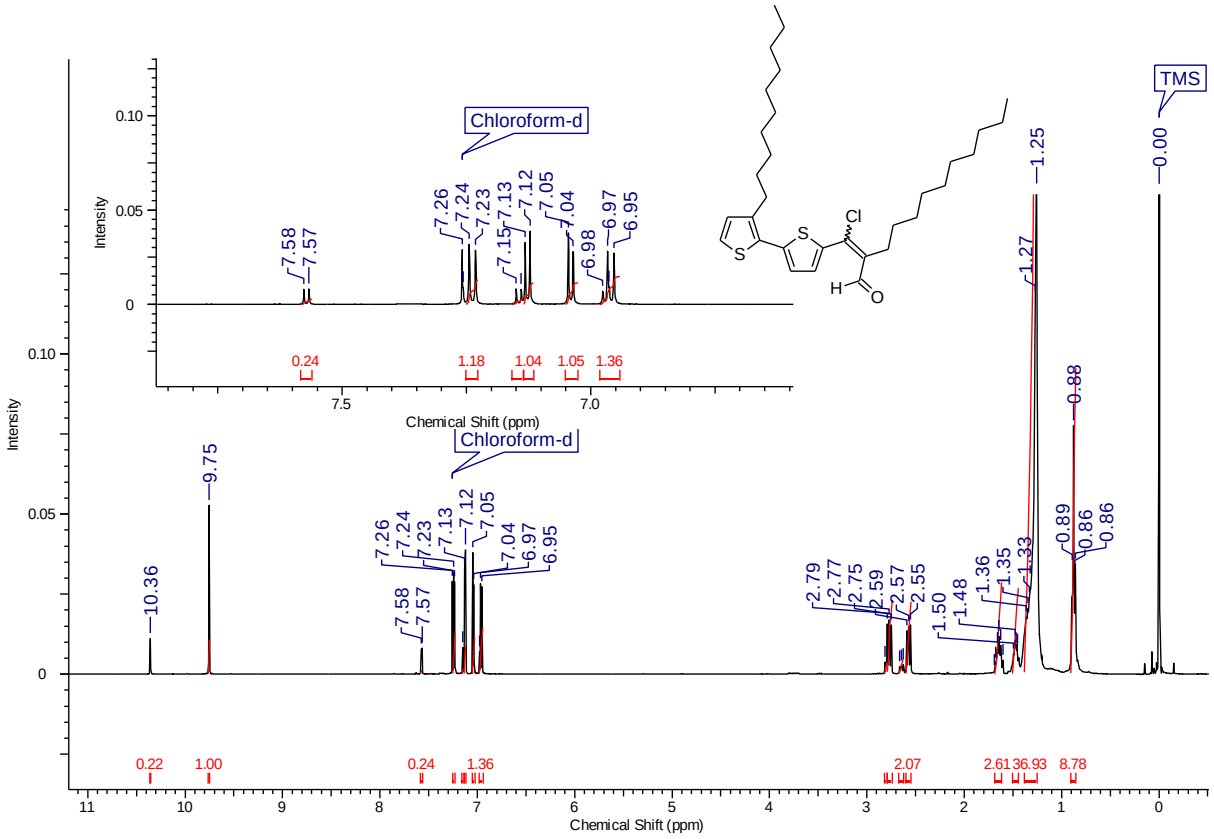


^{13}C NMR (100 MHz, δ, ppm) **(10)**

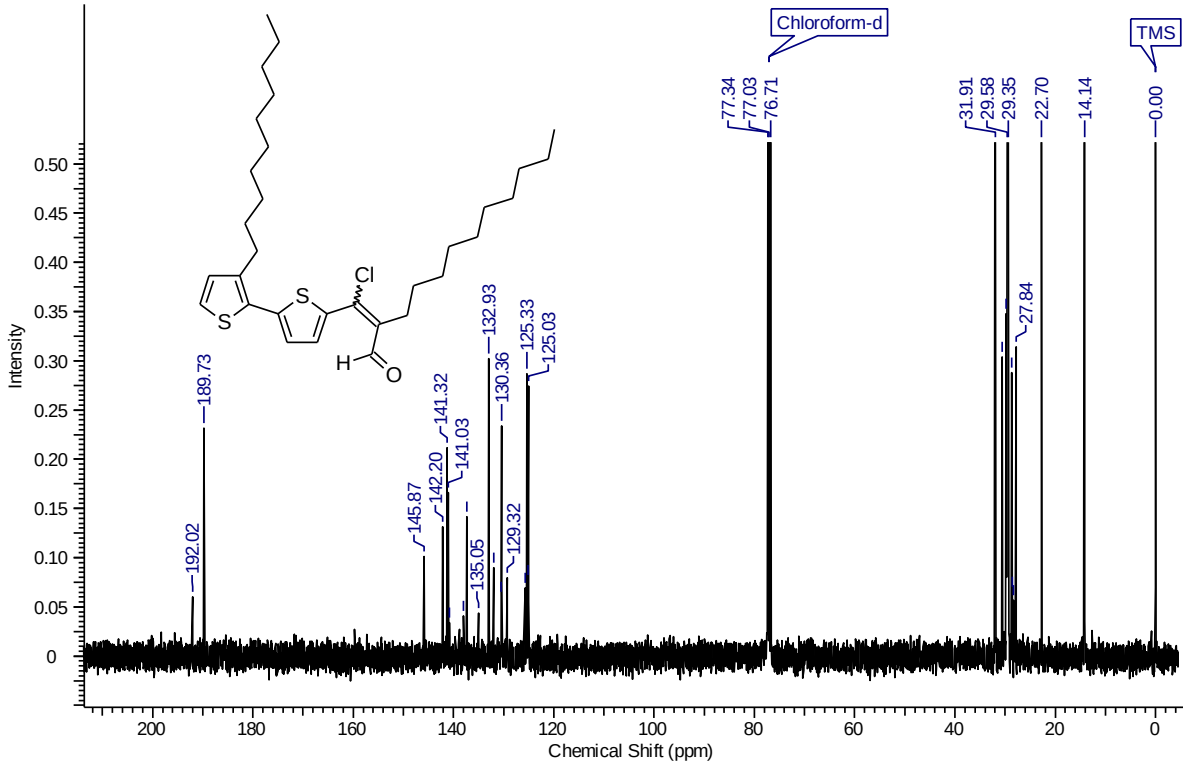


2-(Chloro(3'-decyl-[2,2'-bithiophen]-5-yl)methylene)dodecanal (11)

^{1}H NMR (400 MHz, $CDCl_3$)

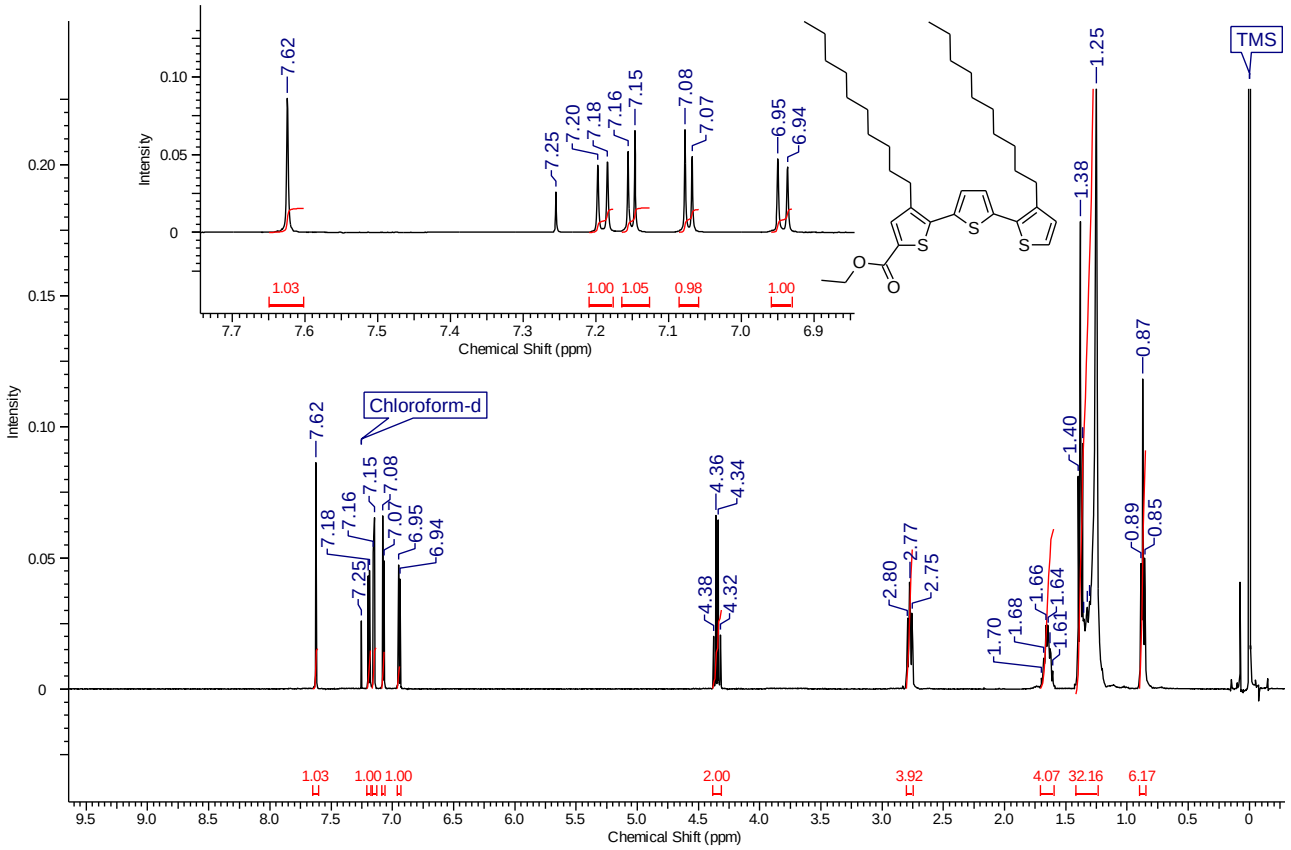


^{13}C NMR (100 MHz, δ, ppm) **(11)**

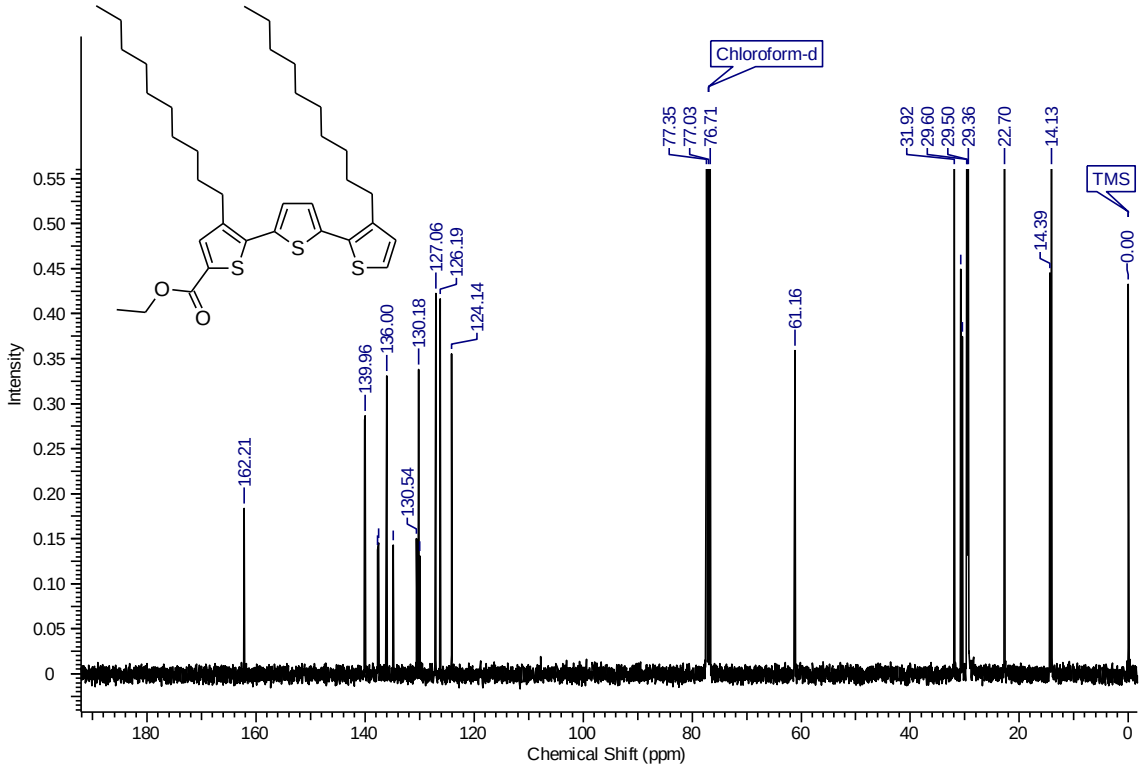


Ethyl 3,3''-didecyl-[2,2':5',2''-terthiophene]-5-carboxylate (7d)

