Materials and Measurements

All reactions and operations were carried out under argon (Ar) atmosphere with the use of standard Schlenk techniques. All chemicals, unless otherwise specified, were purchased from Adamas, Innochem or other commercial resources and used as received. Triethylnmine and dichloromethane were purified by distillation with calcium hydride. TII-diBr and N-hexylthiophen-3-amine were synthesized according to previously reported procedures.[1-3]

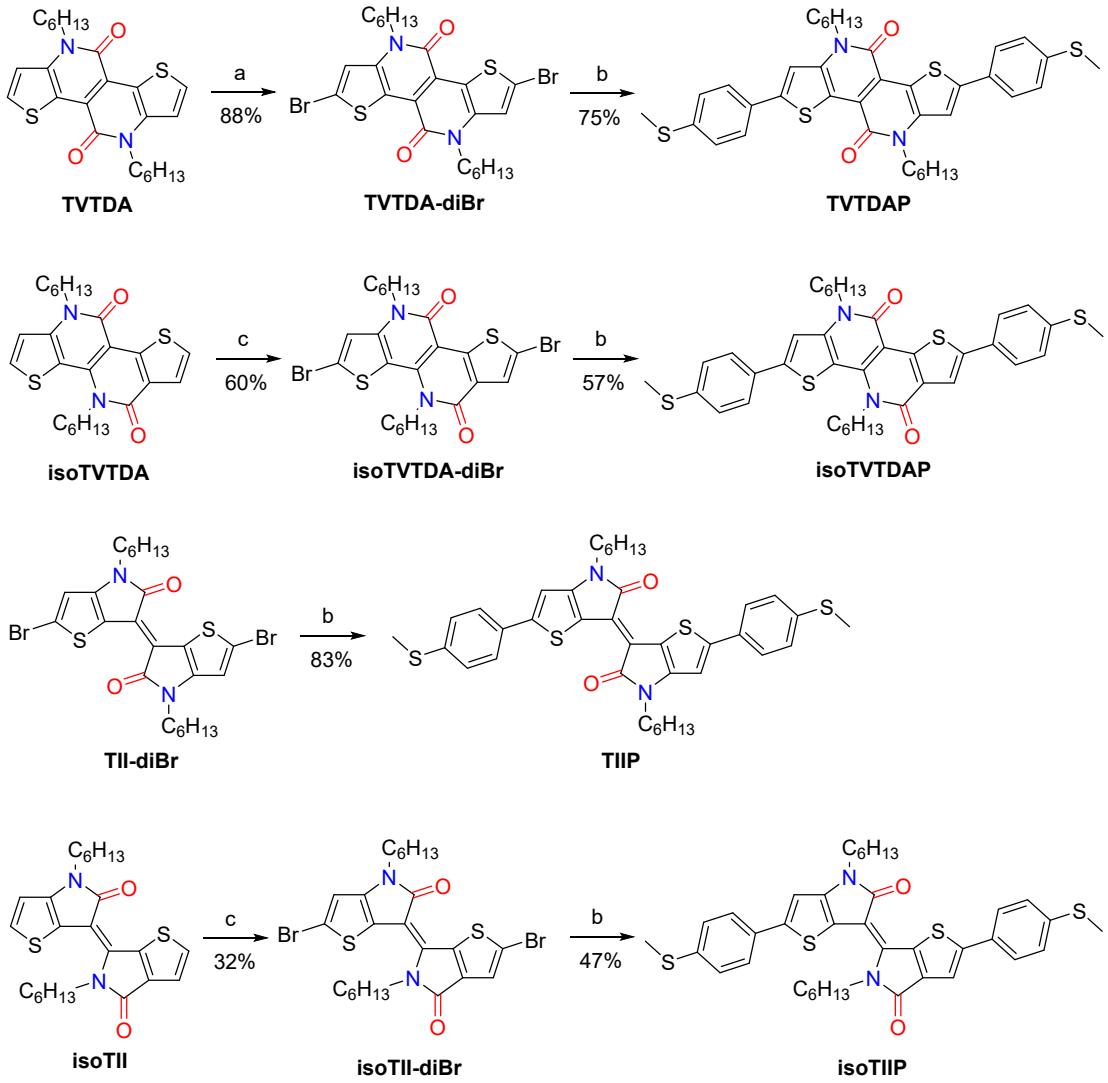
The ^{1}H and ^{13}C NMR spectra were collected on a Bruker AVANCE III HD 400 spectrometer operating at 400 MHz in deuterated chloroform solution with TMS as reference, respectively. High-resolution mass spectroscopy (HRMS) measurements were performed on a Shimadzu LCMS-IT-TOF. UV-vis spectra was measured using a Shimadzu UV-3600 spectrophotometer. Cyclic voltammetry (CV) was conducted using a CHI 760E Electrochemical Analyzer with a standard three-electrode system consisting of Pt disk working electrode, Ag/AgCl reference electrode and Pt wire counter electrode, calibrated against ferrocene. A solution of 0.1 M Bu_4NPF_6 in dichloromethane was used as the electrolyte. The scan rate was 100 mV s^{-1}. HOMO and LUMO energy levels were calculated from the equations: $E_{LUMO} = -(E_{red} - E_{Fc} + 4.8)$ eV and $E_{HOMO} = -(E_{ox} - E_{Fc} + 4.8)$ eV, where E_{red} and E_{ox} are taken from the onset of reduction and oxidation, respectively, and E_{Fc} is the half-wave potential of ferrocene.

Single-molecule conductance measurement: In the Faraday electrostatic shield box, a piece of gold wire (0.25 mm in diameter) with one end burned into a bead was used as a tip, which was fixed on the piezo, while the piezo adhered to the bottom of the stepping motor. A gold-plated silicon wafer washed by piranha was placed below the tip. Then, a small amount of 1,2,4-trichlorobenzene solution containing 0.1 M target molecule was dripped on the substrate, and the tip was also immersed in the solution. In the text, both the tip and the substrate were connected with the external current amplifier and the controller, and a 100 mV bias voltage was applied between them. Using the current between the two electrodes as feedback, the tip was controlled to pull up and down to repeatedly contact/leave the substrate. Single-molecule junctions can be formed during the break junction process so that the single-molecule conductance can be detected.

Theoretical calculations: The geometries of target molecules were optimized by density functional theory (DFT) at the B3LYP/6-31G* level using the Gaussian 09 package and the frontier molecular orbitals (HOMO and LUMO) were calculated. Hexyl side chains in the molecules were replaced by methyl group to simplify the calculations. The transmission spectra of target molecules were obtained by using DFT combined with the none-quilibrium Green's function (NEGF) method as implemented in the Atomistix ToolKit 13.8.0. software package.[4] The optimized target molecule was introduced into the two electrodes to fabricate the gold-molecule-gold model. The initial Au-S distance was 2.65 Å and the adsorption configuration was "top" site of Au

(111) surface. Finally, the geometry of entire scattering region was relaxed until all residual forces on each atom are less than 0.05 eV/Å. The Perdew-Burke-Ernzerhof (PBE) formulation of the generalized gradient approximation (GGA) is adopted as the exchange correlation functional. Single-zeta plus polarization (SZP) basis set was for Au atoms and double-zeta plus polarization (DZP) basis set was for the other atoms. The transmission probability through the single-molecule junction as a function of the applied external bias can be obtained from the Landauer-Büttiker Equation.

Flicker noise measurements: For the conductance noise measurement, the tip is controlled to stabilize for 150 ms after leaving the substrate surface and when the molecular junction is formed. To get the noise power density spectra (PSD), we cut out the conductance feature to perform discrete Fourier transformation, and the data is squared. Then the PSD is integrated from 100 to 1000 Hz. 2D histogram of normalized flicker noise power versus average conductance is constructed from thousands of conductance traces. The 2D Gaussian distribution fitting is applied to determine the scaling power. The conductance power is normalized from $G^{1.0}$ and $G^{2.0}$, and the correlation power is determined by the correlation coefficient, which shows the smallest absolute value in their fitted Gaussian distribution equations.



