Supporting Information

Benzobischalcogeno[3,2-*c*]quinolines: Tuning Electronic and Structural Properties with Group 16 Elements

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1 Experimental Procedures

1.1 General Information

Chemicals were bought from commercial suppliers (abcr, Acros, Alfa Aesar, BLDPharm, Carbolution, Chempur, Fluka, Merck, Sigma Aldrich and TCI) and used as delivered. Anhydrous solvents were dispensed from a solvent purification system MB SPS-800. Solvents were degassed by freeze-pump-thaw technique. Deuterated solvents were bought from Eurisotop and Sigma Aldrich.

Melting points (mp) were measured in open glass capillaries on a Stuart SMP10 melting point apparatus and are uncorrected.

R_f-values were determined by analytical thin layer chromatography (TLC) on aluminium sheets coated with silica gel produced by Macherey-Nagel (ALUGRAM® Xtra SIL G/25 UV_{254}). Detections was accomplished using UV-light (254 and 365 nm) or a TLC staining solution (vanillin and ninhydrine).

Nuclear magnetic resonance (NMR) spectra were, if not mentioned otherwise, recorded at room temperature at the organic chemistry department of Heidelberg University under the supervision of Dr. J. Graf on the following spectrometers: Bruker Avance III 300 (300 MHz), Bruker Avance DRX 300 (300 MHz), Bruker Fourier 300 (300 MHz), Bruker Avance III 400 (400 MHz), Bruker Avance III 500 (500 MHz), Bruker Avance III 600 (600 MHz), Bruker Avance NEO 700 (700 MHz). Chemical shifts δ are given in ppm and coupling constants *J* in Hz. Spectra were referenced to residual solvent protons according to Fulmer *et al.*[1] The following abbreviations were used to describe the observed multiplicities: for ^{1}H NMR spectra: s = singlet, d = doublet, t = triplet, q = quartet, qui = quintet, sext = sextet, sept = septet, m = multiplet, dd = doublet of doublets, td = triplet of doublets, dt = doublet of triplets, br = broad signal; for $^{13}C\{^{1}H\}$ NMR spectra: s = quaternary carbon, d = CH carbon, t = CH_2 carbon and q = CH_3 carbon. $^{13}C\{^{1}H\}$ NMR spectra are proton decoupled and interpreted with help of DEPT- and 2D spectra. All spectra were integrated and processed using MestreNova software.

High-resolution mass spectra (HR-MS) were recorded at the chemistry department of Heidelberg University under the supervision of Dr. J. Gross on the following spectrometers: JEOL AccuTOF GCx (EI), Bruker ApexQe hybrid 9.4 T FT-ICR (ESI, MALDI, DART), Finnigan LCQ (ESI), Bruker AutoFlex Speed (MALDI) and Bruker timsTOFfleX (ESI, MALDI).

Infrared spectra were recorded from a neat powder or oil on a FT-IR spectrometer (Bruker LUMOS) with a Germanium ATR-crystal. For the most significant bands the wave numbers are given.

UV-Vis spectra were recorded on a Jasco UV-Vis V-660. Fluorescence spectra were recorded on a Jasco FP6500. Quantum yields (QY) were recorded on a PTI QuantaMaster 40 with Ulbricht Sphere.

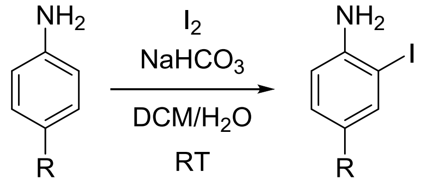
Thermogravimetric Analysis (TGA) / Differential Scanning Calorimetry (DSC) was carried out under nitrogen atmosphere using a Mettler Toledo TGA/DSC 1 device in an aluminium crucible with a heating rate of 10 K min^{-1}. The data was visualized with OriginPro 2023.

X-ray crystallography was carried out at the chemistry department of Heidelberg University under the supervision of Dr. F. Rominger on the following instruments: Bruker Smart APEX II Quazar (with Mo-microsource) and Stoe Stradivari (with Co-microsource and Pilatus detector). The structures were processed with Mercury 4.3.0.

For **flash column chromatography** silica gel (Sigma-Aldrich, pore size 60 Å, 70-230 mesh, 63-200 μm) or aluminium oxide (Honeywell, pore size 60 Å, activated, neutral) was used as stationary phase. As eluents different mixtures of petroleum ether (PE), ethyl acetate (EA) or dichloromethane (DCM) were used.

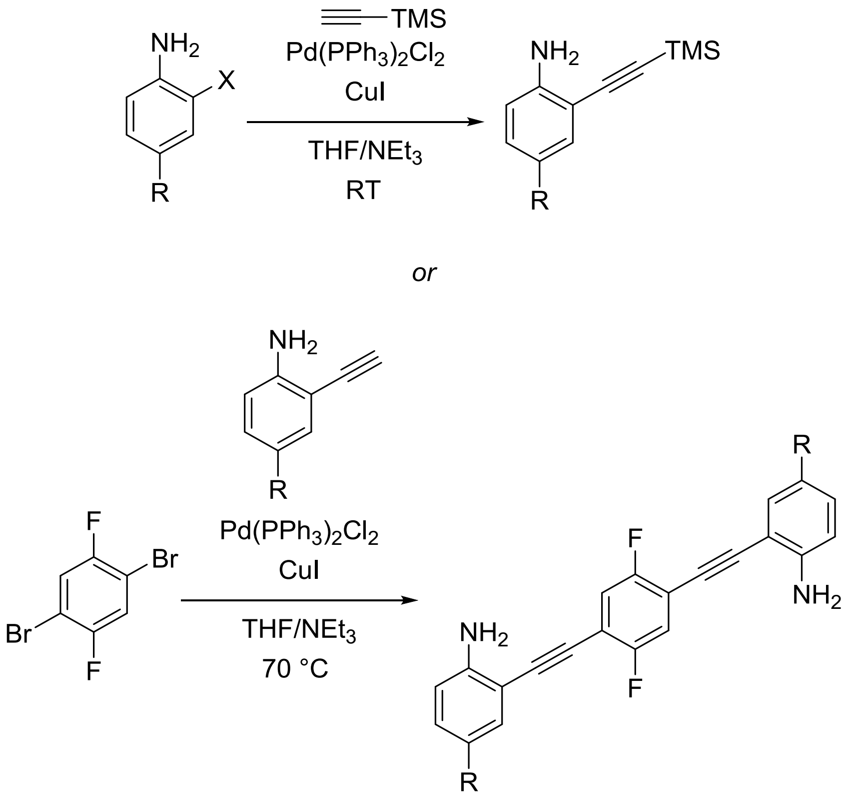
1.2 General Procedures

General Procedure 1 (GP1): Iodination of 4-alkylanilines



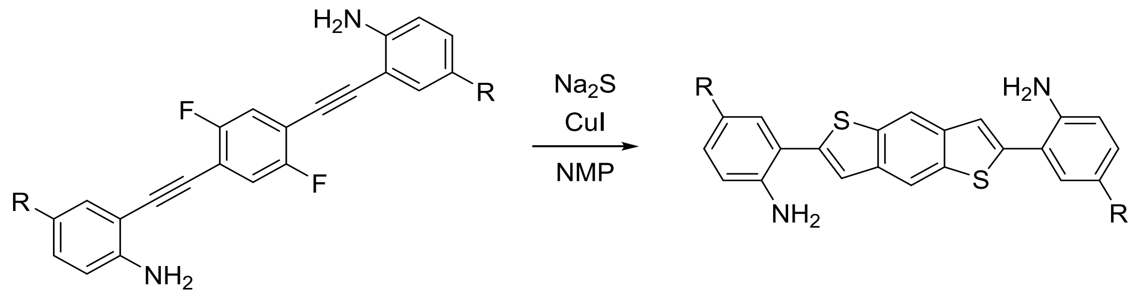
According to a slightly modified procedure of Flynn *et al.*,[2] 4-alkylaniline (1.00 eq.), iodine (1.00 eq.) and $NaHCO_3$ (1.20 eq.) were added to a mixture of DCM (25 ml) and H_2O (25 ml) in the dark. After stirring at rt over night, the reaction was quenched with a sat. solution of sodium sulfite (50 ml). The organic layer was extracted three times with DCM. The combined organic layer was then dried with Na_2SO_4, filtered and the solvent was removed *in vacuo* to obtain 4-alkyl-2-iodoanilines.

General Procedure 2 (GP2): Sonogashira cross coupling



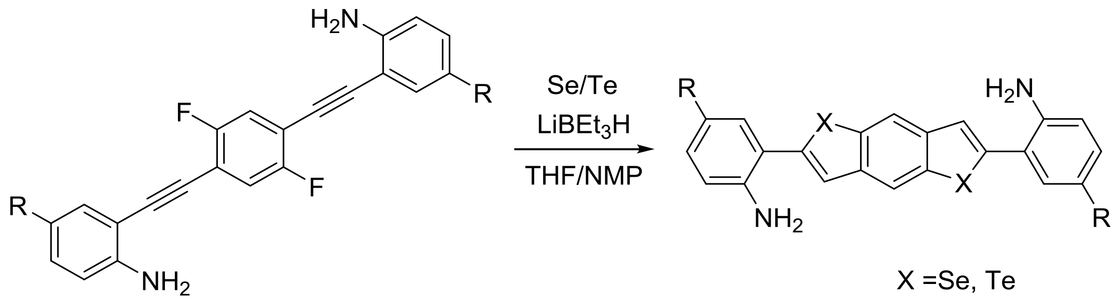
In a heat gun-dried Schlenk flask under an atmosphere of nitrogen, aryl halide (1.00 eq.), $Pd(PPh_3)_2Cl_2$ (2-5 mol %) and CuI (2-5 mol %) were dissolved in a degassed mixture of THF (20 ml) and triethylamine (20 ml). After stirring for 5 min, the corresponding alkyne (1.10-2.10 eq.) was added. The mixture was stirred at RT/70 °C overnight. The reaction was cooled and solvents were removed under reduced pressure. The crude product was purified by flash column chromatography.

General Procedure 3 (GP3): Nucleophilic hydrothiolation



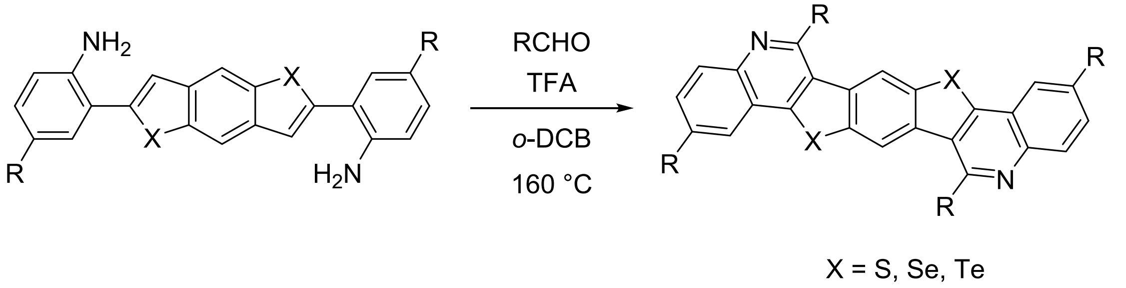
In a crimp vial, 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))dianiline (1.00 eq.), Na_2S (6.00 eq.) and CuI (5 mol %) were dissolved in *N*-methyl-2-pyrrolidon (10 ml). The mixture was stirred at 180 °C overnight. After cooling, EA and a sat. solution of NH_4Cl was added and the organic layer was washed three times with water. The combined organic layer was then dried with Na_2SO_4, filtered and the product was precipitated with methanol to obtain 2,2'-(benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)dianilines.

General Procedure 4 (GP4): Nucleophilic hydroselenation/hydrotelluration



In a heat gun-dried Schlenk flask under an atmosphere of nitrogen, selenium or tellurium (2.20 eq.) was suspended in dry THF (10 ml) and $LiBEt_3H$ (2.50 eq., 1 M in THF) was added dropwise. The solution was stirred for 15 min. Afterwards, 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))dianiline (1.00 eq.) and degassed NMP (10 ml) were added. The THF was driven out at 180 °C and the mixture was stirred at 180 °C overnight. After cooling, EA and a sat. solution of NH_4Cl was added and the organic layer was washed three times with water. The combined organic layer was then dried with Na_2SO_4, filtered and the product was precipitated with PE or filtered over a silica plug (DCM) to obtain 2,2'-(benzo[1,2-*b*:4,5-*b*']diseleno(/telluro)phene-2,6-diyl)dianilines.

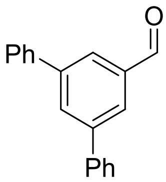
General Procedure 5 (GP5): Pictet-Spengler reaction



In a 4 ml screw-capped vial, 2,2'-(benzo[1,2-*b*:4,5-*b*']dichalcogenophene-2,6-diyl)dianiline (1.00 eq.), the corresponding aldehyde (3.00 eq.) and TFA (0.10 eq.) were dissolved in *ortho*-dichlorobenzene (1 ml). The mixture was stirred at 160 °C overnight. Pentane (2 ml) was added and the mixture was cooled to 0 °C for 1 h. The precipitate was filtered off and washed with Et_2O and pentane to yield the benzobischalcogenopheno[3,2-*c*]quinoline derivative.

1.3 Synthesis of Compounds

3,5-Diphenylbenzaldehyde (S1)

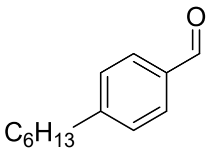


In a heatgun-dried Schlenk-flask under an atmosphere of nitrogen, 3,5-dibromobenzaldehyde (1.00 g, 3.79 mmol, 1.00 eq.), phenylboronic acid (1.85 g, 15.2 mmol, 4.00 eq.), $Pd(OAc)_2$ (85.1 mg, 379 µmol, 0.10 eq.), PPh_3 (398 mg, 1.52 µmol, 0.40 eq.) and Na_2CO_3 (1.20 g, 11.4 mmol, 3.00 eq.) were dissolved in a 1:1 mixture of degassed toluene/water (50 ml) and heated to 100 °C overnight. The reaction was cooled and water was added. The mixture was extracted with EA three times. The organic phase was dried with Na_2SO_4. Purification by flash column chromatography (silica gel, PE/EA 10:1) yielded a colorless solid (910 mg, 3.52 mmol, 93%).

^{1}H NMR (300 MHz, $CDCl_3$): δ= 10.16 (s, 1H), 8.08 (m, 3H), 7.71-7.67 (m, 4H), 7.53-7.48 (m, 4H), 7.45-7.40 (m, 2H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[3]

4-Hexylbenzaldehyde (S2)

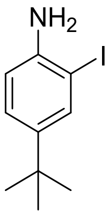


Hexylbenzene (10.0 g, 61.6 mmol, 1.00 eq.) was dissolved in trifluoroacetic acid (70 ml). Hexamethylenetetramine (9.50 g, 67.8 mmol, 1.10 eq.) was added and the mixture was stirred at 80 °C. After cooling, a sat. solution of $NaHCO_3$ was slowly added, the mixture was extracted with Et_2O three times, and the combined organic Phase was dried with Na_2SO_4. Purification by flash column chromatography (silica gel, PE/EA 100:1 → 5:1) yielded a colorless liquid (6.70 g, 35.2 mmol, 57%).

^{1}H NMR (300 MHz, $CDCl_3$): δ= 9.97 (s, 1H), 7.80 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 2.71-2.66 (m, 2H), 1.67-1.59 (m, 2H), 1.36-1.26 (m, 6H), 0.90-0.86 (m, 3H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[4]

2-Iodo-4-*tert*-butylaniline (2a)

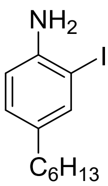


The reaction was carried out according to **GP1** with 4-*tert*-butylaniline (6.00 g, 40.2 mmol, 1.00 eq.), iodine (10.2 g, 40.2 mmol, 1.00 eq.) and $NaHCO_3$ (4.05 g, 48.3 mmol, 1.20 eq.) to obtain a dark brown liquid (11.0 g, 40.0 mmol, 99%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.62 (d, J = 2.2 Hz, 1H), 7.17 (dd, J = 8.4, 2.2 Hz, 1H), 6.70 (d, J = 8.4 Hz, 1H), 3.96 (s, 2H), 1.26 (s, 9H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[5]

2-Iodo-4-hexylaniline (2b)

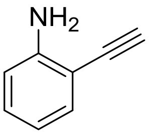


The reaction was carried out according to **GP1** with 4-hexylaniline (4.00 g, 22.6 mmol, 1.00 eq.), iodine (5.73 g, 22.6 mmol, 1.00 eq.) and $NaHCO_3$ (2.27 g, 27.1 mmol, 1.20 eq.) to obtain a dark brown liquid (6.80 g, 22.4 mmol, 99%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.46 (d, J = 1.9 Hz, 1H), 6.95 (dd, J = 8.1, 2.0 Hz, 1H), 6.68 (d, J = 8.1 Hz, 1H), 3.94 (s, 2H), 2.52 – 2.39 (m, 2H), 1.52 (td, J = 8.1, 4.4 Hz, 2H), 1.38 – 1.20 (m, 6H), 0.93 – 0.83 (m, 3H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[2]

2-Ethynylaniline (3a)

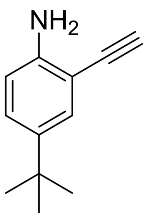


The reaction was carried out according to **GP2** with 2-iodoaniline (10.0 g, 45.7 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (160 mg, 228 µmol, 0.01 eq.), CuI (43.5 mg, 228 µmol, 0.01 eq.) and trimethylsilylacetylene (4.93 g, 50.2 mmol, 1.10 eq.) at rt. The mixture was filtered through Celite® with EA, the solvent was removed under reduced pressure and the residue was dissolved in MeOH (100 ml). K_2CO_3 (15.8 g, 114 mmol, 2.50 eq.) was added and the resulting mixture was stirred at rt overnight. Water was added and the mixture was extracted with DCM three times. The solvent was removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EA 20:1 → 5:1) yielded a light brown oil (4.49 g, 38.3 mmol, 84%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.32 (dd, J = 7.7, 1.6 Hz, 1H), 7.14 (ddd, J = 8.7, 7.4, 1.6 Hz, 1H), 6.79 – 6.61 (m, 2H), 4.25 (s, 2H), 3.38 (s, 1H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[6]

2-Ethynyl-4-*tert*-butylaniline (3b)

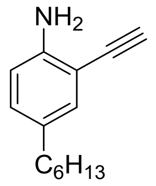


The reaction was carried out according to **GP2** with 2-iodo-4-*tert*-butylaniline **2a** (4.00 g, 14.5 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (204 mg, 291 µmol, 0.02 eq.), CuI (55.4 mg, 291 µmol, 0.02 eq.) and trimethylsilylacetylene (1.71 g, 17.5 mmol, 1.20 eq.) at rt. The mixture was filtered through Celite® with EA, the solvent was removed under reduced pressure and the residue was dissolved in MeOH (100 ml). K_2CO_3 (5.03 g, 36.4 mmol, 2.50 eq.) was added and the resulting mixture was stirred at rt overnight. Water was added and the mixture was extracted with DCM three times. The solvent was removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EA 20:1) yielded a light brown oil (1.87 g, 10.8 mmol, 74%).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.34 (d, J = 2.3 Hz, 1H), 7.19 (dd, J = 8.5, 2.4 Hz, 1H), 6.66 (d, J = 8.5 Hz, 1H), 4.13 (s, 2H), 3.36 (s, 1H), 1.26 (s, 9H) ppm.

The spectroscopic data correspond to those previously reported in the literature.[7]

2-Ethynyl-4-hexylaniline (3c)



The reaction was carried out according to **GP2** with 2-iodo-4-hexylaniline **2b** (3.60 g, 11.9 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (167 mg, 237 µmol, 0.02 eq.), CuI (45.2 mg, 237 µmol, 0.02 eq.) and trimethylsilylacetylene (1.40 g, 14.3 mmol, 1.20 eq.) at rt. The mixture was filtered through Celite® with EA, the solvent was removed under reduced pressure and the residue was dissolved in MeOH (100 ml). K_2CO_3 (4.11 g, 29.7 mmol, 2.50 eq.) was added and the resulting mixture was stirred at rt overnight. Water was added and the mixture was extracted with DCM three times. The solvent was removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EA 20:1) yielded a light brown oil (1.83 g, 9.09 mmol, 77%).

R_f: 0.36 (silica gel, PE/EA = 10:1).

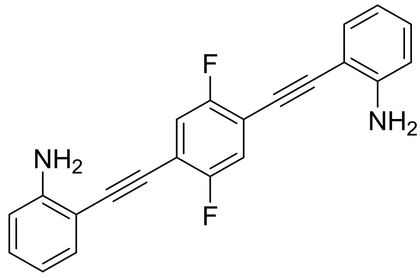
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.15 (d, J = 2.1 Hz, 1H), 6.97 (dd, J = 8.3, 2.1 Hz, 1H), 6.63 (d, J = 8.2 Hz, 1H), 4.12 (s, 2H), 3.36 (s, 1H), 2.52 – 2.40 (m, 2H), 1.61 – 1.49 (m, 2H), 1.38 – 1.23 (m, 6H), 0.95 – 0.83 (m, 3H) ppm.

$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$): δ = 146.52 (s), 132.51 (s), 132.22 (d), 130.53 (d), 114.61 (d), 106.71 (s), 82.16 (d), 81.09 (s), 34.93 (t), 31.86 (t), 31.66 (t), 28.98 (t), 22.74 (t), 14.22 (q) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{14}H_{19}N]^+$, $[M]^+$: 201.15120, found: 201.15423.

IR (ATR): ν [cm^{-1}] = 3473, 3380, 3304, 3022, 2955, 2925, 2854, 2096, 1739, 1620, 1500, 1465, 1421, 1377, 1307, 1262, 1156, 895, 820, 658, 621.

2,2'-((2,5-Difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))dianiline (5a)



The reaction was carried out according to **GP2** with 1,4-dibromo-2,5-difluorobenzene (5.00 g, 18.4 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (516 mg, 736 µmol, 0.04 eq.), CuI (140 mg, 736 µmol, 0.04 eq.) and 2-ethynylaniline **3a** (4.52 g, 38.6 mmol, 2.10 eq.) at 70 °C. The reaction was cooled and solvents were removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EA 10:1 → 5:1 → EA) yielded a light brown solid (4.82 g, 14.0 mmol, 76%).

Mp: 186-188 °C.

R_f: 0.20 (silica gel, PE/EA = 5:1).

^{1}H NMR (700 MHz, $CDCl_3$): δ = 7.37-7.36 (dd, J = 7.7 Hz, 2H), 7.23 (t, J = 7.3 Hz, 2H), 7.18 (td, J = 7.9 Hz, 2H), 6.74-6.71 (m, 4H), 4.35 (s, 4H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 158.82 (s), 157.41 (s), 148.44 (s), 132.25 (d), 130.82 (d), 118.75 (d), 118.09 (d), 114.56 (d), 113.17 (s), 106.82 (s), 94.29 (s), 87.30 (s) ppm.

^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ = -116.17 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{22}H_{14}N_2F_2]^+$, $[M]^+$: 344.11196, found: 344.11276.

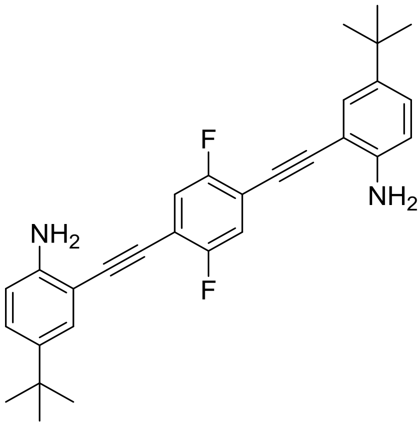
IR (ATR): ν [cm^{-1}] = 3479, 3383, 3070, 3034, 2208, 1938, 1698, 1611, 1565, 1507, 1485, 1455, 1416, 1313, 1285, 1257, 1188, 1167, 1150, 1054, 1025, 940, 881, 823, 751, 738, 634.

UV-VIS (DCM): λ_{max} [nm] = 296, 318, 376.

Fluorescence (DCM): λ_{ex} [nm] = 380, λ_{max} [nm] = 450.

Quantum yield (DCM): Φ = 66 %.

2,2'-((2,5-Difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-(*tert*-butyl)aniline) (5b)



The reaction was carried out according to **GP2** with 1,4-dibromo-2,5-difluorobenzene (1.30 g, 4.78 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (168 mg, 239 µmol, 0.05 eq.), CuI (45.5 mg, 239 µmol, 0.05 eq.) and 2-ethynyl-4-*tert*-butylaniline **3b** (1.74 g, 10.0 mmol, 2.10 eq.) at 70 °C. The reaction was cooled and solvents were removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EE 10:1 → EA) yielded a light brown solid (1.86 g, 4.07 mmol, 85%).

Mp: 211-215 °C.

R_f: 0.25 (silica gel, PE/EA = 10:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37 (d, J = 2.4 Hz, 2H), 7.26-7.21 (m, 4H), 6.69 (d, J = 8.5 Hz, 2H), 4.23 (s, 4H), 1.29 (s, 18H) ppm.

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 159.33 (s), 156.90 (s), 146.13 (s), 141.05 (s), 128.70 (d), 128.28 (d), 118.74 (d), 114.56 (d), 113.19 (s), 106.44 (s), 94.87 (s), 86.83 (s), 34.08 (s), 31.52 (q) ppm.

^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ = -116.21 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{30}H_{30}N_2F_2]^+$, $[M]^+$: 456.23716, found: 456.23676.

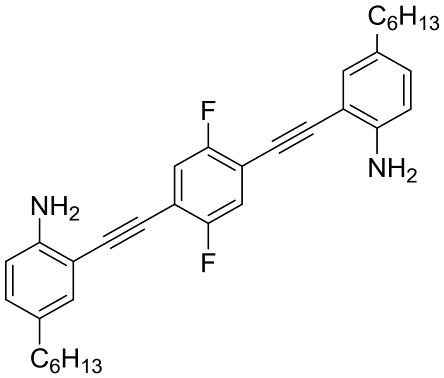
IR (ATR): ν [cm^{-1}] = 3481, 3382, 2949, 2903, 2866 ,2208, 1897, 1774, 1736, 1617, 1596, 1494, 1463, 1428, 1402, 1360, 1314, 1286, 1262, 1203, 1183, 1163, 1136, 931, 892, 878, 826, 768, 739, 694, 648, 625.

UV-VIS (DCM): λ_{max} [nm] = 295, 316, 382.

Fluorescence (DCM): λ_{ex} [nm] = 380, λ_{max} [nm] = 468.

Quantum yield (DCM): Φ = 74 %.

2,2'-((2,5-Difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-hexylaniline) (5c)



The reaction was carried out according to **GP2** with 1,4-dibromo-2,5-difluorobenzene (1.20 g, 4.41 mmol, 1.00 eq.), $Pd(PPh_3)_2Cl_2$ (155 mg, 221 µmol, 0.05 eq.), CuI (42.0 mg, 221 µmol, 0.05 eq.) and 2-ethynyl-4-hexylaniline **3c** (1.87 g, 9.27 mmol, 2.10 eq.) at 70 °C. The reaction was cooled and solvents were removed under reduced pressure. Purification by flash column chromatography (silica gel, PE/EA 10:1 → EA) yielded a light brown solid (1.31 g, 2.56 mmol, 58%).

Mp: 121-122 °C.

R_f: 0.18 (silica gel, PE/EA = 10:1).

^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.21 (t, J = 7.4 Hz, 2H), 7.18 (d, J = 2.1 Hz, 2H), 7.00 (dd, J = 8.2, 2.1 Hz, 2H), 6.67 (d, J = 8.2 Hz, 2H), 4.22 (s, 4H), 2.49 (t, J = 8.1 Hz, 4H), 1.59-1.53 (m, 4H), 1.34-1.25 (m, 12H), 0.90-0.87 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 159.08 (s), 146.34 (s), 132.68 (s), 131.64 (d), 131.17 (d), 118.83 (d), 114.72 (d), 106.76 (s), 94.61 (s), 87.03 (s), 34.98 (t), 31.89 (t), 31.71 (t), 29.01 (t), 22.77 (t), 14.27 (t) ppm.

^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ = -116.24 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{34}H_{38}N_2F_2]^+$, $[M]^+$: 512.29976, found: 512.30075.

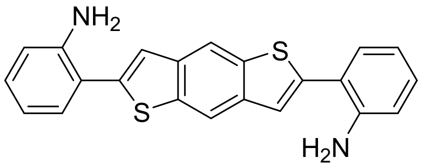
IR (ATR): ν [cm^{-1}] = 3492, 3393, 2957, 2924, 2853, 2211, 1618, 1568, 1509, 1463, 1435, 1377, 1324, 1283, 1259, 1203, 1174, 1154, 1118, 904, 871, 815, 746, 725, 694, 648, 617.

UV-VIS (DCM): λ_{max} [nm] = 295, 317, 382.

Fluorescence (DCM): λ_{ex} [nm] = 380, λ_{max} [nm] = 469.

Quantum yield (DCM): Φ = 61 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)dianiline (6a)



The reaction was carried out according to **GP3** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))dianiline **5a** (500 mg, 1.45 mmol, 1.00 eq.), Na_2S (680 mg, 8.71 mmol, 6.00 eq.) and CuI (13.8 mg, 72.6 µmol, 0.05 eq.) to yield a brown solid (528 mg, 1.42 mmol, 98%).

Mp: 297-299 °C.

^{1}H NMR (600 MHz, DMSO-d6): δ = 8.40 (s, 2H), 7.63 (s, 2H), 7.30 (d, J = 7.5 Hz, 2H), 7.11 (t, J = 7.7 Hz, 2H), 6.86 (d, J = 8.1 Hz, 2H), 6.68 (d, J = 7.3 Hz, 2H), 5.35 (s, 4H) ppm.

^{13}C{^{1}H} NMR (151 MHz, DMSO-d6): δ = 145.88 (s), 141.86 (s), 135.94 (s), 130.21 (d), 129.32 (d), 120.95 (d), 117.92 (s), 116.84 (d), 116.29 (d), 116.16 (d) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{22}H_{16}N_2S_2]^+$, $[M]^+$: 372.07494, found: 372.07446.

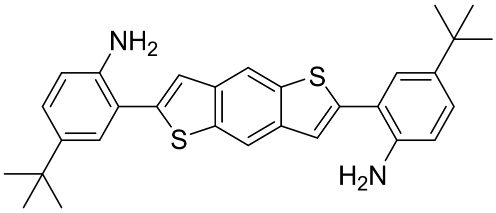
IR (ATR): ν [cm^{-1}] = 3450, 3359, 3030, 1925, 1898, 1614, 1570, 1548, 1487, 1457, 1442, 1387, 1310, 1265, 1236, 1219, 1171, 1140, 1064, 1030, 930, 875, 812, 744, 691, 660.

UV-VIS (DCM): λ_{max} [nm] = 247, 277, 352.

Fluorescence (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 429.

Quantum yield (DCM): Φ = 16 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(4-(*tert*-butyl)aniline) (6b)



The reaction was carried out according to **GP3** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-(*tert*-butyl)aniline) **5b** (1.80 g, 3.94 mmol, 1.00 eq.), Na_2S (1.85 g, 23.7 mmol, 6.00 eq.) and CuI (37.5 mg, 197 µmol, 0.05 eq.) to yield a brown solid (1.60 g, 3.30 mmol, 84%).

Mp: 107-111 °C.

R_f: 0.77 (silica gel, PE/EA = 1:1).

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.22 (s, 2H), 7.46 (s, 2H), 7.42 (d, J = 2.3 Hz, 2H), 7.25 (dd, J = 8.4, 2.3 Hz, 2H), 6.79 (d, J = 8.4 Hz, 2H), 4.08 (s, 4H), 1.34 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 142.71 (s), 141.88 (s), 141.76 (s), 138.25 (s), 137.32 (s), 127.84 (d), 126.88 (d), 121.54 (d), 119.56 (d), 116.30 (d), 116.22 (s), 34.15 (s), 31.63 (q) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{30}H_{32}N_2S_2]^+$, $[M]^+$: 484.20014, found: 484.19885.

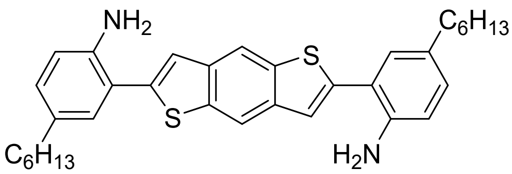
IR (ATR): ν [cm^{-1}] = 3436, 3356, 2958, 2904, 2865, 1735, 1617, 1501, 1461, 1408, 1392, 1361, 1298, 1273, 1203, 1160, 1105, 1066, 970, 872, 820, 748, 716, 693, 659, 632.

UV-VIS (DCM): λ_{max} [nm] = 246, 279, 355.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 441.

Quantum yield (DCM): Φ = 16 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(4-hexylaniline) (6c)



The reaction was carried out according to **GP3** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-hexylaniline) **5c** (1.00 g, 1.95 mmol, 1.00 eq.), Na_2S (913 mg, 11.7 mmol, 6.00 eq.) and CuI (18.6 mg, 97.5 µmol, 0.05 eq.) to yield a brown solid (990 mg, 1.83 mmol, 94%).

Mp: 158-160 °C.

R_f: 0.74 (silica gel, PE/EA = 1:1).

^{1}H NMR (700 MHz, $CDCl_3$): δ = 8.22 (s, 2H), 7.46 (s, 2H), 7.23 (d, J = 2.0 Hz, 2H), 7.02 (dd, J = 8.2, 2.1 Hz, 2H), 6.75 (d, J = 8.2 Hz, 2H), 4.05 (s, 4H), 2.58 – 2.53 (m, 4H), 1.64 – 1.57 (m, 4H), 1.39 – 1.33 (m, 12H), 0.93 – 0.86 (m, 6H) ppm.

^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$): δ = 142.49 (s), 142.08 (s), 138.29 (s), 137.34 (s), 133.51 (s), 130.83 (d), 129.77 (d), 121.51 (d), 119.99 (s), 116.48 (d), 116.30 (d), 35.17 (t), 31.92 (t), 31.86 (t), 29.15 (t), 22.80 (t), 14.27 (q) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{34}H_{40}N_2S_2]^+$, $[M]^+$: 540.26274, found: 540.26432.

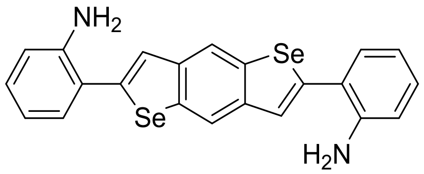
IR (ATR): ν [cm^{-1}] = 3442, 3406, 3356, 3328, 3012, 2953, 2922, 2851, 1618, 1543, 1497, 1468, 1455, 1423, 1377, 1307, 1263, 1235, 1175, 1153, 1114, 1068, 972, 888, 820, 793, 749, 720, 674, 651, 627.

UV-VIS (DCM): λ_{max} [nm] = 245, 276, 356.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 438.

Quantum yield (DCM): Φ = 17 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']diselenophene-2,6-diyl)dianiline (7a)



The reaction was carried out according to **GP4** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))dianiline **5a** (1.00 g, 2.90 mmol, 1.00 eq.), Se (504 mg, 6.39 mmol, 2.20 eq.) and $LiBEt_3H$ (7.26 ml, 7.26 mmol, 2.50 eq.) to yield a brown solid (750 mg, 1.61 mmol, 55%).

Mp: 295-297 °C.

^{1}H NMR (600 MHz, DMSO-d6): δ = 8.43 (s, 2H), 7.74 (s, 2H), 7.27 (dd, J = 7.7, 1.6 Hz, 2H), 7.09 (ddd, J = 8.7, 7.3, 1.6 Hz, 2H), 6.85 (dd, J = 8.1, 1.2 Hz, 2H), 6.67 (td, J = 7.4, 1.2 Hz, 2H), 5.31 (s, 4H) ppm.

^{13}C{^{1}H} NMR (151 MHz, DMSO-d6): δ = 145.39 (s), 144.75 (s), 140.36 (s), 137.14 (s), 130.47 (d), 129.17 (d), 124.45 (d), 121.55 (d), 120.30 (s), 117.03 (d), 116.27 (d) ppm.

^{77}Se{^{1}H} NMR (76 MHz, DMSO-d6): δ = 525.03 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{22}H_{16}N_2Se_2]^+$, $[M]^+$: 467.96384, found: 467.96526.

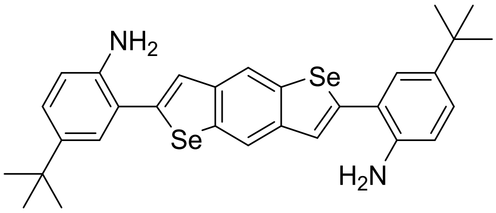
IR (ATR): ν [cm^{-1}] = 3446, 3354, 3058, 3027, 2923, 2852, 1924, 1896, 1612, 1568, 1488, 1451, 1382, 1345, 1308, 1267, 1210, 1175, 1139, 1060, 1044, 915, 881, 801, 744, 645.

UV-VIS (DCM): λ_{max} [nm] = 247, 353.

Fluorescence (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 376.

Quantum yield (DCM): Φ = 2 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']diselenophene-2,6-diyl)bis(4-(*tert*-butyl)aniline) (7b)



The reaction was carried out according to **GP4** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-*tert*-butyl)aniline **5b** (2.00 g, 4.38 mmol, 1.00 eq.), Se (761 mg, 9.64 mmol, 2.20 eq.) and $LiBEt_3H$ (10.9 ml, 10.9 mmol, 2.50 eq.) to yield a brown solid (1.27 g, 2.20 mmol, 50%).

Mp: 102-104 °C.

R_f: 0.70 (silica gel, PE/EA = 1:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.26 (s, 2H), 7.58 (s, 2H), 7.37 (d, J = 2.3 Hz, 2H), 7.23 (dd, J = 8.4, 2.4 Hz, 2H), 6.76 (d, J = 8.4 Hz, 2H), 4.05 (s, 4H) 1.33 (s, 18H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 145.42 (s), 141.82 (s), 141.48 (s), 140.55 (s), 138.51 (s), 127.93 (d), 126.82 (d), 125.43 (d), 121.69 (s), 121.55 (d), 116.21 (d), 31.65 (q), 29.86 (s) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 531.59 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{30}H_{32}N_2Se_2]^+$, $[M]^+$: 580.08904, found: 580.08124.

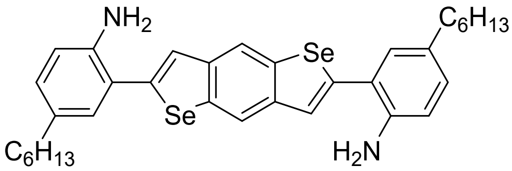
IR (ATR): ν [cm^{-1}] = 3441, 3352, 2957, 2903, 2865, 1616, 1501, 1461, 1406, 1361, 1297, 1272, 1203, 1159, 1099, 1048, 960, 876, 818, 746, 711, 692, 658, 635.

UV-VIS (DCM): λ_{max} [nm] = 242, 264, 356.

Fluorescence (DCM): λ_{ex} [nm] = 360, λ_{max} [nm] = 439.

Quantum yield (DCM): Φ = 2 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']diselenophene-2,6-diyl)bis(4-hexylaniline) (7c)



The reaction was carried out according to **GP4** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-hexyl)aniline **5c** (2.00 g, 3.90 mmol, 1.00 eq.), Se (678 mg, 8.58 mmol, 2.20 eq.) and $LiBEt_3H$ (9.75 ml, 9.75 mmol, 2.50 eq.) to yield a brown solid (813 mg, 1.28 mmol, 33%).

Mp: 165-168 °C.

R_f: 0.61 (silica gel, PE/EA = 2:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.25 (s, 2H), 7.58 (s, 2H), 7.18 (d, J = 2.1 Hz, 2H), 7.01 (dd, J = 8.1, 2.1 Hz, 2H), 6.74 (d, J = 8.1 Hz, 2H), 4.01 (s, 4H), 2.59 – 2.50 (m, 4H), 1.67 – 1.54 (m, 4H), 1.38 – 1.25 (m, 12H), 0.92 – 0.87 (m, 6H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 145.12 (s), 141.66 (s), 140.56 (s), 138.48 (s), 133.54 (s), 130.92 (d), 129.69 (d), 125.38 (d), 122.08 (s), 121.54 (d), 116.47 (d), 35.23 (t), 31.91 (t), 31.85 (t), 29.15 (t), 22.79 (t), 14.26 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 531.85 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{34}H_{40}N_2Se_2]^+$, $[M]^+$: 636.1516, found: 636.1506.

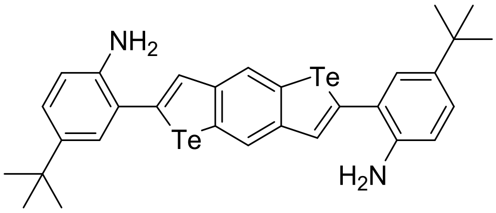
IR (ATR): ν [cm^{-1}] = 3437, 3402, 3350, 3323, 2952, 2923, 2852, 1618, 1552, 1496, 1453, 1423, 1376, 1304, 1262, 1232, 1178, 1153, 1115, 1049, 965, 889, 820, 749, 722, 659, 626.

UV-VIS (DCM): λ_{max} [nm] = 249, 286, 357.

Fluorescence (DCM): λ_{ex} [nm] = 360, λ_{max} [nm] = 446.

Quantum yield (DCM): Φ = 3 %.

2,2'-(Benzo[1,2-*b*:4,5-*b*']ditellurophene-2,6-diyl)bis(4-(*tert*-butyl)aniline) (8)



The reaction was carried out according to **GP4** with 2,2'-((2,5-difluoro-1,4-phenylene)bis(ethyne-2,1-diyl))bis(4-*tert*-butyl)aniline **5b** (500 mg, 1.10 mmol, 1.00 eq.), Te (307 mg, 2.41 mmol, 2.20 eq.) and $LiBEt_3H$ (2.74 ml, 2.74 mmol, 2.50 eq.) to yield a brown solid (186 mg, 275 µmol, 25%).

Mp: 290-292 °C.

$\mathbf{R}_f$: 0.70 (silica gel, PE/EA = 1:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.30 (s, 2H), 7.88 (s, 2H), 7.39 (d, J = 2.3 Hz, 2H), 7.21 (dd, J = 8.3, 2.3 Hz, 2H), 6.76 (d, J = 8.3 Hz, 2H), 3.93 (s, 4H), 1.33 (s, 18H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 145.55 (s), 142.46 (s), 140.34 (s), 137.54 (s), 133.74 (d), 130.64 (d), 129.97 (s), 126.87 (d), 126.37 (s), 126.29 (d), 116.92 (s), 34.21 (s), 31.68 (q) ppm.

^{125}Te{^{1}H} NMR (126 MHz, $CDCl_3$): δ = 756.36 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{30}H_{32}N_2Te_2]^+$, $[M]^+$: 680.0684, found: 680.0639.

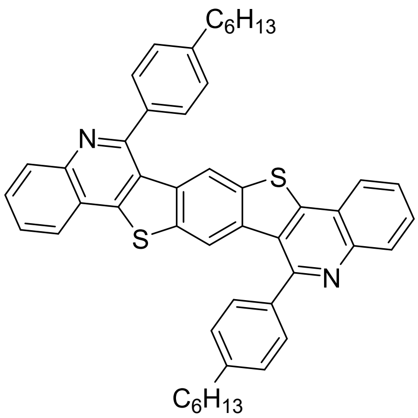
IR (ATR): ν [cm^{-1}] = 3434, 3357, 2950, 2902, 2867, 1871, 1614, 1545, 1498, 1461, 1444, 1411, 1391, 1361, 1294, 1272, 1235, 1203, 1173, 1156, 1048, 959, 876, 854, 817, 741, 705, 688, 655, 635.

UV-VIS (DCM): λ_{max} [nm] = 283, 365, 373, 404.

Fluorescence (DCM): λ_{ex} [nm] = 375, λ_{max} [nm] = 450.

Quantum yield (DCM): Φ = <1 %.

9aa



The reaction was carried out according to **GP5** with **6a** (100 mg, 268 µmol, 1.00 eq.), 4-hexylbenzaldehyde (153 mg, 805 µmol, 3.00 eq.) and TFA (2.63 mg, 26.9 µmol, 0.10 eq.) to yield a light brown solid (94.0 mg, 132 µmol, 49%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.30 – 8.25 (m, 2H), 8.11 – 8.06 (m, 2H), 7.78 (ddd, J = 8.3, 6.9, 1.4 Hz, 2H), 7.71 (s, 2H), 7.65 (ddd, J = 8.2, 6.9, 1.1 Hz, 2H), 7.62-7.61 (m, 4H), 7.49 – 7.47 (m, 4H), 2.86 (t, J = 7.5 Hz, 4H), 1.82 (m, 4H), 1.54 – 1.42 (m, 12H), 1.03 – 0.95 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.83 (s), 148.64 (s), 144.75 (s), 144.39 (s), 137.99 (s), 136.48 (s), 134.26 (s), 130.43 (d), 130.07 (d), 129.39 (d), 128.67 (d), 127.16 (d), 126.28 (s), 123.97 (d), 123.46 (s), 118.57 (d), 36.15 (t), 32.11 (t), 31.77 (t), 29.14 (t), 22.95 (t), 14.44 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{48}H_{44}N_2S_2]^+$, $[M]^+$: 712.2940, found: 712.29390.

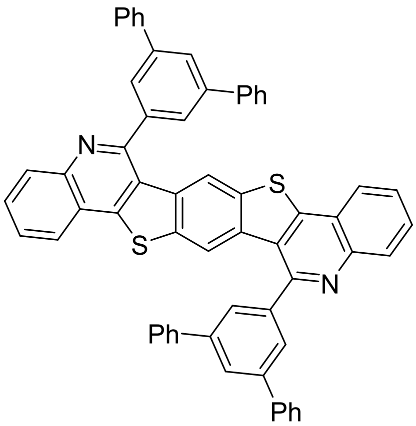
IR (ATR): ν [cm^{-1}] = 3047, 2956, 2923, 2852, 1611, 1556, 1488, 1461, 1394, 1301, 1277, 1216, 1182, 1116, 1079, 1023, 999, 923, 867, 848, 816, 756, 645, 621.

UV-VIS (DCM): λ_{max} [nm] = 273, 308, 334, 353, 370.

Fluorescence (DCM): λ_{ex} [nm] = 335, λ_{max} [nm] = 385.

Quantum yield (DCM): Φ = 4 %.

9ab



The reaction was carried out according to **GP5** with **6a** (100 mg, 268 µmol, 1.00 eq.), 3,5-diphenylbenzaldehyde (208 mg, 805 µmol, 3.00 eq.) and TFA (2.63 mg, 26.9 µmol, 0.10 eq.) to yield a beige solid (126 mg, 148 µmol, 55%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.30 (d, J = 8.3 Hz, 2H), 8.11-8.08 (m, 6H), 7.98-7.97 (m, 4H), 7.79-7.77 (m, 10H), 7.66-7.64 (m, 2H) 7.49-7.46 (m, 8H), 7.40 – 7.38 (m, 4H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.21 (s), 149.16 (s), 144.70 (s), 142.88 (s), 141.37 (s), 140.88 (s), 136.73 (s), 134.22 (s), 130.38 (d), 130.28 (d), 129.09 (d), 127.91 (d), 127.56 (d), 127.42 (d), 127.28 (d), 126.77 (d), 125.98 (s), 124.12 (d), 123.50 (s), 118.68 (d) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{60}H_{36}N_2S_2]^+$, $[M]^+$: 848.23140, found: 848.23220.

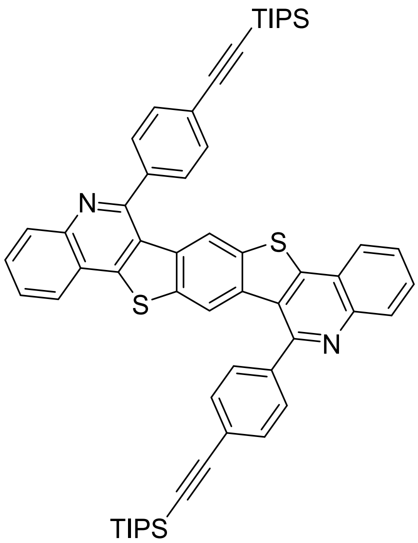
IR (ATR): ν [cm^{-1}] = 3054, 3031, 1594, 1555, 1486, 1423, 1396, 1363, 1295, 1274, 1205, 1156, 1076, 1028, 937, 886, 869, 857, 832, 757, 735, 713, 698, 667, 644, 614.

UV-VIS (DCM): λ_{max} [nm] = 255, 311, 334, 351.

Fluorescence (DCM): λ_{ex} [nm] = 310, λ_{max} [nm] = 387.

Quantum yield (DCM): Φ = 3 %.

9ac



The reaction was carried out according to **GP5** with **6a** (100 mg, 268 µmol, 1.00 eq.), 4-(triisopropylsilyethinyl)benzaldehyde (231 mg, 805 µmol, 3.00 eq.) and TFA (2.63 mg, 26.9 µmol, 0.10 eq.) to yield a light brown solid (100 mg, 110 µmol, 41%).

Mp: >300 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.23 – 8.16 (m, 2H), 8.08 – 8.06 (m, 2H), 7.90 (s, 2H), 7.77 – 7.70 (m, 6H), 7.68 – 7.58 (m, 6H), 1.22 – 1.13 (m, 42H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 155.77 (s), 149.12 (s), 144.80 (s), 140.62 (s), 136.66 (s), 134.18 (s), 132.89 (d), 130.50 (d), 130.28 (d), 129.00 (d), 127.49 (d), 125.74 (s), 124.84 (s), 124.09 (d), 123.49 (s), 118.57 (d), 106.98 (s), 92.53 (s), 18.93 (d), 11.60 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{58}H_{61}N_2S_2Si_2]^+$, $[M+H]^+$: 905.38090, found: 905.37980.

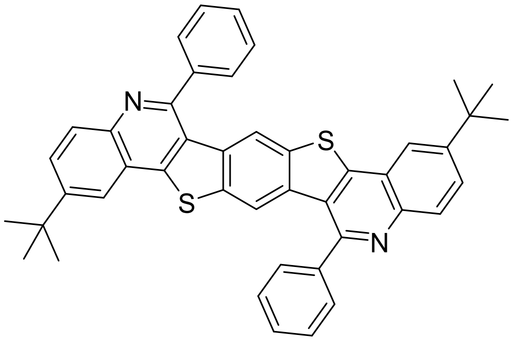
IR (ATR): ν [cm^{-1}] = 2941, 2890, 2863, 2153, 1605, 1556, 1487, 1461, 1401, 1363, 1302, 1277, 1215, 1179, 1104, 1078, 1019, 996, 922, 883, 832, 776, 755, 668, 618.

UV-VIS (DCM): λ_{max} [nm] = 254, 274, 301, 333, 354.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 408.

Quantum yield (DCM): Φ = 2 %.

9ba



The reaction was carried out according to **GP5** with **6b** (50 mg, 103 µmol, 1.00 eq.), benzaldehyde (32.8 mg, 309 µmol, 3.00 eq.) and TFA (1.01 mg, 10.3 µmol, 0.10 eq.) to yield a light yellow solid (66.0 mg, 100 µmol, 97%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.22 (d, J = 8.8 Hz, 2H), 8.01 (d, J = 2.1 Hz, 2H), 7.89 (dd, J = 8.8, 2.2 Hz, 2H), 7.73 – 7.64 (m, 12H), 1.49 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 155.97 (s), 150.56 (s), 148.71 (s), 143.10 (s), 140.87 (s), 136.52 (s), 134.31 (s), 130.69 (d), 129.98 (d), 129.37 (d), 129.28 (d), 129.10 (d), 128.85 (d), 127.86 (d), 126.09 (s), 123.13 (s), 119.18 (d), 118.44 (d), 35.36 (s), 31.42 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{44}H_{36}N_2S_2]^+$, $[M]^+$: 656.23140, found: 656.23120.

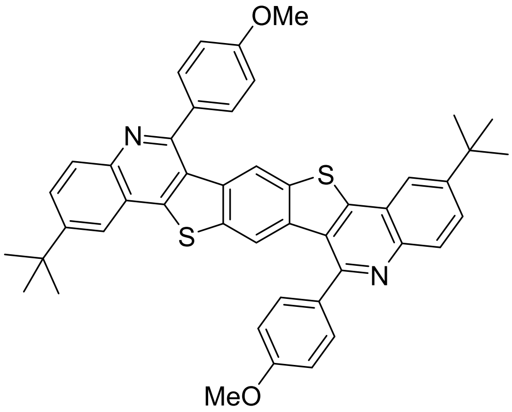
IR (ATR): ν [cm^{-1}] = 3055, 2955, 2903, 2866, 1950, 1723, 1703, 1621, 1553, 1494, 1457, 1440, 1402, 1387, 1364, 1302, 1282, 1253, 1219, 1154, 1127, 1104, 1080, 1026, 951, 917, 866, 842, 791, 767, 750, 707, 670, 646, 617.

UV-VIS (DCM): λ_{max} [nm] = 274, 310, 335, 353, 371.

Fluorescence (DCM): λ_{ex} [nm] = 330, λ_{max} [nm] = 380.

Quantum yield (DCM): Φ = 5 %.

9bb



The reaction was carried out according to **GP5** with **6b** (100 mg, 206 µmol, 1.00 eq.), 4-methoxybenzaldehyde (84.3 mg, 619 µmol, 3.00 eq.) and TFA (2.02 mg, 20.6 µmol, 0.10 eq.) to yield a beige solid (63.0 mg, 87.9 µmol, 43%).

Mp: >300 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.21 (dd, J = 8.8, 0.5 Hz, 2H), 8.01 (dd, J = 2.1, 0.6 Hz, 2H), 7.91 (s, 2H), 7.91 – 7.84 (m, 2H), 7.69 – 7.64 (m, 4H), 7.23 – 7.14 (m, 4H), 4.02 (s, 6H), 1.49 (s, 18H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 160.64 (s), 155.80 (s), 150.38 (s), 148.72 (s), 143.23 (s), 136.51 (s), 134.49 (s), 133.42 (s), 130.35 (d), 129.94 (d), 128.98 (d), 126.23 (s), 123.05 (s), 119.17 (d), 118.52 (d), 114.65 (d), 55.75 (q), 35.35 (s), 31.44 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{46}H_{40}N_2S_2]^+$, $[M]^+$: 716.25260, found: 716.25220.

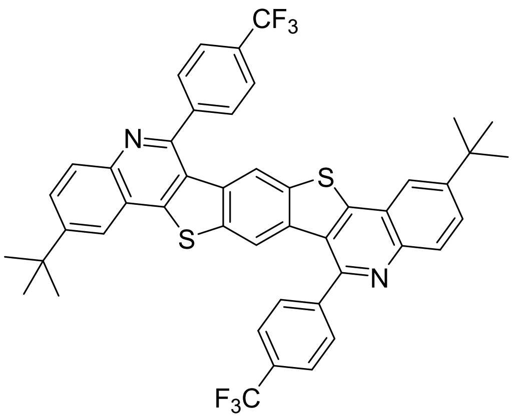
IR (ATR): ν [cm^{-1}] = 2961, 2906, 2869, 2836, 1606, 1577, 1551, 1513, 1493, 1462, 1434, 1383, 1364, 1302, 1245, 1219, 1173, 1107, 1081, 1032, 952, 867, 838, 812, 761, 703, 663, 649, 626.

UV-VIS (DCM): λ_{max} [nm] = 274, 306, 335, 354, 372.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 390.

Quantum yield (DCM): Φ = 4 %.

9bc



The reaction was carried out according to **GP5** with **6b** (50 mg, 103 µmol, 1.00 eq.), 4-trifluoromethylbenzaldehyde (53.9 mg, 309 µmol, 3.00 eq.) and TFA (1.01 mg, 10.3 µmol, 0.10 eq.) to yield a beige solid (66.0 mg, 83.2 µmol, 81%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.21 (d, J = 8.8 Hz, 2H), 8.04 (d, J = 2.1 Hz, 2H), 7.96 (d, J = 8.0 Hz, 4H), 7.92 (dd, J = 8.8, 2.1 Hz, 2H), 7.88 (d, J = 8.0 Hz, 4H), 7.76 (s, 2H), 1.50 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 154.13 (s), 151.20 (s), 149.22 (s), 144.47 (s), 143.03 (s), 136.65 (s), 134.00 (s), 129.96 (d), 129.54 (d), 126.29 (q), 125.44 (s), 123.19 (s), 119.27 (d), 118.18 (d), 35.44 (s), 31.40 (q) ppm.

^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ = -62.40 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{46}H_{34}F_6N_2S_2]^+$, $[M]^+$: 792.20620, found: 792.20550.

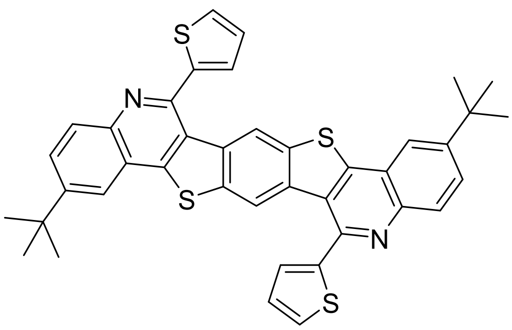
IR (ATR): ν [cm^{-1}] = 2966, 2908, 2870, 1928, 1616, 1549, 1491, 1404, 1384, 1365, 1321, 1251, 1217, 1168, 1127, 1105, 1082, 1073, 1062, 1018, 952, 845, 828, 806, 762, 703, 677, 647, 629.

UV-VIS (DCM): λ_{max} [nm] = 276, 313, 334, 353, 370.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 386.

Quantum yield (DCM): Φ = 4 %.

9bd



The reaction was carried out according to **GP5** with **6b** (100 mg, 206 µmol, 1.00 eq.), thiophen-2-carbaldehyde (69.4 mg, 619 µmol, 3.00 eq.) and TFA (2.02 mg, 20.6 µmol, 0.10 eq.) to yield a black solid (134 mg, 200 µmol, 97%).

Mp: >300 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.22 (d, J = 8.8 Hz, 2H), 8.03 (s, 2H), 8.01 (d, J = 2.1 Hz, 2H), 7.89 (dd, J = 8.9, 2.2 Hz, 2H), 7.68 (dd, J = 5.1, 1.2 Hz, 2H), 7.51 (dd, J = 3.5, 1.2 Hz, 2H), 7.35 (dd, J = 5.1, 3.5 Hz, 2H), 1.50 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 151.01 (s), 149.12 (s), 148.89 (s), 143.09 (s), 141.85 (s), 136.59 (s), 134.31 (s), 130.07 (d), 129.24 (d), 128.21 (d), 127.66 (d), 127.64 (d), 126.77 (s), 123.32 (s), 119.18 (d), 118.31 (d), 35.42 (s), 31.40 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{40}H_{32}N_2S_4]^+$, $[M]^+$: 668.14430, found: 668.14360.

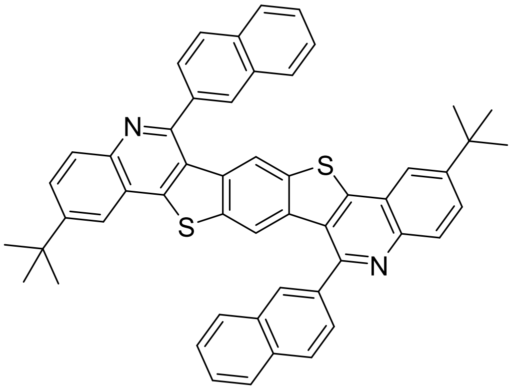
IR (ATR): ν [cm^{-1}] = 2964, 2906, 2869, 1617, 1549, 1493, 1384, 1364, 1323, 1252, 1166, 1124, 1105, 1081, 1062, 1019, 952, 845, 829, 807, 759, 700, 677, 648, 629.

UV-VIS (DCM): λ_{max} [nm] = 273, 313, 336, 356.

Fluorescence (DCM): λ_{ex} [nm] = 360, λ_{max} [nm] = 466.

Quantum yield (DCM): Φ = 4 %.

9be



The reaction was carried out according to **GP5** with **6b** (50 mg, 103 μmol, 1.00 eq.), 2-naphthaldehyde (48.3 mg, 309 μmol, 3.00 eq.) and TFA (1.01 mg, 10.3 μmol, 0.10 eq.) to yield a yellow solid (22.0 mg, 29.0 μmol, 28%).

Mp: >300 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.27 (s, 2H), 8.22 (d, J = 8.8 Hz, 2H), 8.13 (d, J = 8.4 Hz, 2H), 8.10 – 8.05 (m, 2H), 7.99 (d, J = 7.8 Hz, 2H), 7.95 (d, J = 2.0 Hz, 2H), 7.88 (dd, J = 8.8, 2.2 Hz, 2H), 7.83 (s, 2H), 7.80 (dd, J = 8.3, 1.8 Hz, 2H), 7.72 – 7.59 (m, 4H), 1.47 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 155.80 (s), 150.60 (s), 148.93 (s), 143.24 (s), 138.30 (s), 136.57 (s), 134.33 (s), 133.86 (s), 133.82 (s), 130.70 (s), 129.99 (d), 129.10 (d), 128.87 (d), 128.80 (d), 128.37 (d), 128.22 (d), 127.86 (d), 126.96 (d), 126.84 (d), 126.69 (d), 126.03 (s), 123.11 (s), 119.21 (d), 118.56 (d), 35.35 (s), 31.41 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{52}H_{40}N_2S_2]^+$, $[M]^+$: 756.26270, found: 756.26200.

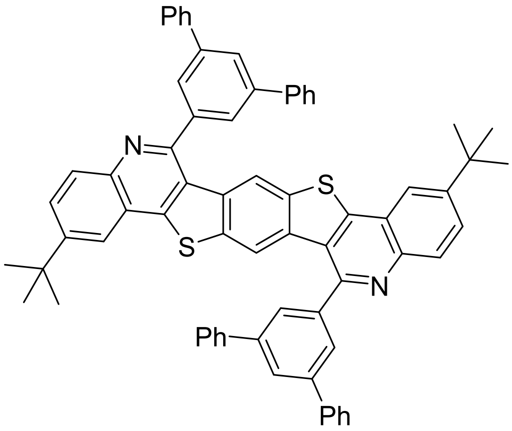
IR (ATR): ν [cm^{-1}] = 3056, 2960, 2904, 2867, 1947, 1738, 1688, 1619, 1548, 1493, 1456, 1433, 1384, 1361, 1299, 1252, 1214, 1192, 1128, 1102, 1079, 1018, 1006, 939, 902, 871, 859, 842, 824, 791, 773, 754, 706, 679, 646, 625.

UV-VIS (DCM): λ_{max} [nm] = 272, 309, 333, 353, 373.

Fluorescence (DCM): λ_{ex} [nm] = 330, λ_{max} [nm] = 405.

Quantum yield (DCM): Φ = 1 %.

9bf



The reaction was carried out according to **GP5** with **6b** (50 mg, 103 µmol, 1.00 eq.), 3,5-diphenylbenzaldehyde (80.0 mg, 309 µmol, 3.00 eq.) and TFA (1.01 mg, 10.3 µmol, 0.10 eq.) to yield a beige solid (58.0 mg, 60.3 µmol, 58%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.24 (d, J = 8.7 Hz, 2H), 8.13 (t, J = 1.7 Hz, 2H), 8.08 (s, 2H), 7.99 (d, J = 2.1 Hz, 2H), 7.97 (d, J = 1.7 Hz, 4H), 7.90 (dd, J = 8.8, 2.2 Hz, 2H), 7.81 – 7.76 (m, 8H), 7.52 – 7.42 (m, 8H), 7.42 – 7.36 (m, 4H), 1.49 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 155.60 (s), 150.66 (s), 149.04 (s), 143.18 (s), 142.84 (s), 141.64 (s), 140.98 (s), 136.75 (s), 134.39 (s), 130.68 (s), 129.98 (d), 129.22 (d), 129.08 (d), 127.87 (d), 127.58 (d), 127.12 (d), 126.79 (d), 126.01 (s), 123.17 (s), 119.27 (d), 118.62 (d), 35.38 (s), 31.41 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{68}H_{52}N_2S_2]^+$, $[M]^+$: 960.35660, found: 960.35600.

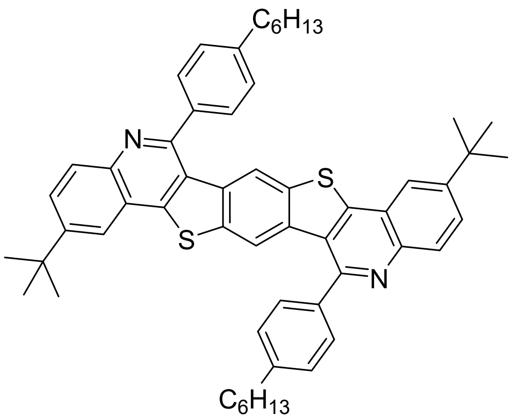
IR (ATR): ν [cm^{-1}] = 3059, 3036, 2962, 2904, 2868, 1595, 1548, 1495, 1462, 1425, 1383, 1363, 1292, 1251, 1214, 1096, 1077, 1031, 1003, 958, 886, 865, 833, 759, 720, 697, 650, 632, 613.

UV-VIS (DCM): λ_{max} [nm] = 274, 316, 343, 361, 377.

Fluorescence (DCM): λ_{ex} [nm] = 360, λ_{max} [nm] = 390.

