Electronic Supplementary Information

Influence of terminal alkyl groups on the structure, electrical and sensory properties of thin films of self-assembling organosilicon derivatives of benzothieno[3,2-b][1]benzothiophene

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1. Synthetic techniques

[1]benzothieno[3,2-b][1]benzothien-2-yl)-ethan-1-one (2). A solution of [1]benzothieno [3,2-b][1]benzothiophene **(1)** (4.0 g, 16.6 mmol) in dry dichloromethane (450 mL) was cooled to -5°C and aluminum chloride (4.1 g, 30.8 mmol) was added in one portion. The mixture was stirred for 1 h under cooling. Thereafter, acetyl chloride (2.42 g, 30.8 mmol) was added dropwise. After 1 h at -5 °C, the reaction mixture was added to water (300 mL) and dichloromethane (300 mL). The organic layer was washed with water and dried over sodium sulfate. The solvent was evaporated under vacuum and the product was purified by column chromatography on silica gel (eluent hot toluene, T=60ºC) to give pure compound **2** (3.01 g, 62 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.55 (dd, J_1 = 1.5 Hz, J_2 =0.6 Hz, 1H), 8.06 (dd, J_1 = 8.5 Hz, J_2 =1.5 Hz, 1H), 7.94 (m, 3H), 7.48 (m, 2H), 3.07 (t, J = 7.3 Hz, 3H).

([1]benzothieno[3,2-b][1]benzothien-2-yl)-butan-1-one (3) was synthesized according to the procedure described for compound **2** using **1** (2.04 g, 8.5 mmol), aluminum chloride (2.1 g, 15.7 mmol), butanoyl chloride (1.67 g, 15.7 mmol) in dry dichloromethane (400 mL). After the standard isolation procedure in dichloromethane the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **3** (1.05 g, 40 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.63 (dd, J_1 = 1.5 Hz, J_2 =0.6 Hz, 1H), 8.04 (dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 7.92 (m, 3H), 7.46 (m, 2H), 3.04 (t, J = 7.3 Hz, 2H). 1.83 (m, 2H), 1.04 (t, J = 7.0 Hz, 3H).

([1]benzothieno[3,2-b][1]benzothien-2-yl)-octan-1-one (4) was synthesized according to the procedure described for compound **2** using **1** (2.8 g, 11.6 mmol), aluminum chloride (2.87 g, 21.5 mmol), octanoyl chloride (3.5 g, 21.5 mmol) in dry dichloromethane (400 mL). After the standard isolation procedure in dichloromethane the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **4** (2.25 g, 52 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.64 (dd, J_1 = 1.5 Hz, J_2 = 0.6 Hz, 1H), 8.05 (dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 7.93 (m, 3H), 7.46 (m, 2H), 3.06 (t, J = 7.3 Hz, 2H), 1.79 (m, 2H), 1.22-1.45 (overlapping peaks, 10H), 0.88 (t, J = 7.0 Hz, 3H).

2-Ethyl-[1]benzothieno[3,2-b][1]benzothiophene (6). To a stirred solution of compound **2** (1.55 g, 5.5 mmol) in dry THF (100 mL) sodium borohydride (1.04 g, 27.4 mmol) and aluminum chloride (1.83 g, 13.7 mmol) were added successively. After the exothermic reaction completion, the mixture was stirred under reflux for 12 h. Thereafter, water (10 mL) was added dropwise. After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **6** (1.2 g, 82 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.88 (dd, J_1 = 14.1 Hz, J_2 = 7.5 Hz, 2H), 7.79 (d, J = 8.2, 1H), 7.73 (s, 1H), 7.41 (m, 2H), 7.30 (dd, J_1 = 8.1 Hz, J_2 = 1.3, 1H), 2.80 (t, J = 7.5 Hz, 2H), 1.33 (t, J = 6.9 Hz, 3 H).

2-Butyl-[1]benzothieno[3,2-b][1]benzothiophene (7) was synthesized according to the procedure described for compound **6** using compound **3** (1.05 g, 3.4 mmol), sodium borohydride (0.64 g, 16.9 mmol) and aluminum chloride (1.13 g, 8.5 mmol) in dry THF (100 mL). After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **7** (0.95 g, 95 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.88 (dd, J_1 = 14.1 Hz, J_2 = 7.5 Hz, 2H), 7.78 (d, J = 8.2, 1H), 7.71 (s, 1H), 7.41 (m, 2H), 7.28 (dd, J_1 = 8.1 Hz, J_2 = 1.3, 1H), 2.76 (t, J = 7.5 Hz, 2H), 1.68 (m, 2H), 1.39 (m, 2H), 0.95 (t, J = 6.9 Hz, 3 H).

2-Octyl-[1]benzothieno[3,2-b][1]benzothiophene (8) was synthesized according to the procedure described for compound **6** using compound **4** (2.25 g, 6.1 mmol), sodium borohydride (1.16 g, 30.7 mmol) and aluminum chloride (2.05 g, 15.3 mmol) in dry THF (100 mL). After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **8** (1.66 g, 77 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.87 (dd, J_1 = 14.1 Hz, J_2 = 7.5 Hz, 2H), 7.78 (d, J = 8.2, 1H), 7.71 (s, 1H), 7.41 (m, 2H), 7.27 (dd, J_1 = 8.1 Hz, J_2 = 1.3, 1H), 2.75 (t, J = 7.5 Hz, 2H), 1.69 (m, 2H), 1.19-1.43 (overlapping peaks, 10H), 0.87 (t, J = 6.9 Hz, 3 H).

10,11-dibromo-1-(7-ethyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecan-1-one (10). A solution of compound **6** (1.2 g, 4.1 mmol) in dry dichloromethane (200 mL) was cooled to -10°C and aluminum chloride (1.1 g, 8.3 mmol) was added in one portion. The mixture was stirred for 1 h at -10°C. Thereafter, the reaction mixture was cooled to -70°C and 10,11-dibromoundecanoyl chloride (3.0 g, 8.3 mmol) was added dropwise. After 2 h at -70°C, the reaction mixture was added to water (200 mL) and dichloromethane (300 mL). After the standard isolation procedure in dichloromethane the product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **10** (1.65 g, 62%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.53 (d, J = 0.9 Hz, 1H), 8.05 (dd, J_1 = 8.4 Hz, J_2 = 1.5 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.74 (s, 1H), 7.31 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 1H), 4.16 (m, 1H), 3.86 (dd, J_1 = 10.3 Hz, J_2 = 4.5 Hz, 1H), 3.62 (t, J = 10.0 Hz, 1H), 3.06 (t, J = 7.5 Hz, 2H), 2.82 (t, J = 7.5 Hz, 2H), 2.12 (m, 1H), 1.70-1.87 (overlapping peaks, 3H), 1.30-1.49 (overlapping peaks, 12H). ^{13}C NMR (75 MHz, CDCl3) δ 199.44, 143.15, 142.55, 141.94, 136.87, 136.34, 133.22, 132.09, 130.59, 125.76, 125.66, 124.57, 124.41, 122.76, 121.73, 121.06, 53.07, 38.65, 36.30, 35.91, 29.27, 29.24, 29.15, 29.04, 28.67, 28.64, 24.39, 15.67. Anal. calcd. for $C_{27}H_{30}Br_2OS_2$: C, 54.55; H, 5.09; Br, 26.88; S, 10.79. Found: C, 54.60; H, 5.13; Br, 26.77; S, 10.67.

10,11-dibromo-1-(7-buthyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecan-1-one (11) was synthesized according to the procedure described for compound **10** using compound **7** (0.8 g, 2.7 mmol), 10,11-dibromoundecanoyl chloride (1.81 g, 5.0

mmol) and aluminum chloride (0.67 g, 5.0 mmol) in dry dichloromethane (150 mL). After the standard isolation procedure in dichloromethane the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **11** (1.27 g, 76%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.53 (d, J = 0.9 Hz, 1H), 8.04 (dd, J_1 = 8.4 Hz, J_2 = 1.5 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.30 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 1H), 4.16 (m, 1H), 3.84 (dd, J_1 = 10.3 Hz, J_2 = 4.5 Hz, 1H), 3.62 (t, J = 10.0 Hz, 1H), 3.06 (t, J = 7.5 Hz, 2H), 2.77 (t, J = 7.9 Hz, 2H), 2.11 (m, 1H), 1.61-1.88 (overlapping peaks, 5H), 1.26-1.48 (overlapping peaks, 11H), 0.95 (t, J = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.46, 143.07, 141.95, 141.25, 136.90, 136.36, 133.22, 132.07, 130.58, 126.12, 124.58, 124.43, 123.36, 121.65, 121.08, 53.07, 38.66, 36.30, 35.91, 35.78, 33.69, 29.27, 29.24, 29.15, 28.67, 26.64, 24.40, 22.28, 13.91. Anal. calcd. for $C_{29}H_{34}Br_2OS_2$: C, 55.95; H, 5.51; Br, 25.67; S, 10.30. Found: C, 55.92; H, 5.59; Br, 25.62; S, 10.24.

10,11-dibromo-1-(7-octyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecan-1-one (12) was synthesized according to the procedure described for compound **10** using compound **8** (1.5 g, 4.3 mmol), 10,11-dibromoundecanoyl chloride (7.64 g, 19.1 mmol) and aluminum chloride (1.7 g, 12.8 mmol) in dry dichloromethane (300 mL). After the standard isolation procedure in dichloromethane the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **12** (2.03 g, 70%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.53 (d, J = 0.9 Hz, 1H), 8.04 (dd, J_1 = 8.4 Hz, J_2 =1.5 Hz, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.30 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 1H), 4.16 (m, 1H), 3.84 (dd, J_1 = 10.3 Hz, J_2 = 4.5 Hz, 1H), 3.62 (t, J = 10.0 Hz, 1H), 3.06 (t, J = 7.5 Hz, 2H), 2.76 (t, J = 7.9 Hz, 2H), 2.11 (m, 1H), 1.63-1.85 (overlapping peaks, 5H), 1.20-1.46 (overlapping peaks, 19H), 0.87 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.45, 143.07, 141.95, 141.30, 136.90, 136.36, 133.23, 132.07, 130.59, 126.11, 124.58, 124.43, 123.35, 121.65, 121.07, 53.06, 38.65, 36.28, 36.09, 35.91, 31.79, 31.56, 29.40, 29.27, 29.24, 29.18, 29.14, 28.66, 26.64, 24.40, 22.59, 14.04. Anal. calcd. for $C_{33}H_{42}Br_2OS_2$: C, 58.41; H, 6.24; Br, 23.55; S, 9.45. Found: C, 58.37; H, 6.19; Br, 23.62; S, 9.51.

10,11-dibromo-1-(7-tridecyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecan-1-one (13) was synthesized according to the procedure described for compound **10** using compound **9** (1.5 g, 3.5 mmol), 10,11-dibromoundecanoyl chloride (5.9 g, 16.0 mmol) and aluminum chloride (1.42 g, 10.6 mmol) in dry dichloromethane (250 mL). After the standard isolation procedure in dichloromethane the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **13** (2.42 g, 54%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.53 (d, J = 0.9 Hz, 1H), 8.04 (dd, J_1 = 8.4 Hz, J_2=1.5 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.73 (s, 1H), 7.30 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 1H), 4.13 (m, 1H), 3.84 (dd, J_1 = 10.3 Hz, J_2 = 4.5 Hz, 1H), 3.62 (t, J = 10.0 Hz, 1H), 3.06 (t, J = 7.5 Hz, 2H), 2.76 (t, J = 7.9 Hz, 2H), 2.08 (m, 1H), 1.62-1.86 (overlapping peaks, 5H), 1.17-1.48

(overlapping peaks, 29H), 0.86 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.48, 143.07, 141.95, 141.32, 136.91, 136.37, 133.23, 132.07, 130.58, 126.12, 124.59, 124.44, 123.36, 121.66, 121.09, 53.07, 38.66, 36.29, 36.09, 35.90, 31.85, 31.56, 29.58, 29.50, 29.43, 29.28, 29.21, 29.14, 28.66, 26.64, 24.40, 22.62, 14.06. Anal. calcd. for $C_{38}H_{52}Br_2OS_2$: C, 60.96; H, 7.00; Br, 21.34; S, 8.56. Found: C, 61.03; H, 7.13; Br, 21.28; S, 8.49.

2-(10,11-dibromoundecyl)-7-ethyl[1]benzothieno[3,2-b][1]benzothiophene (14). To a stirred solution of compound **10** (1.6 g, 2.7 mmol) in dry THF (100 mL), sodium borohydride (0.51 g, 13.5 mmol) and aluminum chloride (0.9 g, 6.7 mmol) were added successively. After the exothermic reaction completion, the mixture was stirred under reflux for 4 h. Thereafter, water (10 mL) was added dropwise. After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **14** (1.2 g, 77 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 2H,), 7.72 (s, 2H), 7.28 (dd, J_1 = 8.2, J_2 = 1.3 Hz, 2H), 4.15 (m, 1H), 3.83 (dd, J_1 = 10.3 Hz, J_2 = 4.4 Hz, 1H), 3.61 (t, J = 10.0 Hz, 1H), 2.76 (t, J = 7.5 Hz, 4H), 2.11 (m, 1H), 1.64-1.83 (overlapping peaks, 3H), 1.20-1.43 (overlapping peaks, 15H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.38, 142.31, 141.27, 139.92, 132.48, 132.44, 131.11, 125.75, 125.30, 123.25, 122.67, 121.08, 121.00, 53.11, 36.31, 36.03, 35.93, 31.61, 29.65, 29.37, 29.35, 29.28, 29.16, 29.00, 28.71, 26.67, 25.79. Anal. calcd. for $C_{27}H_{32}Br_2S_2$: C, 55.87; H, 5.56; Br, 27.53; S, 11.05. Found: C, 55.89; H, 5.51; Br, 27.47; S, 11.11.

2-(10,11-dibromoundecyl)-7-butyl[1]benzothieno[3,2-b][1]benzothiophene (15) was synthesized according to the procedure described for compound **14** using compound **11** (1.2 g, 1.9 mmol), sodium borohydride (0.36 g, 9.6 mmol) and aluminum chloride (0.64 g, 4.8 mmol) in dry THF (80 mL). The reaction was complete after 22 h of stirring at boiling temperature. After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **15** (0.75 g, 64 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75 (d, J = 8.1 Hz, 2H,), 7.70 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.15 (m, 1H), 3.83 (dd, J_1 = 10.3 Hz, J_2 = 4.4 Hz, 1H), 3.61 (t, J = 10.0 Hz, 1H), 2.76(t, J = 7.5 Hz, 4H), 2.11 (m, 1H), 1.63-1.83 (overlapping peaks, 5H), 1.25-1.46 (overlapping peaks, 14H), 0.95 (t, J = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.30, 139.94, 139.91, 132.45, 131.10, 131.08, 125.74, 123.26, 120.99, 53.10, 36.31, 36.03, 35.93, 35.73, 31.61, 29.36, 29.35, 29.27, 29.16, 28.70, 26.66, 22.29, 13.93. Anal. calcd. for $C_{29}H_{36}Br_2S_2$: C, 57.24; H, 5.96; Br, 26.26; S, 10.54. Found: C, 57.19; H, 5.89; Br, 26.31; S, 10.48.

2-(10,11-dibromoundecyl)-7-octyl[1]benzothieno[3,2-b][1]benzothiophene (16) was synthesized according to the procedure described for compound **14** using compound **12** (2.25 g, 3.3 mmol), sodium borohydride (0.63 g, 16.6 mmol) and aluminum chloride (1.1 g, 8.3 mmol) in dry THF (80 mL). The reaction was complete after 8 h of stirring at boiling temperature. After the standard isolation procedure in diethyl

ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **16** (1.94 g, 88 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 2H,), 7.70 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.15 (m, 1H), 3.83 (dd, J_1= 10.3 Hz, J_2 = 4.4 Hz, 1H), 3.61 (t, J = 10.0 Hz, 1H), 2.74 (t, J = 7.5 Hz, 4H), 2.09 (m, 1H), 1.61-1.78 (overlapping peaks, 5H), 1.19-1.42 (overlapping peaks, 22H), 0.87 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.30, 140.00, 139.91, 132.45, 132.44, 131.11, 131.08, 125.75, 123.25, 120.99, 53.10, 36.31, 36.05, 36.03, 35.93, 31.82, 31.66, 31.60, 29.43, 29.36, 29.34, 29.27, 29.26, 29.20, 29.16, 28.70, 26.66, 22.61, 14.06. Anal. calcd. for $C_{33}H_{44}Br_2S_2$: C, 59.63; H, 6.67; Br, 24.04; S, 9.65. Found: C, 59.70; H, 6.72; Br, 23.92; S, 9.57.

2-(10,11-dibromoundecyl)-7-tridecyl[1]benzothieno[3,2-b][1]benzothiophene (17) was synthesized according to the procedure described for compound **14** using compound **13** (2.32 g, 3.1 mmol), sodium borohydride (0.59 g, 15.5 mmol) and aluminum chloride (1.03 g, 7.7 mmol) in dry THF (100 mL). The reaction was completed after 8 h of stirring at boiling temperature. After the standard isolation procedure in diethyl ether the crude product was purified by column chromatography on silica gel (eluent toluene) to give pure compound **17** (1.66 g, 73 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.1 Hz, 2H,), 7.70 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.15 (m, 1H), 3.83 (dd, J_1 = 10.3 Hz, J_2 = 4.4 Hz, 1H), 3.61 (t, J = 10.0 Hz, 1H), 2.75 (t, J = 7.5 Hz, 4H), 2.11 (m, 1H), 1.61-1.86 (overlapping peaks, 6H), 1.20-1.45 (overlapping peaks, 31H), 0.87 (t, J = 6.7 Hz, 3H). Anal. calcd. for $C_{38}H_{54}Br_2S_2$: C, 62.12; H, 7.41; Br, 21.75; S, 8.73. Found: C, 62.08; H, 7.42; Br, 21.71; S, 8.69.

2-ethyl-7-(undec-10-en-1-yl)[1]benzothieno[3,2-b][1]benzothiophene (18). A mixture of compound **14** (0.7 g, 1.2 mmol) and Zn powder (0.16 g, 2.4 mmol) were added to 50 mL mixture of THF-methanol (1:1). The reaction mixture was heated to the boiling point with stirring during 4 h. Then the reaction mixture was cooled to room temperature (23 °C). After the standard isolation procedure in diethyl ether and evaporation of the solvent pure compound **18** (0.77 g, 97 %) was obtained. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H,), 7.70 (s, 2H), 7.29 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 5.81 (m, 1H), 4.94 (m, 2H), 2.78(t, J = 7.5 Hz, 4H), 2.03 (dd, J_1 = 14.2, J_2 = 6.8 Hz, 2H), 1.68 (m, 2H), 1.20-1.46 (overlapping peaks, 15H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.38, 142.31, 141.27, 139.98, 139.18, 132.48, 132.43, 131.11, 131.09, 125.74, 125.29, 123.25, 122.67, 121.07, 120.99, 114.03, 36.04, 33.75, 31.65, 30.87, 29.64, 29.45, 29.43, 29.41, 29.22, 29.06, 28.99, 28.85, 15.77. Anal. calcd. For $C_{27}H_{32}S_2$: C, 77.09; H, 7.67; S, 15.24. Found: C, 77.05; H, 7.63; S, 15.26.

2-butyl-7-(undec-10-en-1-yl)[1]benzothieno[3,2-b][1]benzothiophene (19) was synthesized according to the procedure described for compound **18** using compound **15** (0.65 g, 1.1 mmol) and Zn powder (0.14 g, 2.1 mmol) in 50 mL mixture of THF-methanol (1:1). The reaction was completed after 4 h. After the standard isolation procedure in diethyl ether and evaporation of the solvent pure compound **19** (0.45

g, 94 %) was obtained. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H,), 7.70 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 5.80 (m, 1H), 4.94 (m, 2H), 2.76(t, J = 7.5 Hz, 4H), 2.03 (dd, J_1 = 14.2 Hz, J_2 = 6.8 Hz, 2H,), 1.68 (m, 4H), 1.20-1.48 (overlapping peaks, 16H), 0.95 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.30, 139.96, 139.92, 139.18, 132.44, 131.09, 125.74, 123.25, 120.98, 114.03, 36.04, 35.73, 33.79, 33.74, 31.65, 29.45, 29.43, 29.41, 29.22, 29.06, 28.85, 22.29, 13.91. Anal. calcd. For $C_{29}H_{36}S_2$: C, 77.62; H, 8.09; S, 14.29. Found: C, 77.65; H, 8.11; S, 14.24.

2-octyl-7-(undec-10-en-1-yl)[1]benzothieno[3,2-b][1]benzothiophene (20) was synthesized according to the procedure described for compound **18** using compound **16** (1.85 g, 2.8 mmol) and Zn powder (0.91 g, 13.9 mmol) in 100 mL mixture of THF-methanol (1:1). The reaction was completed after 6 h. After the standard isolation procedure in diethyl ether and evaporation of the solvent pure compound **20** (1.31 g, 93 %) was obtained. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H,), 7.70 (s, 2H), 7.26 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 5.80 (m, 1H), 4.94 (m, 2H), 2.74(t, J = 7.5 Hz, 4H), 2.03 (dd, J_1 = 14.2 Hz, J_2 = 6.8 Hz, 2H,), 1.68 (m, 4H), 1.21-1.43 (overlapping peaks, 22H), 0.87 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.30, 139.98, 139.95, 139.17, 132.44, 131.09, 125.74, 123.24, 120.98, 114.02, 36.04, 33.74, 31.82, 31.65, 30.86, 29.42, 29.25, 29.22, 29.19, 29.05, 28.85, 22.60, 14.05. Anal. calcd. For $C_{33}H_{44}S_2$: C, 78.51; H, 8.78; S, 12.70. Found: C, 78.55; H, 8.82; S, 12.64.

2-tridecyl-7-(undec-10-en-1-yl)[1]benzothieno[3,2-b][1]benzothiophene (21) was synthesized according to the procedure described for compound **18** using compound **17** (1.66 g, 2.3 mmol) and Zn powder (0.74 g, 11.3 mmol) in 100 mL mixture of THF-methanol (1:1). The reaction was completed after 5 h. After the standard isolation procedure in diethyl ether and evaporation of the solvent pure compound **21** (1.26 g, 97 %) was obtained. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H,), 7.70 (s, 2H), 7.26 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 5.77 (m, 1H), 4.94 (m, 2H), 2.76 (t, J = 7.5 Hz, 4H), 2.03 (dd, J_1 = 14.2 Hz, J_2 = 6.8 Hz, 2H,), 1.68 (m, 5H), 1.20-1.42 (overlapping peaks, 41H), 0.87 (t, J = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 142.31, 139.98, 139.95, 139.17, 132.45, 131.09, 125.74, 123.24, 120.98, 114.03, 36.05, 33.74, 31.85, 31.65, 29.60, 29.52, 29.46, 29.44, 29.41, 29.30, 29.24, 29.06, 28.86, 22.63, 14.06. Anal. calcd. For $C_{38}H_{54}S_2$: C, 79.38; H, 9.47; S, 11.15. Found: C, 79.34; H, 9.49; S, 11.09.

1-{11-(7-ethyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (22). 0.4 g (1.0 mmol) compound **18** was dissolved in toluene (40 mL) and 1,1,3,3-tetramethyldisiloxane (3.4 mL, 19 mmol) under argon, after which 40 μl of Karstedt's catalyst was added. The reaction was completed after 16 h of stirring at 50-60 °C. Evaporation of the solvent led to pure compound **22** (0.52 g, 98 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H,), 7.70 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.69 (m, 1H), 2.75 (t, J = 7.5 Hz, 4H), 1.68 (m, 4H), 1.17-1.46

(overlapping peaks, 20H), 0.94 (t, J = 7.0 Hz, 3H), 0.52 (t, J = 7.5 Hz, 2H), 0.15 (d, J = 2.8 Hz, 6H), 0.04 (s, 6H). Anal. calcd. for $C_{31}H_{46}OS_2Si_2$: C, 67.09; H, 8.35; S, 11.56; Si, 10.12. Found: C, 67.13; H, 8.41; S, 11.49; Si, 10.05.

1-{11-(7-butyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (23) was synthesized according to the procedure described for compound **22** using compound **19** (0.28 g, 0.6 mmol), 1,1,3,3-tetramethyldisiloxane (2.2 mL, 12 mmol) and 30 µl of Karstedt's catalyst in toluene (30 mL). The reaction was completed after 10 h of stirring at 50-60 °C. Evaporation of the solvent give pure compound **23** (0.32 g, 98 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H,), 7.71 (s, 2H), 7.28 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.66 (m, 1H), 2.76 (m, 4H), 1.68 (m, 2H), 1.21-1.38 (overlapping peaks, 23H), 0.51 (t, J = 7.5 Hz, 2H), 0.15 (d, J = 2.8, 6H), 0.05 (s, 6H). Anal. calcd. for $C_{33}H_{50}OS_2Si_2$: C, 67.98; H, 8.64; S, 11.00; Si, 9.63. Found: C, 67.93; H, 8.59; S, 11.07; Si, 6.57.

1-{11-(7-octyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (24) was synthesized according to the procedure described for compound **22** using compound **20** (0.31 g, 0.6 mmol), 1,1,3,3-tetramethyldisiloxane (2.2 mL, 12 mmol) and 30 µl of Karstedt's catalyst in toluene (30 mL). The reaction was completed after 9 h of stirring at 50-60 °C. Evaporation of the solvent give compound **24** (0.38 g, 75 %). It was used further without purification. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H,), 7.69 (s, 2H), 7.26 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.67 (m, 1H), 2.74(t, J = 7.3 Hz, 4H), 1.68 (m, 4H), 1.21-1.41 (overlapping peaks, 28H), 0.87 (t, J = 7.0 Hz, 3H), 0.51 (t, J = 7.5 Hz, 2H), 0.16 (d, J = 2.8 Hz, 6H), 0.05 (s, 6H). Anal. calcd. for $C_{34}H_{58}OS_2Si_2$: C, 69.53; H, 9.15; S, 10.03; Si, 8.79. Found: C, 69.47; H, 9.08; S, 10.05; Si, 8.75.

1-{11-(7-tridecyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (25) was synthesized according to the procedure described for compound **22** using compound **21** (0.6 g, 1 mmol), 1,1,3,3-tetramethyldisiloxane (3.7 mL, 20 mmol) and 30 µl of Karstedt's catalyst in toluene (30 mL). The reaction was completed after 5 h of stirring at 50-60 °C. Evaporation of the solvent give compound **25** (0.5 g, 70 %). It was used further without purification. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H,), 7.69 (s, 2H), 7.26 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 4.66 (m, 1H), 2.74 (t, J = 7.3 Hz,4H), 1.68 (m, 4H), 1.15-1.43 (overlapping peaks, 38H), 0.87 (t, J = 7.0 Hz, 3H), 0.51 (t, J = 7.5 Hz, 2H), 0.16 (d, J = 2.8 Hz, 6H), 0.05 (s, 6H). Anal. calcd. for $C_{42}H_{68}OS_2Si_2$: C, 71.12; H, 9.66; S, 9.04; Si, 7.92. Found: C, 71.15; H, 9.68; S, 9.01; Si, 7.89.

1,3-Bis{11-(7-ethyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (D2-Und-BTBT-Et). 0.38 g (0.9 mmol) compound **18** and 0.5 g (0.9 mmol) compound **22** were dissolved in anhydrous toluene (15 mL) under argon, and 25 µl of Karstedt's catalyst was then added. The reaction was completed after the solution was stirred at 55 °C for 15 h. The reaction yield according to GPC

analysis was 85%. The crude product was purified by column chromatography on silica gel (eluent cyclohexane) to give pure **D2-Und-BTBT-Et** (0.39 g, 44 %). ^{1}H NMR (250 MHz, $CDCl_3$) δ 0.03 (s, 12 H), 0.49 (t, 4 H, J = 7.4 Hz), 1.18-1.45 (overlapping peaks, 43H), 1.68 (m, 4H), 2.76 (t, 8H, J = 7.5 Hz), 7.26 (d, 4H, J = 8.1 Hz), 7.70 (s, 4H), 7.76 (d, 4H, J = 8.1 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 0.40, 15.84, 18.41, 23.29, 29.04, 29.34, 29.42, 29.55, 29.62, 29.72, 31.73, 33.45, 36.11, 121.04, 121.13, 122.72, 123.29, 125.34, 125.79, 131.14, 131.18, 132.49, 132.54, 140.04, 141.31, 142.36, 142.44. ^{29}Si (75 MHz, $CDCl_3$) δ 7.33. Anal. calcd. for $C_{58}H_{78}OS_4Si_2$: C, 71.40; H, 8.06; S, 13.15; Si, 5.76. Found: C, 71.38; H, 8.03; S, 13.11; Si, 5.69.

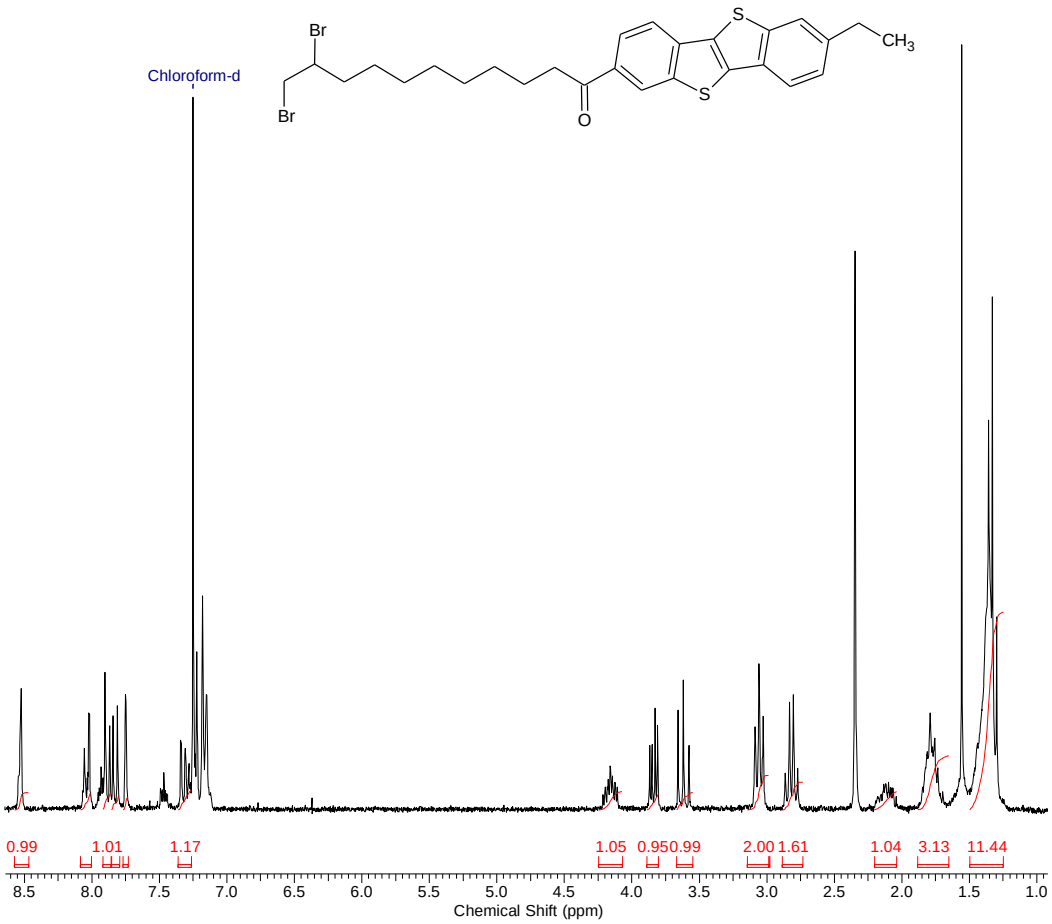
1,3-Bis{11-(7-butyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (D2-Und-BTBT-But) was synthesized according to the procedure described for compound **D2-Und-BTBT-Et** using compounds **23** (0.4 g, 0.7 mmol) and **19** (0.3 g, 0.7 mmol) with 25 µl of Karstedt's catalyst in anhydrous toluene (15 mL). The reaction was complete after 15 h. The reaction yield according to GPC analysis was 70%. The crude product was purified by classical column chromatography on silica gel (eluent cyclohexane) and preparative GPC chromatography to give pure **D2-Und-BTBT-But** (0.086 g, 15%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 0.02 (s, 12H), 0.49 (t, 4H, J = 7.4 Hz), 0.94 (t, 6H, J = 7.3 Hz), 1.15-1.49 (overlapping peaks, 30H), 1.67 (m, 6H), 2.76 (t, 6H, J = 7.5 Hz), 7.26 (d, 4H, J = 8.1 Hz), 7.70 (s, 4H), 7.76 (d, 4H, J = 8.1 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 0.40, 13.98, 18.41, 23.29, 29.41, 29.55, 29.61, 29.72, 31.73, 33.45, 33.84, 35.78, 36.11, 121.03, 123.29, 123.30, 125.79, 131.15, 132.50, 139.97, 140.03, 142.36. ^{29}Si (75 MHz, $CDCl_3$) δ 7.32. Anal. calcd. for $C_{62}H_{86}OS_4Si_2$: C, 72.17; H, 8.40; S, 12.43; Si, 5.44. Found: C, 72.21; H, 8.44; S, 12.39; Si, 5.40.