Scheme S1. The synthetic route of TVTDAP, isoTVTDAP, TIIP and isoTIIP. Conditions: (a) NBS, $CHCl_3$, room temperature; (b) (4-(methylthio)phenyl)boronic acid, $Pd(PPh_3)_4$, Na_2CO_3, 1,4-dioxane/H_2O, 85 °C; (c) Br_2, $FeCl_3$, CH_2Cl_2, room temperature.

Synthesis of methyl 4-hexyl-5-oxo-4,5-dihydrothieno[3,2-b]pyridine-7-carboxylate (TAE)

To a solution of N-hexylthiophen-3-amine (23.5 g, 128 mmol) in tetrahydrofuran (200 mL) was added dimethyl acetylenedicarboxylate (23.64 mL, 193 mmol), and the reaction mixture was heated to 70 °C for 28 hours. After removal of the solvent in vacuo, the crude product was purified through a silica gel column with a mixture of petroleum/ ethyl acetate (8:1) as eluent to give a white solid (17.6 g, 46%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.72 (d, J = 5.6 Hz, 1H), 7.26 (s, 1H), 7.07 (d, J = 5.6 Hz, 1H), 4.28-4.18 (t, 2H), 4.00 (s, 3H), 1.81-1.69 (m, 2H), 1.49-1.23 (m, 6H), 0.94-0.83 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 165.0, 144.5, 133.9, 132.9, 119.7, 166.0, 115.5, 99.9, 53.1, 45.7, 31.5, 28.1, 26.6, 22.5, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{15}H_{19}NO_3S$, 316.0978; found, 316.0944.

Synthesis of 4-hexyl-5-oxo-4,5-dihydrothieno[3,2-b]pyridine-7-carboxylic acid (TAAc)

To a solution of TAE (10.0 g, 34.1 mmol) in ethanol (200 mL) and water (20 mL) was added NaOH (1.64 g, 40.9 mmol), and the reaction mixture was stirred for 12 h at room temperature. The reaction mixture was then acidified with 1 M HCl, extracted with CH_2Cl_2 and washed with brine. The combined organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was washed with hexane to give a white solid (9.22 g, 97%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.82 (d, *J* = 5.5 Hz, 1H), 7.57 (s, 1H), 7.15 (d, *J* = 5.6 Hz, 1H), 4.39 (t, 2H), 1.83 (m, 2H), 1.55-1.21 (m, 6H), 0.97-0.78 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 166.0, 163.8, 144.0, 136.7, 134.7, 119.1, 117.2, 115.3, 46.5, 31.5, 28.1, 26.6, 22.5, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{14}H_{17}NO_3S$, 280.1002; found, 280.0995.

Synthesis of N,4-dihexyl-5-oxo-N-(thiophen-3-yl)-4,5-dihydrothieno[3,2-b]pyridine-7-carboxamide (TAA)

To a solution of TAAc (9.22 g, 33.0 mmol) in $CHCl_3$ (80 mL) were added oxalyl chloride (5.76 mL, 66.0 mmol) and 3 drops of DMF. The mixture was stirred for 2 hours at room temperature. The solvent was removed under vacuum to obtain chloride, which was used in next step without purification. To the solution of N-hexylthiophen-3-amine (7.26 g, 39.6 mmol) and dry triethylnmine (5.49 mL) in dry CH_2Cl_2 (40 mL) at 0 °C was slowly added a solution of chloride in dry CH_2Cl_2 (60 mL). The mixture was stirred at room temperature overnight. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (2:1) as eluent to give a brown solid (14.6 g, 99%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.64 (d, *J* = 5.5 Hz, 1H), 7.20 (dd, *J* = 5.1, 3.1 Hz, 1H), 7.00 (d, *J* = 5.6 Hz, 1H), 6.88 (d, *J* = 20.9 Hz, 2H), 6.25 (s, 1H), 4.18-4.07 (t, 2H), 3.85 (t, 2H), 1.75-1.57 (m, 4H), 1.43-1.23 (m, 12H), 0.95-0.81 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 166.1, 161.4, 143.9, 140.5, 139.8, 131.1, 126.2, 125.4, 120.2, 116.5, 116.1, 115.9, 49.8, 45.2, 31.4, 31.4, 27.9, 26.5, 26.4, 22.5, 22.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{24}H_{32}N_2O_2S_2$, 467.1797; found, 467.1768.

Synthesis of 5,10-dihexyl-5,10-dihydrodithieno[3,2-c:3',2'-h][2,6]naphthyridine-4,9-dione (TVTDA)

To a solution of TAA (14.6 g, 32.9 mmol) in chloroform (150 mL) was added N-bromosuccinimide (5.86 g, 32.9 mmol), and the reaction mixture was stirred for 24 hours at room temperature. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a flash silica gel column with a mixture of petroleum/ethyl acetate (3:1) as eluent to give brown solid. To a solution of the solid in dry acetonitrile (330 mL) were added in portions triphenylphosphine (1.73 g, 6.58 mmol), palladium (II) acetate (739 mg, 3.29 mmol) and dry triethylnmine (9.12

mL, 65.8 mmol). The mixture was refluxed for 8 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2/ethyl acetate (20:10:1) as eluent and then recrystallized from chloroform/methanol to give a yellow solid (13.8 g, 95%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.75 (d, *J* = 5.6 Hz, 2H), 7.20 (d, *J* = 5.6 Hz, 2H), 4.47-4.38 (t, 4H), 1.87 (m, 4H), 1.49 (m, 4H), 1.40-1.30 (m, 8H), 0.90 (t, 6H). ^{13}C NMR (101 MHz, Chloroform-d): δ 159.4, 139.8, 131.3, 122.5, 116.1, 115.0, 46.2, 31.5, 28.1, 26.7, 22.5, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{24}H_{30}N_2O_2S_2$, 465.1641; found, 465.1627.

Synthesis of 2,7-dibromo-5,10-dihexyl-5,10-dihydrodithieno[3,2-c:3',2'-h][2,6]naphthyridine-4,9-dione (TVTDA-diBr)

To a solution of TVTDA (2.63 g, 5.94 mmol) in chloroform (40 mL) was added N-bromosuccinimide (2.33 g, 13.1 mmol), and the reaction mixture was stirred at room temperature overnight. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was recrystallized from CH_2Cl_2/methanol to give a yellow green solid (3.14 g, 88%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.16 (s, 2H), 4.36-4.26 (t, 4H), 1.81 (m, 4H), 1.51-1.23 (m, 12H), 0.95-0.86 (t, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 158.7, 138.9, 121.6, 121.3, 118.0, 117.0, 46.3, 31.5, 28.1, 26.7, 22.6, 14.01. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{24}H_{28}Br_2N_2O_2S_2$, 599.0032; found, 599.0040.

Synthesis of 5,10-dihexyl-2,7-bis(4-(methylthio)phenyl)-5,10-dihydrodithieno[3,2-c:3',2'-h][2,6]naphthyridine-4,9-dione (TVTDAP)

To a solution of TVTDA-diBr (101 mg, 0.168 mmol), (4-(methylthio)phenyl)boronic acid (71 mg, 0.421 mmol) and anhydrous sodium carbonate (90 mg, 0.850 mmol) in a mixture of 1,4-dioxane (10 mL) and water (1 mL) was added $Pd(PPh_3)_4$ (19 mg, 16.8 μmol). The mixture was heated to 85 °C for 20 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2 (1:1.5) as eluent and then recrystallized from chloroform/methanol to give a red solid (87 mg, 75%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.65 (d, *J* = 8.5 Hz, 4H), 7.28 (d, *J* = 8.5 Hz, 4H), 7.26 (s, 2H), 4.42 (t, 4H), 2.54 (s, 6H), 1.92-1.85 (m, 4H), 1.54-1.46 (m, 4H), 1.41-1.33 (m, 8H), 0.91 (t, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 159.2, 148.0, 140.3, 139.6, 130.4, 126.5, 126.1, 121.8, 115.7, 110.0, 46.2, 31.5, 28.1, 26.8, 22.6, 15.4, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{38}H_{42}N_2O_2S_4$, 687.2202; found, 687.2231.