Quantum yield (DCM): Φ = 3 %.

9bg



The reaction was carried out according to **GP5** with **6b** (50 mg, 103 µmol, 1.00 eq.), 4-hexylbenzaldehyde (58.9 mg, 309 µmol, 3.00 eq.) and TFA (1.01 mg, 10.3 µmol, 0.10 eq.) to yield a beige solid (66.0 mg, 80.0 µmol, 78%).

Mp: 195-200 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.52 (d, J = 8.6 Hz, 2H), 8.17 – 8.12 (m, 4H), 7.91 (s, 2H), 7.75 – 7.69 (m, 4H), 7.60 – 7.55 (m, 4H), 2.90 (t, J = 7.7 Hz, 4H), 1.83 (m, 4H), 1.54 – 1.39 (m, 12H), 1.01 – 0.95 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 160.65 (s), 156.11 (s), 154.43 (s), 152.47 (s), 148.18 (s), 137.20 (s), 134.43 (s), 134.14 (s), 133.54 (d), 129.94 (d), 129.02 (d), 128.34 (s), 125.19 (s), 123.15 (d), 123.05 (s), 119.51 (d), 119.09 (d), 36.25 (s), 35.86 (t), 31.92 (t), 31.22 (t), 31.11 (q), 29.07 (t), 22.82 (t), 14.37 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{56}H_{60}N_2S_2]^+$, $[M]^+$: 824.41920, found: 824.41920.

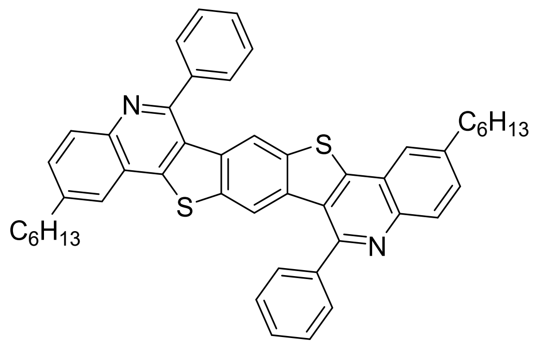
IR (ATR): ν [cm^{-1}] = 2968, 2934, 2860, 1757, 1647, 1610, 1492, 1458, 1427, 1377, 1308, 1199, 1157, 1130, 1022, 953, 876, 834, 795, 781, 724, 701, 669, 650, 633.

UV-VIS (DCM): λ_{max} [nm] = 269, 313, 337, 355, 375.

Fluorescence (DCM): λ_{ex} [nm] = 335, λ_{max} [nm] = 385.

Quantum yield (DCM): Φ = 4 %.

9ca



The reaction was carried out according to **GP5** with **6c** (50 mg, 92.5 µmol, 1.00 eq.), benzaldehyde (29.4 mg, 277 µmol, 3.00 eq.) and TFA (906 µg, 9.25 µmol, 0.10 eq.) to yield a brown solid (35.0 mg, 49.1 µmol, 53%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.23 (d, J = 8.5 Hz, 2H), 7.87 (dd, J = 1.9, 0.7 Hz, 2H), 7.75 – 7.63 (m, 14H), 2.87 (t, J = 7.8 Hz, 4H), 1.80 – 1.70 (m, 4H), 1.46 – 1.28 (m, 12H), 0.94 – 0.86 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 142.81 (s), 136.57 (s), 134.23 (s), 132.07 (d), 129.60 (s), 129.31 (d), 128.90 (d), 125.98 (s), 123.43 (s), 122.51 (d), 118.48 (d), 36.26 (t), 31.86 (t), 31.42 (t), 29.13 (t), 22.75 (t), 14.27 (q) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{48}H_{44}N_2S_2]^+$, $[M]^+$: 712.29400, found: 712.29350.

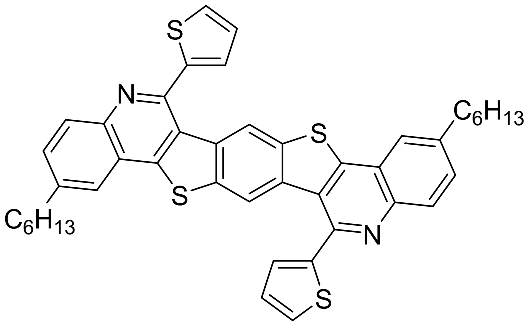
IR (ATR): ν [cm^{-1}] = 3056, 2952, 2927, 2853, 1915, 1621, 1552, 1492, 1457, 1442, 1400, 1383, 1300, 1275, 1212, 1079, 1027, 952, 863, 831, 814, 755, 723, 695, 671, 657, 634, 615.

UV-VIS (DCM): λ_{max} [nm] = 274, 310, 335, 352, 371.

Fluorescence (DCM): λ_{ex} [nm] = 350, λ_{max} [nm] = 382.

Quantum yield (DCM): Φ = 4 %.

9cb



The reaction was carried out according to **GP5** with **6c** (50 mg, 92.5 µmol, 1.00 eq.), 2-thiophencarboxaldehyde (31.1 mg, 277 µmol, 3.00 eq.) and TFA (906 µg, 9.25 µmol, 0.10 eq.) to yield a black solid (49.0 mg, 68.0 µmol, 73%).

Mp: >300 °C.

^{1}H NMR (700 MHz, $CDCl_3$): δ = 8.18 (d, J = 8.4 Hz, 2H), 8.03 (s, 2H), 7.86 (s, 2H), 7.68 (dd, J = 5.2, 1.2 Hz, 2H), 7.64 (dd, J = 8.5, 1.9 Hz, 2H), 7.52 (dd, J = 3.4, 1.2 Hz, 2H), 7.35 (dd, J = 5.3, 3.4 Hz, 2H), 2.87 (t, J = 7.8 Hz, 4H), 1.81 – 1.70 (m, 4H), 1.39 – 1.27 (m, 12H), 0.91 (t, J = 6.9 Hz, 6H) ppm.

^{13}C{^{1}H} NMR (176 MHz, $CDCl_3$): δ = 148.89 (s), 148.42 (s), 143.26 (s), 142.92 (s), 141.82 (s), 136.57 (s), 134.24 (s), 131.84 (d), 130.21 (d), 128.25 (d), 127.68 (d), 127.63 (d), 126.70 (s), 123.61 (s), 122.47 (d), 118.30 (d), 36.28 (t), 31.86 (t), 31.37 (t), 29.13 (t), 22.75 (t), 14.26 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{44}H_{40}N_2S_4]^+$, $[M]^+$: 724.20690, found: 724.20760.

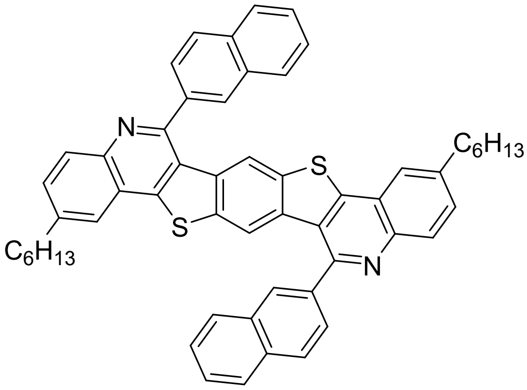
IR (ATR): ν [cm^{-1}] = 2952, 2926, 2853, 1680, 1620, 1551, 1492, 1454, 1384, 1294, 1223, 1197, 1075, 1053, 940, 866, 851, 829, 753, 694, 629.

UV-VIS (DCM): λ_{max} [nm] = 274, 314, 334, 355, 416.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 468.

Quantum yield (DCM): Φ = 8 %.

9cc



The reaction was carried out according to **GP5** with **6c** (50 mg, 92.5 µmol, 1.00 eq.), 2-naphthaldehyde (43.3 mg, 277 µmol, 3.00 eq.) and TFA (906 µg, 9.25 µmol, 0.10 eq.) to yield a light brown solid (25.0 mg, 30.8 µmol, 33%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.28 (d, J = 1.7 Hz, 2H), 8.19 (d, J = 8.5 Hz, 2H), 8.13 (d, J = 8.2 Hz, 2H), 8.07 (d, J = 8.1 Hz, 2H), 7.99 (d, J = 8.0 Hz, 2H), 7.83 – 7.79 (m, 6H), 7.70 – 7.62 (m, 6H), 2.84 (t, J = 7.8 Hz, 4H), 1.78 – 1.68 (m, 4H), 1.43 – 1.30 (m, 12H), 0.91 – 0.88 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 155.56 (s), 148.44 (s), 143.43 (s), 142.51 (s), 138.23 (s), 136.55 (s), 134.27 (s), 133.78 (s), 131.72 (d), 130.15 (d), 128.77 (d), 128.40 (d), 128.20 (d), 126.98 (d), 126.84 (d), 126.68 (d), 126.00 (s), 124.96 (s), 123.41 (s), 122.51 (d), 118.57 (d), 36.23 (t), 31.85 (t), 31.42 (t), 29.13 (t), 22.74 (t), 14.26 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{56}H_{48}N_2S_2]^+$, $[M]^+$: 812.32530, found: 812.32410.

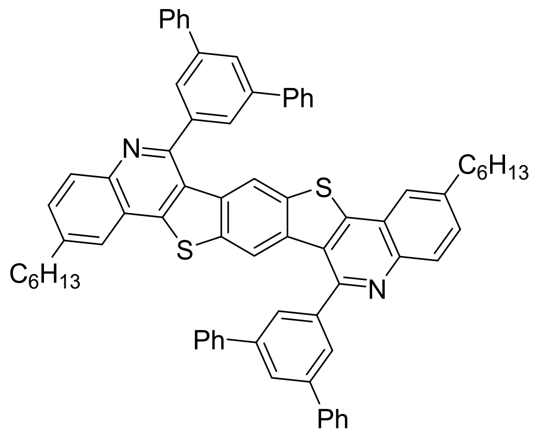
IR (ATR): ν [cm^{-1}] = 3047, 2926, 2852, 1737, 1621, 1549, 1492, 1457, 1384, 1301, 1275, 1209, 1191, 1128, 1079, 1006, 941, 899, 853, 835, 811, 791, 767, 750, 732, 676, 642, 608.

UV-VIS (DCM): λ_{max} [nm] = 273, 310, 334, 354, 375.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 390.

Quantum yield (DCM): Φ = 1 %.

9cd



The reaction was carried out according to **GP5** with **6c** (50 mg, 92.5 µmol, 1.00 eq.), 3,5-diphenylbenzaldehyde (71.6 mg, 277 µmol, 3.00 eq.) and TFA (906 µg, 9.25 µmol, 0.10 eq.) to yield a light brown solid (40.0 mg, 39.3 µmol, 43%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.20 (d, J = 8.4 Hz, 2H), 8.11 (t, J = 1.8 Hz, 2H), 8.07 (s, 2H), 7.97 (d, J = 1.7 Hz, 4H), 7.84 (s, 2H), 7.80 – 7.75 (m, 8H), 7.63 (dd, J = 8.5, 1.9 Hz, 2H), 7.48 (t, J = 7.7 Hz, 8H), 7.42 – 7.36 (m, 4H), 2.86 (t, J = 7.8 Hz, 4H), 1.80 – 1.72 (m, 4H), 1.45 – 1.28 (m, 12H), 0.93 – 0.85 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 155.36 (s), 148.53 (s), 143.38 (s), 142.81 (s), 142.57 (s), 141.60 (s), 140.96 (s), 136.72 (s), 134.30 (s), 131.75 (d), 130.15 (d), 129.08 (d), 127.86 (d), 127.56 (d), 127.08 (d), 126.82 (d), 125.97 (s), 123.48 (s), 122.58 (d), 118.62 (d), 36.25 (t), 31.85 (t), 31.44 (t), 29.16 (t), 22.76 (t), 14.26 (q) ppm.

HR-MS (EI+): *m/z* calculated for $[C_{72}H_{60}N_2S_2]^+$, $[M]^+$: 1016.41920, found: 1016.41900.

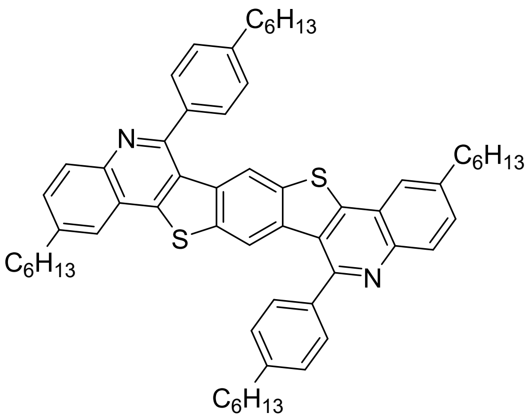
IR (ATR): ν [cm^{-1}] = 3057, 2955, 2926, 2854, 1594, 1551, 1493, 1465, 1423, 1399, 1381, 1289, 1205, 1077, 1029, 866, 827, 756, 712, 697, 644, 614.

UV-VIS (DCM): λ_{max} [nm] = 256, 313, 336, 354, 373.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 383.

Quantum yield (DCM): Φ = 2 %.

9ce



The reaction was carried out according to **GP5** with **6c** (50 mg, 92.5 µmol, 1.00 eq.), 4-hexylbenzaldehyde (52.8 mg, 277 µmol, 3.00 eq.) and TFA (906 µg, 9.25 µmol, 0.10 eq.) to yield a beige solid (67.0 mg, 76.0 µmol, 82%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.18 (d, J = 8.5 Hz, 2H), 7.84 (d, J = 1.8 Hz, 2H), 7.70 (s, 2H), 7.62 (dd, J = 8.7, 2.0 Hz, 2H), 7.60 (d, J = 7.8 Hz, 4H), 7.47 (d, J = 7.8 Hz, 4H), 2.86 (m, 8H), 1.78 (m, 8H), 1.54 – 1.29 (m, 24H), 1.02 – 0.97 (m, 6H), 0.93 – 0.86 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.00 (s), 148.07 (s), 144.20 (s), 143.36 (s), 142.32 (s), 138.13 (s), 136.46 (s), 134.33 (s), 131.57 (d), 130.16 (d), 129.35 (d), 128.70 (d), 126.26 (s), 123.42 (s), 122.46 (d), 118.51 (d), 36.28 (t), 36.15 (t), 32.14 (t), 31.87 (t), 31.75 (t), 31.54 (t), 29.16 (t), 29.11 (t), 22.96 (t), 22.76 (t), 14.48 (q), 14.27 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{60}H_{68}N_2S_2]^+$, $[M]^+$: 880.48180, found: 880.48140.

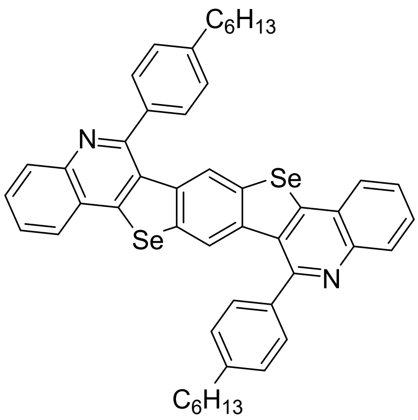
IR (ATR): ν [cm^{-1}] = 2953, 2931, 2860, 1741, 1666, 1615, 1573, 1511, 1468, 1390, 1269, 1207, 1171, 1153, 1022, 893, 838, 792, 778, 725, 704, 673, 618.

UV-VIS (DCM): λ_{max} [nm] = 274, 309, 335, 353, 380.

Fluorescence (DCM): λ_{ex} [nm] = 355, λ_{max} [nm] = 391.

Quantum yield (DCM): Φ = 3 %.

10aa



The reaction was carried out according to **GP5** with **7a** (100 mg, 214 µmol, 1.00 eq.), 4-hexylbenzaldehyde (122 mg, 643 µmol, 3.00 eq.) and TFA (2.10 mg, 21.4 µmol, 0.10 eq.) to yield a brown solid (85.0 mg, 105 µmol, 49%).

Mp: 280-283 °C.

^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.25 (d, J = 8.1 Hz, 2H), 7.91 (dd, J = 8.2, 1.3 Hz, 2H), 7.77 (ddd, J = 8.4, 6.9, 1.4 Hz, 2H), 7.63 (ddd, J = 8.1, 6.9, 1.2 Hz, 2H), 7.57 (d, J = 9.0 Hz, 6H), 7.46 (d, J = 8.0 Hz, 4H), 2.84 (t, J = 7.6 Hz, 4H), 1.86 – 1.76 (m, 4H), 1.56 – 1.40 (m, 12H), 1.03 – 0.95 (m, 6H) ppm.

^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ = 157.53 (s), 151.70 (s), 144.28 (s), 138.27 (s), 136.83 (s), 136.57 (s), 130.35 (d), 130.22 (d), 129.46 (s), 129.40 (d), 128.65 (d), 127.34 (d), 126.01 (s), 125.67 (d), 123.44 (d), 36.12 (t), 32.10 (t), 31.91 (t), 29.16 (t), 22.96 (t), 14.46 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 456.16 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{48}H_{44}N_2Se_2]^+$, $[M]^+$: 808.1829, found: 808.1909.

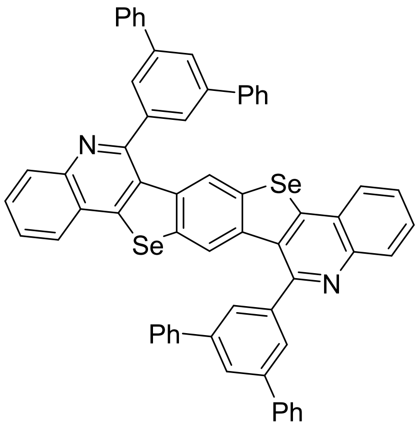
IR (ATR): ν [cm^{-1}] = 2995, 2951, 2925, 2853, 1879, 1607, 1577, 1549, 1511, 1488, 1456, 1437, 1395, 1376, 1357, 1290, 1240, 1208, 1174, 1107, 1078, 1057, 1034, 949, 827, 736, 718, 641.

UV-VIS (DCM): λ_{max} [nm] = 270, 313, 343, 360, 376.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 453.

Quantum yield (DCM): Φ = <1 %.

10ab



The reaction was carried out according to **GP5** with **7a** (100 mg, 214 µmol, 1.00 eq.), 3,5-diphenylbenzaldehyde (166 mg, 643 µmol, 3.00 eq.) and TFA (2.10 mg, 21.4 µmol, 0.10 eq.) to yield a brown solid (87.0 mg, 92.3 µmol, 43%).

Mp: 286-288 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.27 (d, J = 8.3 Hz, 2H), 8.12 – 8.07 (m, 2H), 7.98 (s, 2H), 7.95 – 7.91 (m, 6H), 7.84 – 7.72 (m, 10H), 7.67 – 7.61 (m, 2H), 7.53 – 7.43 (m, 8H), 7.41 – 7.36 (m, 4H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.92 (s), 152.26 (s), 144.29 (s), 142.96 (s), 141.73 (s), 140.93 (s), 136.84 (s), 136.80 (s), 130.41 (d), 130.37 (d), 129.09 (d), 127.91 (s), 127.59 (d), 127.12 (d), 126.83 (d), 126.07 (s), 125.84 (d), 123.59 (d) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 460.26 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{60}H_{37}N_2Se_2]^+$, $[M+H]^+$: 945.1282, found: 945.1285.

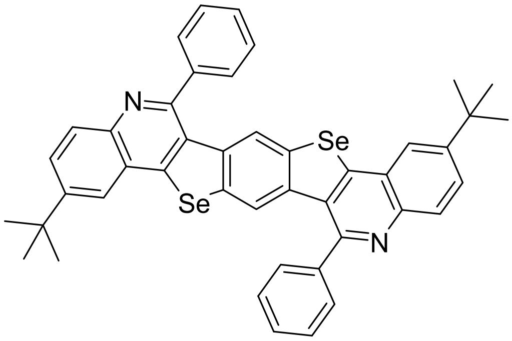
IR (ATR): ν [cm^{-1}] = 3054, 3034, 1950, 1888, 1735, 1594, 1552, 1496, 1480, 1454, 1394, 1289, 1203, 1154, 1065, 1029, 882, 851, 753, 697, 642, 613.

UV-VIS (DCM): λ_{max} [nm] = 252, 318, 343, 362, 378.

Fluorescence (DCM): λ_{ex} [nm] = 360, λ_{max} [nm] = 466.

Quantum yield (DCM): Φ = <1 %.

10ba



The reaction was carried out according to **GP5** with **7b** (100 mg, 214 µmol, 1.00 eq.), benzaldehyde (55.0 mg, 519 µmol, 3.00 eq.) and TFA (1.69 mg, 17.2 µmol, 0.10 eq.) to yield a beige solid (61.0 mg, 81.3 µmol, 47%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.19 (d, J = 8.7 Hz, 2H), 7.88 (dd, J = 8.7, 2.1 Hz, 2H), 7.80 (d, J = 2.0 Hz, 2H), 7.65 (s, 10H), 7.54 (s, 2H), 1.48 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.67 (s), 151.81 (s), 150.70 (s), 142.60 (s), 141.15 (s), 136.87 (s), 136.57 (s), 129.89 (d), 129.28 (d), 129.20 (d), 128.84 (d), 125.66 (s), 124.97 (s), 123.31 (d), 120.85 (d), 35.30 (s), 31.36 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 453.38 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{44}H_{37}N_2Se_2]^+$, $[M+H]^+$: 753.1282, found: 753.1285.

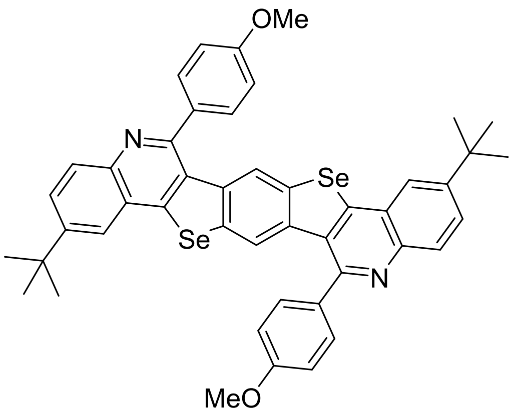
IR (ATR): ν [cm^{-1}] = 3053, 2958, 2903, 2866, 1949, 1687, 1619, 1545, 1492, 1457, 1442, 1380, 1361, 1298, 1248, 1217, 1200, 1154, 1081, 1054, 1026, 947, 915, 866, 840, 791, 763, 738, 702, 661, 641, 614.

UV-VIS (DCM): λ_{max} [nm] = 276, 316, 344, 361, 380.

Fluorescence (DCM): λ_{ex} [nm] = 274, λ_{max} [nm] = 391.

Quantum yield (DCM): Φ = 1 %.

10bb



The reaction was carried out according to **GP5** with **7b** (100 mg, 214 µmol, 1.00 eq.), 4-methoxybenzaldehyde (70.6 mg, 519 µmol, 3.00 eq.) and TFA (1.69 mg, 17.2 µmol, 0.10 eq.) to yield a dark brown solid (78.5 mg, 96.8 µmol, 56%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.17 (d, J = 8.7 Hz, 2H), 7.86 (dd, J = 8.8, 2.1 Hz, 2H), 7.80 (d, J = 2.1 Hz, 2H), 7.77 (s, 2H), 7.62 (d, J = 8.3 Hz, 4H), 7.17 (d, J = 8.5 Hz, 4H), 4.01 (s, 6H), 1.48 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 160.49 (s), 156.48 (s), 151.79 (s), 150.52 (s), 142.70 (s), 137.05 (s), 136.51 (s), 133.64 (s), 130.31 (d), 129.82 (d), 129.35 (s), 129.20 (d), 125.54 (s), 123.39 (d), 120.82 (d), 114.62 (d), 55.76 (q), 35.28 (s), 31.37 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 452.35 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{46}H_{41}N_2O_2Se_2]^+$, $[M+H]^+$: 813.1493, found: 813.1488.

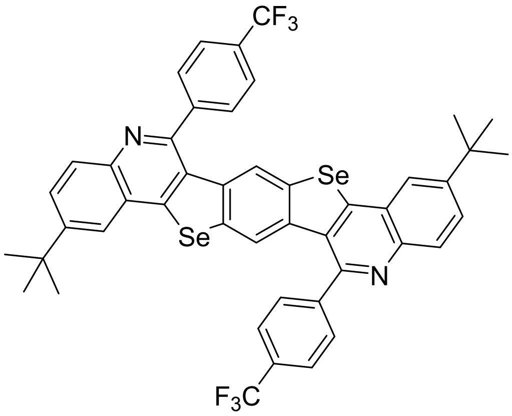
IR (ATR): ν [cm^{-1}] = 3046, 2958, 2904, 2866, 2835, 1729, 1608, 1547, 1511, 1489, 1456, 1426, 1390, 1361, 1291, 1244, 1216, 1173, 1108, 1079, 1055, 1030, 945, 871, 827, 804, 733, 700, 648, 622.

UV-VIS (DCM): λ_{max} [nm] = 275, 310, 343, 359, 379.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 393.

Quantum yield (DCM): Φ = <1 %.

10bc



The reaction was carried out according to **GP5** with **7b** (100 mg, 214 µmol, 1.00 eq.), 4-(trifluoromethyl)benzaldehyde (90.3 mg, 519 µmol, 3.00 eq.) and TFA (1.69 mg, 17.2 µmol, 0.10 eq.) to yield a beige solid (42.9 mg, 48.4 µmol, 28%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.17 (d, J = 8.7 Hz, 2H), 7.93 (d, J = 7.7 Hz, 2H), 7.91 (dd, J = 8.8, 2.1 Hz, 2H), 7.83 (ddd, J = 4.2, 2.1, 1.4 Hz, 8H), 7.60 (s, 2H), 1.49 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 154.85 (s), 152.32 (s), 151.35 (s), 144.76 (s), 142.55 (s), 136.68 (s), 136.59 (s), 129.89 (d), 129.71 (d), 129.58 (d), 128.60 (s), 126.28 (d), 125.73 (s), 124.31 (q), 123.02 (d), 120.91 (d), 35.39 (s), 31.36 (q) ppm.

^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ = -62.41 ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 458.80 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{46}H_{34}F_6N_2Se_2]^+$, $[M]^+$: 888.0951, found: 888.1007.

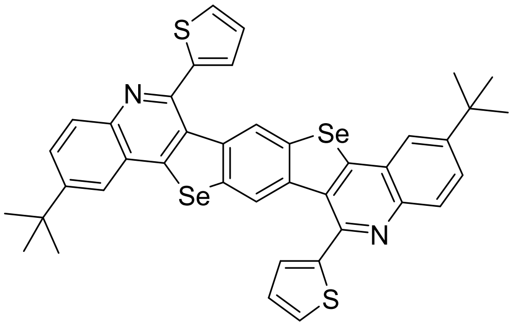
IR (ATR): ν [cm^{-1}] = 3060, 2975, 2958, 2907, 2868, 1615, 1547, 1488, 1457, 1406, 1379, 1365, 1324, 1248, 1217, 1159, 1105, 1079, 1065, 1016, 947, 863, 842, 826, 791, 746, 693, 668, 644, 623.

UV-VIS (DCM): λ_{max} [nm] = 278, 322, 344, 363, 377.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 393.

Quantum yield (DCM): Φ = <1 %.

10bd



The reaction was carried out according to **GP5** with **7b** (100 mg, 214 µmol, 1.00 eq.), thiophen-2-carbaldehyde (58.2 mg, 519 µmol, 3.00 eq.) and TFA (1.69 mg, 17.2 µmol, 0.10 eq.) to yield a black solid (96.2 mg, 126 µmol, 73%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ= 8.19 (d, J = 8.7 Hz, 2H), 7.88 (dd, J = 8.8, 2.1 Hz, 2H), 7.82 (s, 2H), 7.81 (d, J = 2.1 Hz, 2H), 7.66 (dd, J = 5.2, 1.2 Hz, 2H), 7.44 (dd, J = 3.4, 1.2 Hz, 2H), 7.32 (dd, J = 5.2, 3.4 Hz, 2H), 1.48 (s, 18H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ= 151.98 (s), 151.17 (s), 149.69 (s), 142.47 (s), 141.81 (s), 136.82 (s), 136.63 (s), 130.01 (s), 129.90 (d), 129.48 (d), 128.20 (d), 127.64 (d), 127.49 (d), 125.85 (s), 123.11 (d), 120.82 (d), 35.35 (s), 31.33 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ= 455.03 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{40}H_{33}N_2S_2Se_2]^+$, $[M+H]^+$: 765.0410, found: 765.0410.

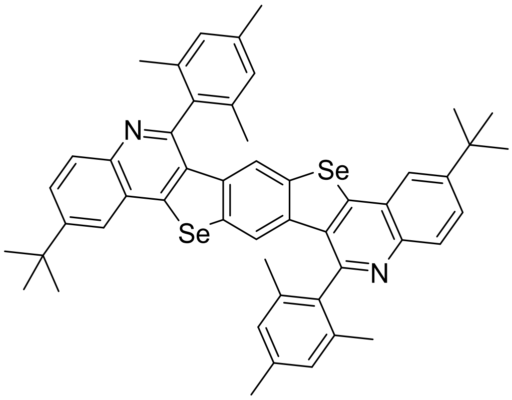
IR (ATR): ν [cm^{-1}] = 3069, 2956, 2903, 2865, 1729, 1617, 1546, 1478, 1461, 1435, 1393, 1362, 1200, 1163, 1064, 977, 931, 848, 832, 696, 644.

UV-VIS (DCM): λ_{max} [nm] = 273, 319, 341, 364.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 435.

Quantum yield (DCM): Φ = <1 %.

10be



The reaction was carried out according to **GP5** with **7b** (100 mg, 214 µmol, 1.00 eq.), 2,4,6-trimethylbenzaldehyde (76.9 mg, 519 µmol, 3.00 eq.) and TFA (1.69 mg, 17.2 µmol, 0.10 eq.) to yield a light brown solid (26.0 mg, 31.1 µmol, 18%).

Mp: >300 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.22 (d, J = 8.7 Hz, 2H), 7.89 (dd, J = 8.8, 2.1 Hz, 2H), 7.86 – 7.84 (m, 2H), 7.32 (s, 2H), 7.12 (s, 2H), 2.52 (s, 6H), 1.93 (s, 12H), 1.50 (s, 18H) ppm.

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 156.59 (s), 151.48 (s), 150.54 (s), 143.37 (s), 138.60 (s), 137.38 (s), 137.09 (s), 136.84 (s), 135.91 (s), 129.97 (d), 129.16 (d), 128.95 (d), 125.60 (s), 121.91 (d), 120.93 (d), 35.32 (s), 31.43 (q), 21.57 (q), 19.89 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 452.99 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{50}H_{49}N_2Se_2]^+$, $[M+H]^+$: 837.2221, found: 837.2221.

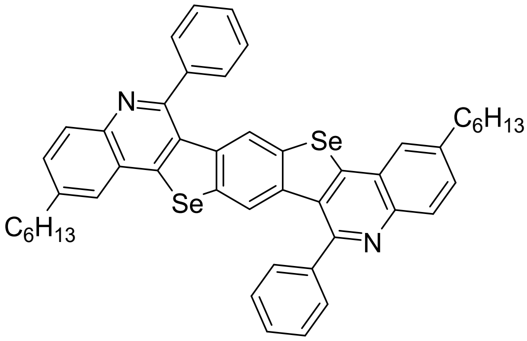
IR (ATR): ν [cm^{-1}] = 3053, 2961, 2916, 2866, 1742, 1612, 1545, 1492, 1460, 1378, 1360, 1294, 1251, 1218, 1165, 1101, 1073, 1051, 1032, 938, 875, 847, 834, 761, 743, 693, 657, 646.

UV-VIS (DCM): λ_{max} [nm] = 276, 316, 344, 363, 378.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 389.

Quantum yield (DCM): Φ = 1 %.

10ca



The reaction was carried out according to **GP5** with **7c** (100 mg, 158 µmol, 1.00 eq.), benzaldehyde (50.2 mg, 473 µmol, 3.00 eq.) and TFA (1.54 mg, 15.8 µmol, 0.10 eq.) to yield a brown solid (73.7 mg, 91.3 µmol, 58%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.15 (d, J = 8.5 Hz, 2H), 7.68 – 7.64 (m, 12H), 7.62 (dd, J = 8.4, 1.9 Hz, 2H), 7.53 (s, 2H), 2.89 – 2.82 (m, 4H), 1.80 – 1.69 (m, 4H), 1.45 – 1.30 (m, 12H), 0.95 – 0.86 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.44 (s), 151.25 (s), 142.83 (s), 142.62 (s), 141.14 (s), 136.82 (s), 136.56 (s), 131.83 (d), 130.08 (d), 129.27 (d), 129.17 (d), 128.87 (d), 125.98 (s), 124.16 (d), 123.31 (d), 36.20 (t), 31.86 (t), 31.41 (t), 29.13 (t), 22.75 (t), 14.27 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 454.74 ppm.

HR-MS (EI+): *m/z* calculated for $[C_{48}H_{45}N_2Se_2]^+$, $[M+H]^+$: 809.1908, found: 809.2031.

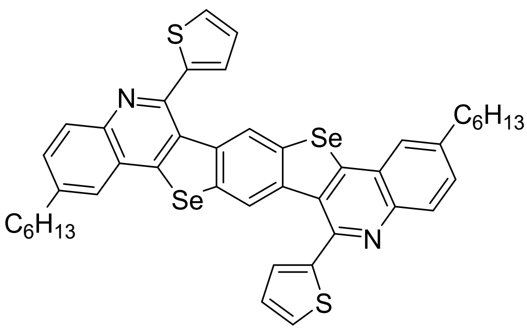
IR (ATR): ν [cm^{-1}] = 3056, 2952, 2927, 2852, 1913, 1724, 1687, 1620, 1547, 1486, 1455, 1439, 1376, 1357, 1294, 1272, 1205, 1078, 1057, 1026, 949, 908, 865, 849, 829, 808, 765, 742, 727, 694, 651, 630, 609.

UV-VIS (DCM): λ_{max} [nm] = 274, 317, 344, 362, 381.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 433.

Quantum yield (DCM): Φ = 1 %.

10cb



The reaction was carried out according to **GP5** with **7c** (100 mg, 158 µmol, 1.00 eq.), thiophen-2-carbaldehyde (53.0 mg, 473 µmol, 3.00 eq.) and TFA (1.54 mg, 15.8 µmol, 0.10 eq.) to yield a black solid (52.0 mg, 63.5 µmol, 40%).

Mp: >300 °C.

^{1}H NMR (600 MHz, CDCl3): δ = 8.16-8.15 (d, J= 8.4 Hz, 2H), 7.83 (s, 2H), 7.67-7.66 (dd, J= 5.2, 1.2 Hz, 2H), 7.64-7.62 (dd, J= 8.5 Hz, 1.9 Hz, 2H), 7.45,-7.43 (m, 2H), 7.33-7.31 (m, 2H), 2.87-2.85 (t, J= 7.8 Hz, 4H) , 1.79-1.74 (m, 4H), 1.42-1.25 (m, 12H), 0.92-0.89 (m, 6H) ppm.

^{13}C{^{1}H} NMR (150 MHz, CDCl3): δ = 151.37 (s), 149.53 (s), 143.08 (s), 142.76 (s), 141.95 (s), 136.78 (s), 136.62 (s), 131.98 (d), 130.15 (d), 129.95 (s), 128.20 (d), 127.63 (d), 127.48 (d), 126.16 (s), 124.14 (d), 123.11 (d), 36.23 (t), 31.86 (t), 31.36 (t), 29.13 (t), 22.76 (t), 14.27 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, CDCl3): δ = 456.09 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{44}H_{41}N_2S_2Se_2]^+$, $[M+H]^+$: 821.1036, found: 821.1057.

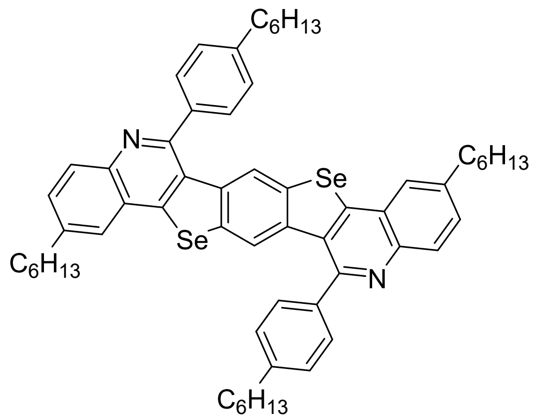
IR (ATR): ν [cm^{-1}] = 3068, 2952, 2926, 2852, 1913, 1730, 1619, 1548, 1485, 1455, 1376, 1289, 1234, 1190, 1063, 935, 867, 850, 826, 737, 690, 625.

UV-VIS (DCM): λ_{max} [nm] = 233, 275, 318, 343, 364.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 408.

Quantum yield (DCM): Φ = <1 %.

10cc



The reaction was carried out according to **GP5** with **7c** (100 mg, 158 µmol, 1.00 eq.), 4-hexylbenzaldehyde (89.9 mg, 473 µmol, 3.00 eq.) and TFA (1.54 mg, 15.8 µmol, 0.10 eq.) to yield a light brown solid (20.0 mg, 20.5 µmol, 13%).

Mp: >300 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.15 (d, J = 8.4 Hz, 2H), 7.63 (s, 2H), 7.61 (dd, J = 8.5, 1.9 Hz, 2H), 7.55 (d, J = 8.0 Hz, 4H), 7.52 (s, 2H), 7.45 (d, J = 8.1 Hz, 4H), 2.84 (t, J = 7.7 Hz, 8H), 1.84 – 1.78 (m, 4H), 1.78 – 1.72 (m, 4H), 1.54 – 1.44 (m, 12H), 1.43 – 1.30 (m, 12H), 1.04 – 0.95 (m, 6H), 0.94 – 0.84 (m, 6H) ppm.

^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ = 156.67 (s), 151.07 (s), 144.10 (s), 142.85 (s), 142.48 (s), 138.39 (s), 136.87 (s), 136.51 (s), 131.73 (d), 130.05 (d), 129.40 (s), 129.34 (d), 128.70 (d), 125.95 (s), 124.12 (d), 123.37 (d), 36.23 (t), 36.14 (t), 32.17 (t), 31.92 (t), 31.86 (t), 31.49 (t), 29.16 (t), 22.98 (t), 22.76 (t), 14.50 (q), 14.26 (q) ppm.

^{77}Se{^{1}H} NMR (76 MHz, $CDCl_3$): δ = 452.82 ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{60}H_{69}N_2Se_2]^+$, $[M+H]^+$: 977.3786, found: 977.3784.

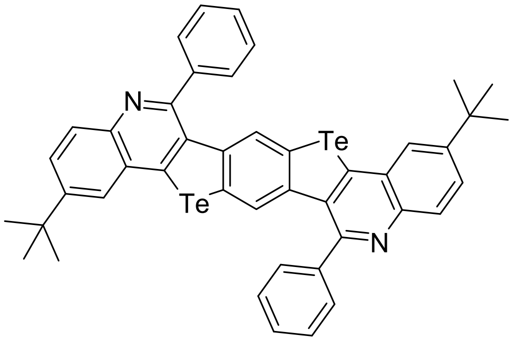
IR (ATR): ν [cm^{-1}] = 2954, 2922, 2853, 1920, 1612, 1547, 1514, 1487, 1455, 1396, 1377, 1294, 1273, 1210, 1181, 1140, 1116, 1077, 1056, 1020, 949, 871, 824, 789, 728, 644.

UV-VIS (DCM): λ_{max} [nm] = 274, 317, 344, 361, 381.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 392.

Quantum yield (DCM): Φ = 1 %.

11ba



The reaction was carried out according to **GP5** with **8** (50 mg, 74.0 µmol, 1.00 eq.), benzaldehyde (23.6 mg, 222 µmol, 3.00 eq.) and TFA (725 µg, 7.40 µmol, 0.10 eq.) to yield an orange solid (29.0 mg, 34.2 µmol, 46%).

Mp: >300 °C.

^{1}H NMR (400 MHz, CDCl3): δ = 8.17 (d, J = 8.8 Hz, 2H), 7.88 (dd, J = 8.8, 2.1 Hz, 2H), 7.62 (s, 10H), 7.44 (d, J = 2.0 Hz, 2H), 7.38 (s, 2H), 1.46 (s, 18H) ppm.

^{13}C{^{1}H} NMR (100 MHz, CDCl3): δ = 157.18 (s), 151.07 (s), 147.72 (s), 142.52 (s), 141.07 (s), 135.74 (s), 132.62 (d), 130.14 (s), 129.70 (s), 129.47 (d), 129.25 (d), 129.05 (d), 128.97 (d), 126.58 (d), 125.59 (s), 123.95 (d), 35.21 (s), 31.31 (q) ppm.

HR-MS (MALDI+): *m/z* calculated for $[C_{44}H_{36}N_2Te_2]^+$, $[M]^+$: 850.0980, found: 850.0997.

IR (ATR): ν [cm^{-1}] = 3046, 2957, 2903, 2865, 1682, 1617, 1546, 1487, 1442, 1372, 1288, 1241, 1197, 1081, 1026, 942, 872, 833, 789, 769, 755, 701, 655, 635, 614.

UV-VIS (DCM): λ_{max} [nm] = 289, 325, 339, 359, 409.

Fluorescence (DCM): λ_{ex} [nm] = 340, λ_{max} [nm] = 468.

Quantum yield (DCM): Φ = <1 %.

Due to the low solubility of the product, no signal in the ^{125}Te{^{1}H} NMR could be obtained. As a substitute, the expected molecular structure was confirmed *via* X-ray single crystal analysis (see Chapter **5**, Table **S10**).

2 NMR Spectra

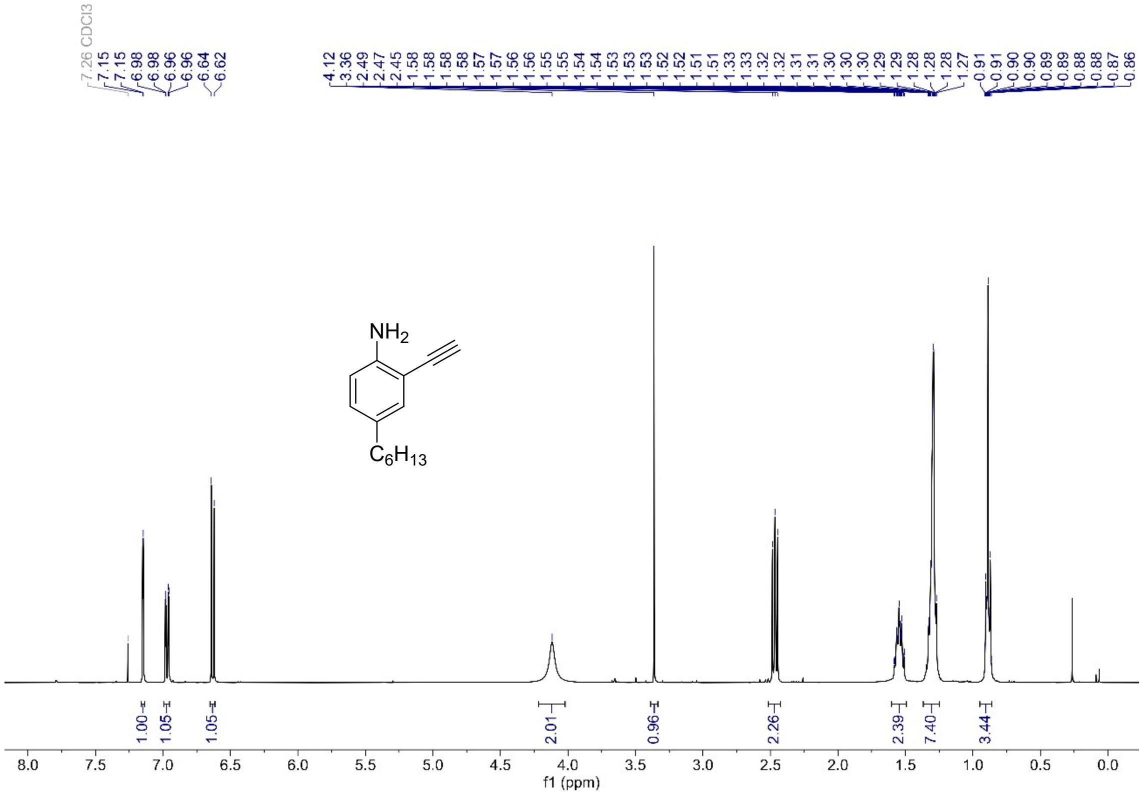


Figure S1. [1]H NMR spectrum (400 MHz, $CDCl_3$) of **3c**.

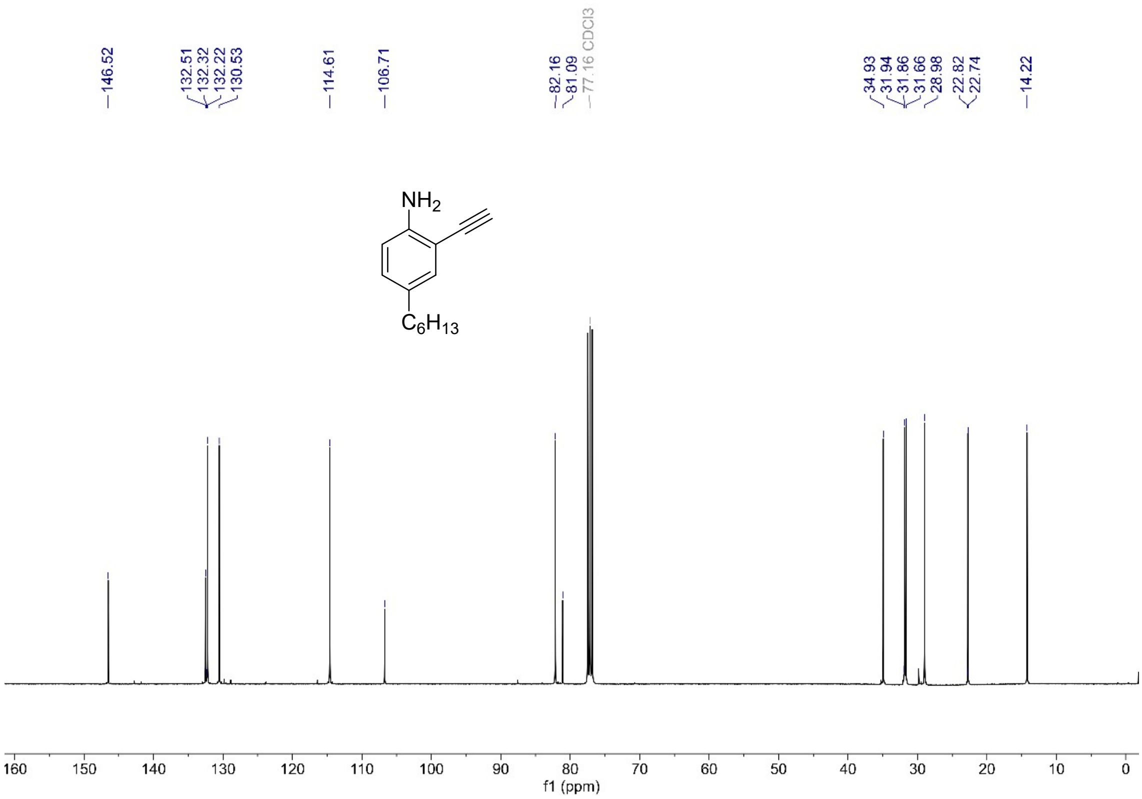


Figure S2. [13]C{[1]H} NMR spectrum (101 MHz, $CDCl_3$) of **3c**.

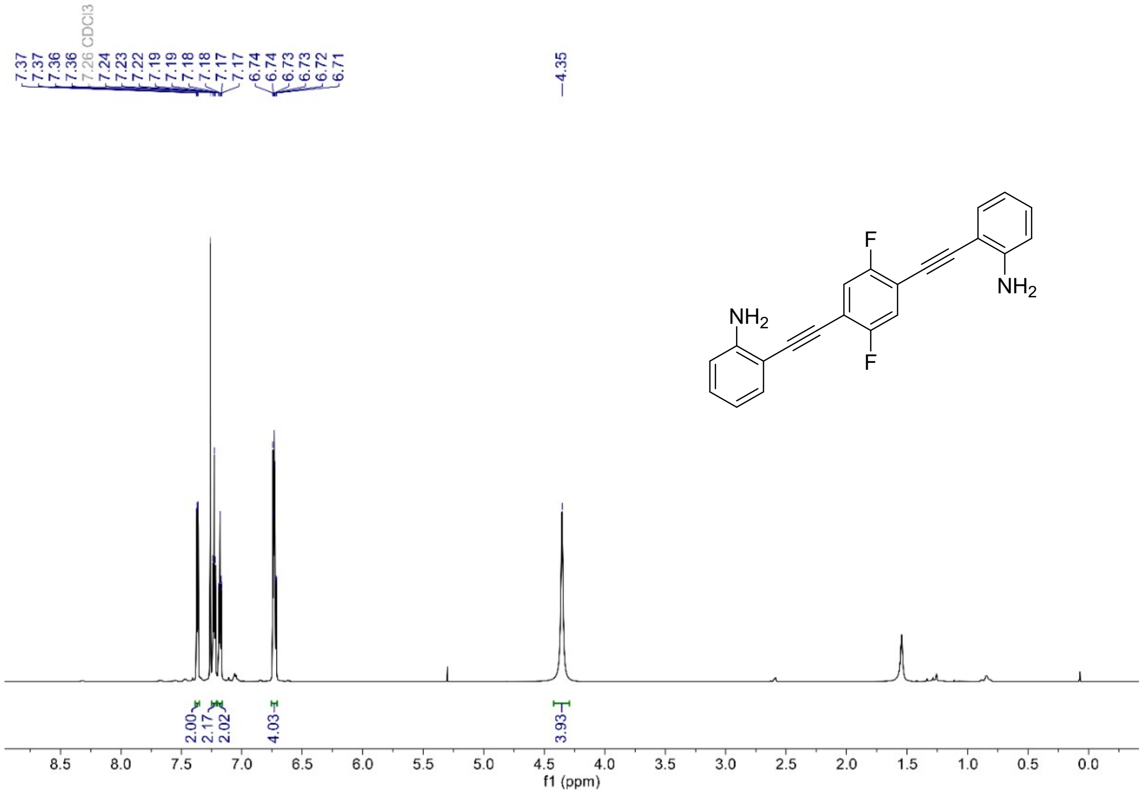


Figure S3. [1]H NMR spectrum (700 MHz, $CDCl_3$) of **5a**.

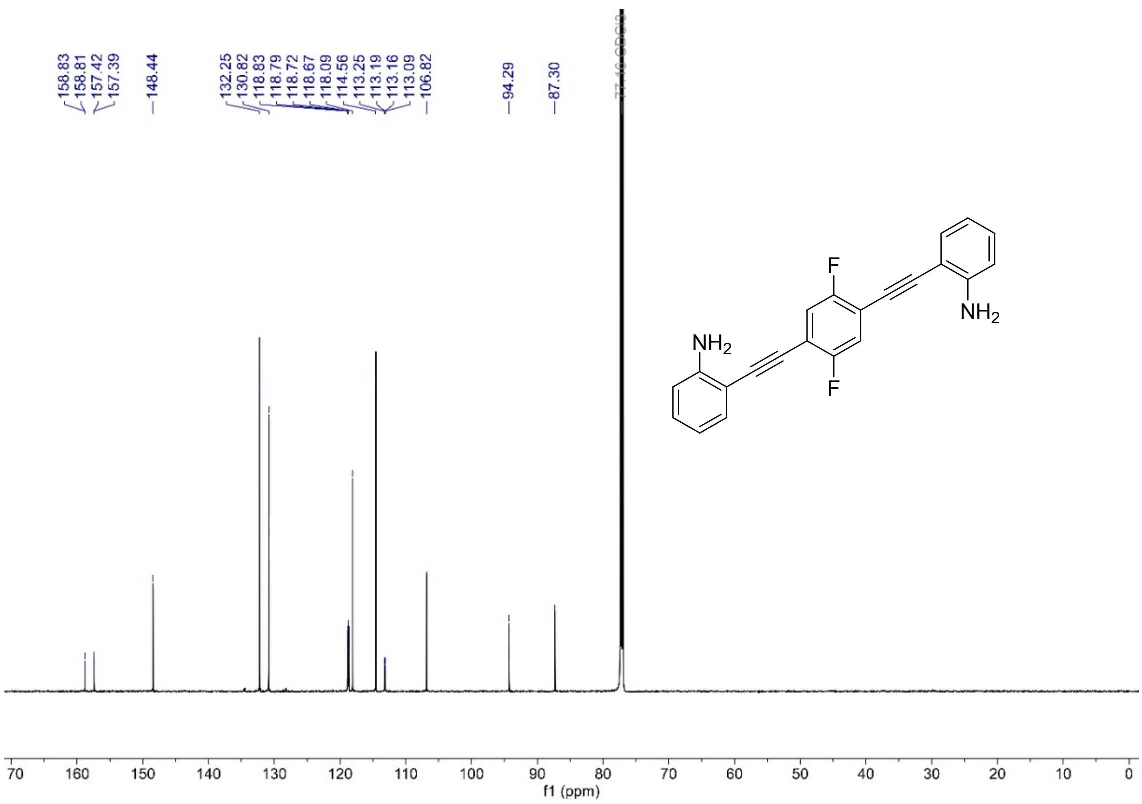


Figure S4. [13]C{[1]H} NMR spectrum (176 MHz, $CDCl_3$) of **5a**.

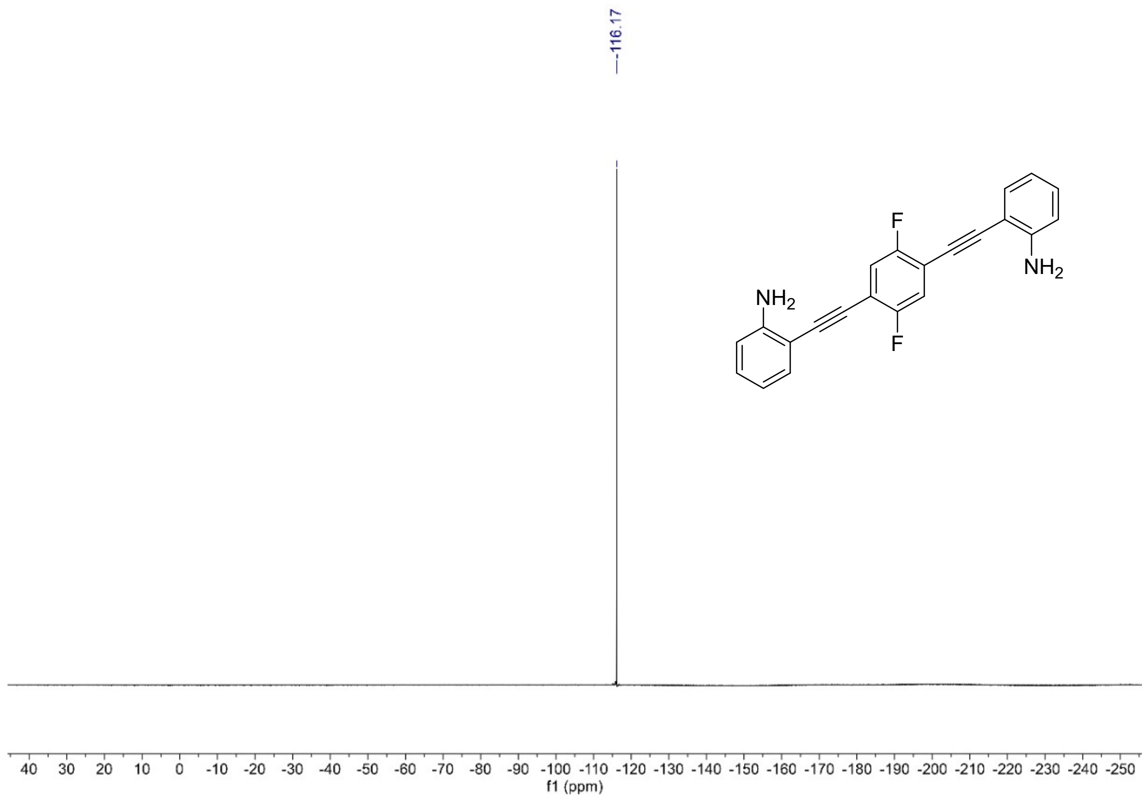


Figure S5. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **5a**.

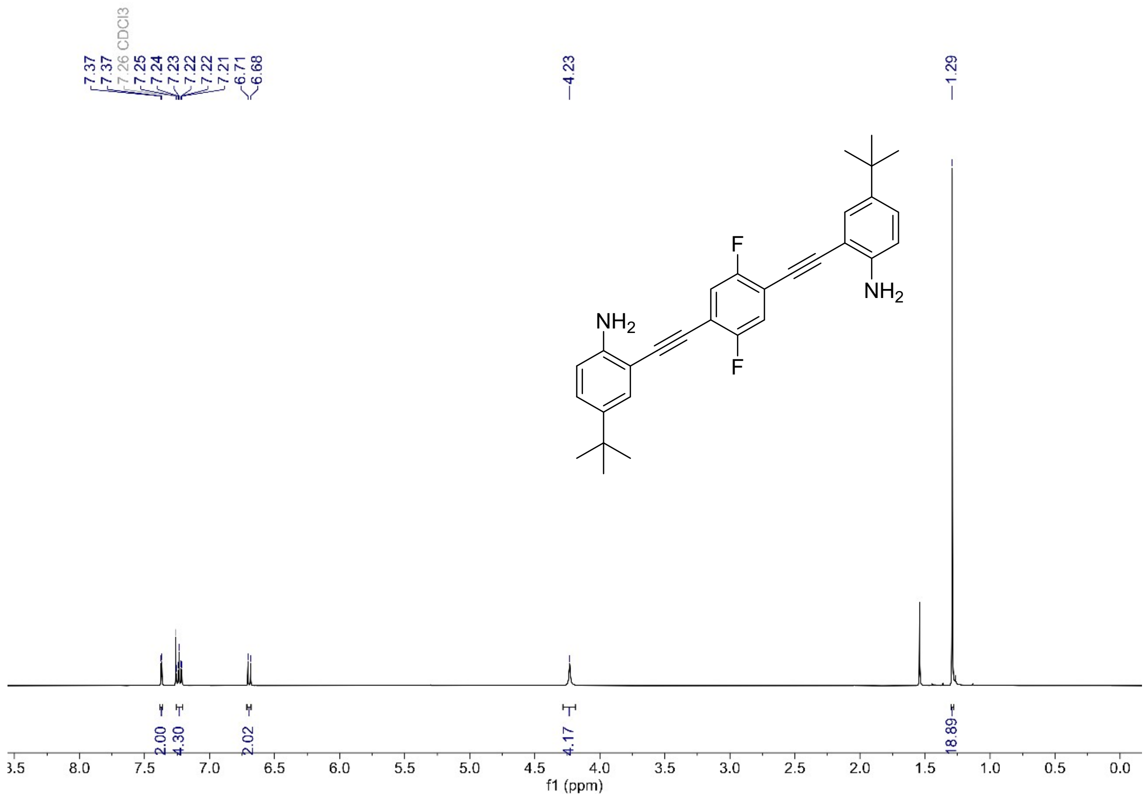


Figure S6. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **5b**.

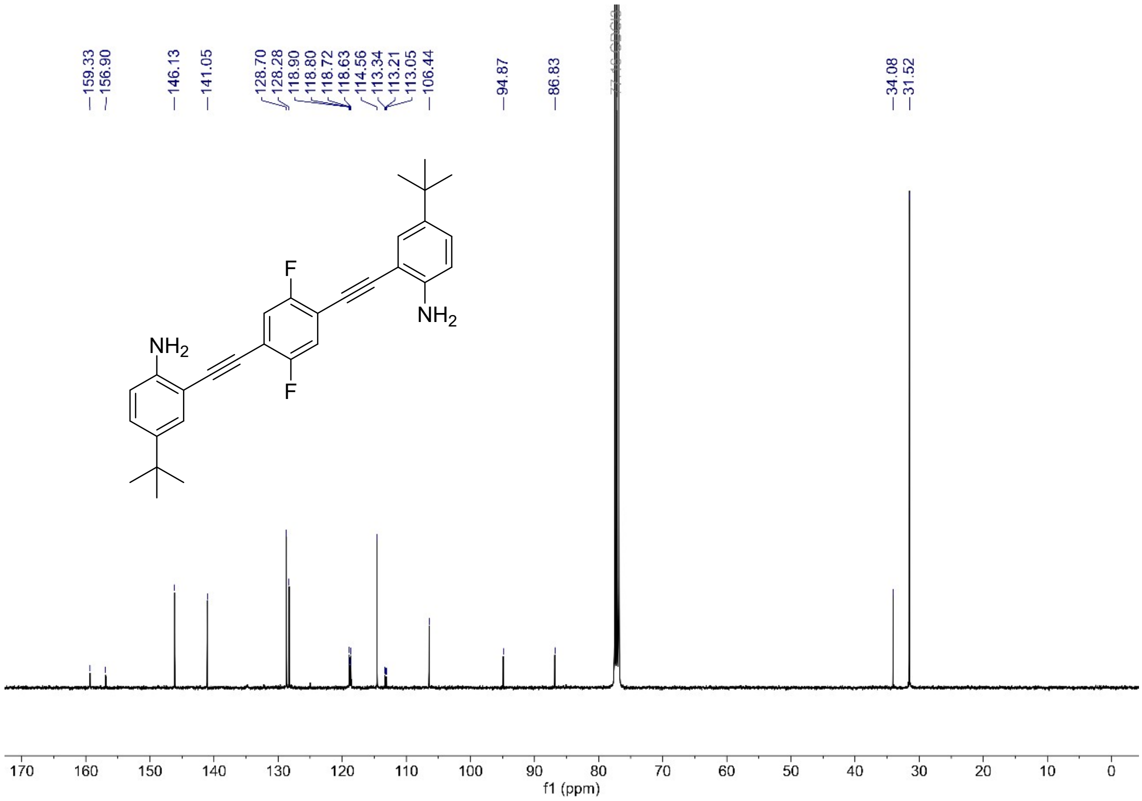


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **5b**.

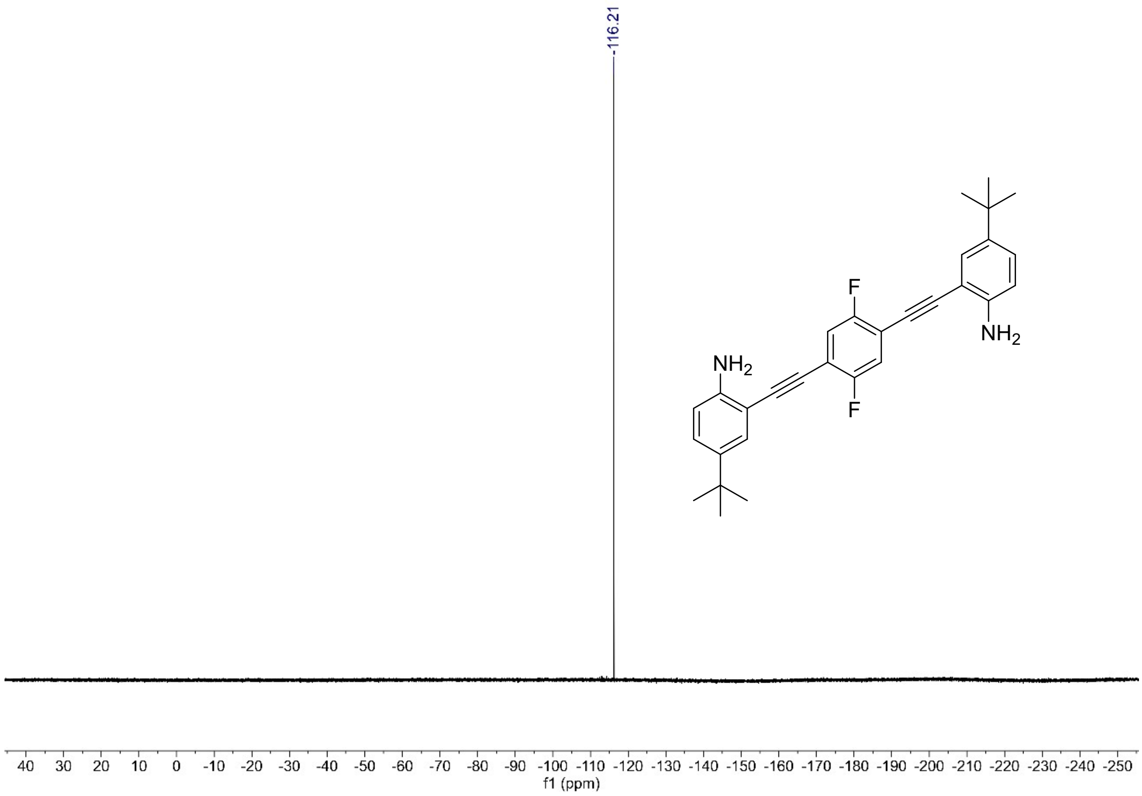


Figure S8. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **5b**.