^{1}H NMR (400 MHz, $CDCl_3$)

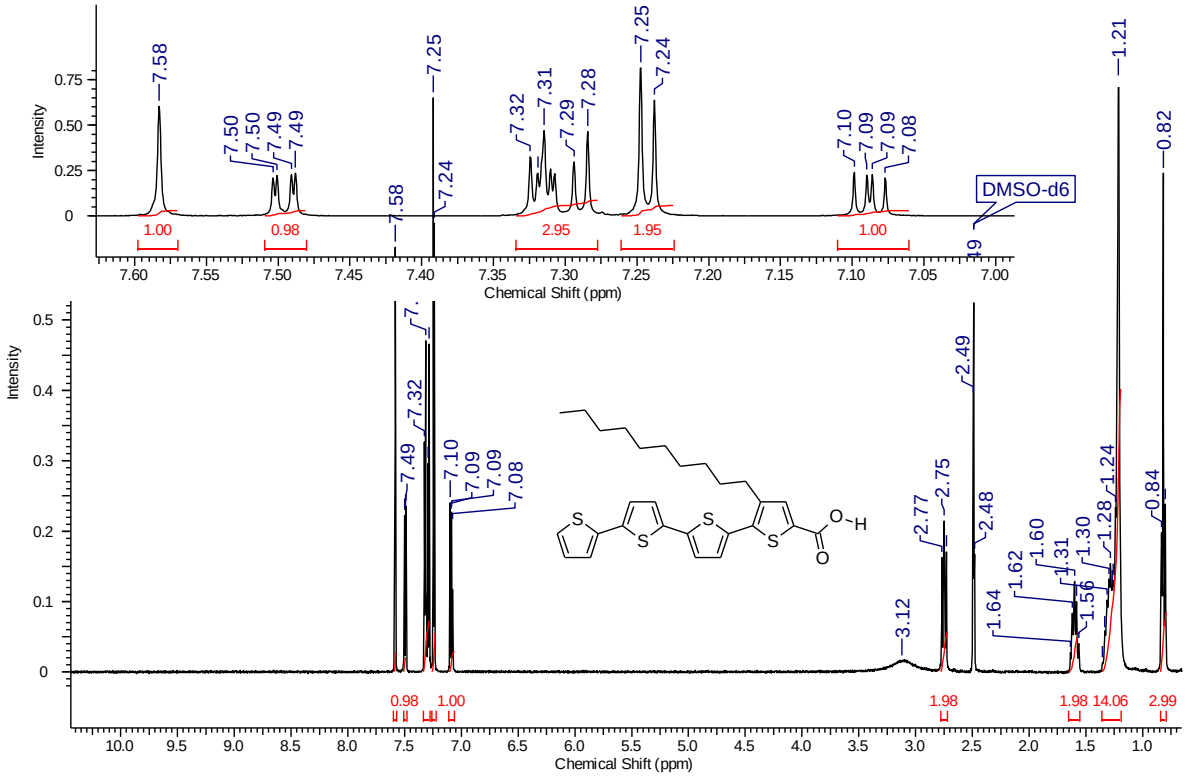


^{13}C NMR (100 MHz, δ, ppm) **(7d)**

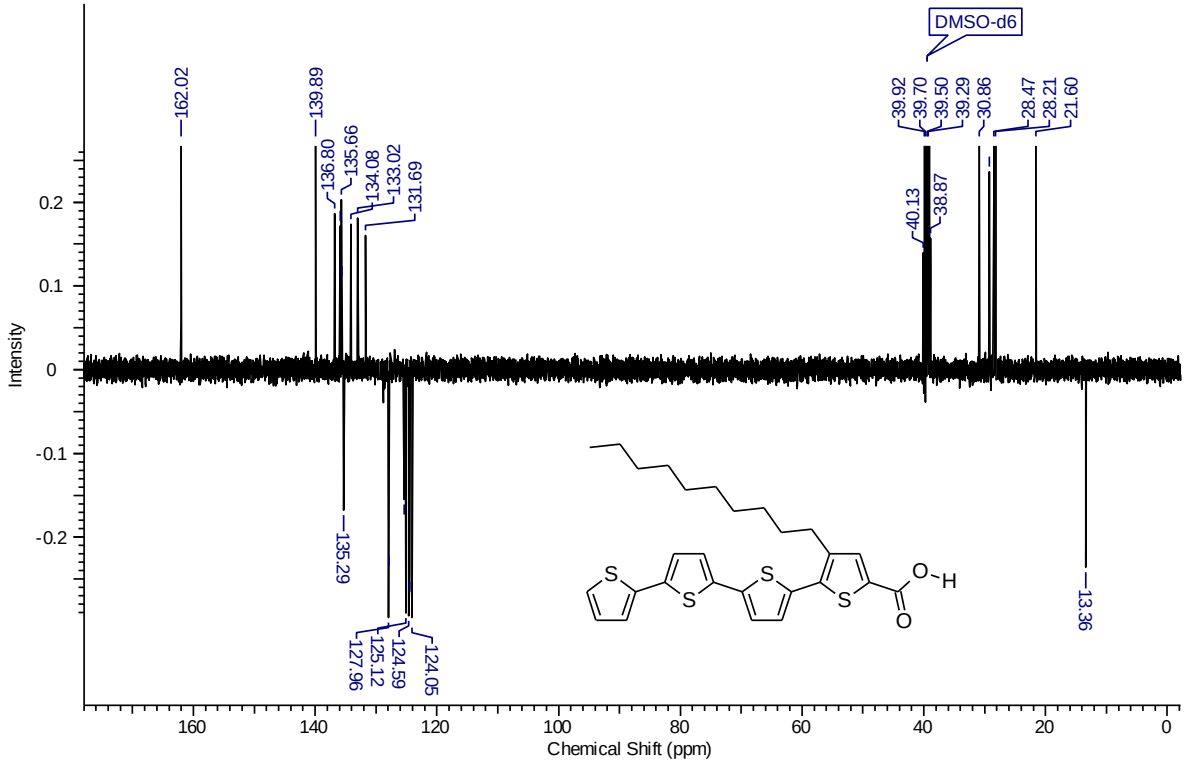


3-Decyl-[2,2':5',2'':5'',2'''-quaterthiophene]-5-carboxylic acid (12c)

^{1}H NMR (400 MHz, DMSO-d6)

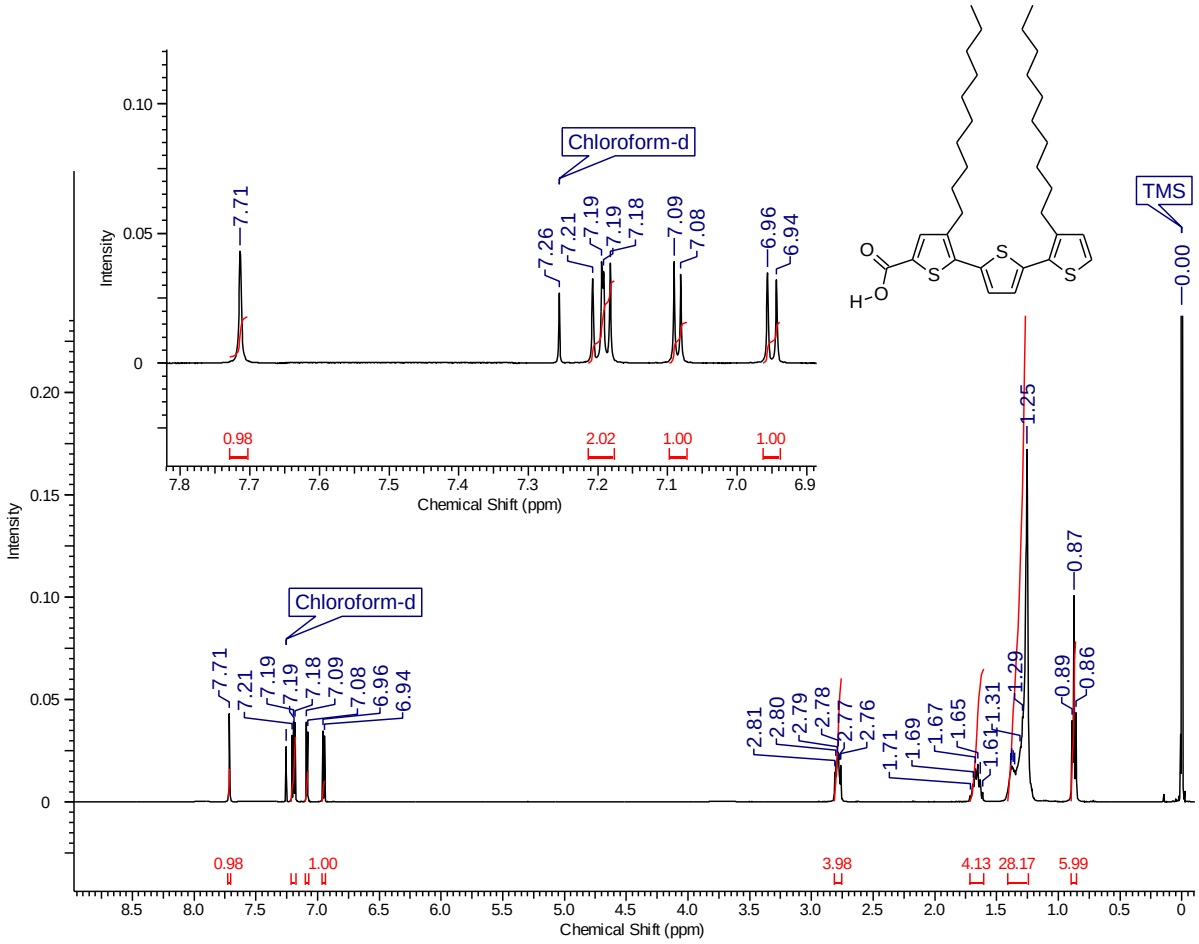


^{13}C NMR (100 MHz, δ, ppm) **(12c)**

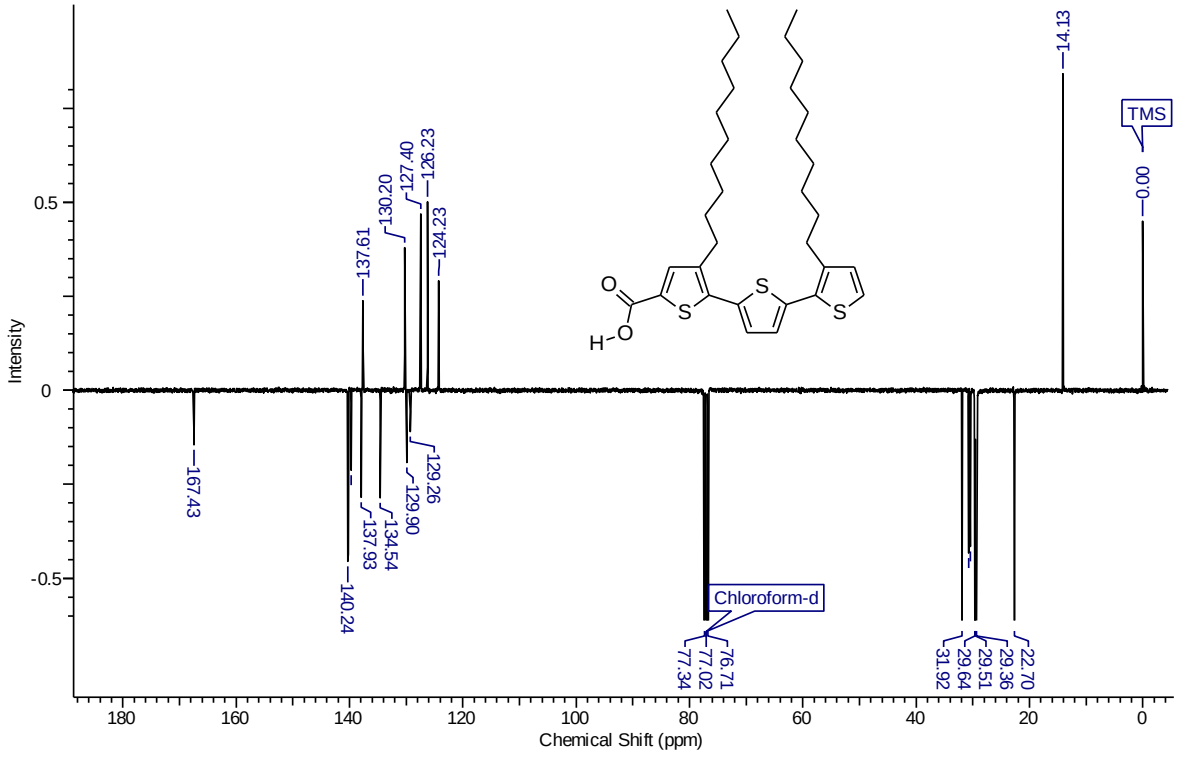


3,3''-didecyl-[2,2':5',2''-terthiophene]-5-carboxylic acid (12d)