Synthesis of tert-butyl (4-hexyl-5-oxo-4,5-dihydrothieno[3,2-b]pyridin-7-yl)carbamate (TA-Boc)

To a solution of TAAc (1.08 g, 3.86 mmol) and dry triethylamine (1.07 mL, 7.72 mmol) in dry tert-butyl alcohol (20 mL) was added diphenylphosphoryl azide (0.92 mL, 4.25 mmol), and the reaction mixture was heated to 80 °C for 17 hours. After cooling to room temperature, the mixture was poured into water and extracted with ethyl acetate three times and washed with Na_2CO_3. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (5:1) as eluent to give a white solid (1.15 g, 85%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.52 (d, *J* = 5.4 Hz, 1H), 7.14 (s, 1H), 7.05 (d, *J* = 5.4 Hz, 1H), 6.45 (s, 1H), 4.15 (t, 2H), 1.71 (m, 2H), 1.54 (s, 9H), 1.45-1.23 (m, 6H), 0.87 (t, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 163.2, 151.3, 143.5, 141.4, 127.3, 117.2, 111.6, 102.5, 82.4, 44.9, 31.5, 28.3, 28.1, 26.6, 22.5, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{18}H_{26}N_2O_3S$, 351.1737; found, 351.1744.

Synthesis of tert-butyl hexyl(4-hexyl-5-oxo-4,5-dihydrothieno[3,2-b]pyridin-7-yl)carbamate (TA-Boc-H)

To a solution of TA-Boc (1.15 g, 3.29 mmol) in dry DMF (16 mL) was added NaH (263 mg, 6.58 mmol) at 0 °C. After stirring at room temperature for 30 min, 1-bromohexane (0.92 mL, 6.58 mmol) was added. The mixture was stirred at room temperature overnight. Then, the mixture was quenched with water at 0 °C, and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (6:1) as eluent to give a colorless oil (1.34 g, 94%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.57 (d, *J* = 5.5 Hz, 1H), 7.02 (d, *J* = 5.5 Hz, 1H), 6.41 (s, 1H), 4.18 (t, 2H), 3.63 (t, 2H), 1.79-1.72 (m, 2H), 1.59-1.50 (m, 2H), 1.40 (s, 9H), 1.37-1.20 (m, 12H), 0.86 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 163.1, 153.0, 147.4, 143.5, 129.4, 119.2, 116.2, 114.3, 81.3, 49.8, 45.3, 31.5, 31.4, 28.9, 28.2, 28.1, 26.6, 26.4, 22.5, 22.5, 14.0, 13.9. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{24}H_{38}N_2O_3S$, 435.2676; found, 435.2680.

Synthesis of 4-hexyl-7-(hexylamino)thieno[3,2-b]pyridin-5(4H)-one (TA-H)

To a solution of TA-Boc-H (1.34 g, 3.09 mmol) in $CHCl_3$ (14 mL) was added trifluoroacetic acid (7 mL), and the reaction mixture was stirred for 12 h at room temperature. Then, the mixture was neutralized with Na_2CO_3 at 0 °C, and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (3:1) as eluent to give a white solid (982 mg, 95%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.44 (d, *J* = 5.4 Hz, 1H), 7.01 (d, *J* = 5.4 Hz, 1H), 5.64 (s, 1H), 4.18-4.03 (m, 3H), 3.24-3.19 (m, 2H), 1.75-1.61 (m, 4H), 1.46-1.23 (m, 12H), 0.88 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 163.9, 149.2, 143.1, 126.3, 117.3, 111.1, 90.5, 44.4, 43.2, 31.6, 31.5, 28.8, 28.6, 26.7, 26.6, 22.5, 22.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{19}H_{30}N_2OS$, 335.2152; found, 335.2153.

Synthesis of 4,10-dihexyldithieno[3,2-c:3',2'-h][1,6]naphthyridine-5,9(4H,10H)-dione (isoTVTDA)

A solution of 2-bromothiophene-3-carboxylic acid (381 mg, 1.84 mmol) in thionyl chloride (10 mL) was refluxed for 6 hours. The solvent was removed under vacuum to obtain chloride, which was used in next step without purification. To the solution of TA-H (360 mg, 1.08 mmol) and diisopropylethylamine (1 mL) in dry CH_2Cl_2 (5 mL) at 0 °C was slowly added a solution of chloride in dry CH_2Cl_2 (10 mL). The mixture was stirred at room temperature overnight. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a flash silica gel column with a mixture of petroleum/ethyl acetate (4:1) as eluent to give a brown oil. To a solution of the oil in dry acetonitrile (10 mL) were added in portions triphenylphosphine (1.304 g, 4.97 mmol), palladium (II) acetate (253 mg, 1.13 mmol) and dry triethylnmine (1.57 mL, 11.3 mmol). The mixture was refluxed for 9 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (10:1) as eluent and then recrystallized from chloroform/methanol to give a light yellow solid (338 mg, 71%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.74 (d, *J* = 5.4 Hz, 2H), 7.49 (d, *J* = 5.4 Hz, 1H), 7.22 (d, *J* = 5.7 Hz, 1H), 4.73 (t, 2H), 4.37 (t, 2H), 1.96-1.88 (m, 2H), 1.86-1.79 (m, 2H), 1.57-1.53 (m, 2H), 1.52-1.43 (m, 2H), 1.43-1.29 (m, 8H), 0.93-0.88 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 159.2, 159.1, 144.5, 142.7, 140.0, 129.7, 128.4, 127.9, 124.0, 116.7, 109.2, 104.5, 45.8, 45.2, 31.5, 31.4, 29.4, 28.1, 26.7, 26.4, 22.6, 22.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{24}H_{30}N_2O_2S_2$, 443.1821; found, 443.1824.

Synthesis of 2,7-dibromo-4,10-dihexyldithieno[3,2-c:3',2'-h][1,6]naphthyridine-5,9(4H,10H)-dione (isoTVTDA-diBr)

To a solution of isoTVTDA (49 mg, 0.111 mmol) in dry CH_2Cl_2 (10 mL) was added slowly bromine (0.02 mL, 0.443 mmol), then iron trichloride (1 mg) was added to the reaction mixture. The mixture was stirred for 2 hours in the dark before saturated sodium sulfite solution was added and stirring continued for 0.5 h. The resulting mixture was extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2/ethyl acetate (2:1:0.2) as eluent to give a light yellow solid (40 mg, 60%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.63 (s, 1H), 7.19 (s, 1H), 4.54 (t, 2H), 4.26 (t, 2H), 1.92-1.81 (m, 2H), 1.81-1.72 (m, 2H), 1.57-1.51 (m, 2H), 1.49-1.43 (m, 2H), 1.38-1.35 (m, 8H), 0.94-0.89 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 158.5, 157.6, 145.5, 142.2, 139.2, 127.8, 126.1, 119.9, 119.8, 117.6, 110.0, 104.0, 45.9, 45.4, 31.5, 31.4, 29.4, 28.1, 26.6, 26.3, 22.6, 22.5, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{24}H_{28}Br_2N_2O_2S_2$, 599.0032; found, 599.0016.