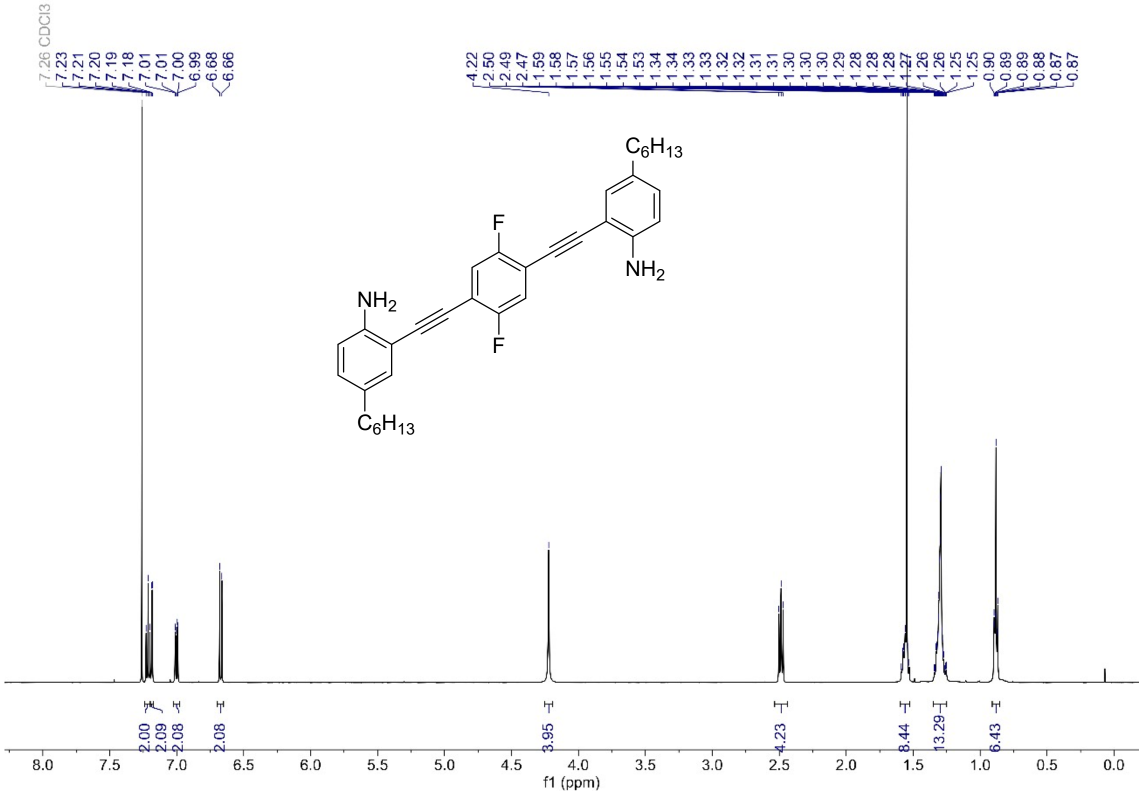


Figure S9. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **5c**.

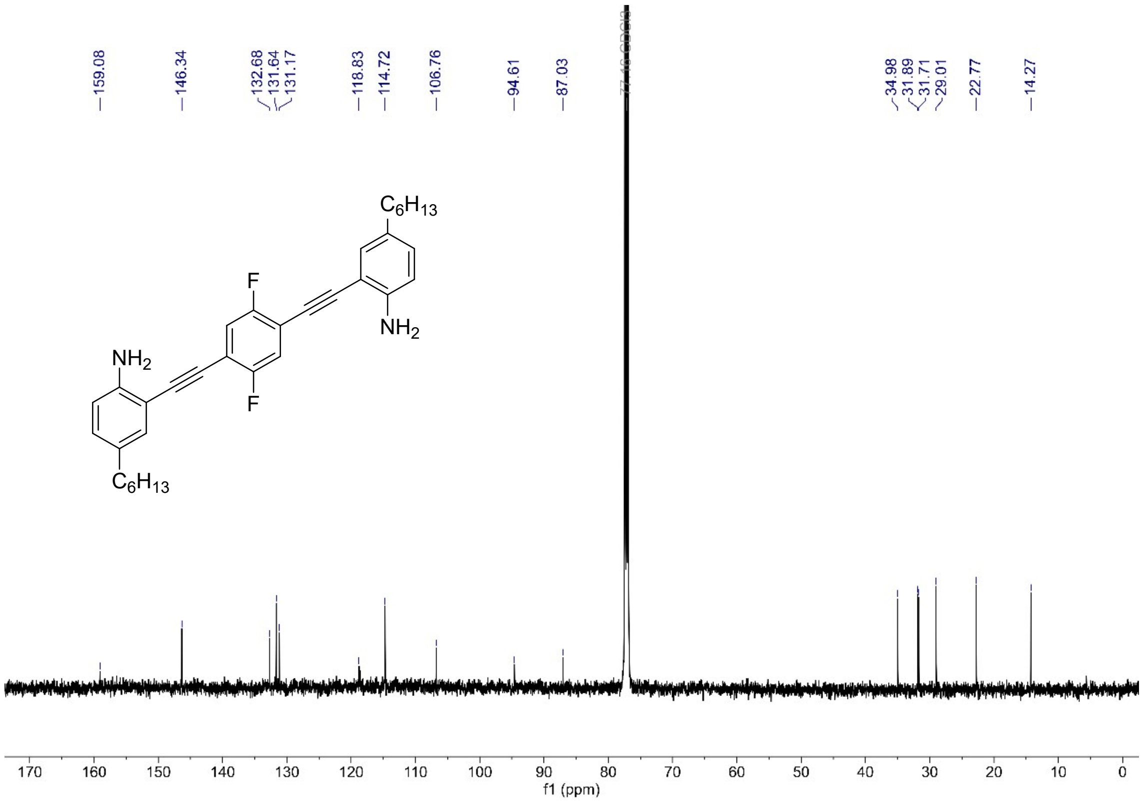


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, $CDCl_3$) of **5c**.

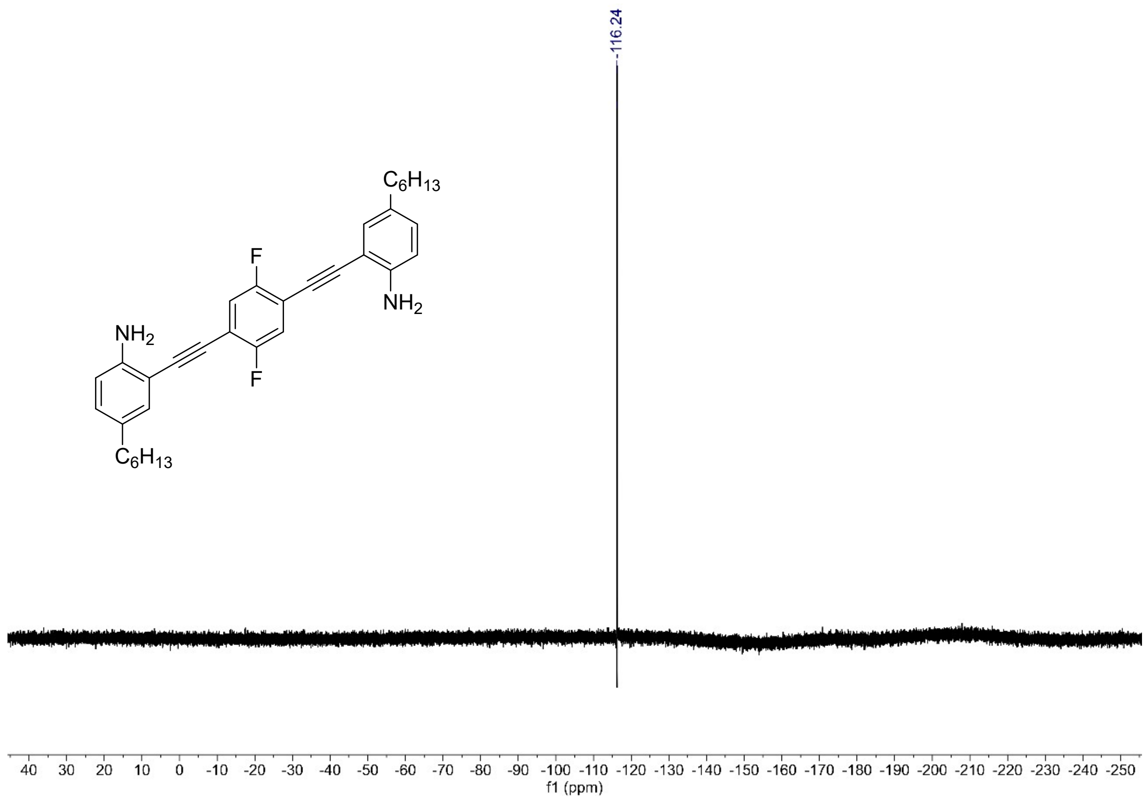


Figure S11. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **5c**.

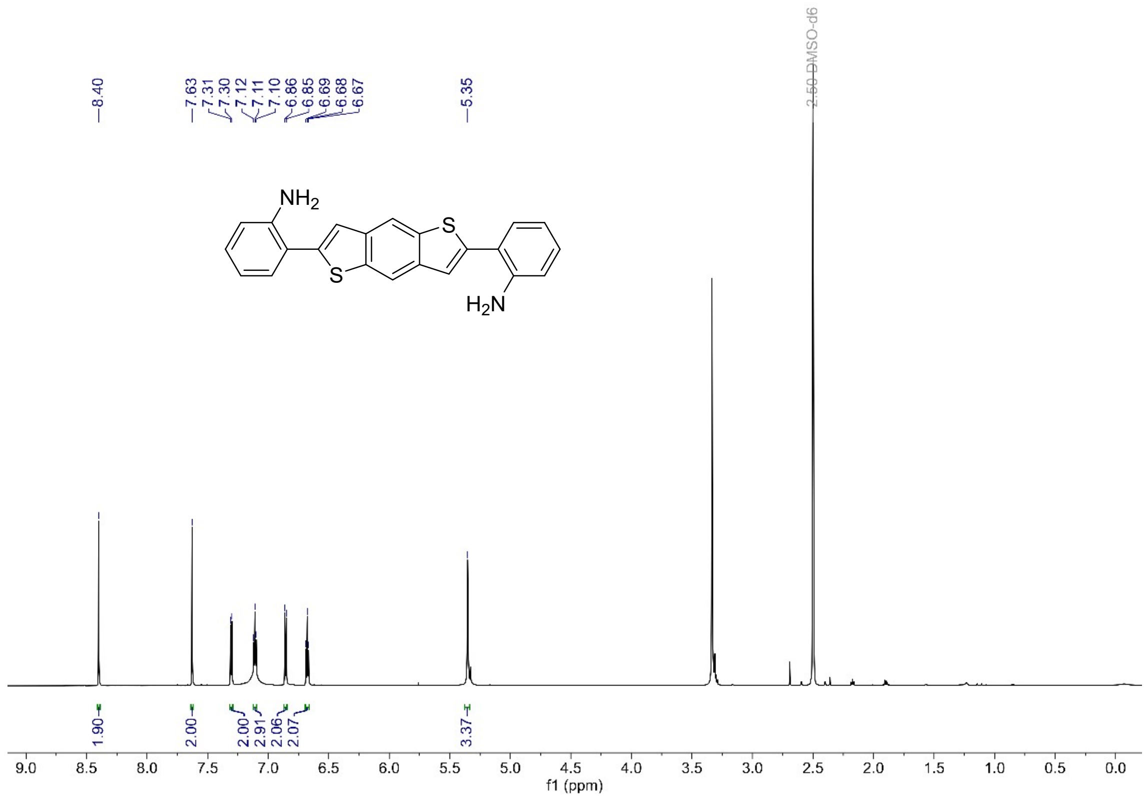


Figure S12. ^{1}H NMR spectrum (700 MHz, DMSO-d6) of **6a**.

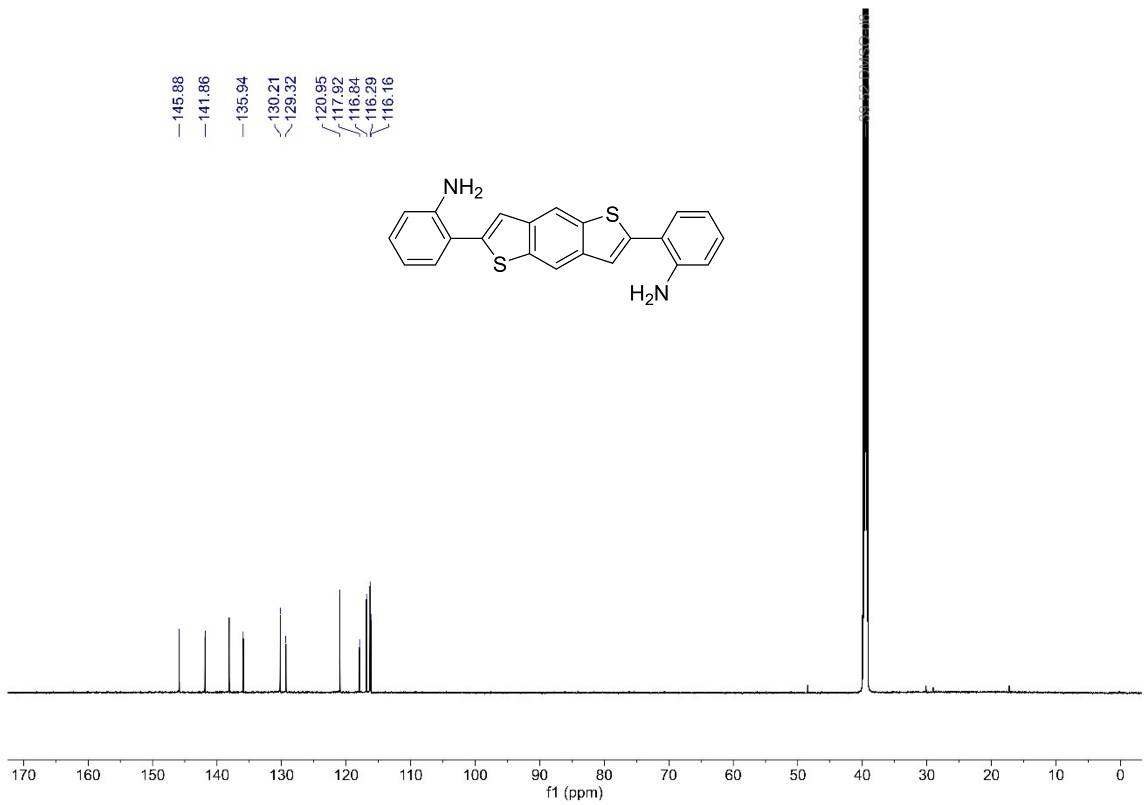


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, DMSO-d6) of **6a**.

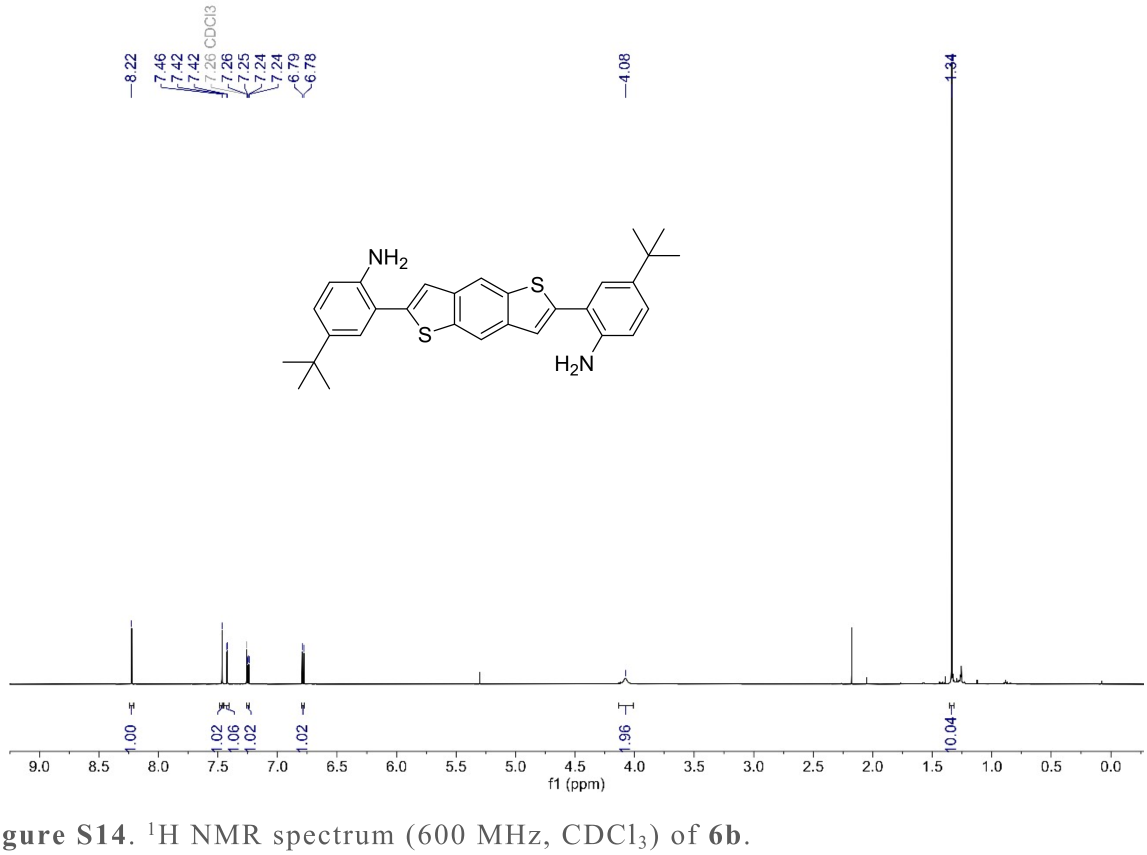


Figure S14. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **6b**.

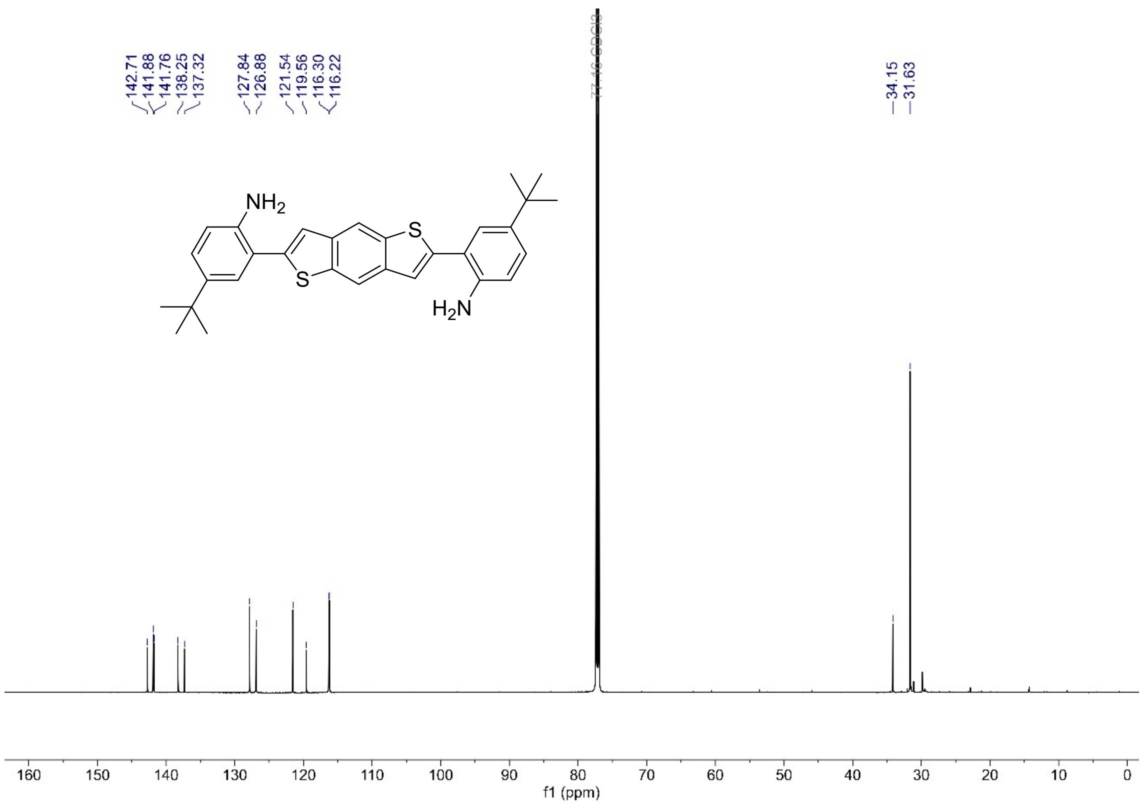


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **6b**.

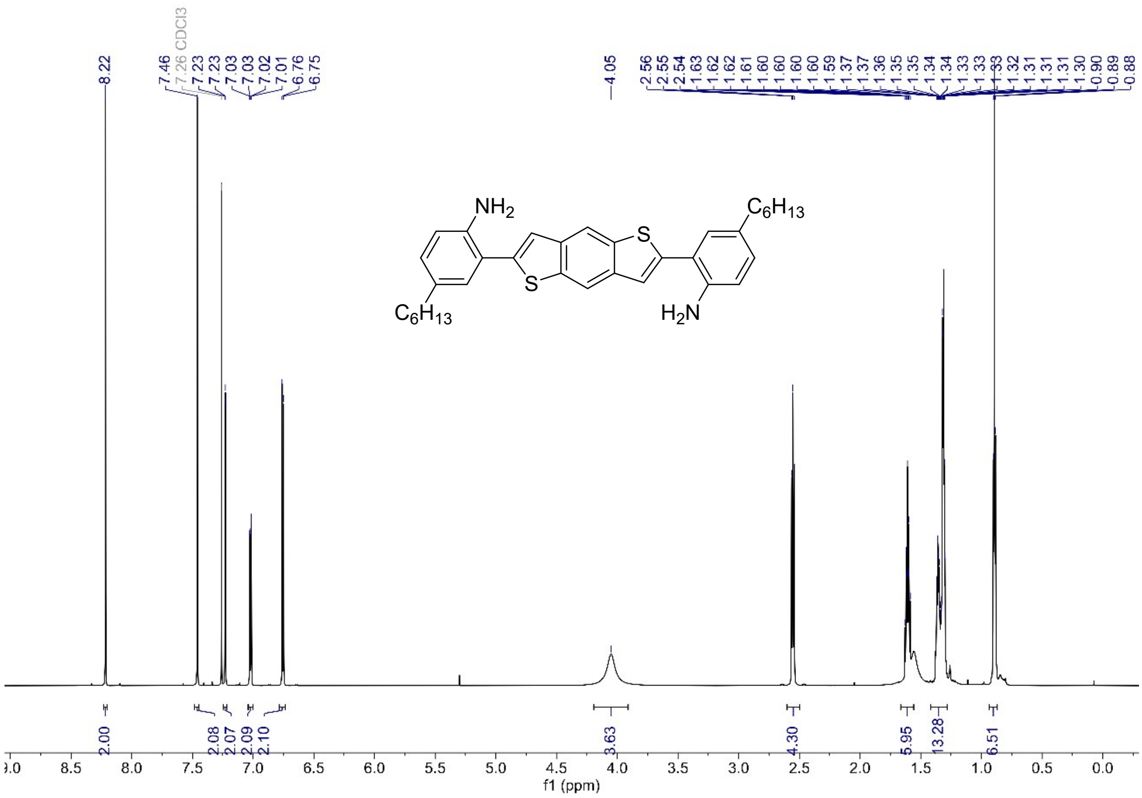


Figure S16. ^{1}H NMR spectrum (700 MHz, $CDCl_3$) of **6c**.

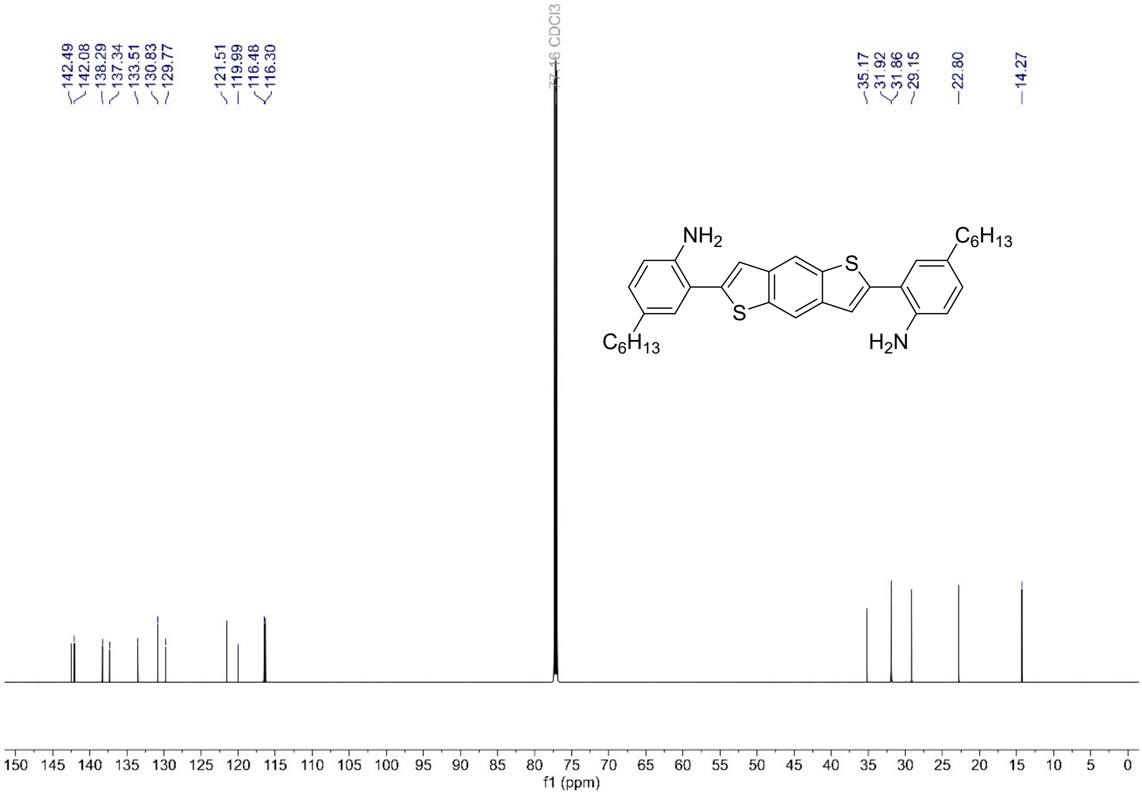


Figure S17. $^{13}C\{^1H\}$ NMR spectrum (176 MHz, $CDCl_3$) of **6c**.

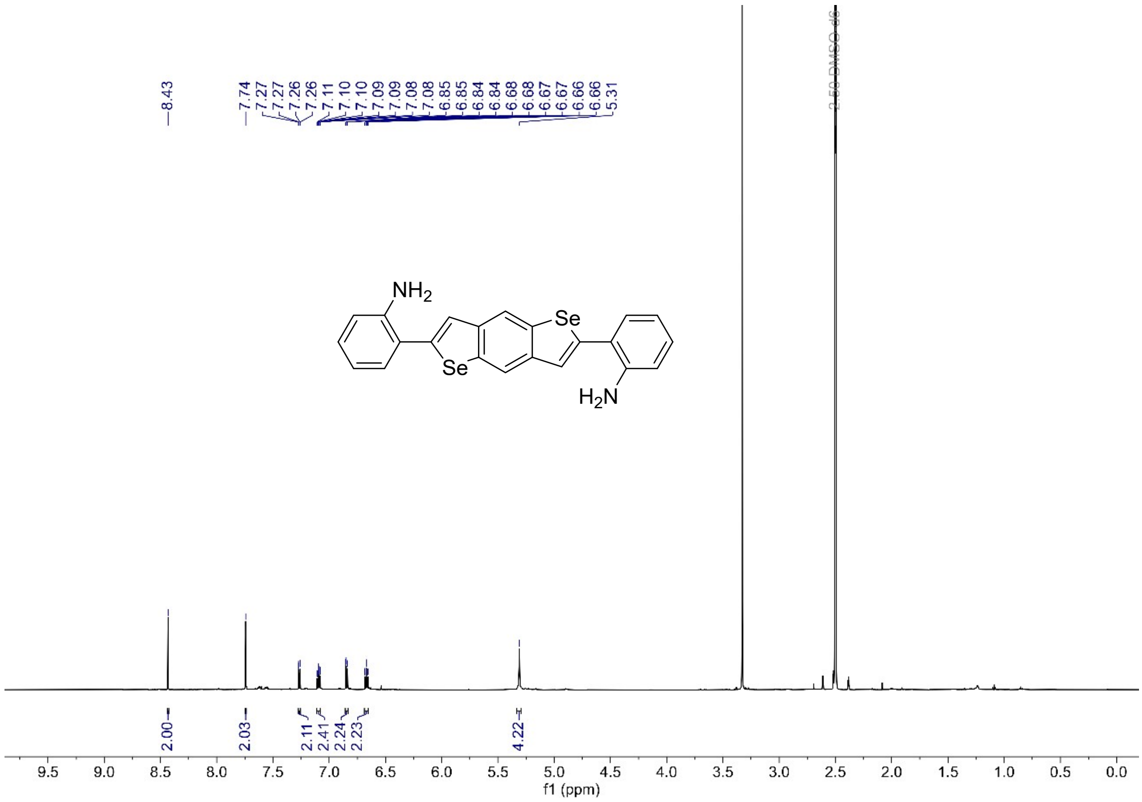


Figure S18. ^1H NMR spectrum (600 MHz, DMSO-d6) of **7a**.

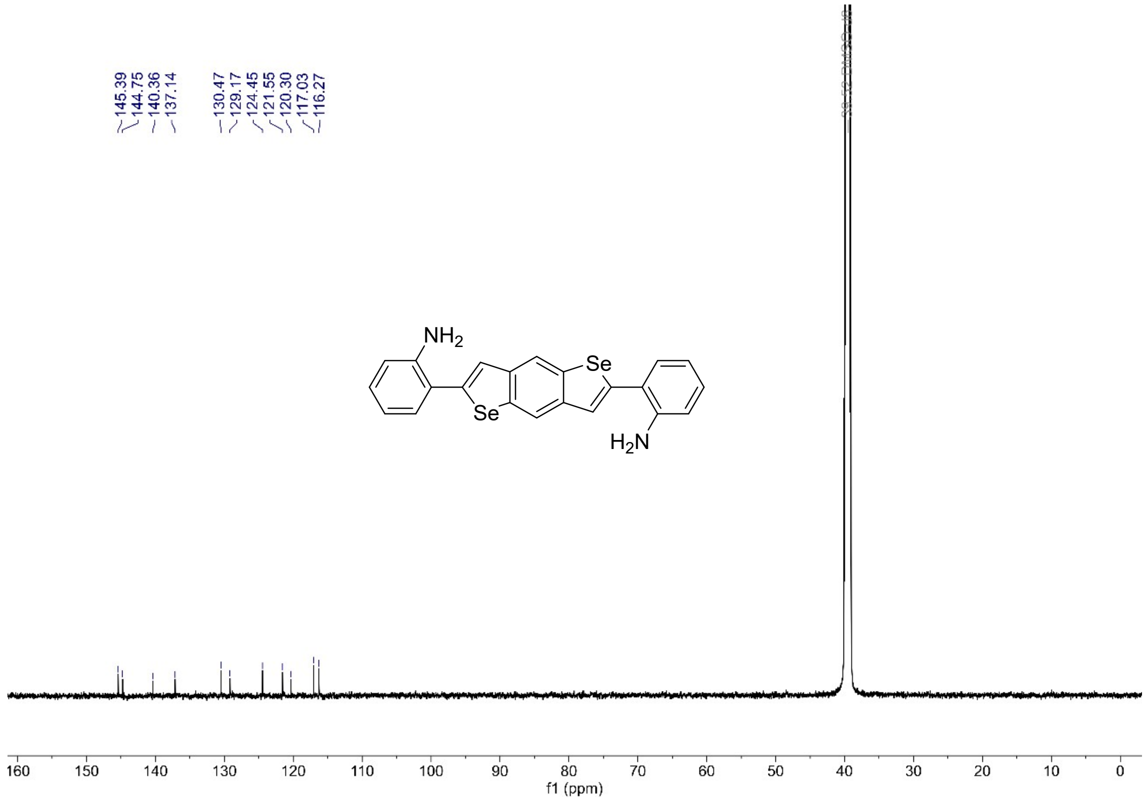


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, DMSO-d6) of **7a**.

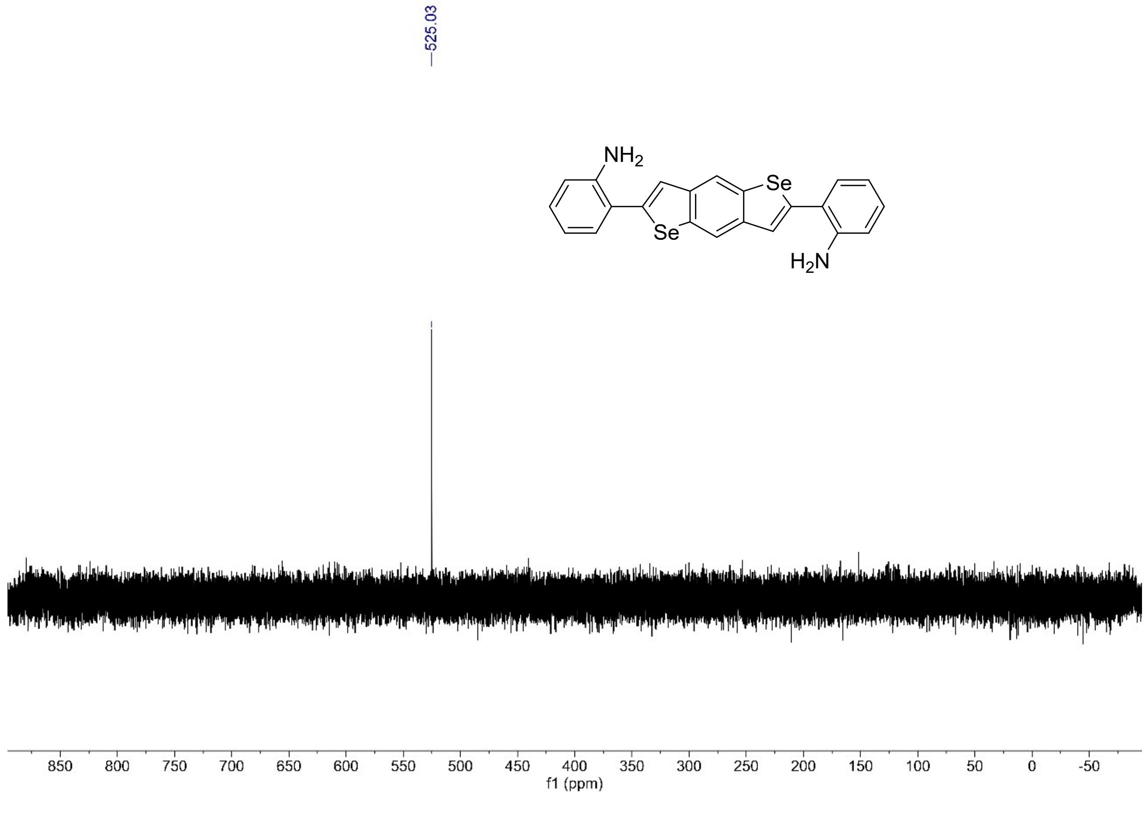


Figure S20. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, DMSO-d6) of **7a**.

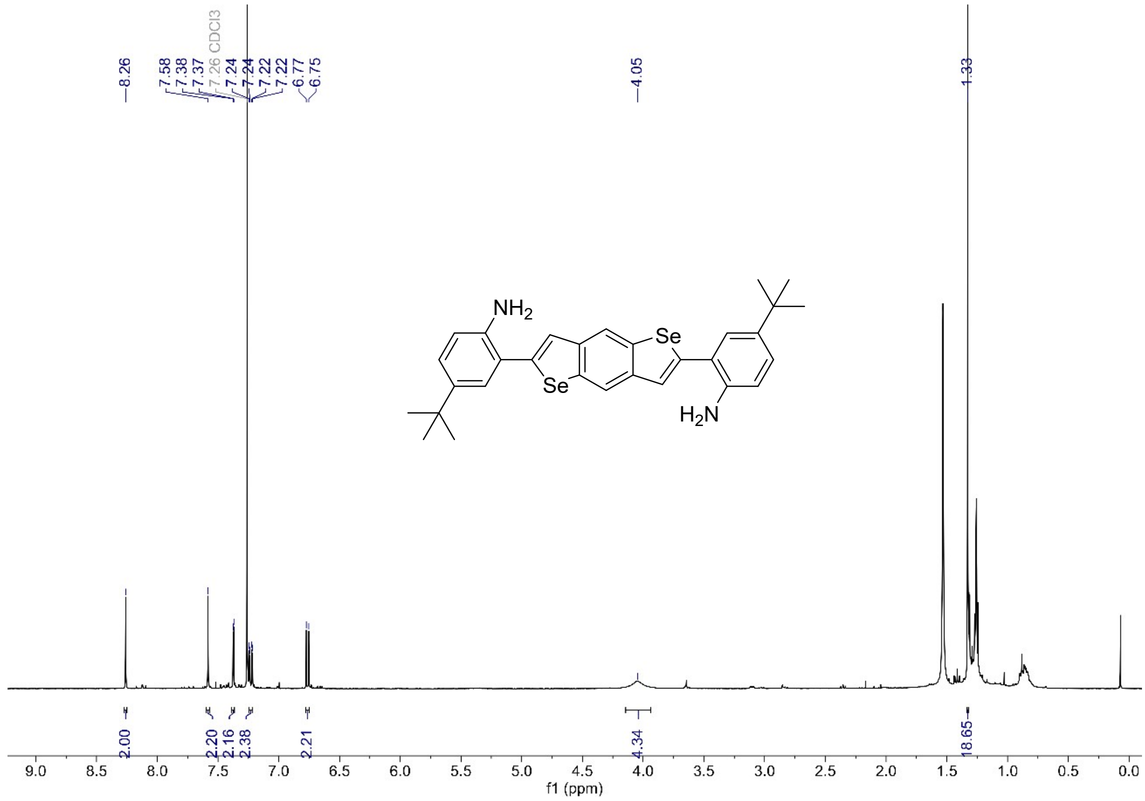


Figure S21. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **7b**.

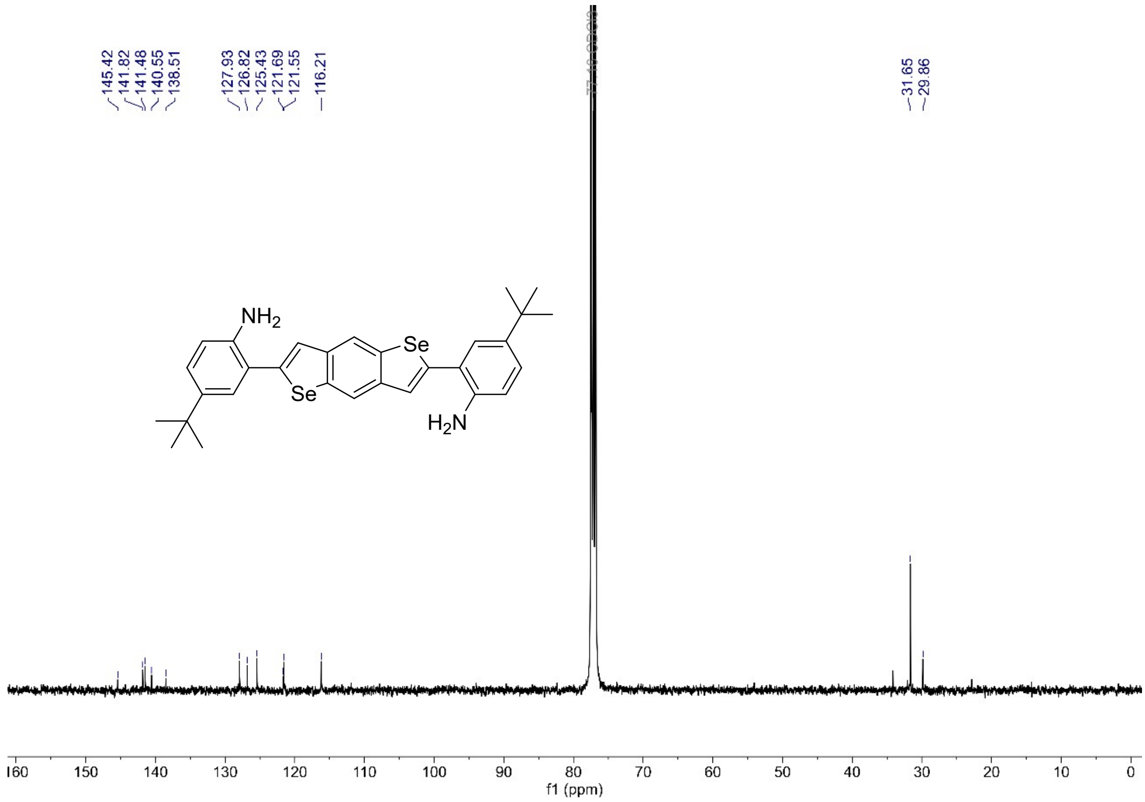


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **7b**.

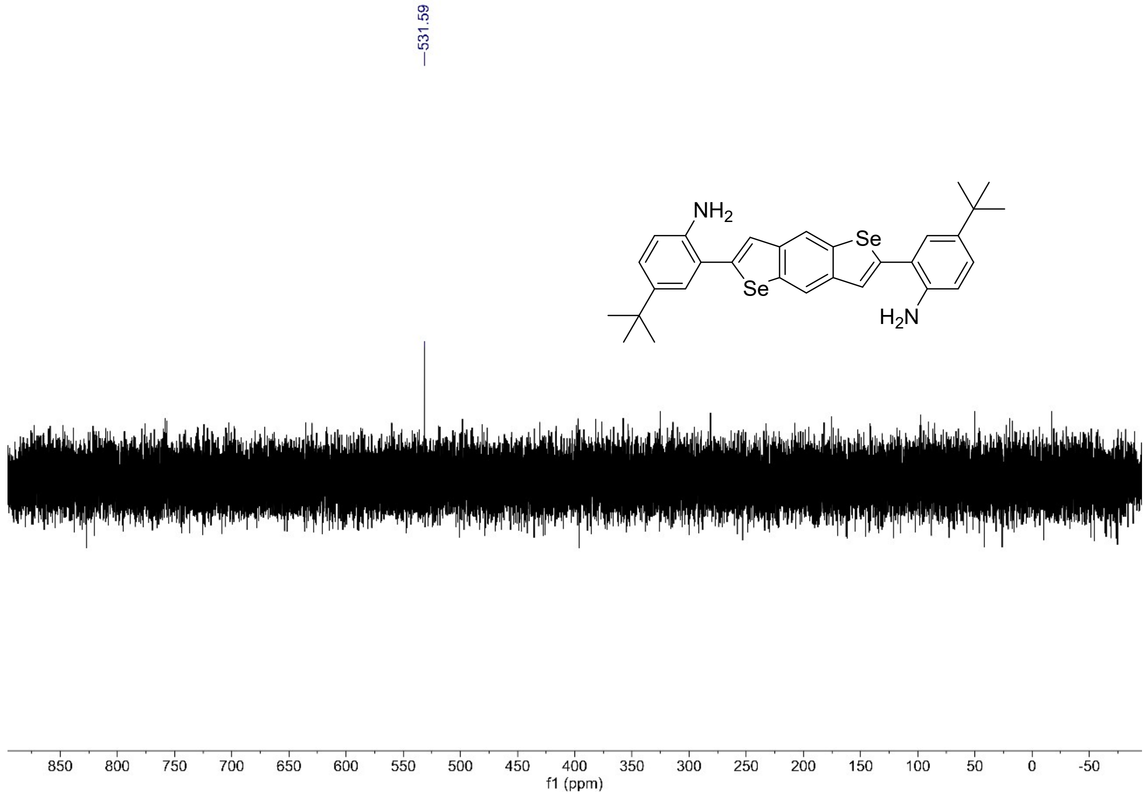


Figure S23. $^{77}Se\{^1H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **7b**.

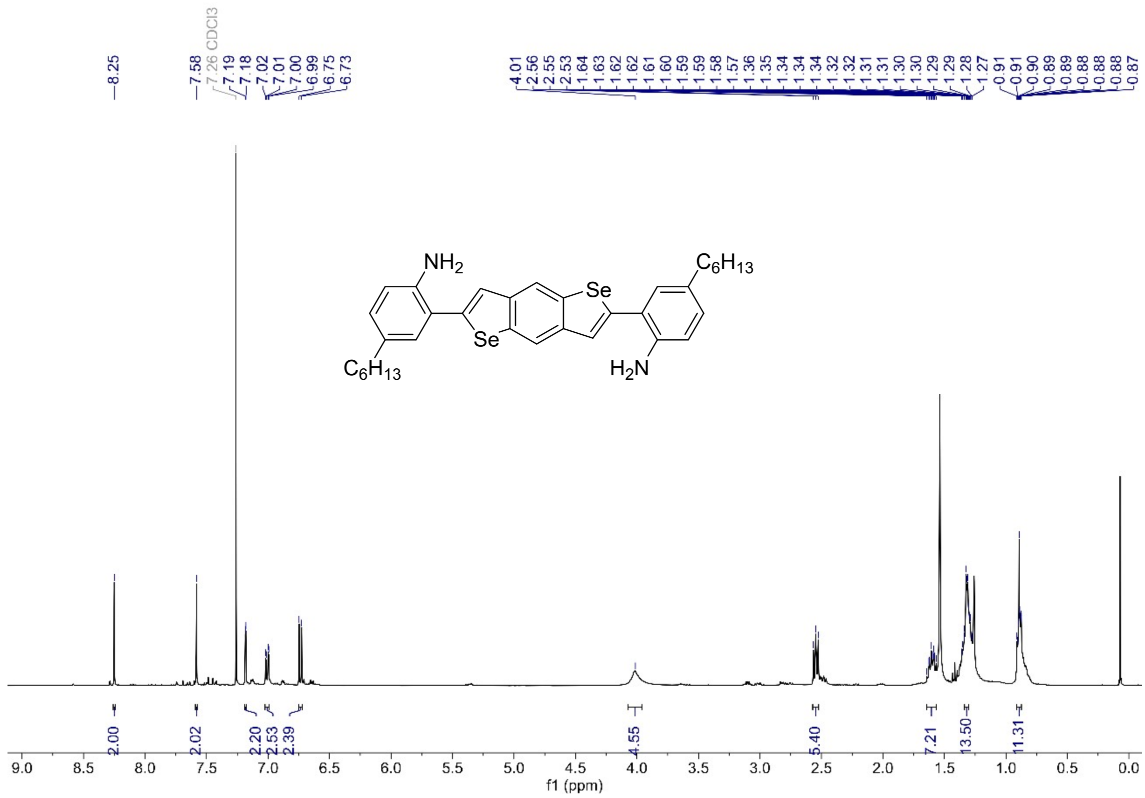


Figure S24. ^1H NMR spectrum (400 MHz, $CDCl_3$) of **7c**.

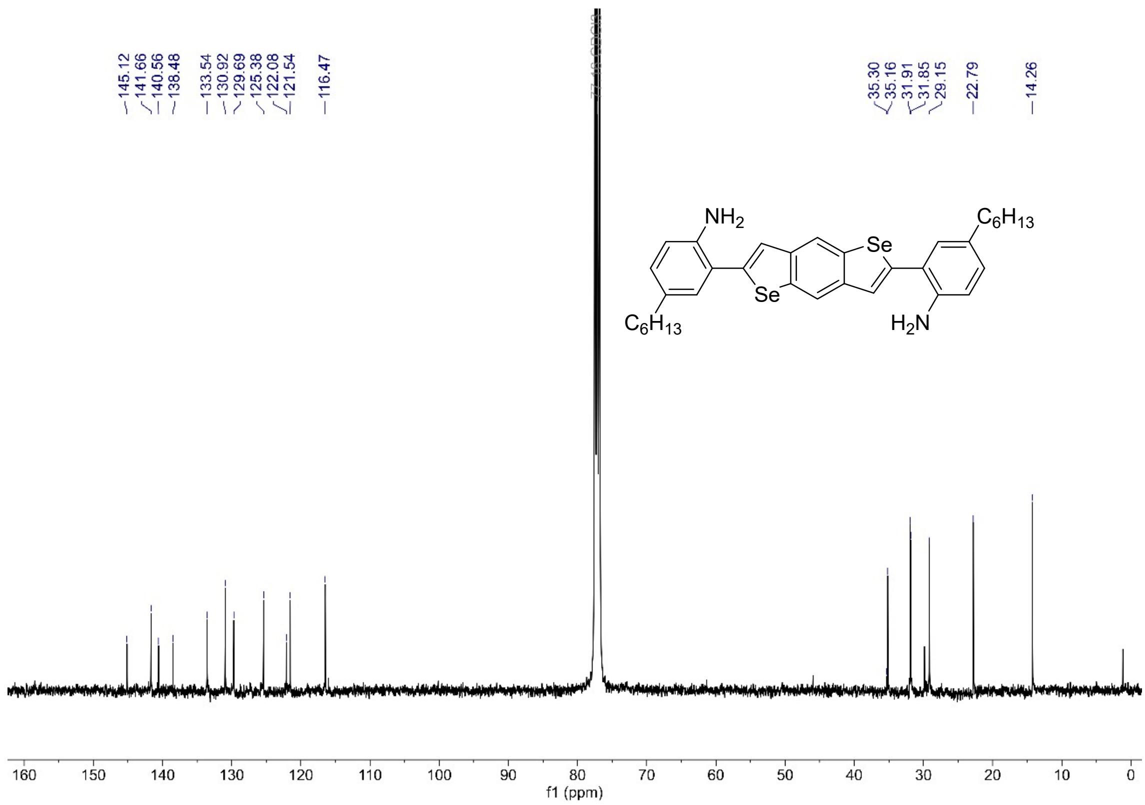


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **7c**.

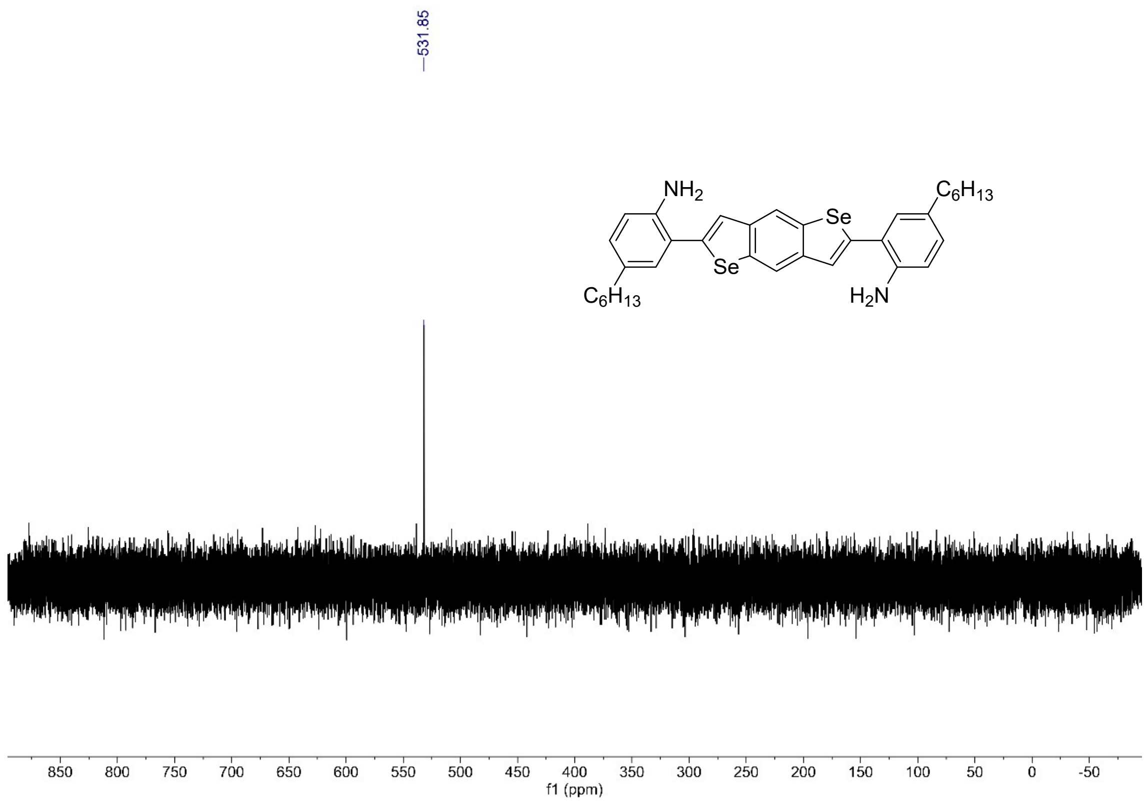


Figure S26. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **7c**.

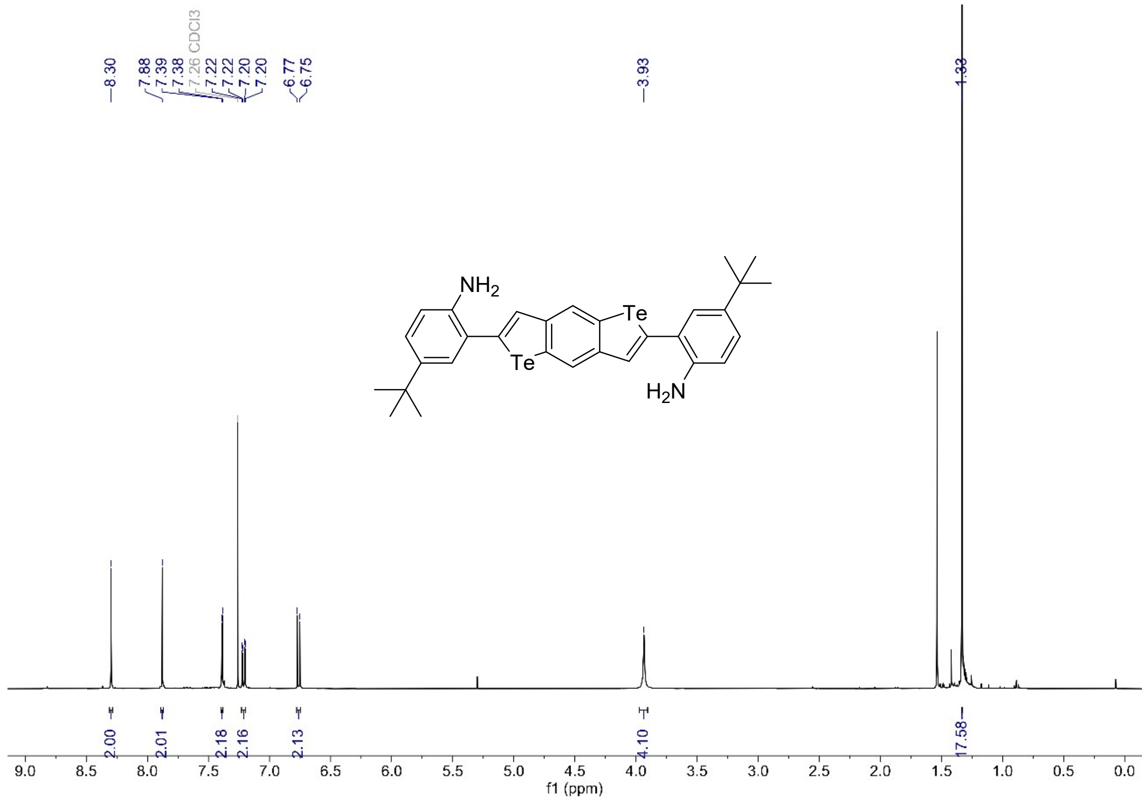


Figure S27. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **8**.

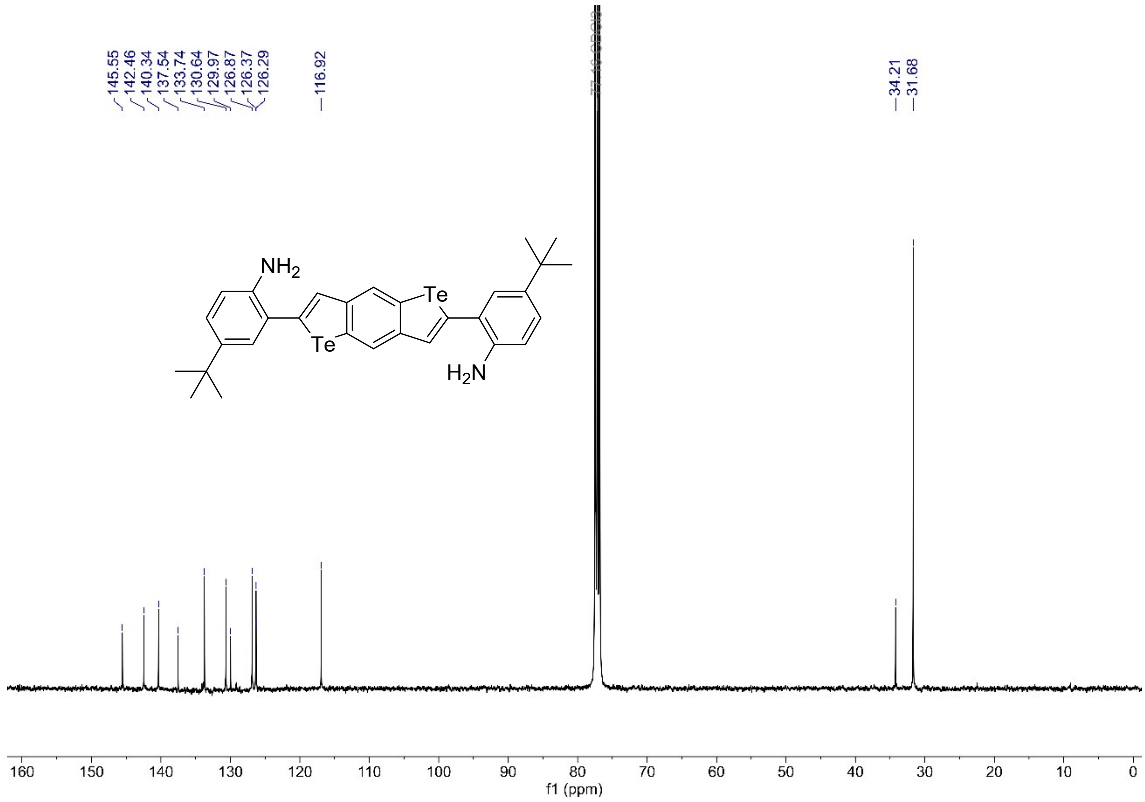


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **8**.

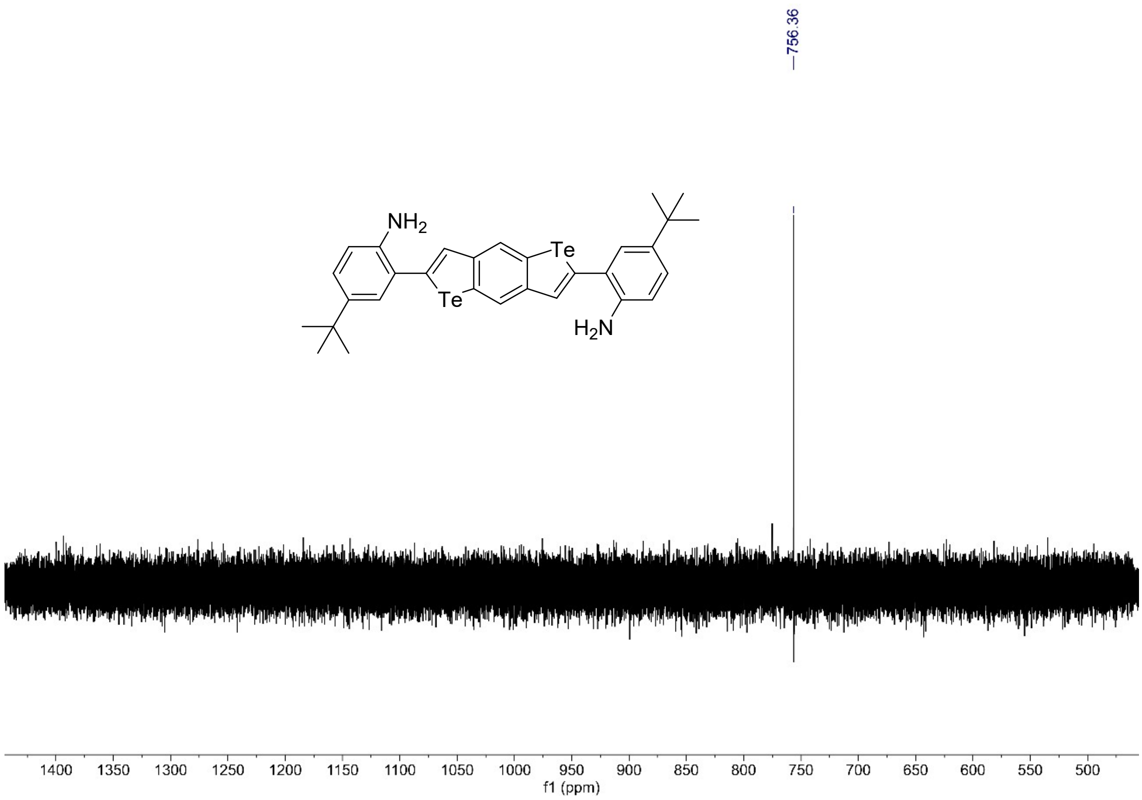


Figure S29. ^{125}Te{^{1}H} NMR spectrum (126 MHz, $CDCl_3$) of **8**.

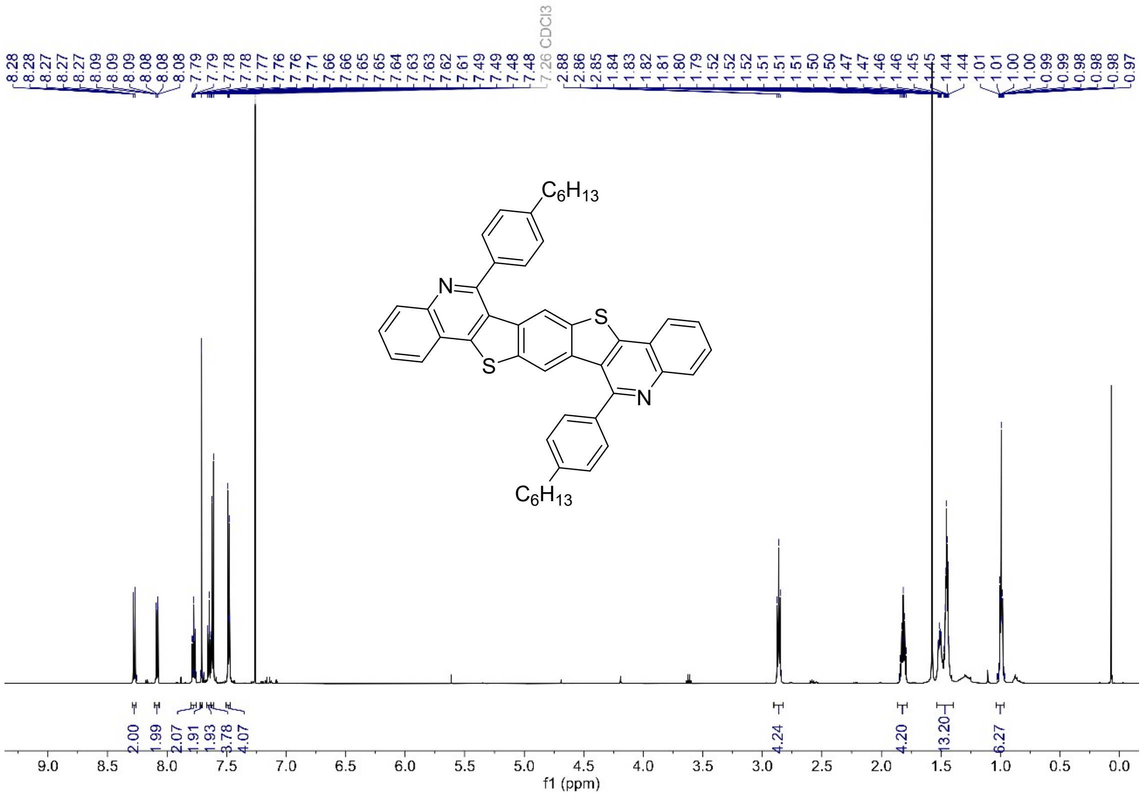


Figure S30. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9aa**.