^{1}H NMR (400 MHz,$CDCl_3$)

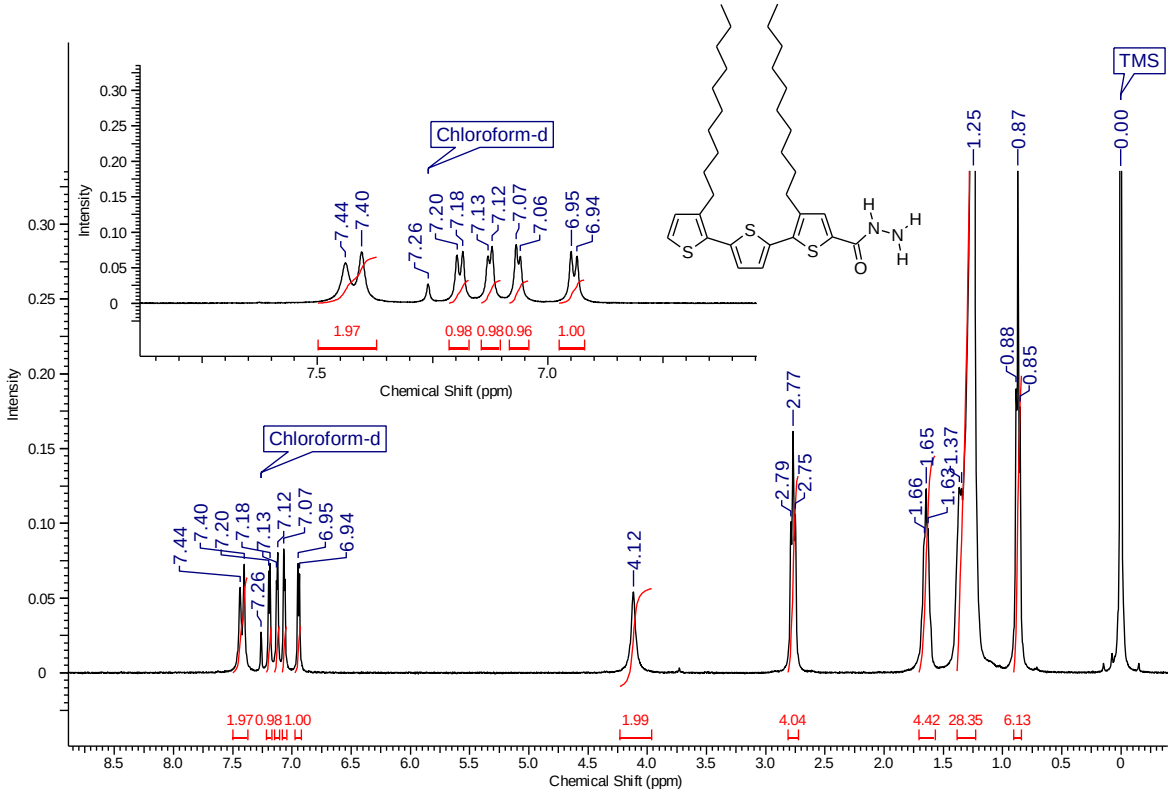


^{13}C NMR (100 MHz, δ, ppm) **(12d)**

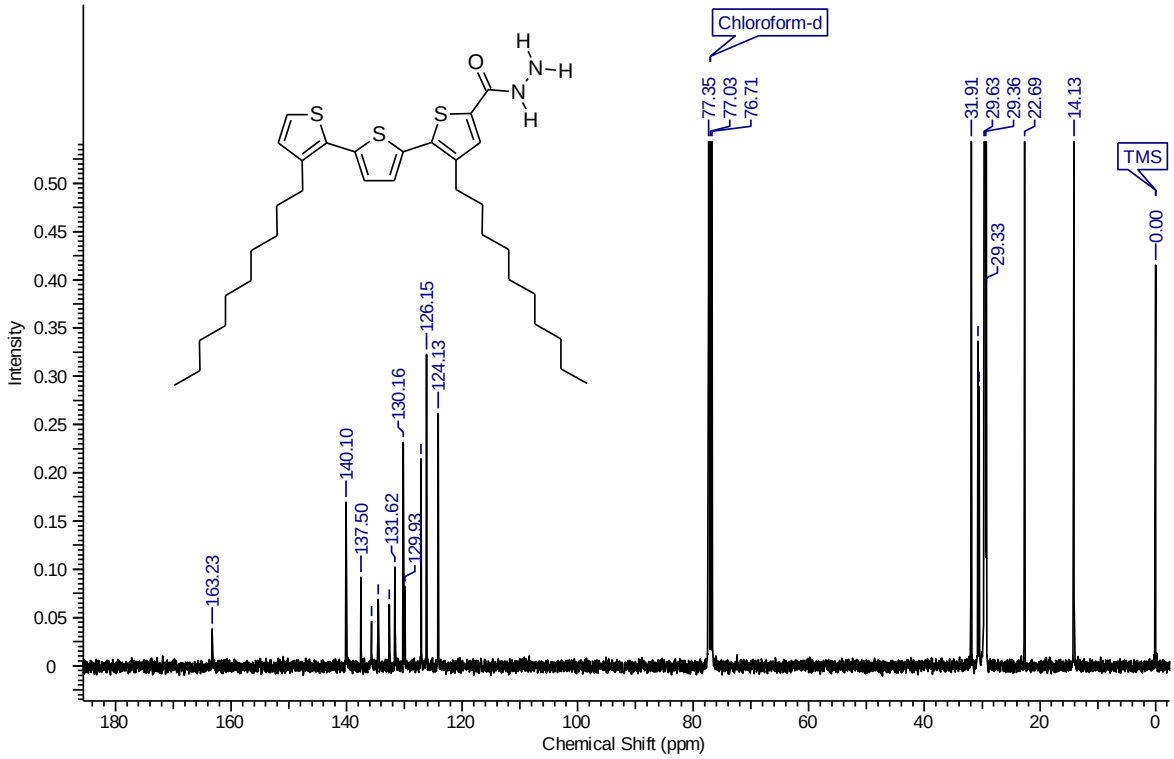


3,3''-Didecyl-[2,2':5',2''-terthiophene]-5-carbohydrazide (13d)

^{1}H NMR (400 MHz, $CDCl_3$)