Synthesis of 4,10-dihexyl-2,7-bis(4-(methylthio)phenyl)dithieno[3,2-c:3',2'-h][1,6]naphthyridine-5,9(4H,10H)-dione (isoTVTDAP)

To a solution of isoTVTDA-diBr (20 mg, 0.0333 mmol), (4-(methylthio)phenyl)boronic acid (22 mg, 0.133 mmol) and anhydrous sodium

carbonate (18 mg, 0.167 mmol) in a mixture of 1,4-dioxane (10 mL) and water (2 mL) was added $Pd(PPh_3)_4$ (4 mg, 3.33 μmol). The mixture was heated to 85 °C for 20 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2/ethyl acetate (2:1:0.05) as eluent and then recrystallized from chloroform/methanol to give a yellow solid (13 mg, 57%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.79 (s, 1H), 7.61 (d, *J* = 8.1 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 7.19 (s, 1H), 4.70 (t, 2H), 4.36 (t, 2H), 2.54 (s, 3H), 2.51 (s, 3H), 1.98-1.87 (m, 2H), 1.86-1.77 (m, 2H), 1.59-1.47 (m, 4H), 1.46-1.29 (m, 8H), 0.94-0.90 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 158.8, 158.8, 147.1, 145.1, 143.5, 143.2, 141.1, 139.6, 138.6, 130.6, 128.6, 128.5, 126.6, 126.4, 126.2, 126.2, 118.7, 111.3, 104.1, 45.8, 45.2, 31.5, 31.5, 29.5, 28.1, 26.7, 26.4, 22.6, 22.5, 15.6, 15.3, 14.1, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{38}H_{42}N_2O_2S_4$, 687.2202; found, 687.2184.

Synthesis of (E)-4,4'-dihexyl-2,2'-bis(4-(methylthio)phenyl)-[6,6'-bithieno[3,2-b]pyrrolylidene]-5,5'(4H,4'H)-dione (TIIP)

To a solution of TII-diBr (57 mg, 0.0949 mmol), (4-(methylthio)phenyl)boronic acid (64 mg, 0.380 mmol) and anhydrous sodium carbonate (50 mg, 0.475 mmol) in a mixture of 1,4-dioxane (10 mL) and water (2 mL) was added $Pd(PPh_3)_4$ (11 mg, 9.49 μmol). The mixture was heated to 85 °C for 18 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2 (1:1) as eluent and then recrystallized from chloroform/methanol to give a black green solid (54 mg, 83%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.61 (d, *J* = 8.5 Hz, 4H), 7.23 (d, *J* = 8.5 Hz, 4H), 6.94 (s, 2H), 3.80 (t, 4H), 2.52 (s, 6H), 1.77-1.70 (m, 4H), 1.45-1.24 (m, 12H), 0.88 (t, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 170.8, 151.9, 151.5, 139.5, 131.0, 126.5, 125.9, 119.7, 113.9, 106.7, 41.8, 31.5, 28.7, 26.7, 22.6, 15.5, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{38}H_{42}N_2O_2S_4$, 687.2202; found, 687.2177.

Synthesis of ethyl (E)-3-(2-bromo-N-hexylthiophene-3-carboxamido)acrylate (T-AE)

A solution of 2-bromothiophene-3-carboxylic acid (3.61 g, 17.5 mmol) in thionyl chloride (10 mL) was refluxed for 9 hours. The solvent was removed under vacuum to obtain chloride, which was used in next step without purification. To a solution of hexylamine (2.54 mL, 19.2 mmol) in dry CH_2Cl_2 (38 mL) was added ethyl propiolate (1.95 mL, 19.2 mmol). After the mixture was stirred at room termperature for 9 hours, the diisopropylethylamine (6.10 mL, 35.0 mmol) was added and then a solution of chloride in dry CH_2Cl_2 (20 mL) was slowly added at 0 °C. The mixture was stirred at room temperature overnight. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After

removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (20:1) as eluent to give a light yellow oil (2.24 g, 33%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.77 (d, *J* = 13.8 Hz, 1H), 7.35 (d, *J* = 5.7 Hz, 1H), 6.98 (d, *J* = 5.7 Hz, 1H), 5.38 (d, *J* = 13.9 Hz, 1H), 4.16 (q, 2H), 3.77 (t, 2H), 1.69-1.62 (m, 2H), 1.41-1.29 (m, 6H), 1.26 (t, 3H), 0.89 (t, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 167.2, 165.6, 143.0, 134.8, 127.9, 127.7, 113.7, 99.8, 60.2, 43.9, 31.4, 26.6, 26.5, 22.6, 14.3, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{16}H_{22}BrNO_3S$, 410.0396; found, 410.0370.

Synthesis of ethyl (E)-2-(5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)acetate (TPYE)

To a solution of T-AE (908 mg, 2.34 mmol) in dry DMF (16 mL) were added in portions triphenylphosphine (153 mg, 0.585 mmol), palladium (II) acetate (53 mg, 0.234 mmol) and anhydrous sodium carbonate (496 mg, 4.68 mmol). The mixture was heated to 150 °C for 5 hours. After cooling to room temperature, the mixture was poured into water and extracted with ethyl acetate three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (10:1) as eluent to give a yellow solid (460 mg, 64%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.59 (d, *J* = 5.0 Hz, 1H), 7.30 (d, *J* = 5.0 Hz, 1H), 5.59 (s, 1H), 4.31 (q, 2H), 3.70 (t, 2H), 1.67-1.60 (m, 2H), 1.37 (t, 3H), 1.35-1.26 (m, 6H), 0.91-0.86 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 166.9, 163.4, 145.6, 141.9, 139.3, 135.8, 120.3, 94.9, 60.7, 40.0, 31.5, 28.4, 26.5, 22.6, 14.4, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{16}H_{21}NO_3S$, 330.1134; found, 330.1150.

Synthesis of (E)-2-(5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)acetic acid (TPYAc)

To a solution of TPYE (455 mg, 1.48 mmol) in a mixture of ethanol (6 mL) and water (6 mL) was added NaOH (71 mg, 1.78 mmol), and the reaction mixture was heated to 80 °C for 3 hours. After cooling to room temperature, the mixture was acidified with 1 M HCl, extracted with ethyl acetate and washed with brine. The combined organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was washed with hexane to give a light yellow solid (335 mg, 81%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.63 (d, *J* = 5.1 Hz, 1H), 7.32 (d, *J* = 5.0 Hz, 1H), 5.63 (s, 1H), 3.73 (t, 2H), 1.65 (m, 2H), 1.33 (m, 6H), 0.89 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 171.8, 163.4, 147.6, 141.7, 139.4, 136.4, 120.5, 93.5, 40.2, 31.4, 28.3, 26.5, 22.5, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{14}H_{17}NO_3S$, 302.0821; found, 302.0824.

Synthesis of (E)-N-hexyl-2-(5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)-N-(thiophen-3-yl)acetamide (TPYA)

To a solution of TPYAc (884 mg, 3.16 mmol) in dry CH_2Cl_2 (25 mL) were added oxalyl chloride (0.88 mL, 10.1 mmol) and 3 drops of DMF. The mixture was stirred for 10 hours at room temperature. The solvent was removed under vacuum to obtain chloride, which was used in next step without purification. To the solution of N-hexylthiophen-

3-amine (705 mg, 3.85 mmol) and diisopropylethylamine (619 mg, 4.79 mmol) in dry CH_2Cl_2 (10 mL) at 0 °C was slowly added a solution of chloride in dry CH_2Cl_2 (10 mL). The mixture was stirred at room temperature overnight. Then, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (16:1) as eluent to give a tawny solid (1.00 g, 71%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.55 (d, *J* = 5.1 Hz, 1H), 7.41 (dd, *J* = 5.1, 3.2 Hz, 1H), 7.27 (s, 1H), 7.16 (dd, *J* = 3.2, 1.4 Hz, 1H), 6.99 (dd, *J* = 5.1, 1.4 Hz, 1H), 5.46 (s, 1H), 3.78 (t, 2H), 3.42 (t, 2H), 1.42-1.08 (m, 16H), 0.94-0.78 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 165.6, 163.4, 143.0, 142.3, 141.0, 138.9, 135.6, 126.6, 126.4, 121.4, 120.1, 96.5, 48.8, 39.8, 31.6, 31.4, 28.2, 28.1, 26.5, 26.4, 22.6, 22.5, 14.1, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{24}H_{32}N_2O_2S_2$, 467.1797; found, 467.1778.