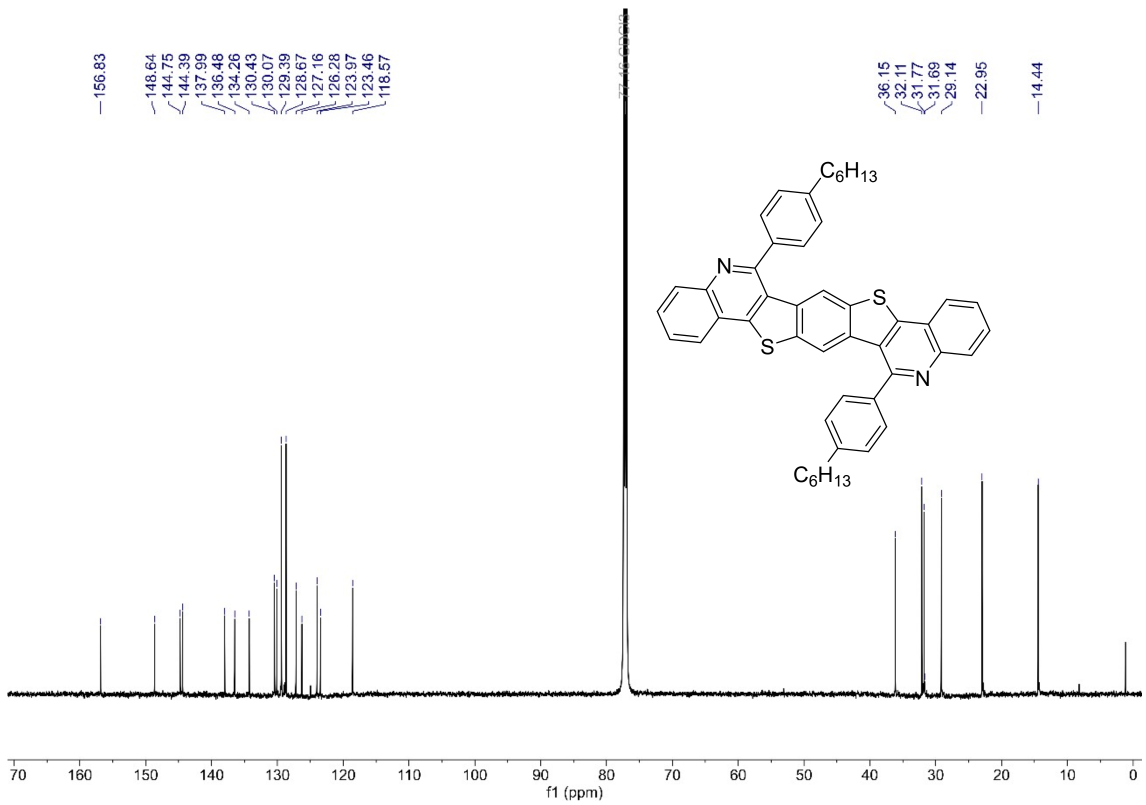


Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9aa**.

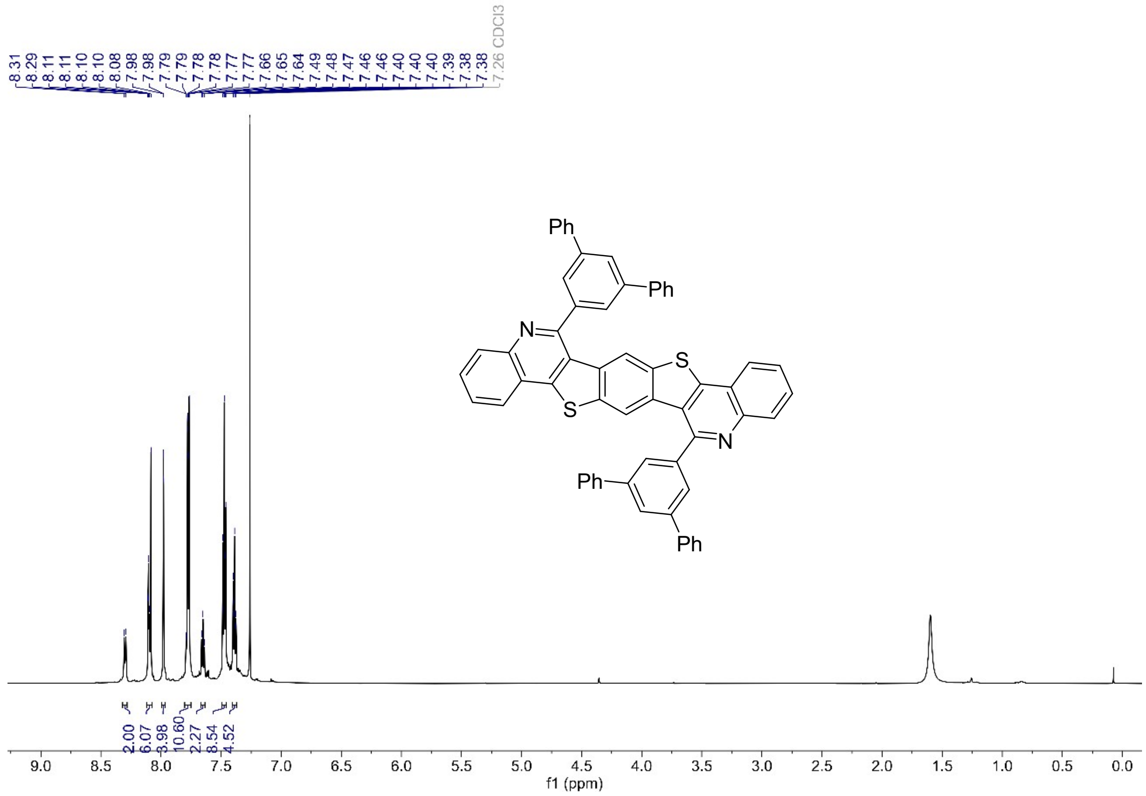


Figure S32. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9ab**.

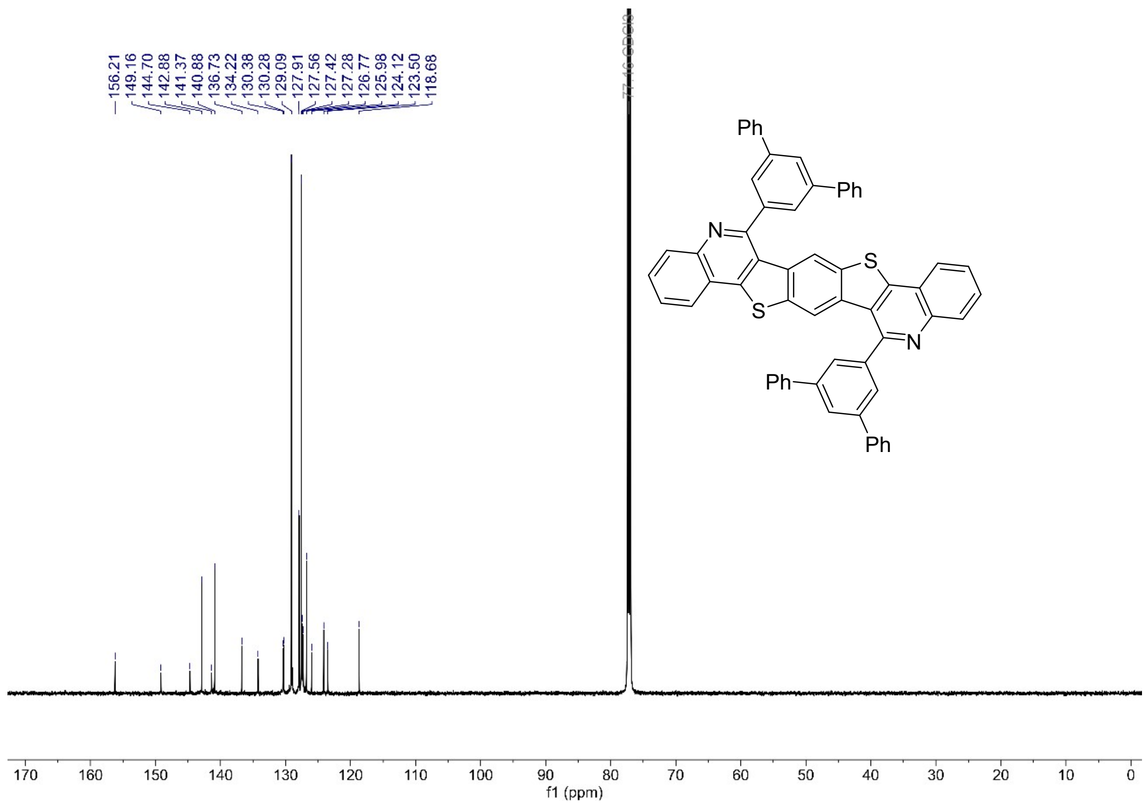


Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9ab**.

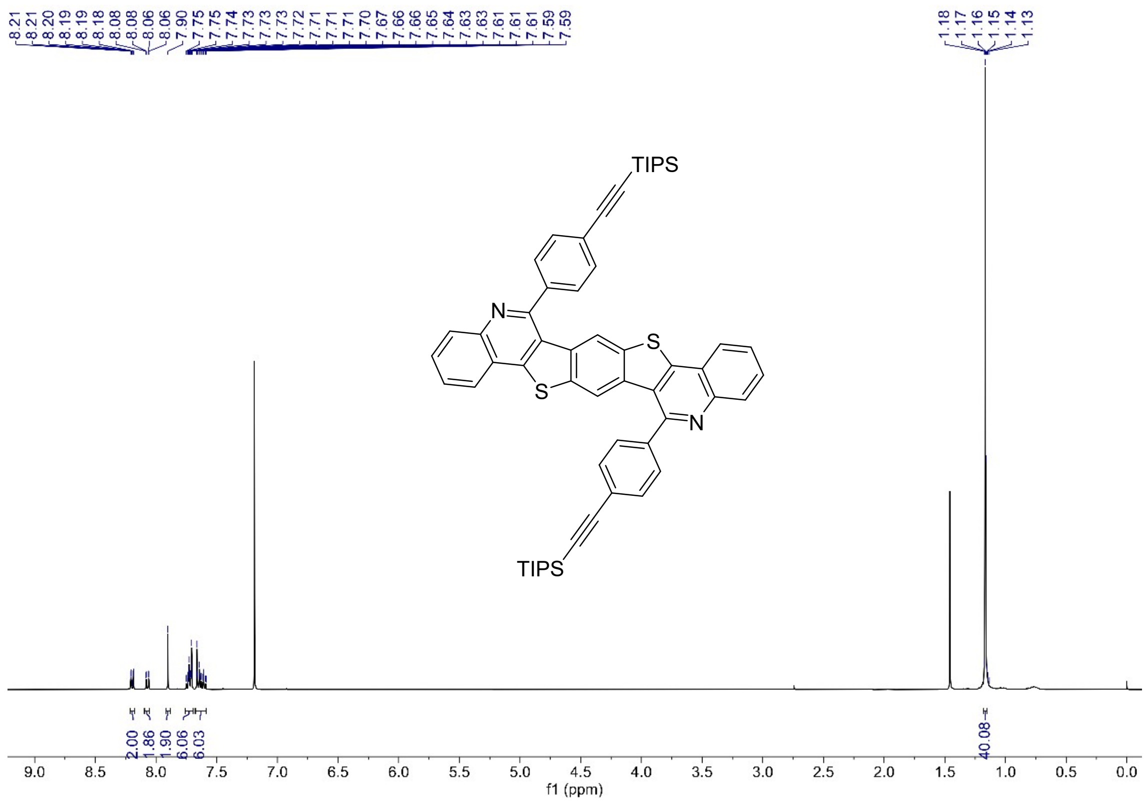


Figure S34. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9ac**.

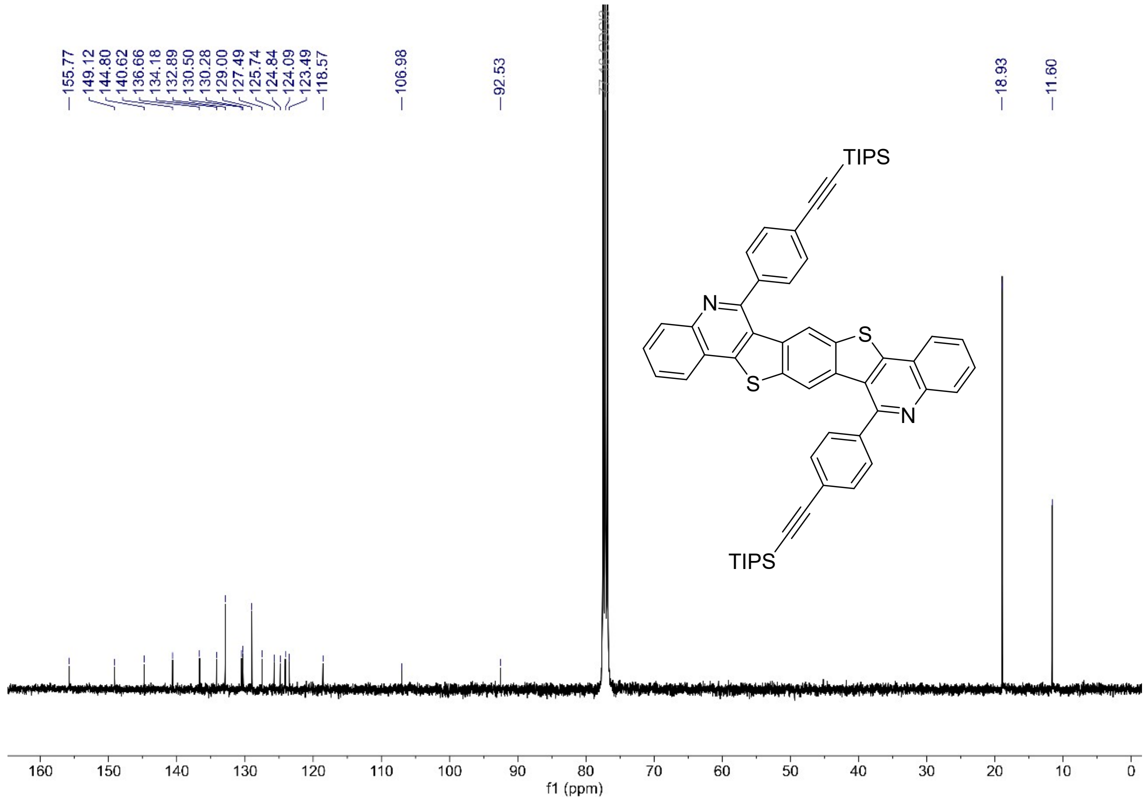


Figure S35. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **9ac**.

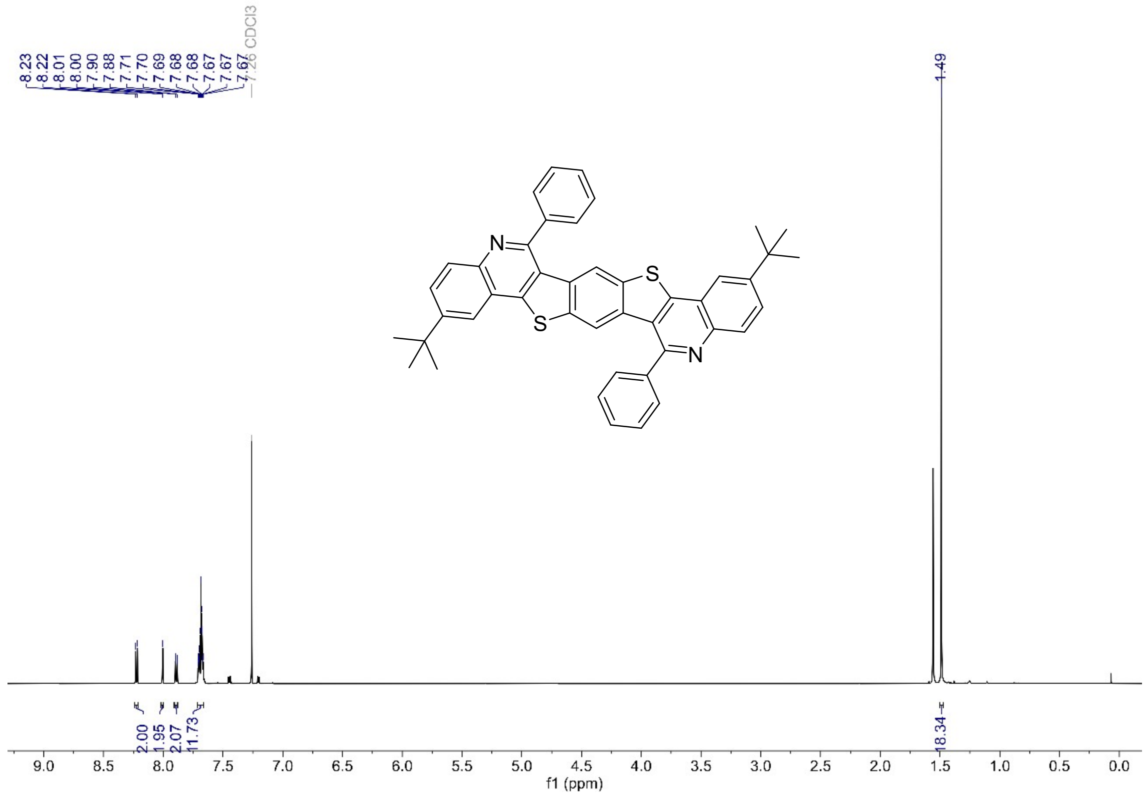


Figure S36. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9ba**.

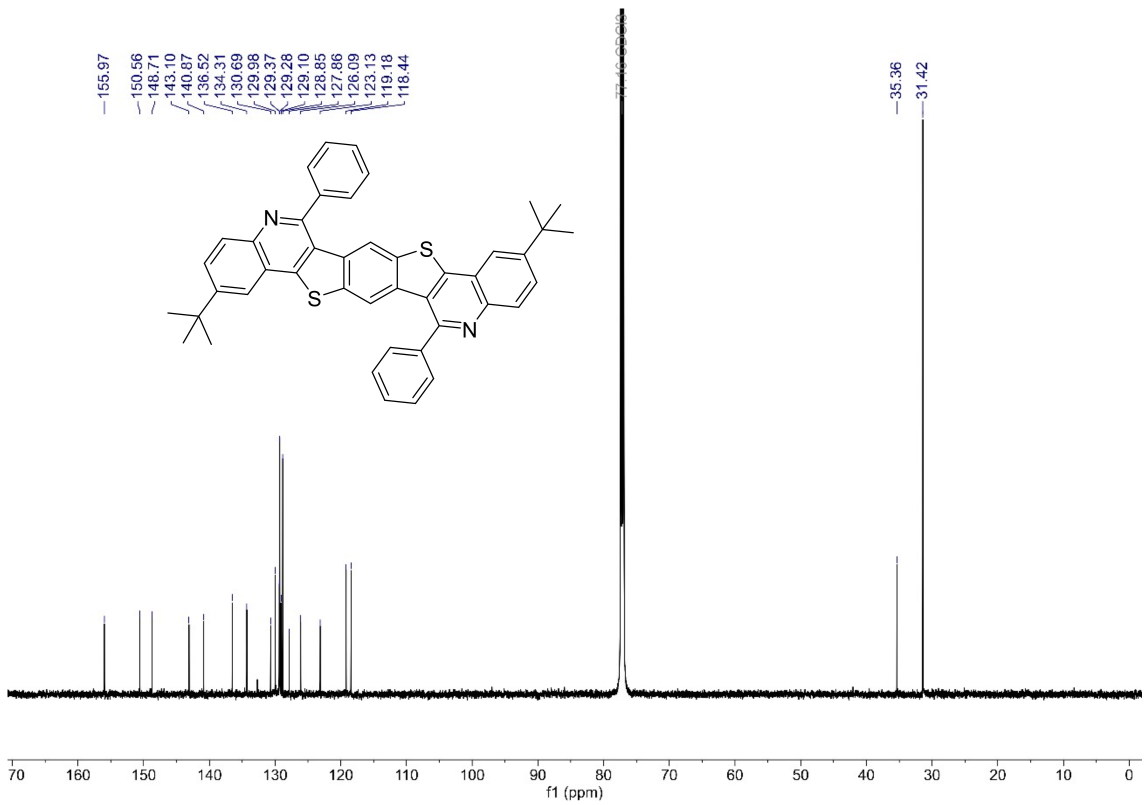


Figure S37. $^{13}C\{^1H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9ba**.

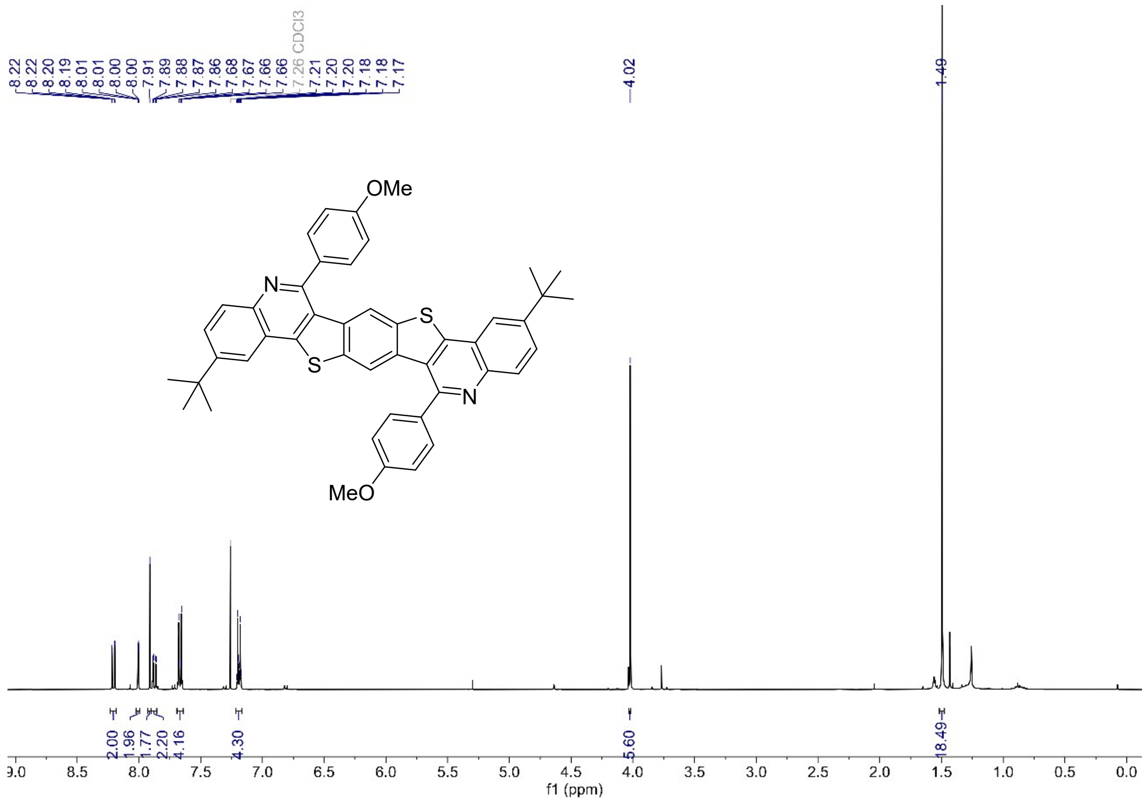


Figure S38. ^1H NMR spectrum (400 MHz, $CDCl_3$) of **9bb**.

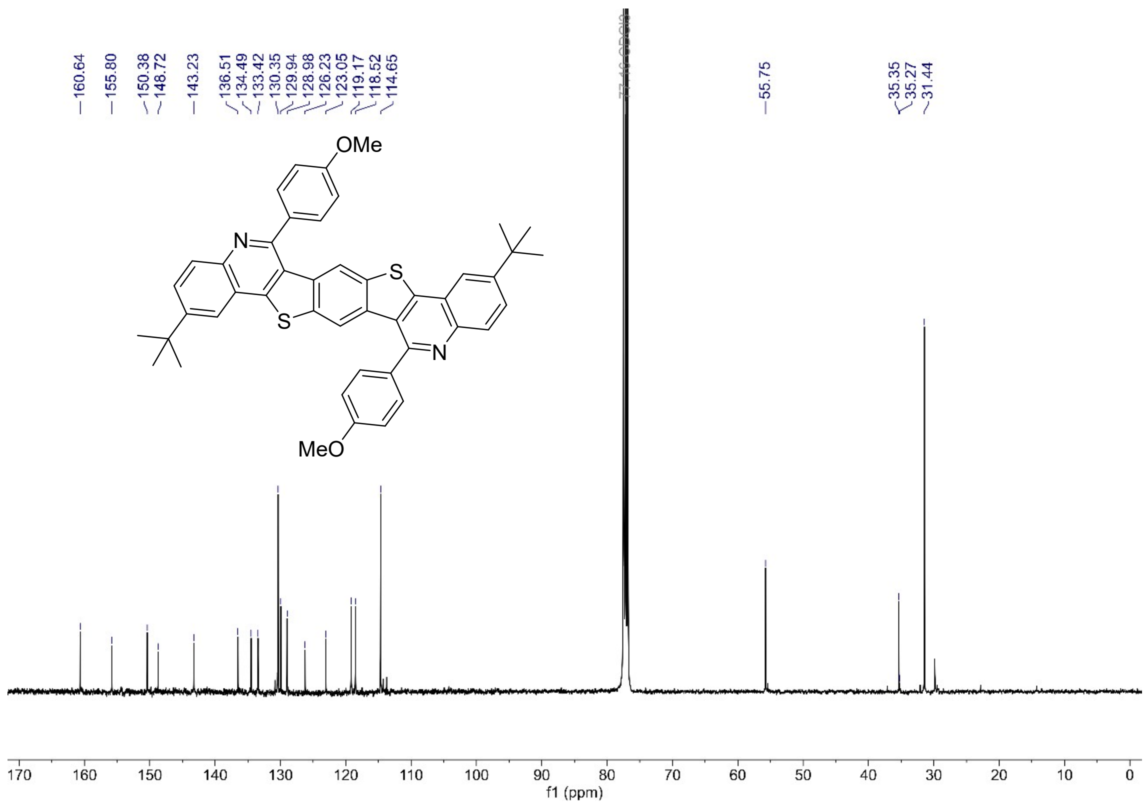


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **9bb**.

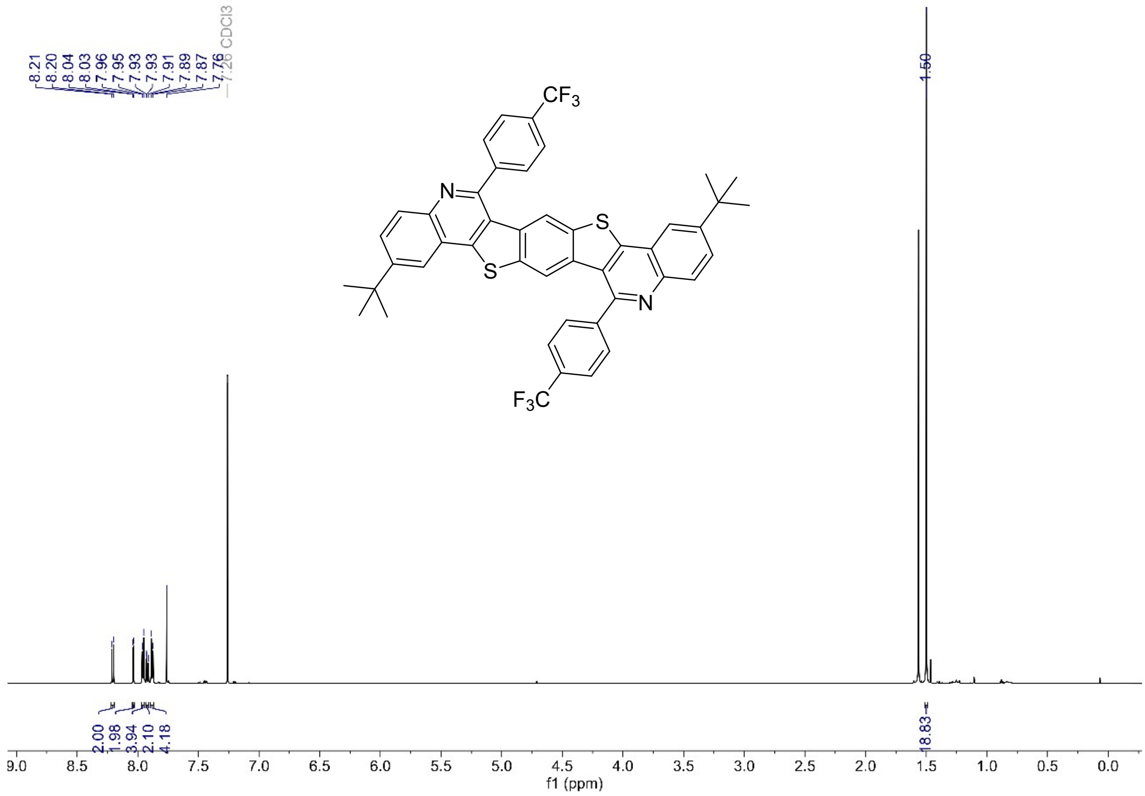


Figure S40. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9bc**.

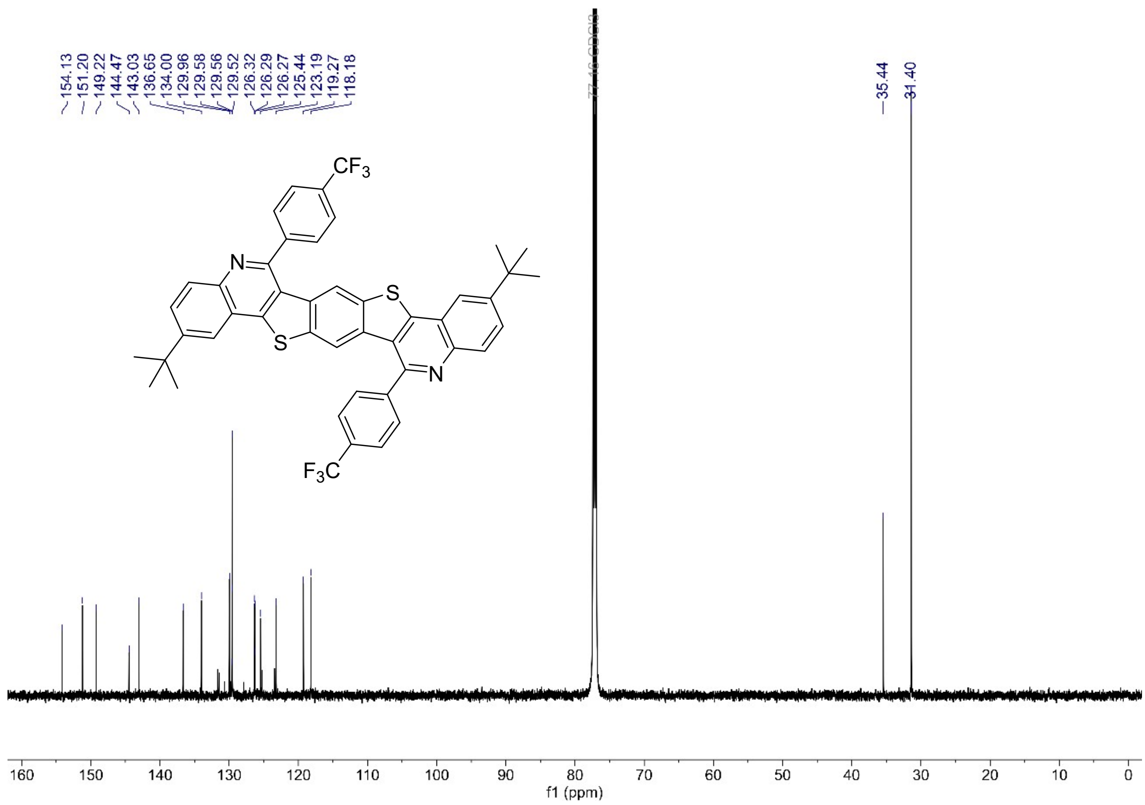


Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9bc**.

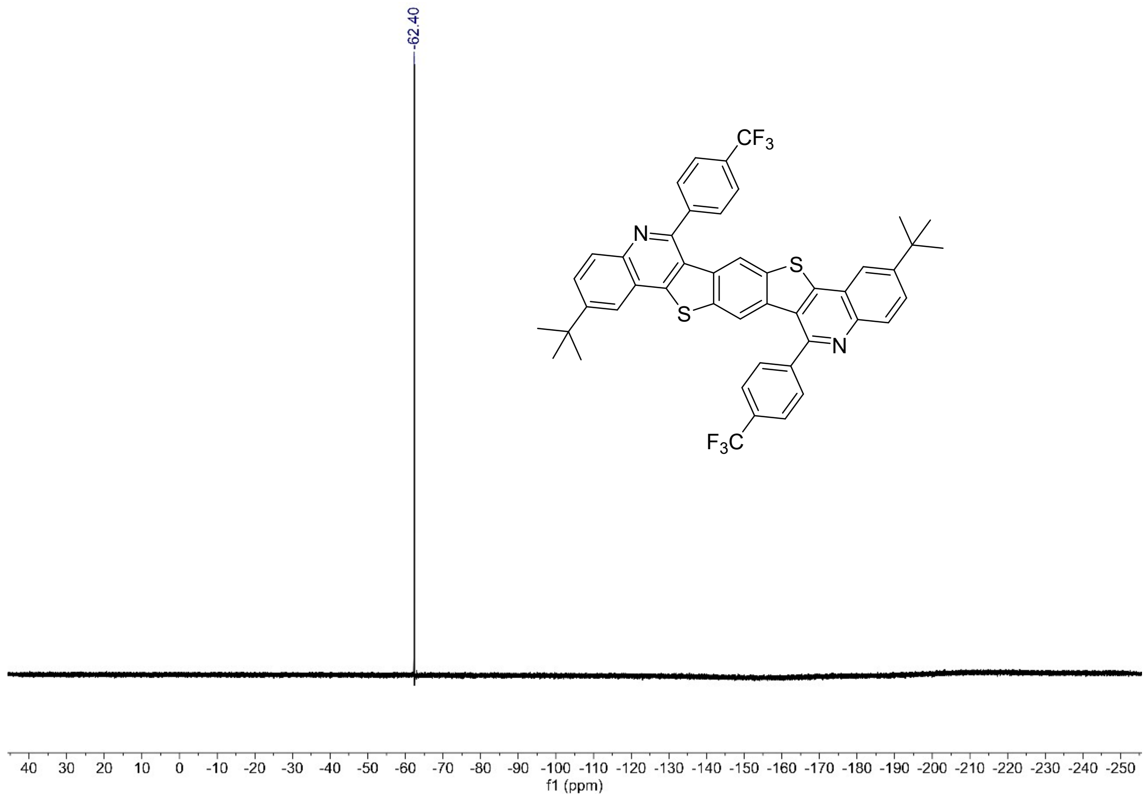


Figure S42. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **9bc**.

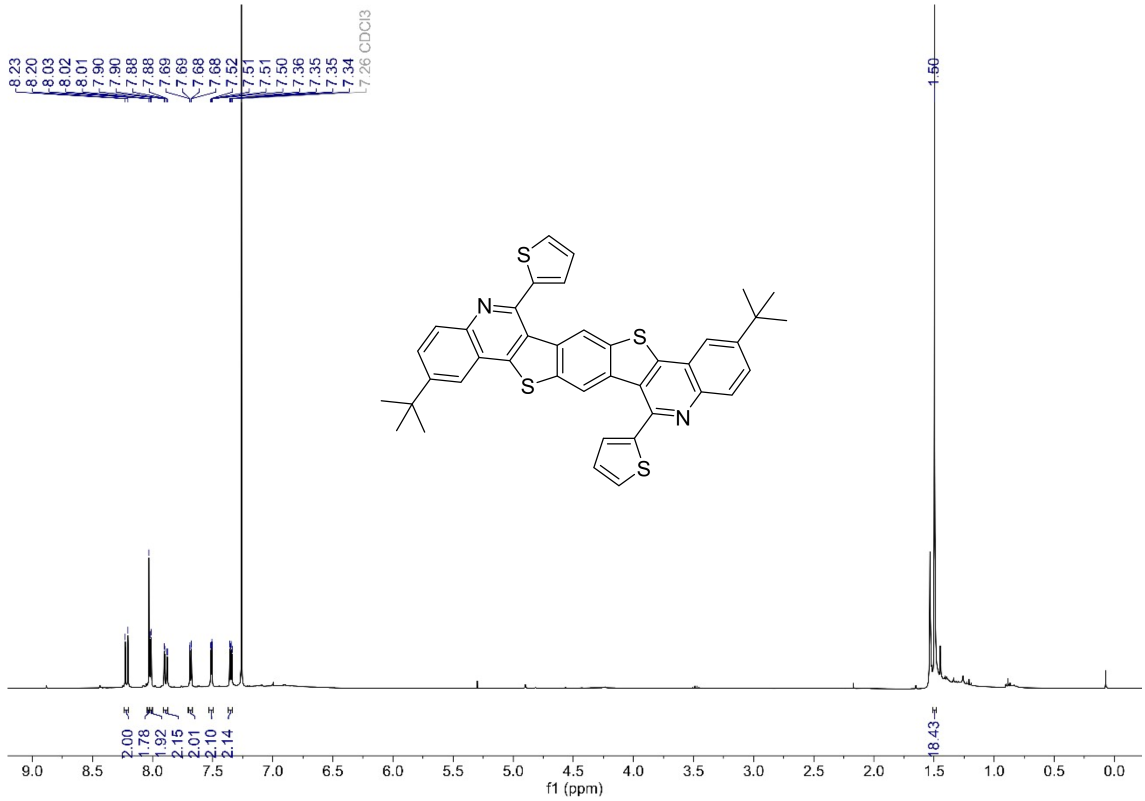


Figure S43. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9bd**.

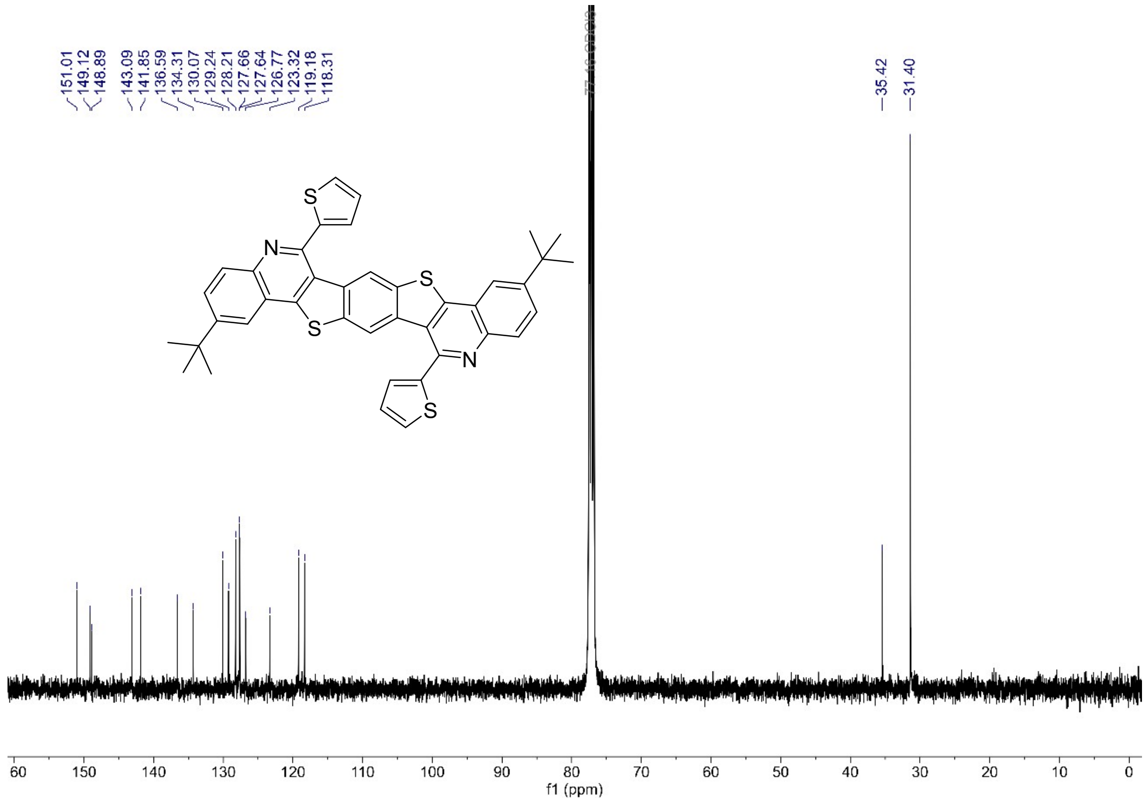


Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **9bd**.

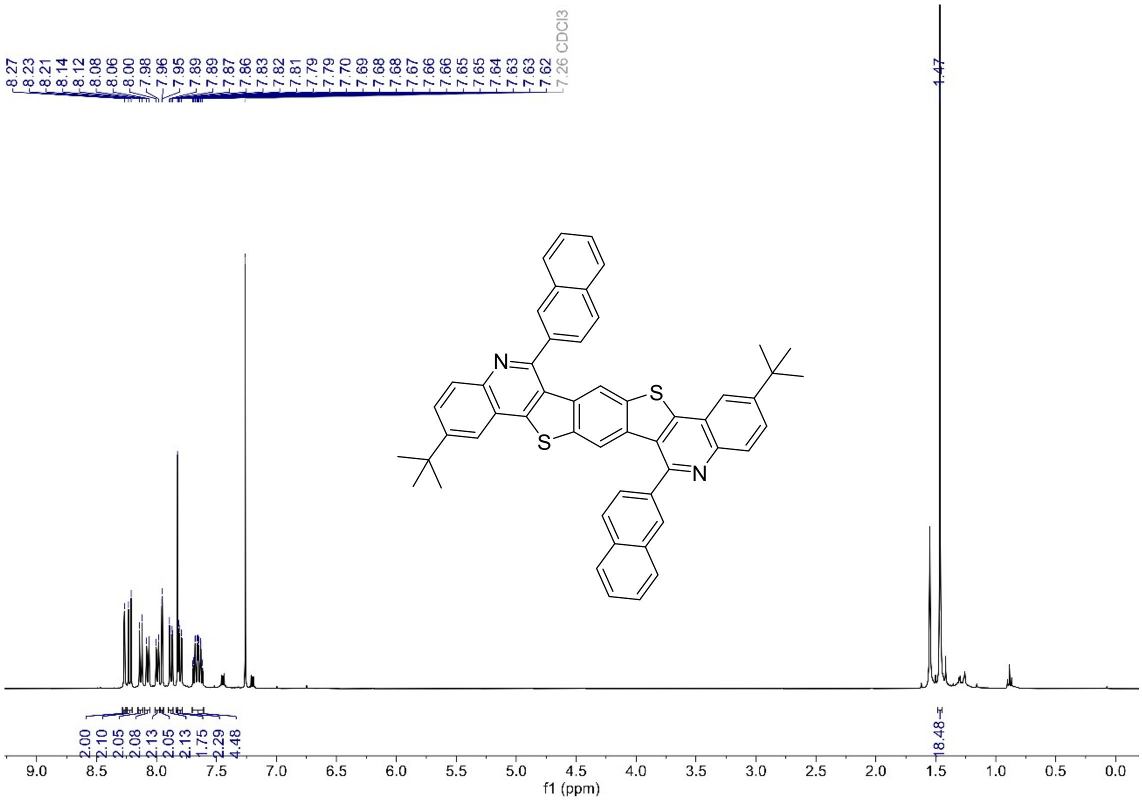


Figure S45. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9be**.

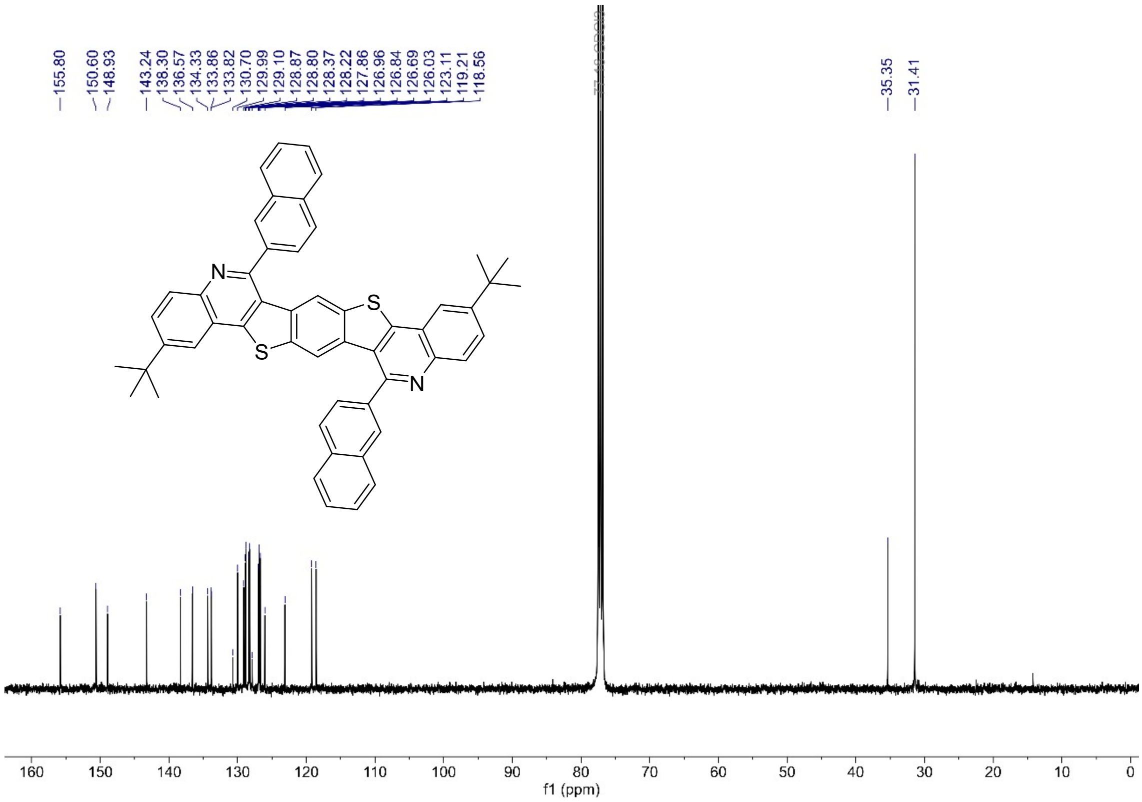


Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **9be**.

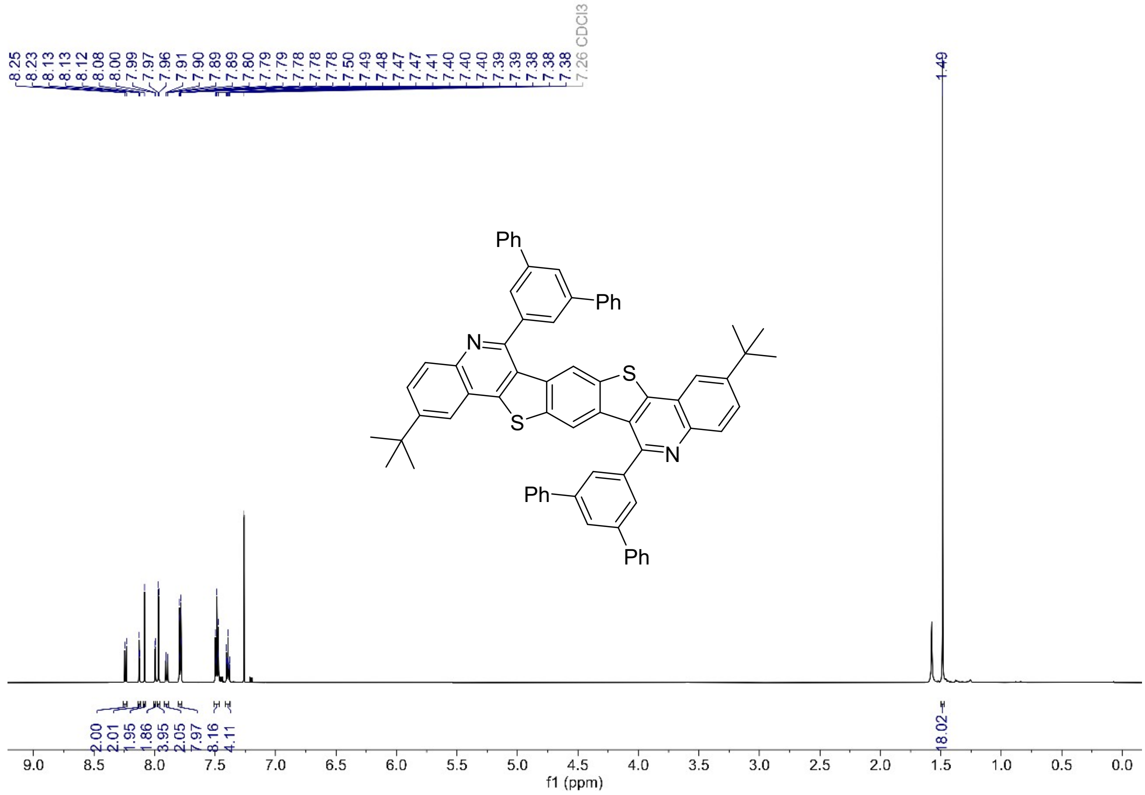


Figure S47. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9bf**.

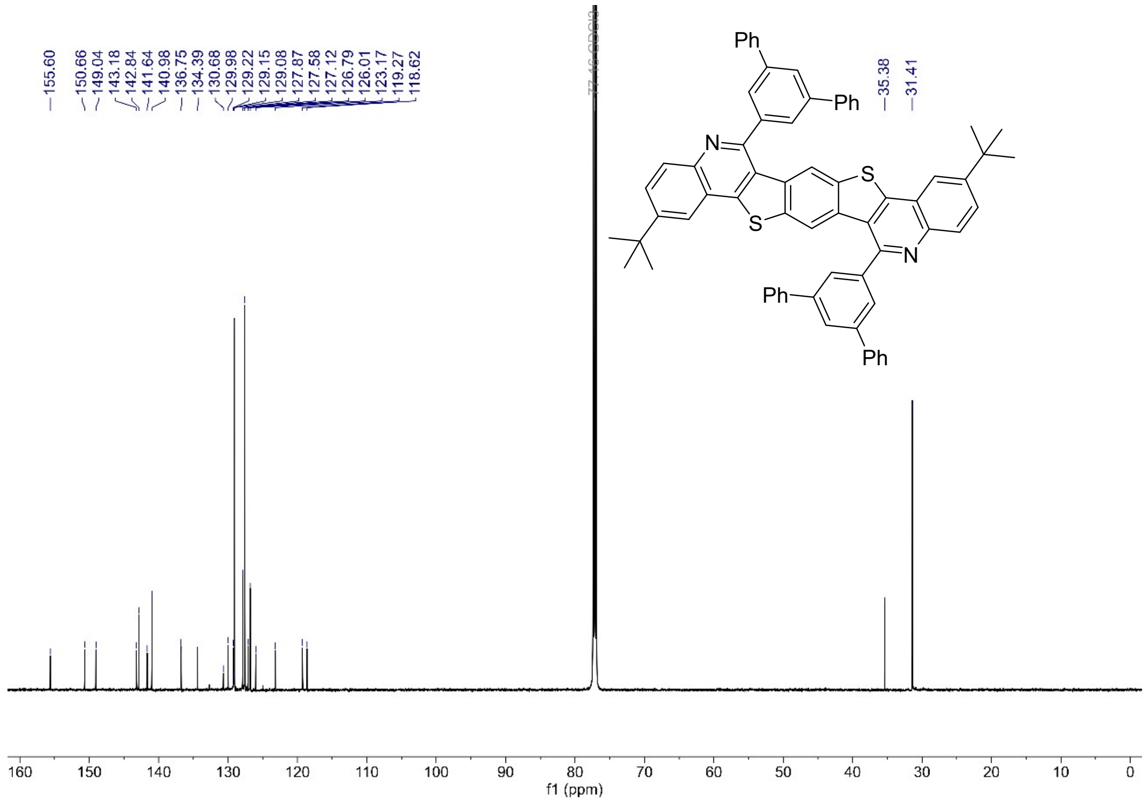


Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9bf**.

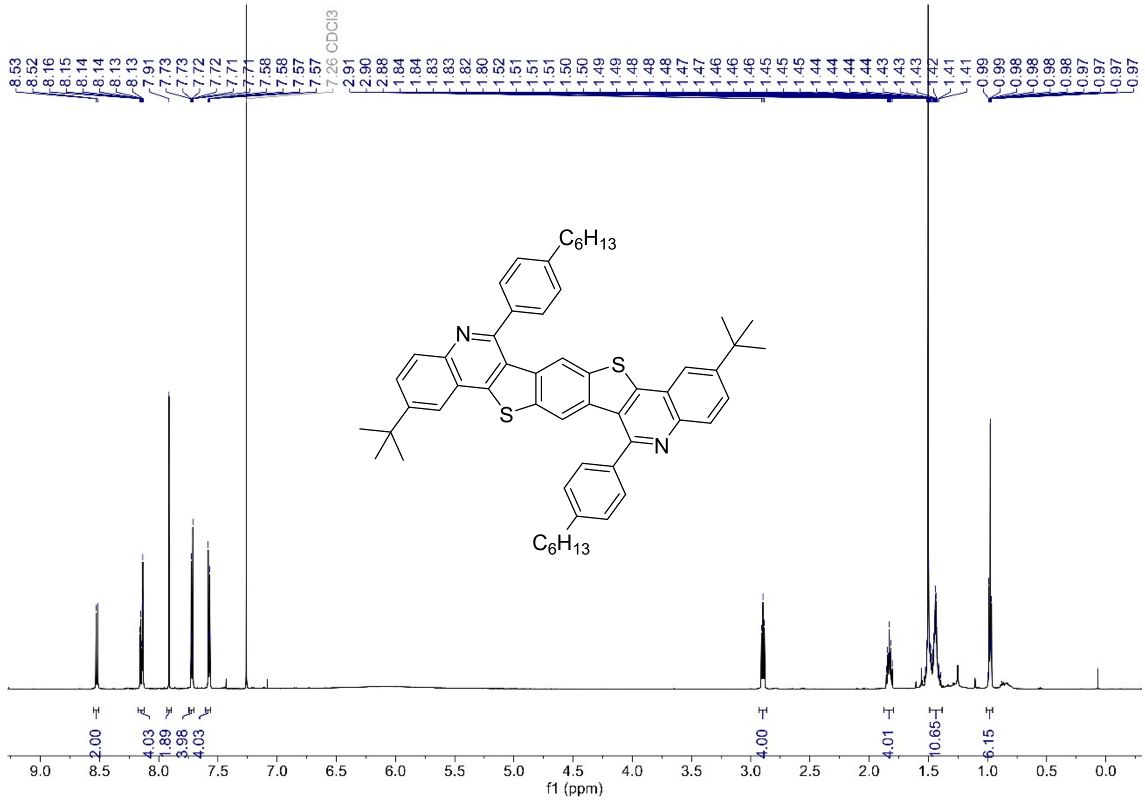


Figure S49. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9bg**.

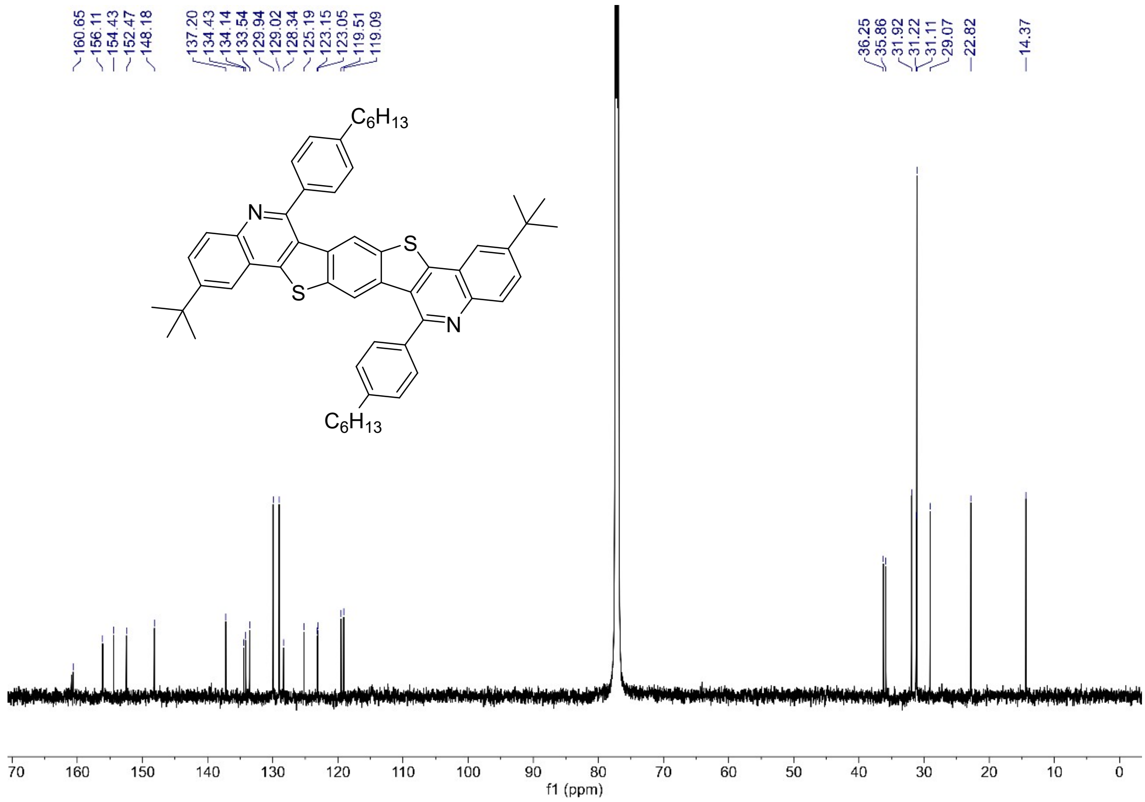


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9bg**.

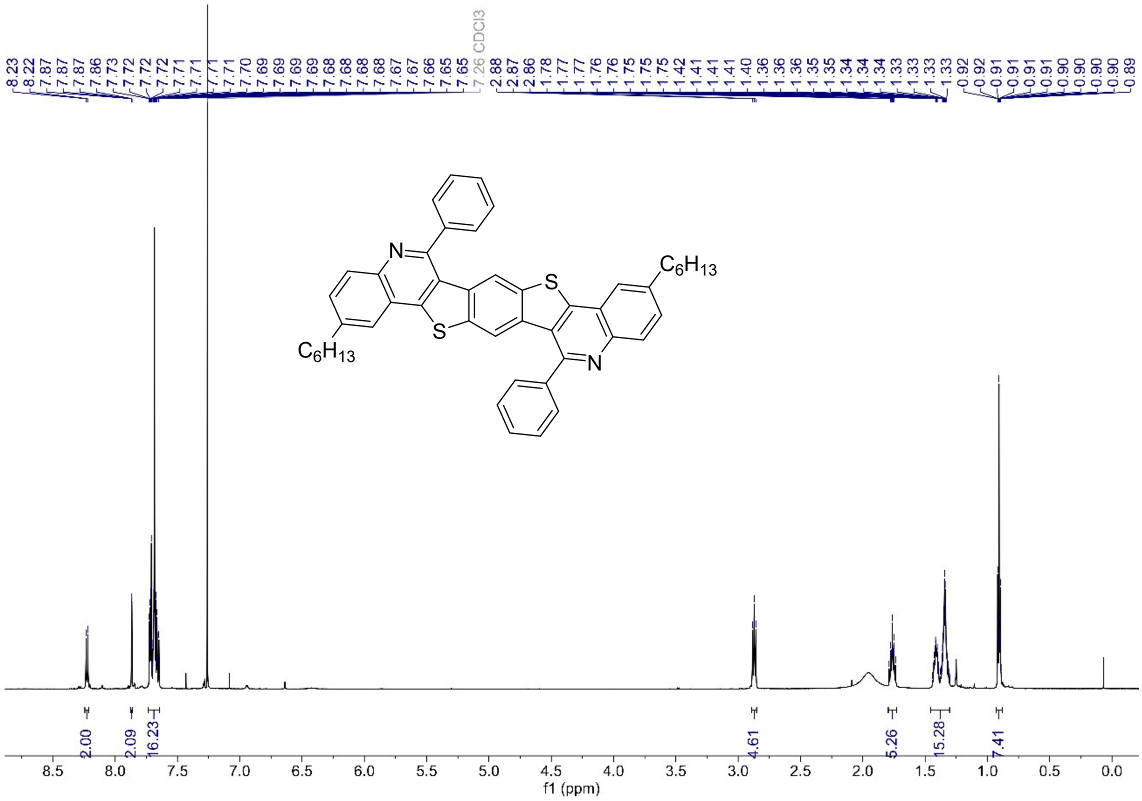


Figure S51. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9ca**.

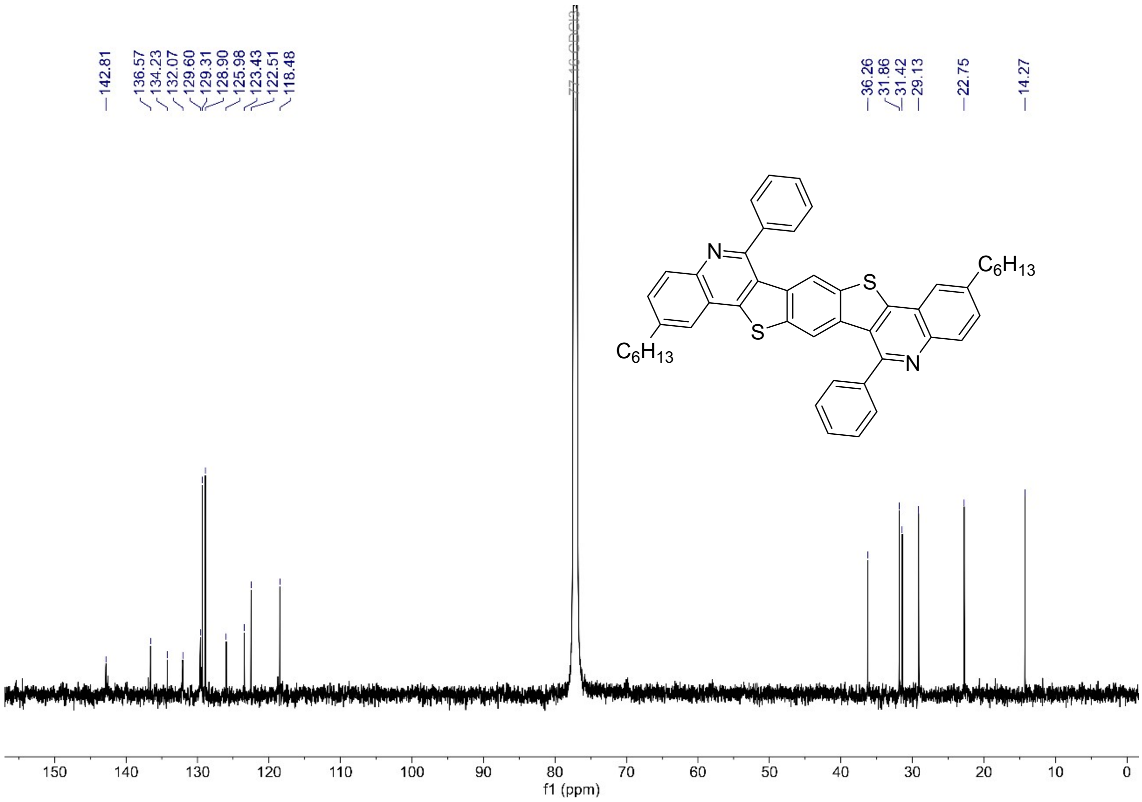


Figure S52. $^{13}C\{^1H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9ca**.

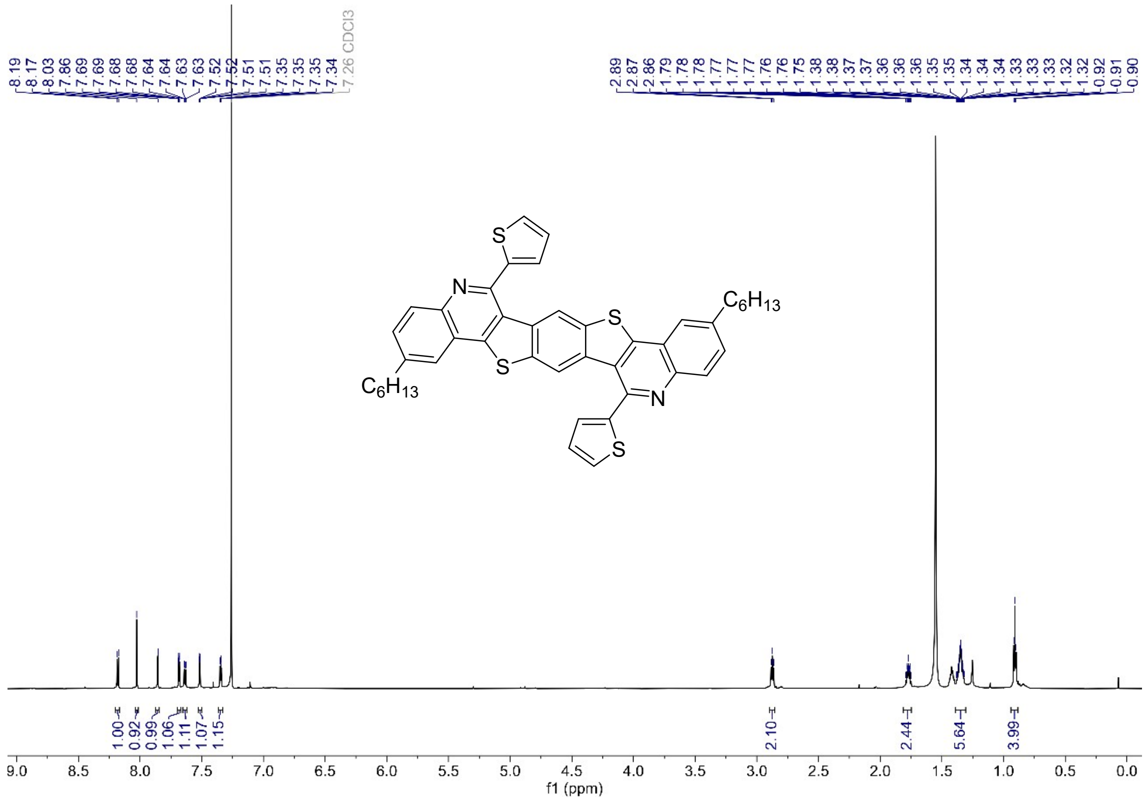


Figure S53. ^{1}H NMR spectrum (700 MHz, $CDCl_3$) of **9cb**.