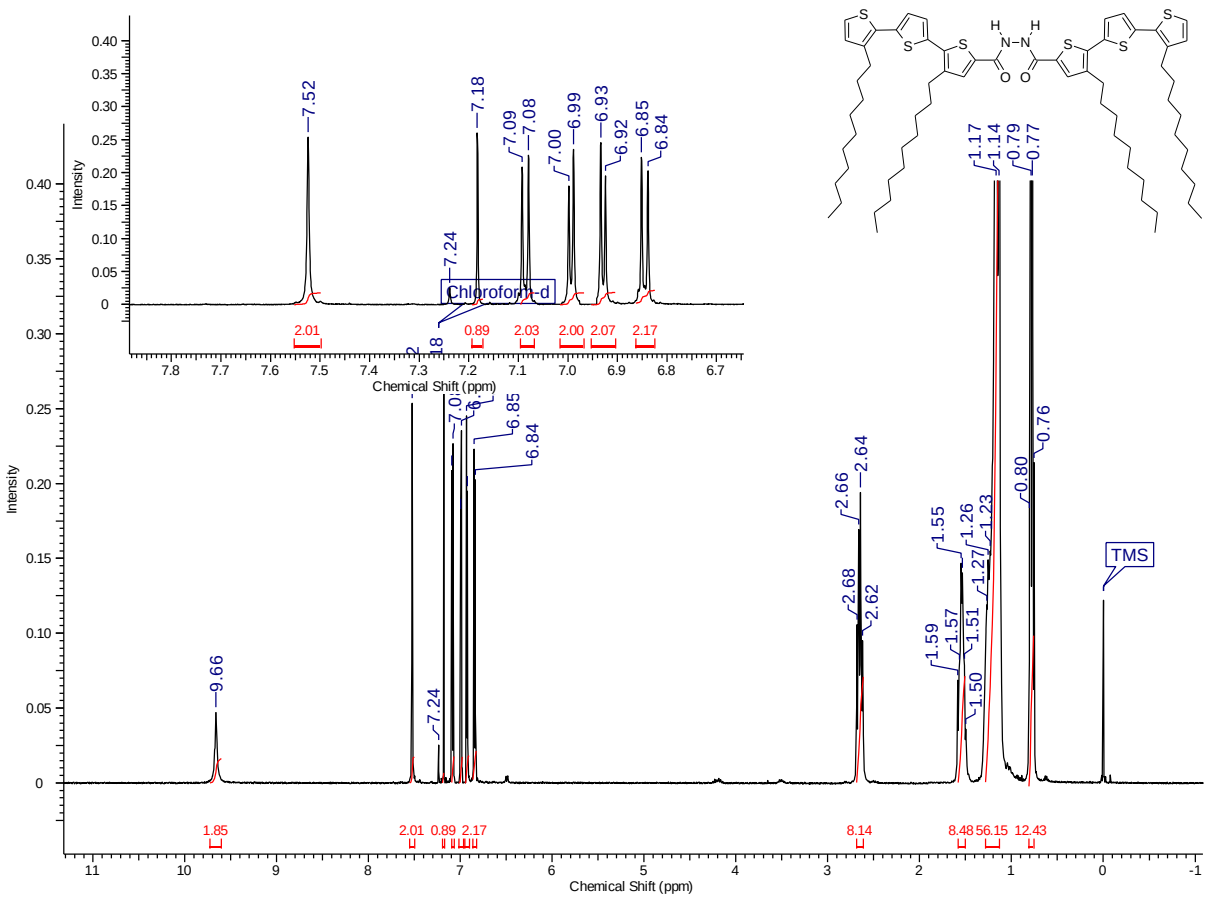


^{13}C NMR (100 MHz, δ, ppm) **(13d)**

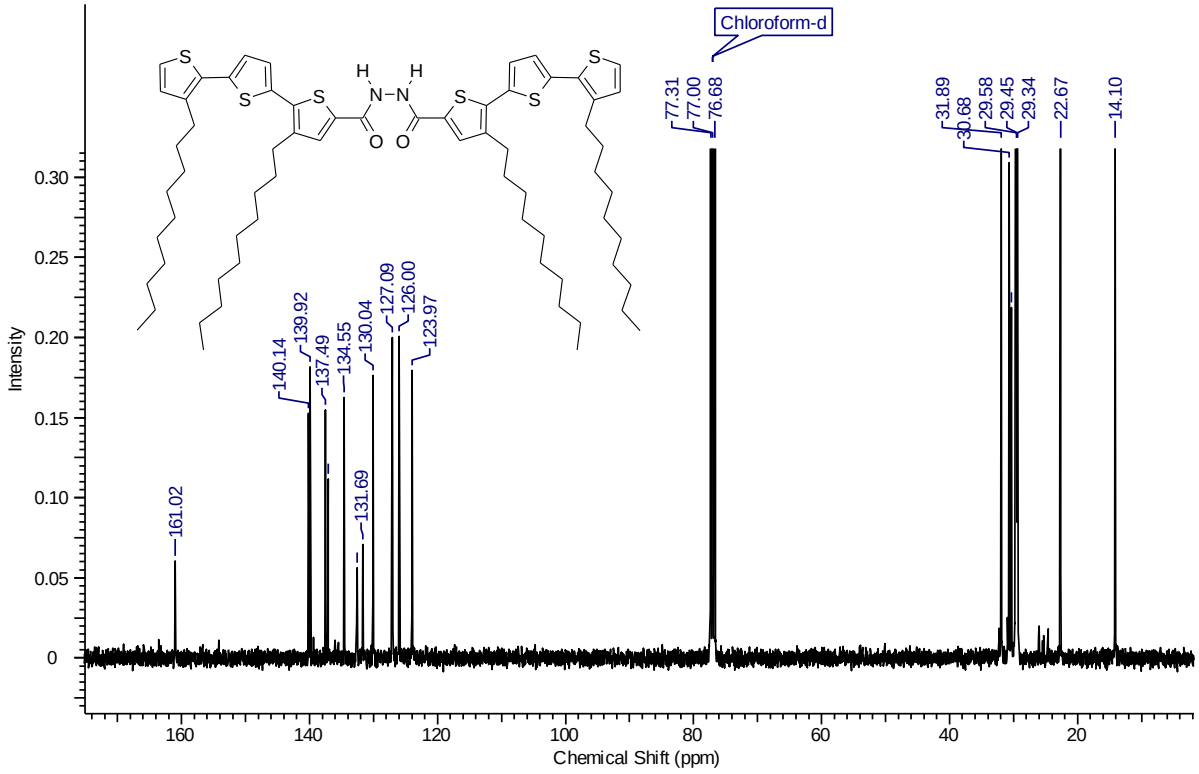


N,N’-Bis(3,3’’-decyl-2,2':5',2''-terthiophene-5-oyl)hydrazine (14d)

^{1}H NMR (400 MHz, $CDCl_3$)

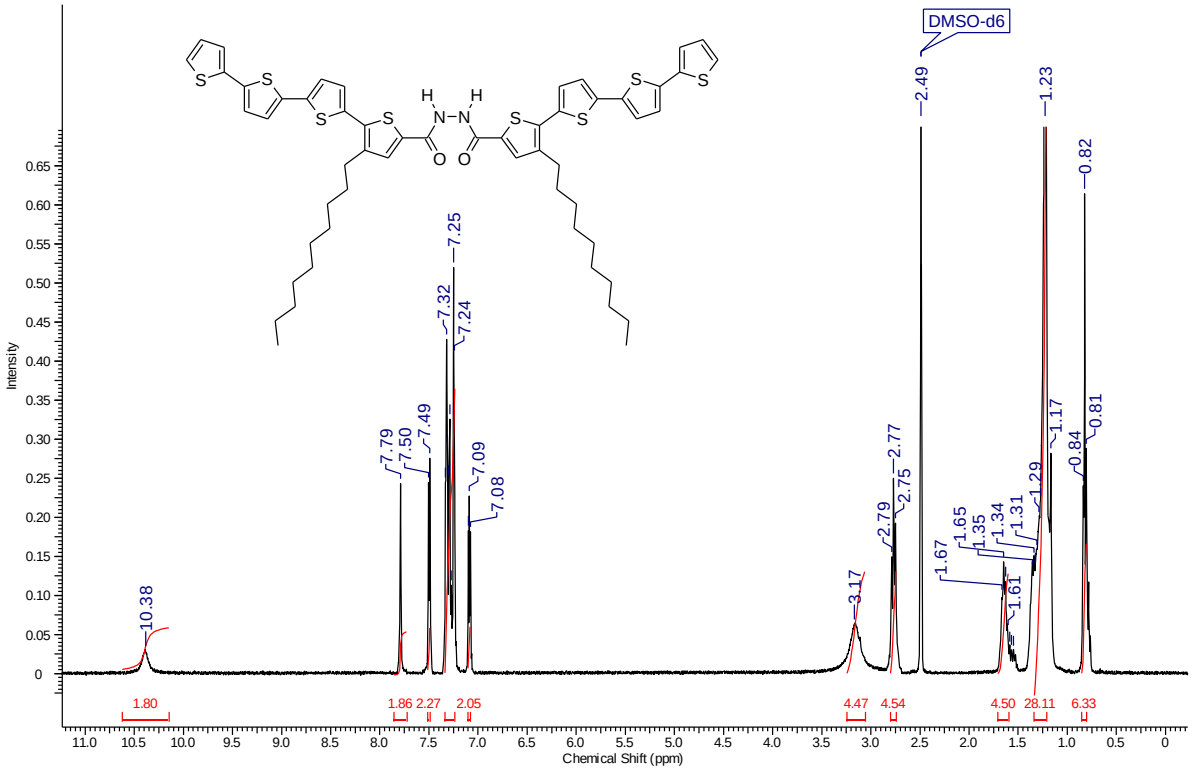


^{13}C NMR (100 MHz, δ, ppm) **(14d)**

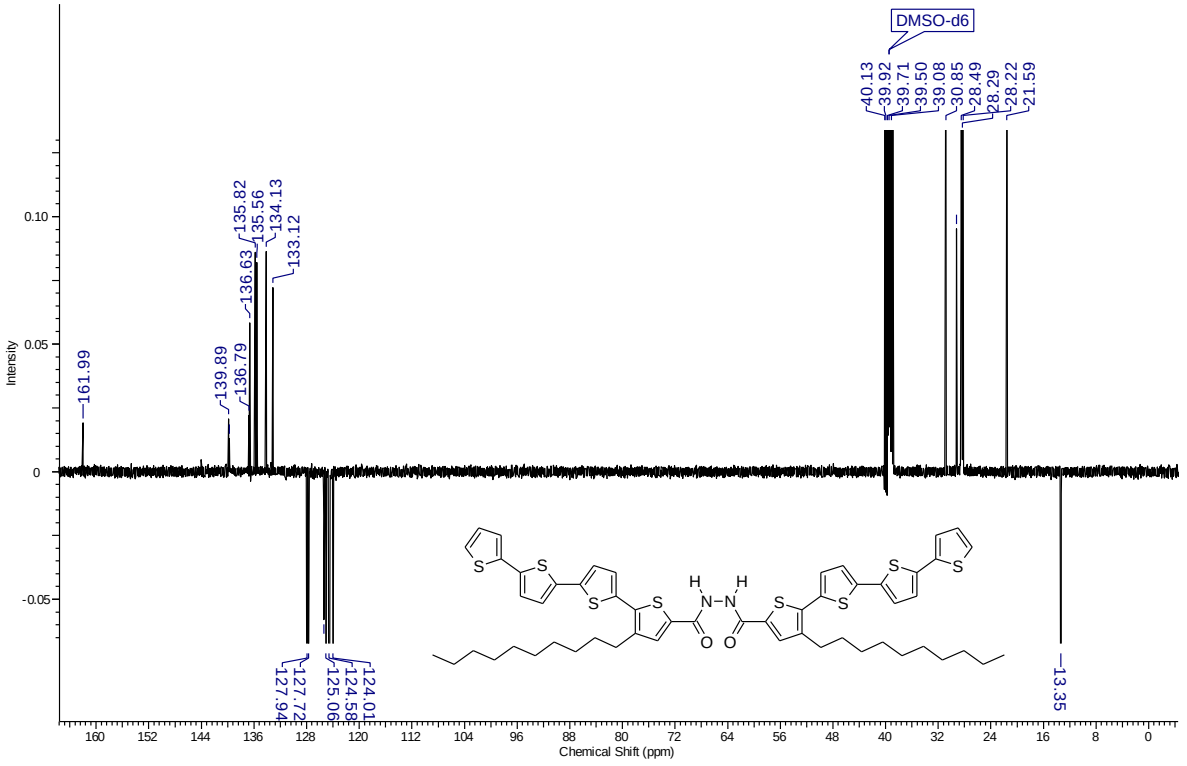


N,N’-Bis(3-decyl-2,2':5',2'':5'',2'''-quaterthiophene -5-oyl)hydrazine (14c)

^{1}H NMR (400 MHz, DMSO-d6)