Synthesis of (E)-N-(2-bromothiophen-3-yl)-N-hexyl-2-(5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)acetamide (TPYA-Br)

To a solution of TPYA (940 mg, 2.11 mmol) in a mixture of chloroform (24 mL) and acetic acid (12 mL) was added N-bromosuccinimide (380 mg, 2.11 mmol), and the reaction mixture was stirred for 12 hours at room temperature. Then, the mixture was poured into water, extracted with CH_2Cl_2 three times and washed with $NaHCO_3$. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a flash silica gel column with a mixture of petroleum/ethyl acetate (16:1) as eluent to give a tawny oil (1.07 g, 97%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.55 (d, *J* = 5.0 Hz, 1H), 7.40 (d, *J* = 5.7 Hz, 1H), 7.26 (d, *J* = 5.1 Hz, 1H), 6.89 (d, *J* = 5.7 Hz, 1H), 5.30 (s, 1H), 3.84-3.68 (m, 2H), 3.60-3.48 (m, 1H), 3.39-3.27 (m, 1H), 1.62-1.53 (m, 2H), 1.44-1.10 (m, 14H), 0.94-0.78 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 165.4, 163.4, 143.6, 142.2, 140.2, 138.9, 135.6, 127.0, 126.4, 120.1, 111.7, 95.6, 48.0, 39.8, 31.6, 31.4, 28.2, 28.1, 26.6, 26.5, 22.6, 22.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{24}H_{31}BrN_2O_2S_2$, 545.0903; found, 545.0909.

Synthesis of (Z)-4-hexyl-6-(5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)-4,6-dihydro-5H-thieno[3,2-b]pyrrol-5-one (isoTII)

To a solution of TPYA-Br (1.01 g, 1.93 mmol) in dry DMF (20 mL) were added in portions triphenylphosphine (127 mg, 0.484 mmol), palladium (II) acetate (46 mg, 0.202 mmol) and anhydrous sodium carbonate (410 mg, 3.87 mmol). The mixture was heated to 150 °C for 5 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/ethyl acetate (12:1) as eluent and then recrystallized from chloroform/methanol to give a red solid (525 mg, 64%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.56 (d, *J* = 5.1 Hz, 1H), 7.41 (d, *J* = 5.2 Hz, 1H), 7.36 (d, *J* = 5.1 Hz, 1H), 6.84 (d, *J* = 5.2 Hz, 1H), 4.25 (t, 2H), 3.83 (t, 2H), 1.75-1.67 (m, 4H), 1.45-1.18 (m, 12H), 0.89-0.82 (m, 6H). ^{13}C NMR (101 MHz,

Chloroform-*d*): δ 170.2, 164.5, 147.1, 143.0, 137.4, 136.7, 135.5, 129.6, 120.2, 111.6, 111.6, 106.8, 42.0, 41.9, 31.5, 31.4, 30.2, 28.5, 26.6, 26.0, 22.5, 22.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+Na]^+$, calcd. for $C_{24}H_{30}N_2O_2S_2$, 465.1641; found, 465.1637.

Synthesis of (Z)-2-bromo-6-(2-bromo-5-hexyl-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)-4-hexyl-4,6-dihydro-5H-thieno[3,2-b]pyrrol-5-one (isoTII-diBr)

To a solution of isoTII (140 mg, 0.316 mmol) in chloroform (20 mL) was added slowly bromine (0.06 mL 1.27 mmol), then iron trichloride (1 mg) was added to the reaction mixture. The mixture was stirred for 2 hours in the dark before saturated sodium sulfite solution was added and stirring continued for 0.5 h. The resulting mixture was extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2 (2:1) as eluent to give a red solid (60 mg, 32%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.36 (s, 1H), 6.87 (s, 1H), 4.10 (t, 2H), 3.77 (t, 2H), 1.73-1.62 (m, 4H), 1.43-1.21 (m, 12H), 0.90-0.84 (m, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 169.4, 163.3, 146.0, 142.2, 136.1, 136.0, 123.9, 122.8, 117.8, 115.2, 111.7, 106.0, 42.1, 41.8, 31.4, 31.4, 30.2, 28.5, 26.5, 25.9, 22.5, 22.4, 14.0, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{24}H_{28}Br_2N_2O_2S_2$, 599.0032; found, 599.0028.

Synthesis of (Z)-4-hexyl-6-(5-hexyl-2-(4-(methylthio)phenyl)-4-oxo-4,5-dihydro-6H-thieno[2,3-c]pyrrol-6-ylidene)-2-(4-(methylthio)phenyl)-4,6-dihydro-5H-thieno[3,2-b]pyrrol-5-one (isoTIIP)

To a solution of isoTII-diBr (30 mg, 0.0500 mmol), (4-(methylthio)phenyl)boronic acid (34 mg, 0.200 mmol) and anhydrous sodium carbonate (53 mg, 0.500 mmol) in a mixture of 1,4-dioxane (10 mL) and water (2 mL) was added $Pd(PPh_3)_4$ (6 mg, 5.00 μmol). The mixture was heated to 85 °C for 20 hours. After cooling to room temperature, the mixture was poured into water and extracted with CH_2Cl_2 three times. The organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified through a silica gel column with a mixture of petroleum/CH_2Cl_2 (1:1) as eluent and then recrystallized from chloroform/methanol to give a black purple solid (16 mg, 47%). ^{1}H NMR (400 MHz, Chloroform-*d*): δ 7.64 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.51 (s, 1H), 7.27 (d, *J* = 7.0 Hz, 4H), 6.98 (s, 1H), 4.26 (t, 2H), 3.85 (t, 2H), 2.61-2.42 (m, 6H), 1.79-1.71 (m, 4H), 1.48-1.18 (m, 12H), 0.89 (t, 3H), 0.85 (t, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*): δ 164.7, 153.2, 148.3, 147.6, 140.4, 139.6, 139.5, 137.9, 136.2, 130.6, 130.3, 126.7, 126.6, 126.4, 125.7, 115.5, 110.5, 107.0, 106.7, 42.0, 31.5, 31.5, 30.2, 29.7, 28.7, 26.6, 26.1, 22.6, 22.5, 15.5, 14.0, 14.0. HRMS (ESI, m/z): $[M+H]^+$, calcd. for $C_{38}H_{42}N_2O_2S_4$, 687.2202; found, 687.2182.