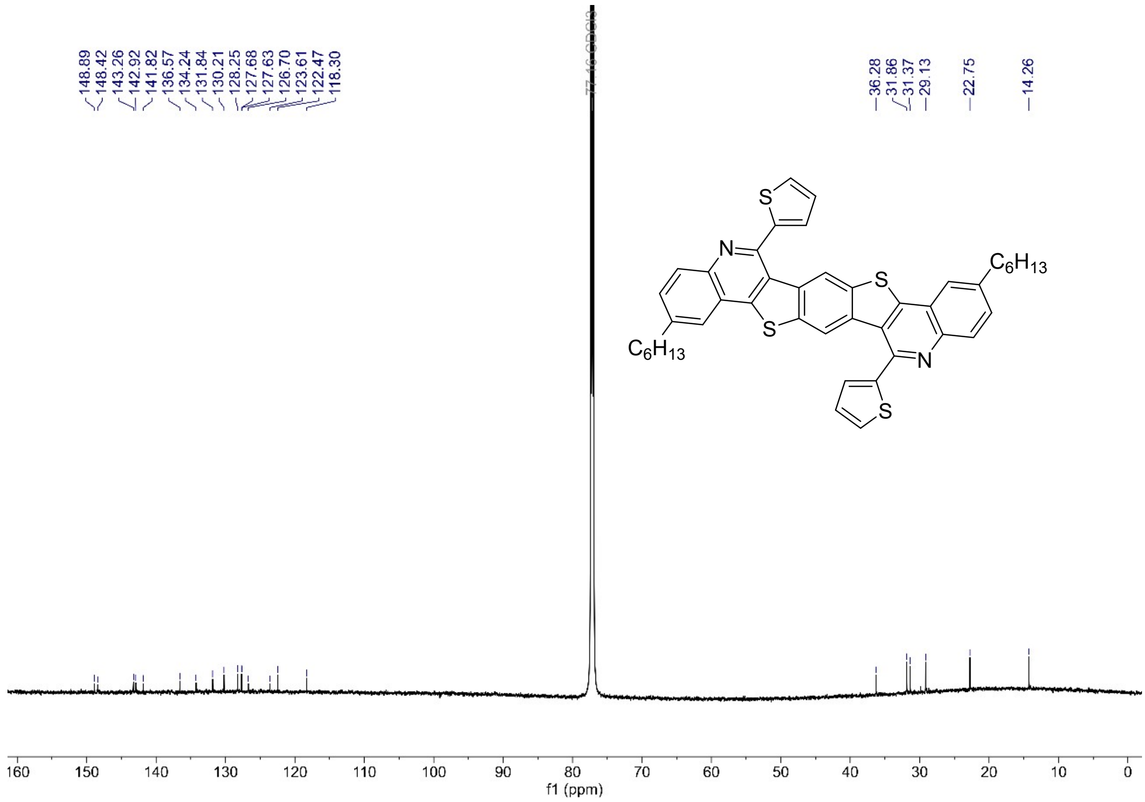


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum (176 MHz, $CDCl_3$) of **9cb**.

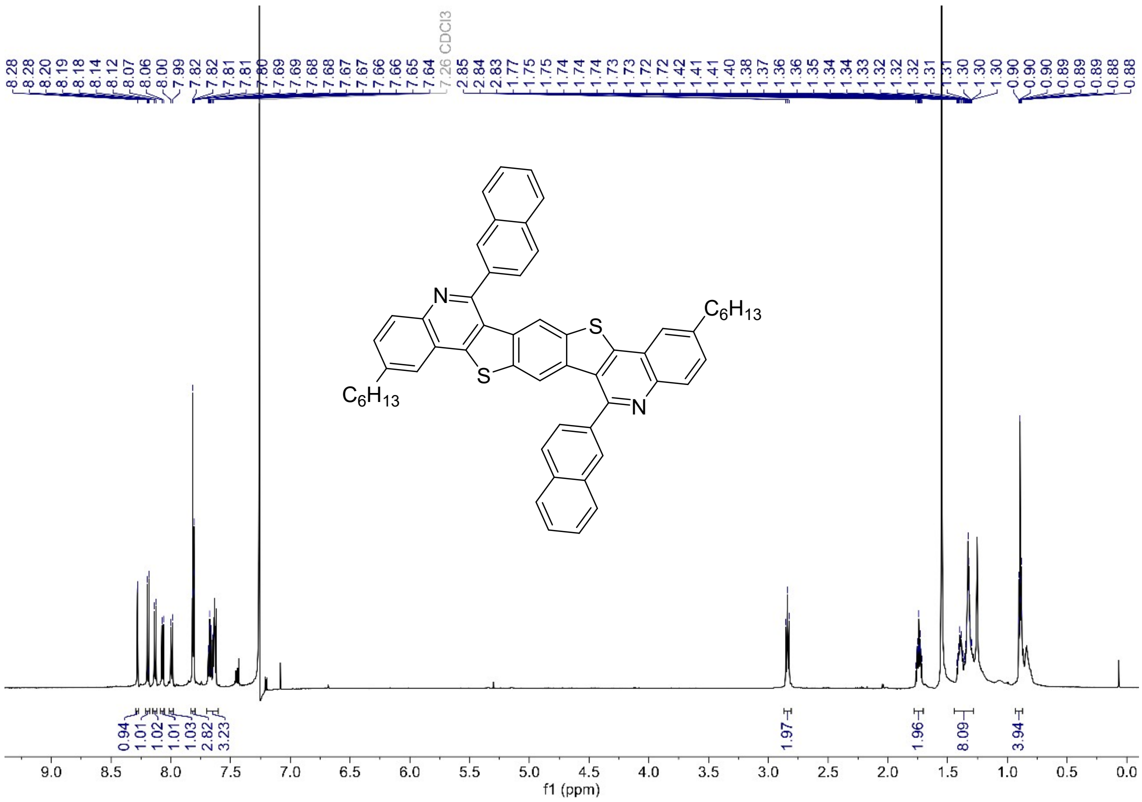


Figure S55. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9cc**.

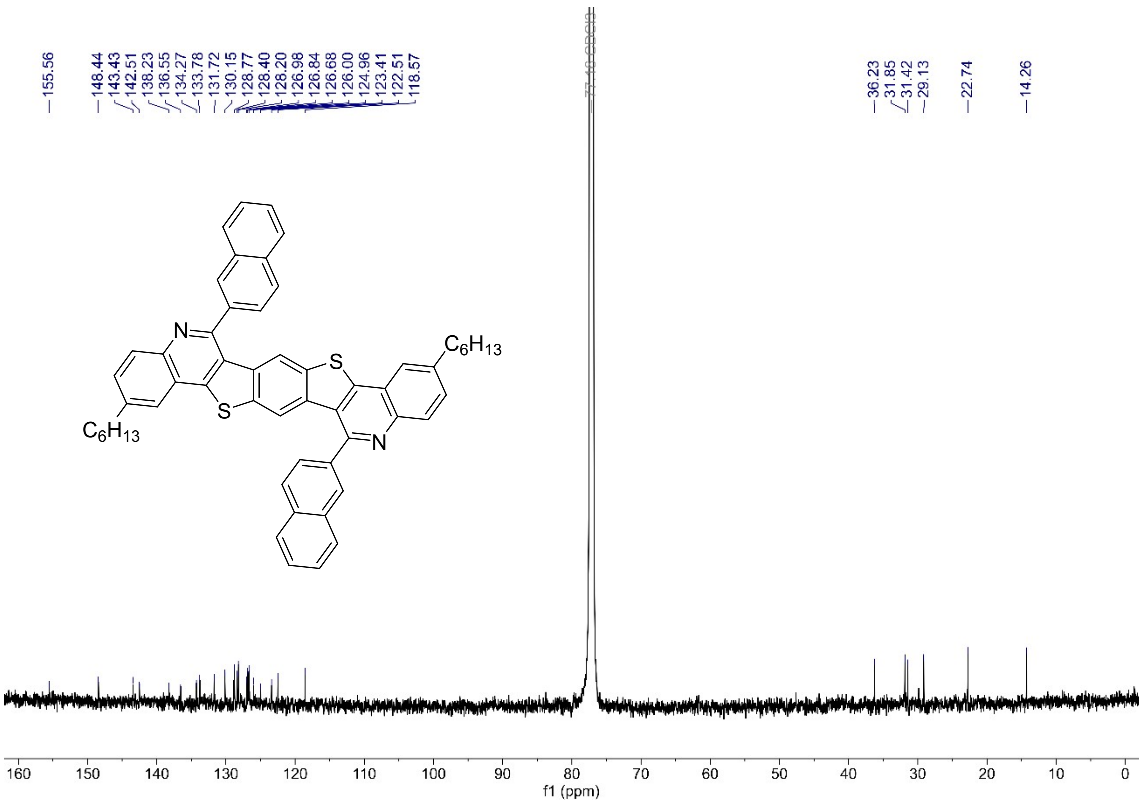


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9cc**.

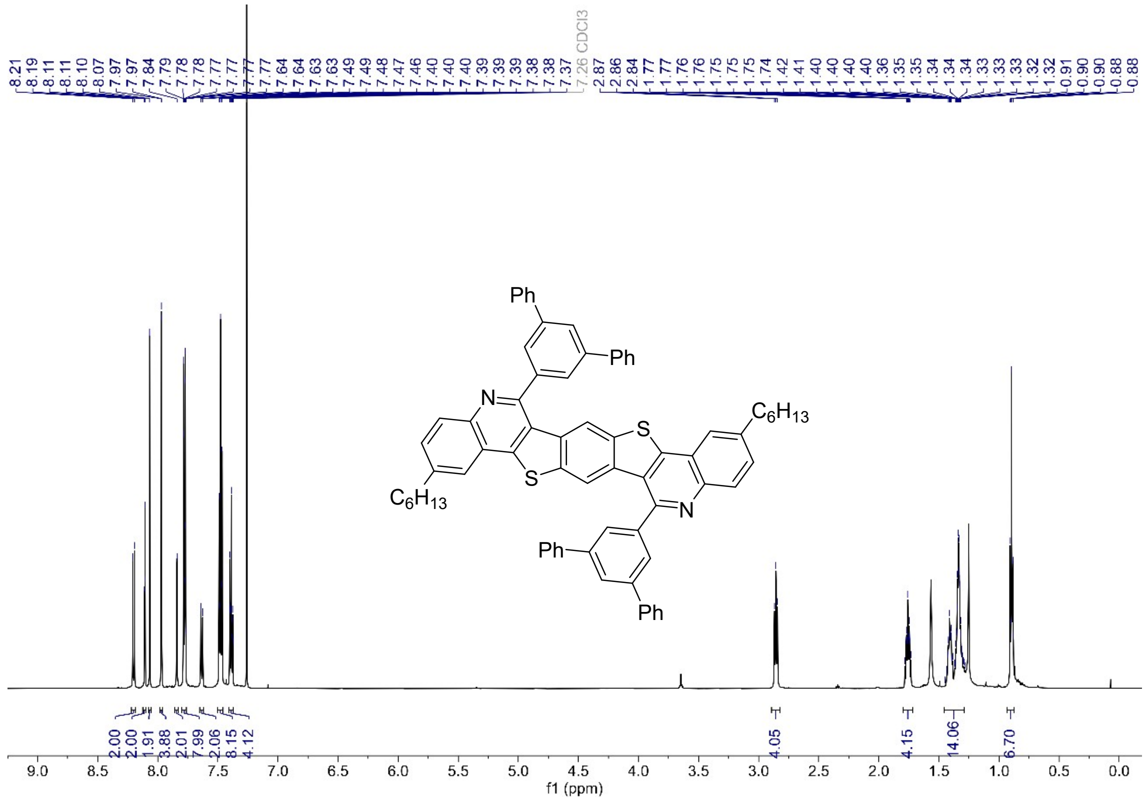


Figure S57. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9cd**.

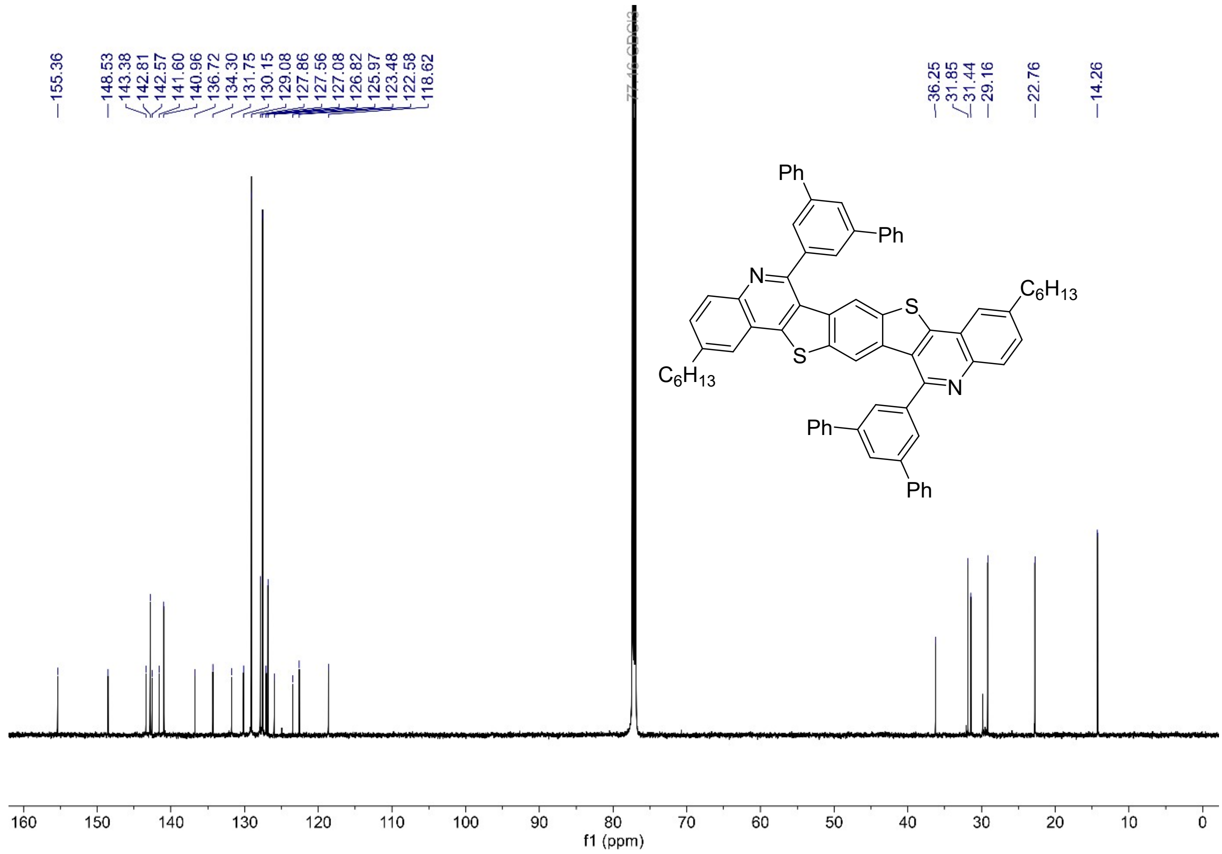


Figure S58. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9cd**.

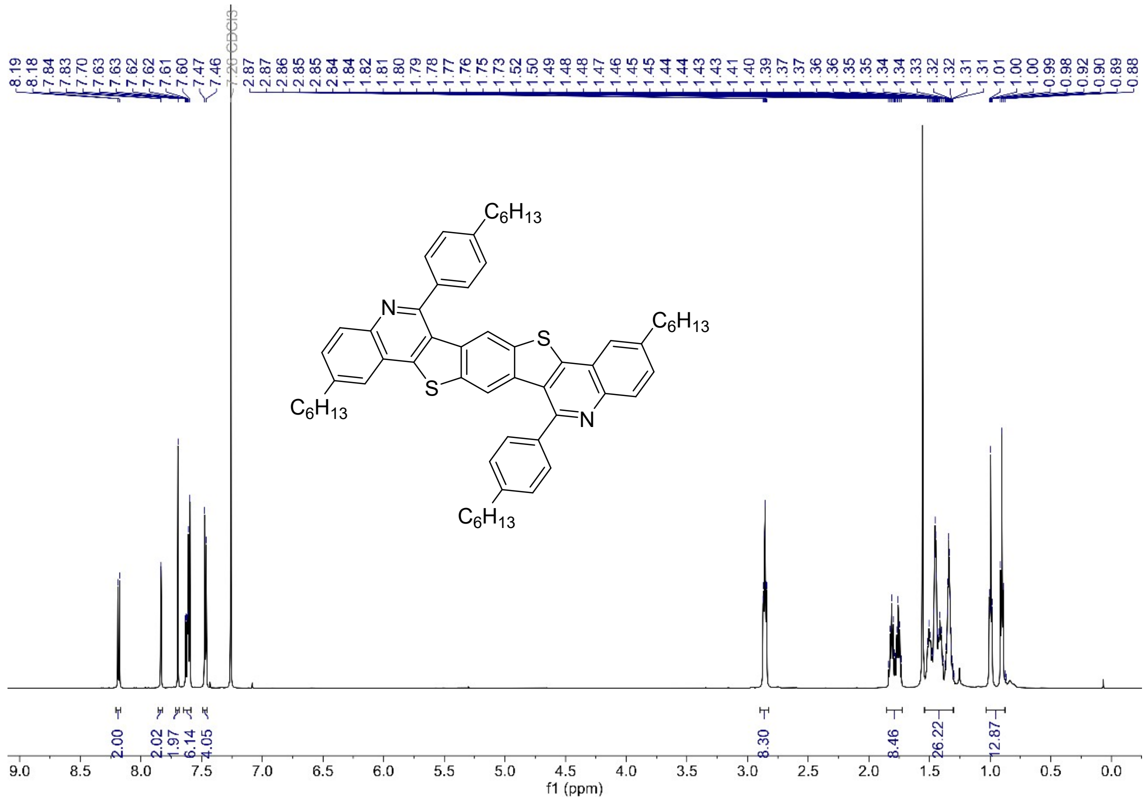


Figure S59. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **9ce**.

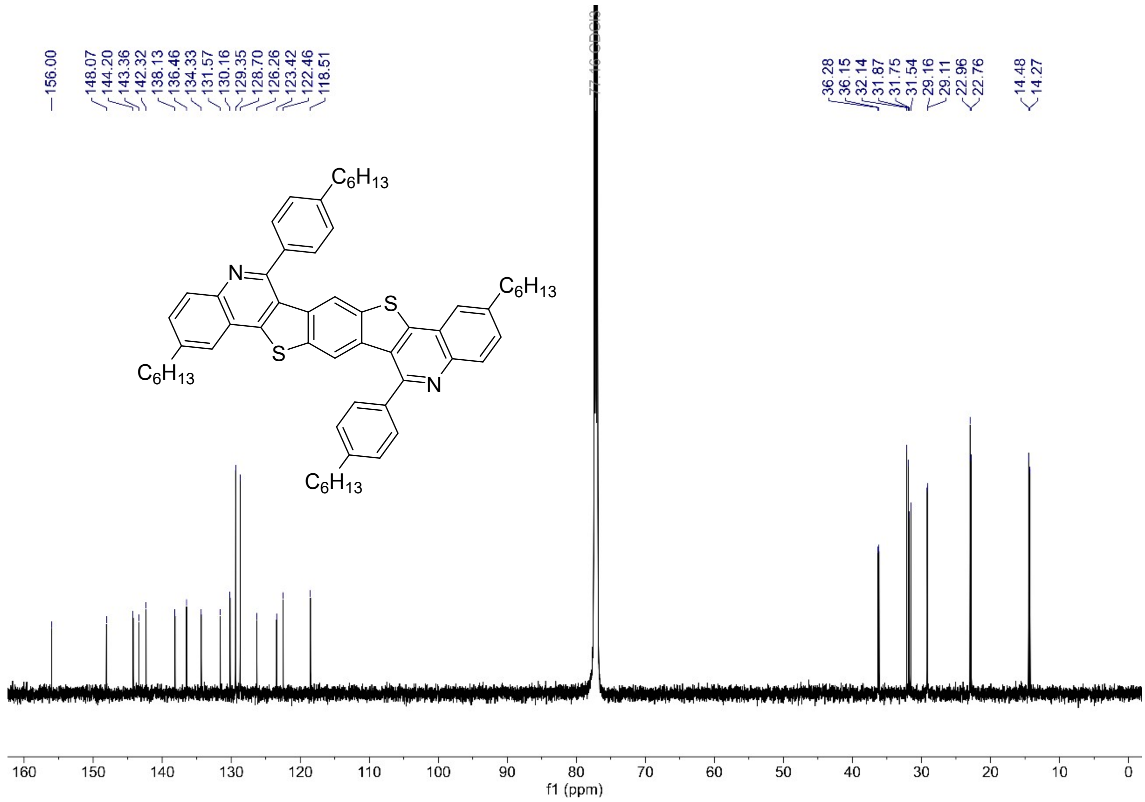


Figure S60. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **9ce**.

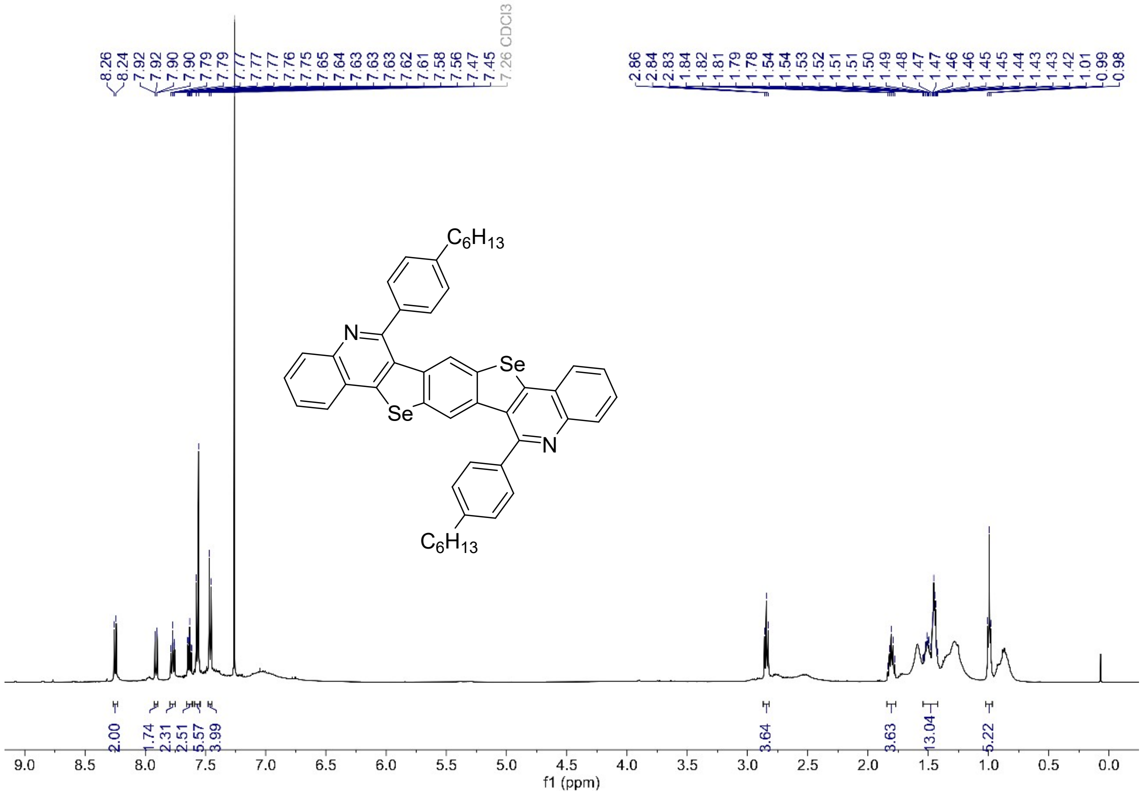


Figure S61. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **10aa**.

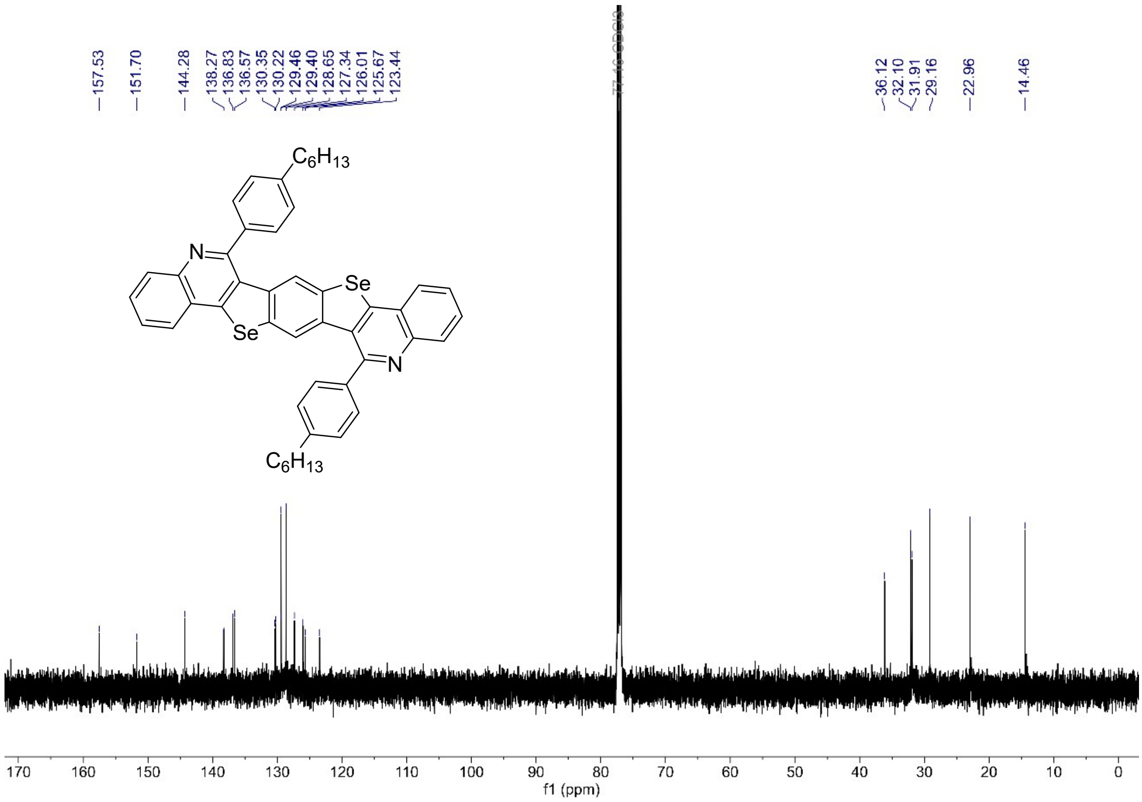


Figure S62. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, $CDCl_3$) of **10aa**.

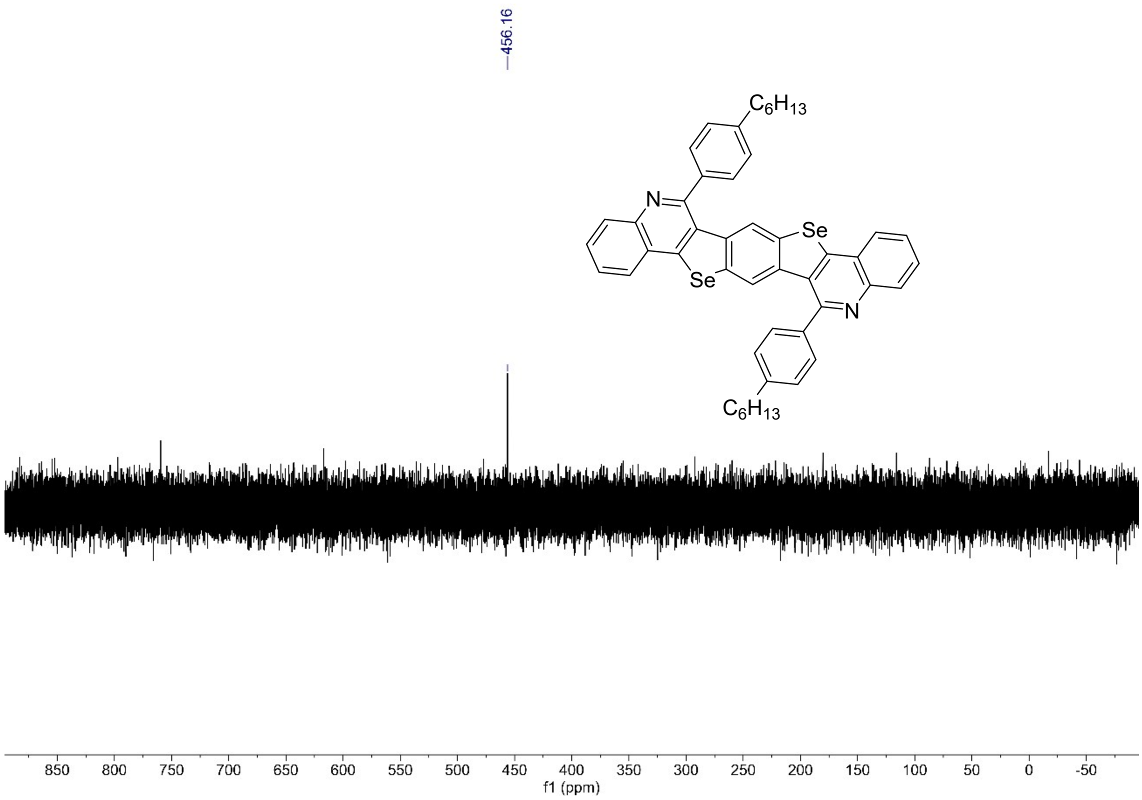


Figure S63. $^{77}Se\{^1H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10aa**.

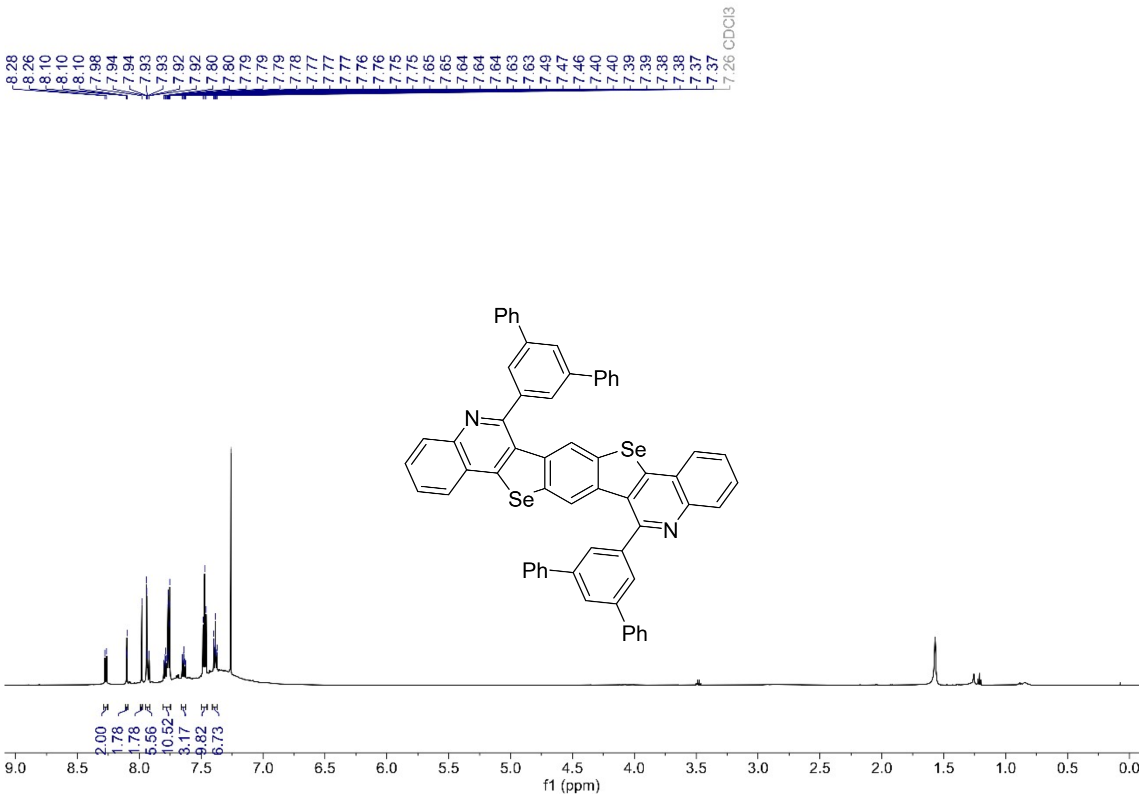


Figure S64. ^1H NMR spectrum (600 MHz, $CDCl_3$) of **10ab**.

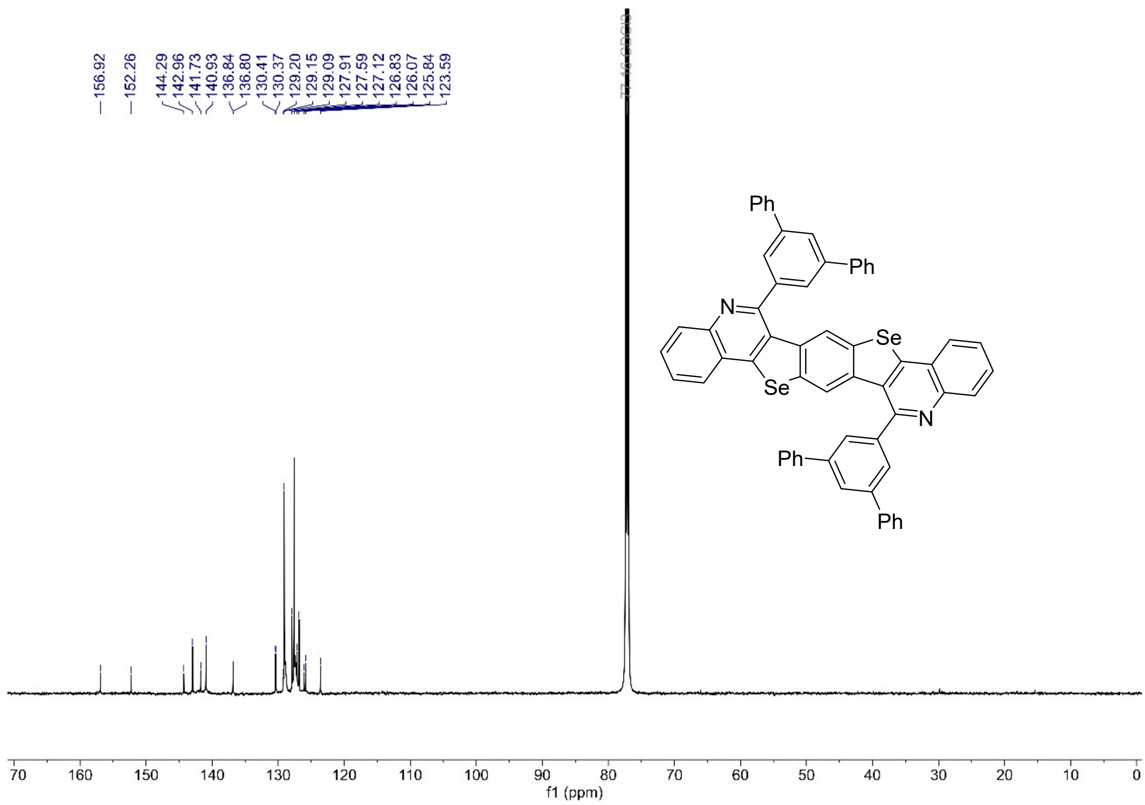


Figure S65. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10ab**.

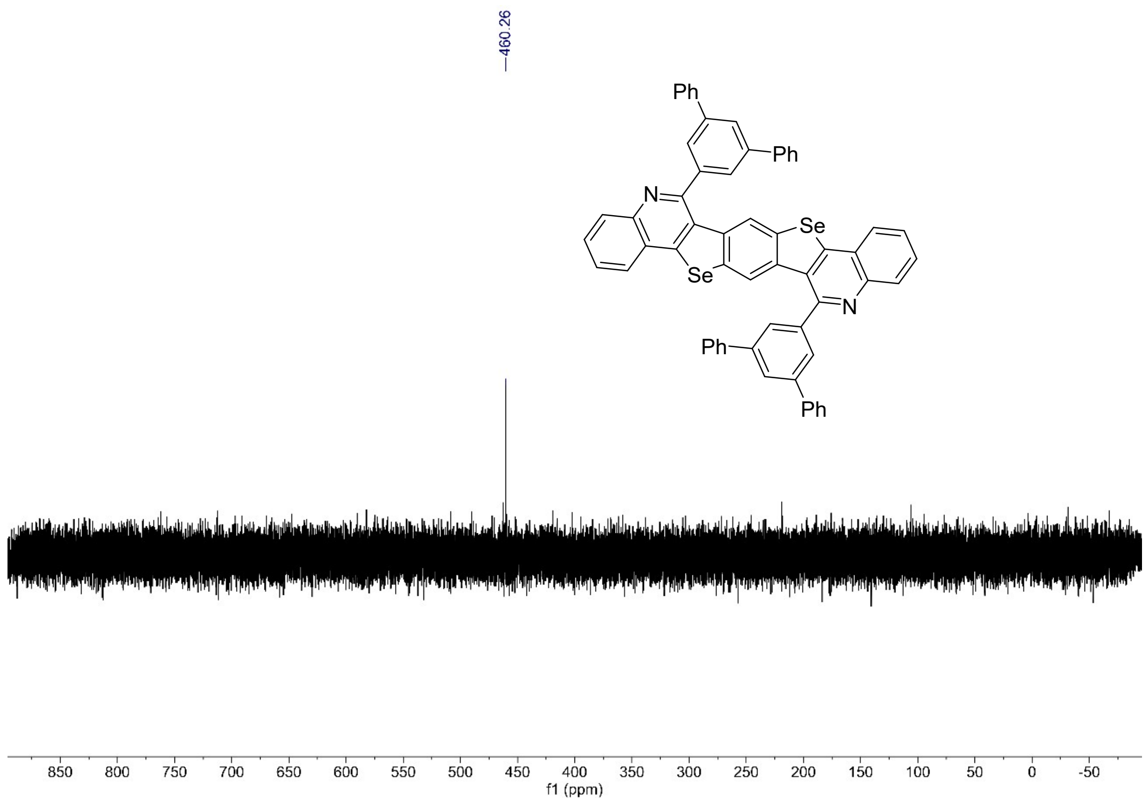


Figure S66. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10ab**.

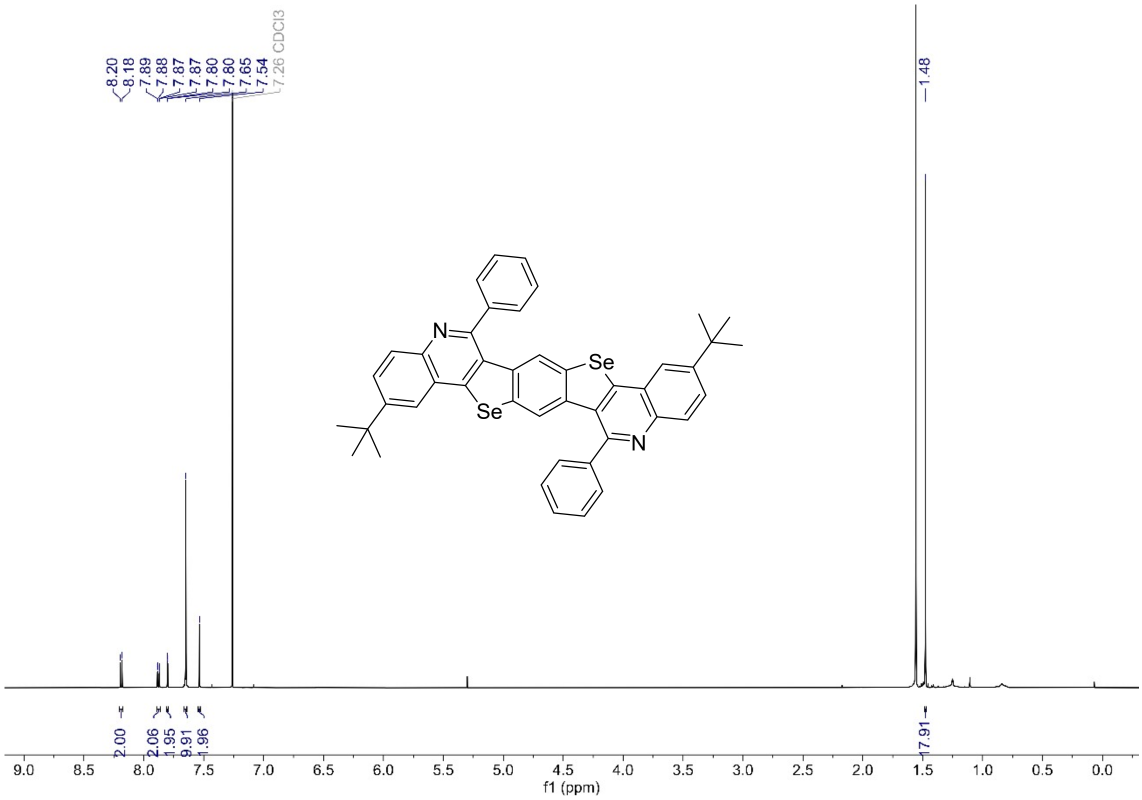


Figure S67. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10ba**.

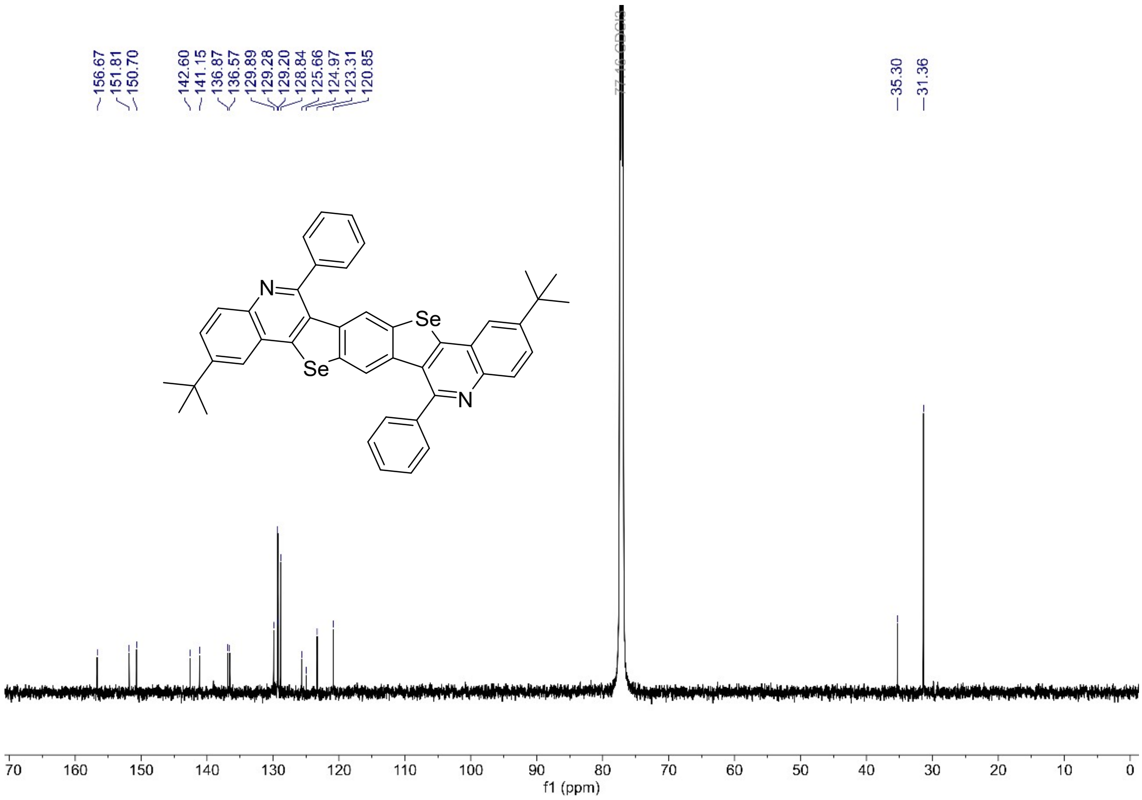


Figure S68. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10ba**.

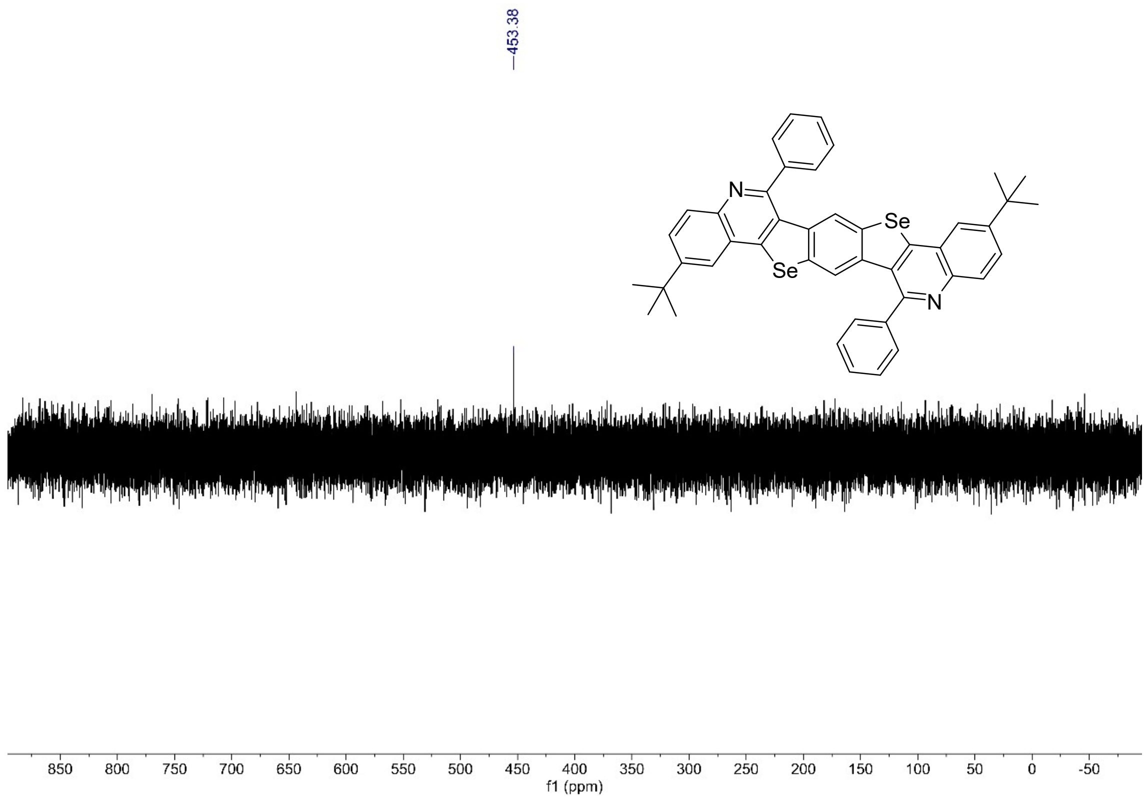


Figure S69. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10ba**.

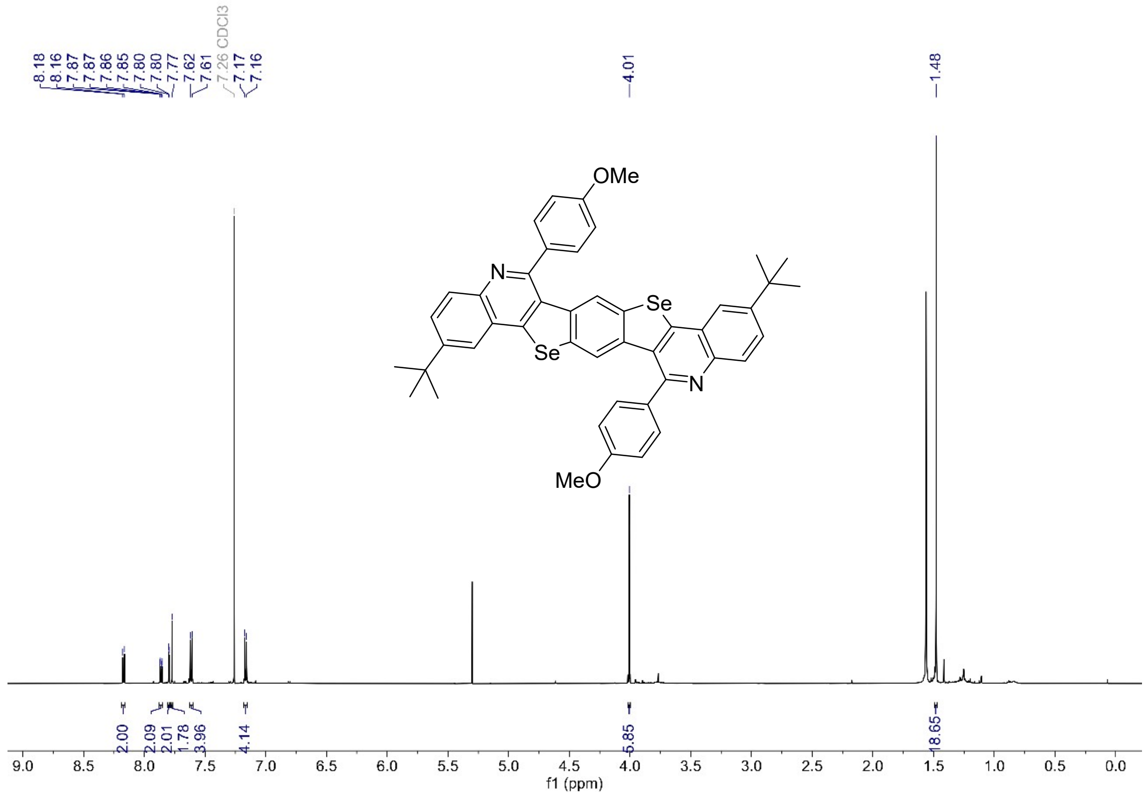


Figure S70. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10bb**.

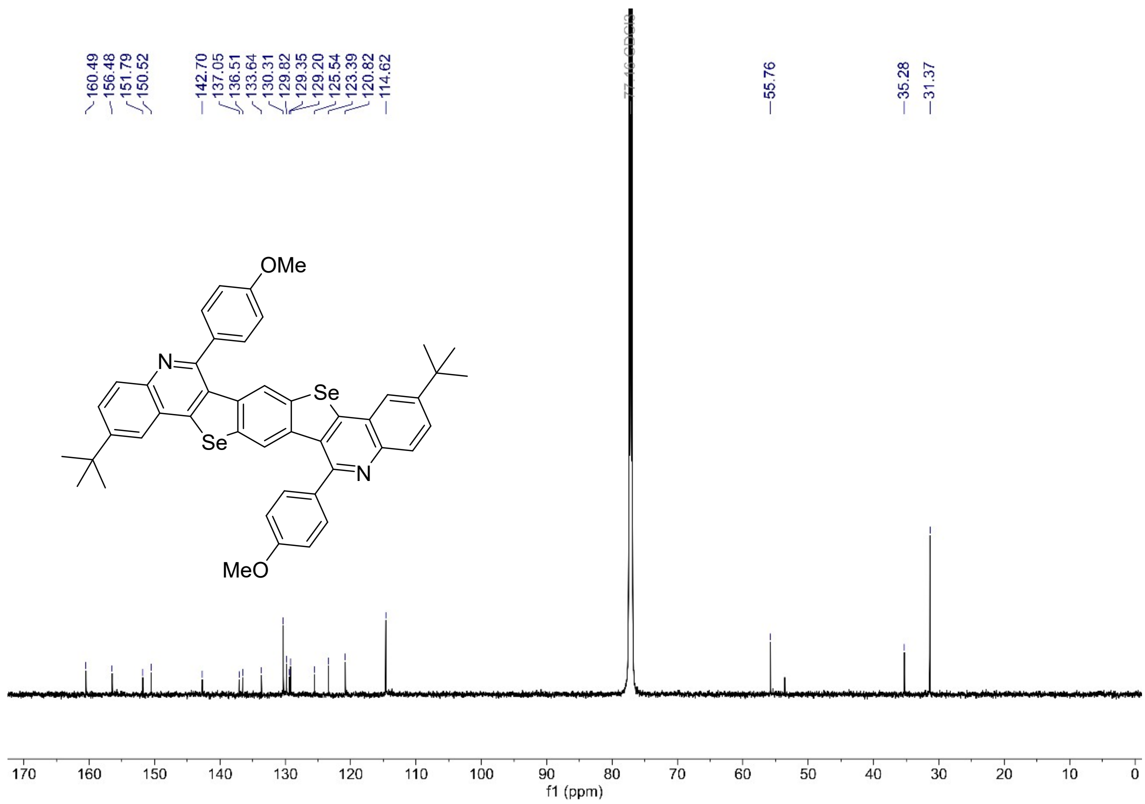


Figure S71. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10bb**.

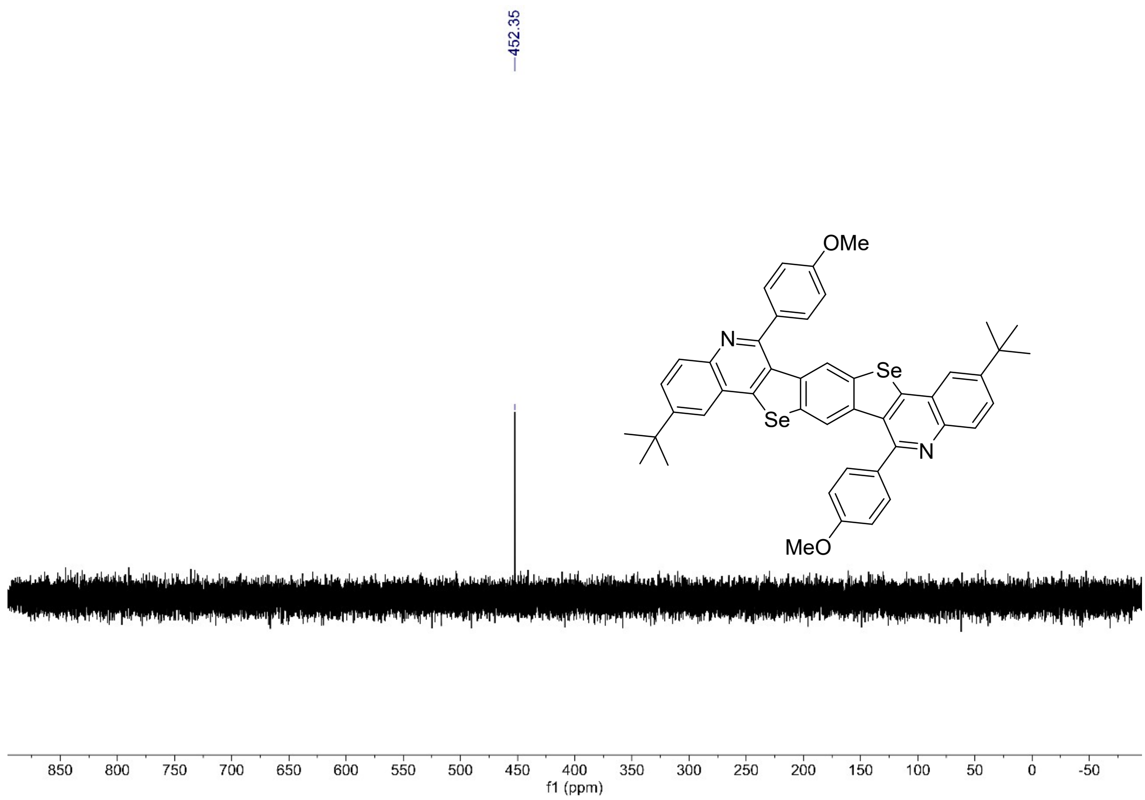


Figure S72. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10bb**.

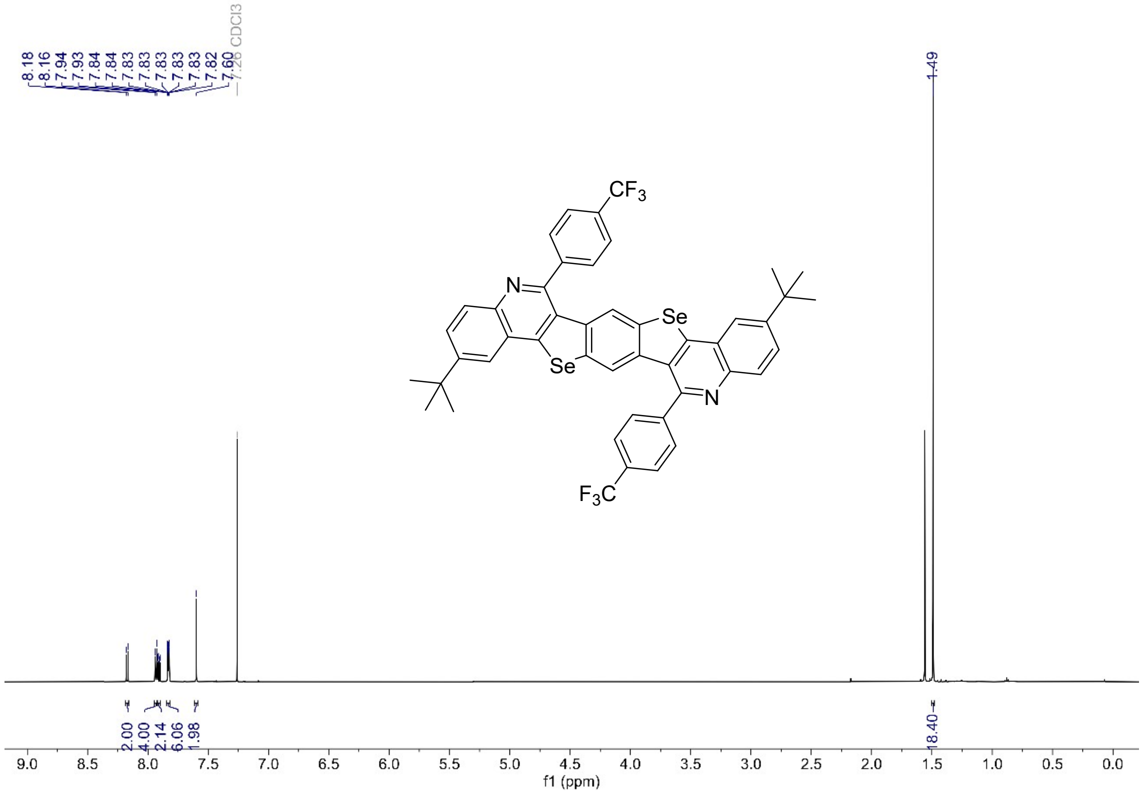


Figure S73. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10bc**.

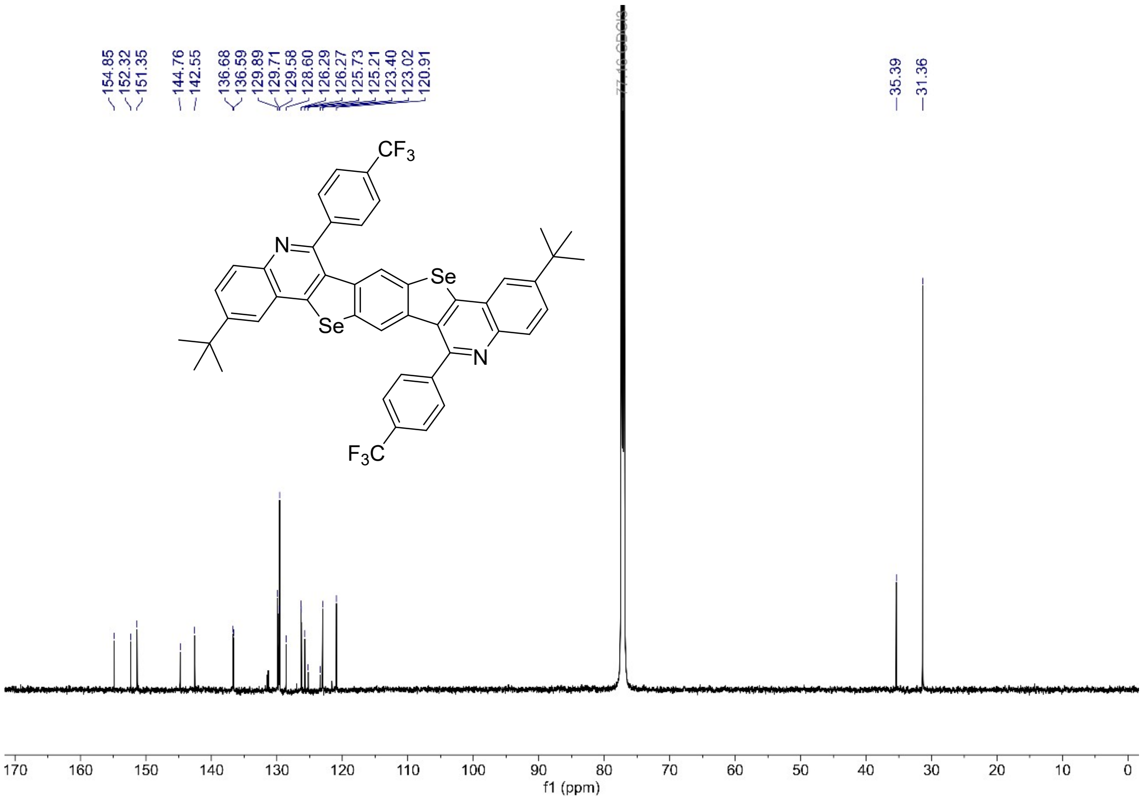


Figure S74. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10bc**.

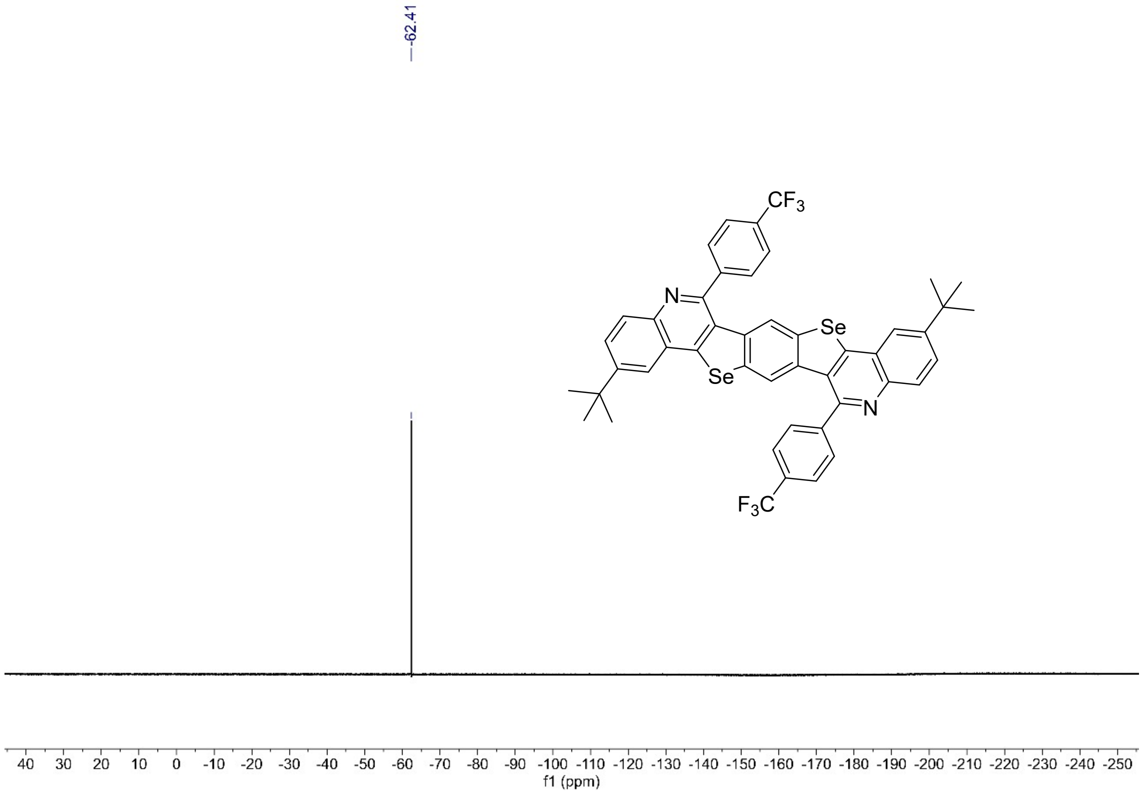


Figure S75. $^{19}F\{^{1}H\}$ NMR spectrum (283 MHz, $CDCl_3$) of **10bc**.