1,3-Bis{11-(7-octyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (D2-Und-BTBT-Oct) was synthesized according to the procedure described for compound **D2-Und-BTBT-Et** using compounds **20** (0.23 g, 0.4 mmol) and **24** (0.29 g, 0.4 mmol) with 25 µl of Karstedt's catalyst in anhydrous toluene (15 mL). The reaction was completed after 8 h. The reaction yield according to GPC analysis was 85%. The crude product was purified by preparative GPC chromatography to give pure **D2-Und-BTBT-Oct** (0.23 g, 46%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 0.01 (s, 12H), 0.48 (t, 4H, J = 7.4 Hz), 0.87 (t, 6H, J = 7.3 Hz), 1.14-1.40 (overlapping peaks, 55H), 1.68 (m, 8H), 2.73 (t, 8H, J = 7.5 Hz), 7.26 (d, 4H, J = 8.1 Hz), 7.68 (s, 4H), 7.73 (d, 4H, J = 8.1 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 0.39, 14.11, 22.66, 23.28, 29.26, 29.32, 29.41, 29.49, 29.55, 29.61, 29.72, 31.73, 31.88, 33.45, 36.11, 121.02, 123.29, 125.79, 131.15, 132.49, 140.02, 142.36. ^{29}Si (75 MHz, $CDCl_3$) δ 7.32. Anal. calcd. for $C_{70}H_{102}OS_4Si_2$: C, 73.49; H, 8.99; S, 11.21; Si, 4.91. Found: C, 73.40; H, 8.95; S, 11.24; Si, 4.89.

1,3-Bis{11-(7-tridecyl[1]benzothieno[3,2-b][1]benzothien-2-yl)undecyl}-1,1,3,3-tetramethyl-disiloxane (D2-Und-BTBT-TriD) was synthesized according to the

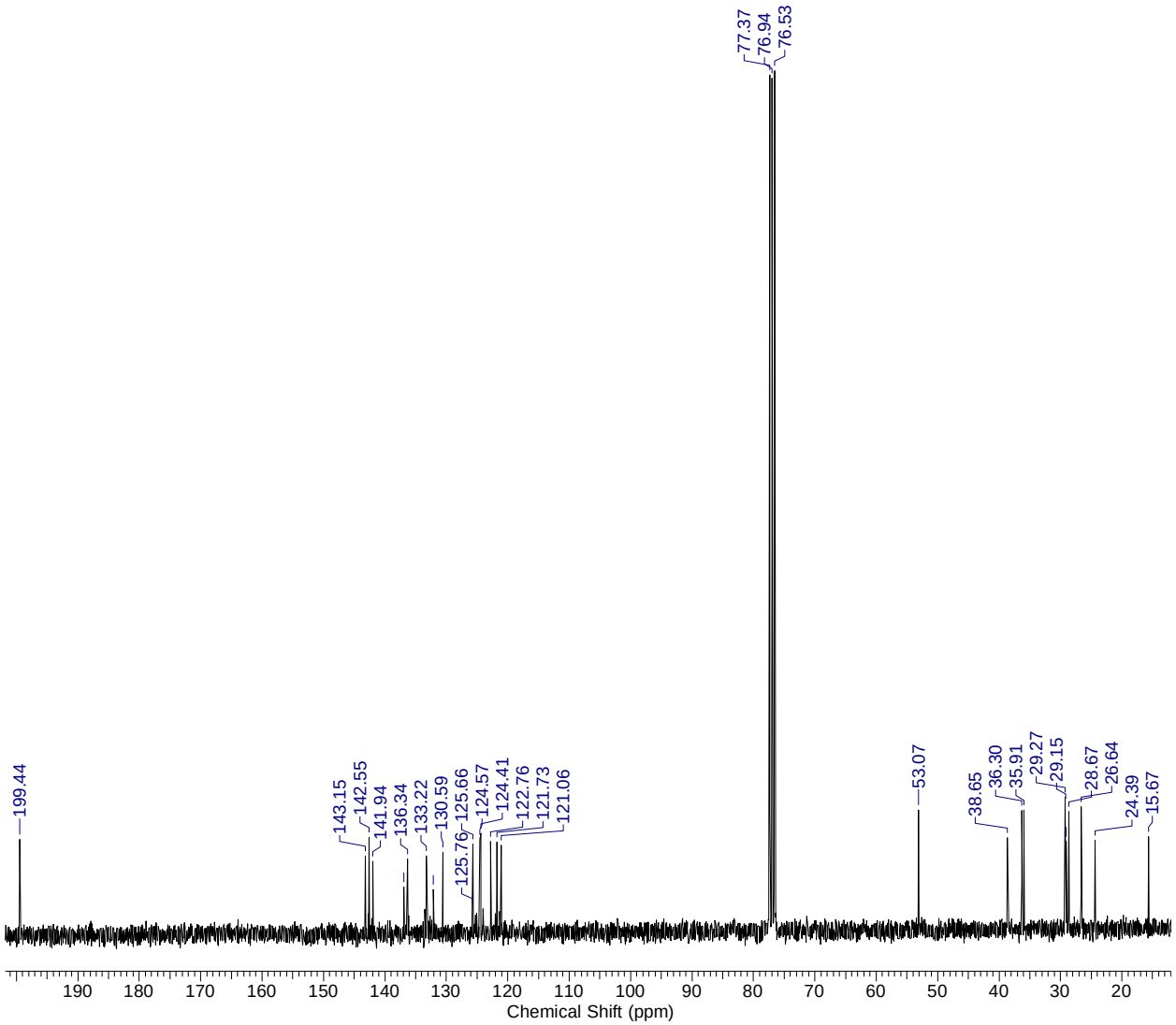
procedure described for compound **D2-Und-BTBT-Et** using compounds **21** (0.4 g, 0.7 mmol) and **25** (0.49 g, 0.7 mmol) with 25 μl of Karstedt's catalyst in anhydrous toluene (15 mL). The reaction was completed after 8 h. The reaction yield according to GPC analysis was 78%. The crude product was purified by column chromatography on silica gel (eluent cyclohexane) followed by recrystallization from hexane. As a result, compound **D2-Und-BTBT-TriD** was obtained with the yield of 0.23 g (26%). ^{1}H NMR (250 MHz, $CDCl_3$) δ 0.01 (s, 12H), 0.48 (t, 4H, J = 7.4 Hz), 0.87 (t, 6H, J = 7.3 Hz), 1.17-1.43 (overlapping peaks, 73H), 1.68 (m, 8H), 2.73 (t, 8H, J = 7.5 Hz), 7.26 (d, 4H, J = 8.1 Hz), 7.68 (s, 4H), 7.74 (d, 4H, J = 8.1 Hz). ^{13}C NMR (75 MHz, CDCl3) δ 0.39, 14.13, 18.40, 22.69, 23.29, 29.31, 29.36, 29.41, 29.52, 29.55, 29.61, 29.67, 29.72, 31.72, 31.92, 33.45, 36.11, 121.02, 123.29, 125.79, 131.15, 132.49, 140.02, 142.35. ^{29}Si (75 MHz, $CDCl_3$) δ 7.32. Anal. calcd. for $C_{80}H_{122}OS_4Si_2$: C, 74.82; H, 9.58; S, 9.99; Si, 4.37. Found: C, 74.83; H, 9.57; S, 9.93; Si, 4.31.

2. ^{1}H, ^{13}C and ^{29}Si NMR spectra of final and intermediate compounds



No.	(ppm)	Value	Absolute Value
1	[1.25 .. 1.50]	11.435	1.20774e+8
2	[1.65 .. 1.88]	3.129	3.30459e+7
3	[2.04 .. 2.20]	1.042	1.10038e+7
4	[2.73 .. 2.89]	1.608	1.69848e+7
5	[2.98 .. 2.98]	0.002	2.42790e+4
6	[2.98 .. 3.14]	2.000	2.11235e+7
7	[3.55 .. 3.67]	0.994	1.05021e+7
8	[3.80 .. 3.89]	0.954	1.00722e+7
9	[4.07 .. 4.24]	1.048	1.10669e+7
10	[7.26 .. 7.36]	1.171	1.23656e+7
11	[7.73 .. 7.77]	0.749	7.90794e+6
12	[7.79 .. 7.86]	0.814	8.59191e+6
13	[7.86 .. 7.92]	1.009	1.06573e+7
14	[8.00 .. 8.08]	0.995	1.05094e+7
15	[8.47 .. 8.57]	0.992	1.04759e+7

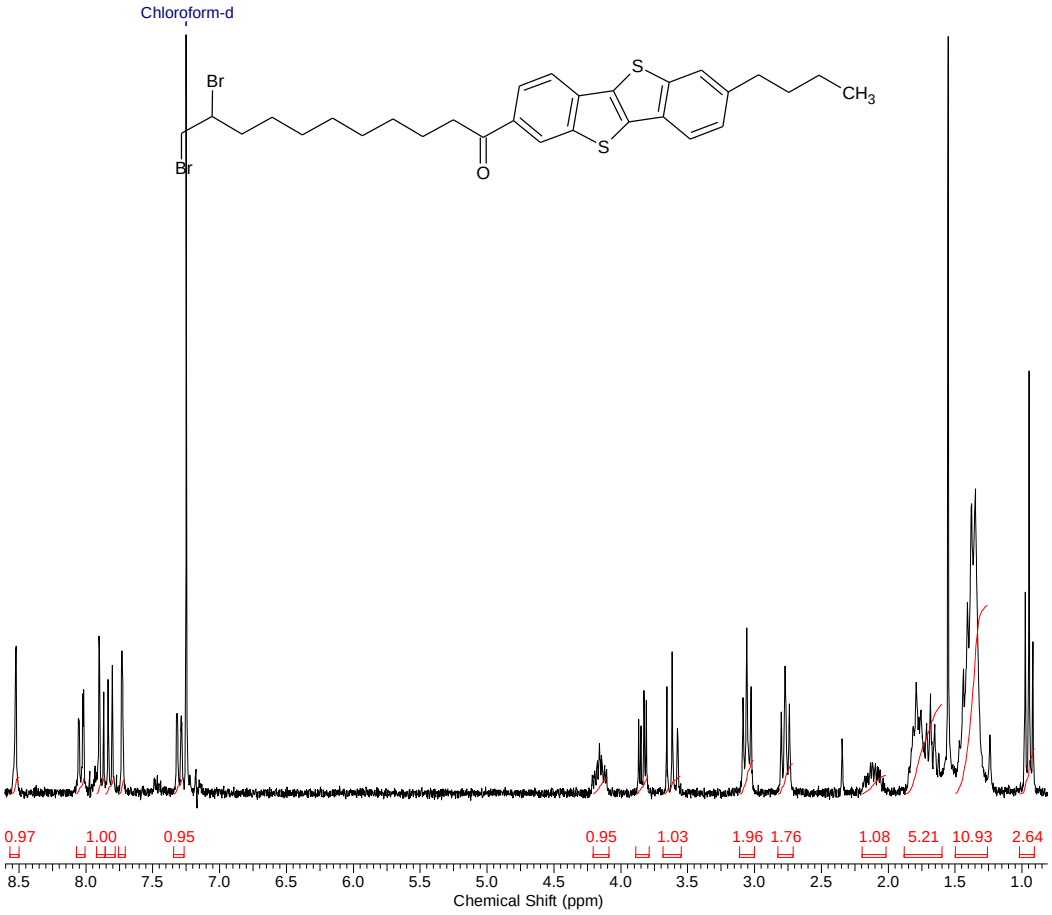
Figure S1. ^{1}H NMR spectrum of compound **10** in $CDCl_3$



No.	(ppm)	(Hz)	Height
1	15.67	1182.9	0.1082
2	24.39	1840.8	0.1036
3	26.64	2011.1	0.1430
4	28.67	2163.7	0.1372
5	29.04	2191.9	0.1028
6	29.15	2200.1	0.1469
7	29.24	2207.3	0.1474
8	29.27	2209.5	0.1539
9	35.91	2710.4	0.1391
10	36.30	2739.7	0.1383
11	38.65	2917.2	0.1067
12	53.07	4005.8	0.1390
13	76.53	5776.1	1.0000
14	76.94	5807.6	0.9911
15	77.37	5839.7	0.9952
16	121.06	9137.6	0.0985

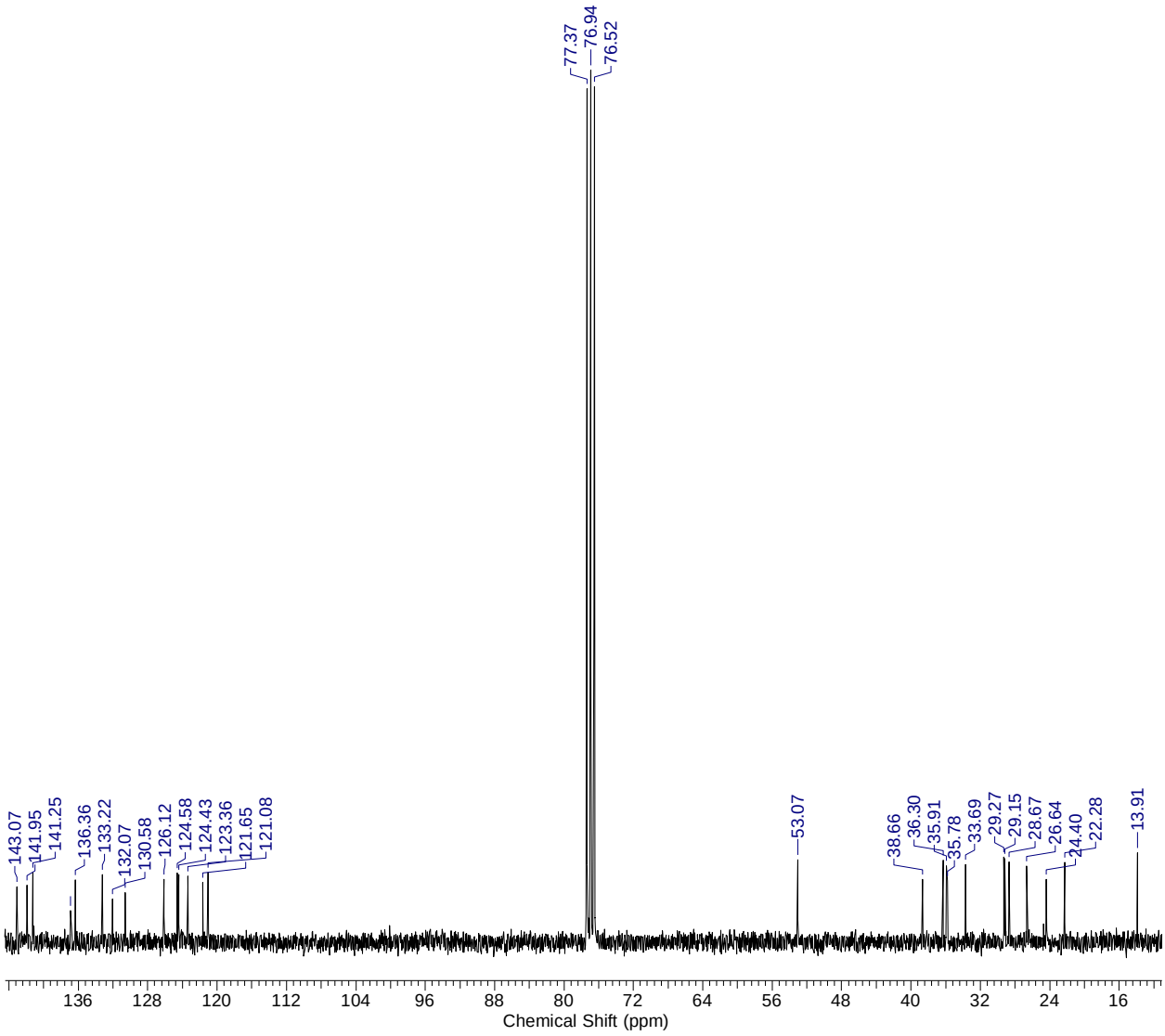
No.	(ppm)	(Hz)	Height
17	121.73	9187.9	0.1020
18	122.76	9265.8	0.1027
19	124.41	9390.2	0.1116
20	124.57	9402.4	0.1050
21	125.66	9484.8	0.0996
22	125.76	9492.0	0.0248
23	130.59	9856.9	0.0898
24	132.09	9969.6	0.0468
25	133.22	10054.8	0.0858
26	136.34	10290.9	0.0821
27	136.87	10330.7	0.0496
28	141.94	10713.3	0.0798
29	142.55	10759.7	0.1075
30	143.15	10804.5	0.0857
31	199.44	15053.3	0.1047

Figure S2. ^{13}C NMR spectrum of compound **10** in $CDCl_3$



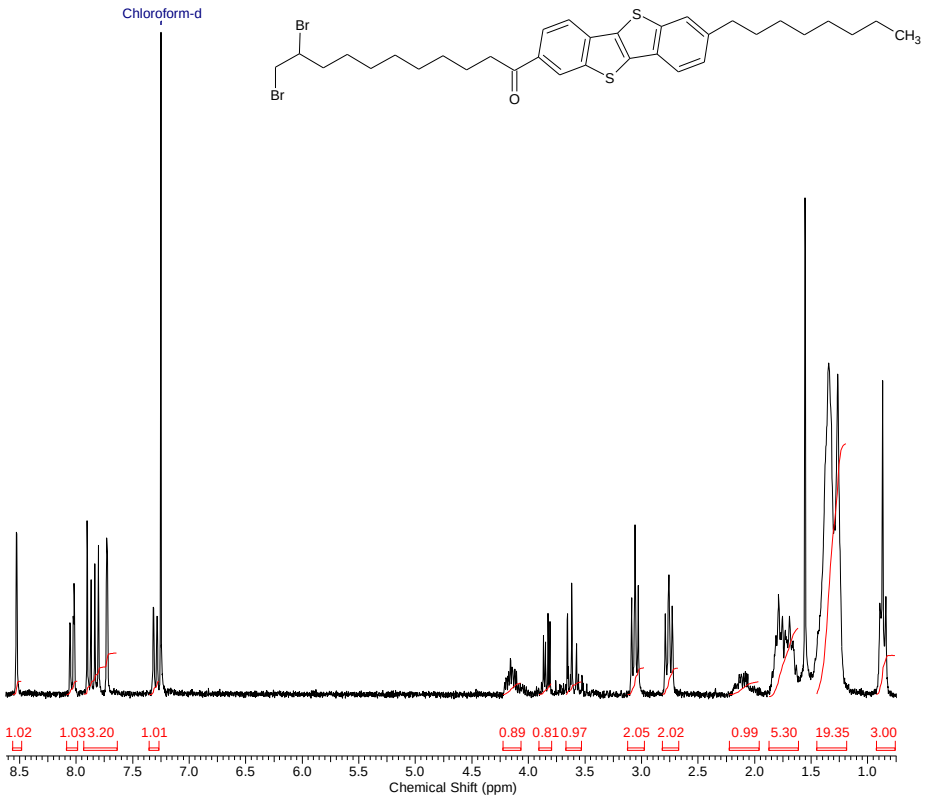
No.	(ppm)	Value	Absolute Value
1	[0.91 .. 1.02]	2.644	2.39677e+7
2	[1.26 .. 1.50]	10.927	9.90697e+7
3	[1.60 .. 1.88]	5.205	4.71941e+7
4	[2.02 .. 2.20]	1.080	9.79581e+6
5	[2.71 .. 2.83]	1.764	1.59968e+7
6	[3.00 .. 3.11]	1.957	1.77422e+7
7	[3.55 .. 3.68]	1.031	9.35079e+6
8	[3.79 .. 3.89]	0.999	9.05466e+6
9	[4.09 .. 4.21]	0.949	8.60649e+6
10	[7.27 .. 7.35]	0.946	8.57585e+6
11	[7.70 .. 7.75]	0.863	7.82327e+6
12	[7.78 .. 7.85]	0.928	8.41162e+6
13	[7.86 .. 7.92]	0.996	9.02628e+6
14	[8.01 .. 8.07]	0.966	8.75831e+6
15	[8.50 .. 8.57]	0.975	8.83934e+6

Figure S3. ^{1}H NMR spectrum of compound **11** in $CDCl_3$



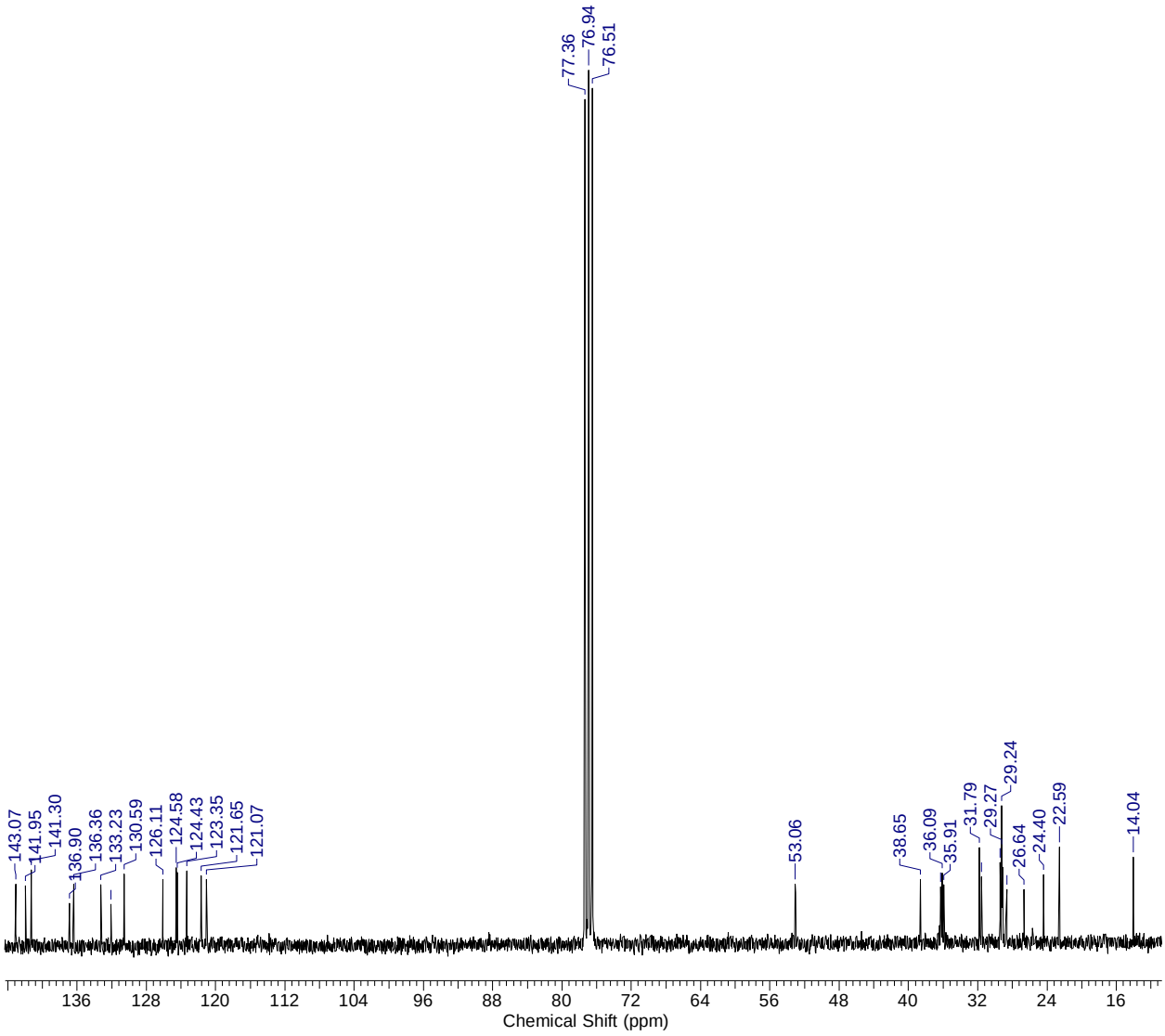
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.91	1049.6	0.1026	17	77.37	5839.7	0.9789
2	22.28	1681.6	0.0914	18	121.08	9138.7	0.0797
3	24.40	1841.3	0.0719	19	121.65	9181.8	0.0686
4	26.64	2011.1	0.0875	20	123.36	9311.2	0.0754
5	28.67	2163.7	0.0919	21	124.43	9391.9	0.0776
6	29.15	2200.1	0.0960	22	124.58	9403.0	0.0794
7	29.24	2207.3	0.0909	23	126.12	9519.1	0.0720
8	29.27	2209.5	0.0975	24	130.58	9855.8	0.0567
9	33.69	2542.9	0.0891	25	132.07	9968.0	0.0498
10	35.78	2700.5	0.0705	26	133.22	10054.8	0.0774
11	35.91	2710.4	0.0878	27	136.36	10292.0	0.0711
12	36.30	2739.7	0.0940	28	136.90	10332.9	0.0359
13	38.66	2917.8	0.0719	29	141.25	10661.3	0.0800
14	53.07	4005.8	0.0943	30	141.95	10713.8	0.0655
15	76.52	5775.6	0.9809	31	143.07	10799.0	0.0634
16	76.94	5807.6	1.0000	32	199.46	15055.0	0.0758

Figure S4. ^{13}C NMR spectrum of compound **11** in $CDCl_3$



No.	(ppm)	Value	Absolute Value
1	[0.76 .. 0.92]	3.001	3.02979e+7
2	[1.19 .. 1.45]	19.349	1.95346e+8
3	[1.61 .. 1.87]	5.299	5.34956e+7
4	[1.96 .. 2.22]	0.986	9.95119e+6
5	[2.67 .. 2.82]	2.019	2.03789e+7
6	[2.97 .. 3.12]	2.046	2.06583e+7
7	[3.53 .. 3.67]	0.967	9.76002e+6
8	[3.79 .. 3.91]	0.812	8.20023e+6
9	[4.07 .. 4.22]	0.885	8.93645e+6
10	[7.27 .. 7.35]	1.011	1.02023e+7
11	[7.64 .. 7.93]	3.205	3.23546e+7
12	[7.99 .. 8.08]	1.026	1.03601e+7
13	[8.48 .. 8.56]	1.018	1.02792e+7

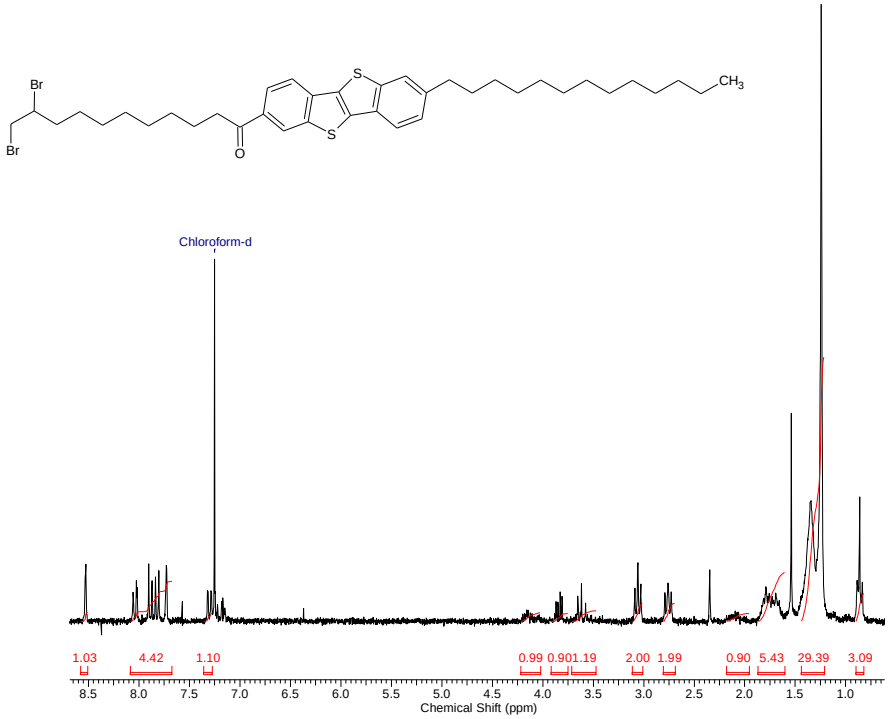
Figure S5. ^{1}H NMR spectrum of compound **12** in $CDCl_3$



No.	(ppm)	(Hz)	Height
1	14.04	1059.6	0.0976
2	22.59	1704.8	0.1094
3	24.40	1841.3	0.0779
4	26.64	2010.5	0.0607
5	28.66	2163.1	0.0606
6	29.14	2199.6	0.0863
7	29.18	2202.4	0.1124
8	29.24	2206.8	0.1567
9	29.27	2209.0	0.1069
10	29.40	2218.9	0.0917
11	31.56	2382.0	0.0755
12	31.79	2399.7	0.1090
13	35.91	2710.4	0.0661
14	36.09	2724.3	0.0794
15	36.28	2738.6	0.0636
16	38.65	2917.2	0.0720
17	53.06	4004.7	0.0668
18	76.51	5775.0	0.9792