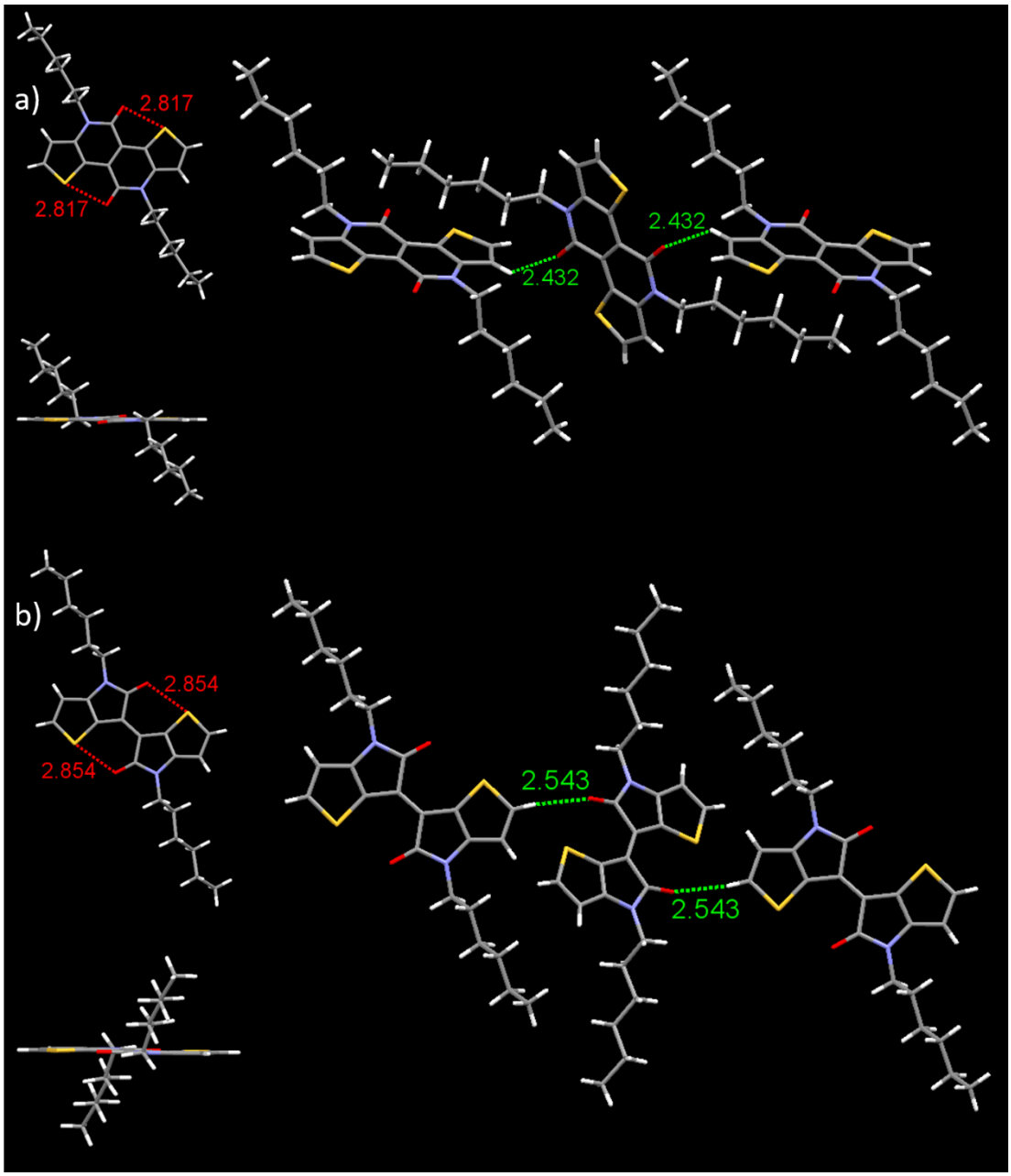


Figure S1. Single crystal structure and molecular stacking of a) TVTDA (CCDC 2068472) and b) TII (CCDC 1061786). C (grey), H (white), O (red), N (blue), S (yellow). S···O and H···O distances are marked and the unit is Å.

Table S1. Crystallographic data of TVTDA single crystal.

Identification code	TVTDA
Empirical formula	$C_{24}H_{30}N_2O_2S_2$
Formula weight	442.62
Temperature	293.15 K
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.6340(6) Å α = 84.340(5)° b = 10.2270(6) Å β = 78.779(5)° c = 12.2687(6) Å γ = 76.395(5)°
Volume	1150.66(12) $Å^3$
Z	2
Density (calculated)	1.278 g/cm^3
Absorption coefficient	0.254 mm^{-1}
F(000)	472.0
Crystal size	0.4 × 0.35 × 0.25 mm^3
Radiation	MoKα (λ = 0.71073)
Theta range for data collection	6.03 to 52.732°
Index ranges	$-11 \leq h \leq 12$, $-12 \leq k \leq 12$, $-15 \leq l \leq 15$
Reflections collected	7037
Data/restraints/parameters	7037/1/274
Goodness-of-fit on F^2	0.958
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0668$, $wR_2 = 0.1684$
Final R indexes [all data]	$R_1 = 0.1260$, $wR_2 = 0.1931$
Largest diff. peak and hole	0.70/-0.43 e $Å^{-3}$

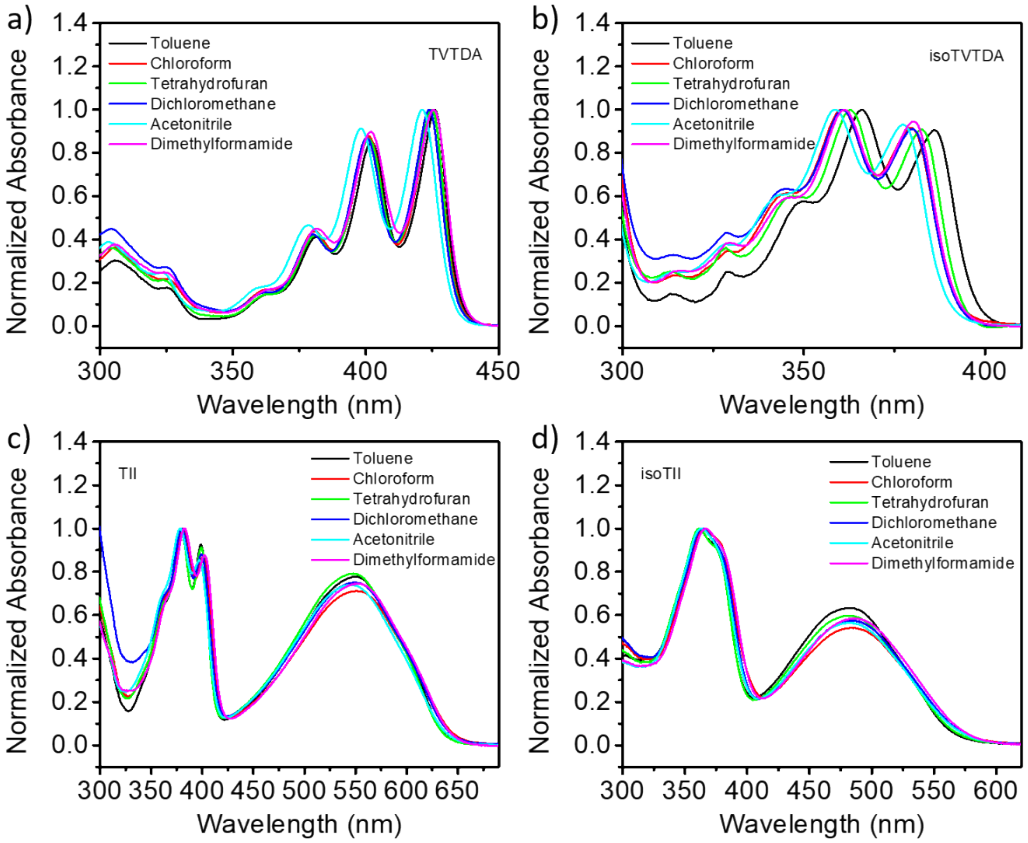


Figure S2. UV-vis absorption spectra of a) TVTDA, b) isoTVTDA, c) TII and d) isoTII in various solution.