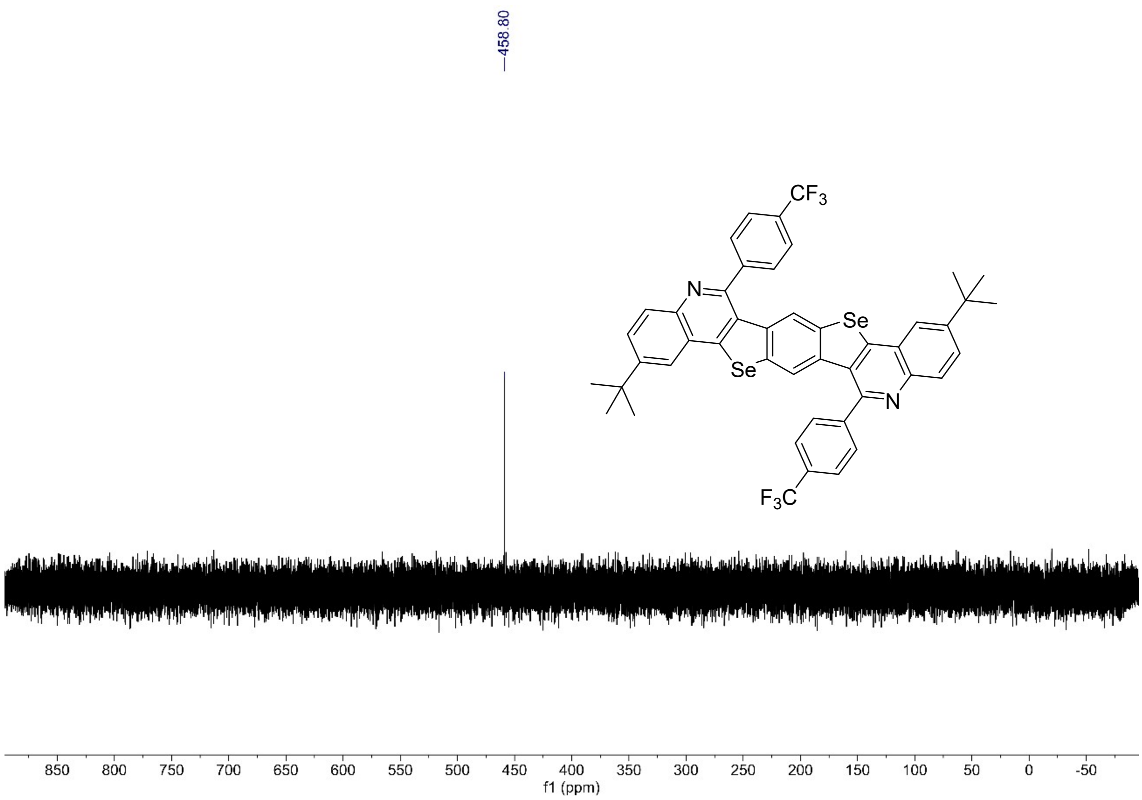


Figure S76. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10bc**.

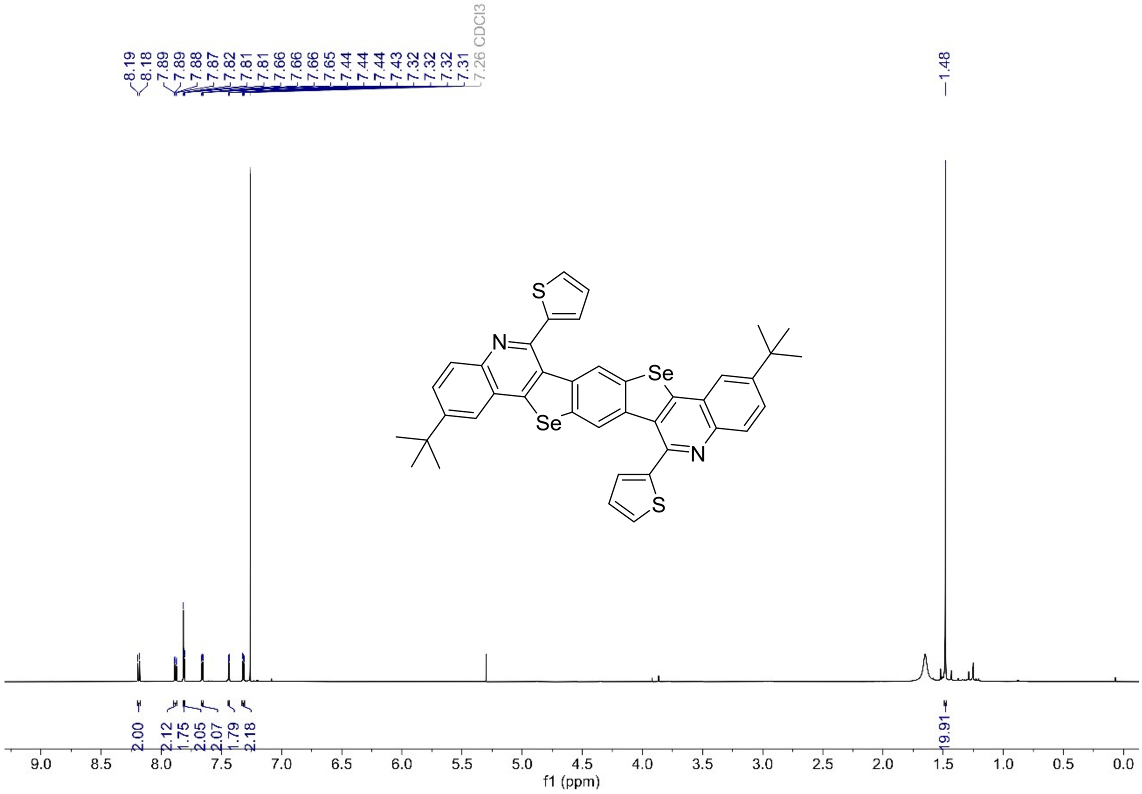


Figure S77. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10bd**.

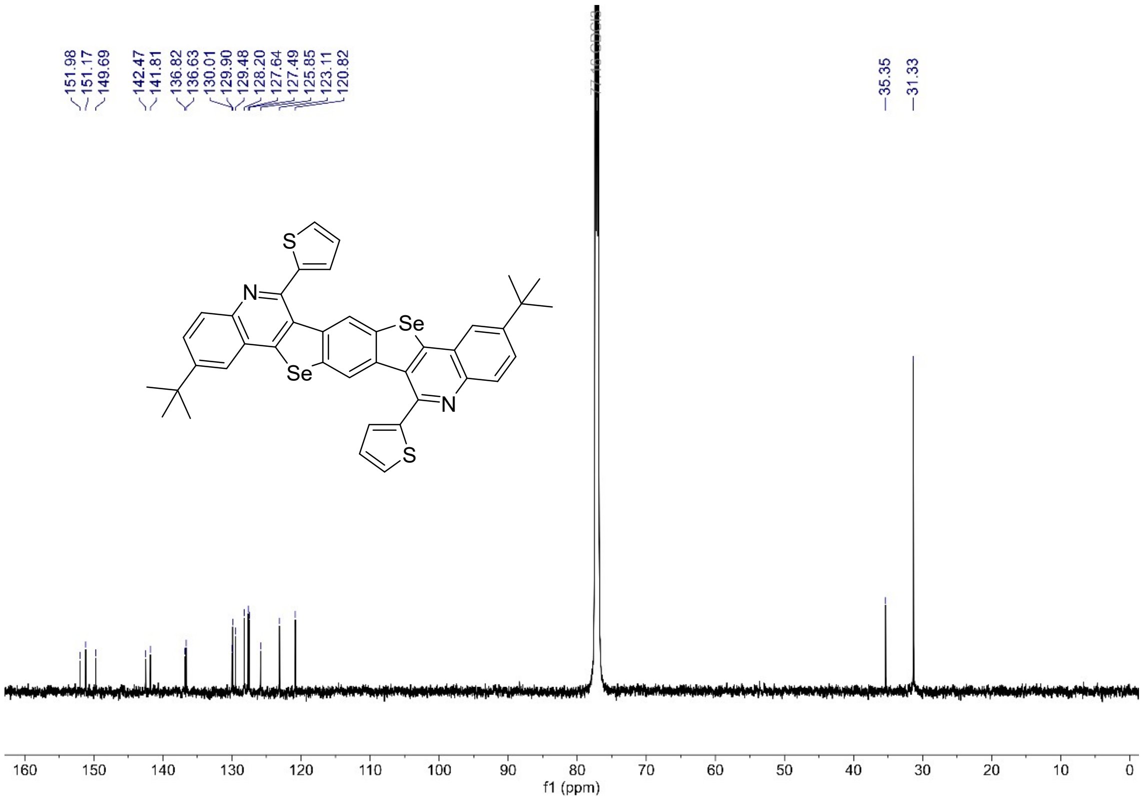


Figure S78. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10bd**.

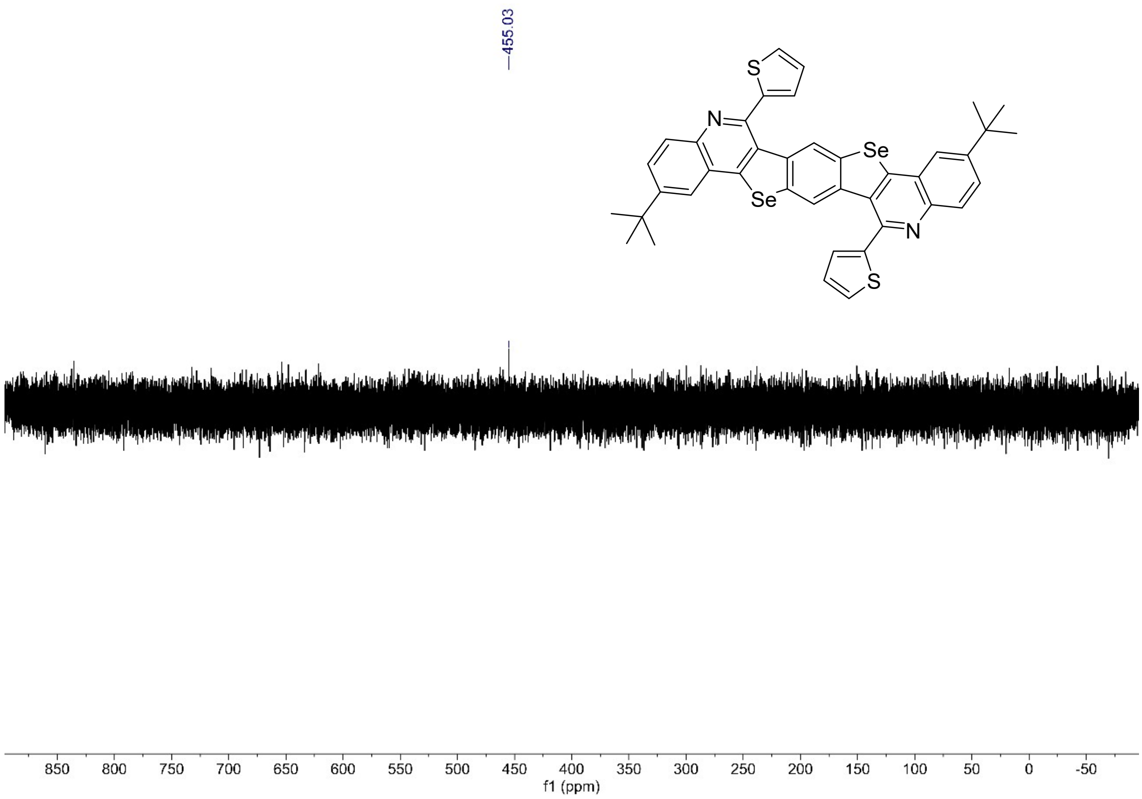


Figure S79. $^{77}Se\{^1H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10bd**.

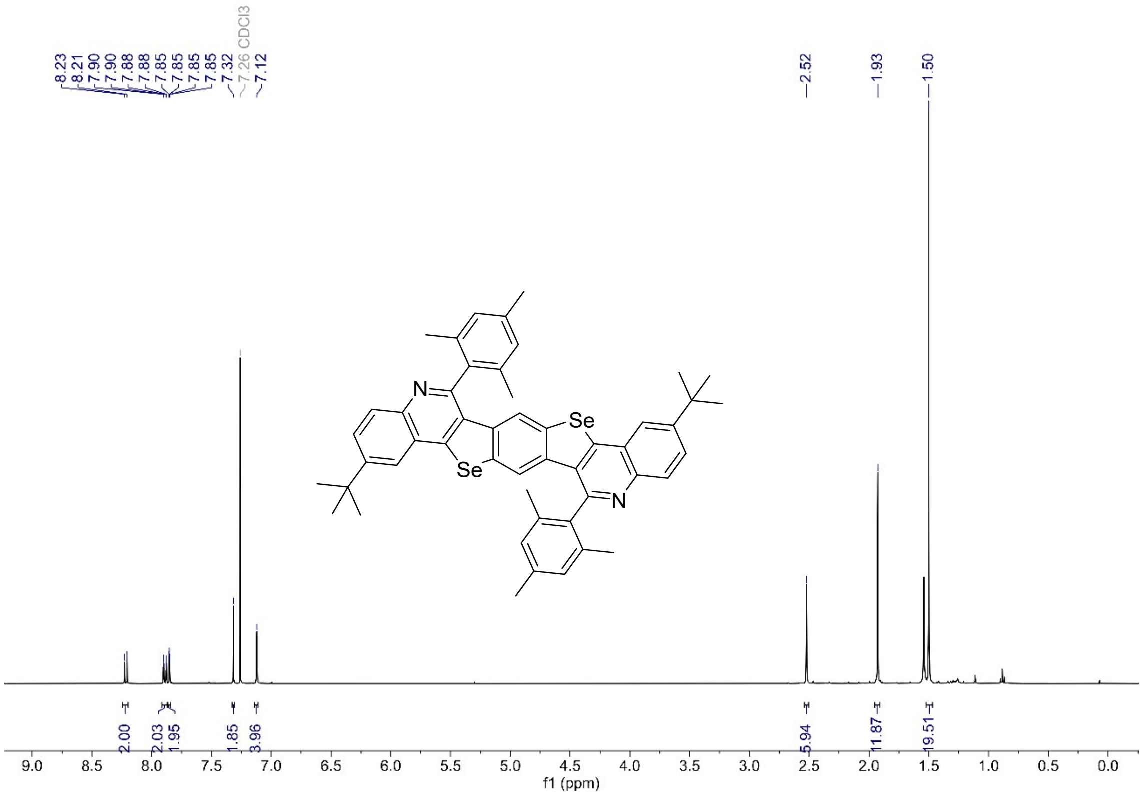


Figure S80. ^1H NMR spectrum (400 MHz, $CDCl_3$) of **10be**.

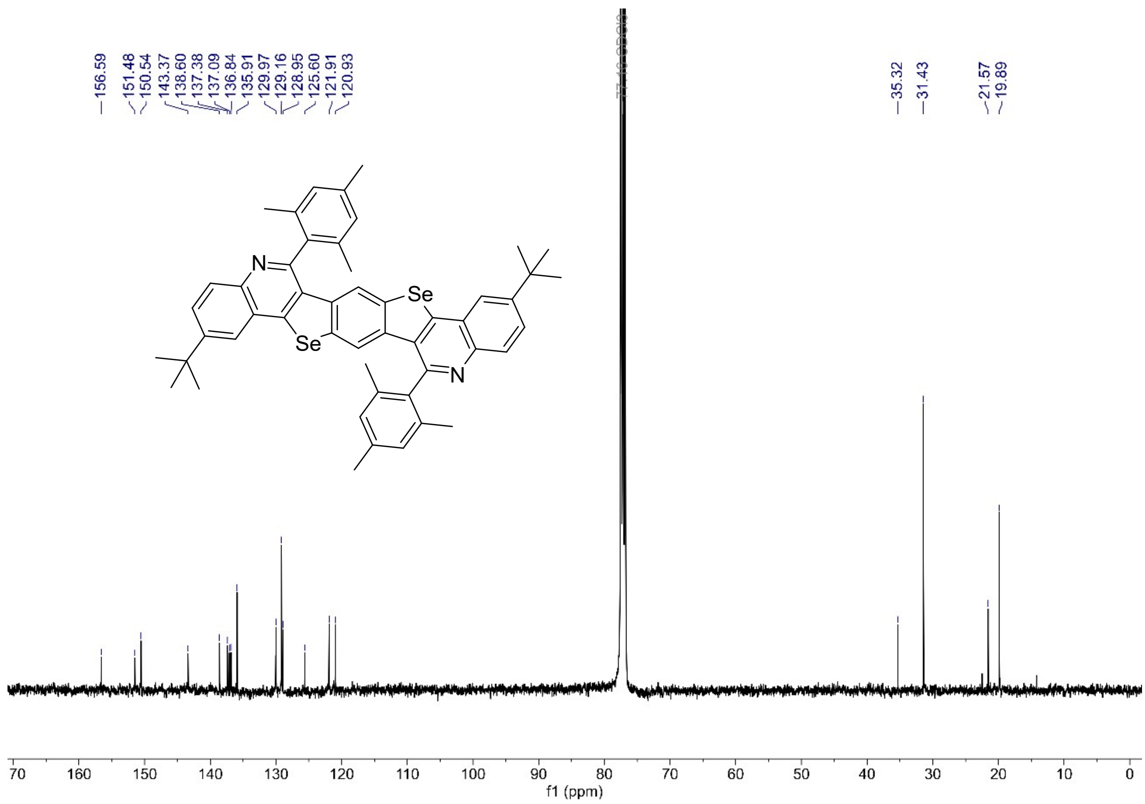


Figure S81. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **10be**.

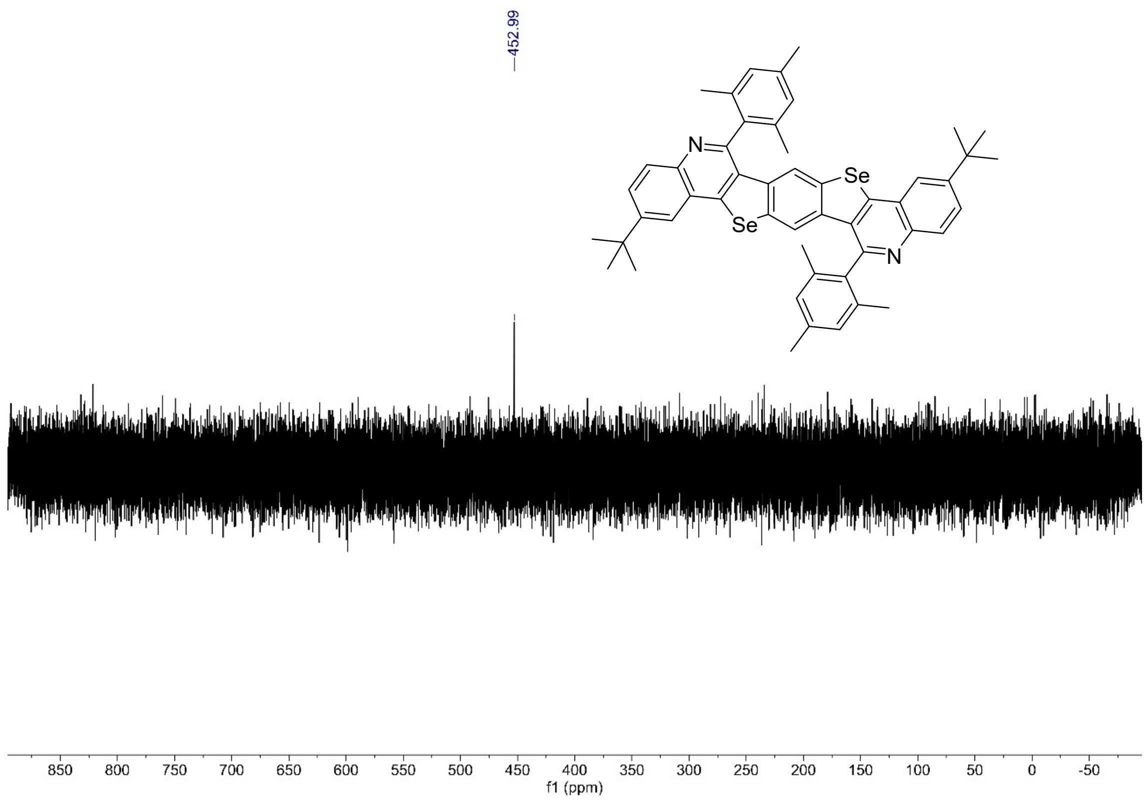


Figure S82. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10be**.

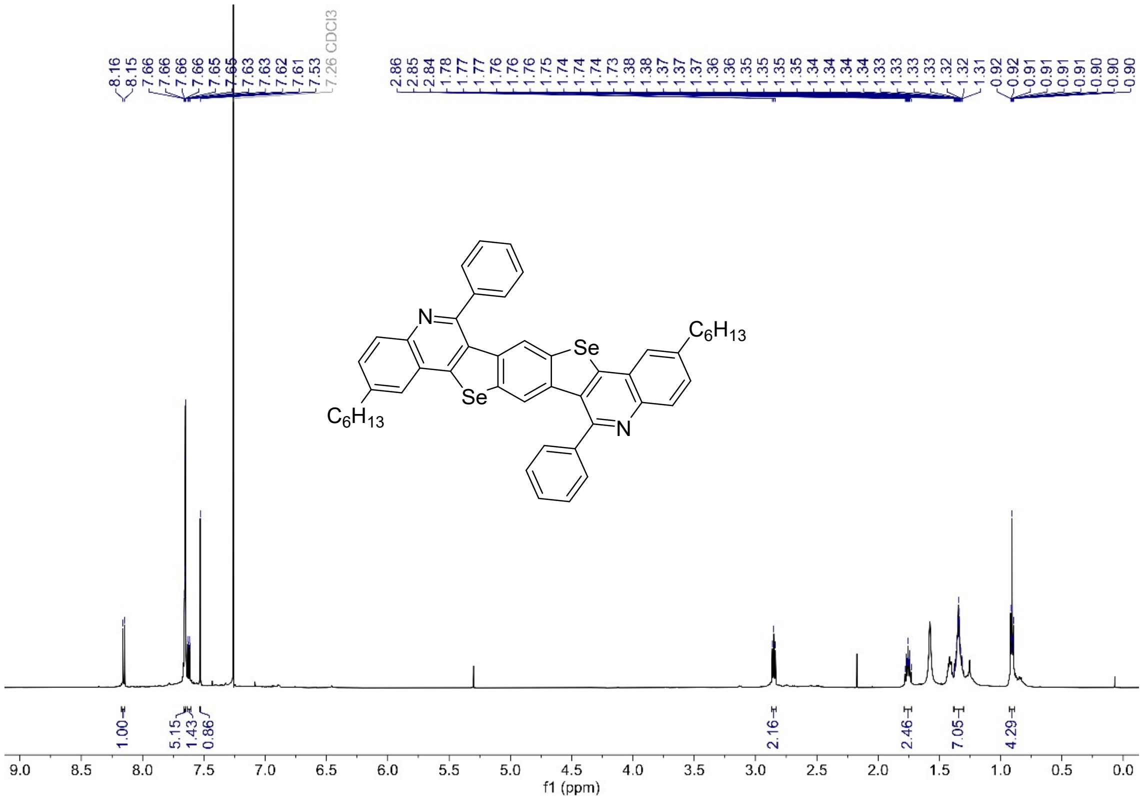


Figure S83. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10ca**.

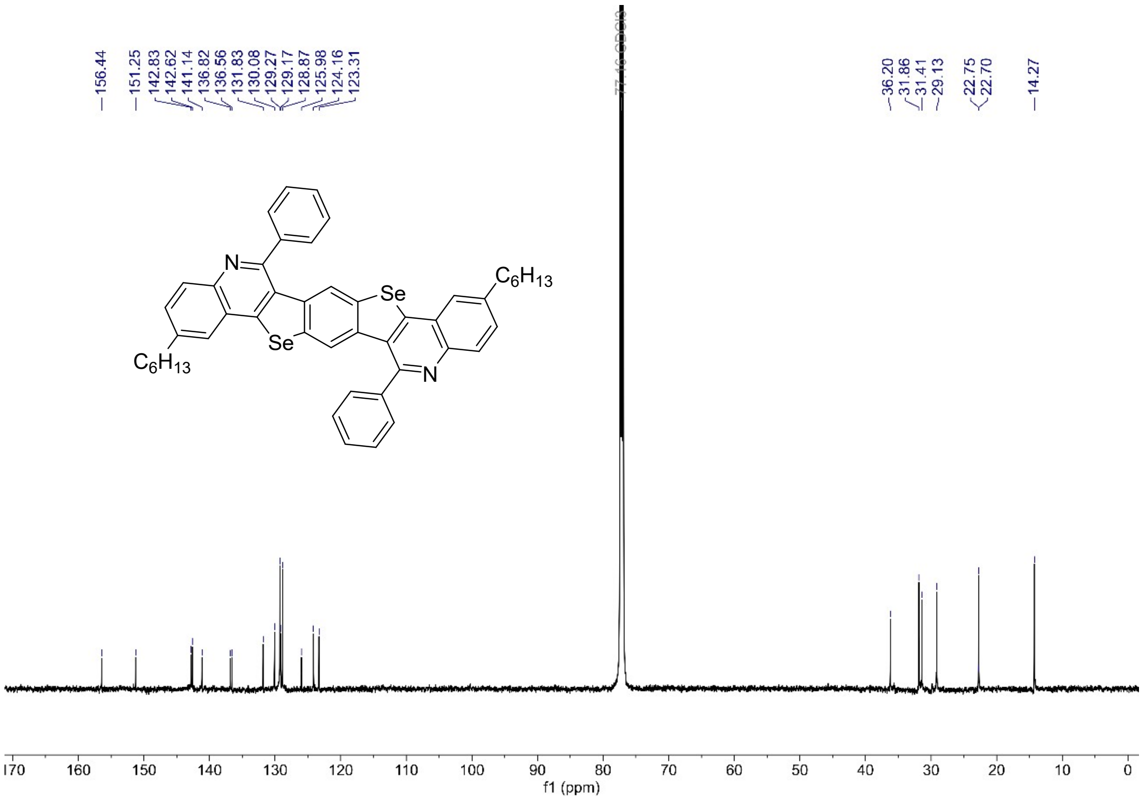


Figure S84. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10ca**.

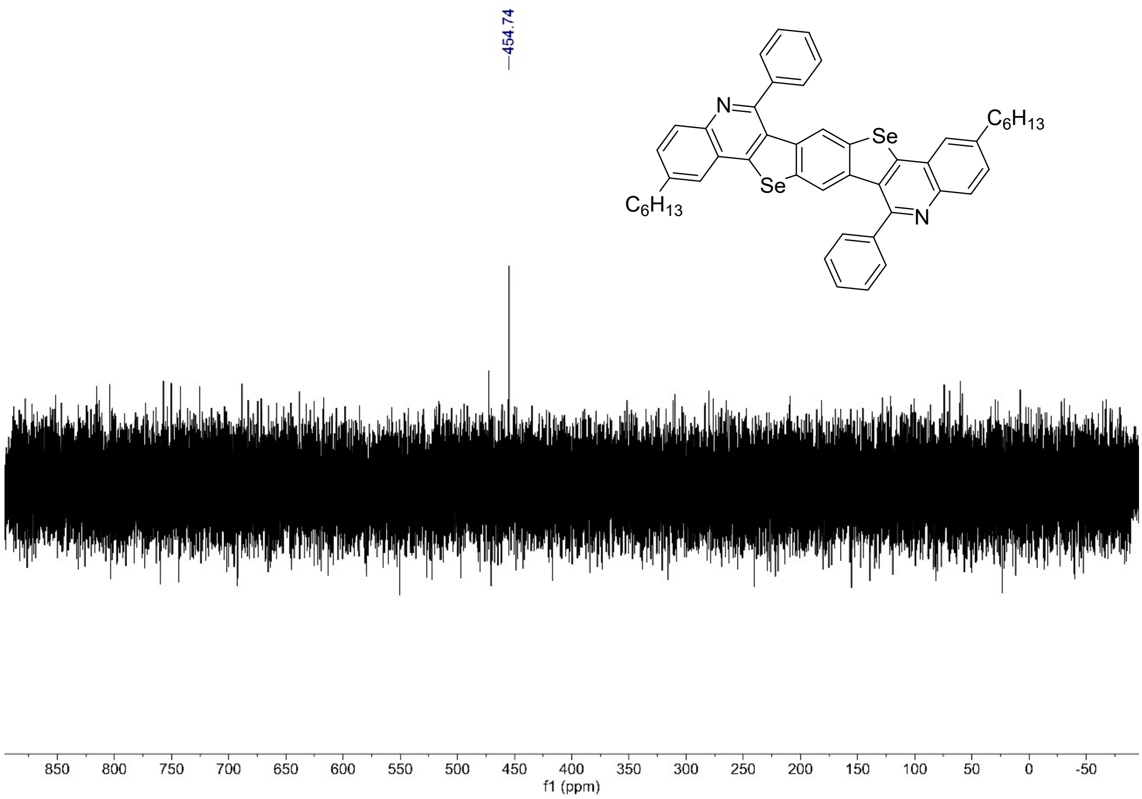


Figure S85. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10ca**.

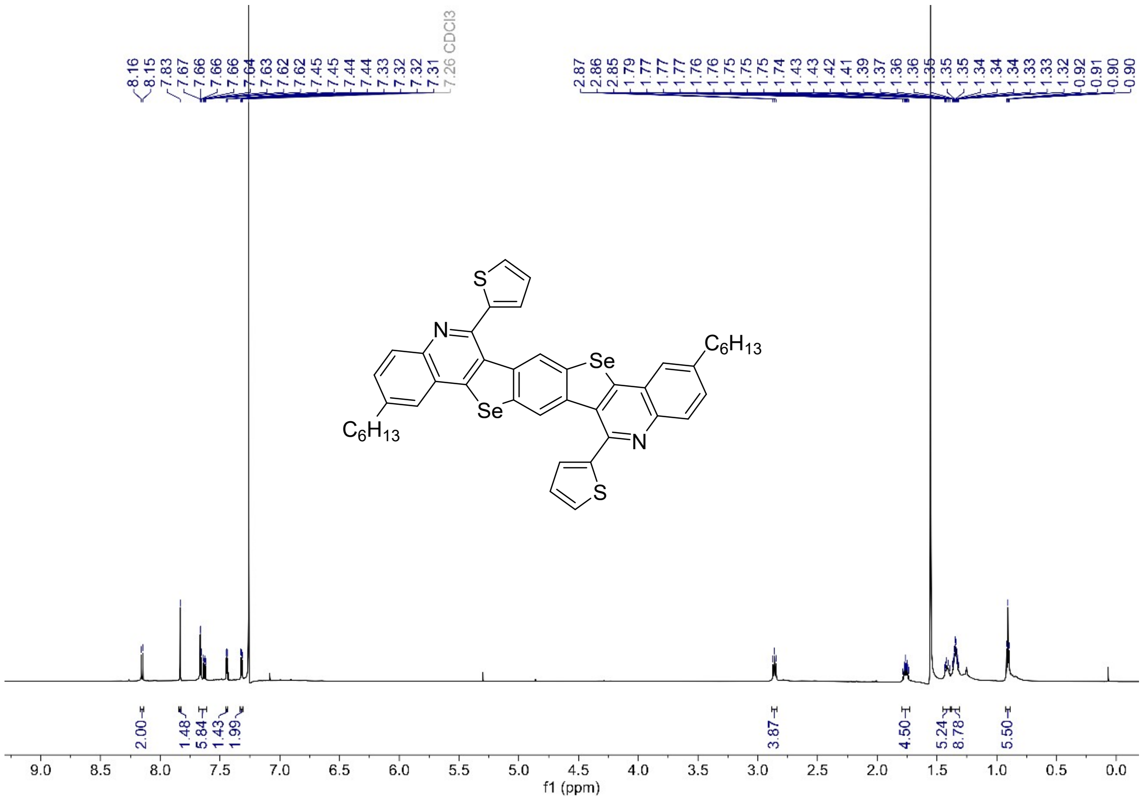


Figure S86. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10cb**.

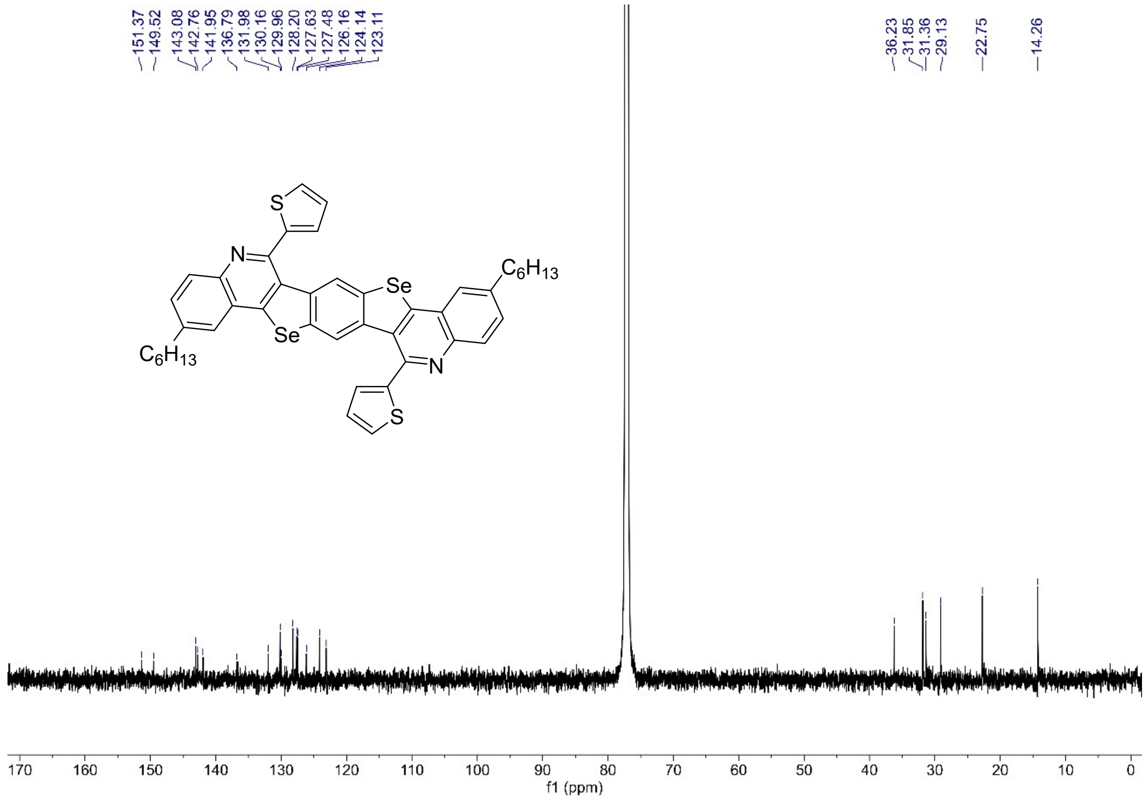


Figure S87. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10cb**.

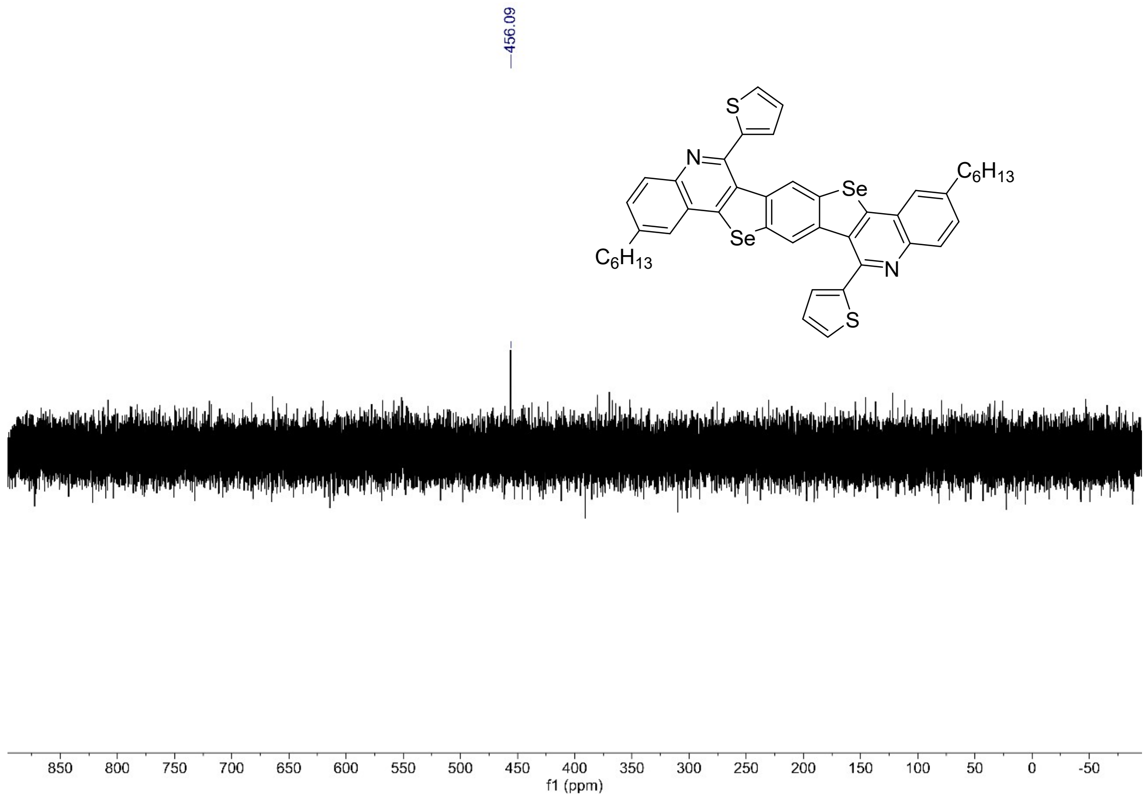


Figure S88. $^{77}Se\{^{1}H\}$ NMR spectrum (76 MHz, $CDCl_3$) of **10cb**.

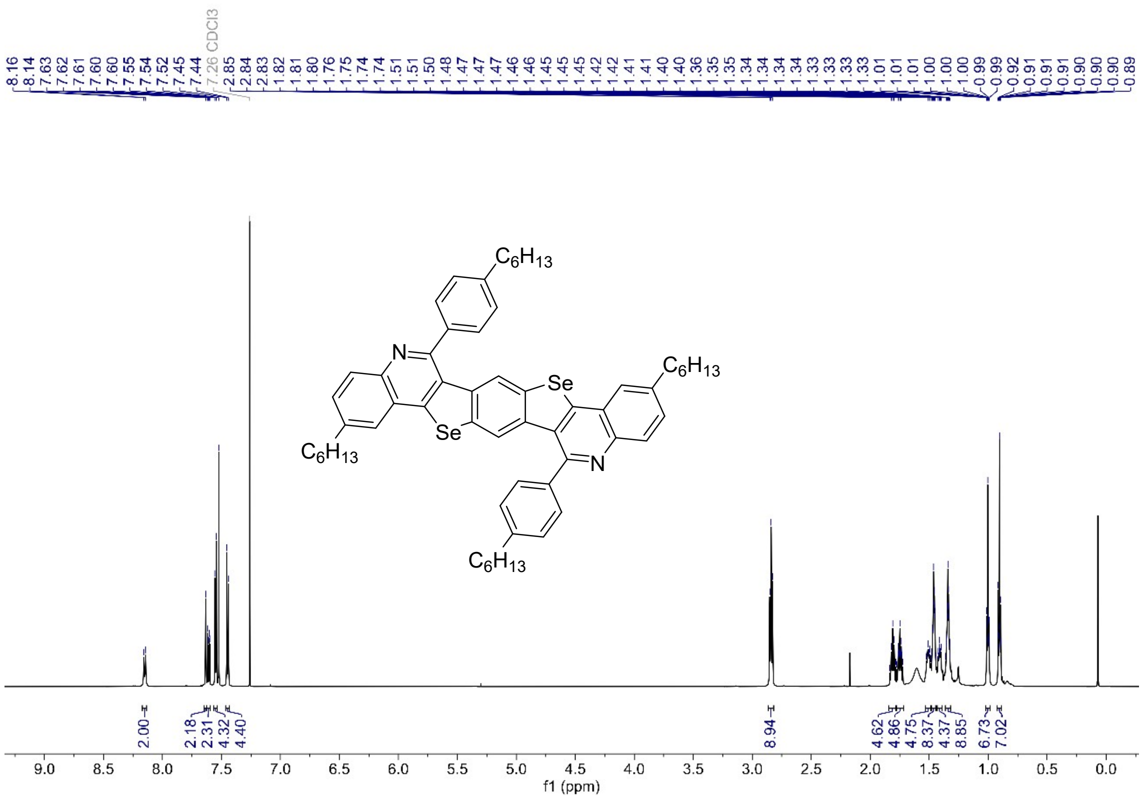


Figure S89. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of **10cc**.

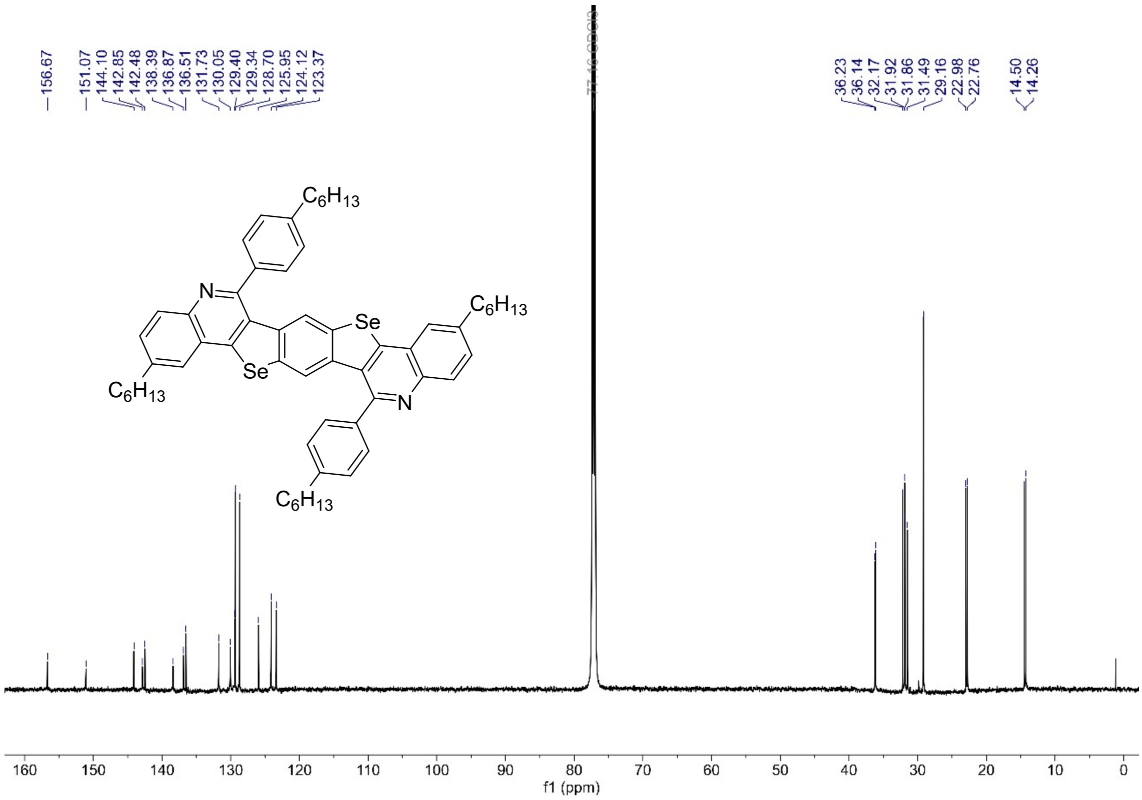


Figure S90. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, $CDCl_3$) of **10cc**.

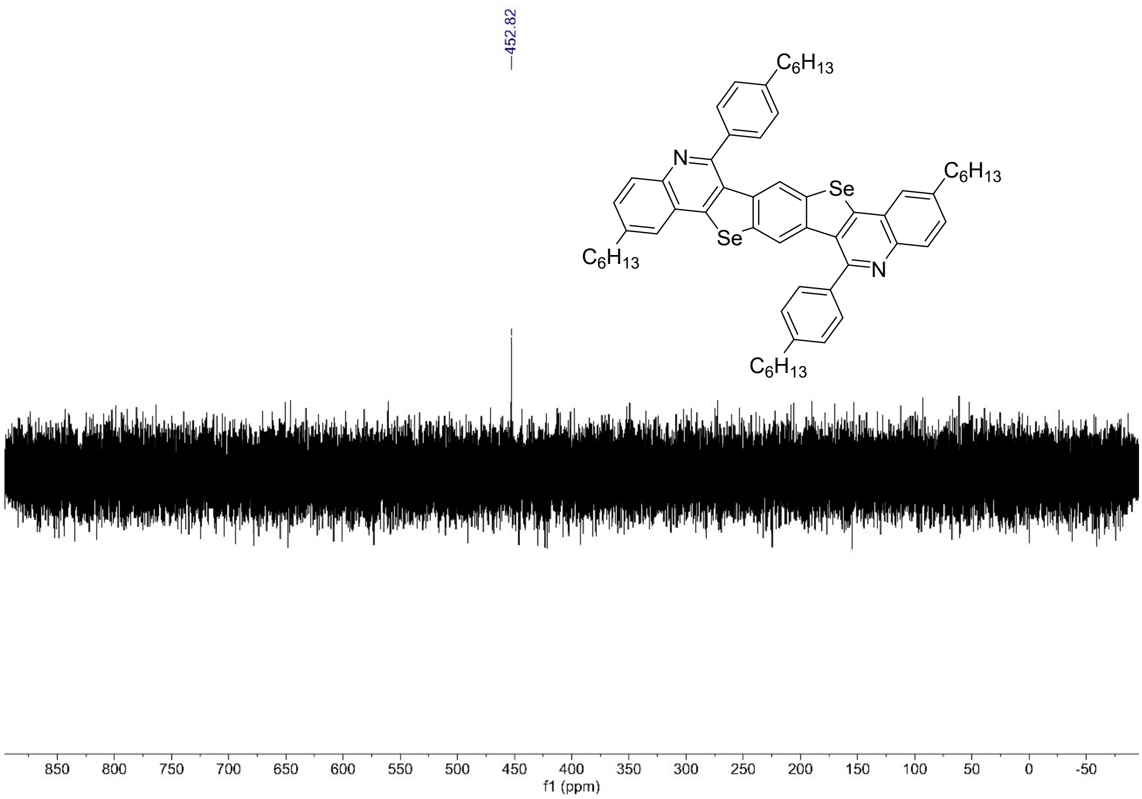


Figure S91. ^{77}Se{^{1}H} NMR spectrum (76 MHz, $CDCl_3$) of **10cc**.

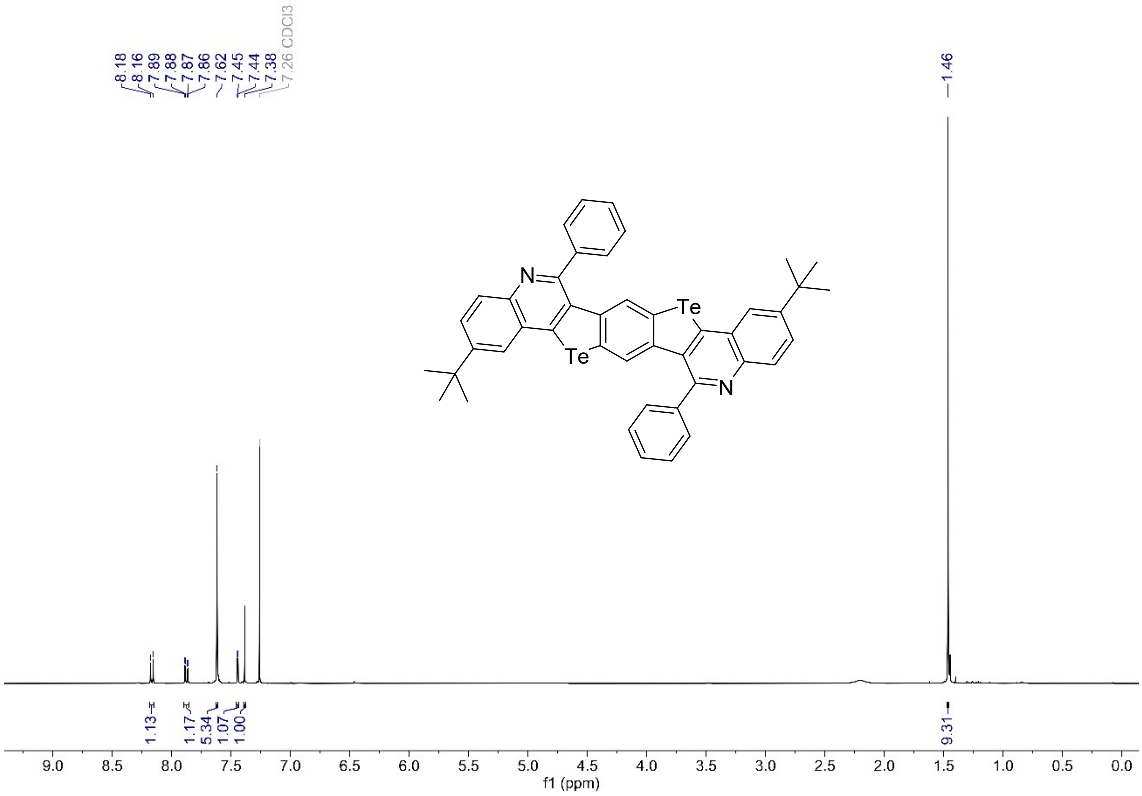


Figure S92. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **11ba**.

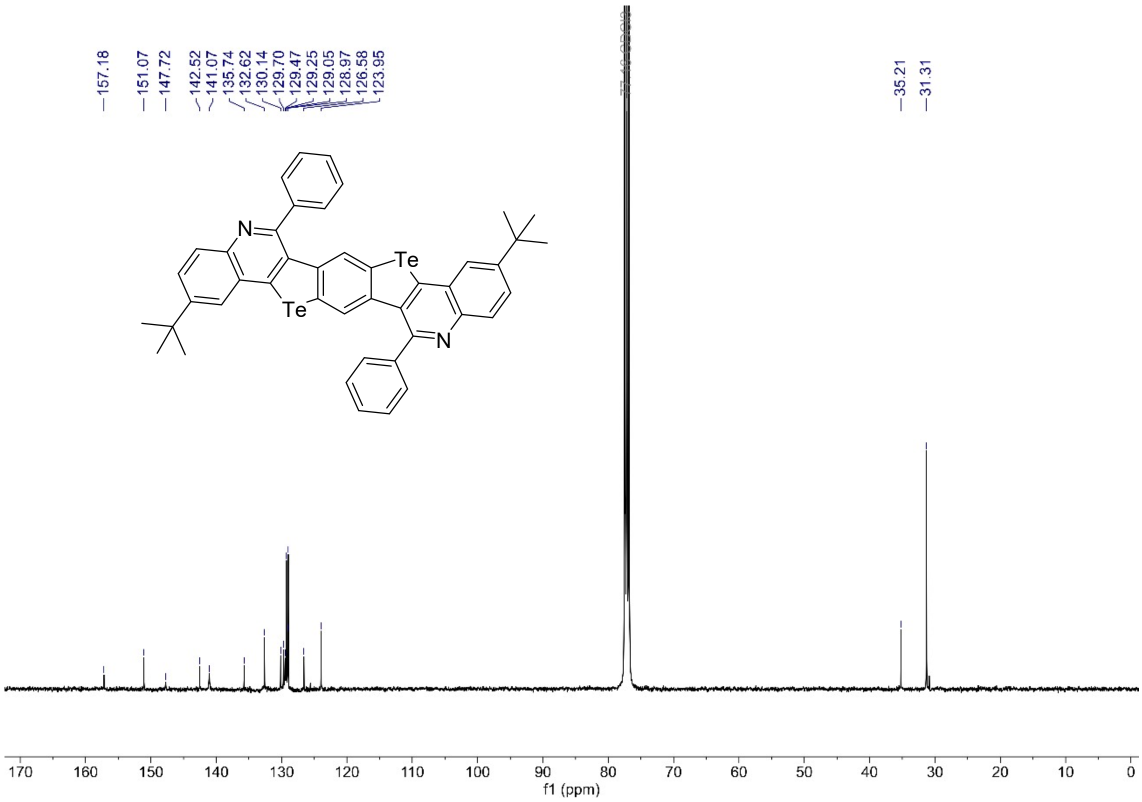


Figure S93. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **11ba**.

3 UV-Vis and Fluorescence Spectra

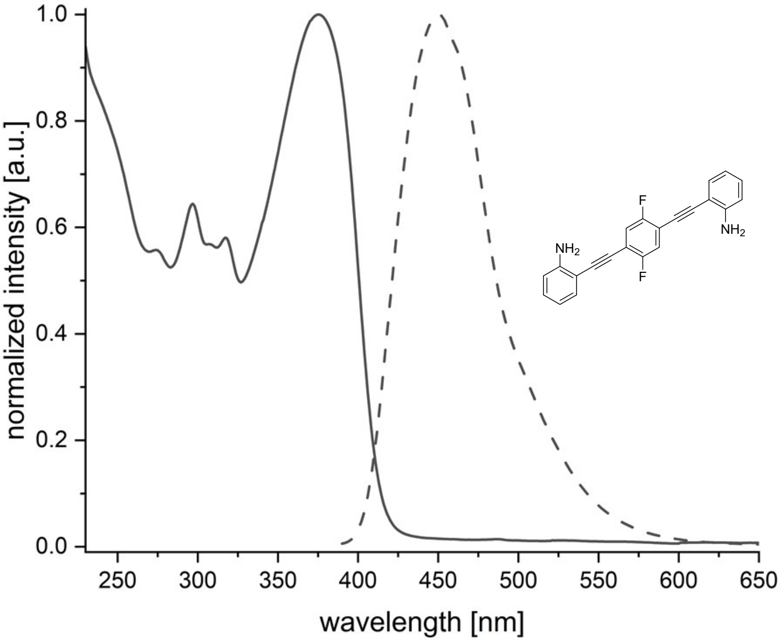


Figure S94. Absorption (solid line) and emission (dashed line) spectra of **5a** in DCM.

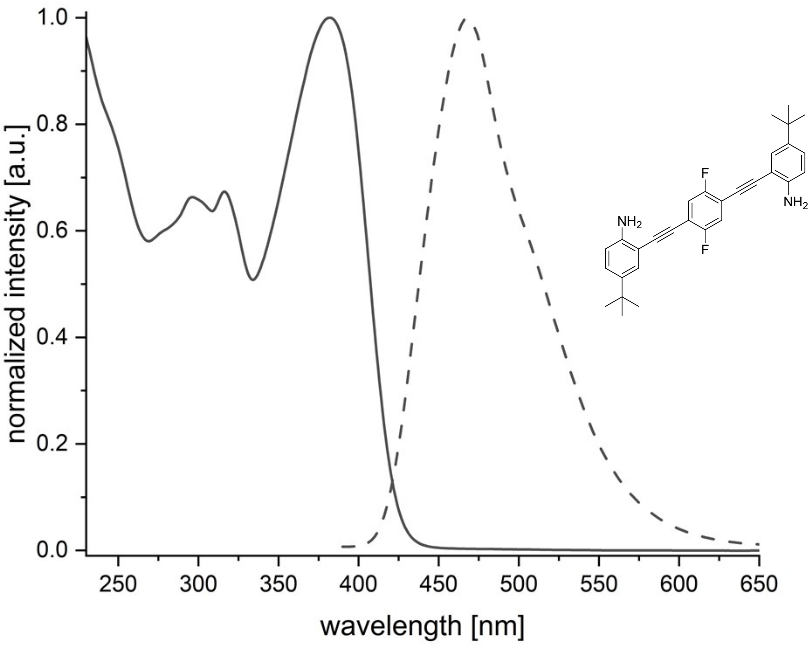


Figure S95. Absorption (solid line) and emission (dashed line) spectra of **5b** in DCM.

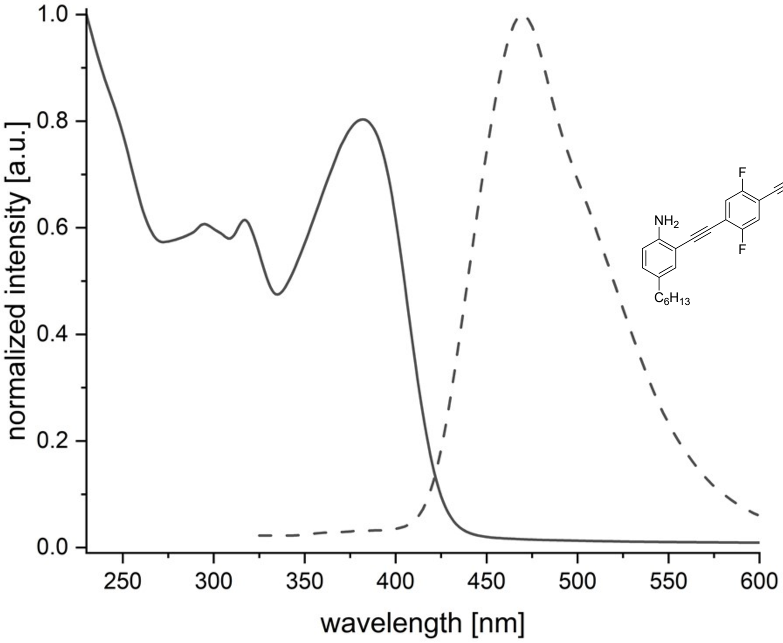


Figure S96. Absorption (solid line) and emission (dashed line) spectra of **5c** in DCM.

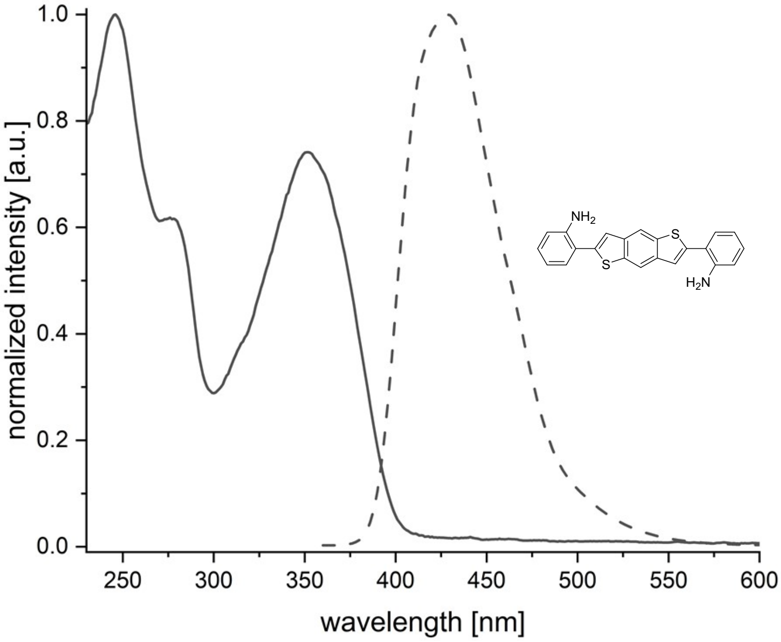


Figure S97. Absorption (solid line) and emission (dashed line) spectra of **6a** in DCM.

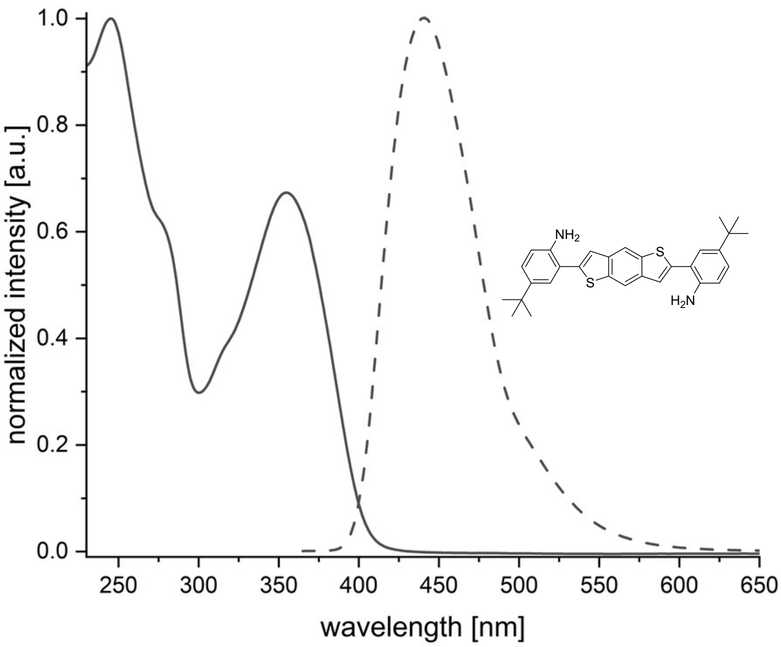


Figure S98. Absorption (solid line) and emission (dashed line) spectra of **6b** in DCM.

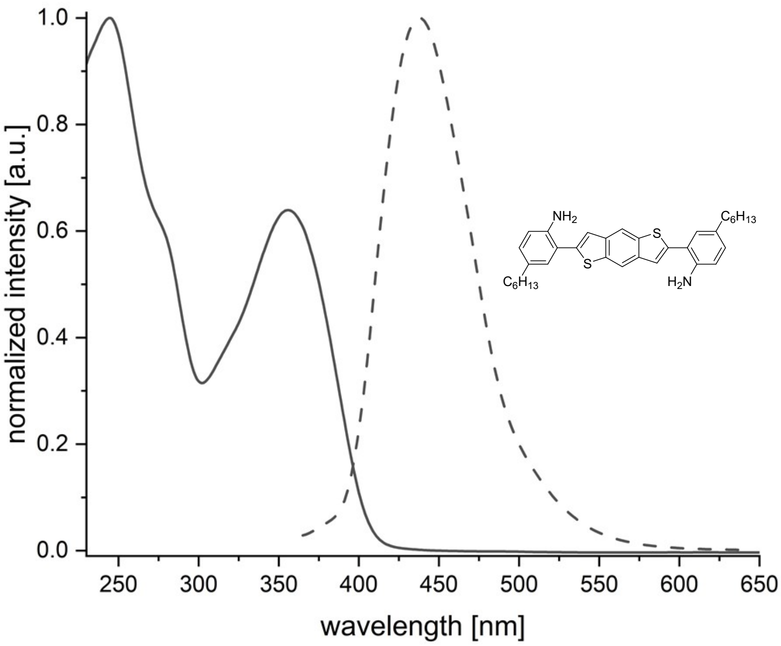


Figure S99. Absorption (solid line) and emission (dashed line) spectra of **6c** in DCM.

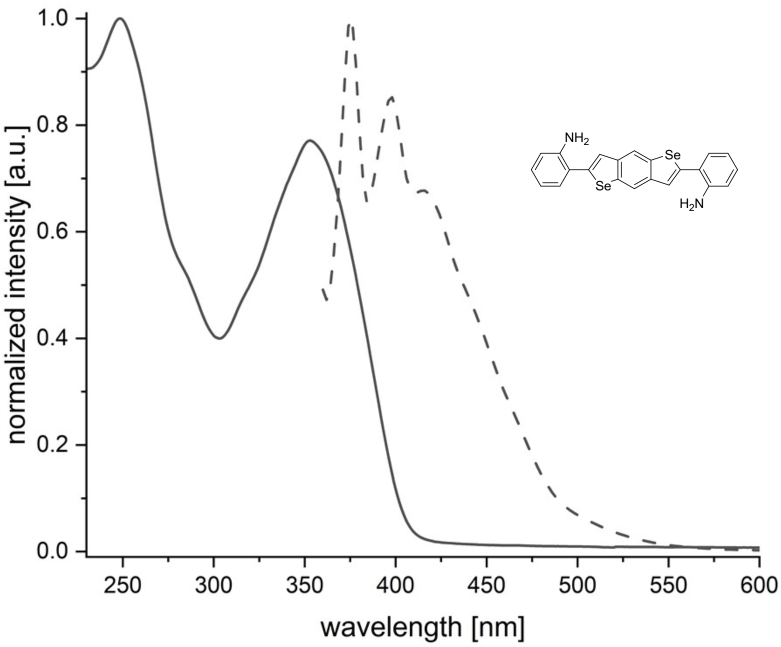


Figure S100. Absorption (solid line) and emission (dashed line) spectra of **7a** in DCM.

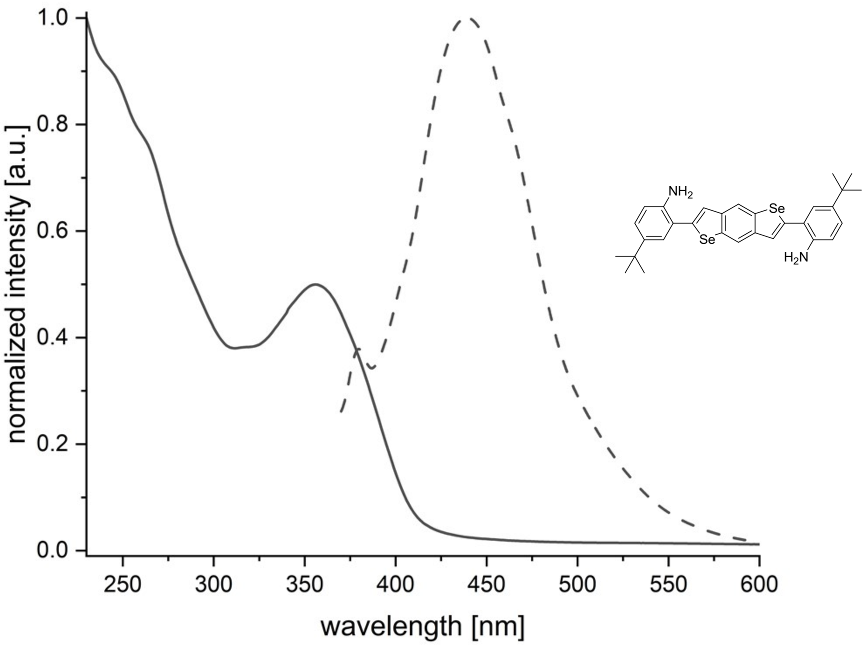


Figure S101. Absorption (solid line) and emission (dashed line) spectra of **7b** in DCM.