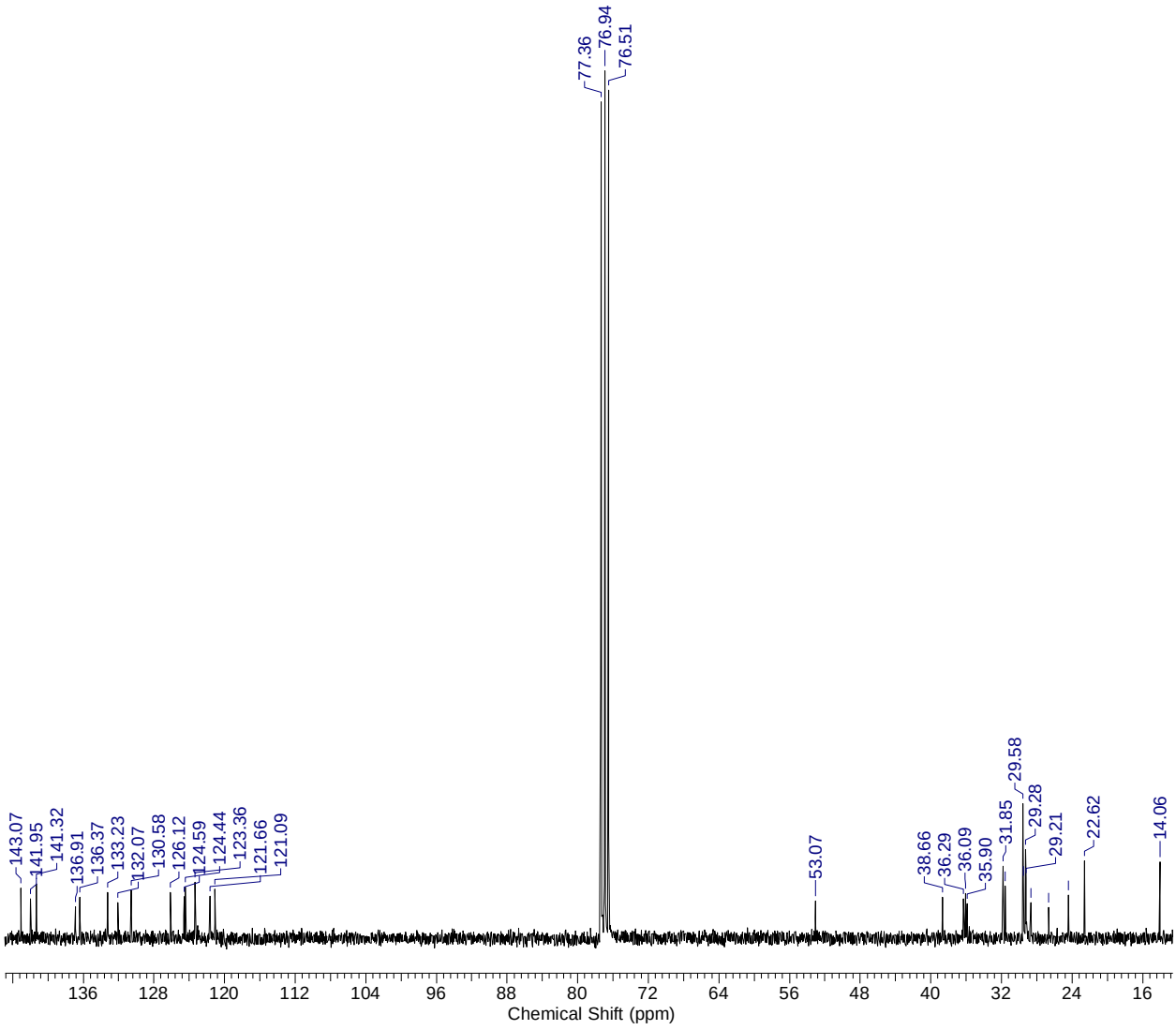
No.	(ppm)	(Hz)	Height
19	76.94	5807.1	1.0000
20	77.36	5839.1	0.9667
21	121.07	9138.1	0.0724
22	121.65	9181.8	0.0765
23	123.35	9310.1	0.0819
24	124.43	9391.3	0.0802
25	124.58	9403.0	0.0855
26	126.11	9518.5	0.0722
27	130.59	9856.3	0.0786
28	132.07	9968.0	0.0440
29	133.23	10055.9	0.0660
30	136.36	10292.5	0.0666
31	136.90	10332.9	0.0447
32	141.30	10665.2	0.0831
33	141.95	10714.4	0.0649
34	143.07	10799.0	0.0669
35	199.45	15053.9	0.0512

Figure S6. ^{13}C NMR spectrum of compound **12** in $CDCl_3$



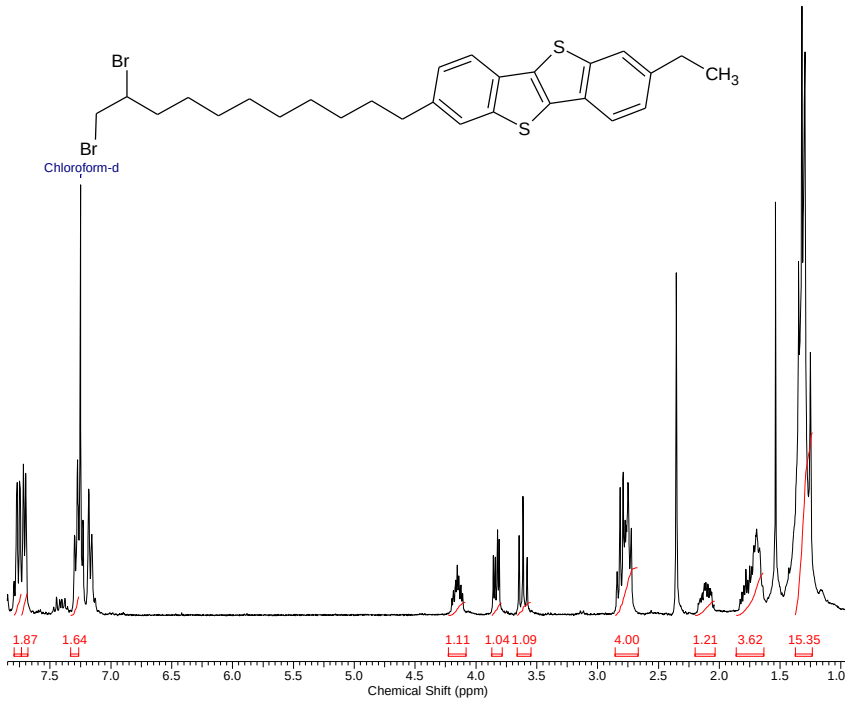
No.	(ppm)	Value	Absolute Value
1	[0.82 .. 0.90]	3.093	9.31838e+6
2	[1.21 .. 1.44]	29.386	8.85287e+7
3	[1.60 .. 1.87]	5.429	1.63561e+7
4	[1.95 .. 2.18]	0.898	2.70569e+6
5	[2.69 .. 2.80]	1.988	5.98789e+6
6	[3.01 .. 3.11]	2.000	6.02528e+6
7	[3.47 .. 3.71]	1.190	3.58498e+6
8	[3.75 .. 3.92]	0.900	2.71253e+6
9	[4.02 .. 4.22]	0.992	2.98995e+6
10	[7.27 .. 7.36]	1.097	3.30350e+6
11	[7.67 .. 8.08]	4.418	1.33099e+7
12	[8.51 .. 8.58]	1.029	3.10092e+6

Figure S7. ^{1}H NMR spectrum of compound **13** in $CDCl_3$



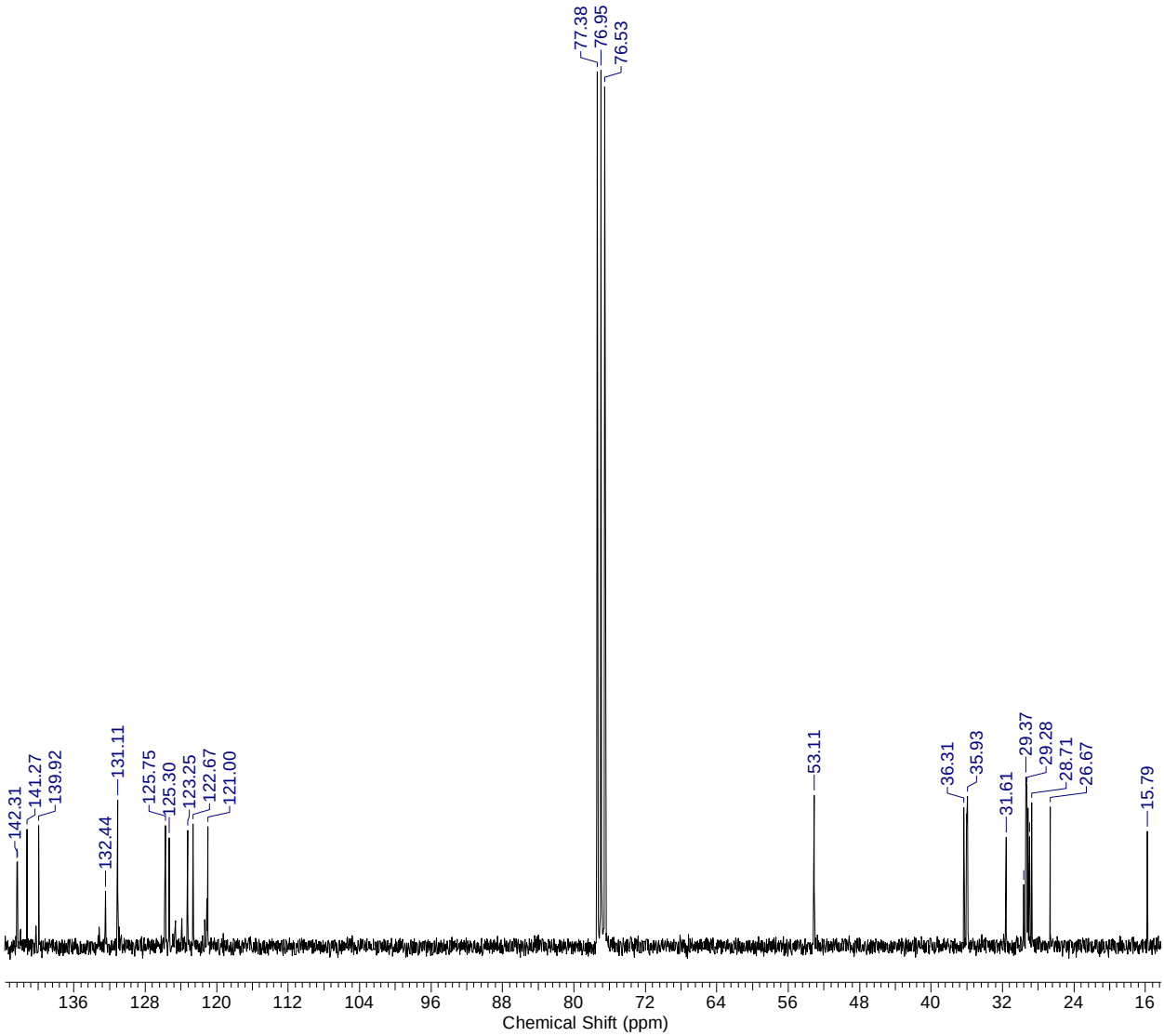
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.06	1061.2	0.0880	19	76.51	5775.0	0.9776
2	22.62	1707.0	0.0890	20	76.94	5807.1	1.0000
3	24.40	1841.3	0.0499	21	77.36	5839.1	0.9642
4	26.64	2010.5	0.0355	22	121.09	9139.2	0.0563
5	28.66	2163.1	0.0412	23	121.66	9182.4	0.0484
6	29.14	2199.6	0.0545	24	123.36	9311.2	0.0645
7	29.21	2204.6	0.0695	25	124.44	9392.5	0.0592
8	29.28	2210.1	0.1019	26	124.59	9403.5	0.0475
9	29.43	2221.2	0.0607	27	126.12	9519.1	0.0527
10	29.50	2226.7	0.0666	28	130.58	9855.8	0.0555
11	29.58	2232.8	0.1551	29	132.07	9968.0	0.0410
12	31.56	2382.0	0.0599	30	133.23	10055.9	0.0528
13	31.85	2403.6	0.0829	31	136.37	10293.1	0.0472
14	35.90	2709.9	0.0396	32	136.91	10333.4	0.0363
15	36.09	2724.3	0.0518	33	141.32	10666.3	0.0627
16	36.29	2739.2	0.0456	34	141.95	10714.4	0.0455
17	38.66	2917.8	0.0475	35	143.07	10799.0	0.0578
18	53.07	4005.3	0.0431	36	199.48	15056.1	0.0519

Figure S8. ^{13}C NMR spectrum of compound **13** in $CDCl_3$



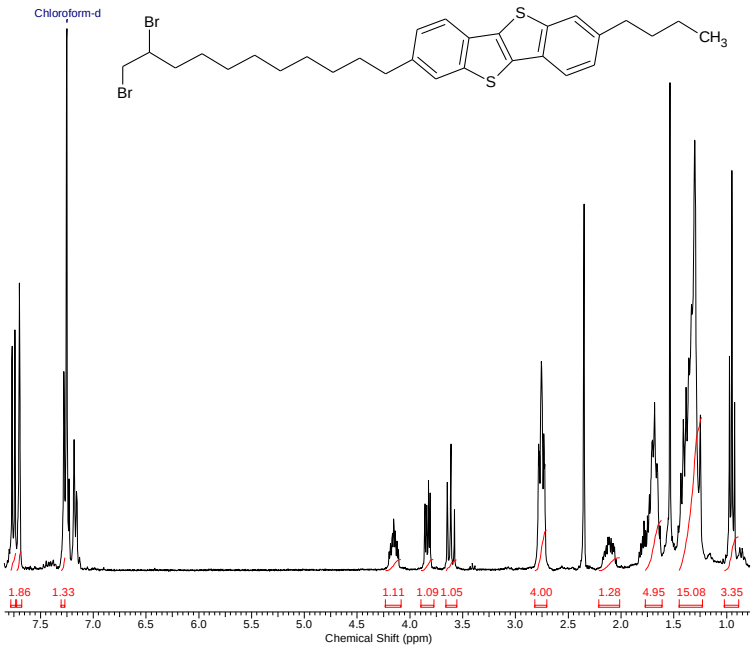
No.	(ppm)	Value	Absolute Value
1	[1.23 .. 1.38]	15.349	1.68723e+10
2	[1.63 .. 1.86]	3.617	3.97574e+9
3	[2.03 .. 2.20]	1.210	1.33034e+9
4	[2.66 .. 2.85]	4.000	4.39701e+9
5	[3.55 .. 3.66]	1.088	1.19569e+9
6	[3.79 .. 3.87]	1.045	1.14818e+9
7	[4.08 .. 4.23]	1.111	1.22172e+9
8	[7.26 .. 7.33]	1.644	1.80689e+9
9	[7.68 .. 7.74]	1.868	2.05380e+9
10	[7.74 .. 7.80]	1.806	1.98520e+9

Figure S9. ^{1}H NMR spectrum of compound **14** in $CDCl_3$



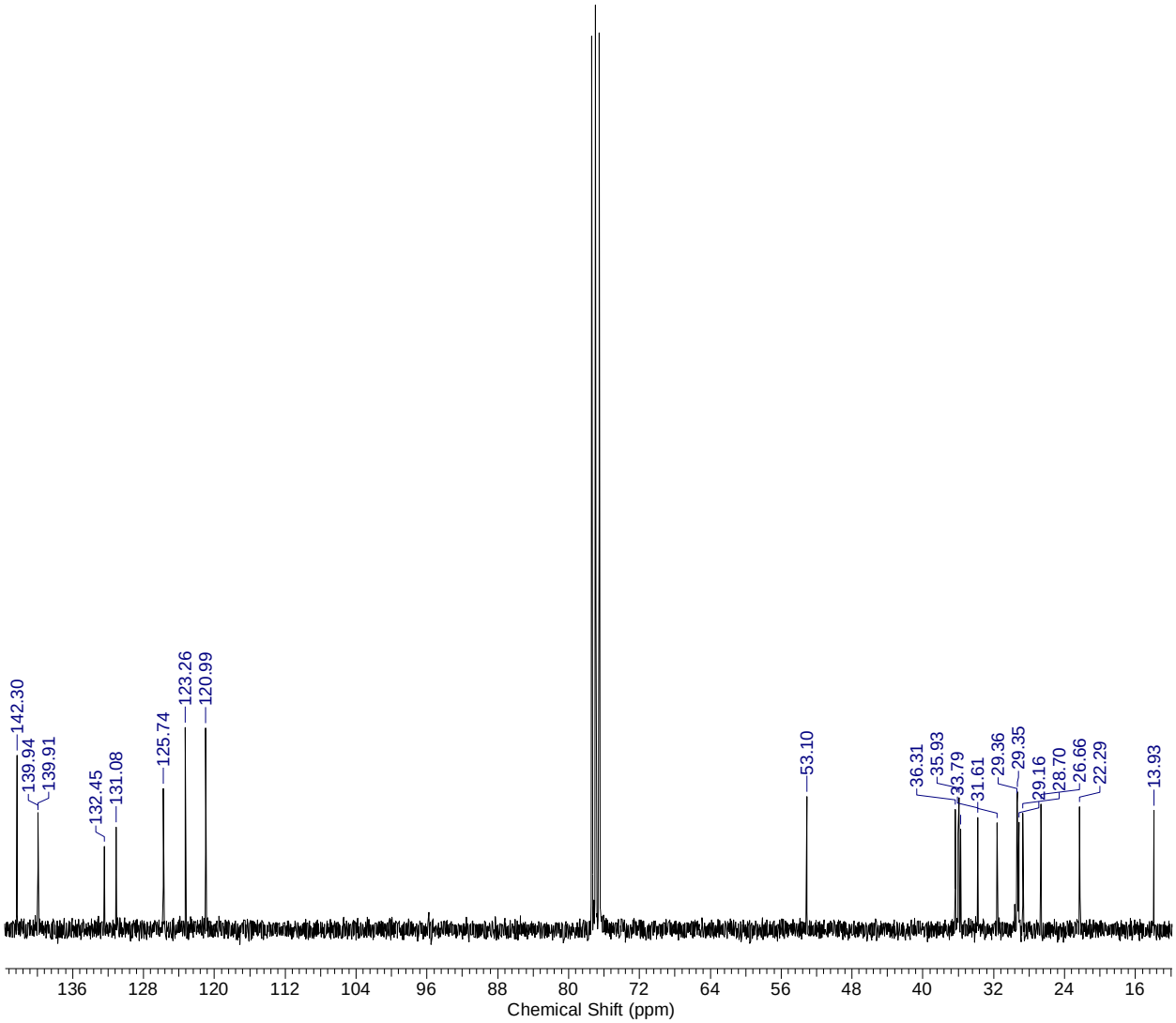
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	15.79	1191.7	0.1309	16	76.95	5808.2	1.0000
2	26.67	2012.7	0.1589	17	77.38	5840.3	0.9979
3	28.71	2167.0	0.1640	18	121.00	9133.2	0.1367
4	29.00	2188.5	0.1248	19	121.08	9138.7	0.1292
5	29.16	2201.3	0.1576	20	122.67	9259.2	0.1398
6	29.28	2210.1	0.1817	21	123.25	9302.9	0.1321
7	29.35	2215.1	0.1906	22	125.30	9457.7	0.1236
8	29.37	2216.7	0.1929	23	125.75	9491.4	0.1379
9	29.65	2237.7	0.0703	24	131.11	9895.6	0.1667
10	31.61	2385.9	0.1244	25	132.44	9996.2	0.0623
11	35.93	2711.6	0.1711	26	132.48	9999.0	0.0591
12	36.03	2719.3	0.1355	27	139.92	10561.2	0.1378
13	36.31	2740.9	0.1585	28	141.27	10662.9	0.1337
14	53.11	4008.6	0.1724	29	142.31	10740.9	0.0966
15	76.53	5776.7	0.9812	30	142.38	10746.4	0.0950

Figure S10. ^{13}C NMR spectrum of compound **14** in $CDCl_3$



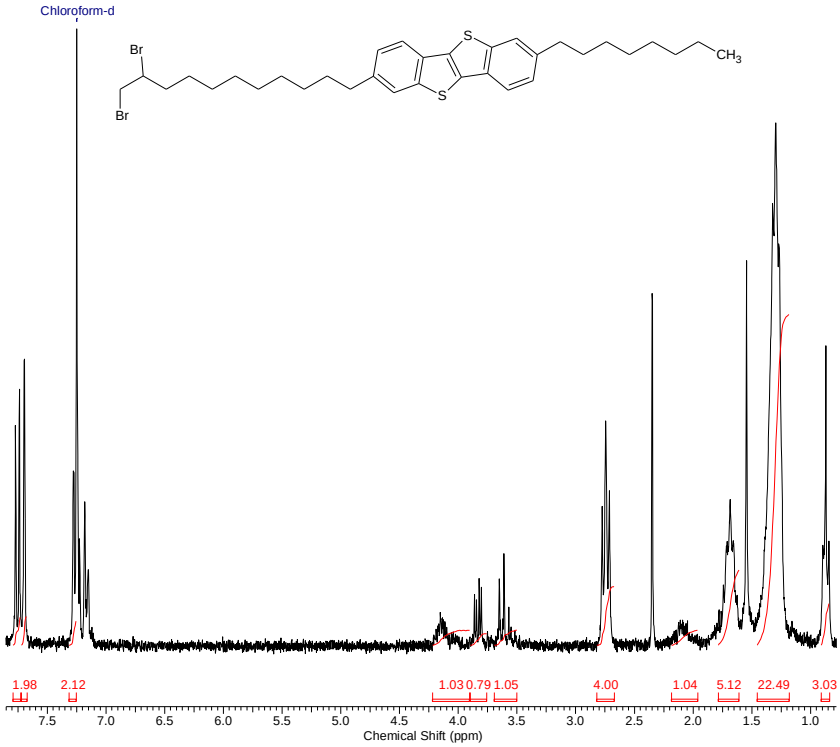
No.	(ppm)	Value	Absolute Value
1	[0.89 .. 1.02]	3.349	3.32280e+9
2	[1.23 .. 1.45]	15.081	1.49652e+10
3	[1.61 .. 1.77]	4.947	4.90900e+9
4	[2.01 .. 2.21]	1.280	1.26992e+9
5	[2.70 .. 2.82]	4.000	3.96929e+9
6	[3.55 .. 3.66]	1.053	1.04506e+9
7	[3.77 .. 3.90]	1.093	1.08456e+9
8	[4.08 .. 4.23]	1.106	1.09729e+9
9	[7.27 .. 7.30]	1.330	1.31992e+9
10	[7.68 .. 7.72]	1.856	1.84143e+9
11	[7.74 .. 7.78]	1.728	1.71492e+9

Figure S11. ^{1}H NMR spectrum of compound **15** in $CDCl_3$



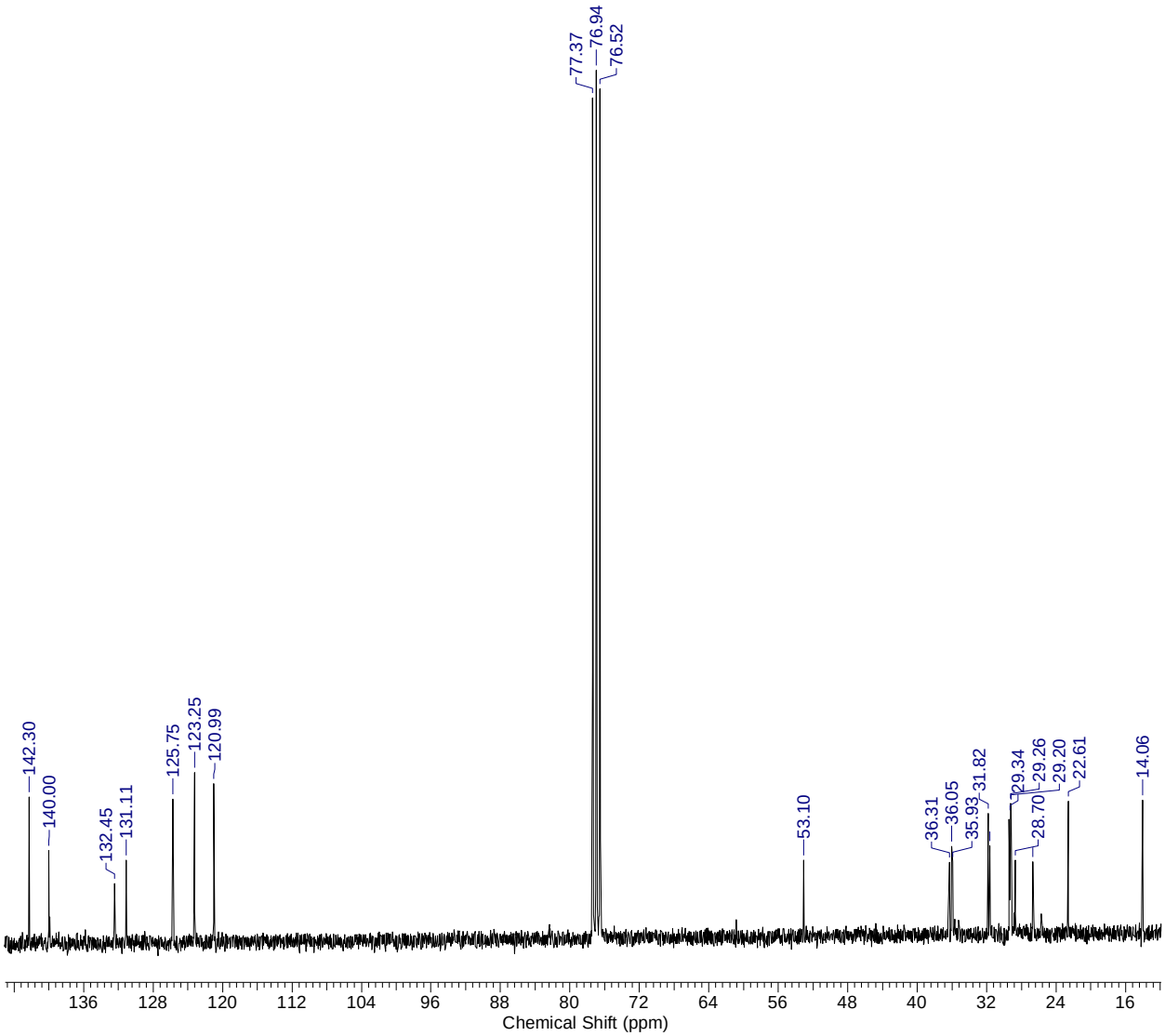
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.93	1051.3	0.1286	13	36.03	2719.3	0.1035
2	22.29	1682.7	0.1326	14	36.31	2740.9	0.1297
3	26.66	2012.2	0.1357	15	53.10	4008.0	0.1437
4	28.70	2166.4	0.1258	16	120.99	9132.0	0.2178
5	29.16	2201.3	0.1159	17	123.26	9303.4	0.2184
6	29.27	2209.5	0.1269	18	125.74	9490.9	0.1526
7	29.35	2215.1	0.1489	19	131.08	9893.9	0.1110
8	29.36	2216.2	0.1421	20	131.10	9895.0	0.1087
9	31.61	2385.9	0.1153	21	132.45	9996.7	0.0897
10	33.79	2550.7	0.1210	22	139.91	10560.1	0.1264
11	35.73	2696.6	0.1083	23	139.94	10562.3	0.1241
12	35.93	2711.6	0.1427	24	142.30	10740.4	0.1885

Figure S12. ^{13}C NMR spectrum of compound **15** in $CDCl_3$



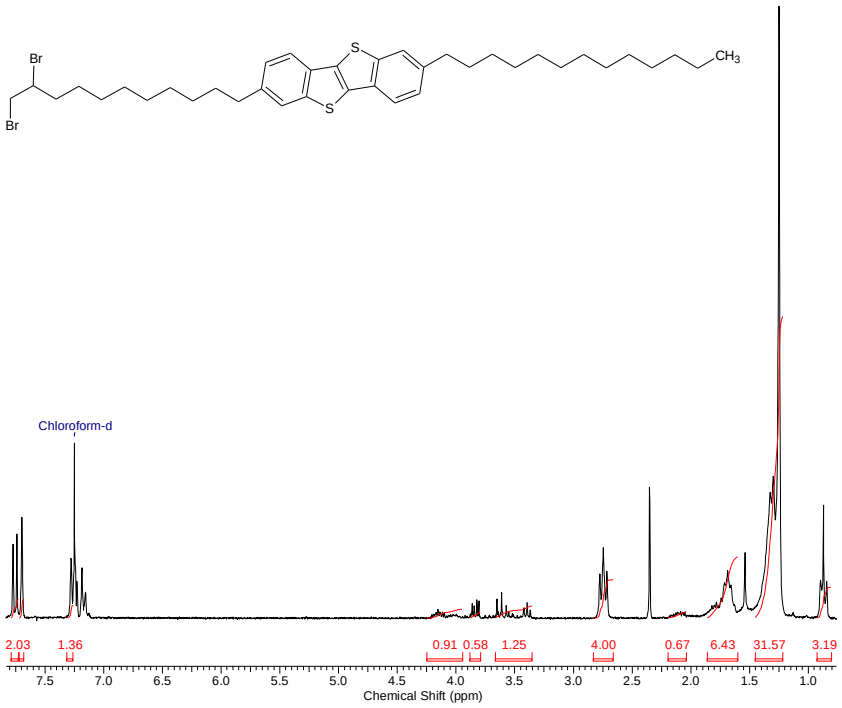
No.	(ppm)	Value	Absolute Value
1	[0.84 .. 0.91]	3.029	2.52522e+7
2	[1.18 .. 1.45]	22.487	1.87492e+8
3	[1.61 .. 1.78]	5.116	4.26600e+7
4	[1.96 .. 2.18]	1.043	8.69607e+6
5	[2.67 .. 2.82]	4.000	3.33514e+7
6	[3.50 .. 3.69]	1.048	8.73979e+6
7	[3.76 .. 3.90]	0.790	6.59085e+6
8	[3.90 .. 4.22]	1.034	8.62545e+6
9	[7.25 .. 7.31]	2.116	1.76418e+7
10	[7.67 .. 7.72]	1.981	1.65162e+7
11	[7.73 .. 7.79]	1.974	1.64557e+7

Figure S13. ^{1}H NMR spectrum of compound **16** in $CDCl_3$



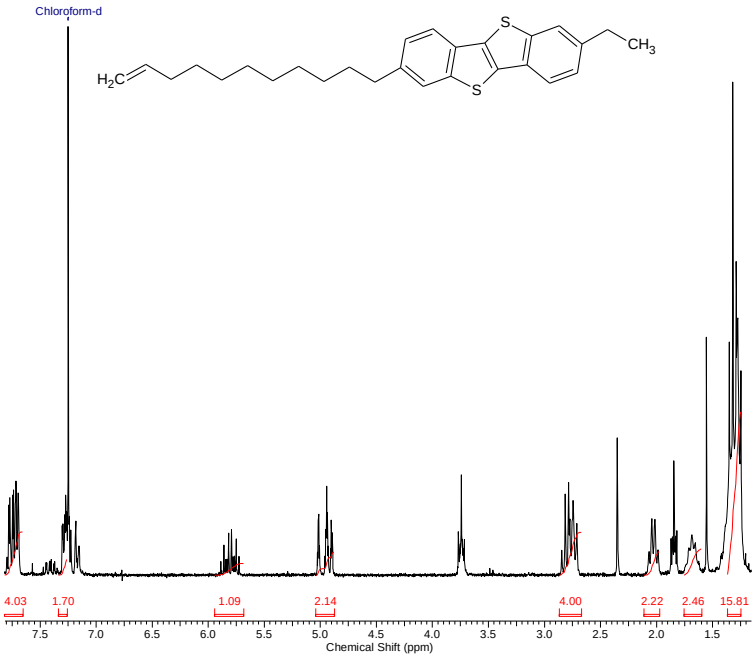
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.06	1061.2	0.1561	17	36.05	2721.0	0.1029
2	22.61	1706.4	0.1550	18	36.31	2740.3	0.0841
3	26.66	2012.2	0.0849	19	53.10	4008.0	0.0870
4	28.70	2166.4	0.0870	20	76.52	5775.6	0.9783
5	29.16	2201.3	0.1123	21	76.94	5807.6	1.0000
6	29.20	2204.0	0.1514	22	77.37	5839.7	0.9682
7	29.26	2208.4	0.1523	23	120.99	9132.0	0.1749
8	29.27	2209.5	0.1340	24	123.25	9302.3	0.1878
9	29.34	2214.5	0.1387	25	125.75	9491.4	0.1571
10	29.36	2216.2	0.1326	26	131.08	9893.4	0.0850
11	29.43	2221.2	0.1340	27	131.11	9895.6	0.0865
12	31.60	2385.4	0.0915	28	132.44	9996.2	0.0595
13	31.66	2389.8	0.1031	29	132.45	9997.3	0.0600
14	31.82	2401.4	0.1410	30	139.91	10560.1	0.0856
15	35.93	2711.6	0.0850	31	140.00	10566.7	0.0976
16	36.03	2719.3	0.0994	32	142.30	10740.4	0.1598