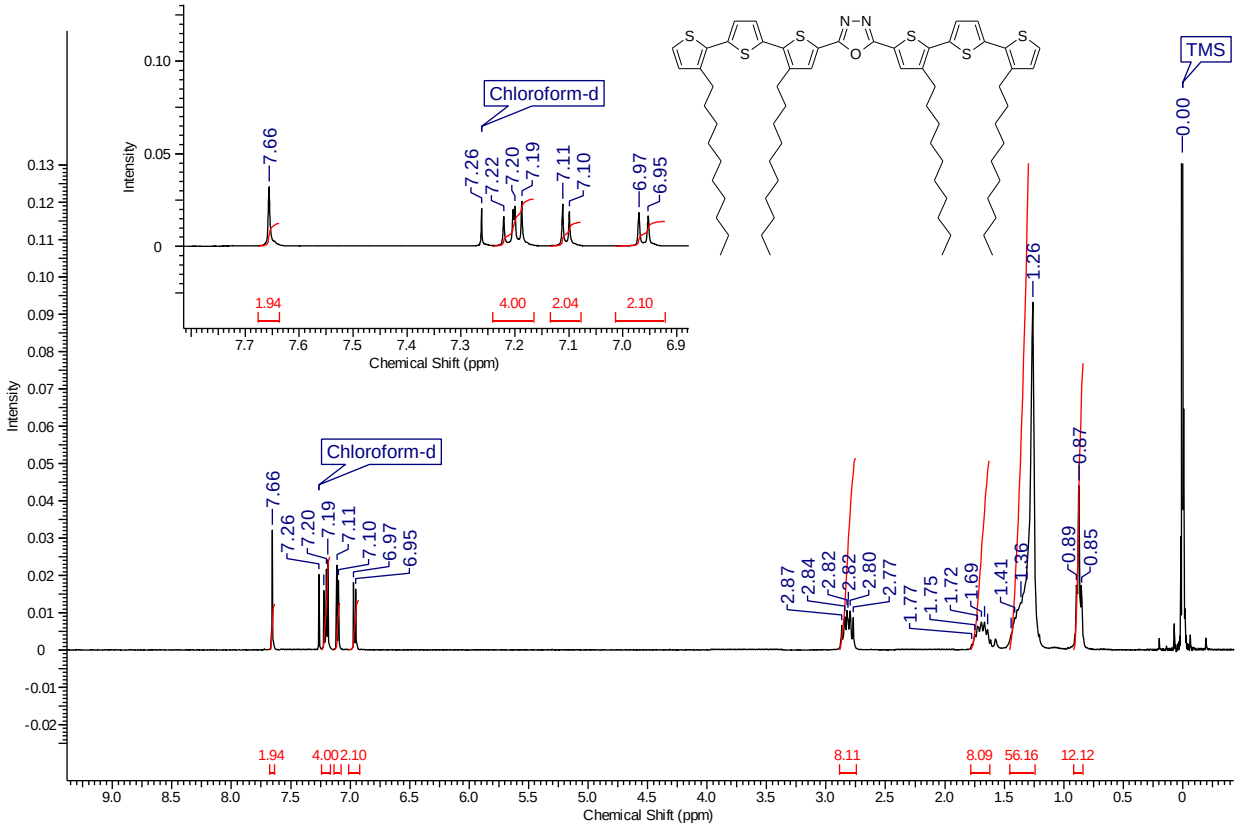


^{13}C NMR (100 MHz, δ, ppm) **(14c)**

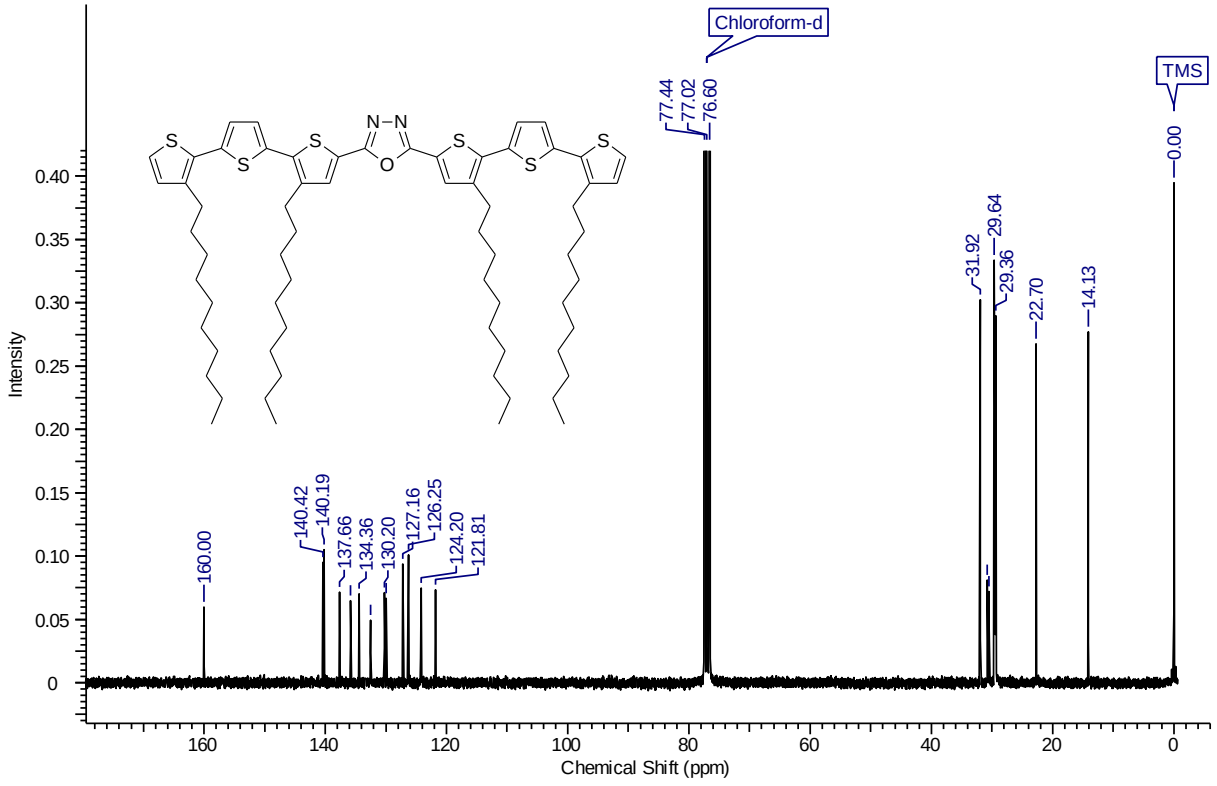


2,5-Bis(3,3''-didecyl-[2,2':5',2''-terthiophen]-5-yl)-1,3,4-oxadiazole (2)

^{1}H NMR (400 MHz, $CDCl_3$)

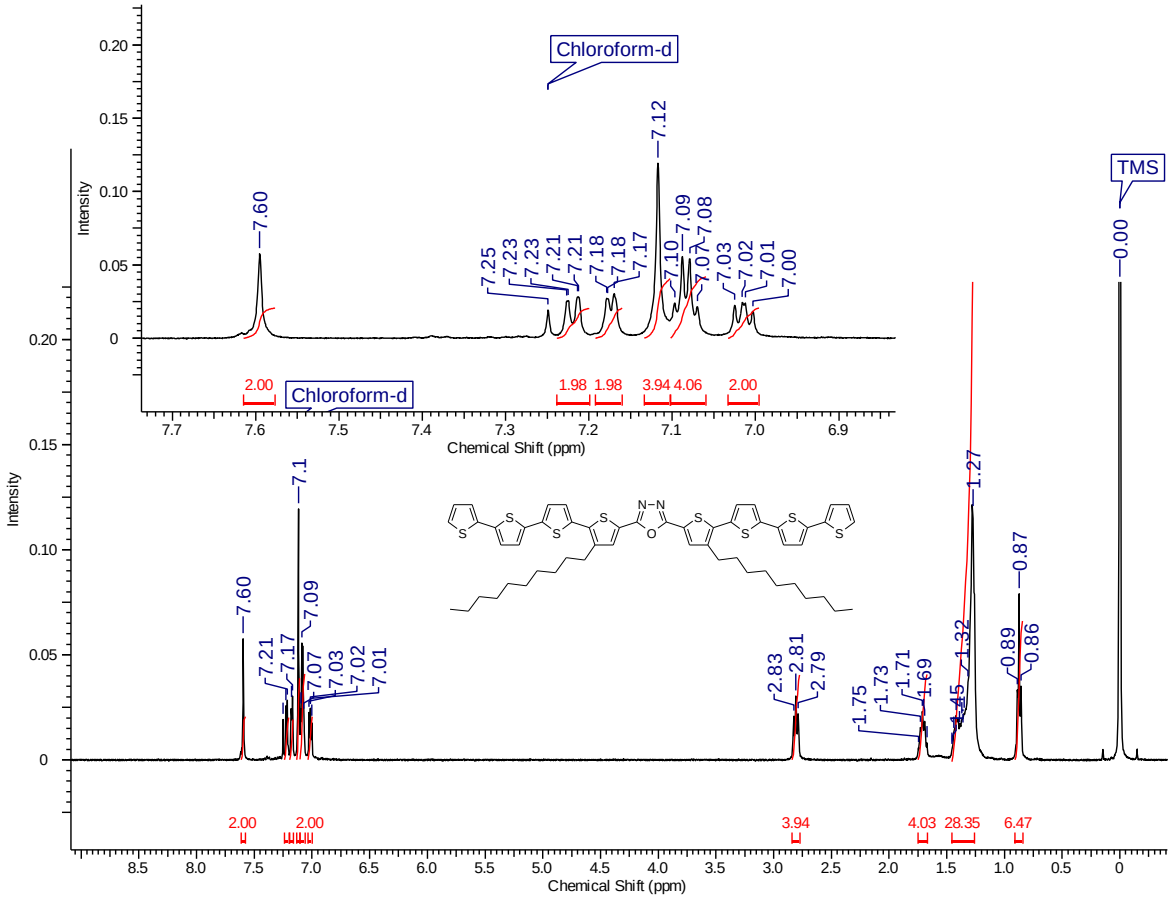


^{13}C NMR (100 MHz, δ, ppm) **(2)**

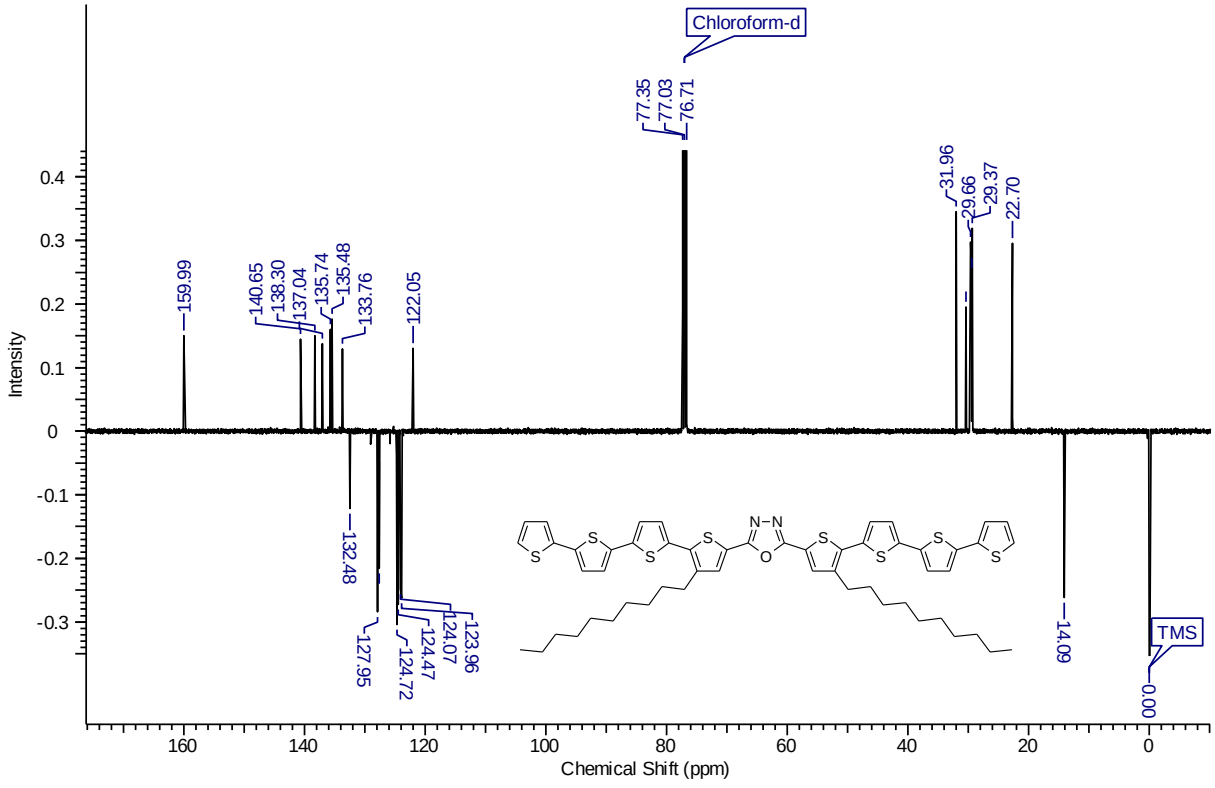


2,5-Bis(3-decyl-[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl)-1,3,4-oxadiazole (1)

^{1}H NMR (400 MHz, $CDCl_3$)