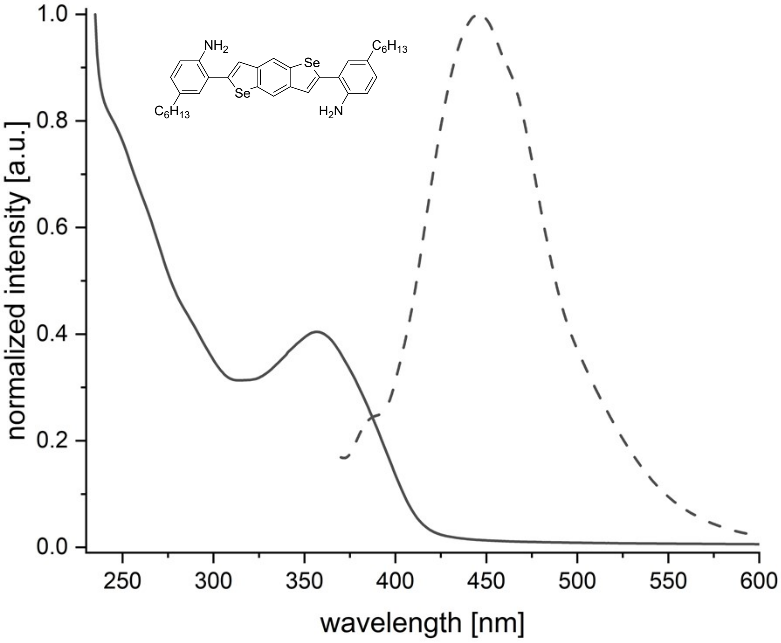


Figure S102. Absorption (solid line) and emission (dashed line) spectra of **7c** in DCM.

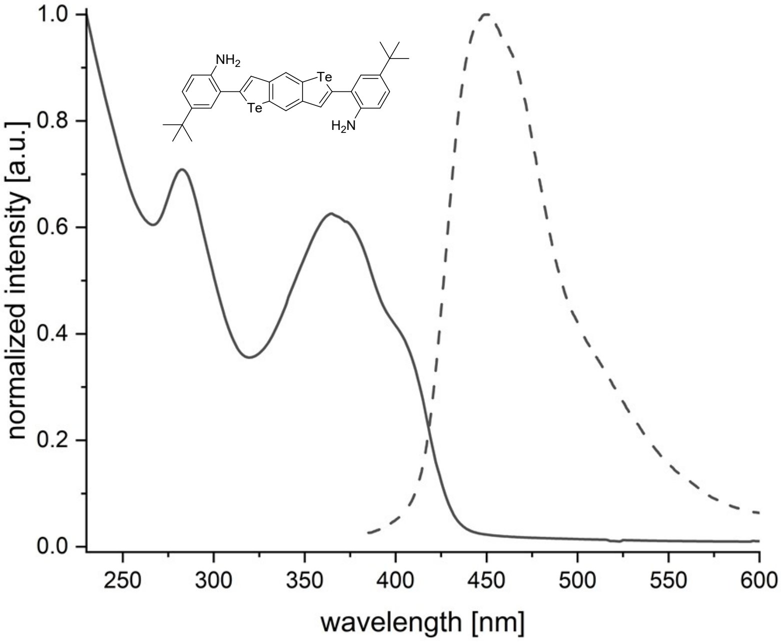


Figure S103. Absorption (solid line) and emission (dashed line) spectra of **8** in DCM.

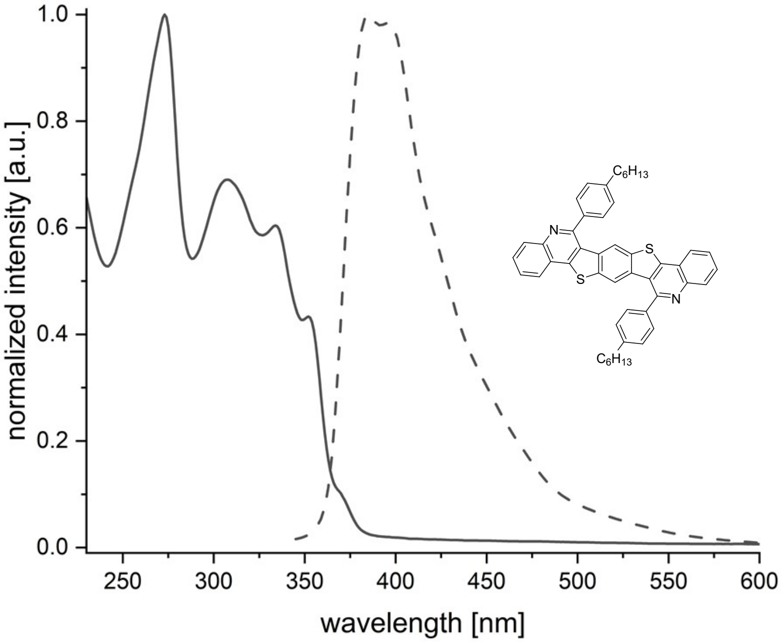


Figure S104. Absorption (solid line) and emission (dashed line) spectra of **9aa** in DCM.

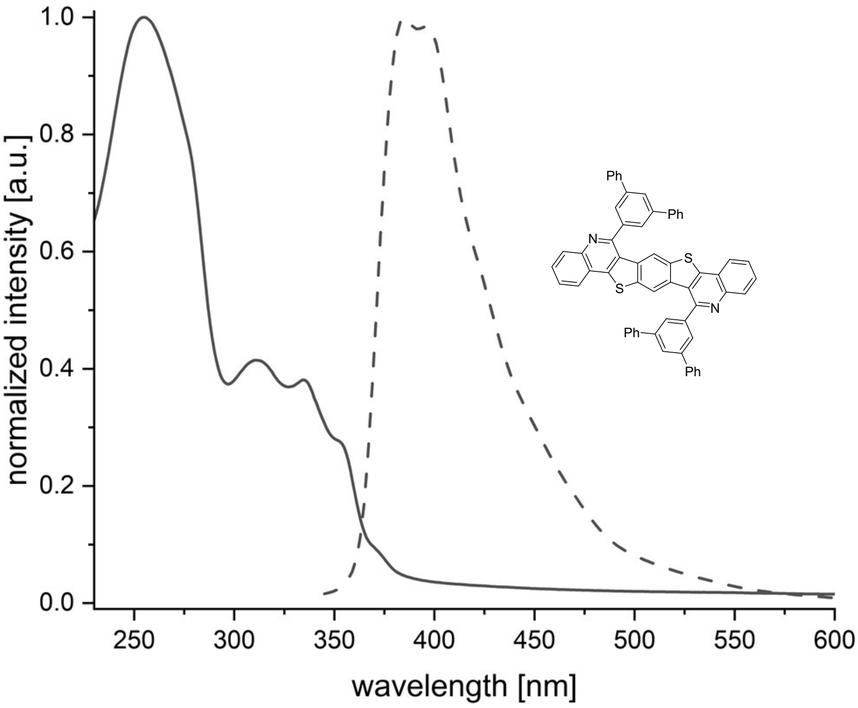


Figure S105. Absorption (solid line) and emission (dashed line) spectra of **9ab** in DCM.

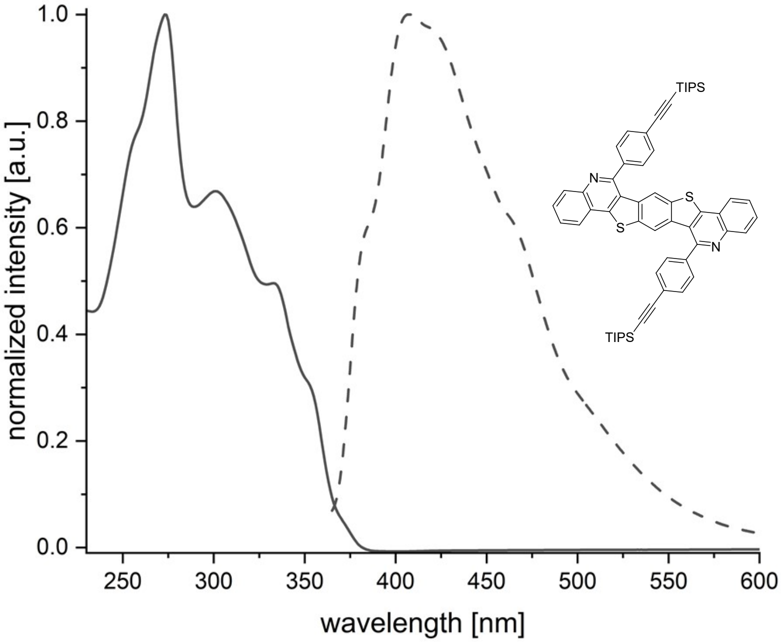


Figure S106. Absorption (solid line) and emission (dashed line) spectra of **9ac** in DCM.

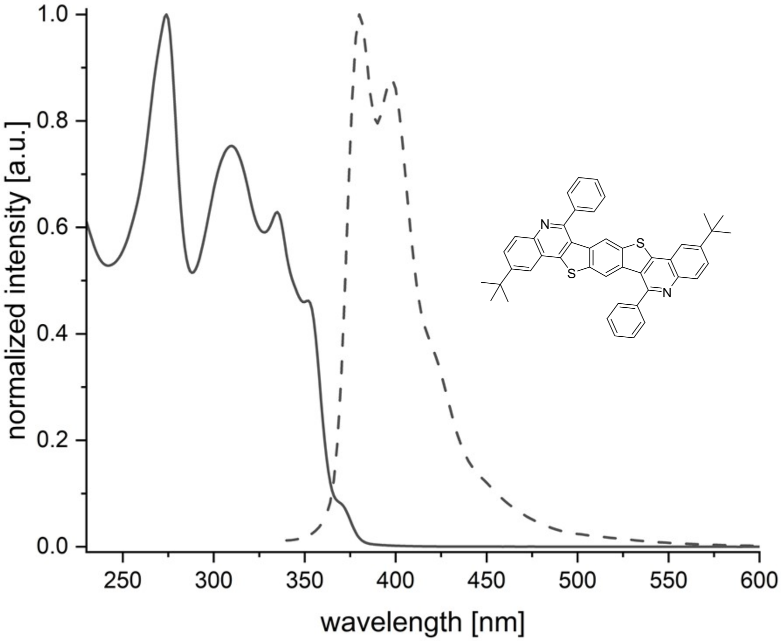


Figure S107. Absorption (solid line) and emission (dashed line) spectra of **9ba** in DCM.

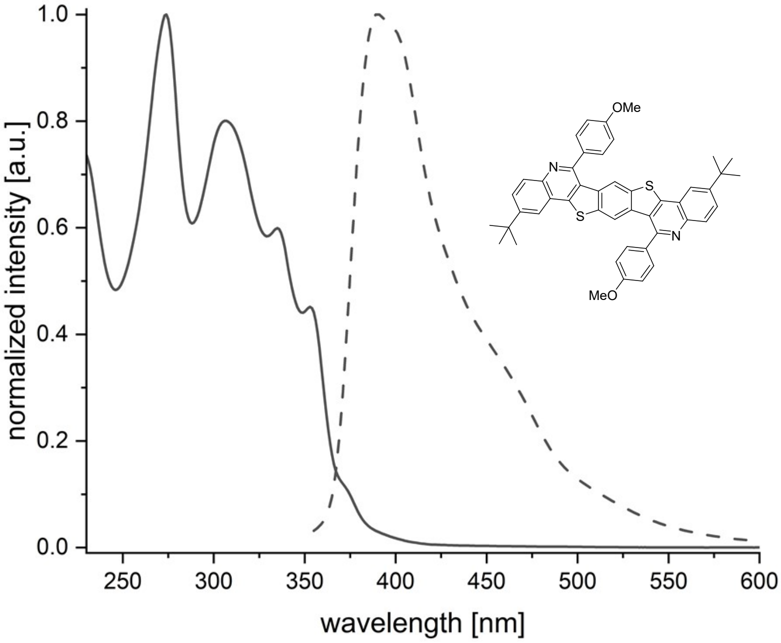


Figure S108. Absorption (solid line) and emission (dashed line) spectra of **9bb** in DCM.

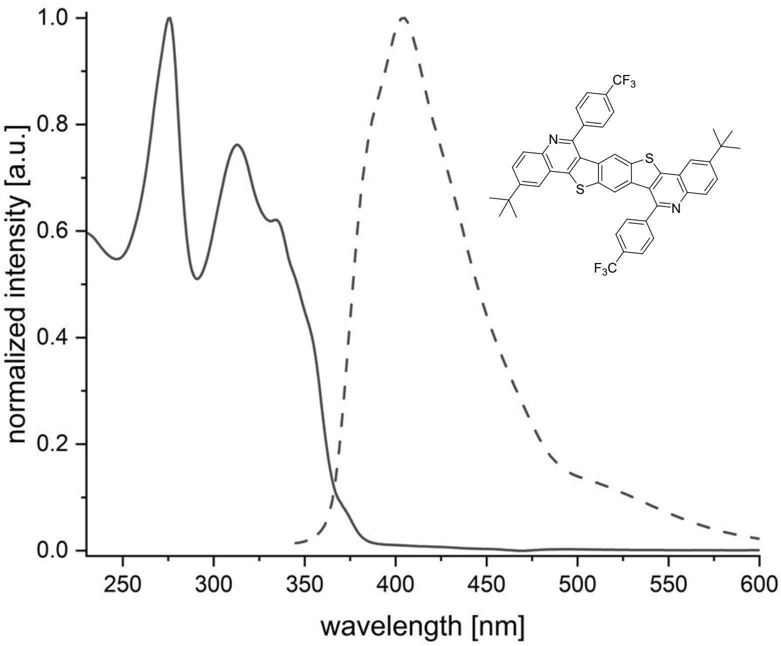


Figure S109. Absorption (solid line) and emission (dashed line) spectra of **9bc** in DCM.

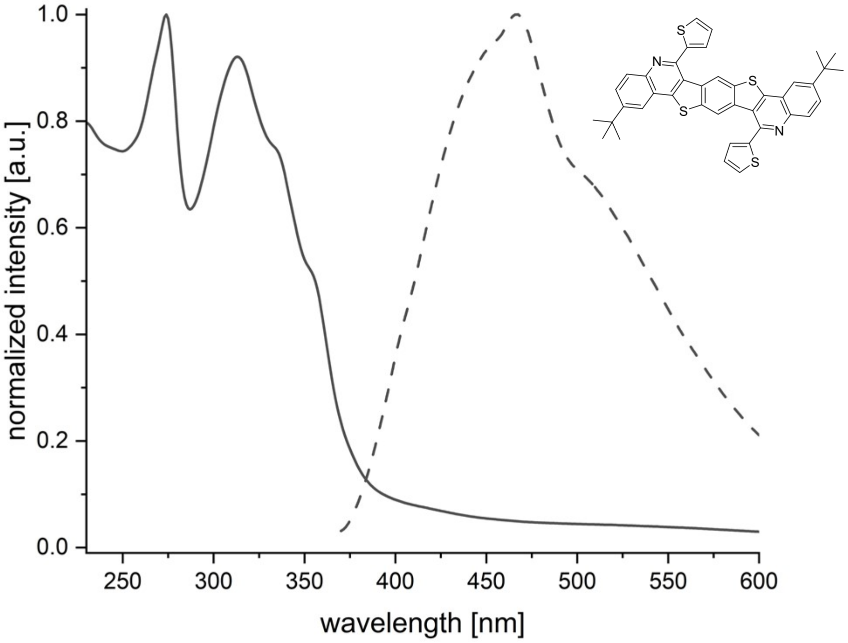


Figure S110. Absorption (solid line) and emission (dashed line) spectra of **9bd** in DCM.

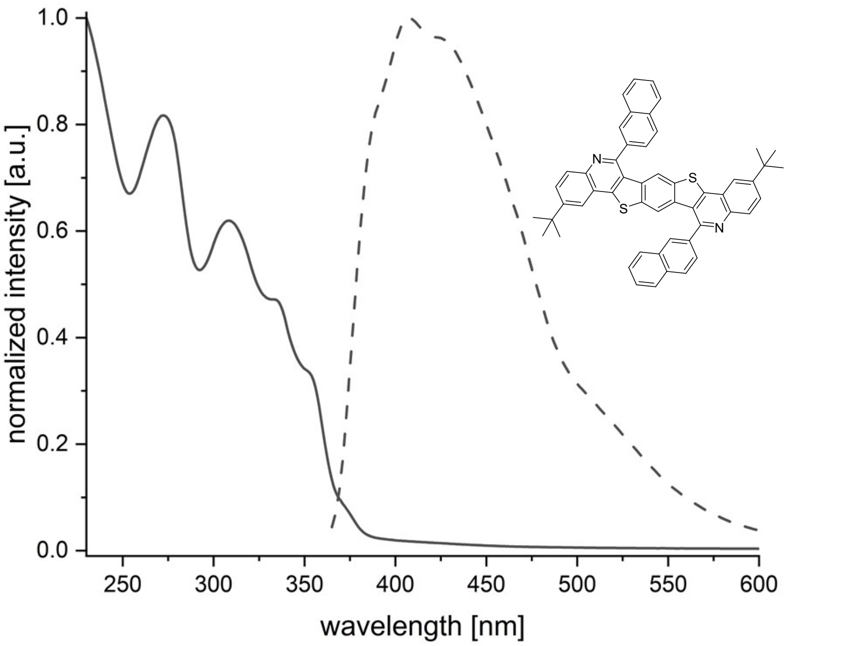


Figure S111. Absorption (solid line) and emission (dashed line) spectra of **9be** in DCM.

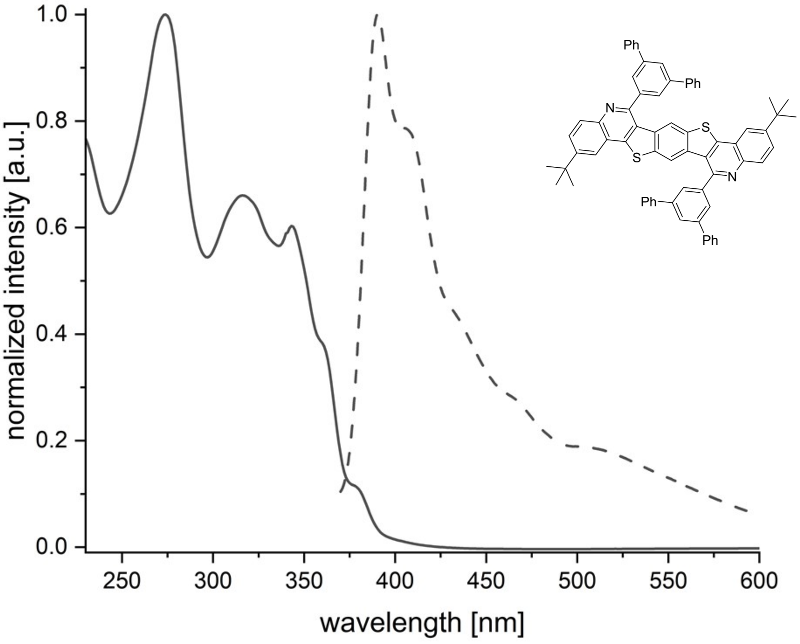


Figure S112. Absorption (solid line) and emission (dashed line) spectra of **9bf** in DCM.

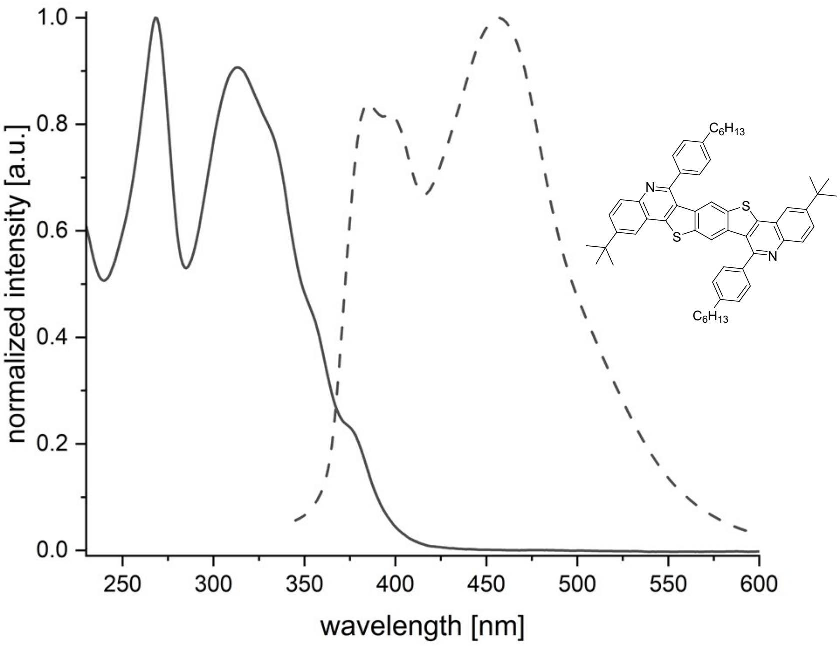


Figure S113. Absorption (solid line) and emission (dashed line) spectra of **9bg** in DCM.

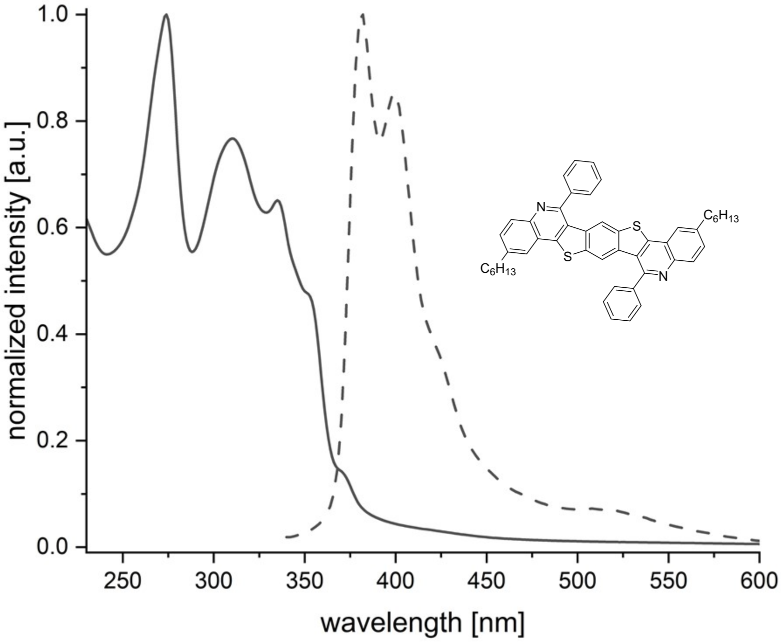


Figure S114. Absorption (solid line) and emission (dashed line) spectra of **9ca** in DCM.

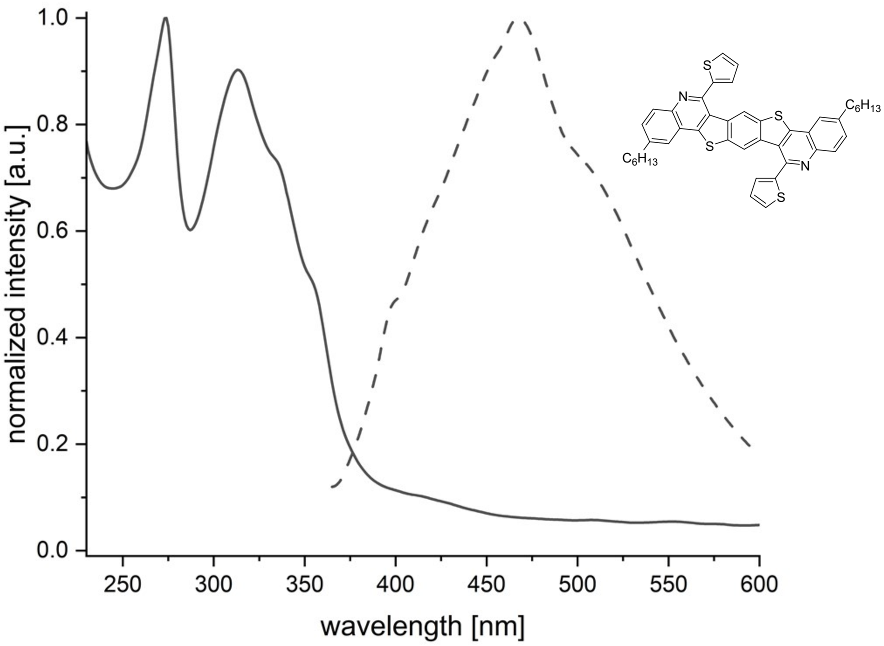


Figure S115. Absorption (solid line) and emission (dashed line) spectra of **9cb** in DCM.

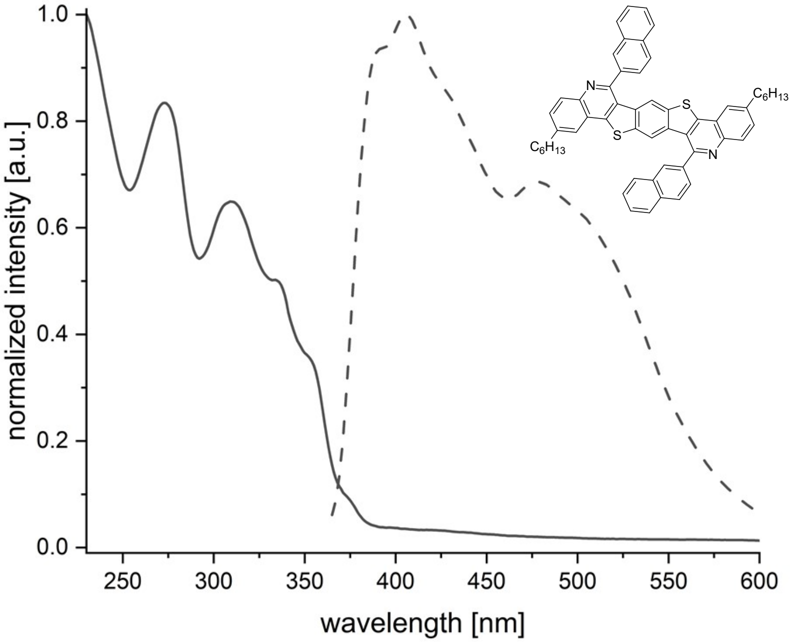


Figure S116. Absorption (solid line) and emission (dashed line) spectra of **9cc** in DCM.

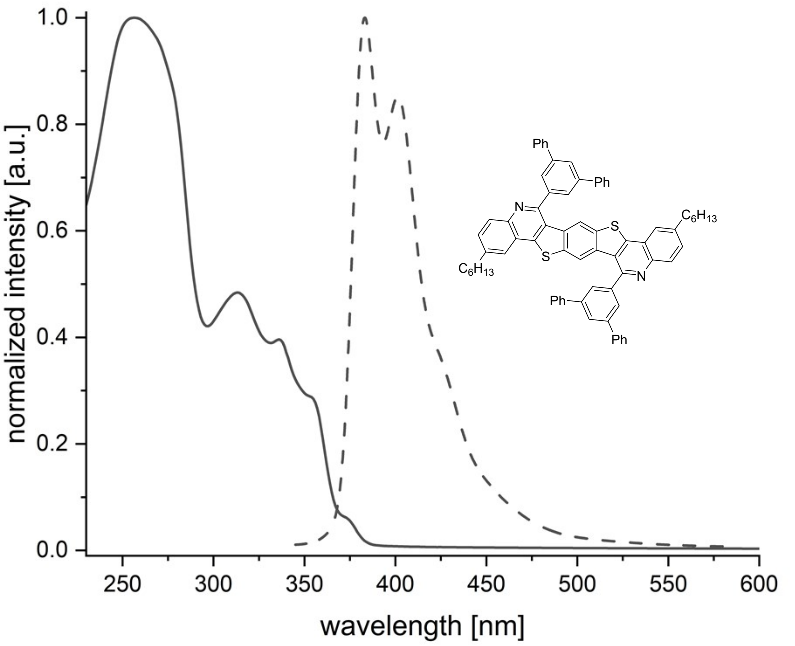


Figure S117. Absorption (solid line) and emission (dashed line) spectra of **9cd** in DCM.

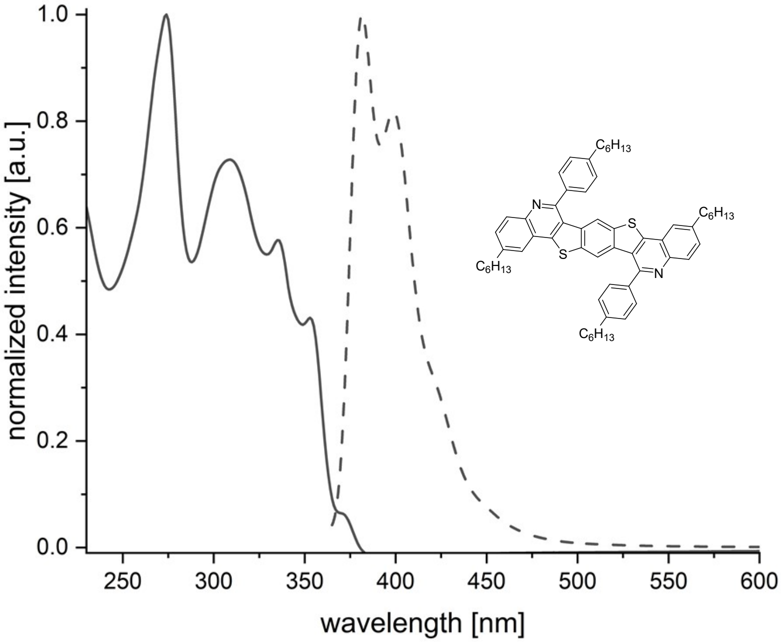


Figure S118. Absorption (solid line) and emission (dashed line) spectra of **9ce** in DCM.

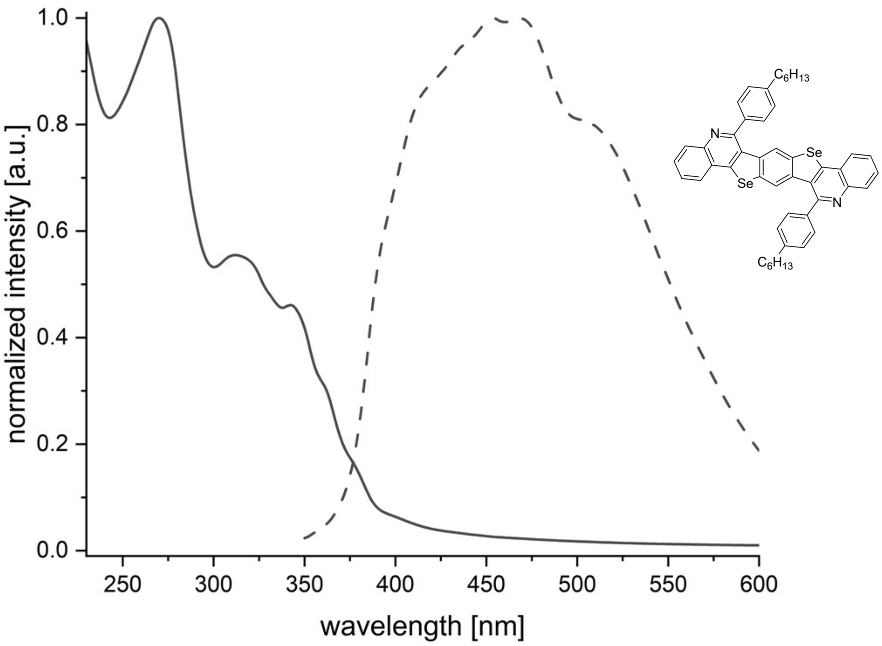


Figure S119. Absorption (solid line) and emission (dashed line) spectra of **10aa** in DCM.

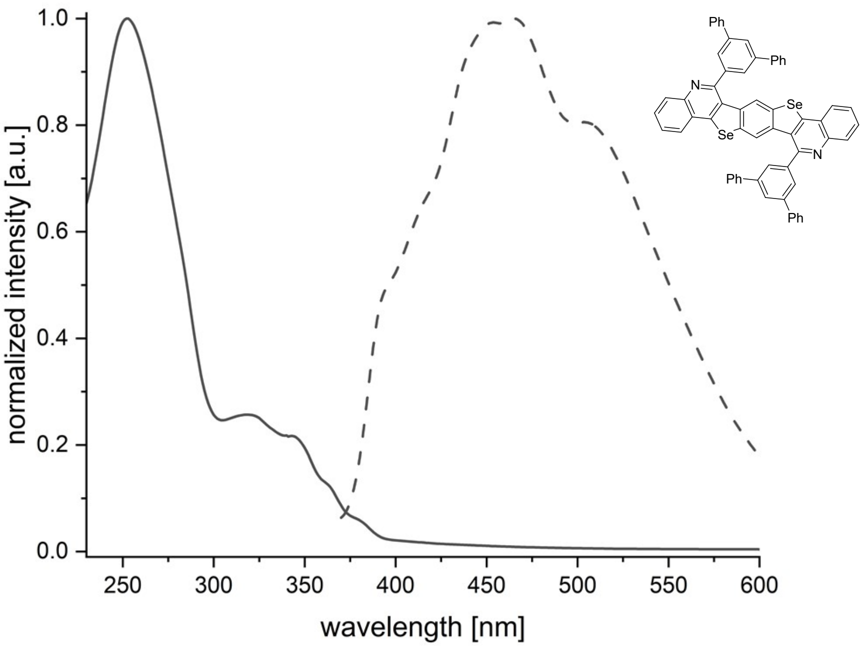


Figure S120. Absorption (solid line) and emission (dashed line) spectra of **10ab** in DCM.

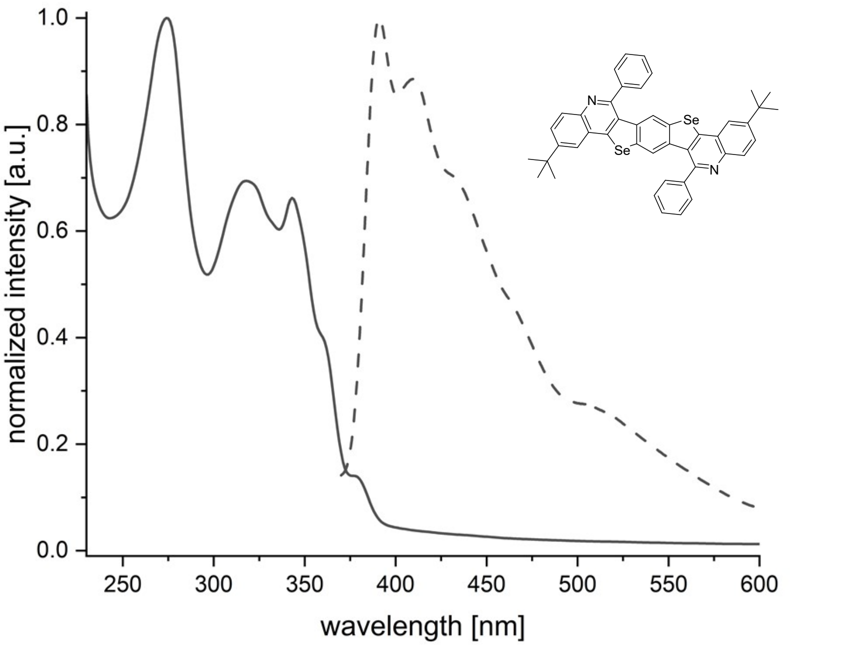


Figure S121. Absorption (solid line) and emission (dashed line) spectra of **10ba** in DCM.

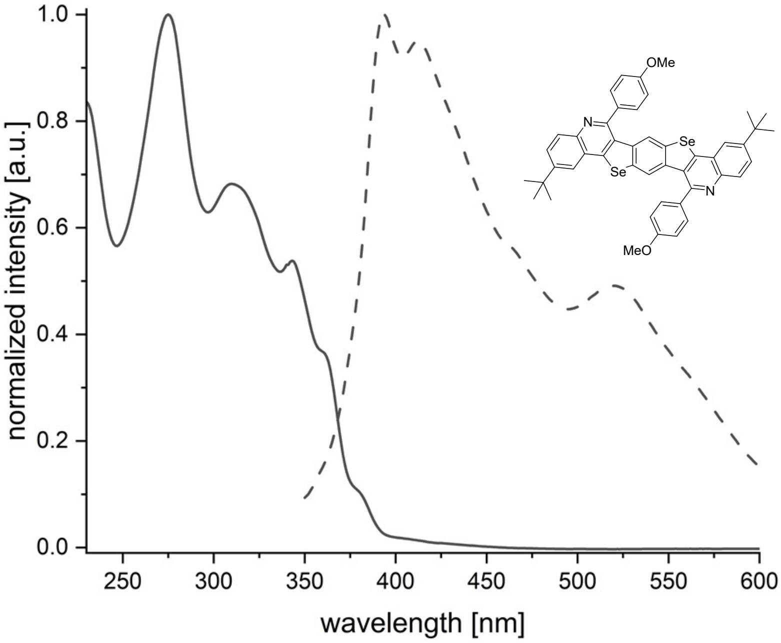


Figure S122. Absorption (solid line) and emission (dashed line) spectra of **10bb** in DCM.

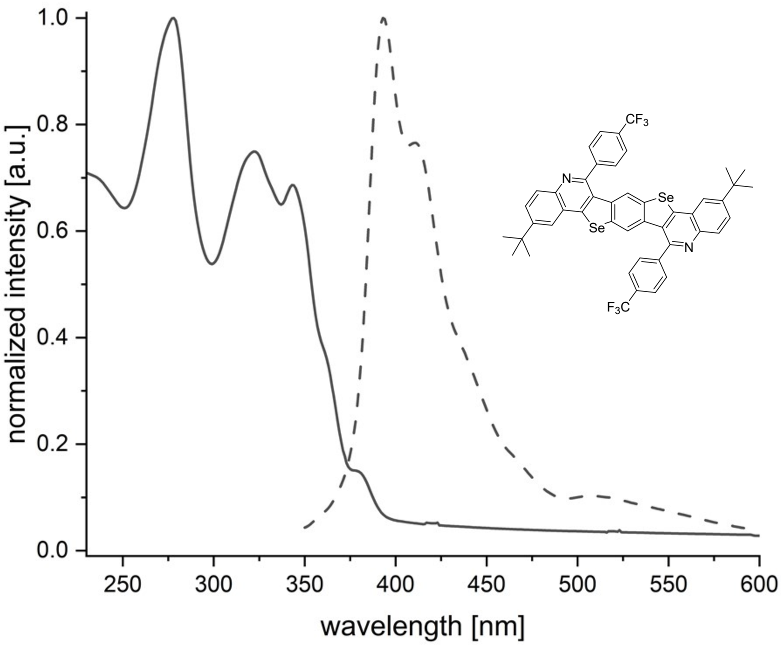


Figure S123. Absorption (solid line) and emission (dashed line) spectra of **10bc** in DCM.

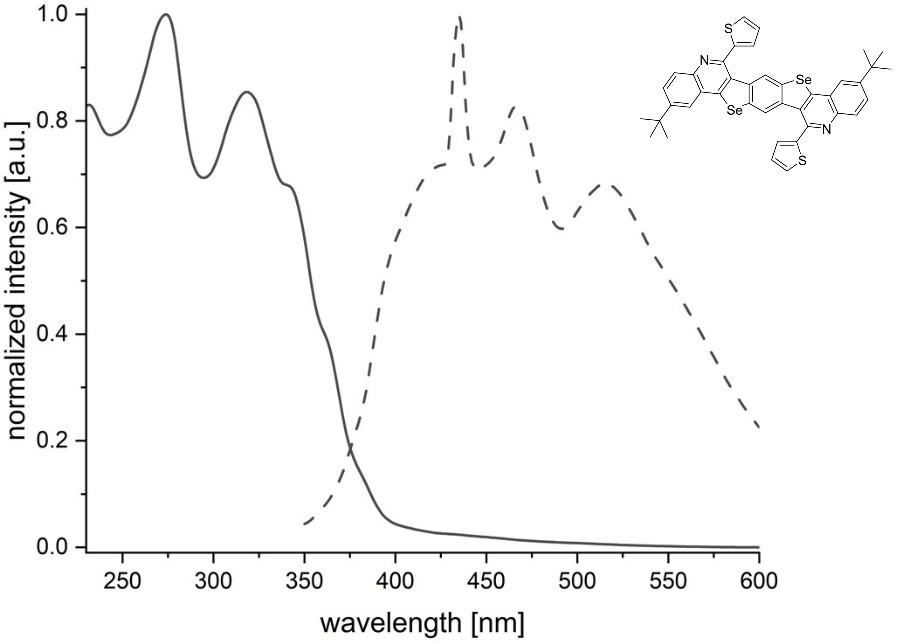


Figure S124. Absorption (solid line) and emission (dashed line) spectra of **10bd** in DCM.

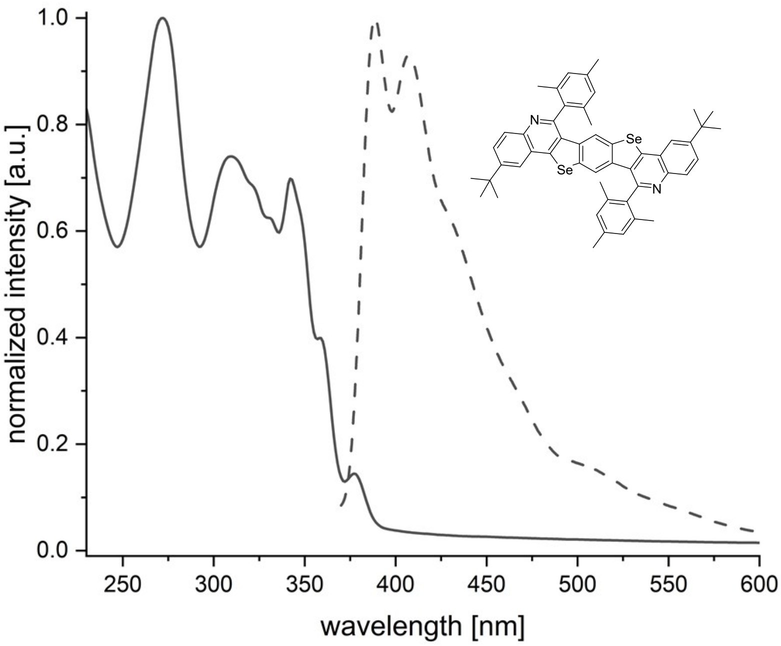


Figure S125. Absorption (solid line) and emission (dashed line) spectra of **10be** in DCM.

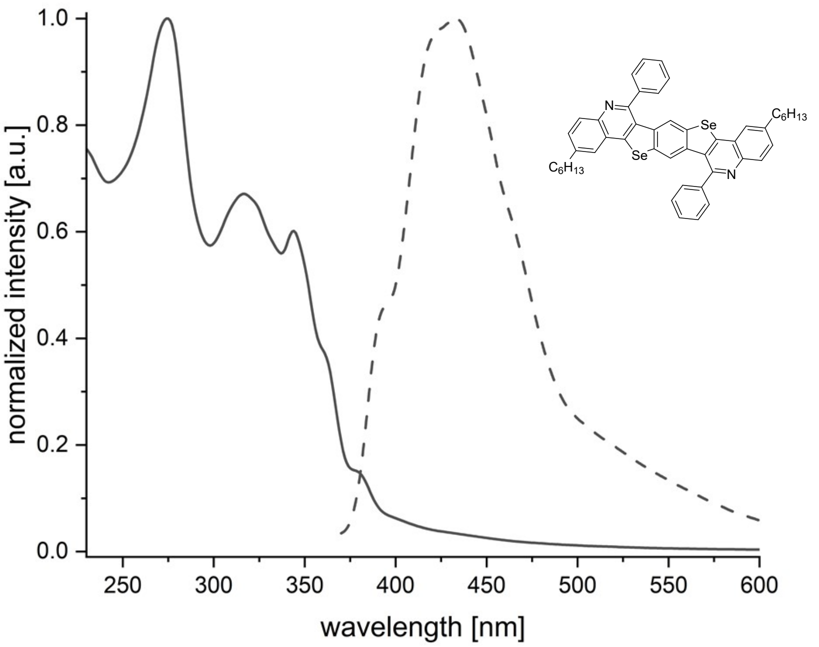


Figure S126. Absorption (solid line) and emission (dashed line) spectra of **10ca** in DCM.

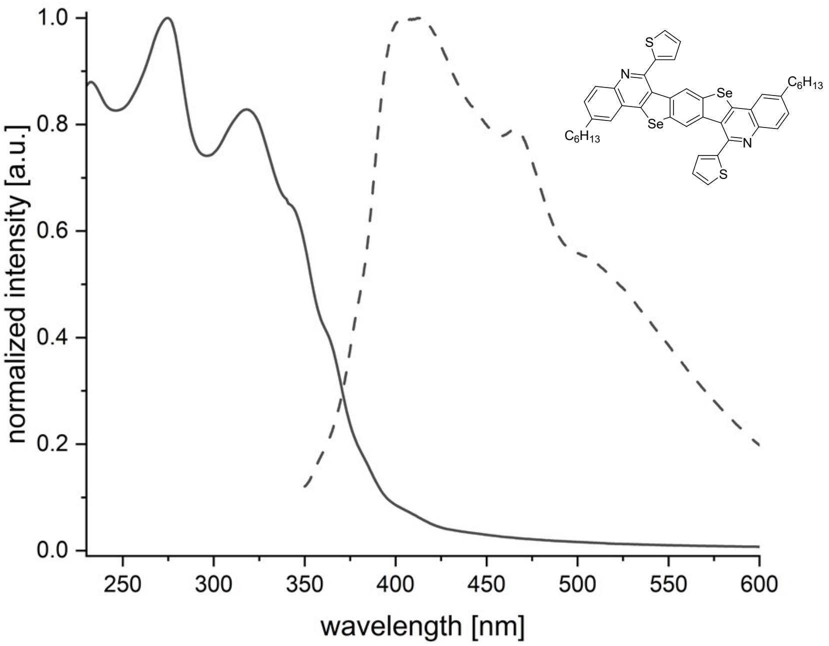


Figure S127. Absorption (solid line) and emission (dashed line) spectra of **10cb** in DCM.

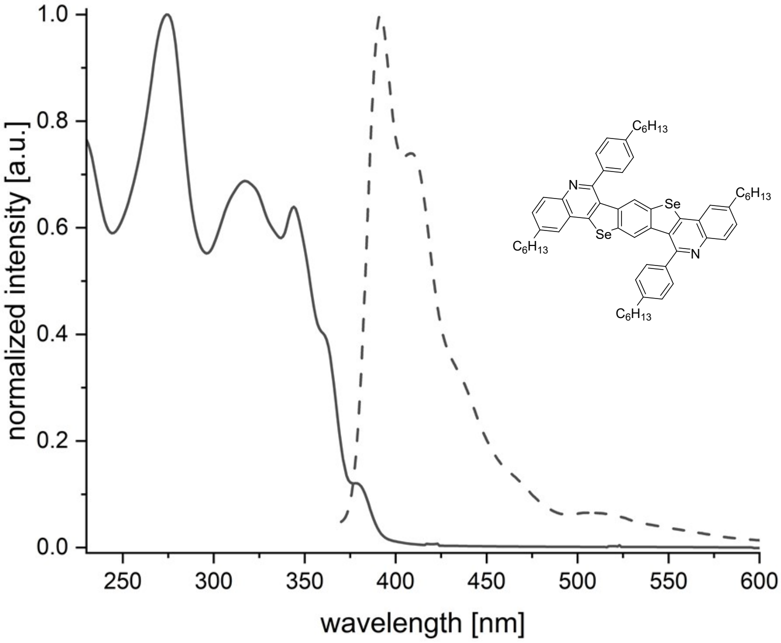


Figure S128. Absorption (solid line) and emission (dashed line) spectra of **10cc** in DCM.

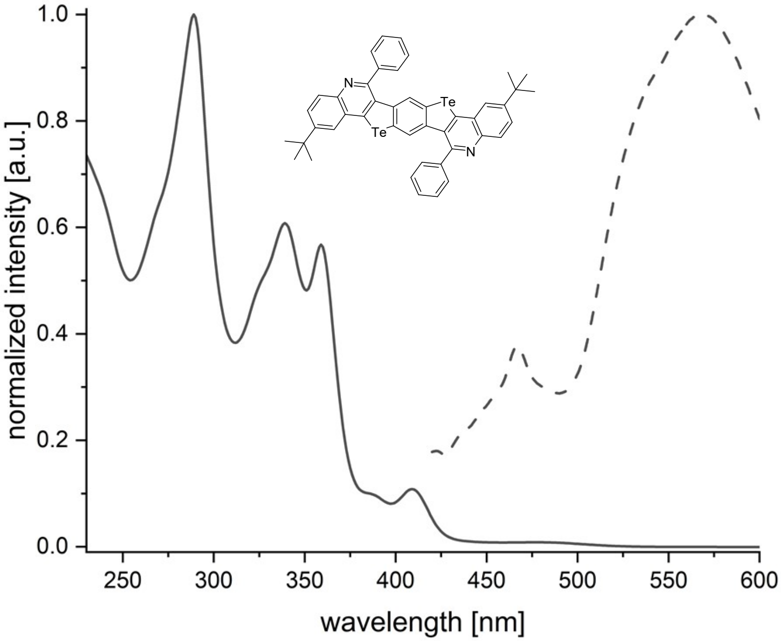


Figure S129. Absorption (solid line) and emission (dashed line) spectra of **11ba** in DCM.

4 Thermogravimetric Analysis / Differential Scanning Calorimetry (TGA/DSC)

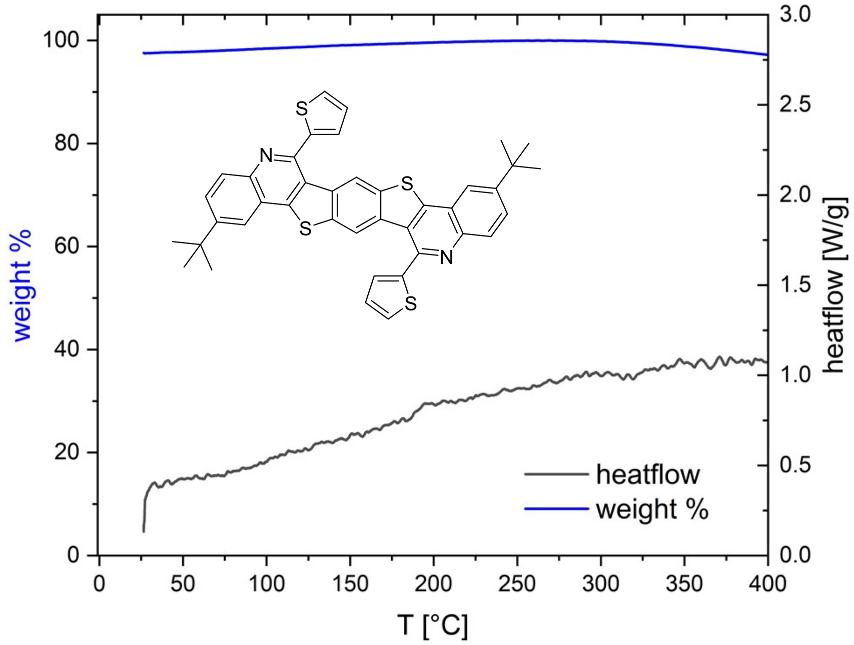


Figure S130. TGA/DSC plot of **9bd** under nitrogen atmosphere.

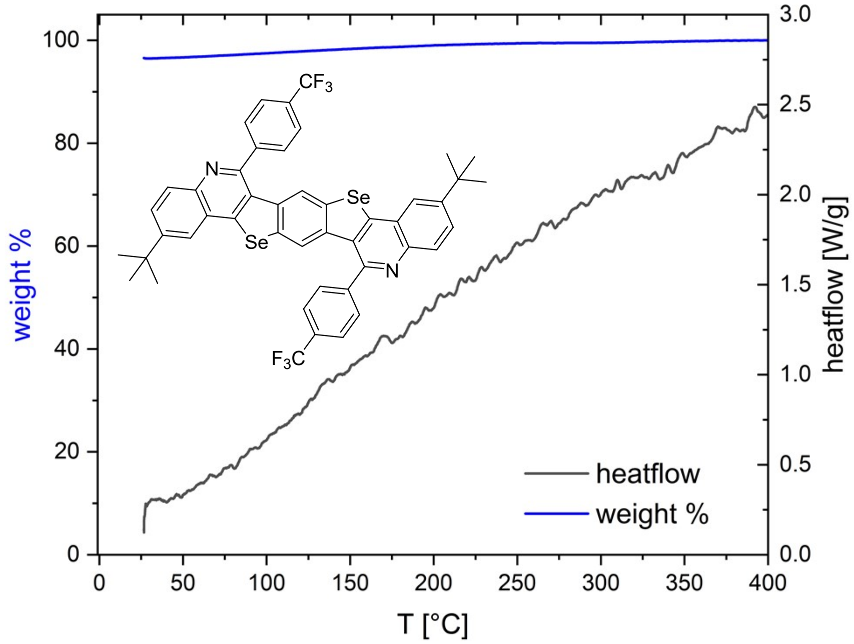


Figure S131. TGA/DSC plot of **10bc** under nitrogen atmosphere.

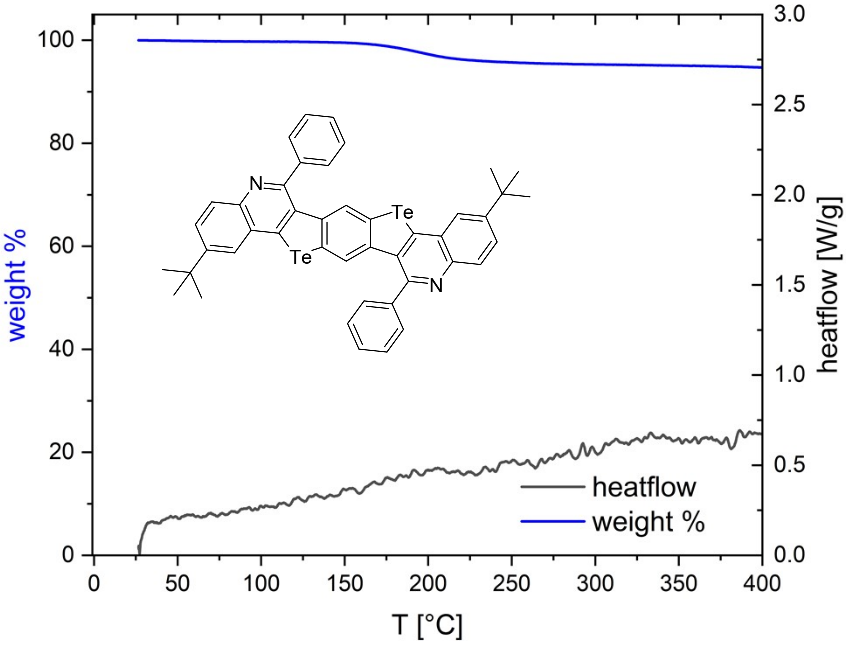
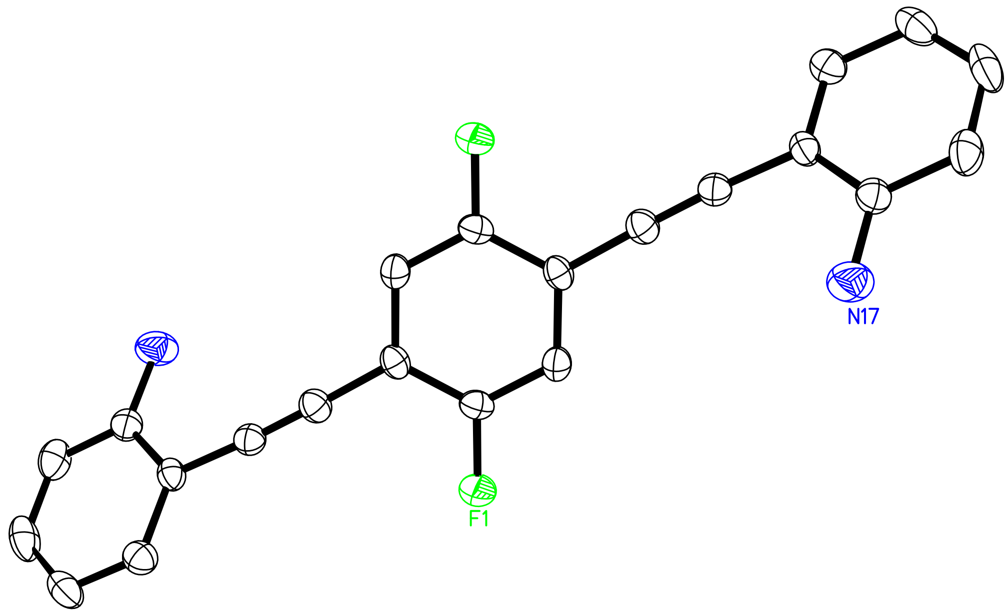


Figure S132. TGA/DSC plot of **11ba** under nitrogen atmosphere.

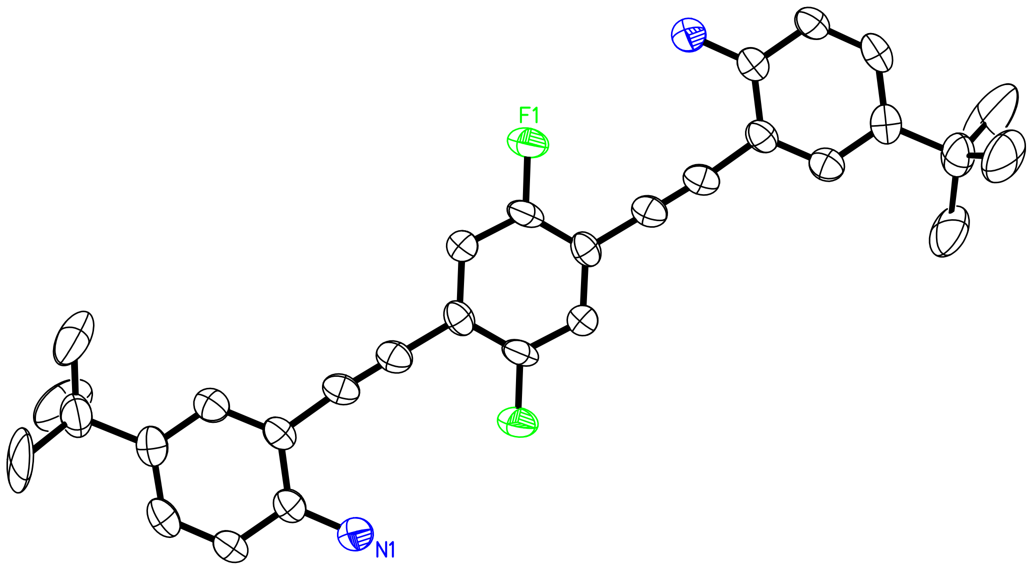
5 Crystallographic Data

Table S1. Crystal structure, crystal data and structure refinement of **5a** (CCDC 2380037).



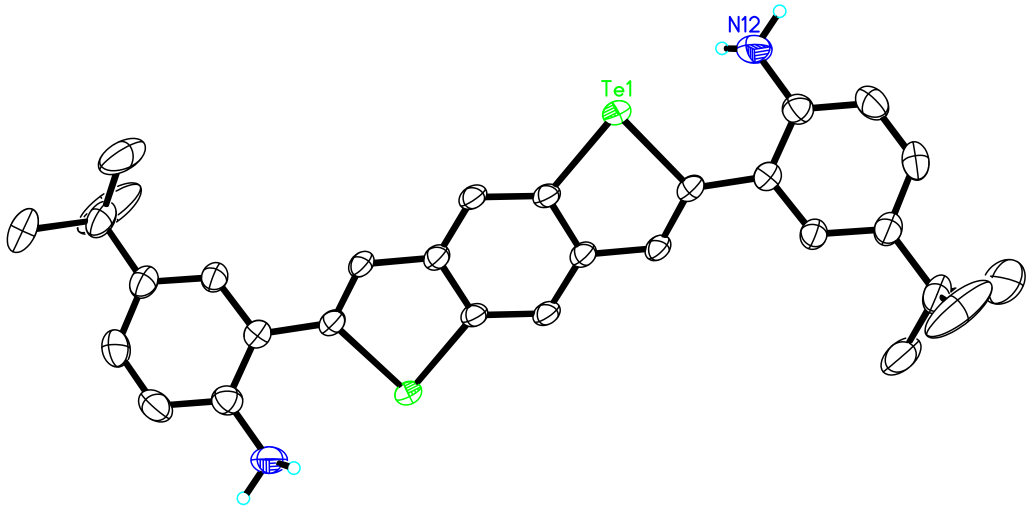
Empirical formula	$C_{22}H_{14}F_2N_2$	
Formula weight	344.35	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	2	
Unit cell dimensions	a = 5.9473(5) Å	α = 95.1290(19) deg.
	b = 7.4852(7) Å	β = 98.8424(18) deg.
	c = 18.7512(16) Å	γ = 90.5733(17) deg.
Volume	821.28(12) $Å^3$	
Density (calculated)	1.39 g/cm^3	
Absorption coefficient	0.10 mm^{-1}	
Crystal shape	plank	
Crystal size	0.210 x 0.150 x 0.046 mm^3	
Crystal colour	yellow	
Theta range for data collection	2.2 to 28.4 deg.	
Index ranges	$-7 \le h \le 7$, $-9 \le k \le 9$, $-24 \le l \le 23$	
Reflections collected	11889	
Independent reflections	3682 (R(int) = 0.0341)	
Observed reflections	2732 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.92	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3682 / 6 / 248	
Goodness-of-fit on F^2	1.05	
Final R indices (I>2sigma(I))	R1 = 0.046, wR2 = 0.101	
Largest diff. peak and hole	0.24 and -0.20 $eÅ^{-3}$	

Table S2. Crystal structure, crystal data and structure refinement of **5b** (CCDC 2380038).



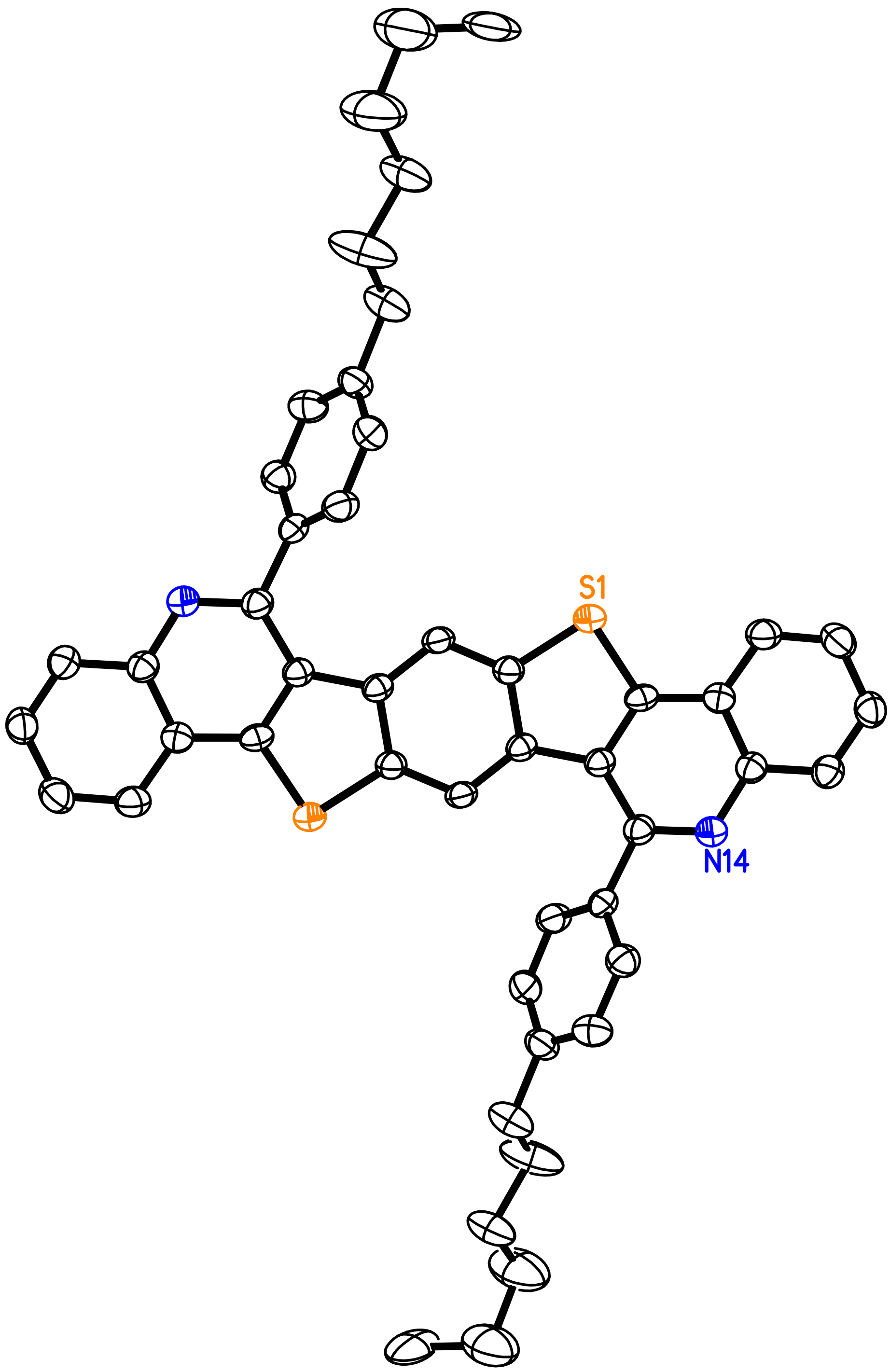
Empirical formula	$C_{30}H_{30}F_2N_2$	
Formula weight	456.56	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	4	
Unit cell dimensions	a = 22.061(4) Å	α = 90 deg.
	b = 6.1949(10) Å	β = 118.425(3) deg.
	c = 21.030(3) Å	γ = 90 deg.
Volume	2527.6(7) $Å^3$	
Density (calculated)	1.20 g/cm^3	
Absorption coefficient	0.08 mm^{-1}	
Crystal shape	plate	
Crystal size	0.140 x 0.096 x 0.018 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.0 to 20.2 deg.	
Index ranges	$-21 \leq h \leq 21$, $-6 \leq k \leq 6$, $-20 \leq l \leq 20$	
Reflections collected	16704	
Independent reflections	2408 (R(int) = 0.0936)	
Observed reflections	1681 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.88	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	2408 / 379 / 325	
Goodness-of-fit on F^2	1.06	
Final R indices (I>2sigma(I))	R1 = 0.055, wR2 = 0.109	
Largest diff. peak and hole	0.18 and -0.20 $eÅ^{-3}$	

Table S3. Crystal structure, crystal data and structure refinement of **8** (CCDC 2380039).