Figure S14. ^{13}C NMR spectrum of compound **16** in $CDCl_3$



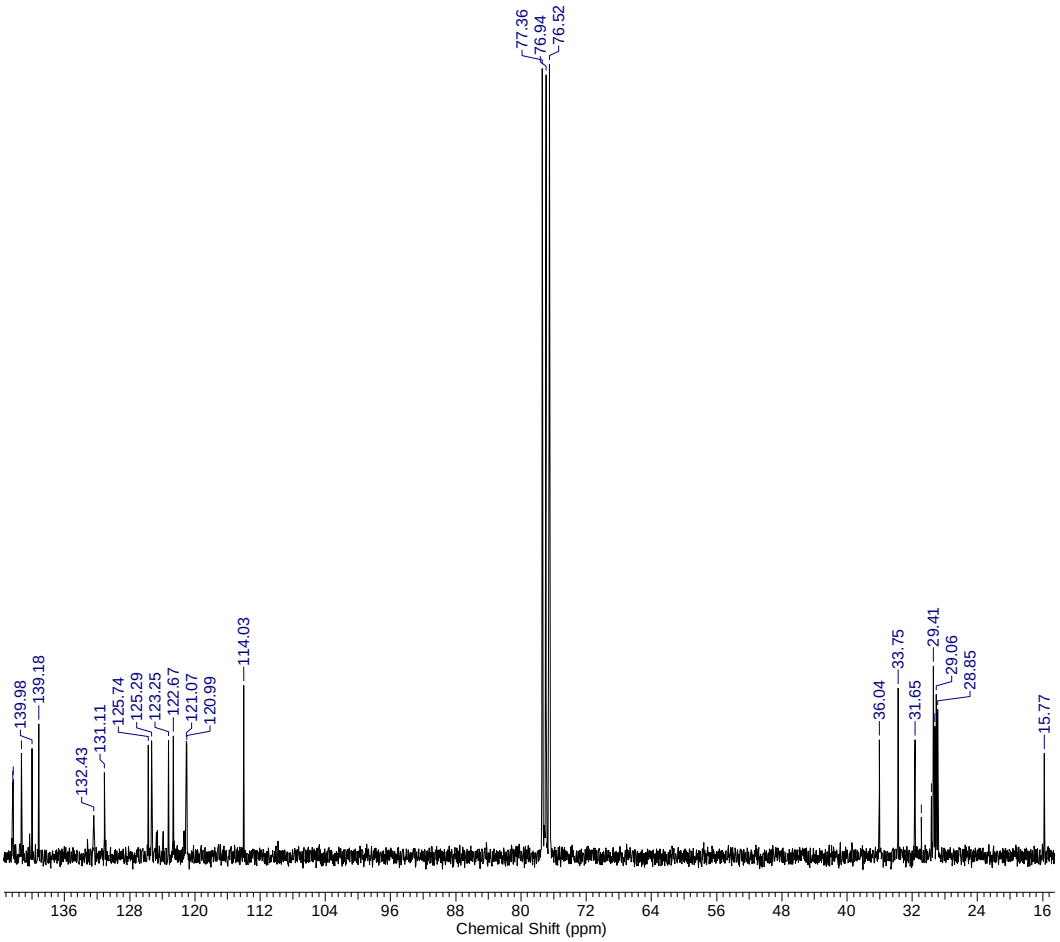
No.	(ppm)	Value	Absolute Value
1	[0.80 .. 0.92]	3.195	1.16002e+7
2	[1.22 .. 1.45]	31.572	1.14644e+8
3	[1.60 .. 1.86]	6.432	2.33545e+7
4	[2.04 .. 2.19]	0.672	2.43962e+6
5	[2.66 .. 2.83]	4.000	1.45250e+7
6	[3.35 .. 3.66]	1.255	4.55568e+6
7	[3.79 .. 3.88]	0.580	2.10770e+6
8	[3.94 .. 4.25]	0.906	3.28984e+6
9	[7.26 .. 7.31]	1.362	4.94667e+6
10	[7.68 .. 7.72]	1.964	7.13159e+6
11	[7.72 .. 7.79]	2.027	7.36034e+6

Figure S15. ^{1}H NMR spectrum of compound **17** in $CDCl_3$



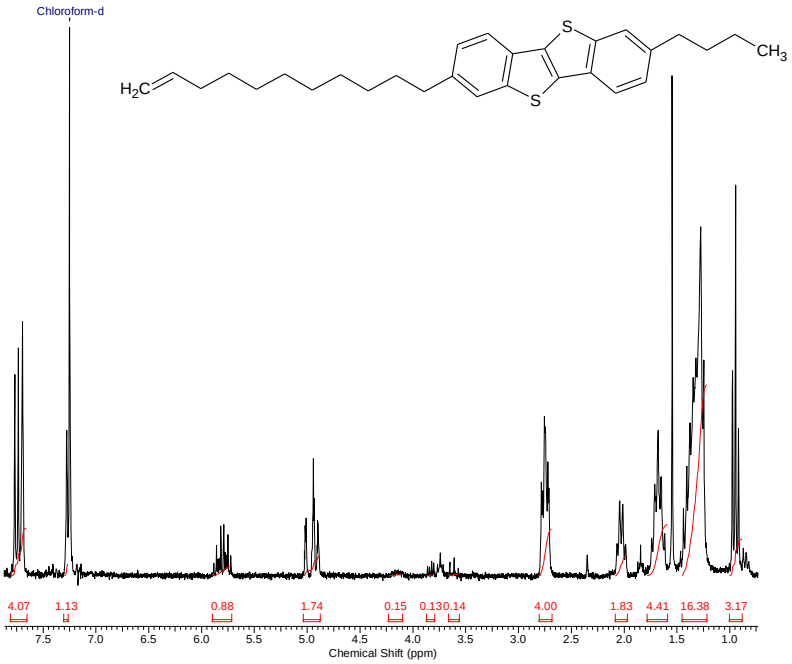
No.	(ppm)	Value	Absolute Value
1	[1.25 .. 1.37]	15.810	1.07853e+8
2	[1.60 .. 1.75]	2.460	1.67810e+7
3	[1.97 .. 2.11]	2.218	1.51298e+7
4	[2.67 .. 2.87]	4.000	2.72868e+7
5	[4.87 .. 5.04]	2.140	1.45984e+7
6	[5.68 .. 5.94]	1.092	7.44588e+6
7	[7.26 .. 7.34]	1.696	1.15704e+7
8	[7.65 .. 7.82]	4.031	2.74976e+7

Figure S16. ^{1}H NMR spectrum of compound **18** in $CDCl_3$



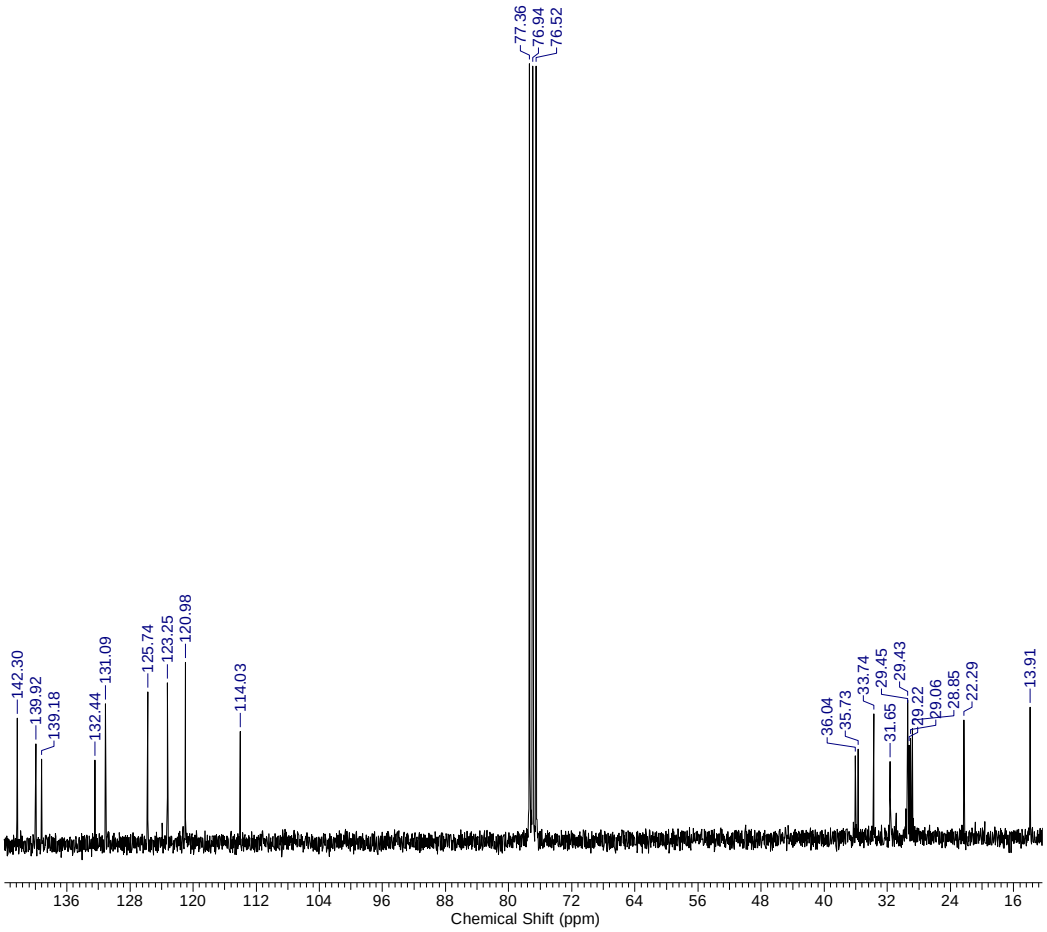
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	15.77	1190.6	0.1298	17	114.03	8606.8	0.2156
2	28.85	2177.5	0.1852	18	120.99	9132.0	0.1416
3	28.99	2188.0	0.1295	19	121.07	9138.1	0.1453
4	29.06	2193.5	0.2041	20	122.67	9258.7	0.1517
5	29.22	2205.7	0.1642	21	123.25	9302.3	0.1461
6	29.41	2220.0	0.2401	22	125.29	9456.6	0.1454
7	29.43	2221.2	0.2388	23	125.74	9490.9	0.1402
8	29.45	2222.8	0.2220	24	131.09	9894.5	0.1046
9	29.64	2237.2	0.0758	25	131.11	9896.1	0.1056
10	30.87	2330.1	0.0488	26	132.43	9995.6	0.0512
11	31.65	2388.7	0.1469	27	132.48	9999.5	0.0484
12	33.75	2547.3	0.2118	28	139.18	10504.8	0.1667
13	36.04	2720.4	0.1468	29	139.98	10565.1	0.1358
14	76.52	5775.6	1.0000	30	141.27	10662.4	0.1301
15	76.94	5807.6	0.9865	31	142.31	10740.9	0.0967
16	77.36	5839.1	0.9943	32	142.38	10746.4	0.0913

Figure S17. ^{13}C NMR spectrum of compound **18** in $CDCl_3$



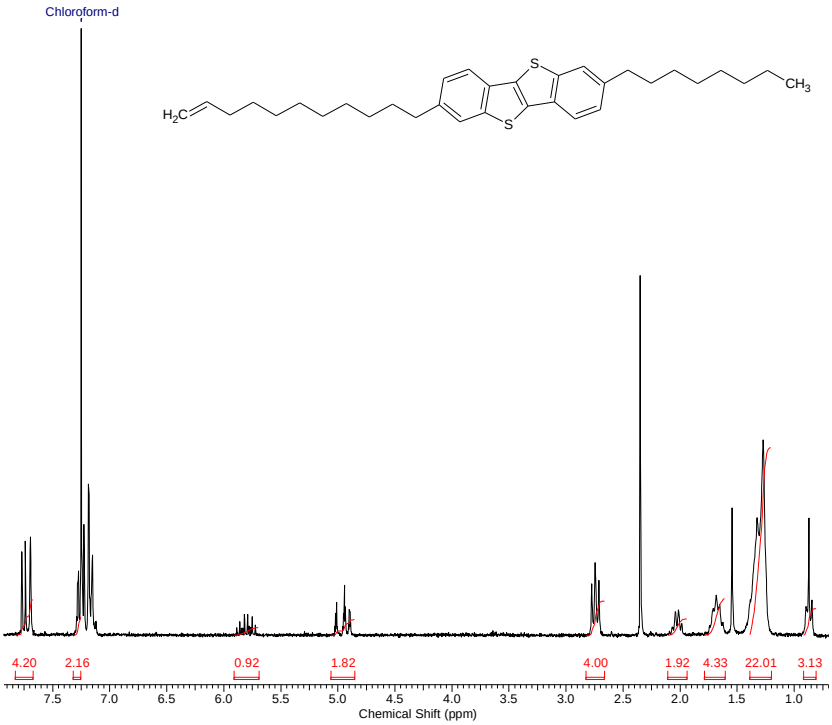
No.	(ppm)	Value	Absolute Value
1	[0.88 .. 1.00]	3.174	2.10720e+7
2	[1.22 .. 1.45]	16.375	1.08730e+8
3	[1.59 .. 1.78]	4.406	2.92541e+7
4	[1.97 .. 2.09]	1.832	1.21673e+7
5	[2.68 .. 2.81]	4.000	2.65593e+7
6	[3.56 .. 3.66]	0.140	9.26642e+5
7	[3.79 .. 3.87]	0.129	8.58645e+5
8	[4.10 .. 4.23]	0.147	9.74060e+5
9	[4.88 .. 5.04]	1.744	1.15781e+7
10	[5.72 .. 5.90]	0.880	5.84417e+6
11	[7.26 .. 7.30]	1.128	7.49202e+6
12	[7.65 .. 7.81]	4.067	2.70046e+7

Figure S18. ^{1}H NMR spectrum of compound **19** in $CDCl_3$



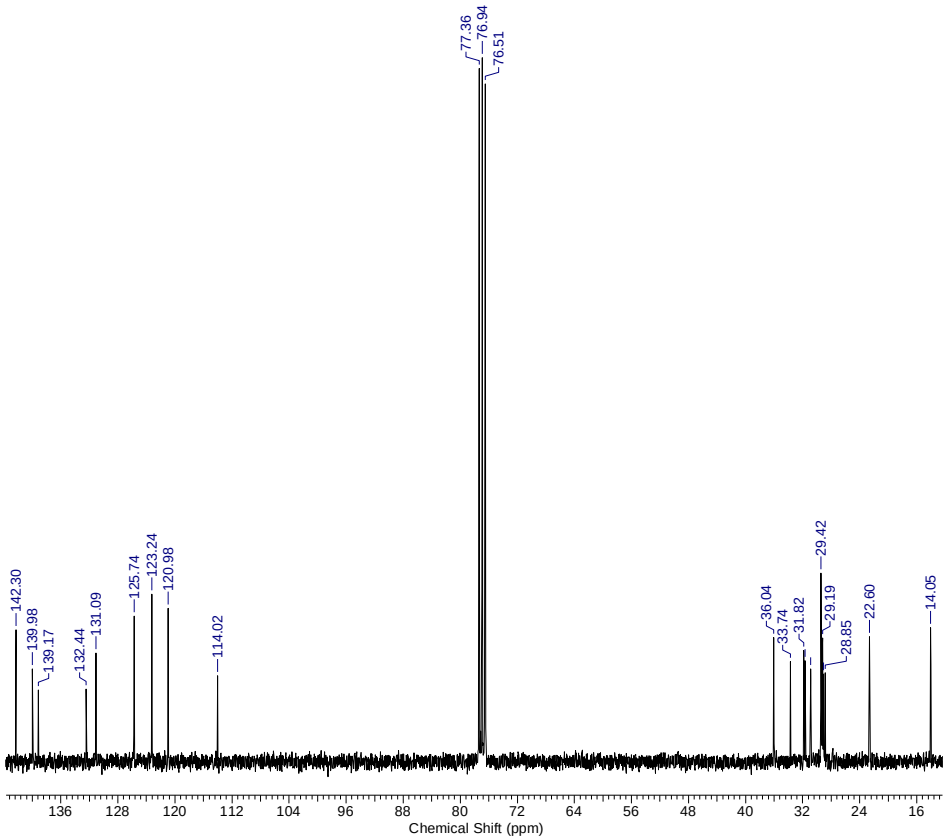
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.91	1050.2	0.1682	14	76.52	5775.6	0.9971
2	22.29	1682.1	0.1520	15	76.94	5807.1	0.9966
3	28.85	2177.5	0.1410	16	77.36	5839.1	1.0000
4	29.06	2193.5	0.1286	17	114.03	8606.8	0.1368
5	29.22	2205.7	0.1194	18	120.98	9131.5	0.2262
6	29.41	2220.0	0.1659	19	123.25	9302.9	0.2002
7	29.43	2221.2	0.1776	20	125.74	9490.9	0.1882
8	29.45	2222.8	0.1686	21	131.09	9894.5	0.1730
9	31.65	2388.7	0.0985	22	132.44	9996.2	0.1000
10	33.74	2546.8	0.1601	23	139.18	10504.8	0.1015
11	33.79	2550.1	0.1404	24	139.92	10561.2	0.1207
12	35.73	2696.6	0.1144	25	139.96	10564.0	0.1039
13	36.04	2720.4	0.1056	26	142.30	10740.4	0.1542

Figure S19. ^{13}C NMR spectrum of compound **19** in $CDCl_3$



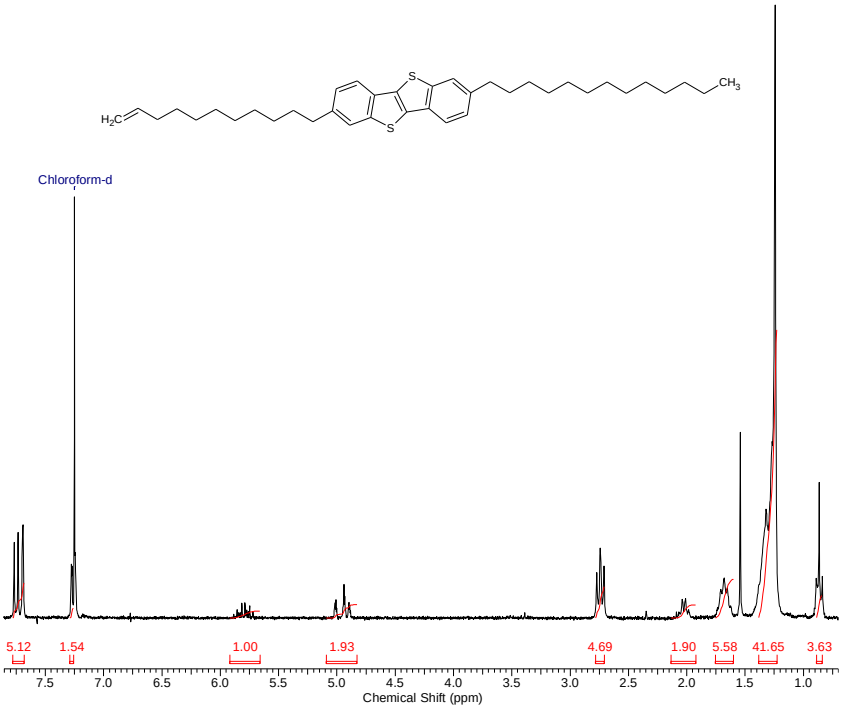
No.	(ppm)	Value	Absolute Value
1	[0.81 .. 0.92]	3.129	1.34128e+7
2	[1.20 .. 1.39]	22.013	9.43595e+7
3	[1.61 .. 1.79]	4.327	1.85467e+7
4	[1.94 .. 2.11]	1.917	8.21715e+6
5	[2.66 .. 2.82]	4.000	1.71460e+7
6	[4.85 .. 5.06]	1.816	7.78274e+6
7	[5.69 .. 5.91]	0.919	3.94044e+6
8	[7.25 .. 7.32]	2.165	9.28007e+6
9	[7.67 .. 7.83]	4.199	1.79982e+7

Figure S20. ^{1}H NMR spectrum of compound **20** in $CDCl_3$



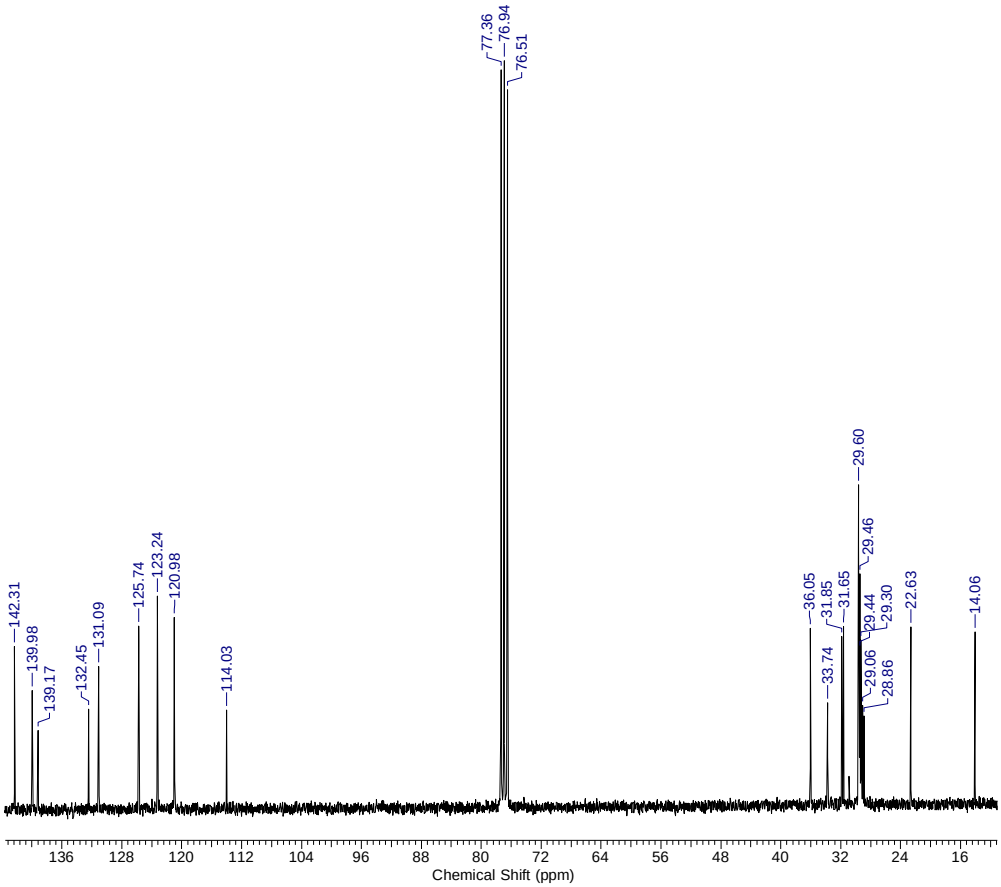
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.05	1060.1	0.1902	14	76.51	5775.0	0.9625
2	22.60	1705.9	0.1776	15	76.94	5807.1	1.0000
3	28.85	2177.5	0.1263	16	77.36	5839.1	0.9847
4	29.05	2193.0	0.1243	17	114.02	8606.3	0.1220
5	29.19	2203.5	0.1756	18	120.98	9130.9	0.2174
6	29.22	2205.7	0.1375	19	123.24	9301.8	0.2380
7	29.25	2207.9	0.1587	20	125.74	9490.3	0.2065
8	29.42	2220.6	0.2679	21	131.09	9894.5	0.1540
9	30.86	2329.5	0.1319	22	132.44	9996.2	0.1028
10	31.65	2389.2	0.1433	23	139.17	10504.3	0.1021
11	31.82	2401.4	0.1578	24	139.95	10563.4	0.1123
12	33.74	2546.8	0.1423	25	139.98	10565.6	0.1315
13	36.04	2720.4	0.1762	26	142.30	10740.4	0.1872

Figure S21. ^{13}C NMR spectrum of compound **20** in $CDCl_3$



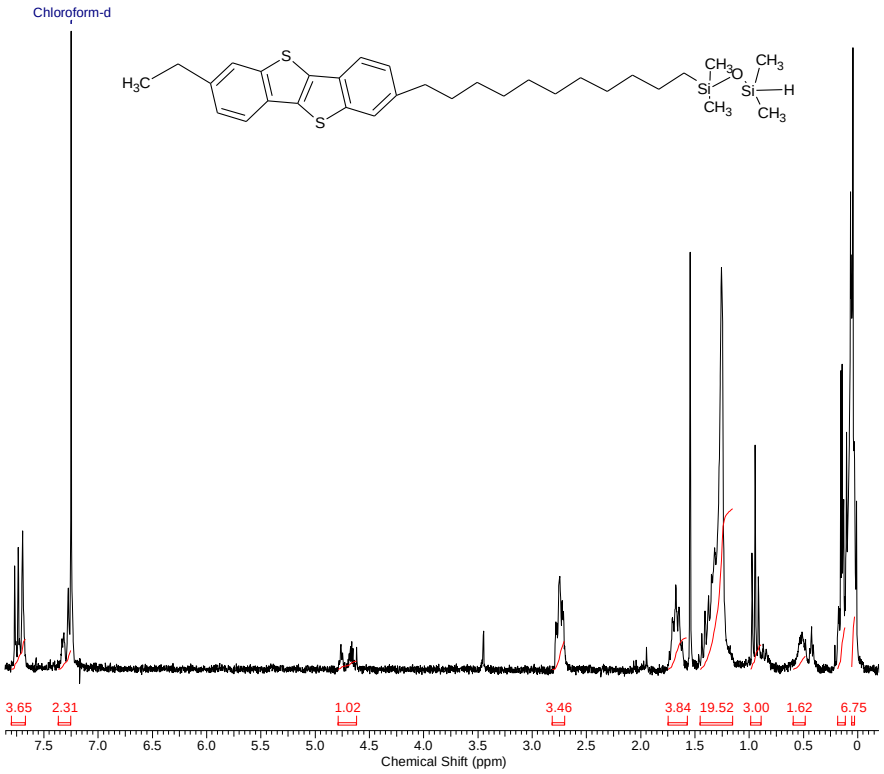
No.	(ppm)	Value	Absolute Value
1	[0.84 .. 0.89]	3.627	6.67821e+6
2	[1.22 .. 1.38]	41.655	7.66958e+7
3	[1.60 .. 1.75]	5.576	1.02660e+7
4	[1.92 .. 2.14]	1.901	3.50006e+6
5	[2.71 .. 2.78]	4.693	8.64092e+6
6	[4.83 .. 5.09]	1.925	3.54460e+6
7	[5.66 .. 5.92]	1.000	1.84122e+6
8	[7.26 .. 7.29]	1.544	2.84224e+6
9	[7.68 .. 7.78]	5.118	9.42354e+6

Figure S22. ^{1}H NMR spectrum of compound **21** in $CDCl_3$



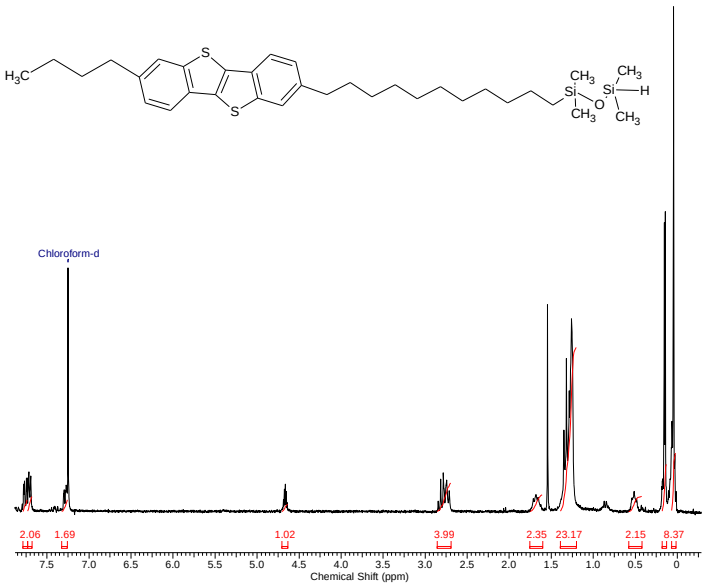
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.06	1061.2	0.2285	15	36.05	2721.0	0.2333
2	22.63	1708.1	0.2356	16	76.51	5775.0	0.9608
3	28.86	2178.0	0.1153	17	76.94	5807.1	1.0000
4	29.06	2193.5	0.1294	18	77.36	5839.1	0.9875
5	29.24	2206.8	0.2116	19	114.03	8606.8	0.1232
6	29.30	2211.2	0.2177	20	120.98	9130.9	0.2480
7	29.41	2220.0	0.1816	21	123.24	9301.8	0.2773
8	29.44	2221.7	0.2046	22	125.74	9490.3	0.2366
9	29.46	2223.4	0.3073	23	131.09	9894.5	0.1820
10	29.52	2228.3	0.1933	24	132.45	9996.7	0.1247
11	29.60	2234.4	0.4273	25	139.17	10504.3	0.0957
12	31.65	2388.7	0.2362	26	139.95	10563.4	0.1089
13	31.85	2404.2	0.2228	27	139.98	10565.1	0.1496
14	33.74	2546.8	0.1333	28	142.31	10740.9	0.2092

Figure S23. ^{13}C NMR spectrum of compound **21** in $CDCl_3$



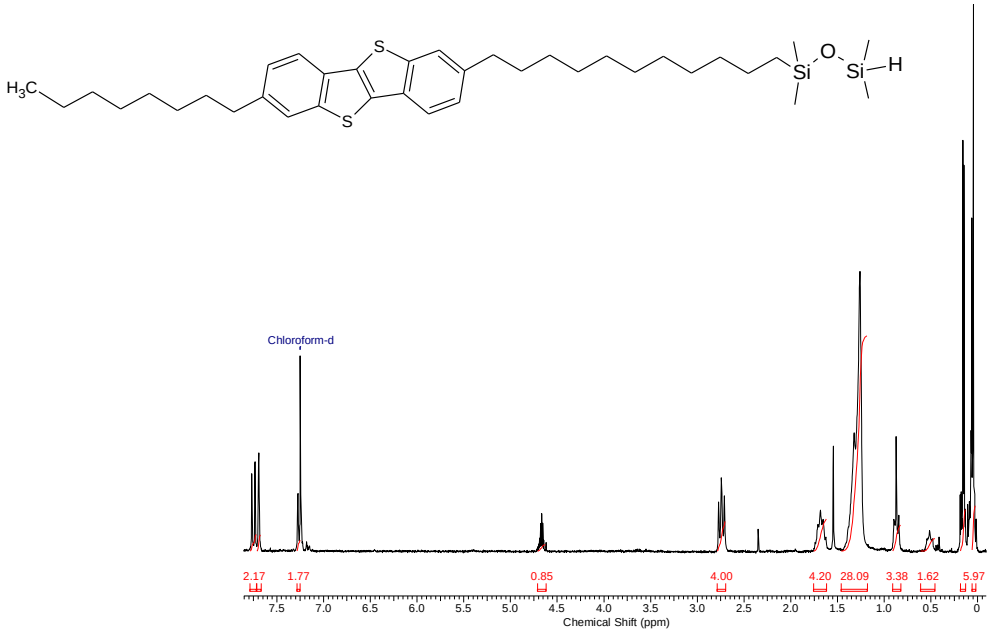
No.	(ppm)	Value	Absolute Value
1	[0.03 .. 0.06]	6.748	4.96782e+7
2	[0.11 .. 0.19]	5.208	3.83417e+7
3	[0.48 .. 0.60]	1.619	1.19163e+7
4	[0.89 .. 0.99]	3.000	2.20851e+7
5	[1.15 .. 1.45]	19.515	1.43666e+8
6	[1.57 .. 1.75]	3.842	2.82865e+7
7	[2.70 .. 2.81]	3.461	2.54793e+7
8	[4.62 .. 4.79]	1.020	7.50965e+6
9	[7.25 .. 7.36]	2.313	1.70259e+7
10	[7.67 .. 7.80]	3.654	2.69010e+7