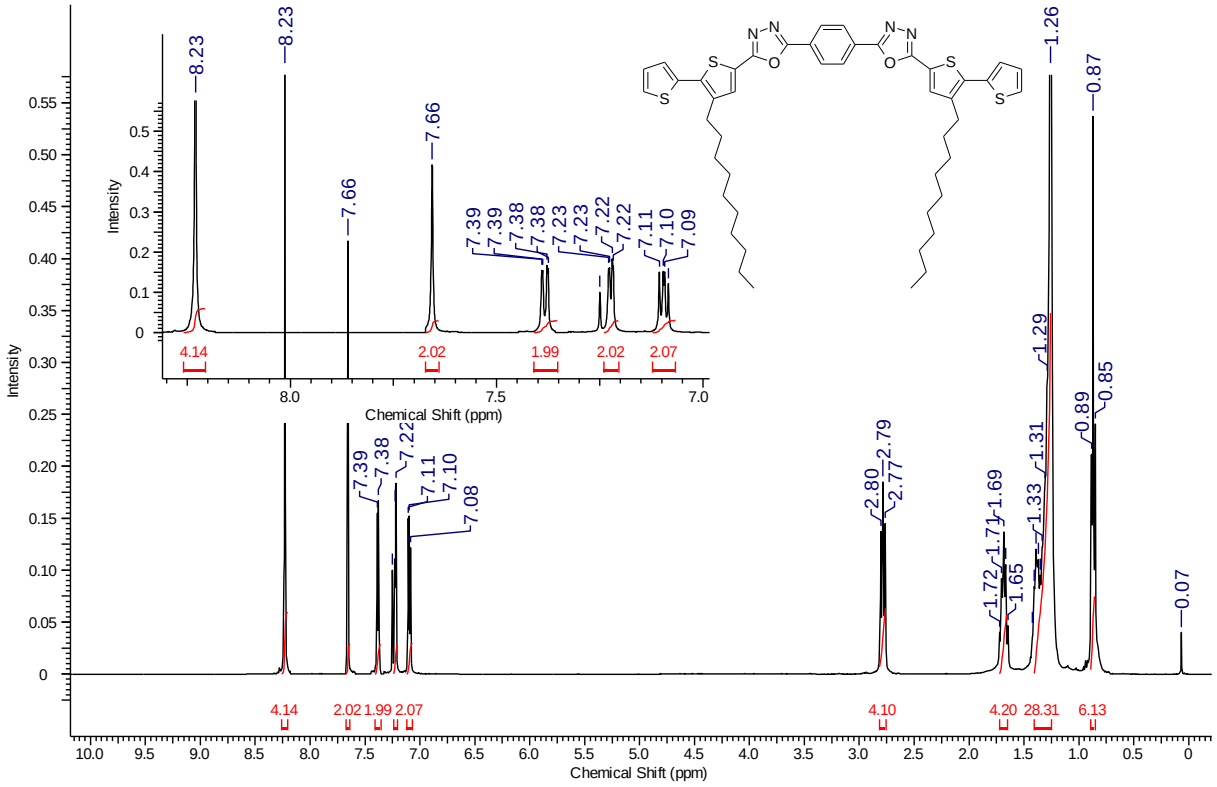


^{13}C NMR (100 MHz, δ, ppm) **(1)**

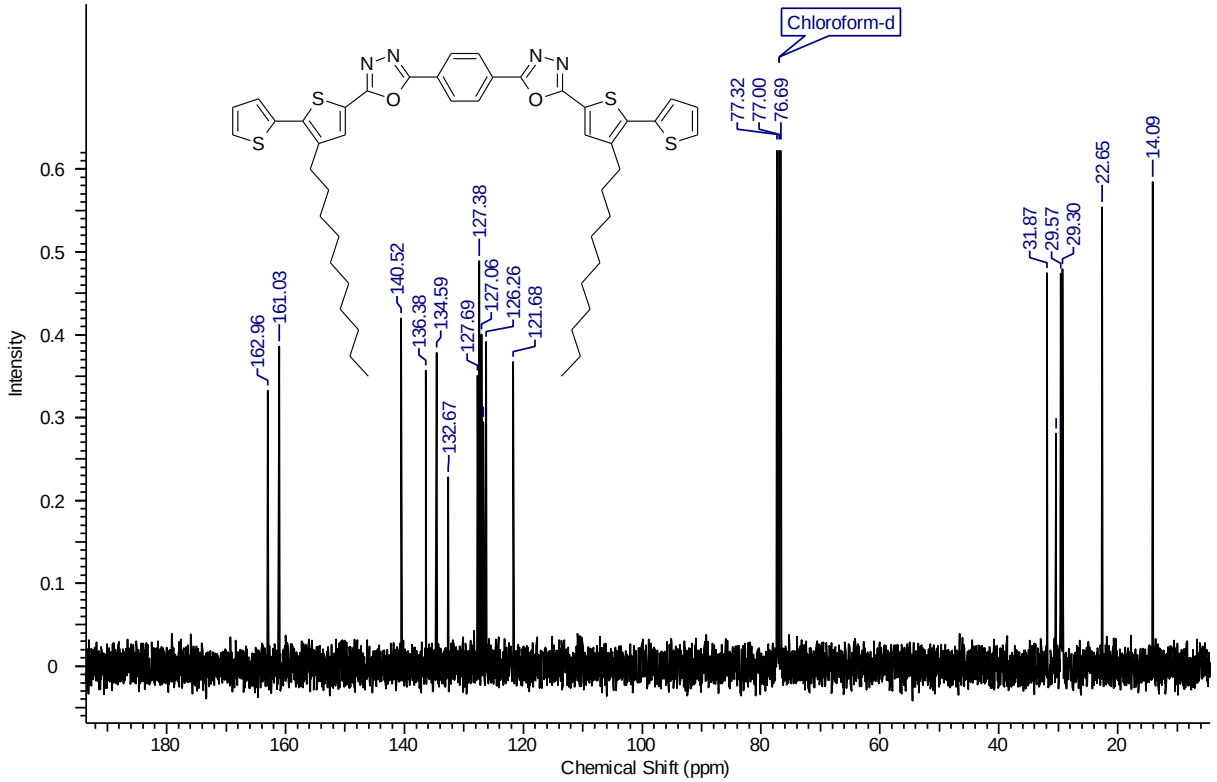


1,4-bis(5-(3-decyl-[2,2'-bithiophen]-5-yl)-1,3,4-oxadiazol-2-yl)benzene (5)

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, δ, ppm) **(5)**



Auxiliary electrochemical, spectroelectrochemical, and quantum computational data

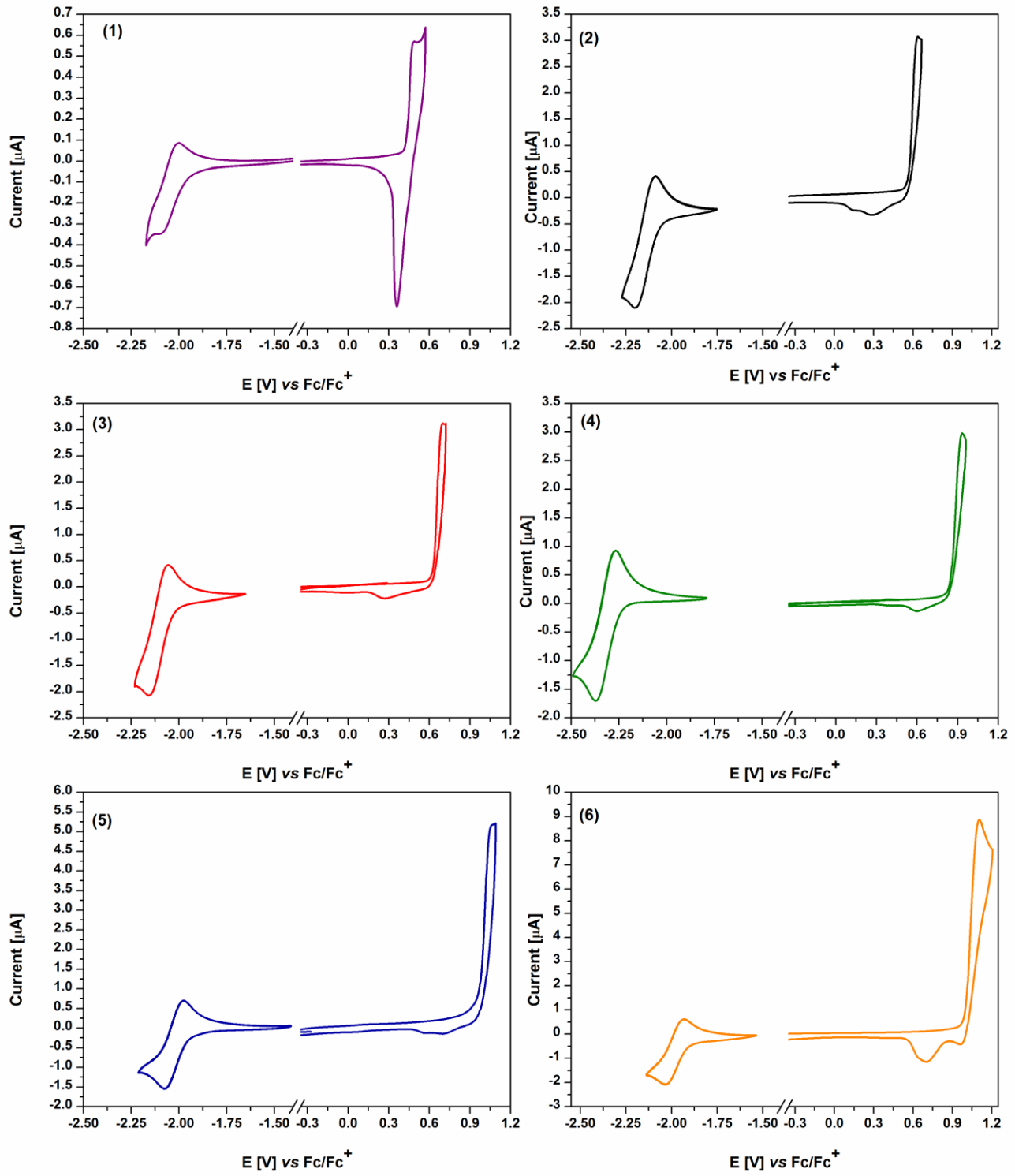


Fig.S1. Cyclic voltammograms of the monomers registered in 0.1 M Bu_4NPF_6 in dichloromethane for the anodic potential range and in tetrahydrofuran for cathodic potential range, set to a common current scale for each compound. Scan rate: 100 mV/s.

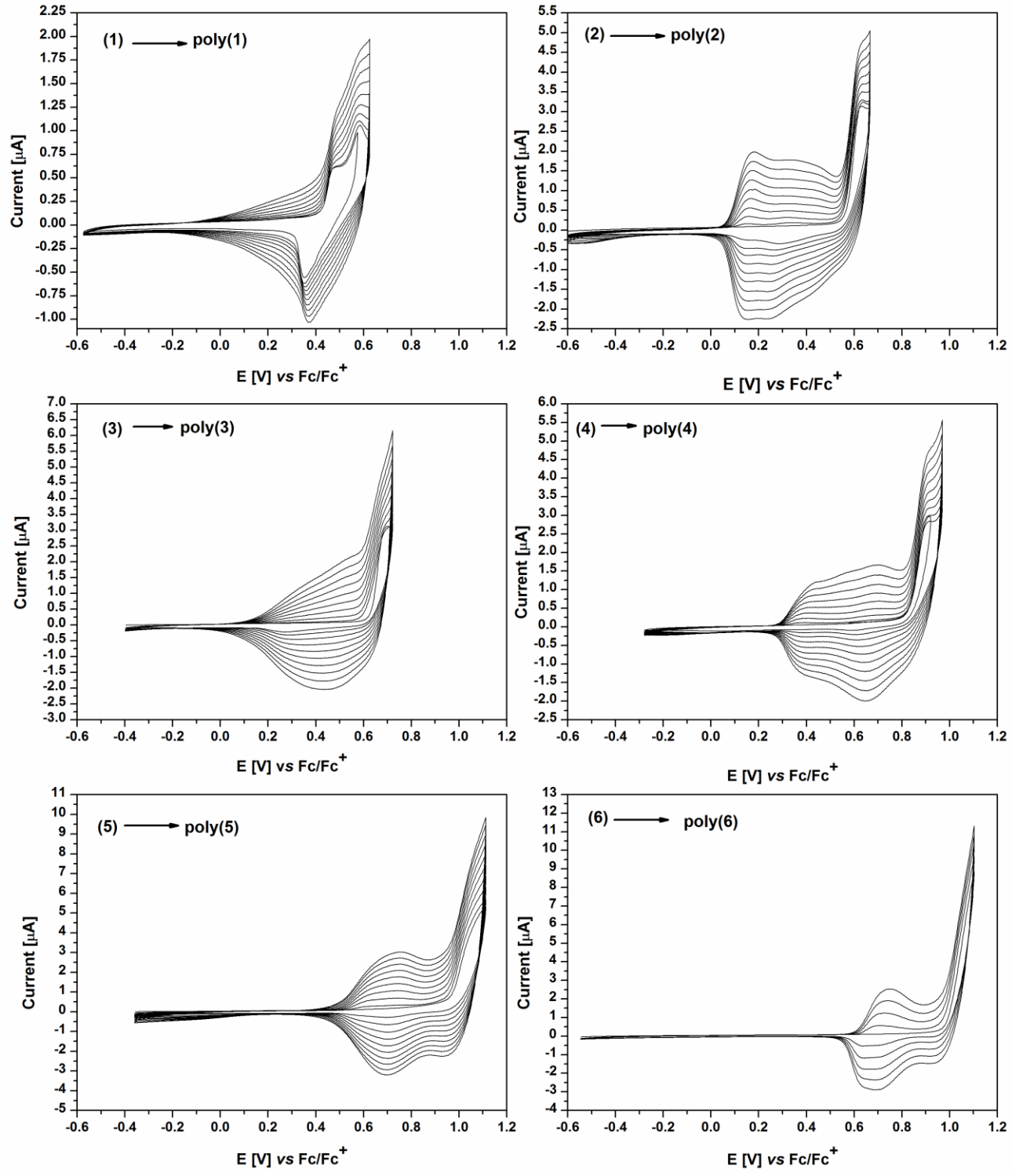


Fig.S2. Cyclic voltammogram of polymerization process registered in 0.1 M Bu_4NPF_6 in dichloromethane for the anodic potential range. Scan rate: 100 mV/s.