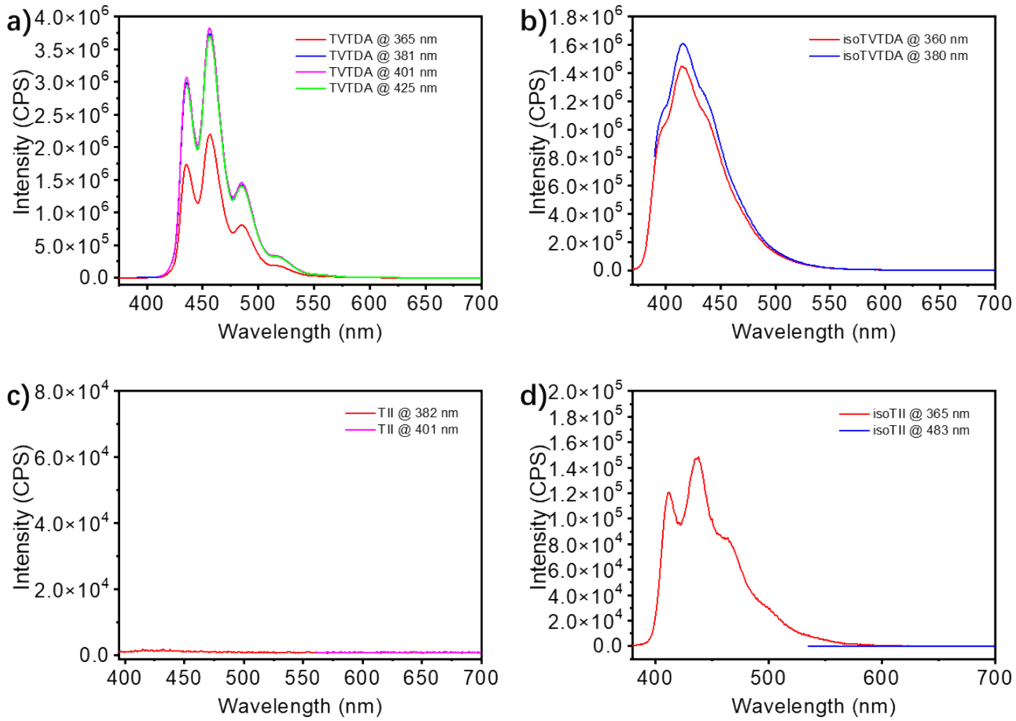


Figure S3. PL spectra of a) TVTDA, b) isoTVTDA, c) TII and d) isoTII in chloroform solution with different excitation wavelengths. c = 1.88×10^{-5} M.

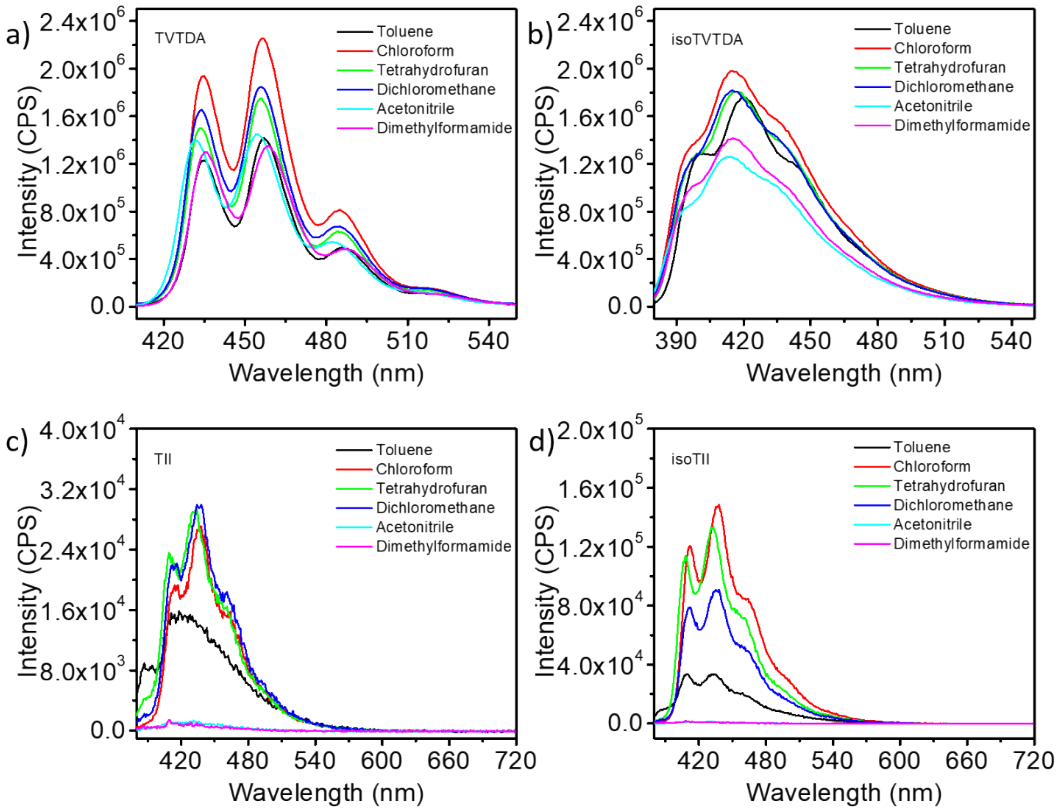


Figure S4. PL spectra of a) TVTDA, b) isoTVTDA, c) TII and d) isoTII in various solution. Excited at 365 nm. c = 1.88×10^{-5} M.

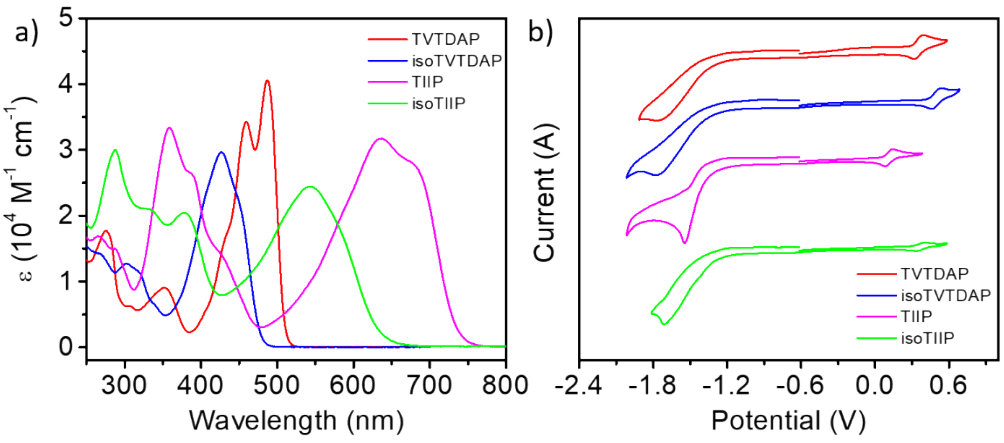


Figure S5. a) UV-vis absorption spectra and b) CV curves of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

Table S2. Photophysical and electrochemical properties of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

Compound	$\lambda_{abs.}$ (nm)	ε ($M^{-1}cm^{-1}$)	$E_g^{opt.}$ (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g^{cv} (eV)
TVTDAP	351, 459, 487	4.06×10^4	2.42	-5.10	-3.48	1.62
isoTVTDAP	302, 427	2.97×10^4	2.58	-5.23	-3.45	1.78
TIIP	359, 637	3.34×10^4	1.68	-4.87	-3.44	1.43
isoTIIP	288, 377, 541	3.00×10^4	1.95	-5.11	-3.47	1.64