Figure S24. ^{1}H NMR spectrum of compound **22** in $CDCl_3$



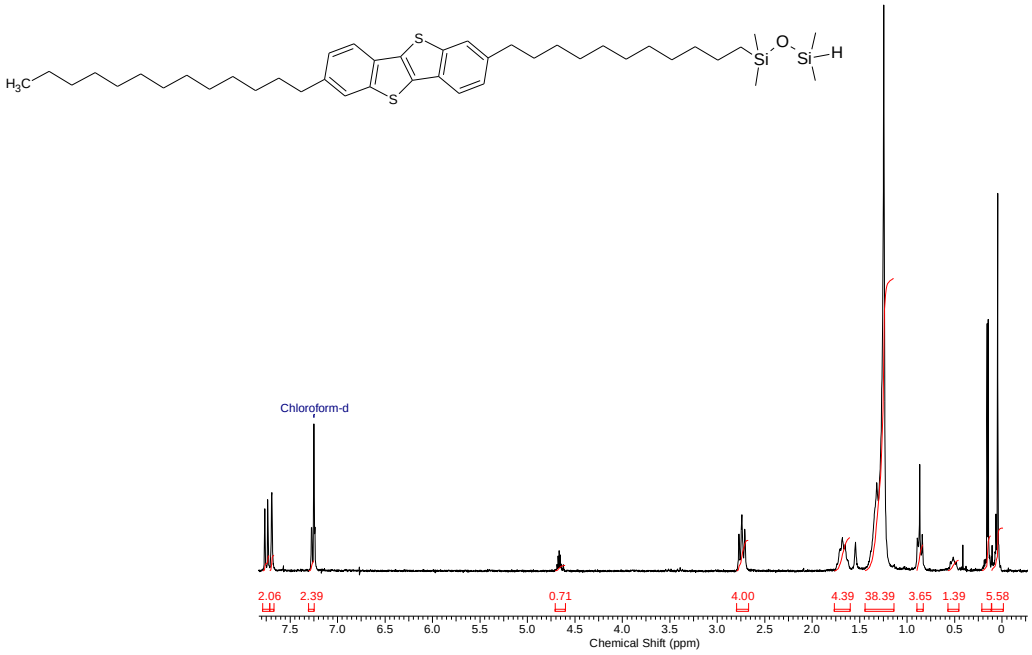
No.	(ppm)	Value	Absolute Value
1	[0.02 .. 0.07]	8.367	2.50237e+7
2	[0.13 .. 0.18]	6.707	2.00594e+7
3	[0.42 .. 0.58]	2.149	6.42845e+6
4	[1.20 .. 1.39]	23.167	6.92857e+7
5	[1.60 .. 1.75]	2.350	7.02788e+6
6	[2.69 .. 2.86]	3.994	1.19446e+7
7	[4.64 .. 4.71]	1.025	3.06518e+6
8	[7.26 .. 7.33]	1.693	5.06271e+6
9	[7.68 .. 7.73]	2.058	6.15384e+6
10	[7.73 .. 7.79]	1.888	5.64789e+6

Figure S25. ^{1}H NMR spectrum of compound **23** in $CDCl_3$



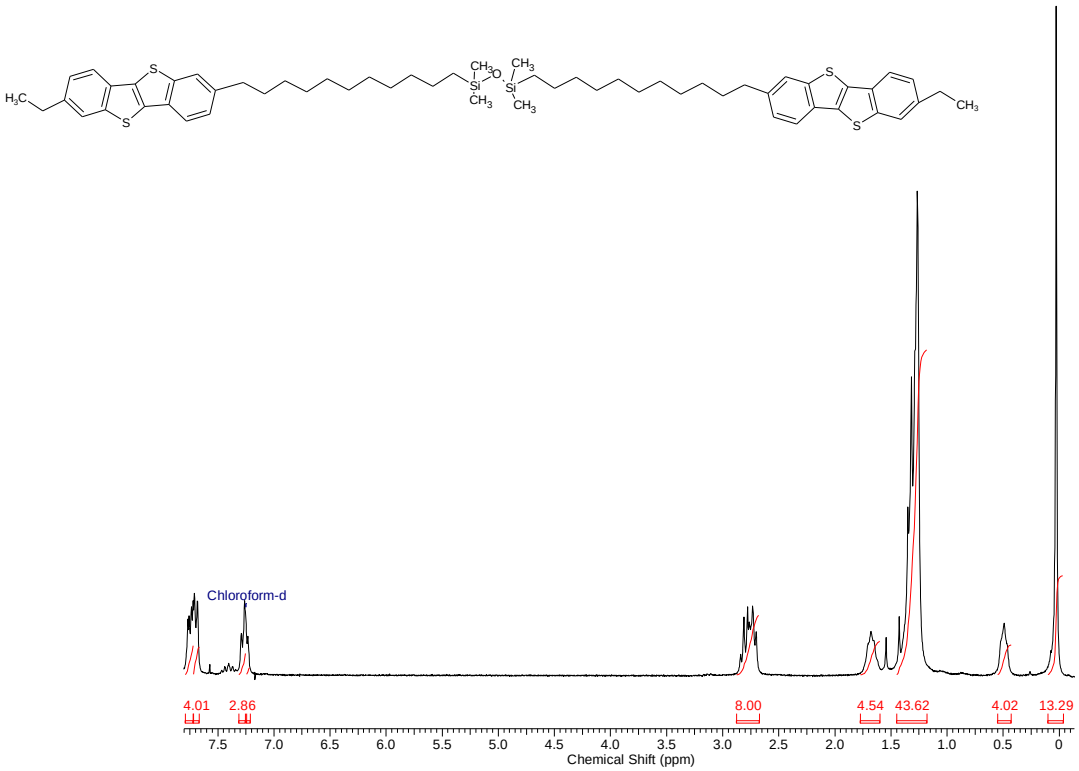
No.	(ppm)	Value	Absolute Value
1	[0.02 .. 0.06]	5.966	2.16932e+7
2	[0.13 .. 0.18]	5.601	2.03663e+7
3	[0.46 .. 0.61]	1.623	5.90282e+6
4	[0.82 .. 0.91]	3.384	1.23032e+7
5	[1.18 .. 1.46]	28.088	1.02124e+8
6	[1.62 .. 1.76]	4.195	1.52528e+7
7	[2.70 .. 2.79]	4.000	1.45437e+7
8	[4.62 .. 4.71]	0.853	3.10084e+6
9	[7.25 .. 7.29]	1.770	6.43477e+6
10	[7.67 .. 7.72]	2.128	7.73761e+6
11	[7.72 .. 7.79]	2.170	7.88826e+6

Figure S26. ^{1}H NMR spectrum of compound **24** in $CDCl_3$



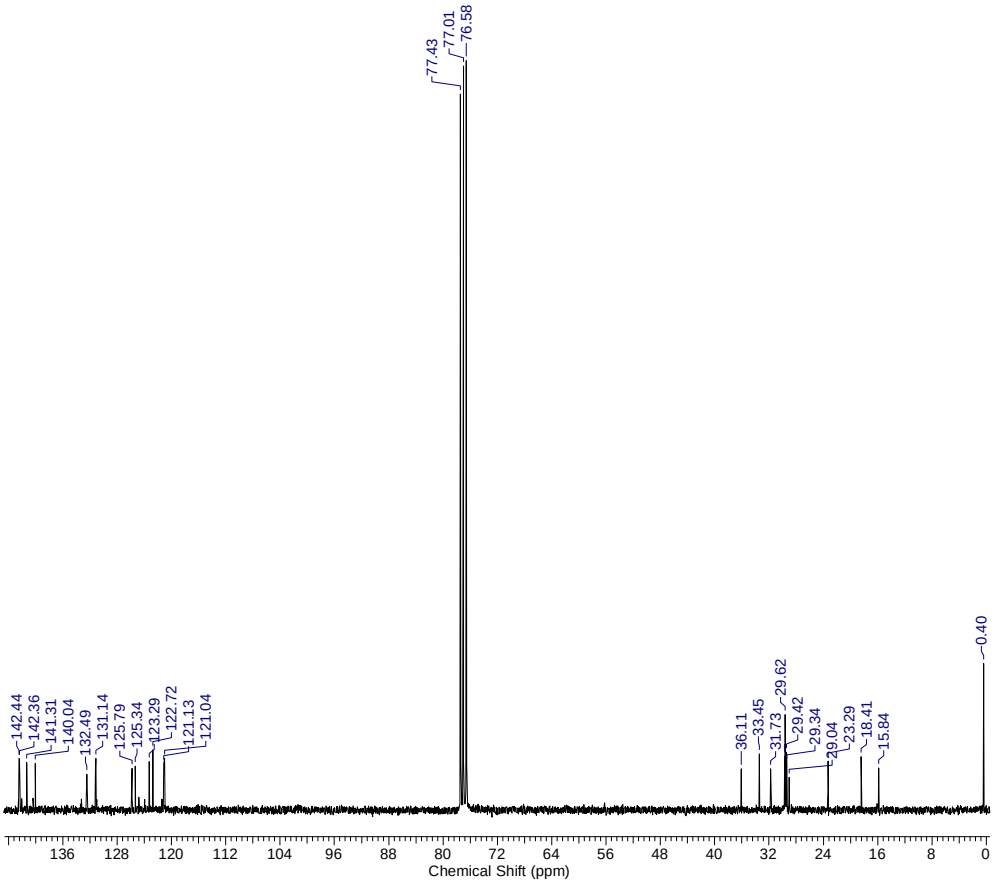
No.	(ppm)	Value	Absolute Value
1	[-0.01 .. 0.11]	5.577	1.34130e+7
2	[0.11 .. 0.21]	4.719	1.13507e+7
3	[0.45 .. 0.57]	1.390	3.34332e+6
4	[0.83 .. 0.90]	3.653	8.78691e+6
5	[1.14 .. 1.44]	38.391	9.23376e+7
6	[1.60 .. 1.76]	4.394	1.05672e+7
7	[2.67 .. 2.79]	4.000	9.62068e+6
8	[4.60 .. 4.71]	0.709	1.70474e+6
9	[7.25 .. 7.30]	2.387	5.74207e+6
10	[7.67 .. 7.71]	2.045	4.91896e+6
11	[7.71 .. 7.79]	2.061	4.95600e+6

Figure S27. ^{1}H NMR spectrum of compound **25** in $CDCl_3$



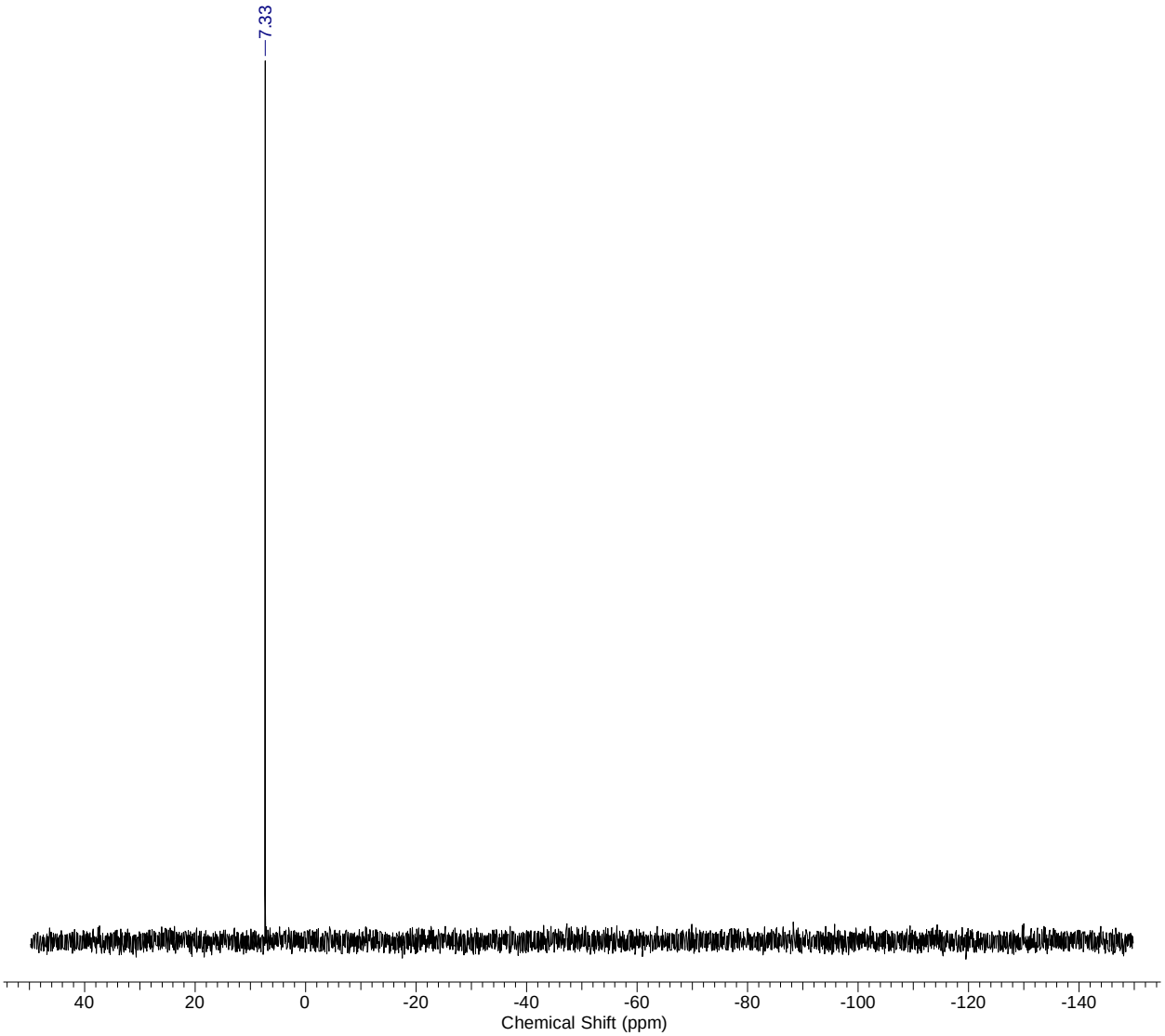
No.	(ppm)	Value	Absolute Value
1	[-0.04 .. 0.10]	13.286	5.16723e+7
2	[0.43 .. 0.55]	4.022	1.56419e+7
3	[1.18 .. 1.45]	43.623	1.69660e+8
4	[1.60 .. 1.77]	4.538	1.76497e+7
5	[2.67 .. 2.87]	8.000	3.11134e+7
6	[7.21 .. 7.24]	0.983	3.82124e+6
7	[7.25 .. 7.31]	2.857	1.11110e+7
8	[7.67 .. 7.72]	3.748	1.45749e+7
9	[7.72 .. 7.79]	4.010	1.55941e+7

Figure S28. ^{1}H NMR spectrum of **D2-Und-BTBT-Et** in $CDCl_3$



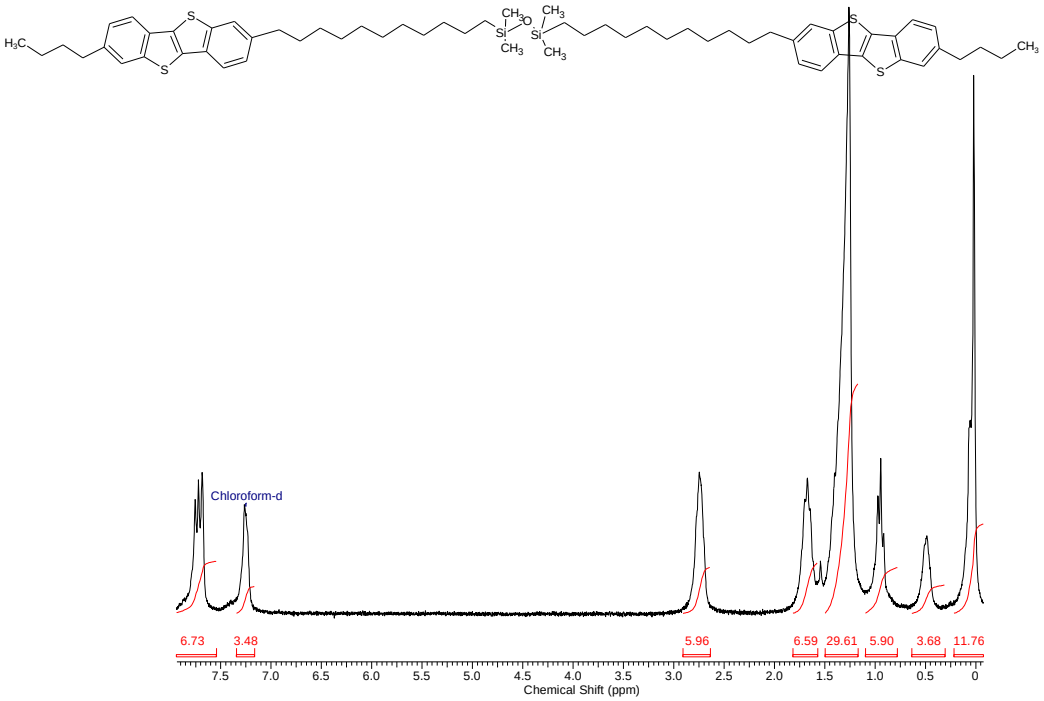
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.40	30.5	0.1956	16	77.43	5843.9	0.9552
2	15.84	1195.4	0.0562	17	121.04	9135.7	0.0691
3	18.41	1389.4	0.0712	18	121.13	9142.4	0.0613
4	23.29	1757.7	0.0653	19	122.72	9262.3	0.0805
5	29.04	2192.2	0.0435	20	123.29	9305.5	0.0648
6	29.34	2214.3	0.0626	21	125.34	9460.3	0.0587
7	29.42	2220.4	0.0773	22	125.79	9494.5	0.0555
8	29.55	2230.4	0.0716	23	131.14	9898.1	0.0686
9	29.62	2235.3	0.1275	24	131.18	9900.9	0.0583
10	29.72	2243.1	0.0721	25	132.49	9999.9	0.0477
11	31.73	2395.1	0.0549	26	132.54	10003.7	0.0457
12	33.45	2525.0	0.0748	27	140.04	10569.9	0.0624
13	36.11	2725.7	0.0547	28	141.31	10665.5	0.0635
14	76.58	5780.3	1.0000	29	142.36	10745.1	0.0682
15	77.01	5812.4	0.9926	30	142.44	10751.2	0.0687

Figure S29. ^{13}C NMR spectrum of **D2-Und-BTBT-Et** in $CDCl_3$



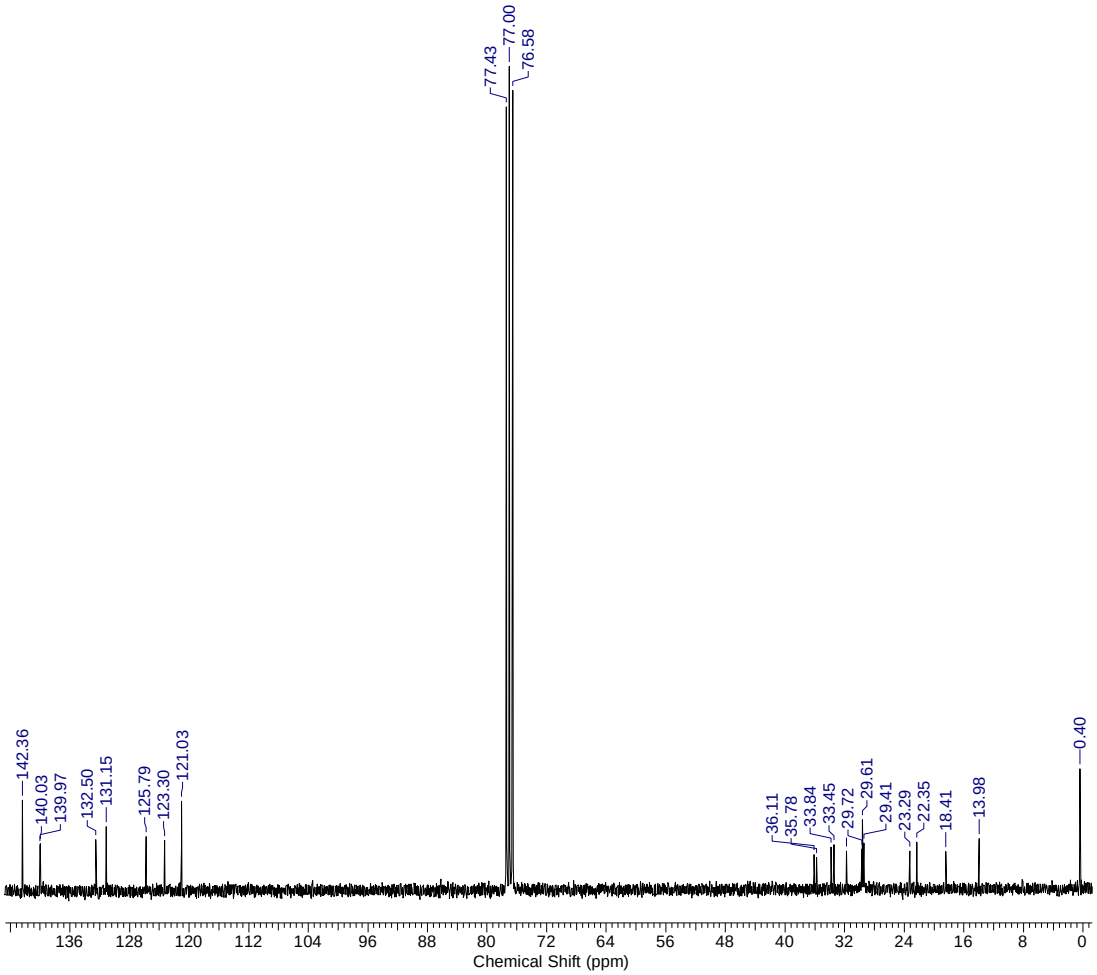
No.	(ppm)	(Hz)	Height
1	7.33	436.9	1.0000

Figure S30. ^{29}Si NMR spectrum of **D2-Und-BTBT-Et** in $CDCl_3$



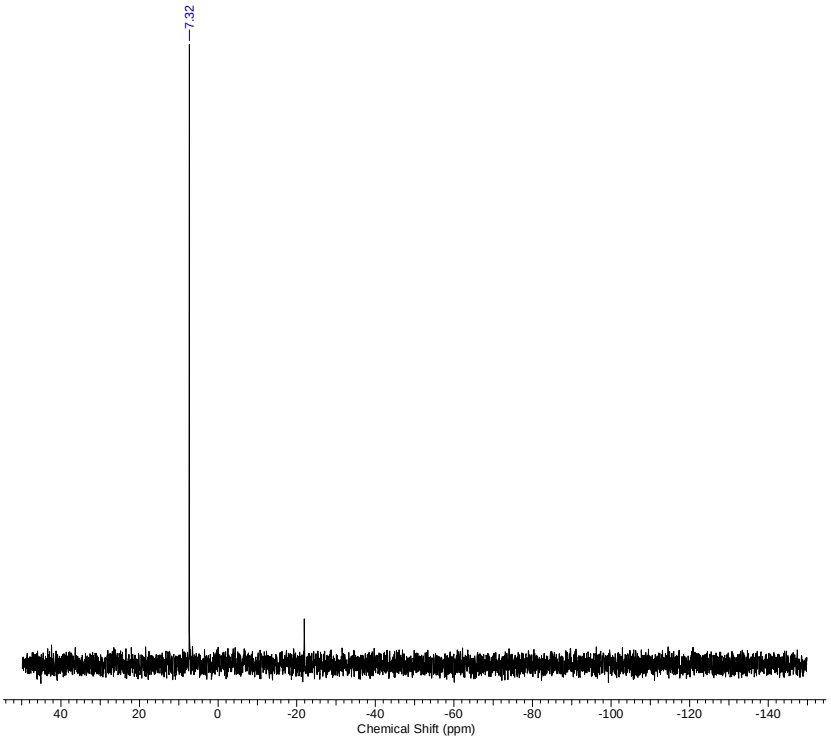
No.	(ppm)	Value	Absolute Value
1	[-0.15 .. 0.22]	11.764	1.58913e+8
2	[0.31 .. 0.64]	3.678	4.96888e+7
3	[0.78 .. 1.10]	5.900	7.97034e+7
4	[1.17 .. 1.50]	29.613	4.00037e+8
5	[1.57 .. 1.82]	6.591	8.90381e+7
6	[2.64 .. 2.91]	5.956	8.04628e+7
7	[7.16 .. 7.35]	3.482	4.70385e+7
8	[7.54 .. 8.02]	6.730	9.09153e+7

Figure S31. ^{1}H NMR spectrum of **D2-Und-BTBT-But** in $CDCl_3$



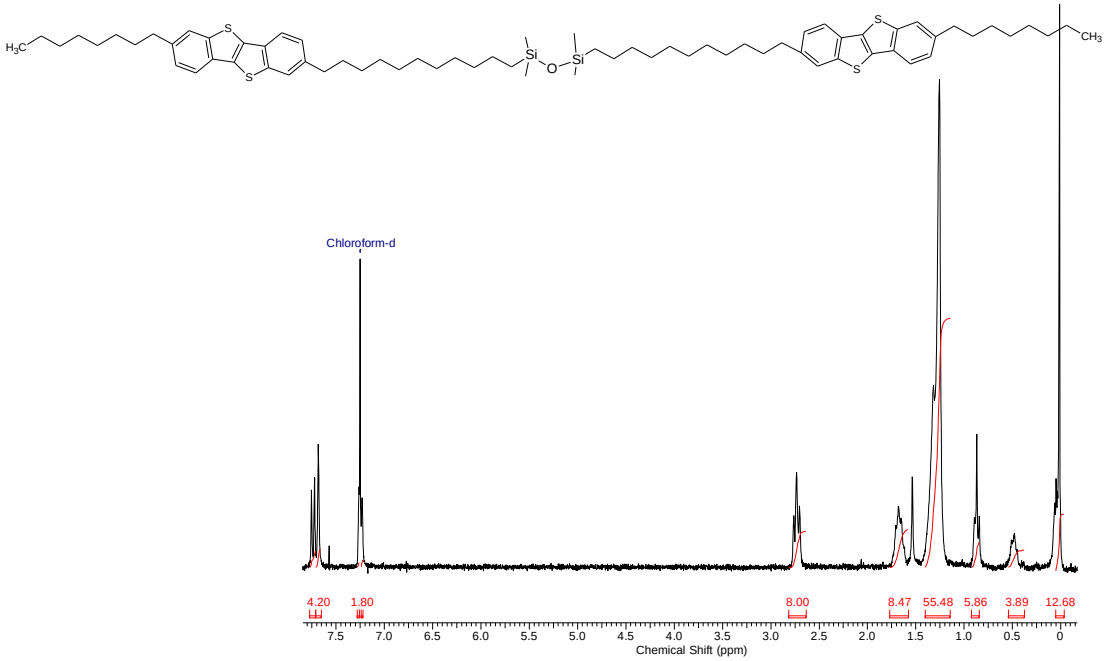
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.40	29.9	0.1502	14	36.11	2725.7	0.0459
2	13.98	1055.0	0.0653	15	76.58	5779.8	0.9713
3	18.41	1389.4	0.0495	16	77.00	5811.9	1.0000
4	22.35	1686.9	0.0615	17	77.43	5843.9	0.9512
5	23.29	1757.7	0.0502	18	121.03	9135.2	0.1110
6	29.41	2219.9	0.0603	19	123.29	9305.5	0.0610
7	29.55	2230.4	0.0512	20	123.30	9306.6	0.0629
8	29.61	2234.8	0.0884	21	125.79	9494.5	0.0678
9	29.72	2243.1	0.0531	22	131.15	9898.7	0.0798
10	31.73	2395.1	0.0506	23	132.50	10001.0	0.0646
11	33.45	2524.5	0.0582	24	139.97	10564.3	0.0597
12	33.84	2554.3	0.0550	25	140.03	10569.3	0.0569
13	35.78	2700.8	0.0427	26	142.36	10745.1	0.1117

Figure S32. ^{13}C NMR spectrum of **D2-Und-BTBT-But** in $CDCl_3$



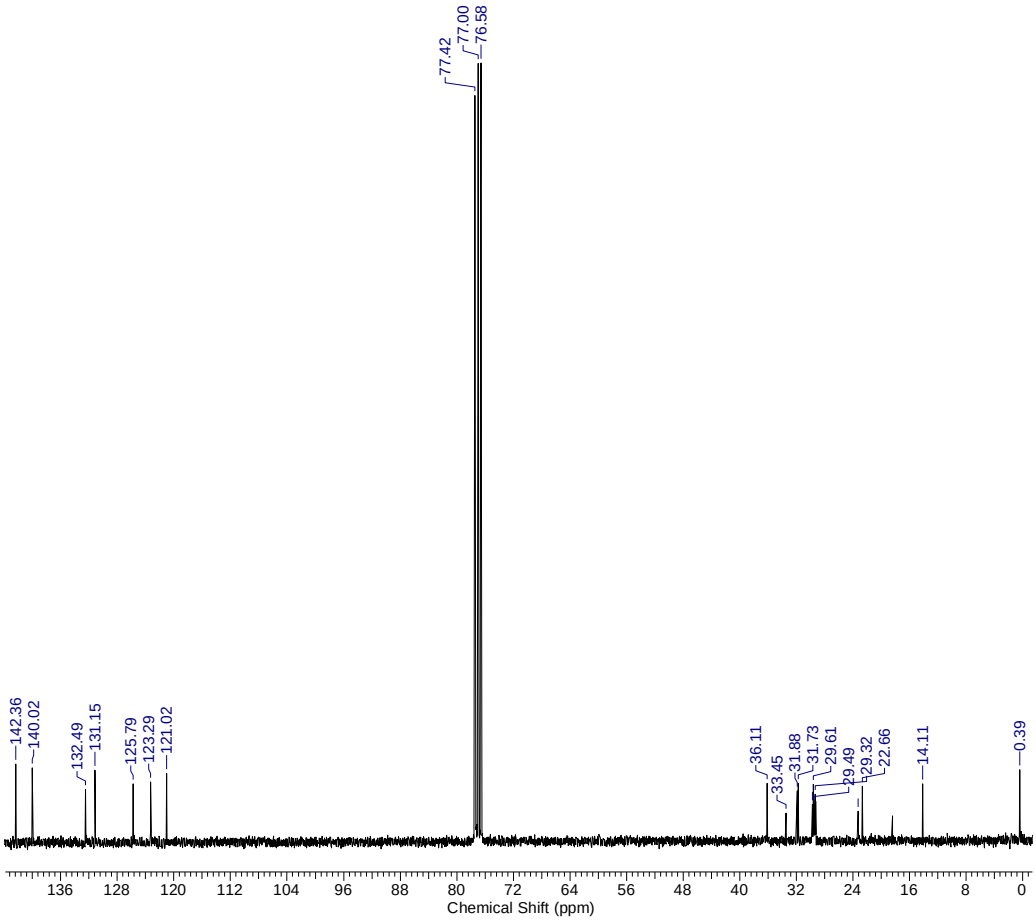
No.	(ppm)	(Hz)	Height
1	7.32	436.5	1.0000