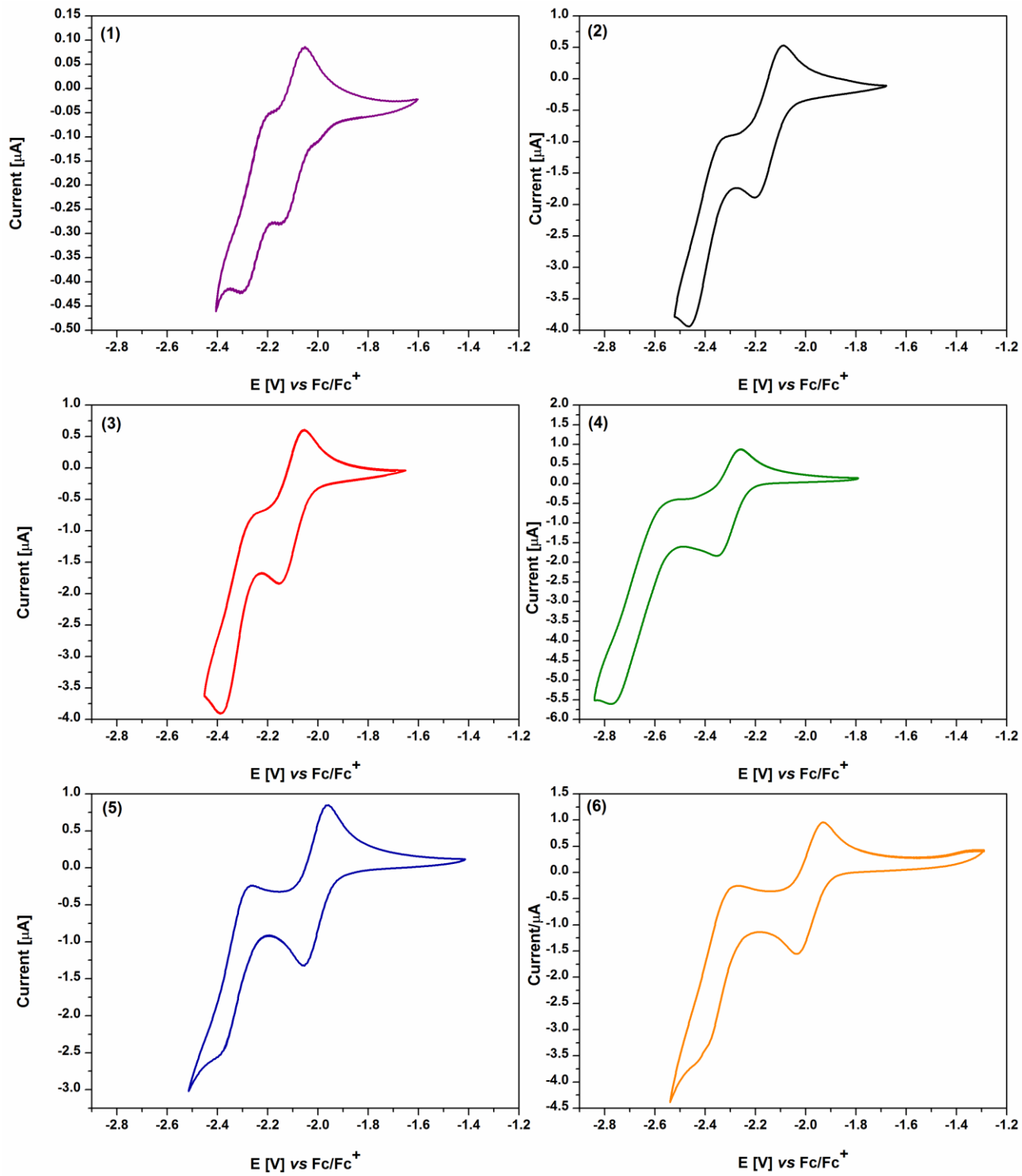


Fig.S3. Cyclic voltammogram of investigated monomers registered in 0.1 M Bu_4NPF_6 in tetrahydrofuran in extended cathodic potential range. Scan rate: 100 mV/s.

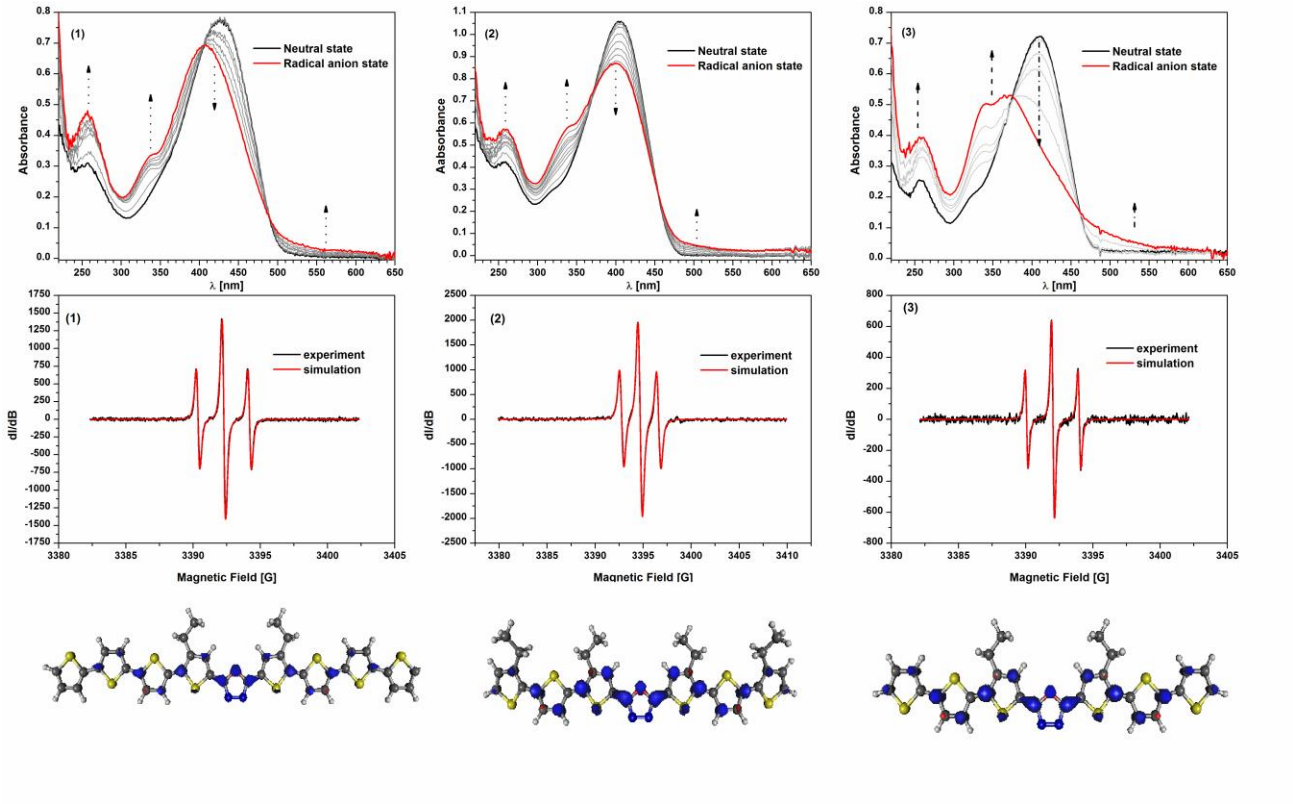


Fig.S4. Changes in UV-Vis and EPR spectra upon electrochemical generation of radical anions, registered in 0.1 M Bu_4NPF_6 in tetrahydrofuran with the monomer concentration equal to 1mmol/dm^3 for (2) and (3) and 0.25 mmol/dm^3 for (1).

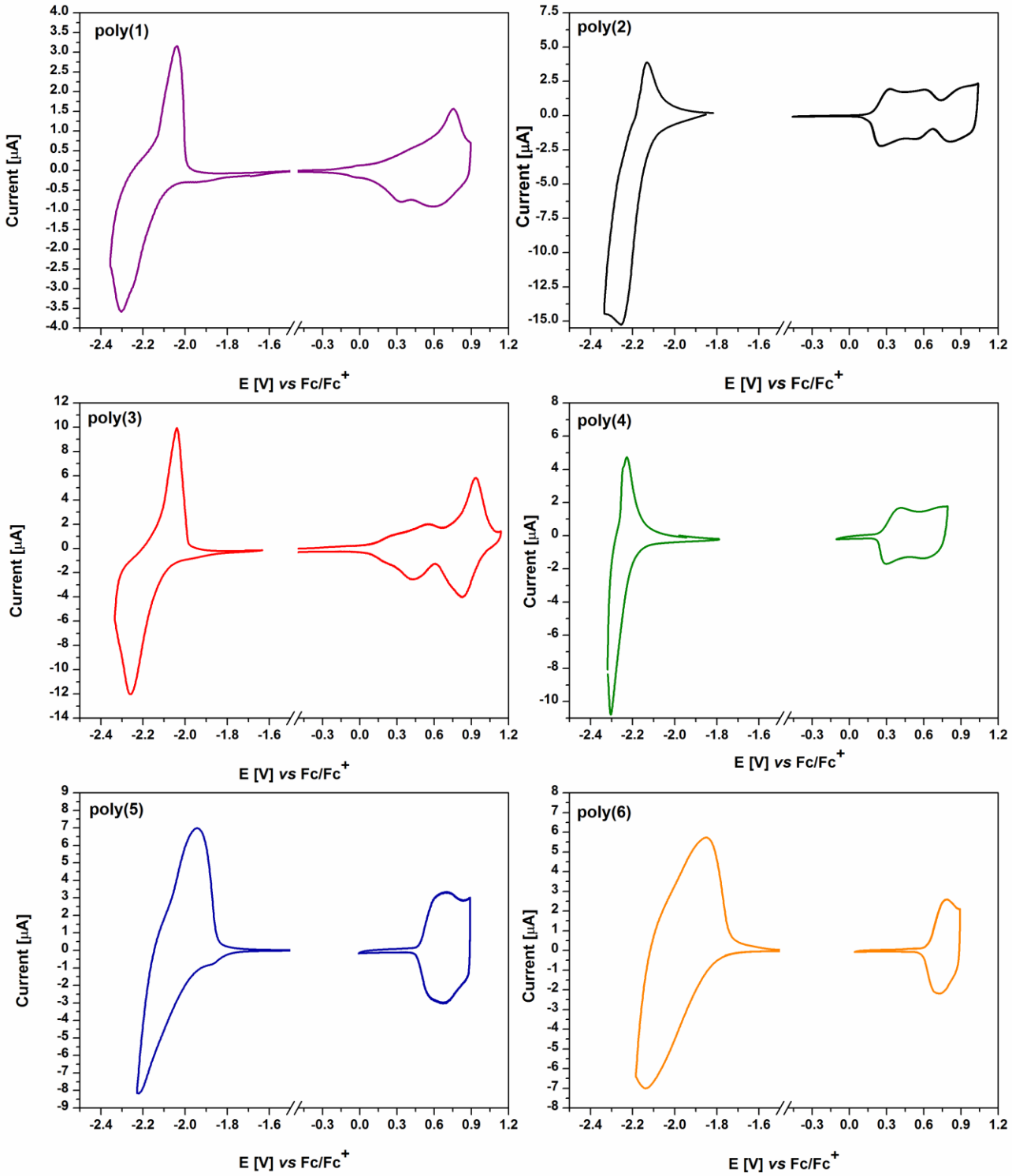
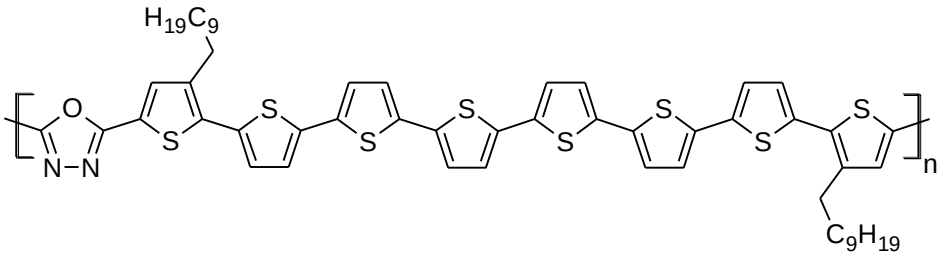
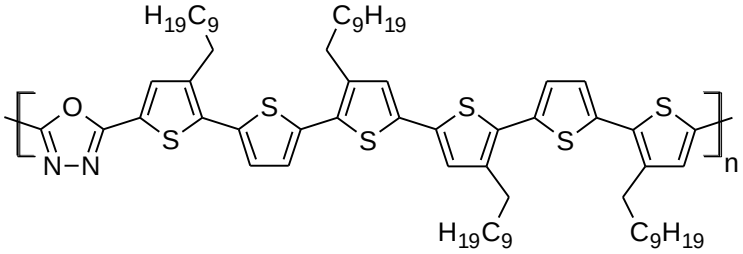