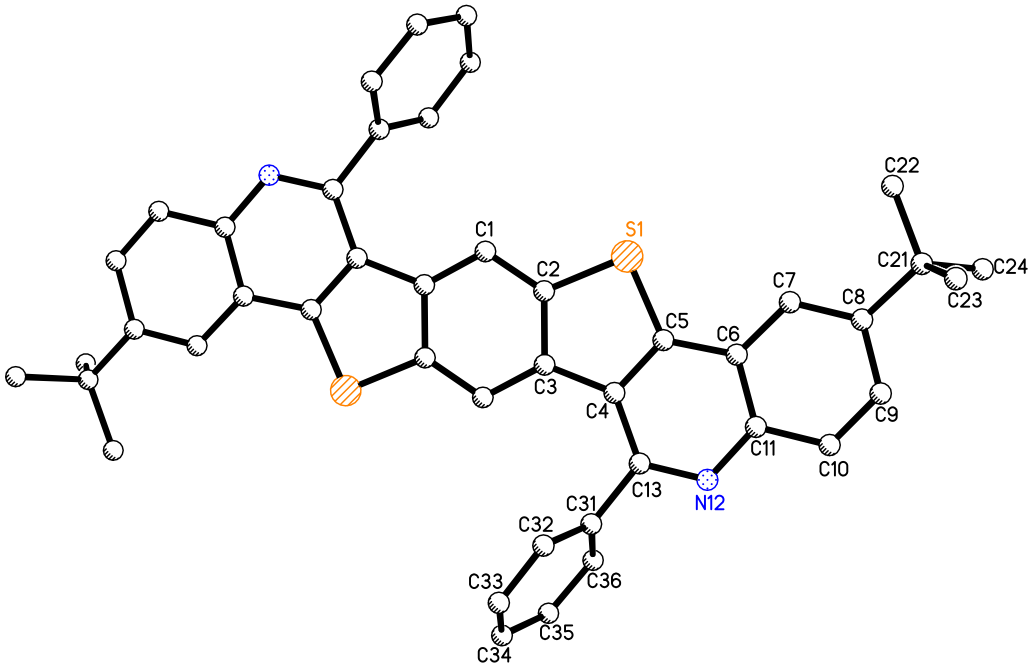
Empirical formula	$C_{30}H_{32}N_2Te_2$
Formula weight	675.77
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	$P\bar{1}$
Z	1
Unit cell dimensions	a = 5.9242(6) Å α = 97.2719(14) deg.
	b = 6.7487(6) Å β = 98.0695(13) deg.
	c = 17.7181(17) Å γ = 101.6422(13) deg.
Volume	678.12(11) Å^3
Density (calculated)	1.65 g/cm^3
Absorption coefficient	2.17 mm^{-1}
Crystal shape	prism
Crystal size	0.218 x 0.042 x 0.034 mm^3
Crystal colour	yellow
Theta range for data collection	2.4 to 30.1 deg.
Index ranges	$-8 \le h \le 8$, $-9 \le k \le 9$, $-25 \le l \le 25$
Reflections collected	13809
Independent reflections	3689 (R(int) = 0.0281)
Observed reflections	3296 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.85
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3689 / 205 / 194
Goodness-of-fit on F^2	1.07
Final R indices (I>2sigma(I))	R1 = 0.025, wR2 = 0.054
Largest diff. peak and hole	0.64 and -0.33 eÅ^{-3}

Table S4. Crystal structure, crystal data and structure refinement of **9aa** (CCDC 2380040).



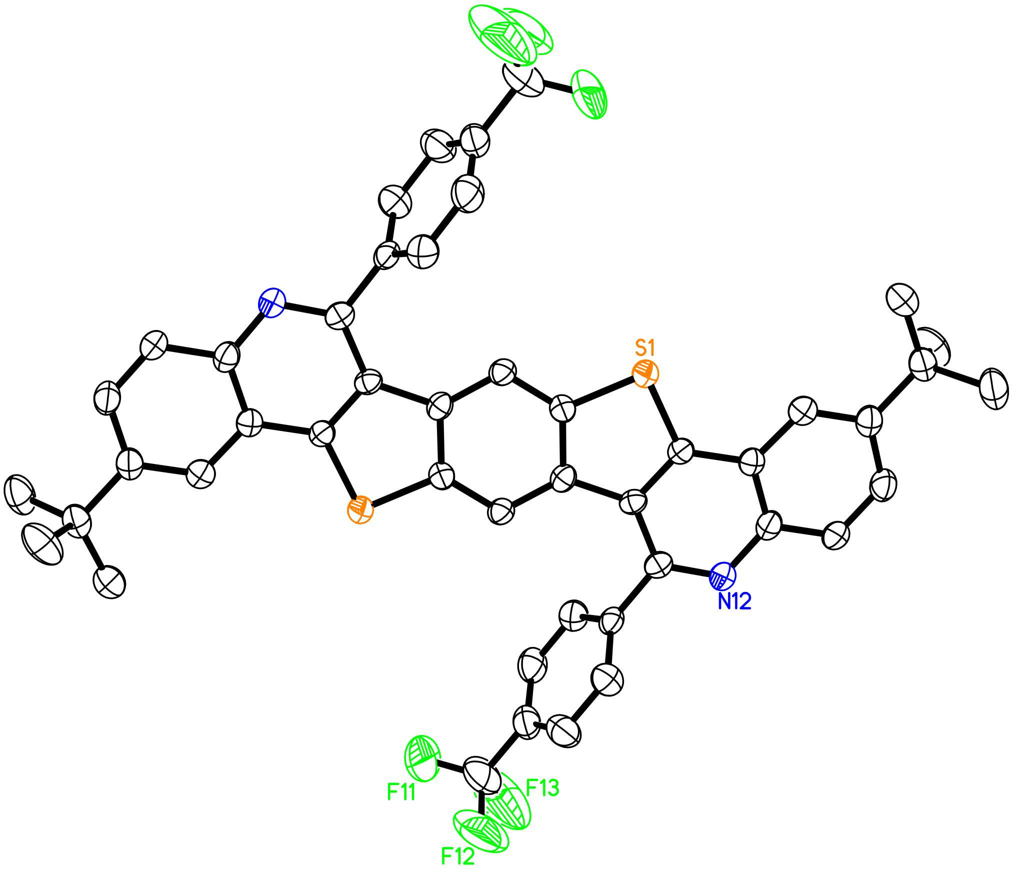
Empirical formula	$C_{48}H_{44}N_2S_2$	
Formula weight	712.97	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	1	
Unit cell dimensions	a = 5.9858(3) Å	α = 82.696(4) deg.
	b = 10.7692(6) Å	β = 88.046(5) deg.
	c = 14.9923(8) Å	γ = 78.685(4) deg.
Volume	939.92(9) $Å^3$	
Density (calculated)	1.26 g/cm^3	
Absorption coefficient	1.56 mm^{-1}	
Crystal shape	needle	
Crystal size	0.273 x 0.020 x 0.010 mm^3	
Crystal colour	colourless	
Theta range for data collection	3.0 to 62.0 deg.	
Index ranges	$-6 \leq h \leq 5$, $-12 \leq k \leq 11$, $-14 \leq l \leq 17$	
Reflections collected	9036	
Independent reflections	2870 (R(int) = 0.0416)	
Observed reflections	1966 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.98 and 0.90	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	2870 / 443 / 283	
Goodness-of-fit on F^2	1.05	
Final R indices (I>2sigma(I))	R1 = 0.049, wR2 = 0.094	
Largest diff. peak and hole	0.23 and -0.22 $eÅ^{-3}$	

Table S5. Crystal structure, crystal data and structure refinement of **9ba** (CCDC 2380041).



Empirical formula	$C_{44}H_{36}N_2S_2$	
Formula weight	656.87	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P $\bar{1}$	
Z	1	
Unit cell dimensions	a = 5.9420(7) Å	α = 94.938(3) deg.
	b = 10.9486(14) Å	β = 92.627(3) deg.
	c = 13.5387(16) Å	γ = 101.794(3) deg.
Volume	857.17(18) $Å^3$	
Density (calculated)	1.27 g/cm^3	
Absorption coefficient	0.19 mm^{-1}	
Crystal shape	rhomboid	
Crystal size	0.262 x 0.059 x 0.014 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.5 to 29.2 deg.	
Index ranges	$-8 \le h \le 8$, $-14 \le k \le 14$, $-18 \le l \le 18$	
Reflections collected	16548	
Independent reflections	4271 (R(int) = 0.0577)	
Observed reflections	2879 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.90	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	4271 / 0 / 220	
Goodness-of-fit on F^2	1.08	
Final R indices (I>2sigma(I))	R1 = 0.049, wR2 = 0.118	
Largest diff. peak and hole	0.36 and -0.34 $eÅ^{-3}$	

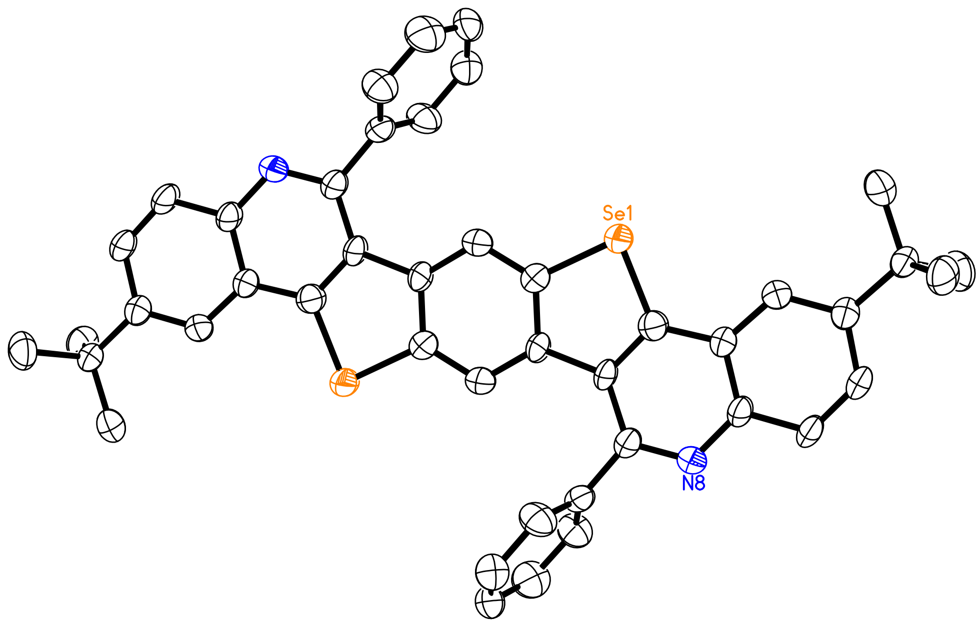
Table S6. Crystal structure, crystal data and structure refinement of **9bc** (CCDC 2380042).



Empirical formula	$C_{46}H_{34}F_6N_2S_2$	
Formula weight	792.87	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	2	
Unit cell dimensions	a = 16.739(2) Å	α = 90 deg.
	b = 5.9610(7) Å	β =101.617(3) deg.
	c = 19.559(3) Å	γ = 90 deg.
Volume	1911.7(4) $Å^3$	
Density (calculated)	1.38 g/cm^3	
Absorption coefficient	0.20 mm^{-1}	
Crystal shape	brick	
Crystal size	0.086 x 0.071 x 0.051 mm^3	
Crystal colour	colourless	
Theta range for data collection	1.8 to 25.4 deg.	
Index ranges	$-20 \le h \le 20$, $-7 \le k \le 7$, $-23 \le l \le 23$	
Reflections collected	17512	
Independent reflections	3493 (R(int) = 0.0867)	
Observed reflections	2120 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	

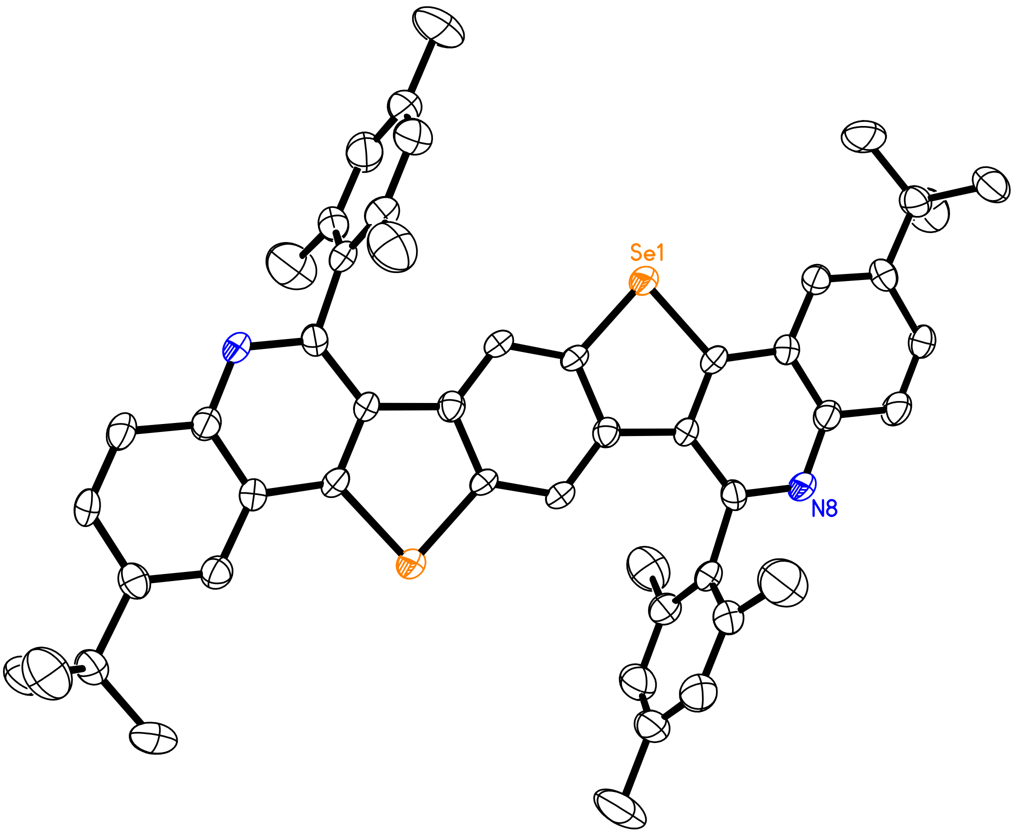
Max. and min. transmission	0.96 and 0.89
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3493 / 0 / 256
Goodness-of-fit on F^2	1.03
Final R indices (I>2sigma(I))	R1 = 0.070, wR2 = 0.159
Largest diff. peak and hole	0.81 and -0.62 eÅ^{-3}

Table S7. Crystal structure, crystal data and structure refinement of **10ba** (CCDC 2380043).



Empirical formula	$C_{44}H_{36}N_2Se_2$	
Formula weight	750.67	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	1	
Unit cell dimensions	a = 5.8232(4) Å	α = 99.647(5) deg.
	b = 11.2843(7) Å	β = 90.681(5) deg.
	c = 13.7511(8) Å	γ = 102.214(5) deg.
Volume	869.60(10) $Å^3$	
Density (calculated)	1.43 g/cm^3	
Absorption coefficient	2.91 mm^{-1}	
Crystal shape	plate	
Crystal size	0.037 x 0.035 x 0.018 mm^3	
Crystal colour	pale yellow	
Theta range for data collection	3.3 to 62.2 deg.	
Index ranges	$-6 \le h \le 6$, $-8 \le k \le 12$, $-15 \le l \le 14$	
Reflections collected	10186	
Independent reflections	2633 (R(int) = 0.0639)	
Observed reflections	1669 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.94 and 0.82	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	2633 / 0 / 220	
Goodness-of-fit on F^2	0.99	
Final R indices (I>2sigma(I))	R1 = 0.047, wR2 = 0.095	
Largest diff. peak and hole	0.59 and -0.44 $eÅ^{-3}$	

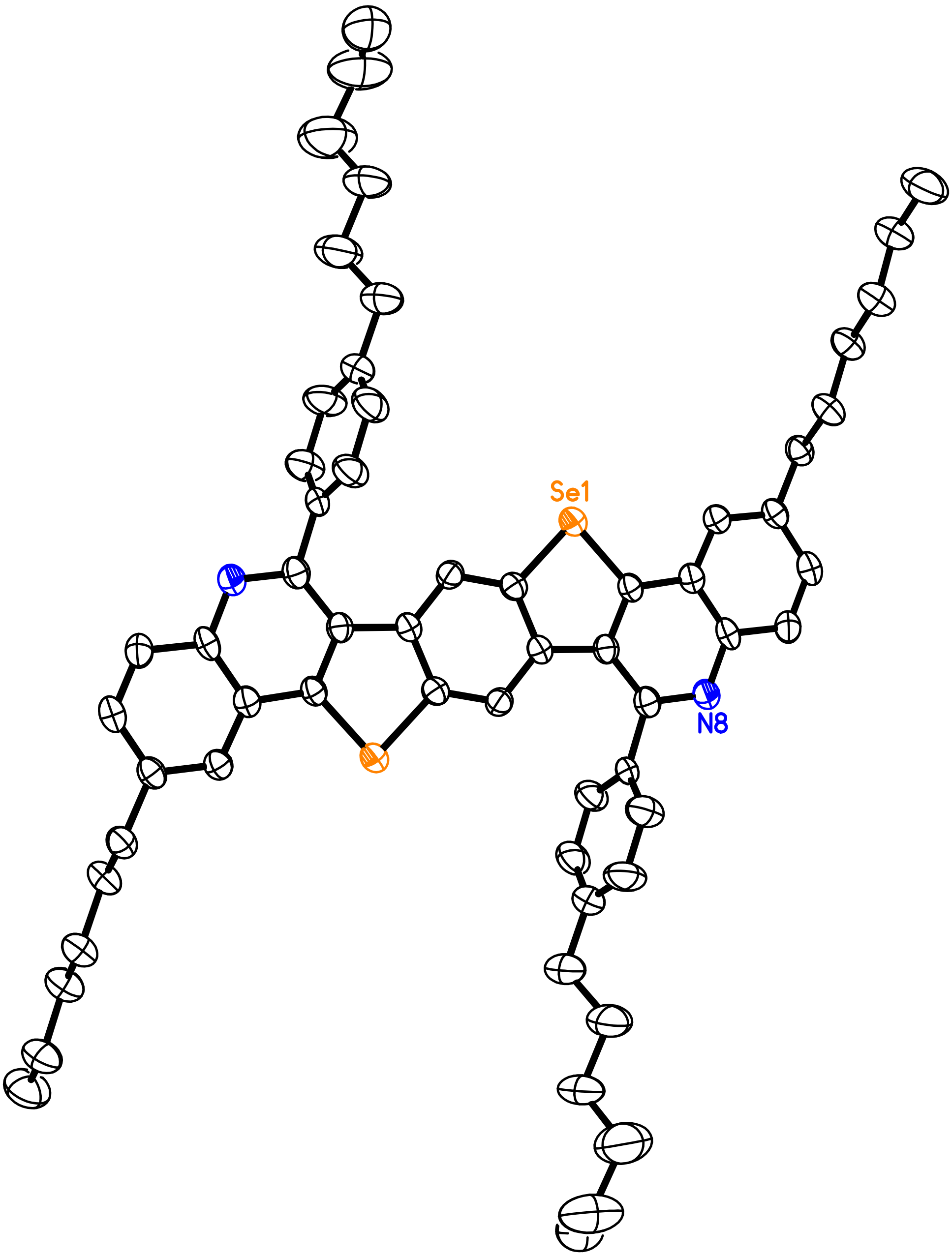
Table S8. Crystal structure, crystal data and structure refinement of **10be** (CCDC 2380044).



Empirical formula	$C_{51}H_{50}Cl_2N_2Se_2$	
Formula weight	919.75	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Z	4	
Unit cell dimensions	a = 26.6788(10) Å	α = 90 deg.
	b = 10.4142(4) Å	β = 92.530(3) deg.
	c = 16.3568(7) Å	γ = 90 deg.
Volume	4540.1(3) $Å^3$	
Density (calculated)	1.35 g/cm^3	
Absorption coefficient	1.78 mm^{-1}	
Crystal shape	irregular	
Crystal size	0.088 x 0.080 x 0.035 mm^3	
Crystal colour	yellow	
Theta range for data collection	1.5 to 25.1 deg.	
Index ranges	$-31 \leq h \leq 31$, $-12 \leq k \leq 12$, $-19 \leq l \leq 19$	
Reflections collected	20865	
Independent reflections	4020 (R(int) = 0.1105)	
Observed reflections	2500 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.96 and 0.83
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4020 / 0 / 264
Goodness-of-fit on F^2	1.04
Final R indices (I>2sigma(I))	R1 = 0.055, wR2 = 0.121
Largest diff. peak and hole	0.67 and -0.79 eÅ^{-3}

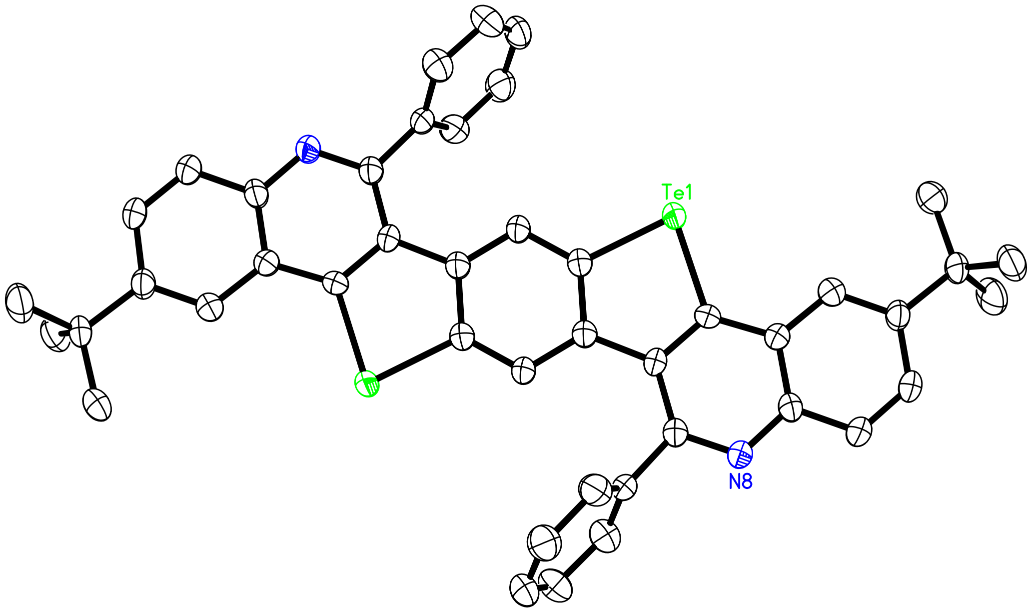
Table S9. Crystal structure, crystal data and structure refinement of **10cc** (CCDC 2380045).



Empirical formula	$C_{60}H_{68}N_2Se_2$
Formula weight	975.08
Temperature	200(2) K
Wavelength	1.54178 Å
Crystal system	monoclinic

Space group	$P2_1/c$	
Z	2	
Unit cell dimensions	a = 17.8271(8) Å	α = 90 deg.
	b = 4.9029(2) Å	β = 98.823(3) deg.
	c = 28.5940(12) Å	γ = 90 deg.
Volume	2469.67(18) $Å^3$	
Density (calculated)	1.31 g/cm^3	
Absorption coefficient	2.17 mm^{-1}	
Crystal shape	column	
Crystal size	0.264 x 0.016 x 0.014 mm^3	
Crystal colour	pale brown	
Theta range for data collection	2.5 to 61.1 deg.	
Index ranges	$-19 \leq h \leq 19$, $-5 \leq k \leq 4$, $-23 \leq l \leq 32$	
Reflections collected	17278	
Independent reflections	3681 (R(int) = 0.0683)	
Observed reflections	2286 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.97 and 0.83	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3681 / 0 / 291	
Goodness-of-fit on F^2	0.89	
Final R indices (I>2sigma(I))	R1 = 0.040, wR2 = 0.077	
Largest diff. peak and hole	0.36 and -0.33 $eÅ^{-3}$	

Table S10. Crystal structure, crystal data and structure refinement of **11ba** (CCDC 2380046).



Empirical formula	$C_{44}H_{36}N_2Te_2$	
Formula weight	847.95	
Temperature	200(2) K	
Wavelength	1.54178 Å	
Crystal system	triclinic	
Space group	P $\bar{1}$	
Z	1	
Unit cell dimensions	a = 5.7584(2) Å	α = 77.226(3) deg.
	b = 11.4517(5) Å	β = 88.956(3) deg.
	c = 14.1958(5) Å	γ = 77.594(3) deg.
Volume	891.21(6) $Å^3$	
Density (calculated)	1.58 g/cm^3	
Absorption coefficient	13.16 mm^{-1}	
Crystal shape	plate	
Crystal size	0.066 x 0.044 x 0.010 mm^3	
Crystal colour	yellow	
Theta range for data collection	3.2 to 68.4 deg.	
Index ranges	$-6 \leq h \leq 6$, $-12 \leq k \leq 13$, $-10 \leq l \leq 17$	
Reflections collected	10474	
Independent reflections	3156 (R(int) = 0.0216)	
Observed reflections	2828 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.68 and 0.54	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3156 / 0 / 220	
Goodness-of-fit on F^2	1.04	
Final R indices (I>2sigma(I))	R1 = 0.036, wR2 = 0.085	
Largest diff. peak and hole	1.99 and -0.67 $eÅ^{-3}$	

6 Computational Investigation

6.1 Computational Details

All quantum chemical calculations were performed using Orca 5.0.3.[8] The structures were optimized using the B3LYP/G[9,10] functional with the def2-TZVP[11,12] basis set, as used for the calculation of BBPQs, previously published.[13]

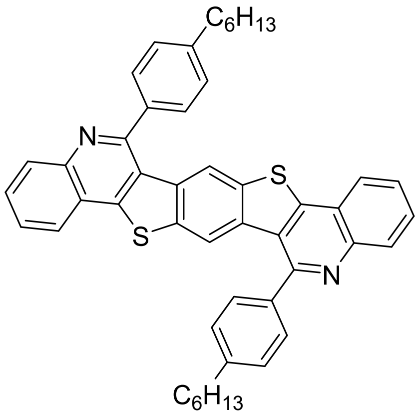
6.2 Overview of the Computed Molecules

Table S11. Energies of all computed structures.

Compound	$\mathbf{E_{HOMO}}$ **[eV]**	$\mathbf{E_{LUMO}}$ **[eV]**	$\mathbf{E_{g(calc)}}$ **[eV]**
9aa	-5.88	-2.00	3.88
9ab	-5.99	-2.11	3.88
9ac	-6.02	-2.17	3.85
9ba	-5.85	-1.97	3.88
9bb	-5.91	-2.04	3.86
9bc	-6.00	-2.14	3.86
9bd	-5.95	-2.11	3.84
9be	-5.84	-1.98	3.87
9bf	-5.77	-2.14	3.63
9bg	-5.93	-2.05	3.88
9ca	-5.92	-2.04	3.88
9cb	-5.96	-2.07	3.89
9cc	-5.92	-2.09	3.83
9cd	-5.94	-2.11	3.83
9ce	-5.92	-2.07	3.85
10aa	-5.94	-2.13	3.81
10ab	-5.92	-2.15	3.77
10ba	-5.87	-2.11	3.77
10bb	-5.84	-2.08	3.77
10bc	-5.93	-2.17	3.76
10bd	-5.90	-2.14	3.76
10be	-5.86	-2.07	3.79
10ca	-5.87	-2.11	3.75
10cb	-5.89	-2.16	3.73
10cc	-5.85	-2.10	3.75
11ba	-5.66	-2.14	3.52

6.3 Coordinates of the Optimized Geometries

9aa



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6	3.803184000	2.946474000	-0.581982000
6	4.088940000	4.348576000	-0.630002000
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1	0.116031000	1.728375000	-0.529356000
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6	5.160076000	6.461717000	-0.774450000
16	3.479939000	6.902439000	-0.553879000
6	6.634838000	4.572229000	-1.050848000
6	6.191444000	7.370375000	-0.932390000
6	7.666222000	5.480875000	-1.208741000

6	7.479746000	6.887732000	-1.168444000
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1	6.830105000	3.513689000	-1.100177000
16	9.346398000	5.040168000	-1.428911000
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6	13.704693000	8.314138000	-1.585875000
1	14.700598000	8.737089000	-1.605392000
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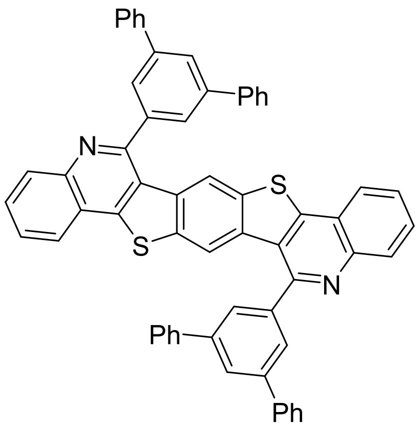

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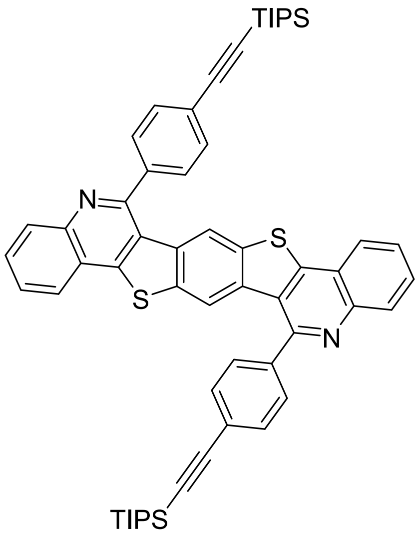

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C	2.02294763487918	1.00022024044044	-3.35358897433908
C	2.95268282789622	1.92278549396844	-2.80558270330994
C	2.57904397495841	3.30222394396631	-2.71527710202161
N	4.15241281102908	1.45661688001329	-2.36117848877608
C	5.04189104140281	2.27959306481935	-1.84729788095817
C	4.83448268572804	3.70371003094353	-1.80865376050915
C	3.57688296966925	4.17825699146367	-2.21029162859444
H	-0.57540629942698	3.10784091647616	-4.01732833290129
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C	5.73789753518316	4.79537137147973	-1.45791226432418
C	5.07999802380514	6.05936819513630	-1.53260981254331
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C	5.71075697916057	7.26515885295181	-1.24352420298380

C	7.74122160924709	5.99174694423846	-0.87375642649494
C	7.06413947672554	7.24771423121096	-0.87154484776613
H	5.16472631332623	8.20197142712451	-1.32547448429208
H	7.67391765998691	3.85654752332167	-1.14925378412805
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C	7.97294250589731	8.34166872421374	-0.54257591937545
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C	11.72781324554866	8.42372136536994	-0.05443856374037
C	12.70711839781470	9.38725127630185	0.08320357163915
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H	13.14935628116374	11.51272475206175	0.19171076829896
H	10.75289540844440	12.20405729561670	-0.03976510006302
H	11.99394122413991	7.36387255566130	-0.06188860930954
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C	6.96356481689348	0.68164153337134	-2.02397600702326
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C	8.52894379404177	0.35747328428703	-0.18989963866308
C	7.79646268159326	1.29174006480899	0.57182728175890
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H	6.61385272357788	0.43636614576963	-3.02805267962692
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C	5.40062113147995	9.82164007030030	0.53439213159798
C	6.05034916190376	11.45758853000373	-1.12221598695538

C	4.13696997726067	10.39762651493441	0.61538697408950
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H	6.81506951498092	11.87569700813031	-1.77869624164620
H	5.64480035746667	8.96439015082354	1.16488249865273
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C	2.50013064183575	12.08369596586047	-0.12592156314882
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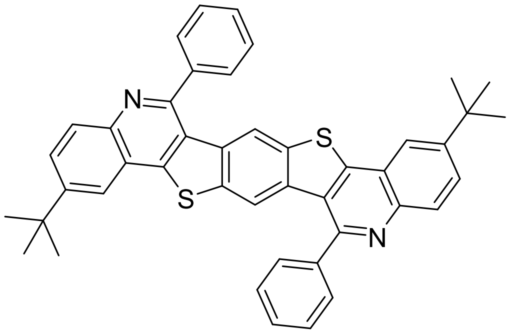

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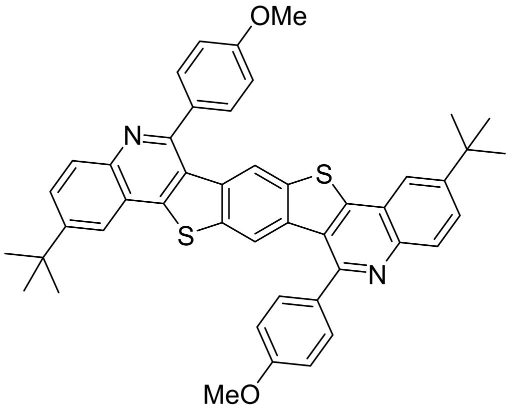

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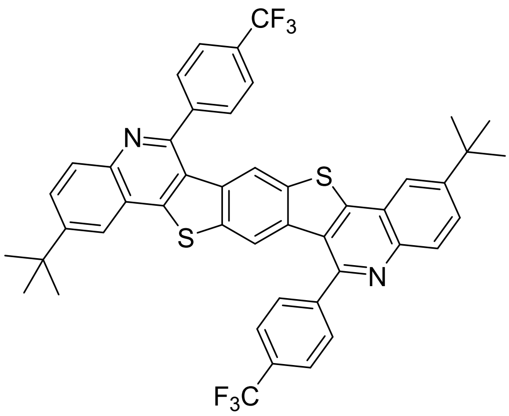

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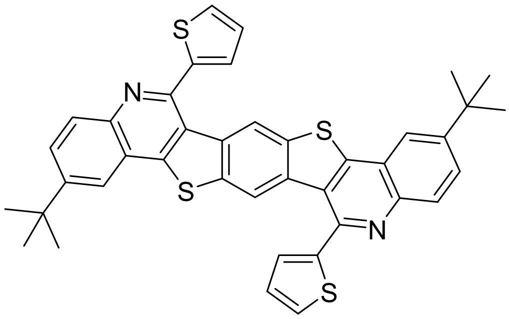

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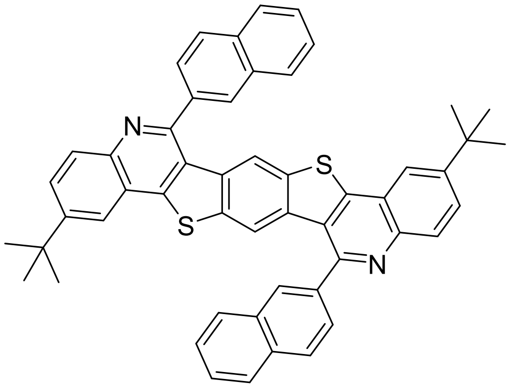

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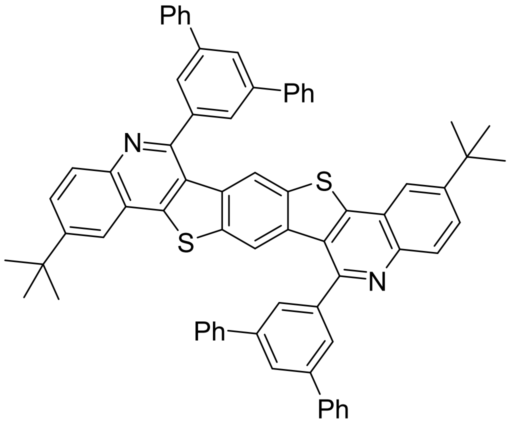

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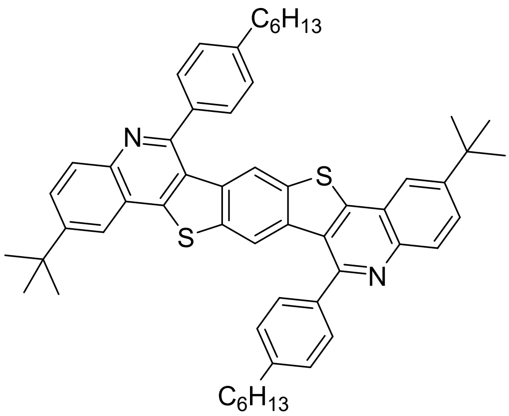

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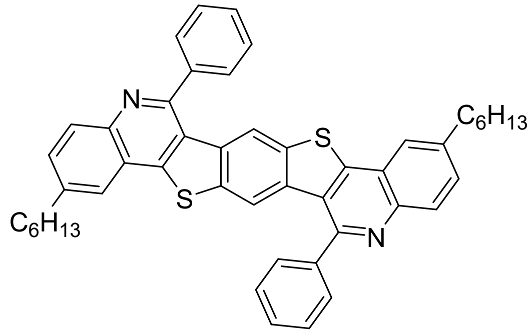

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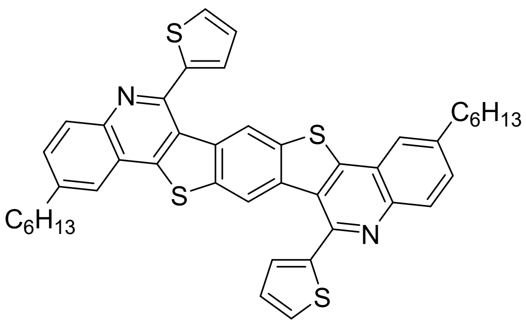

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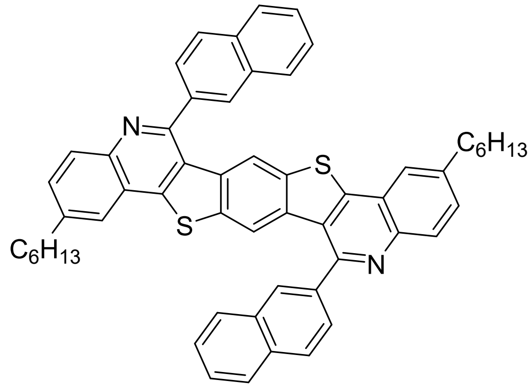

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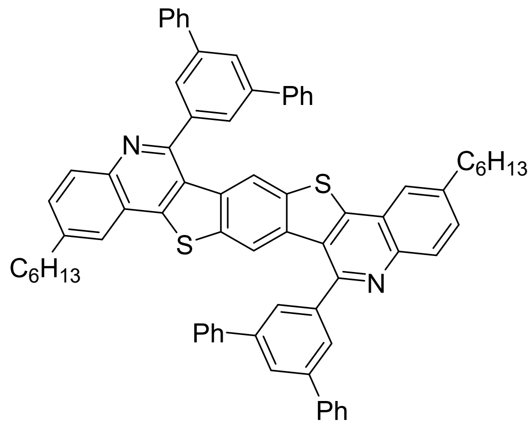

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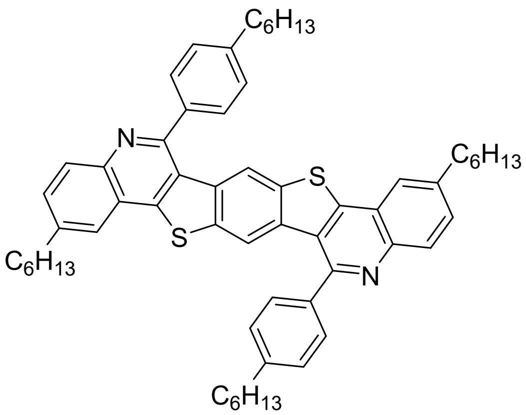

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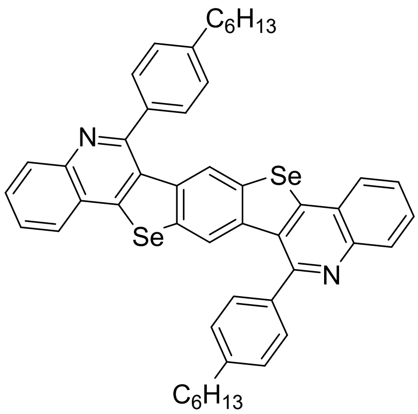

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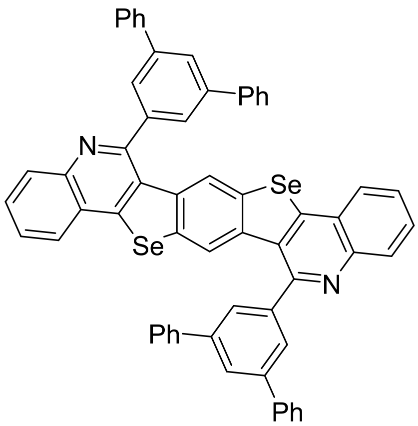

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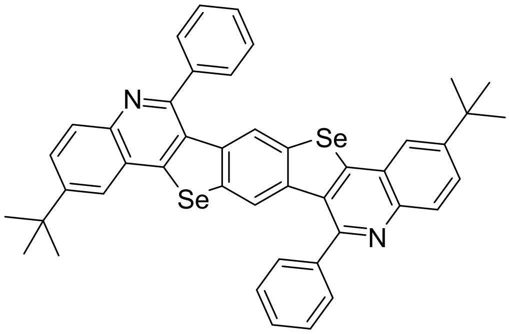

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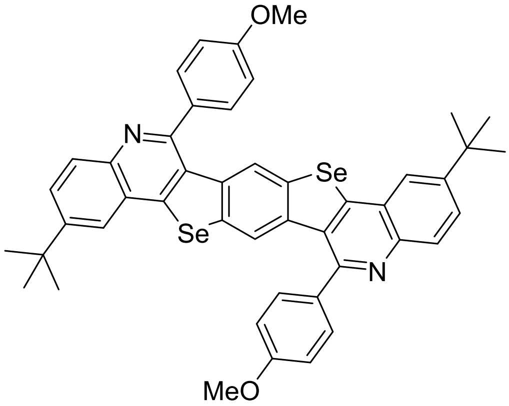

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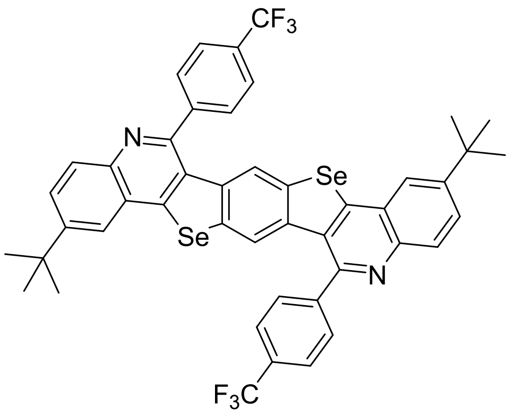

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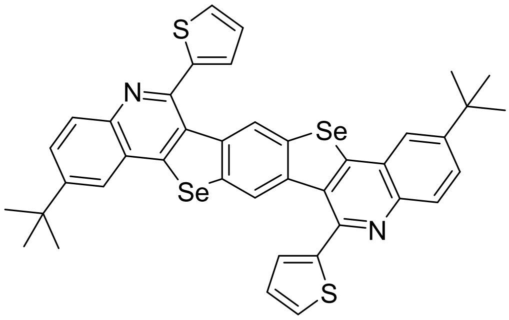

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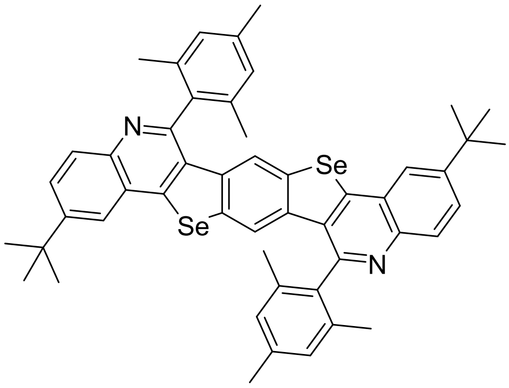

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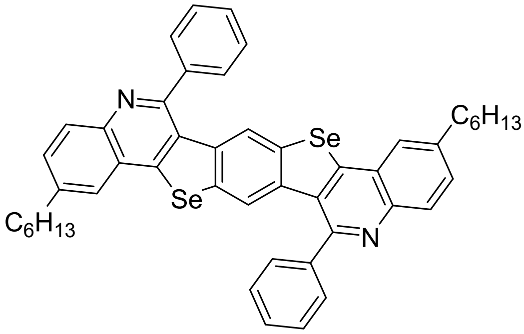

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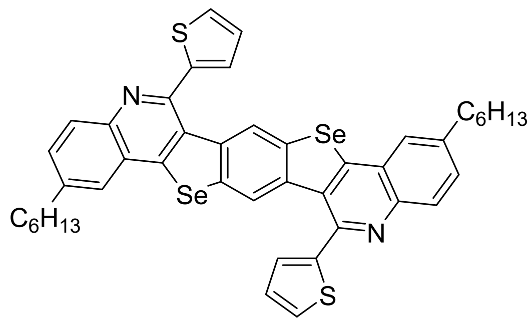

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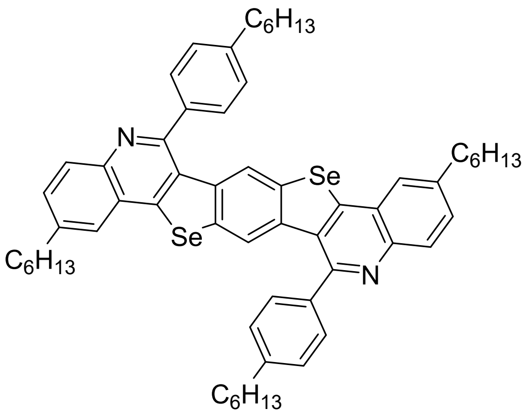

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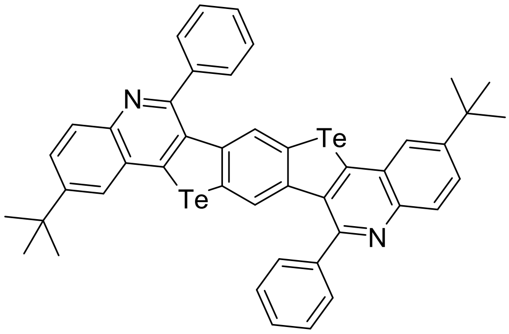

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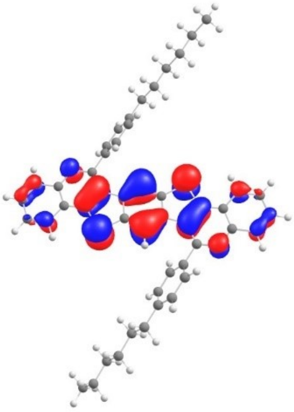
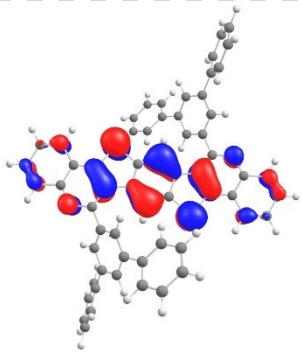
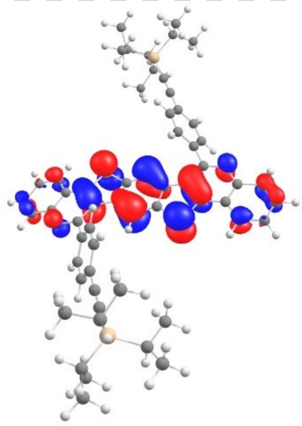
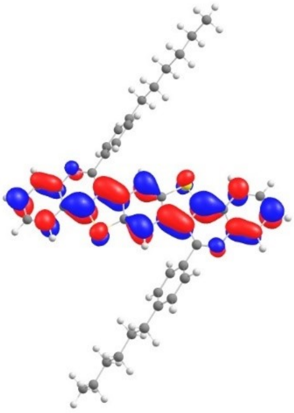
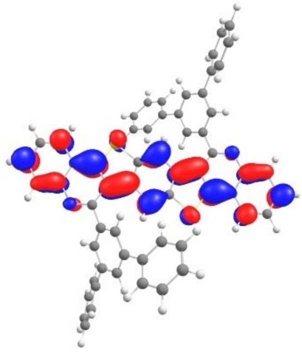
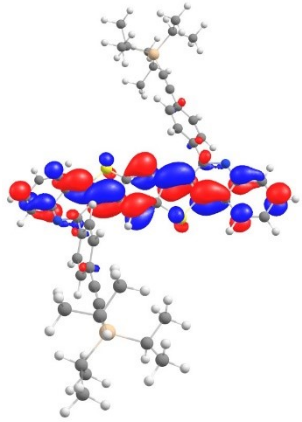
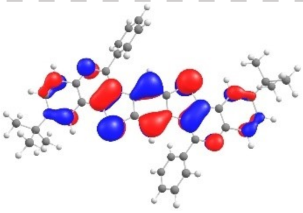
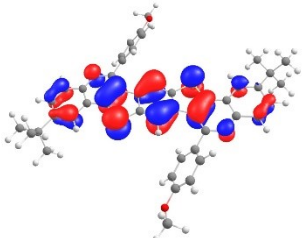
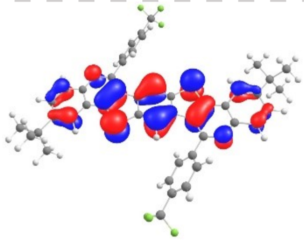
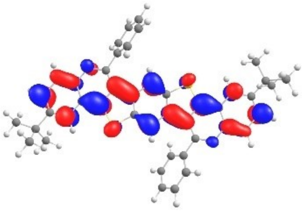
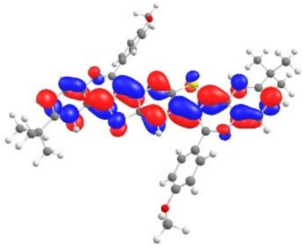
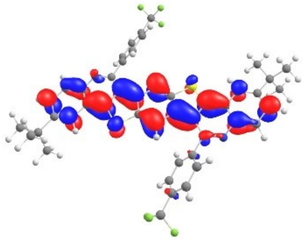
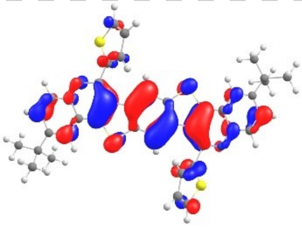
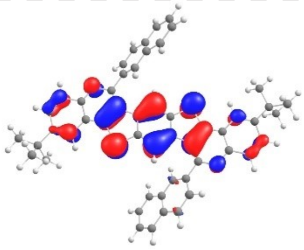
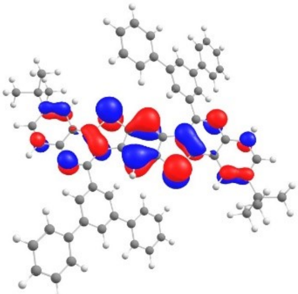
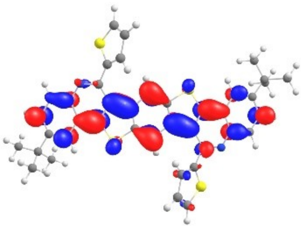
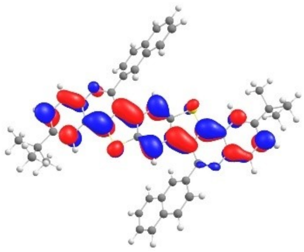
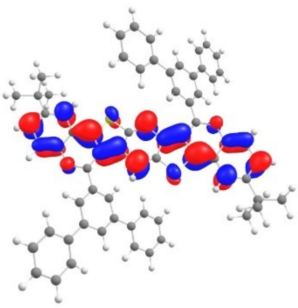
6	8.788380000	7.772503000	-1.192615000
6	8.984536000	9.205678000	-1.254766000
6	11.237132000	7.562492000	-1.330218000
6	11.294663000	8.988136000	-1.235254000
7	10.176231000	9.760970000	-1.228524000
6	12.568471000	9.605508000	-1.194259000
6	12.442854000	6.826611000	-1.406407000
6	13.688316000	7.436785000	-1.372897000
6	13.724757000	8.853975000	-1.259018000
1	14.683435000	9.370129000	-1.227103000
1	12.598455000	10.694083000	-1.121207000
1	12.376301000	5.737974000	-1.481374000
6	4.867848000	2.274401000	-0.215521000
6	5.023816000	1.195315000	-1.096156000
6	5.751109000	2.406125000	0.867867000
6	6.070103000	0.286562000	-0.921476000
6	6.957278000	0.434373000	0.148754000
6	6.788753000	1.491332000	1.049578000
6	7.851230000	10.161736000	-1.424969000
6	6.966982000	10.033439000	-2.507927000
6	7.693604000	11.235545000	-0.538274000
6	5.926707000	10.946474000	-2.683378000
6	5.756474000	11.998016000	-1.776551000
6	6.644627000	12.142412000	-0.706671000
1	5.626903000	3.239179000	1.563130000
1	4.316617000	1.079920000	-1.919526000
1	7.092246000	9.204258000	-3.207625000
1	8.401391000	11.348242000	0.284975000
1	7.468966000	1.603364000	1.897189000
1	6.191201000	-0.543335000	-1.621945000

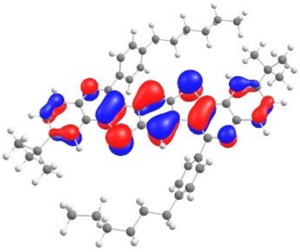
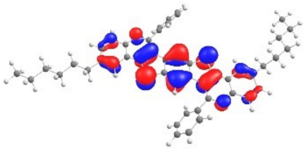
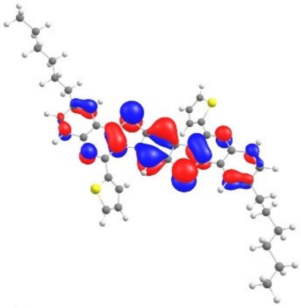
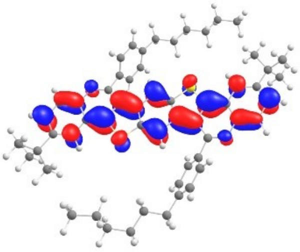
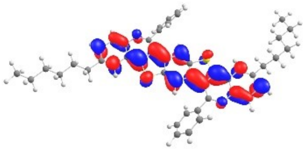
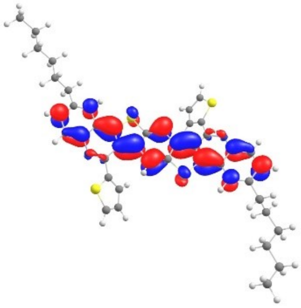
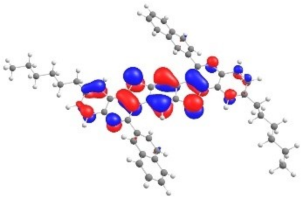
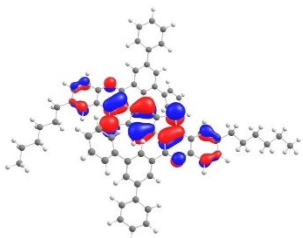
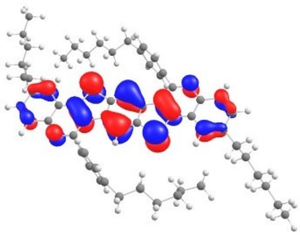
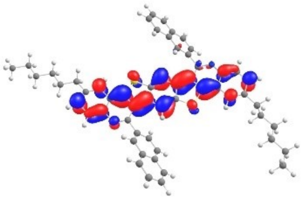
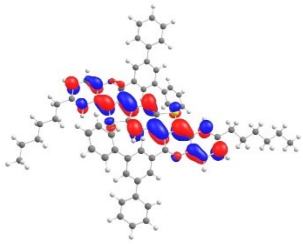
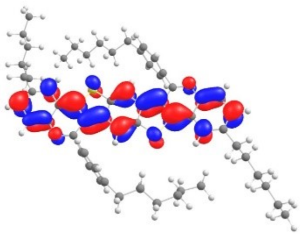
1	6.522140000	12.968099000	-0.001486000
1	5.245608000	10.837147000	-3.530625000
1	7.774499000	-0.277800000	0.286221000
1	4.937079000	12.708635000	-1.909003000
6	-2.280625000	5.792001000	-0.237253000
6	-3.094668000	5.522785000	-1.520807000
1	-4.048104000	6.074478000	-1.492135000
1	-3.330205000	4.454904000	-1.640919000
1	-2.536771000	5.846736000	-2.413165000
6	-2.048633000	7.305974000	-0.119975000
1	-1.489744000	7.563786000	0.792797000
1	-3.016457000	7.828355000	-0.075370000
1	-1.496816000	7.702772000	-0.986024000
6	-3.087118000	5.326747000	0.993982000
1	-3.321153000	4.252735000	0.949197000
1	-4.041054000	5.874835000	1.056050000
1	-2.524498000	5.510005000	1.922597000
6	14.962491000	6.579687000	-1.452032000
6	14.956500000	5.778916000	-2.771382000
1	14.086738000	5.108490000	-2.838317000
1	15.864455000	5.159203000	-2.848540000
1	14.926844000	6.454535000	-3.640335000
6	14.992555000	5.603692000	-0.256647000
1	14.122745000	4.929950000	-0.258271000
1	14.989867000	6.152523000	0.697934000
1	15.900553000	4.980214000	-0.292236000
6	16.240207000	7.432417000	-1.411298000
1	16.288898000	8.137518000	-2.255262000
1	17.123755000	6.778782000	-1.473344000
1	16.319010000	8.008232000	-0.476424000

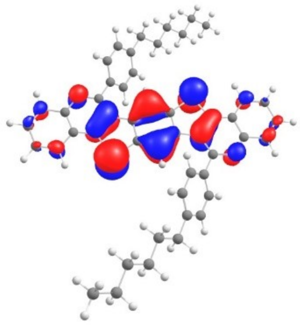
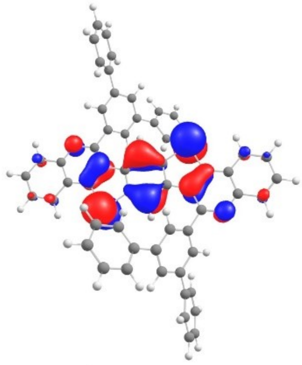
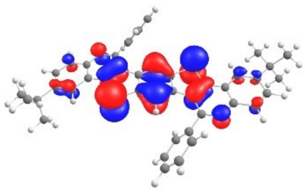
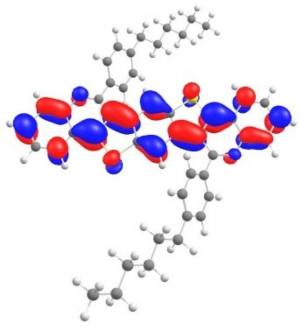
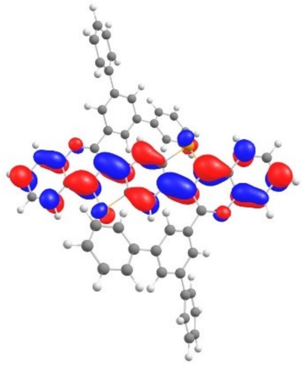
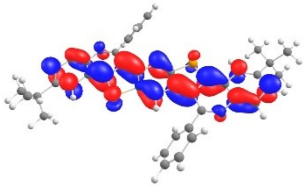
6.4 Visualization of the Frontier Molecular Orbitals

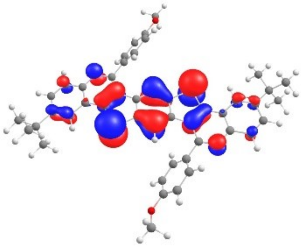
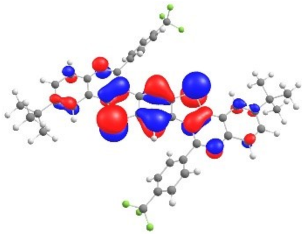
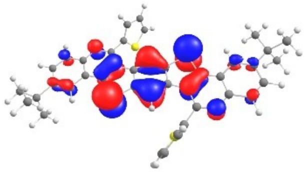
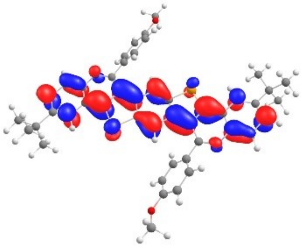
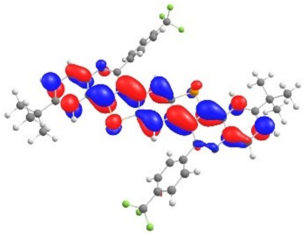
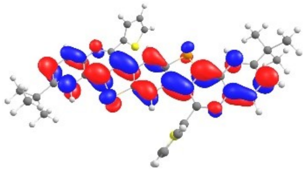
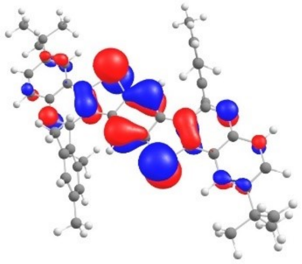
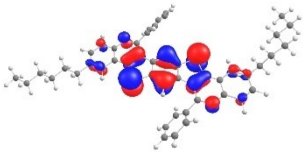
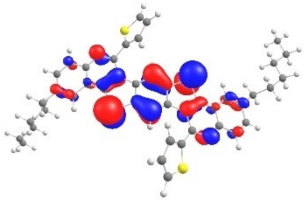
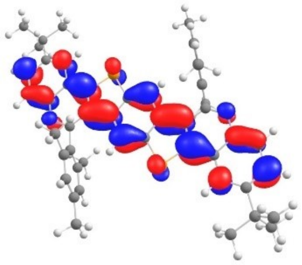
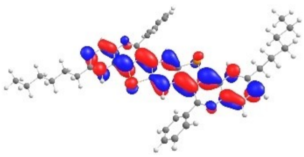
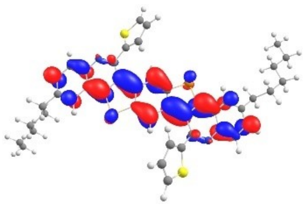
Table S12. Visualization of the HOMO and LUMO Orbitals of **9-11**.

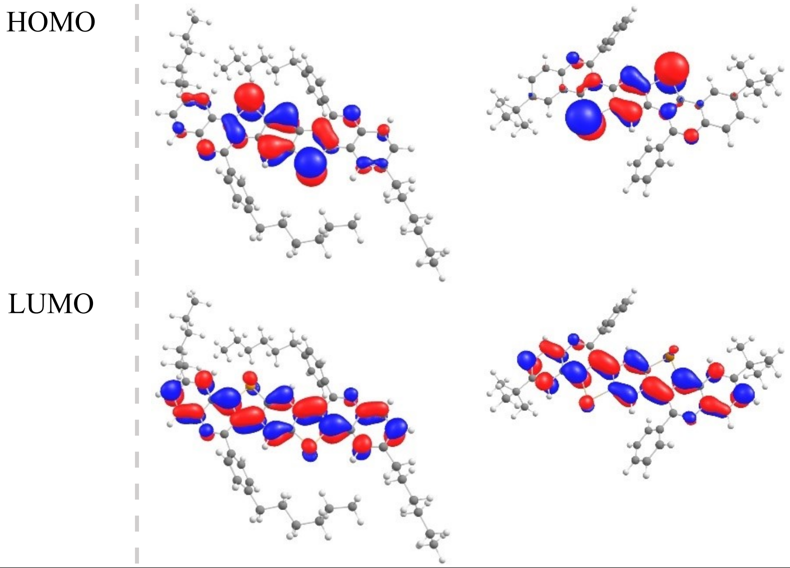
Compound	**9aa**	**9ab**	**9ac**
HOMO			
LUMO			
Compound	**9ba**	**9bb**	**9bc**
HOMO			
LUMO			
Compound	**9bd**	**9be**	**9bf**

HOMO			
LUMO			
Compound	**9bg**	**9ca**	**9cb**

HOMO			
LUMO			
Compound	**9cc**	**9cd**	**9ce**
HOMO			
LUMO			
Compound	**10aa**	**10ab**	**10ba**

HOMO			
LUMO			
Compound	**10bb**	**10bc**	**10bd**

HOMO			
LUMO			
Compound	**10be**	**10ca**	**10cb**
HOMO			
LUMO			
Compound	**10cc**	**11ba**	


HOMO
LUMO

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