Figure S33. ^{29}Si NMR spectrum of **D2-Und-BTBT-But** in $CDCl_3$



No.	(ppm)	Value	Absolute Value
1	[-0.04 .. 0.05]	12.680	4.43506e+7
2	[0.37 .. 0.54]	3.894	1.36218e+7
3	[0.84 .. 0.92]	5.861	2.05004e+7
4	[1.14 .. 1.40]	55.475	1.94042e+8
5	[1.57 .. 1.77]	8.466	2.96127e+7
6	[2.63 .. 2.82]	8.000	2.79826e+7
7	[7.22 .. 7.24]	1.802	6.30244e+6
8	[7.26 .. 7.28]	1.594	5.57712e+6
9	[7.65 .. 7.71]	4.203	1.47030e+7
10	[7.71 .. 7.77]	3.866	1.35226e+7

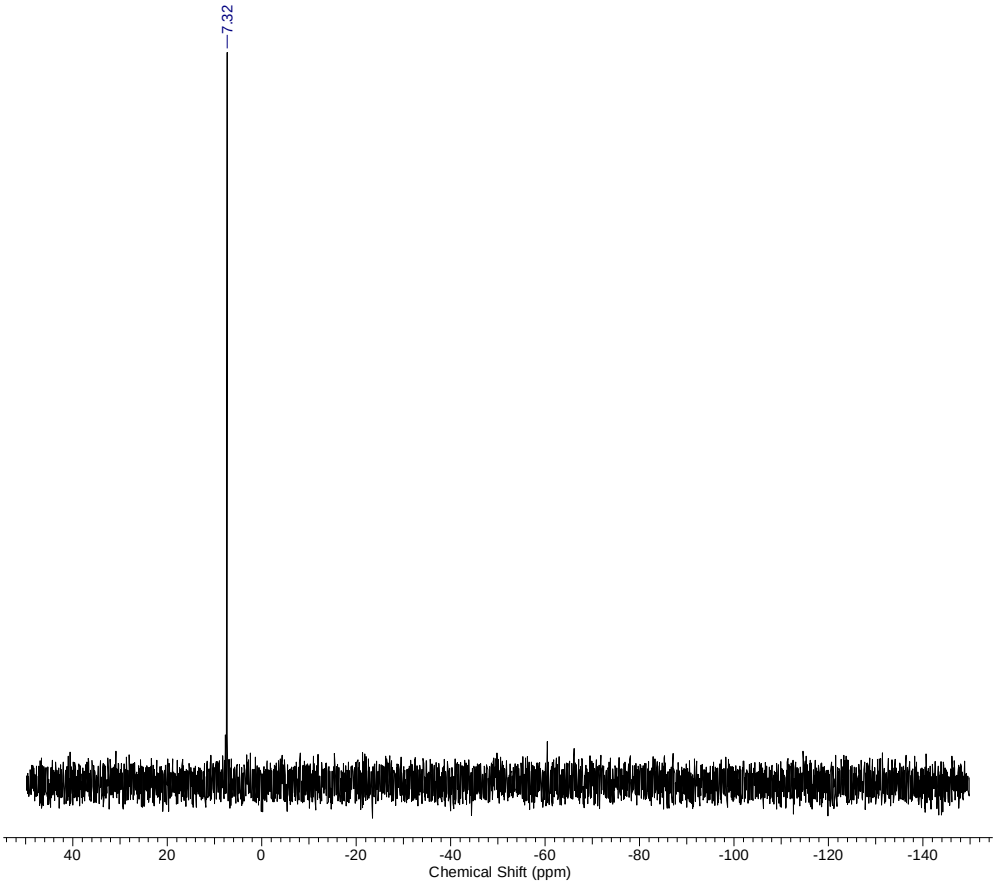
Figure S34. ^{1}H NMR spectrum of **D2-Und-BTBT-Oct** in $CDCl_3$



No.	(ppm)	(Hz)	Height
1	0.39	29.4	0.0952
2	14.11	1064.9	0.0772
3	22.66	1710.7	0.0745
4	23.28	1757.1	0.0421
5	29.26	2208.8	0.0549
6	29.32	2213.2	0.0643
7	29.41	2219.9	0.0455
8	29.49	2225.9	0.0500
9	29.55	2230.4	0.0480
10	29.61	2234.8	0.0767
11	29.72	2243.1	0.0508
12	31.73	2394.6	0.0777
13	31.88	2406.2	0.0686

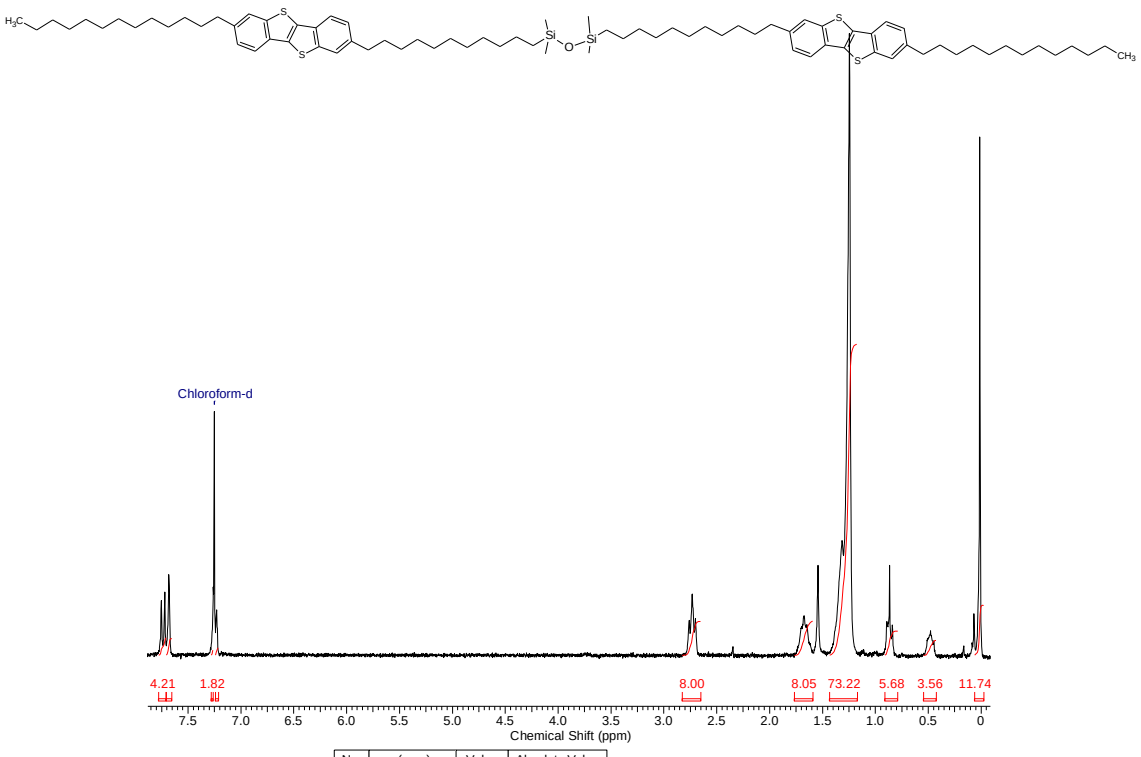
No.	(ppm)	(Hz)	Height
14	33.45	2524.5	0.0402
15	36.11	2725.7	0.0780
16	76.58	5779.8	1.0000
17	77.00	5811.9	0.9990
18	77.42	5843.4	0.9581
19	121.02	9134.6	0.0905
20	123.29	9305.5	0.0795
21	125.79	9494.0	0.0772
22	131.15	9898.7	0.0947
23	132.49	10000.4	0.0703
24	140.02	10568.8	0.0978
25	142.36	10745.1	0.1025

Figure S35. ^{13}C NMR spectrum of **D2-Und-BTBT-Oct** in $CDCl_3$



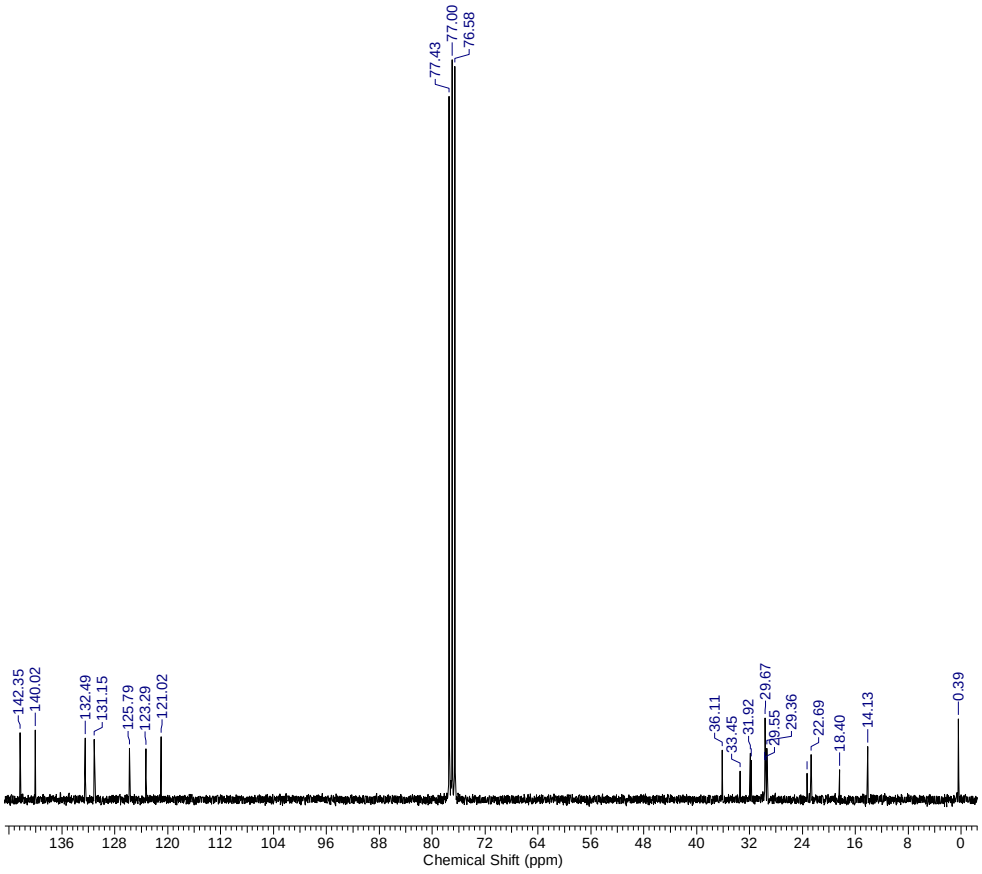
No.	(ppm)	(Hz)	Height
1	7.32	436.5	1.0000

Figure S36. ^{29}Si NMR spectrum of **D2-Und-BTBT-Oct** in $CDCl_3$



No.	(ppm)	Value	Absolute Value
1	[-0.03 .. 0.06]	11.741	2.40983e+7
2	[0.42 .. 0.55]	3.560	7.30615e+6
3	[0.79 .. 0.91]	5.678	1.16547e+7
4	[1.17 .. 1.43]	73.219	1.50277e+8
5	[1.59 .. 1.76]	8.052	1.65270e+7
6	[2.65 .. 2.82]	8.000	1.64195e+7
7	[7.21 .. 7.24]	1.822	3.73866e+6
8	[7.26 .. 7.28]	1.822	3.73937e+6
9	[7.65 .. 7.71]	3.982	8.17295e+6
10	[7.71 .. 7.78]	4.210	8.64017e+6

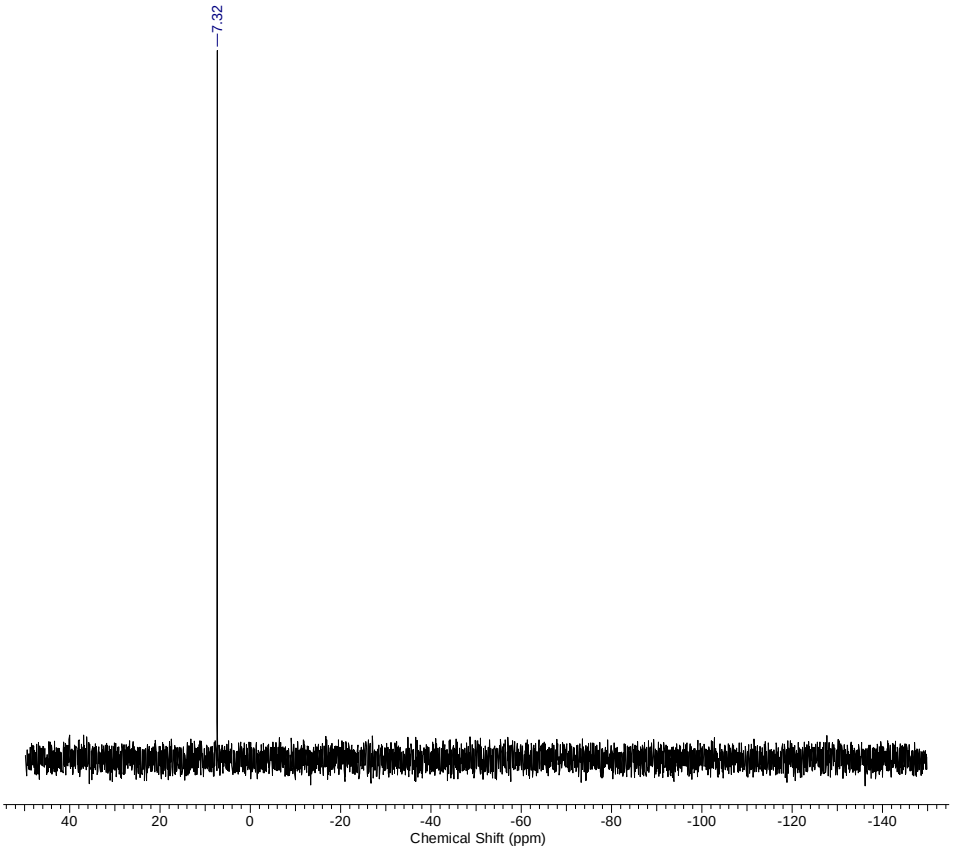
Figure S37. ^{1}H NMR spectrum of **D2-Und-BTBT-Trid** in $CDCl_3$



No.	(ppm)	(Hz)	Height
1	0.39	29.4	0.1089
2	14.13	1066.6	0.0713
3	18.40	1388.9	0.0402
4	22.69	1712.3	0.0604
5	23.29	1757.7	0.0352
6	29.31	2212.1	0.0422
7	29.36	2216.0	0.0689
8	29.41	2219.9	0.0427
9	29.52	2228.1	0.0442
10	29.55	2230.4	0.0476
11	29.61	2234.8	0.0742
12	29.67	2239.2	0.1103
13	29.72	2243.1	0.0477
14	31.72	2394.0	0.0529

No.	(ppm)	(Hz)	Height
15	31.92	2408.9	0.0624
16	33.45	2524.5	0.0381
17	36.11	2725.7	0.0668
18	76.58	5779.8	0.9907
19	77.00	5811.9	1.0000
20	77.43	5843.9	0.9503
21	121.02	9134.6	0.0850
22	123.29	9305.5	0.0686
23	125.79	9494.0	0.0689
24	131.15	9898.7	0.0814
25	132.49	10000.4	0.0829
26	140.02	10568.8	0.0941
27	142.35	10744.6	0.0904