Fig.S5. Cyclic voltammograms of electrodeposited polymers registered in 0.1 M Bu_4NPF_6 in dichloromethane for the anodic potential range and in tetrahydrofuran for cathodic potential range, set to a common current scale for each polymer. Scan rate: 100 mV/s

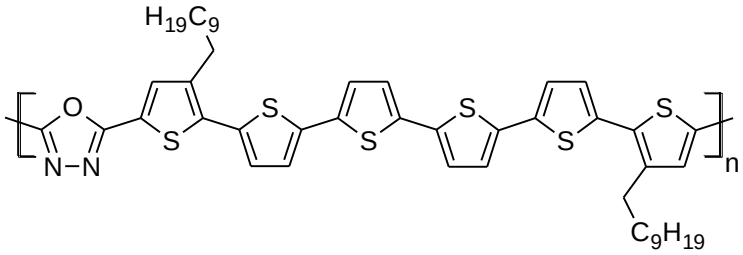
poly(**1**)



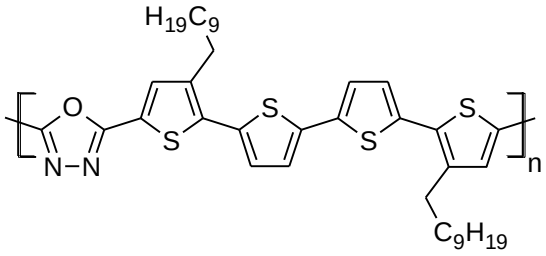
poly(**2**)



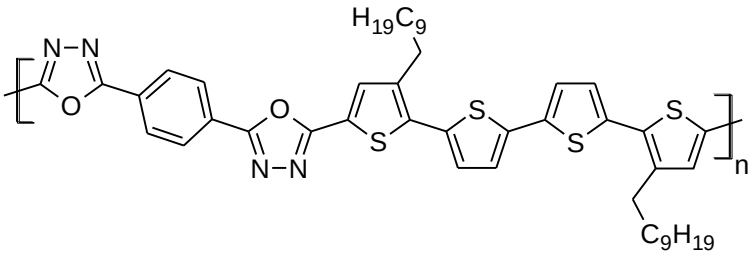
poly(**3**)



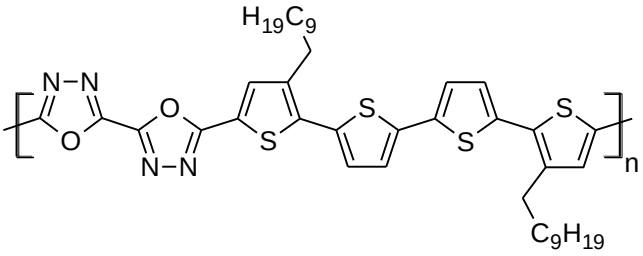
poly(**4**)



poly(**5**)



poly(**6**)



Scheme S1. Structures of the repeating unit of electrochemically generated polymers of compounds **1** to **6**.

Table S1. Description of the most important optical transitions simulated with B3LYP/6-31G(d)/PCM(THF) method.

Comp.	No. of transition	Wavelength [nm]	Oscillator strength	Composition
(**1**)	1	565	3.0470	HOMO -> LUMO (93%) HOMO-1 -> LUMO+1 (5%)
(**2**)	1	512	2.2891	HOMO -> LUMO (96%) HOMO-1 -> LUMO+1 (3%)
(**3**)	1	518	2.3327	HOMO -> LUMO (97%) HOMO-1 -> LUMO+1 (3%)
(**4**)	1	448	1.6243	HOMO -> LUMO (99%)
(**5**)	1	455	2.1027	HOMO -> LUMO (95%) HOMO-1 -> LUMO+1 (4%)
(**6**)	1	462	1.7547	HOMO -> LUMO (97%) HOMO-1 -> LUMO+1 (2%)

Table S2. Description of the most important optical transitions simulated with CAM- B3LYP/6-31G(d)/PCM(THF) method.

Compound	No. of transition	Wavelength [nm]	Oscillator strength	Composition
(**1**)	1	411	3.5630	HOMO -> LUMO (76%) HOMO-1 -> LUMO+1 (25%)
(**2**)	1	375	2.4326	HOMO -> LUMO (74%) HOMO-1 -> LUMO+1 (15%)
(**3**)	1	391	2.6540	HOMO -> LUMO (73%) HOMO-1 -> LUMO+1 (19%)
(**4**)	1	342	1.7000	HOMO -> LUMO (85%) HOMO-1 -> LUMO+1 (11%)
(**5**)	1	353	2.7205	HOMO -> LUMO (63%) HOMO-1 -> LUMO+1 (24%)
(**6**)	1	360	2.1728	HOMO -> LUMO (71%) HOMO-1 -> LUMO+1 (21%)

Table S3. Selected dihedral angles of the molecules investigated at the ground and first excited state. Geometries were obtained with B3LYP/6-31G(d)/PCM(THF) method.

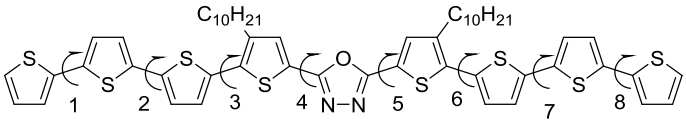
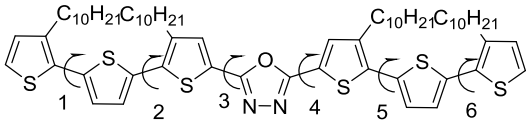
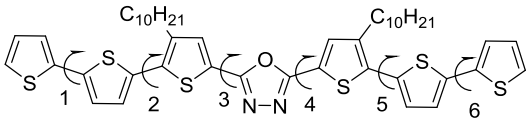
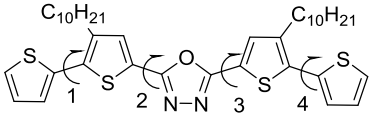
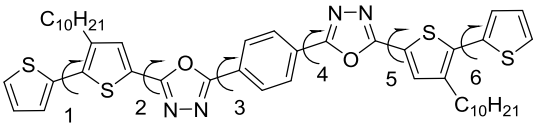
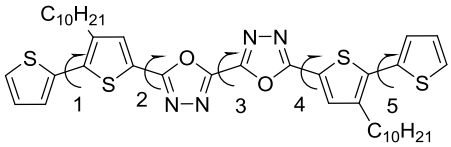
Compound	Dihedral angle no.	Dihedral angle in ground state	Dihedral angle in S_1 excited state
	1	13.710	0.000
	2	12.301	0.009
	3	20.495	0.000
	4	0.793	0.000
	5	0.791	0.000
	6	20.493	0.000
	7	12.304	0.009
	8	13.701	0.001
	1	25.958	0.010
	2	24.560	0.007
	3	0.760	0.003
	4	0.759	0.003
	5	24.556	0.007
	6	25.928	0.011
	1	15.682	0.002
	2	22.009	0.000
	3	0.675	0.000
	4	0.678	0.000
	5	22.010	0.000
	6	15.720	0.002
	1	26.591	0.019
	2	0.693	0.001
	3	0.682	0.001
	4	26.654	0.020
	1	30.465	0.030
	2	0.857	0.000
	3	0.020	0.000
	4	0.002	0.000
	5	0.725	0.001
	6	26.618	0.017
	1	25.637	0.003
	2	1.284	0.000
	3	0.157	0.000
	4	1.384	0.002
	5	29.254	0.004

Table S4. Description of the most important optical transitions for radical anions of the molecules investigated, simulated with CAM- B3LYP/6-31G(d)/PCM(THF) method.

Species	No. of transition	Wavelength [nm]	Oscillator strength	Composition
(**1**)$^{\bullet-}$	1	4462	1.3320	SOMO(A) -> LUMO(A)
	3	823	0.1141	HOMO-1(B) -> LUMO(B) HOMO(B) -> SOMO(B)
	5	659	1.2796	SOMO(A) -> LUMO+2(A)
(**2**)$^{\bullet-}$	1	4988	1.0555	SOMO(A) -> LUMO(A)
	3	667	0.2917	HOMO(B) -> SOMO(B)
	5	559	0.9600	SOMO(A) -> LUMO+2(A)
(**3**)$^{\bullet-}$	1	13094	1.1120	SOMO(A) -> LUMO(A)
	3	702	0.2839	HOMO(B) -> SOMO(B)
	5	575	1.0195	SOMO(A) -> LUMO+2(A)
(**4**)$^{\bullet-}$	1	2766	0.7892	SOMO(A) -> LUMO(A)
	3	573	0.4920	HOMO(B) -> SOMO(B)
	5	458	0.5545	SOMO(A) -> LUMO+2(A)
(**5**)$^{\bullet-}$	1	1655	0.9814	SOMO(A) -> LUMO(A)
	3	642	0.3462	HOMO-1(B) -> LUMO(B) HOMO(B) -> SOMO(B)
	7	433	1.2010	HOMO(B) -> SOMO(B)
(**6**)$^{\bullet-}$	1	2638	0.8077	SOMO(A) -> LUMO(A)
	3	602	0.3157	HOMO-1(B) -> LUMO(B) HOMO(B) -> SOMO(B)
	5	438	0.6508	SOMO(A) -> LUMO+2(A)

Table S5. Comparison of electron structure parameters of compounds **1** to **6** and their electro-generated polymers.

Structure	**Monomer**			**Polymer**			**$\Delta(IP_P\text{-}IP_M)$**	**$\Delta(EA_P\text{-}EA_M)$**	**$\Delta(Eg_P\text{-}Eg_M)$**
	IP	**EA**	**E_g^{el} [eV]**	**IP**	**EA**	**E_g^{el} [eV]**			
(**1**)	5,53	3,15	2,38	4,98	2,99	1,99	-0,55	-0,16	-0,39
(**2**)	5,66	3,03	2,63	5,28	2,91	2,37	-0,38	-0,12	-0,26
(**3**)	5,73	3,07	2,66	5,17	2,95	2,22	-0,56	-0,12	-0,44
(**4**)	5,93	2,85	3,08	5,33	2,89	2,44	-0,6	+0,04	-0,64
(**5**)	6,06	3,14	2,92	5,57	3,13	2,44	-0,49	-0,01	-0,48
(**6**)	6,09	3,19	2,9	5,73	3,29	2,44	-0,36	+0,1	-0,46

References

1 A. S. Kostyuchenko, A. M. Averkov and A. S. Fisyuk, *Org. Lett.*, 2014, **16**, 1833–1835.

2 K. Kotwica, E. Kurach, G. Louarn, A. S. Kostyuchenko, A. S. Fisyuk, M. Zagorska and A. Pron, *Electrochim. Acta*, 2013, **111**, 491–498.

3 A. S. Kostyuchenko, G. Wiosna-Salyga, A. Kurowska, M. Zagorska, B. Luszczynska, R. Grykien, I. Glowacki, A. S. Fisyuk, W. Domagala and A. Pron, *J. Mater. Sci.*, 2016, **51**, 2274–2282.

4 A. S. Kostyuchenko, V. L.Yurpalov, A. Kurowska, W. Domagala, A. Pron and A. S. Fisyuk, *Beilstein J. Org. Chem.*, 2014, **10**, 1596–1602.

5 R. B. Phillips, S. A. Herbert and A. J. Robichaud, *Synth. Commun.*, 1986, **16**, 411–417.

6 H. Wynberg and J. Metselaar, *Synth. Commun.*, 1984, **14**, 1–9.

7 A. V. Kluchnikova, O. A., Udashkin, *Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya*, 2005, vol. 48.

8 A. S. Kostyuchenko, E. A. Drozdova and A. S. Fisyuk, *Chem. Heterocycl. Compd.*, 2017, **53**, 92–96.

9 A. S. Kostyuchenko, T. Y. Zheleznova, A. J. Stasyuk, A. Kurowska, W. Domagala, A. Pron and A. S. Fisyuk, *Beilstein J. Org. Chem.*, 2017, **13**, 313–322.