Figure S38. ^{13}C NMR spectrum of **D2-Und-BTBT-Trid** in $CDCl_3$



No.	(ppm)	(Hz)	Height
1	7.32	436.5	1.0000

Figure S39. ^{29}Si NMR spectrum of **D2-Und-BTBT-Trid** in $CDCl_3$

3. TGA-data for thermal and thermal-oxidative stability

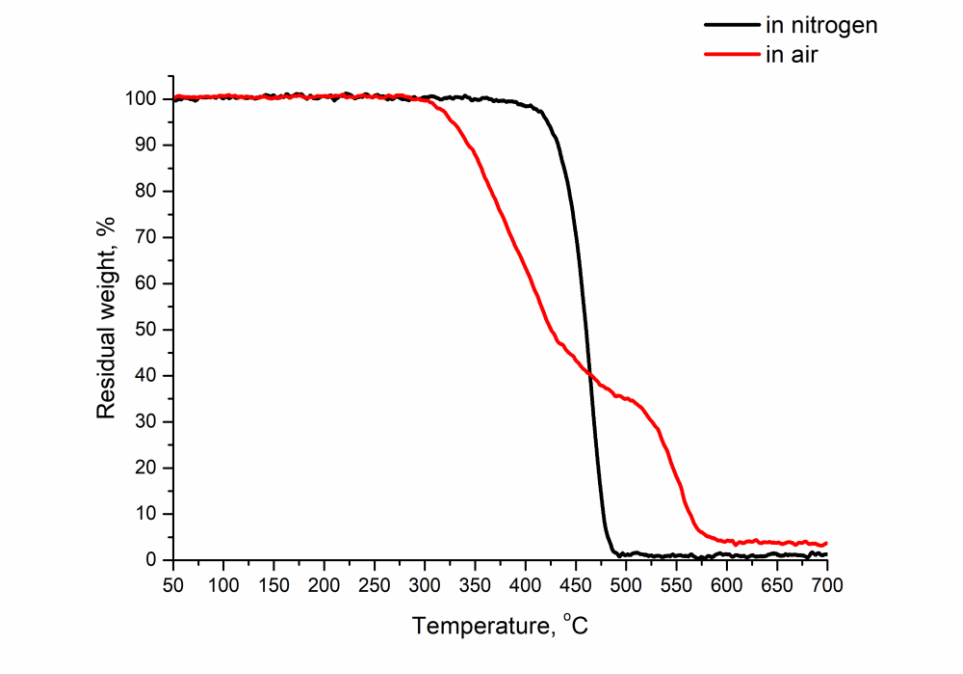


Figure S40. TGA-curves of **D2-Und-BTBT-Et**

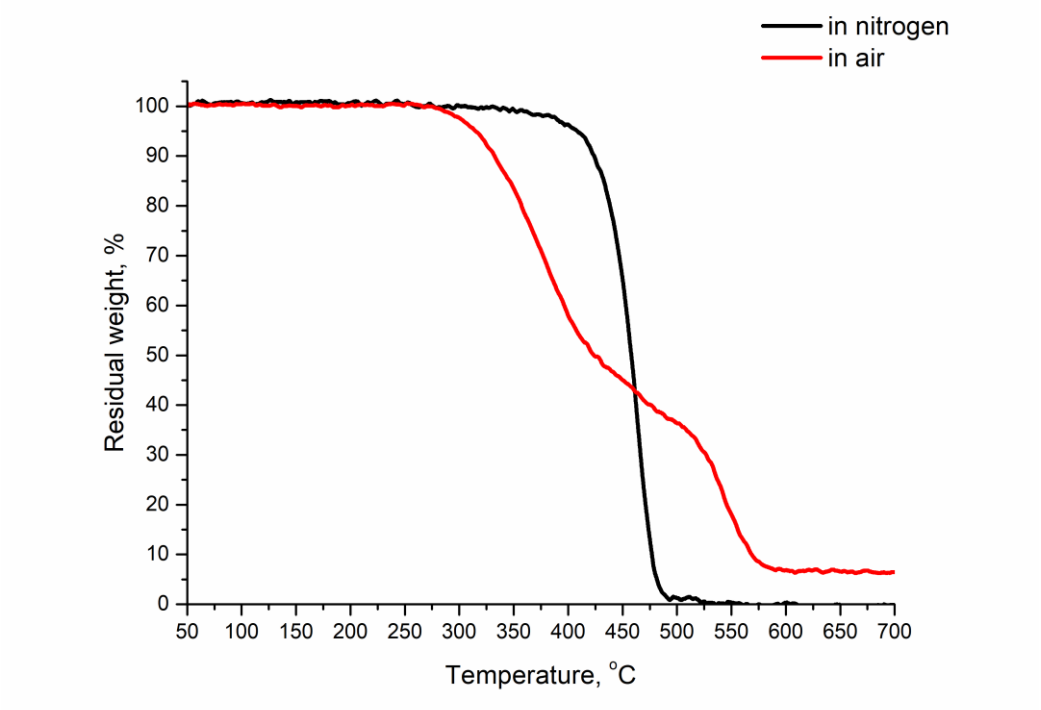


Figure S41. TGA-curves of **D2-Und-BTBT-But**

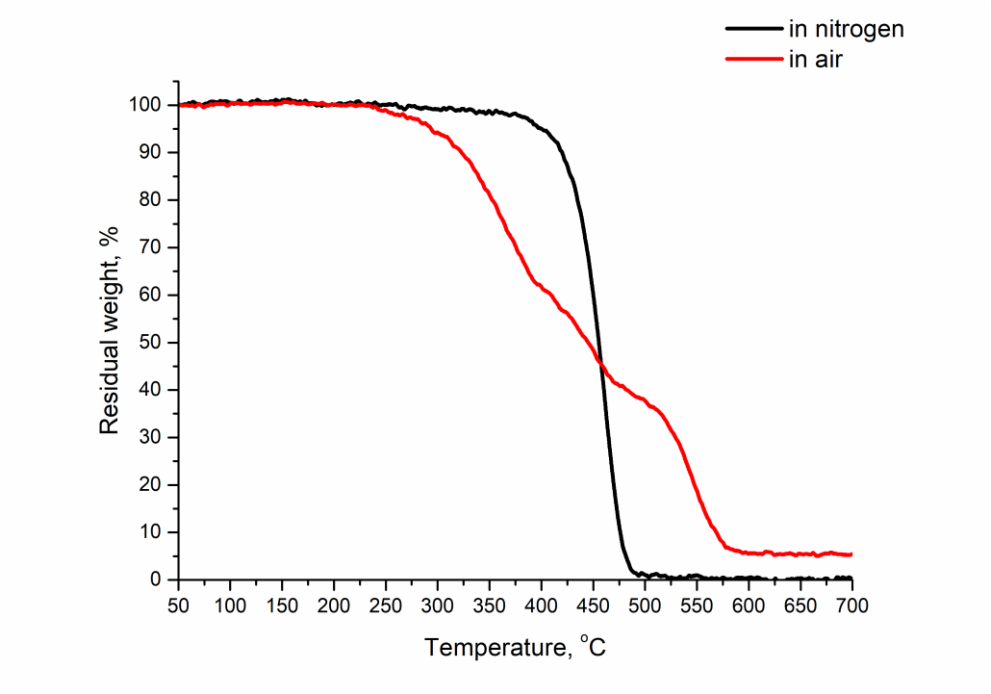


Figure S42. TGA-curves of **D2-Und-BTBT-Oct**

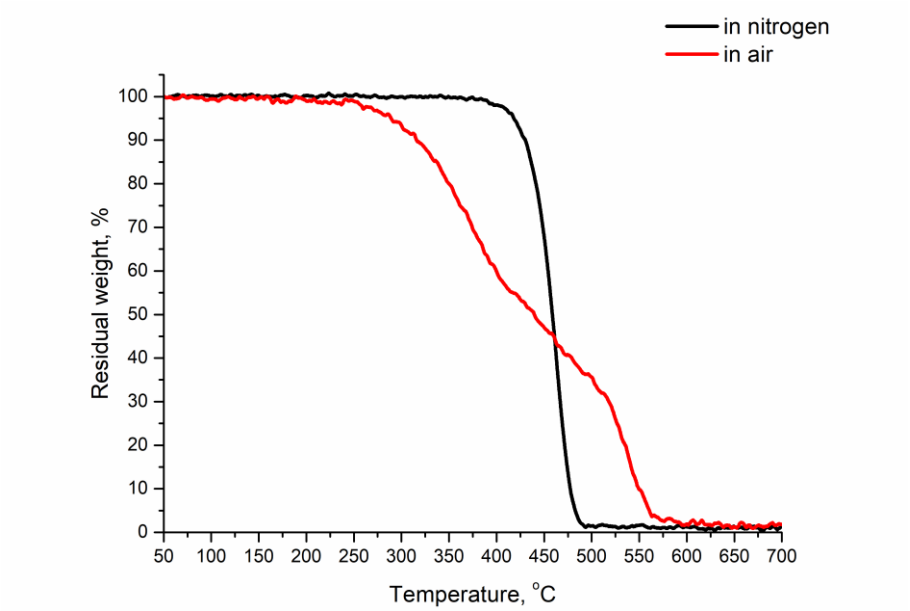


Figure S43. TGA-curves of **D2-Und-BTBT-TriD**

4. DSC curves

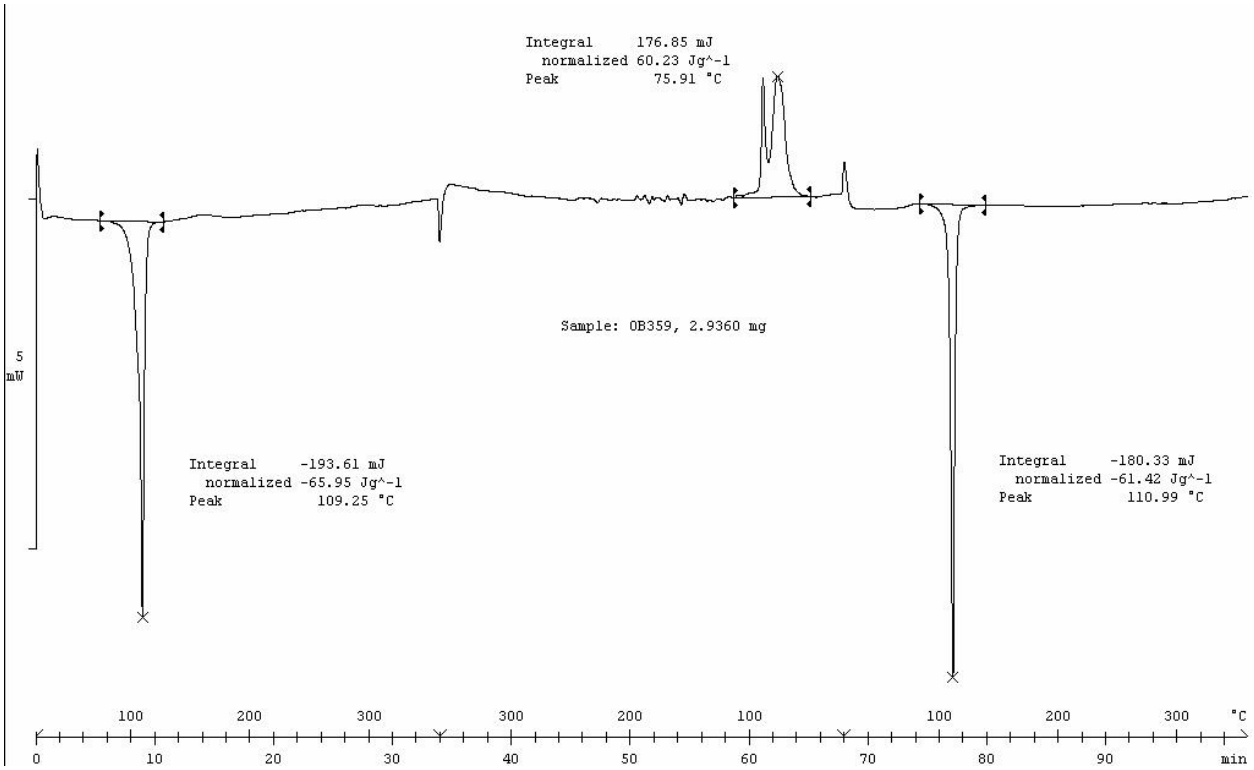


Figure S44. DSC-curve of **D2-Und-BTBT**

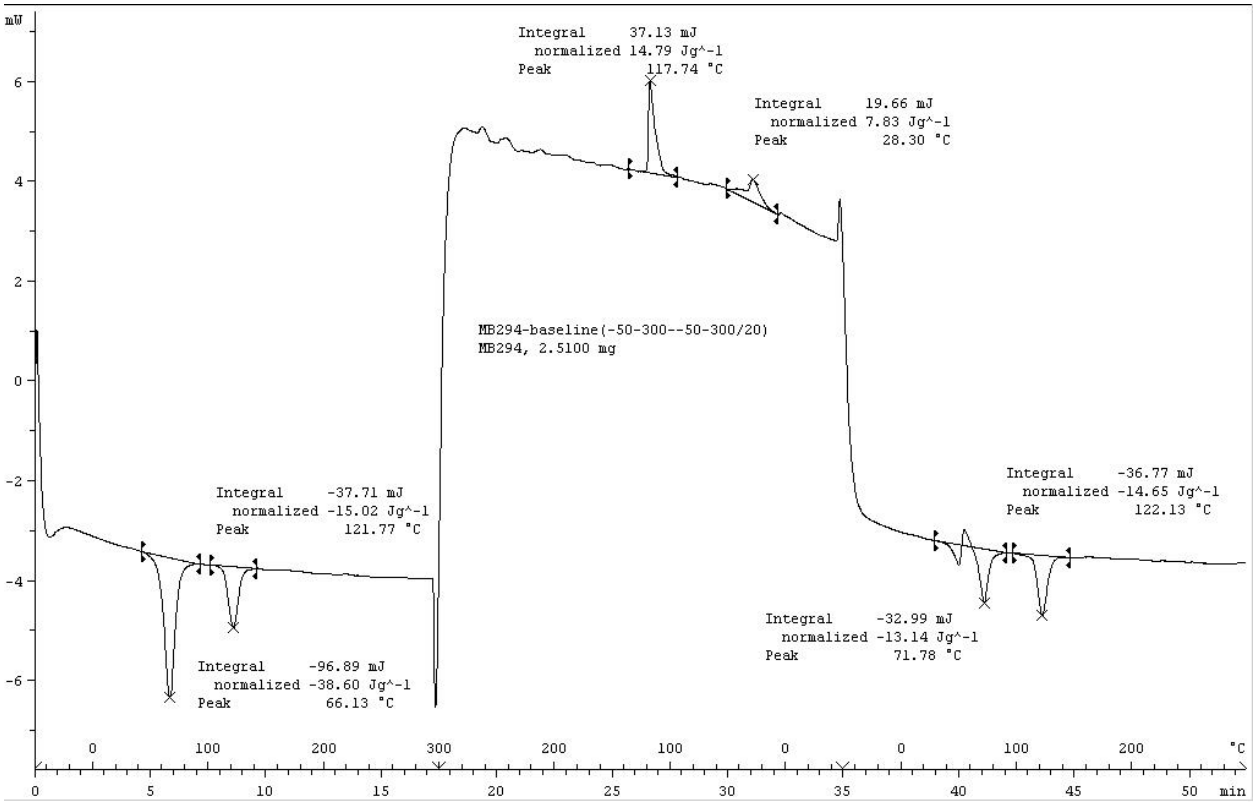


Figure S45. DSC-curve of **D2-Und-BTBT-Et**

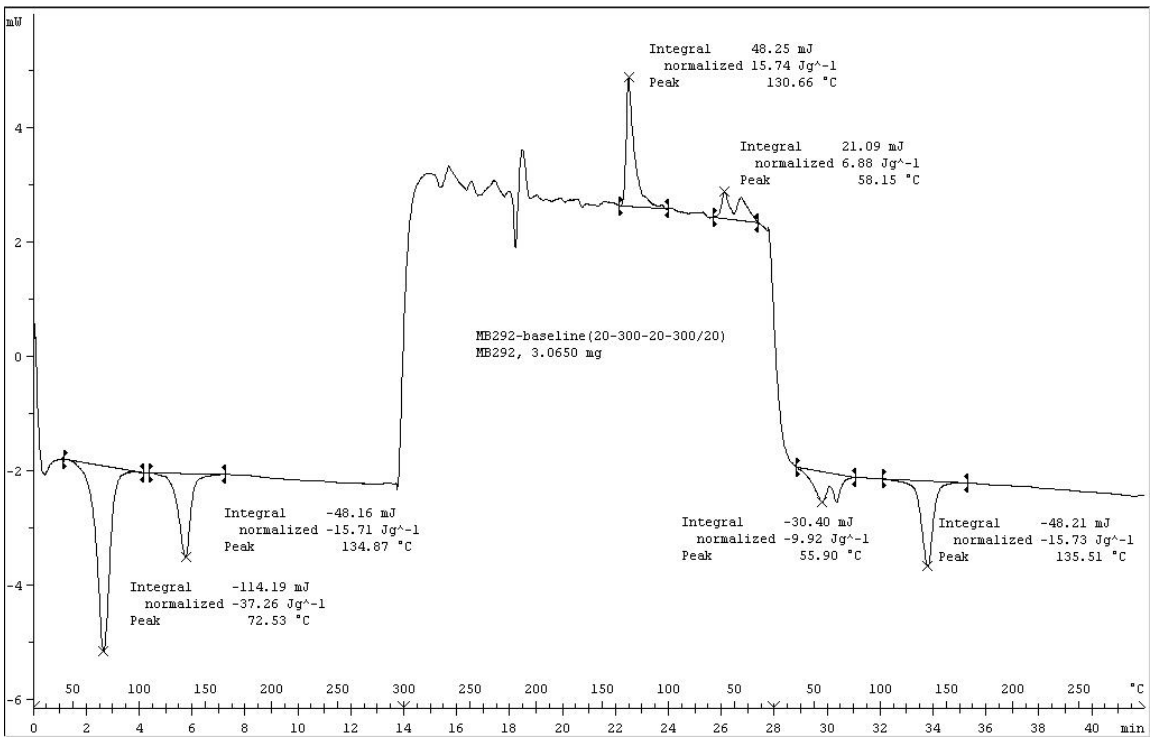


Figure S46. DSC-curve of **D2-Und-BTBT-But**

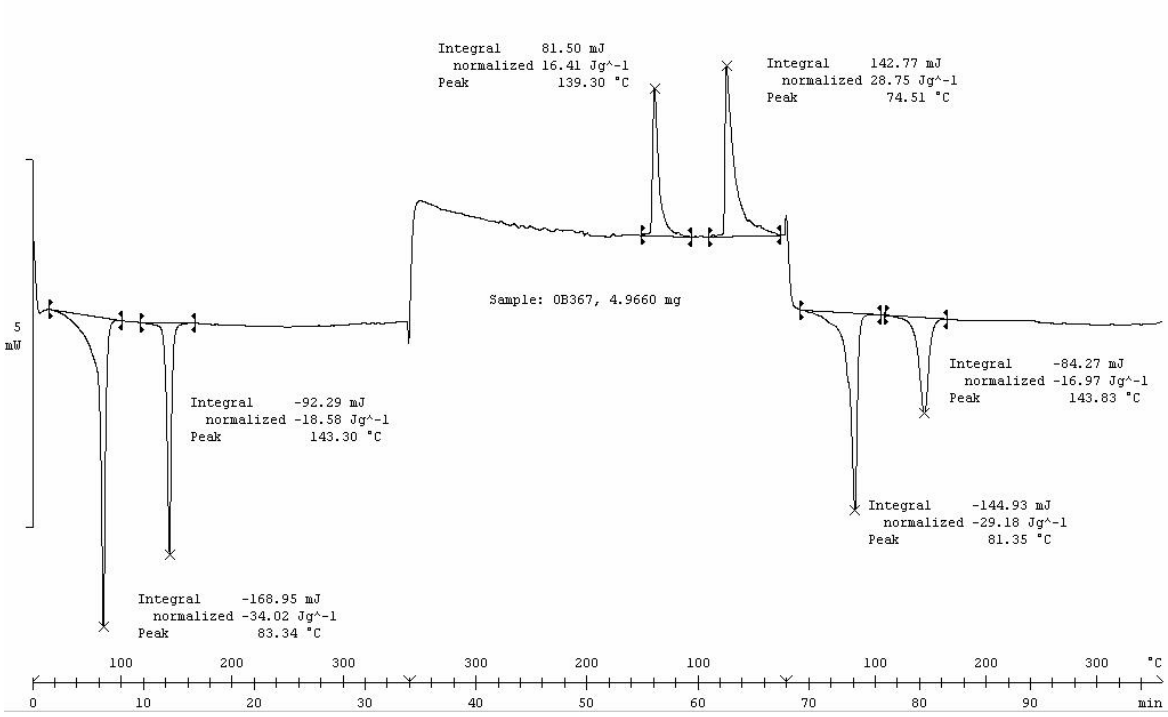


Figure S47. DSC-curve of **D2-Und-BTBT-Hex**

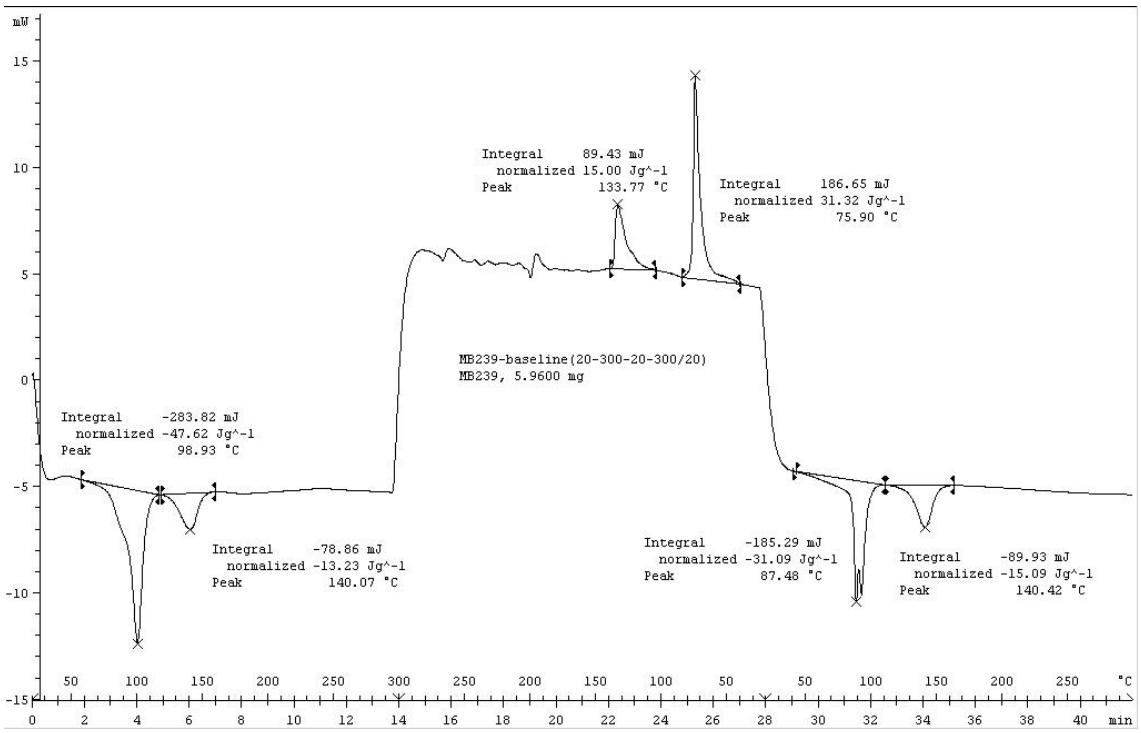


Figure S48. DSC-curve of **D2-Und-BTBT-Oct**

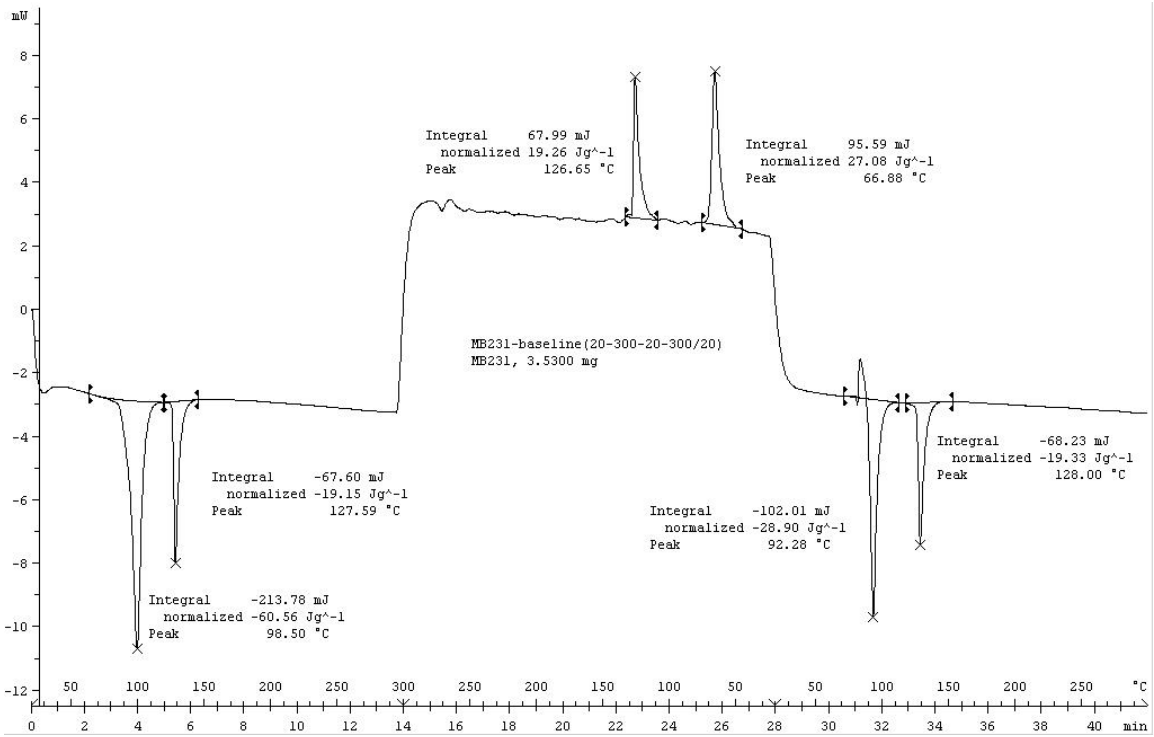


Figure S49. DSC-curve of **D2-Und-BTBT-TriD**

5. XRD curves

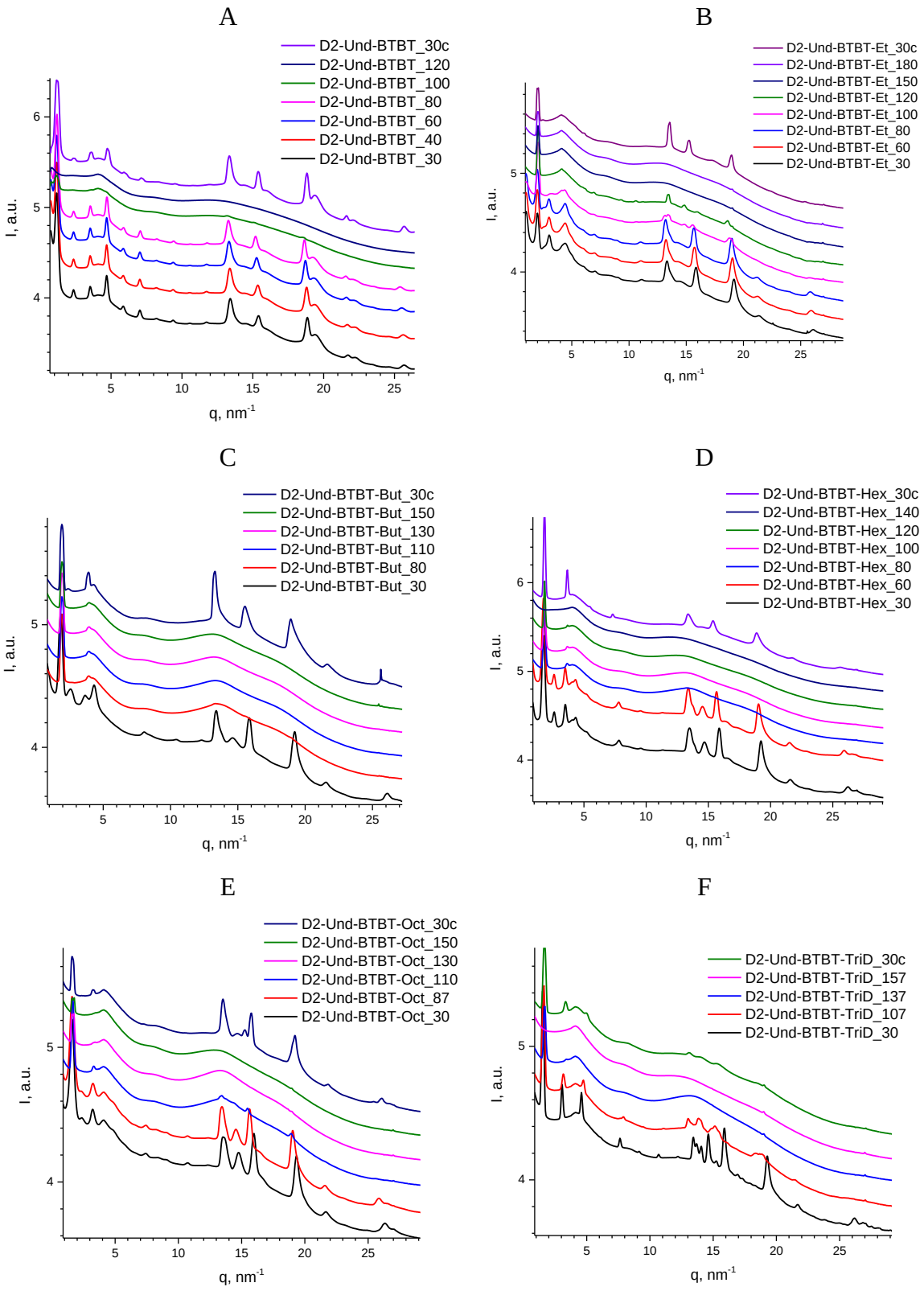


Figure S50. XRD curves for **D2-Und-BTBT** (a), **D2-Und-BTBT-Et** (b), **D2-Und-BTBT-But** (c), **D2-Und-BTBT-Hex** (d), **D2-Und-BTBT-Oct** (e), **D2-Und-BTBT-TriD** (f) at varied temperatures. Curves presented in log scale and shifted for clarity.

6. Additional electrical characteristics of the OFETs

Table S1. Electrical performance dataset for **D2-Und-BTBT**-based OFETs.

№	μ_{ave} (μ_{max})*, $cm^2V^{-1}s^{-1}$	V_{th}**, V	I_{on}/I_{off}***	Hysteresis, V
1	$7•10^{-3}$ ($1.7•10^{-2}$)	-11…-17	$10^4…10^6$	2
2	$7•10^{-5}$ ($2.9•10^{-4}$)	-8…-15	$10^1…10^2$	3
3	$3.5•10^{-4}$ ($7.5•10^{-4}$)	-3…-16	$10^2…10^4$	2
4	$2.1•10^{-5}$ ($7.7•10^{-5}$)	-9…-20	$10^1…10^2$	3
5	$3.2•10^{-4}$ ($6.9•10^{-4}$)	-4…-17	$10^2…10^4$	2

*μ_{ave} (μ_{max}) – average (maximum) saturated charge carrier mobility; **V_{th} – average threshold voltage; ***I_{on}/I_{off} – on/off ratio.

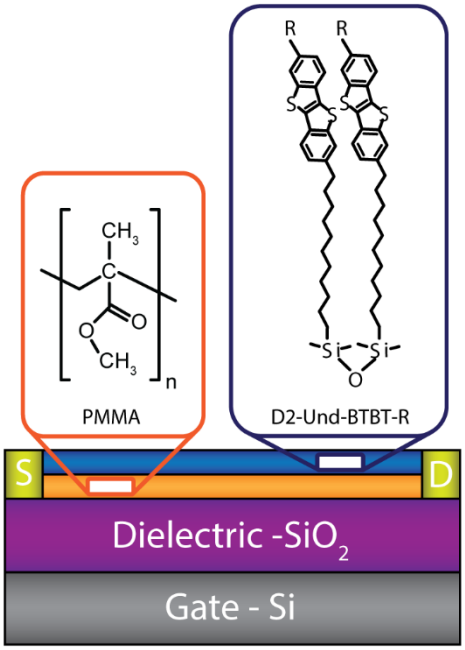


Figure S51. The schematic of the OFET-based gas sensor used in this work.

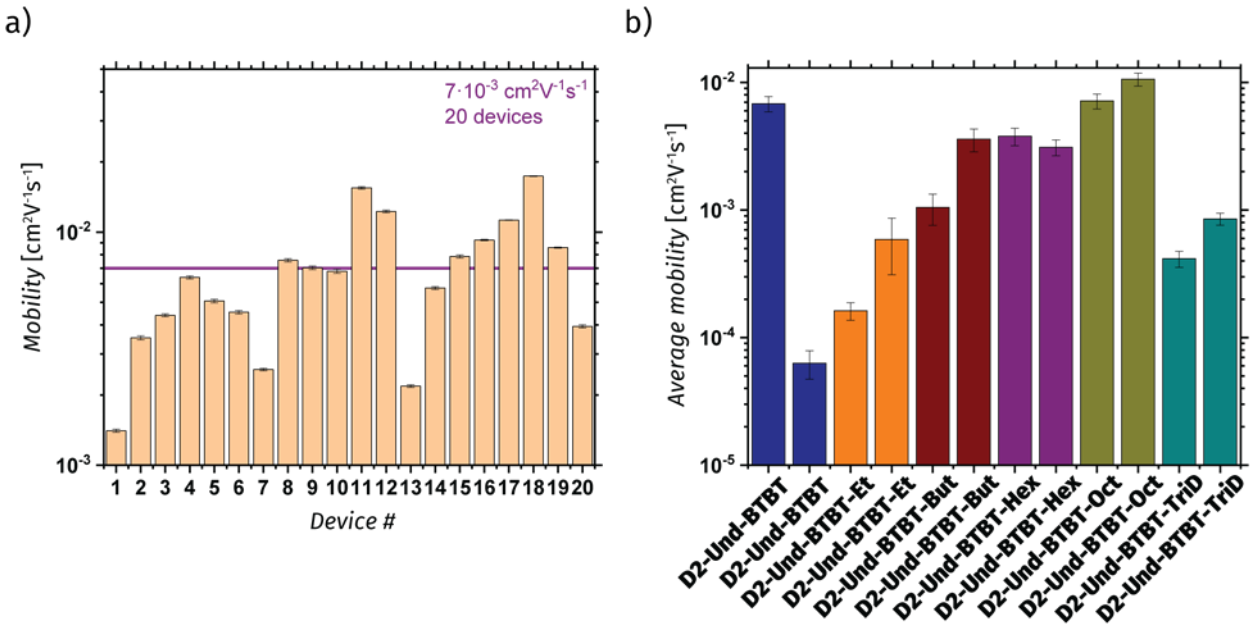


Figure S52. Additional charge carrier mobility distribution for the OFETs based on dimer **D2-Und-BTBT-Oct** (a). Dependence of the average mobility on terminal end-group length (b) of the dimers investigated – presented for two substrates for each dimer investigated.

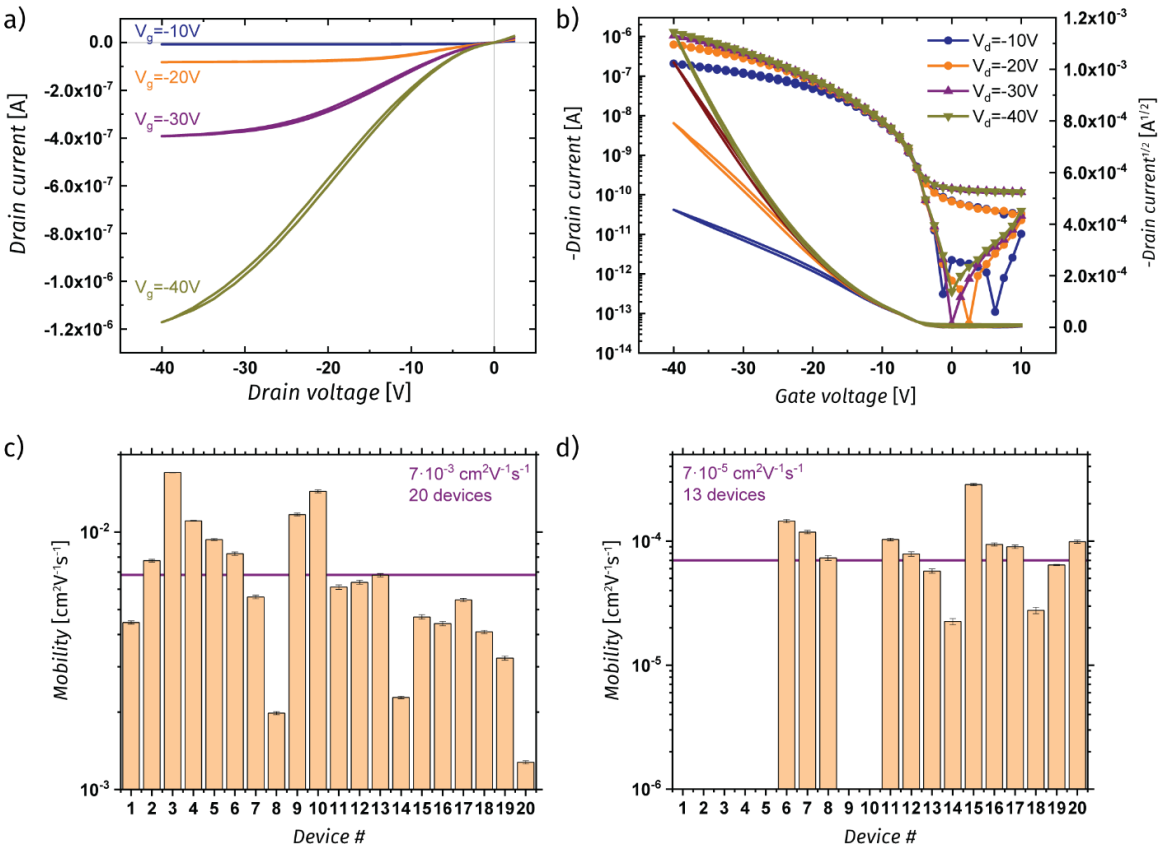


Figure S53. Typical output (a) transfer (b) characteristics and charge carrier mobility distribution (c-d) for two OFETs based on dimer **D2-Und-BTBT**.

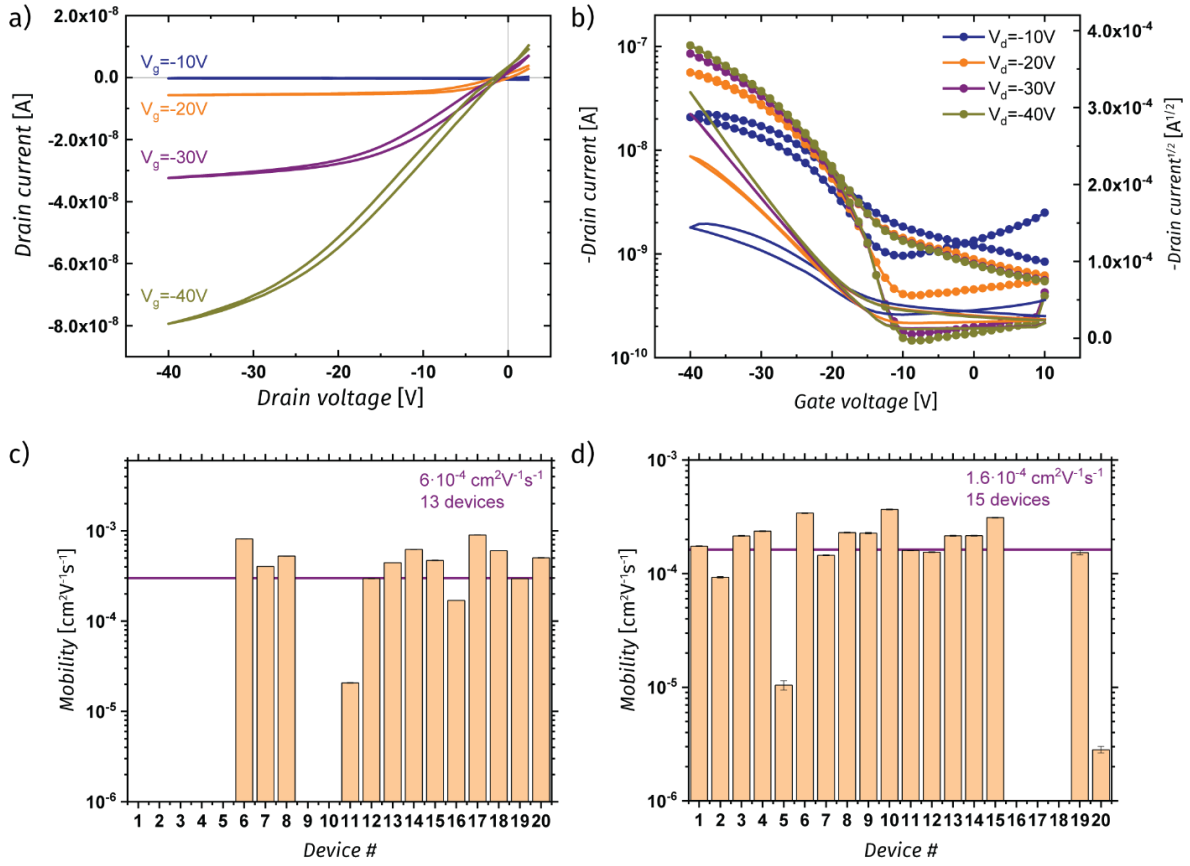


Figure S54. Typical output (a) transfer (b) characteristics and charge carrier mobility distribution (c) for two OFETs based on dimer **D2-Und-BTBT-Et**.

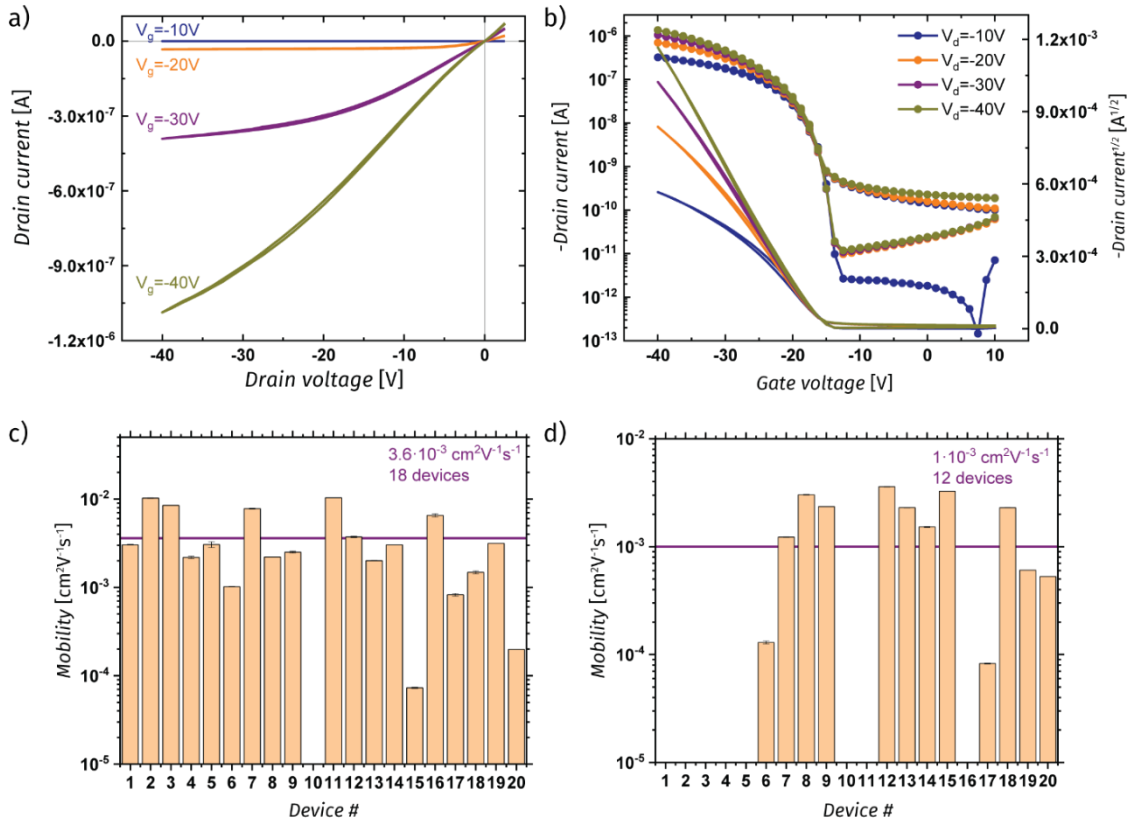


Figure S55. Typical output (a) transfer (b) characteristics and charge carrier mobility distribution (c) for two OFETs based on dimer **D2-Und-BTBT-But**.

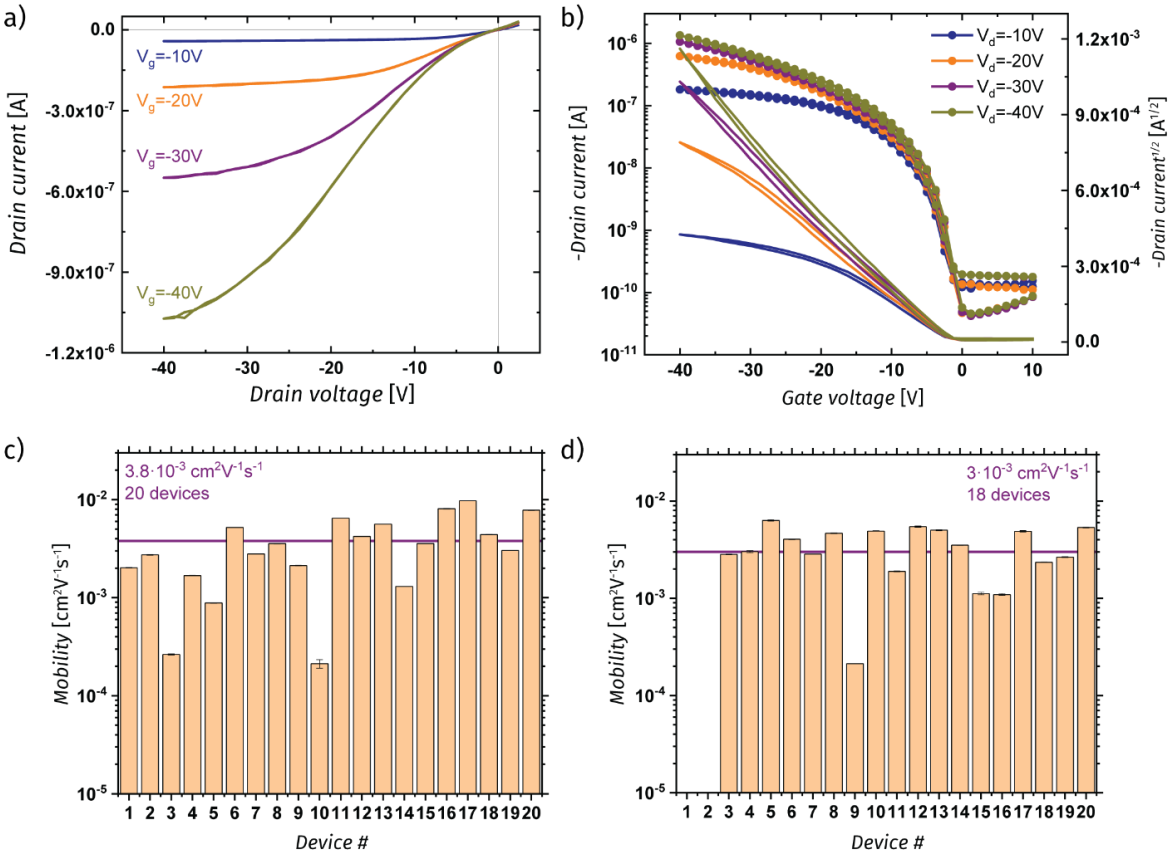


Figure S56. Typical output (a) transfer (b) characteristics and charge carrier mobility distribution (c) for two OFETs based on dimer **D2-Und-BTBT-Hex.**

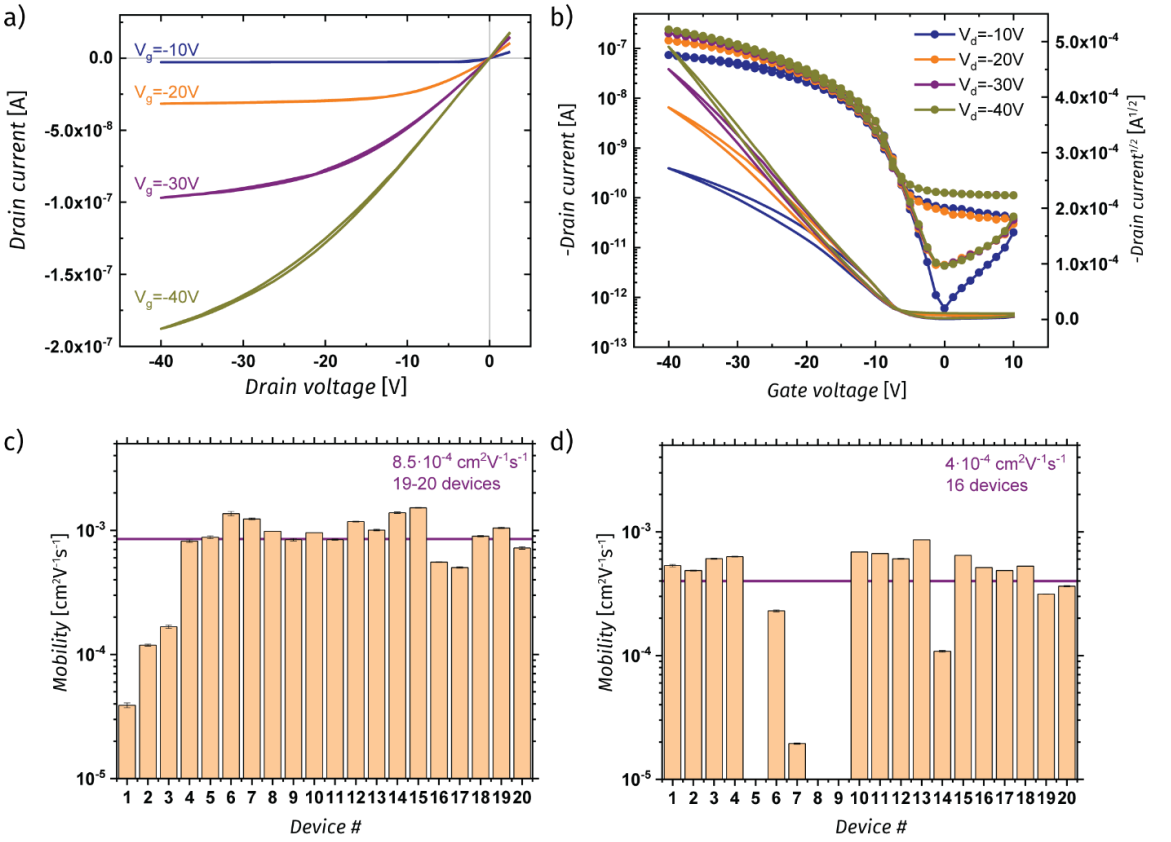


Figure S57. Typical output (a) transfer (b) characteristics and charge carrier mobility distribution (c) for two OFETs based on dimer **D2-Und-BTBT-TriD.**

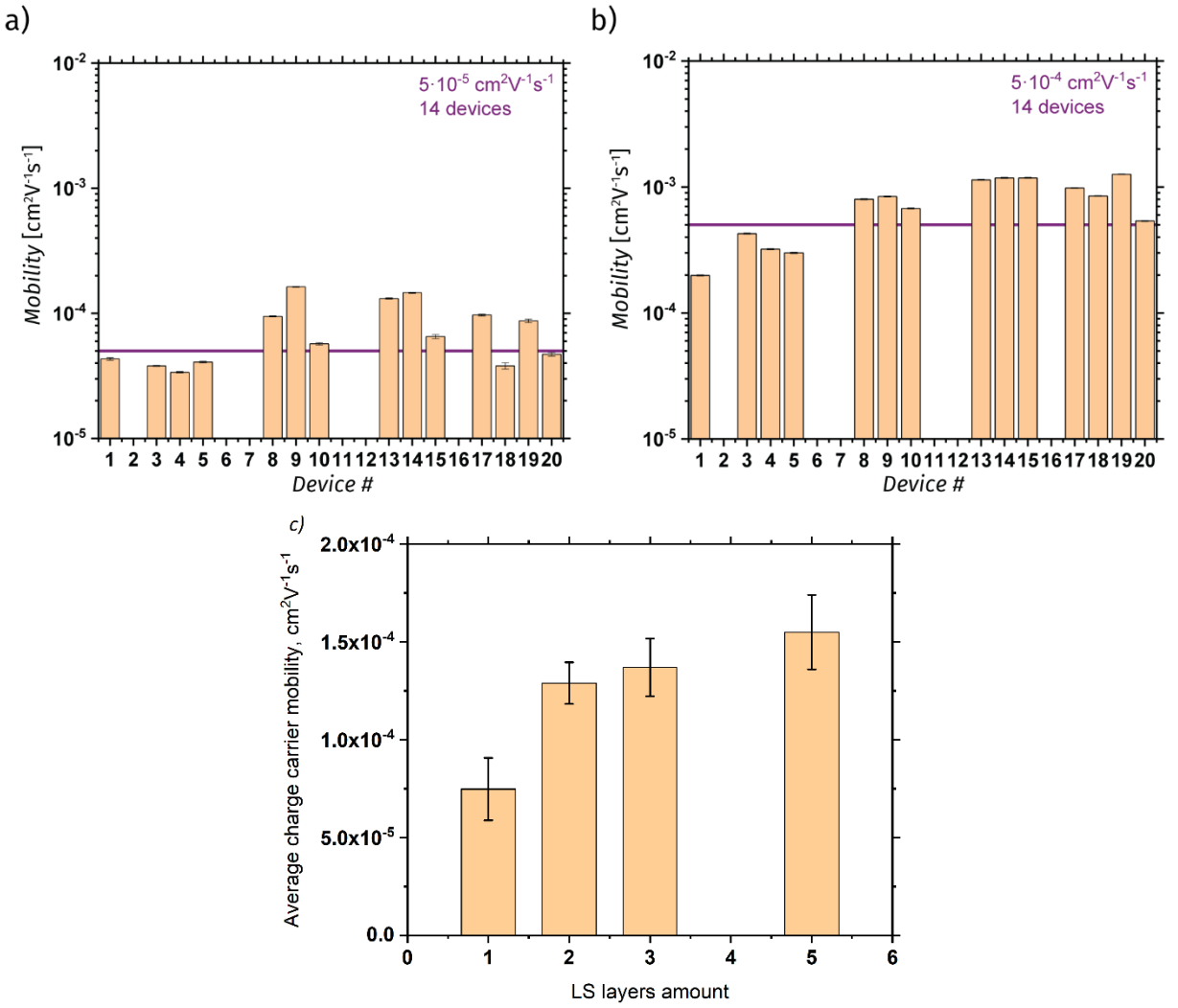


Figure S58. Charge carrier mobility distribution for the OFETs based on **D2-Und-BTBT-Et** transferred in one (a) or two (b) layers. Dependence of charge carrier mobility on LS layer amount for OFETs based on **D2-Und-BTBT-Et** (c).

7. Additional sensory characteristics of the OFETs

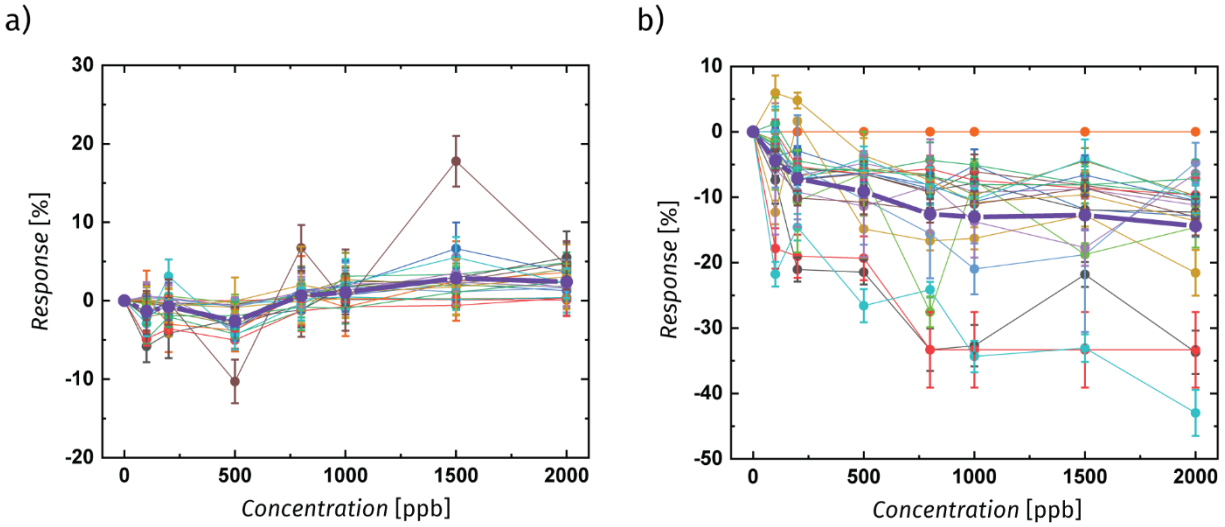


Figure S59. Typical response curves of OFETs based on dimer **D2-Und-BTBT** with high (a) and low (b) charge carrier mobility. The violet curves represent the average response curves.

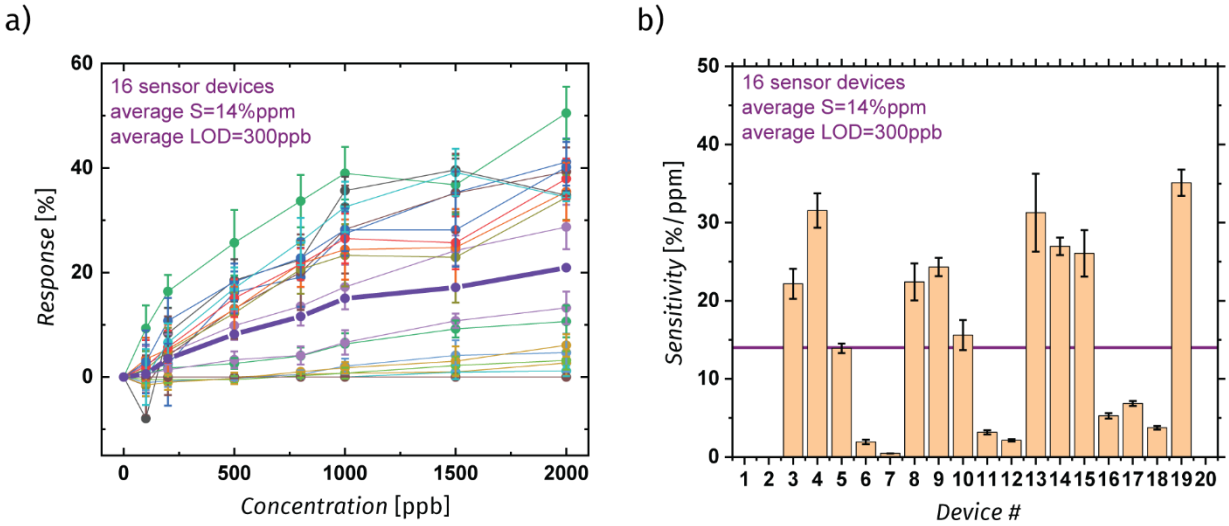


Figure S60. Typical response curves (a) and corresponding sensitivity distribution (b) of OFETs based on dimer **D2-Und-BTBT-Et**. The violet curve and horizontal line represent the average response curve and sensitivity.

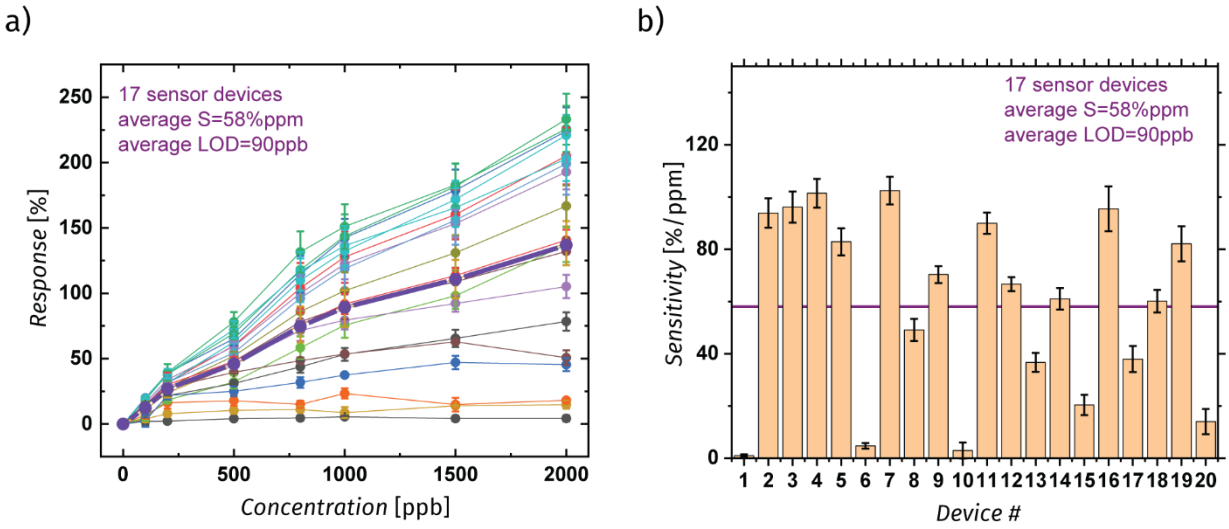


Figure S61. Typical response curves (a) and corresponding sensitivity distribution (b) of OFETs based on dimer **D2-Und-BTBT-But**. The violet curve and horizontal line represent the average response curve and sensitivity.

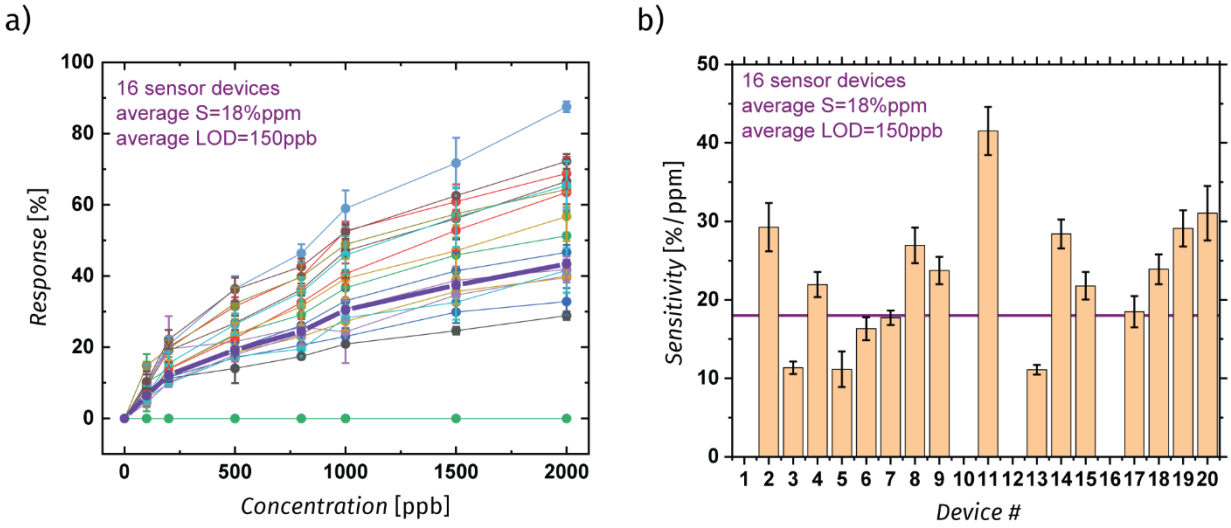


Figure S62. Typical response curves (a) and corresponding sensitivity distribution (b) of OFETs based on dimer **D2-Und-BTBT-Hex**. The violet curve and horizontal line represent the average response curve and sensitivity.

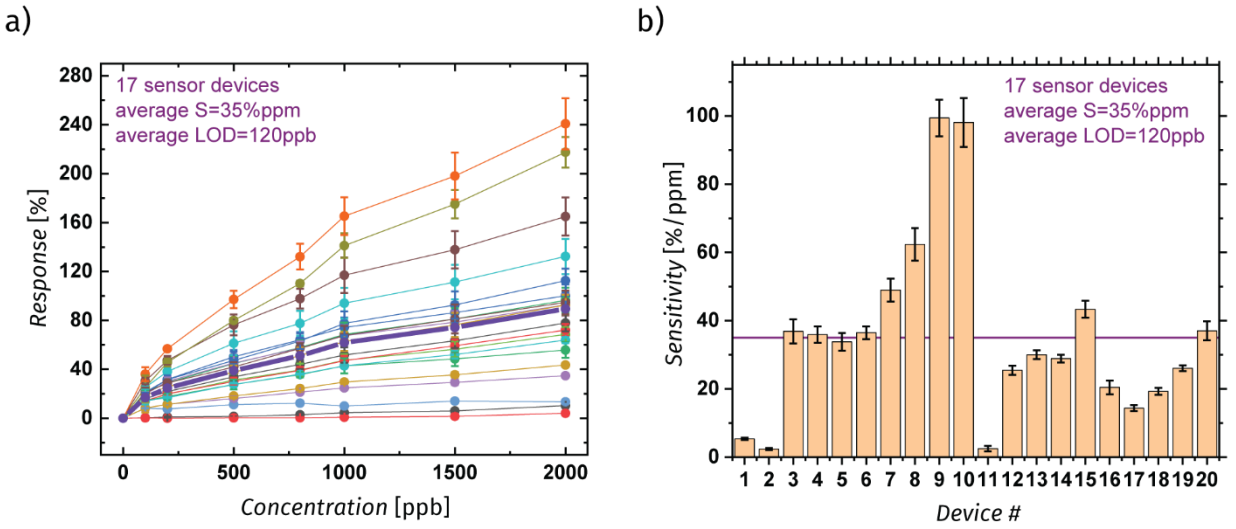


Figure S63. Typical response curves (a) and corresponding sensitivity distribution (b) of OFETs based on dimer **D2-Und-BTBT-TriD**. The violet curve and horizontal line represent the average response curve and sensitivity.

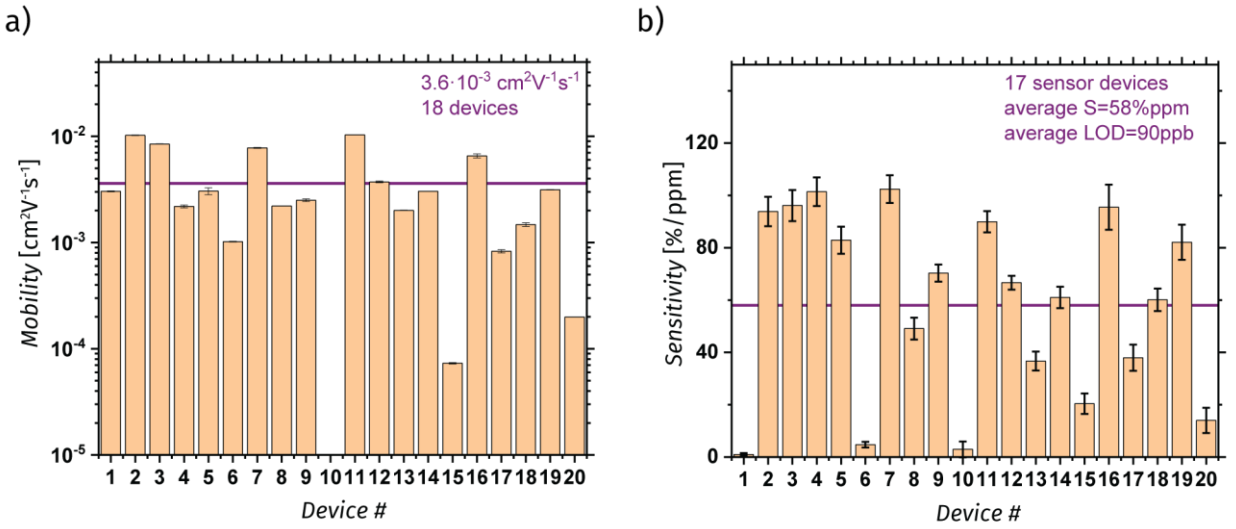


Figure S64. Distribution of charge carrier mobility (a) and sensitivity (b) for the OFTEs based on **D2-Und-BTBT-But**.

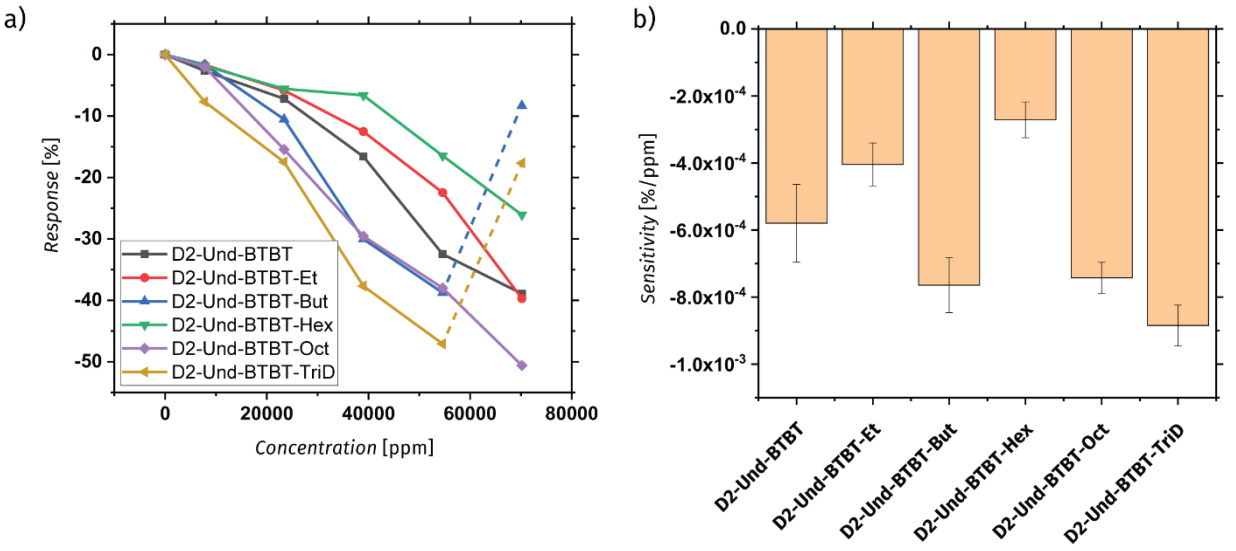


Figure S65. Typical response curves (a) and corresponding sensitivities (b) to isopropanol for the OFETs based on dimers investigated.

Table S2. Comparison of the performance for recently reported OFET-based sensors to NO_2

Active layer material	Device type	Response (Concentration)	LOD, ppm (Response)	Measured concentration range, ppm	Reference
D2-Und-BTBT-(H/Et/But/Hex/Oct/TriD)	OFET	14-134% (1 ppm)	0.05 - 0.3 (depending on alkyl chain length)	0.1−2	[this work]
PCDTBT	OFET	16% (1 ppm)	1	1−60	1
P3HT/PVK	OFET	700% (600 ppb)	0.3	0.3−30	2
a-IGZO	FET	20% (1 ppm)	0.1	0.1−5	3
ZnPc	OFET	220% (20 ppm)	0.05	0.05−20	4
PDVT-10/MOF-A	OFET	1500% (50 ppm)	0.008	0.025−50	5
TIPS-Pentacene	chemiresistor	6300% (5 ppm)	0.3 (170%)**	1-20	6
VOPc /PTCDI-Ph	chemiresistor	670% (30 ppm)	5*	5-30	7
ZnPc nano fibers	chemiresistor	94% (30 ppm)	5*	5-30	8
ZnO nanowires	chemiresistor	6200% (5 ppm)	0.5	0.5-20	9
PANI fibers	chemiresistor	80% (1 ppm)	0.050 (15%)**	1-50	10

**not discussed in the reference, estimated from the data reported.*

***not measured, but approximated LOD*

8. Additional AFM images of the OFETs

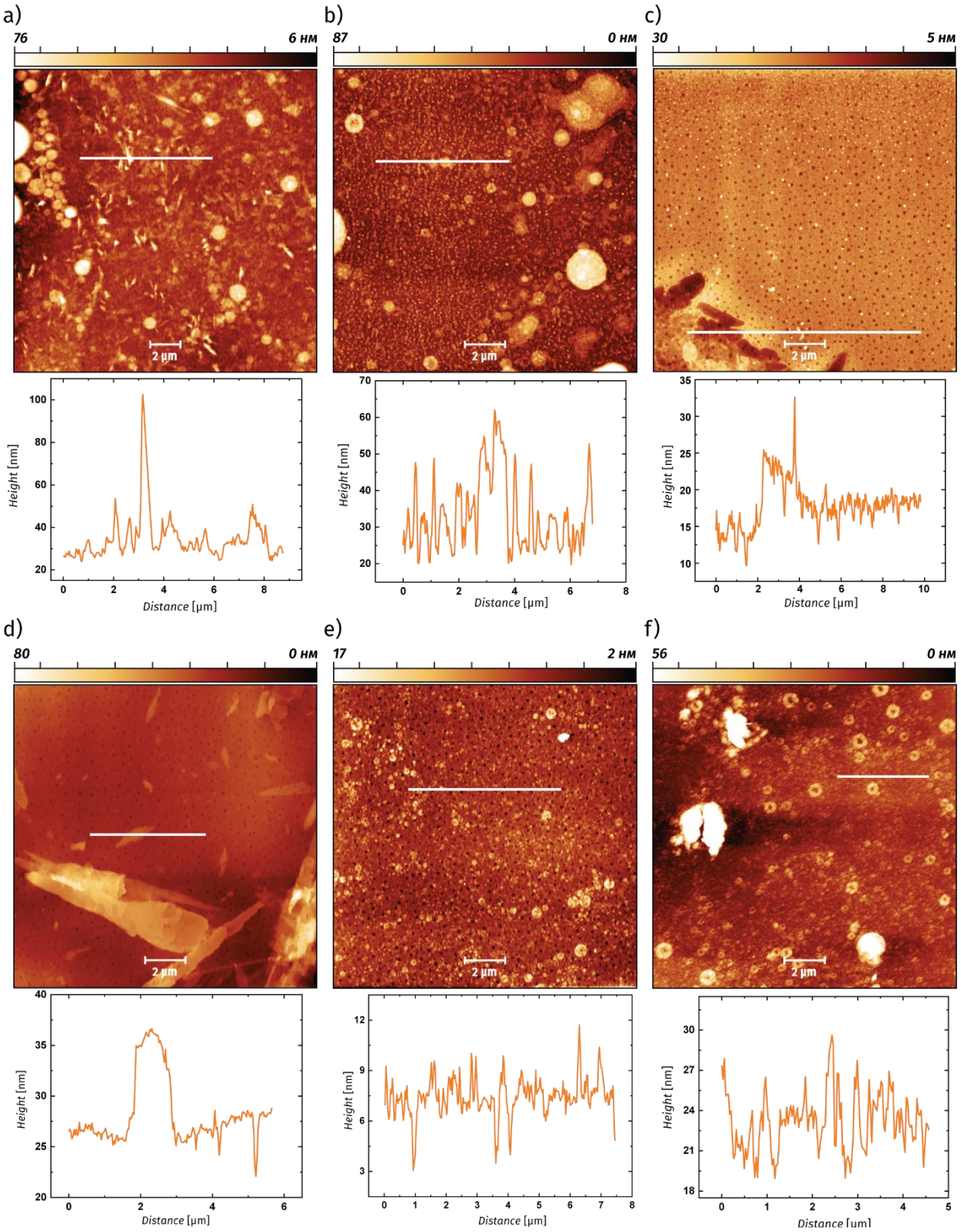


Figure S66. AFM images (topology) with corresponding cross-sections of the OFETs channels fabricated from dimer **D2-Und-BTBT** (a), **D2-Und-BTBT-Et** (b), **D2-Und-BTBT-But** (c), **D2-Und-BTBT-Hex** (d), **D2-Und-BTBT-Oct** (e), **D2-Und-BTBT-TriD** (f).

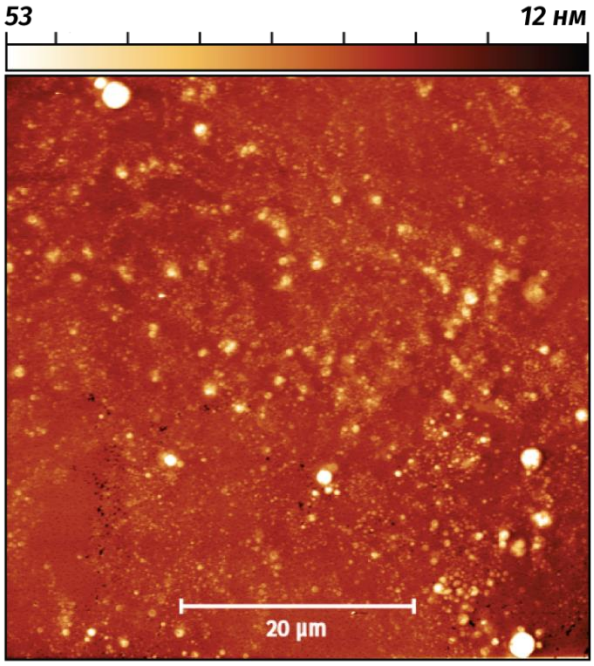


Figure S67. AFM image (topology) of the OFET fabricated from dimer **D2-Und-BTBT-Oct** at large scale.

References:

(1) Kumar, A.; Jha, P.; Singh, A.; Chauhan, A.; Gupta, S.; Aswal, D.; Muthe, K.; Gadkari, S., Modeling of gate bias controlled NO2 response of the PCDTBT based organic field effect transistor. *Chemical Physics Letters* **2018,** *698*, 7-10.

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(6) Wang, Z.; Huang, L.; Zhu, X.; Zhou, X.; Chi, L., An Ultrasensitive Organic Semiconductor NO2 Sensor Based on Crystalline TIPS-Pentacene Films. *Advanced materials* **2017,** *29* (38), 1703192.

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(10) Zhang, Y.; Kim, J. J.; Chen, D.; Tuller, H. L.; Rutledge, G. C., Electrospun polyaniline fibers as highly sensitive room temperature chemiresistive sensors for ammonia and nitrogen dioxide gases. *Advanced Functional Materials* **2014,** *24* (25), 4005-4014.