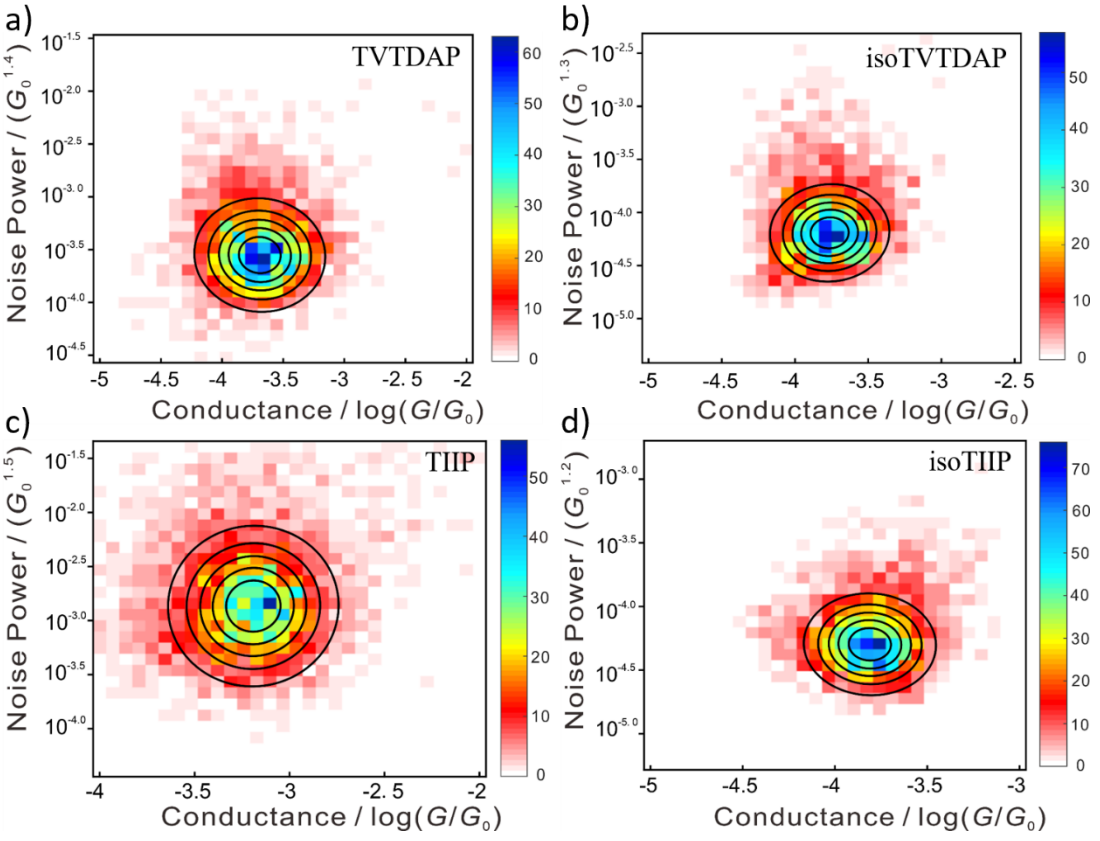


Figure S6. The noise power versus averaged conductance for a) TVTDAP, b) isoTVTDAP, c) TIIP and d) isoTIIP.

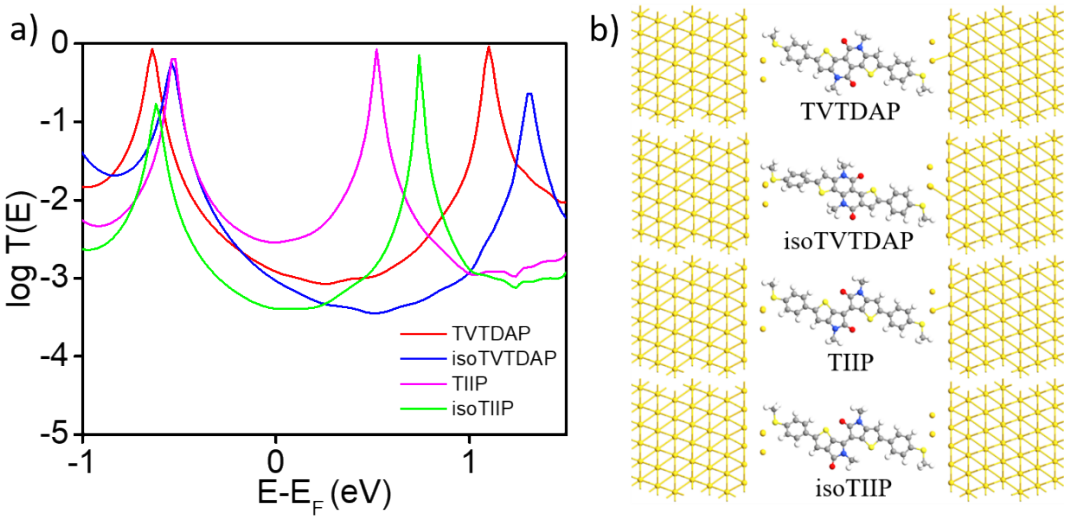


Figure S7. a) The calculated transmission curves and b) the optimized single-molecule device configurations of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

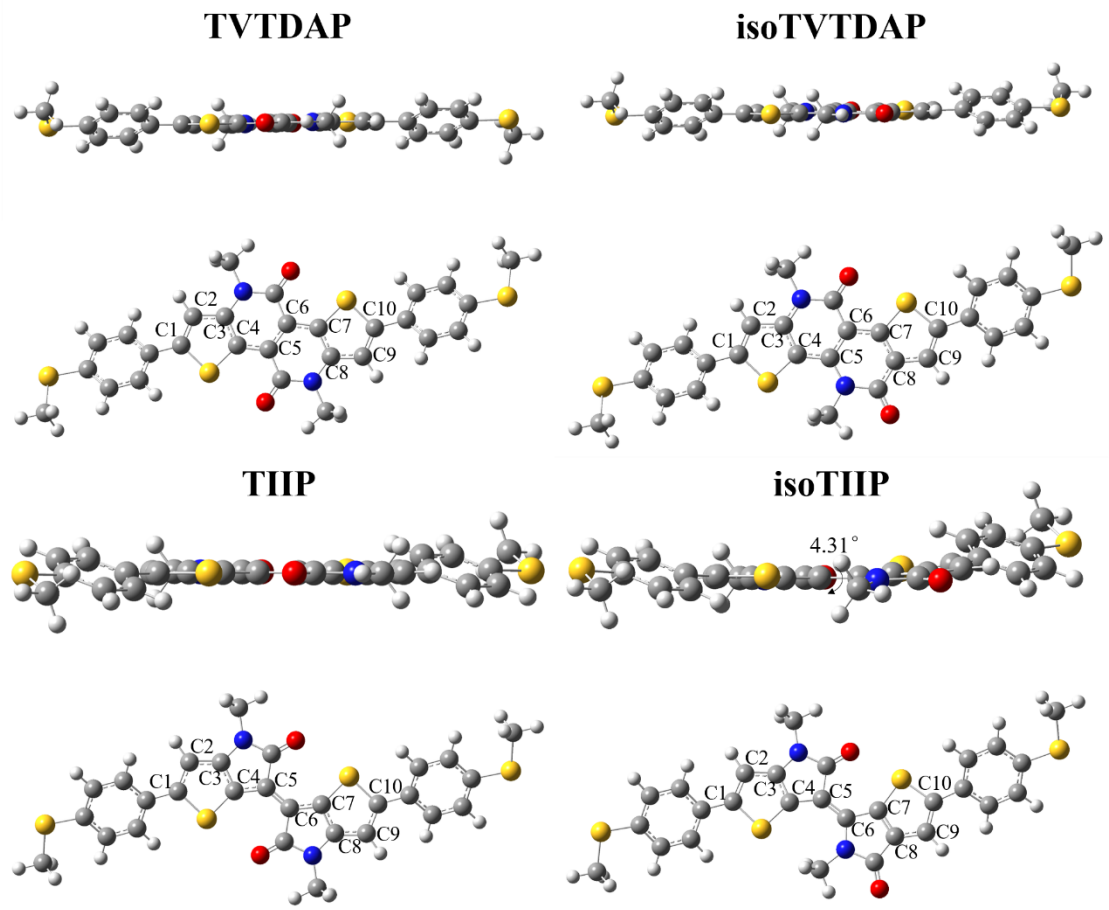


Figure S8. Optimized geometries of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

Table S3. Bond length and molecular length of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

Compound	C1-C2 (Å)	C2-C3 (Å)	C3-C4 (Å)	C4-C5 (Å)	C5-C6 (Å)	C6-C7 (Å)	C7-C8 (Å)	C8-C9 (Å)	C9-C10 (Å)	Molecular length[a] (Å)
TVTDAP	1.379	1.421	1.395	1.417	1.397	1.417	1.395	1.421	1.379	20.8
isoTVTDAP	1.374	1.423	1.402	1.436	1.409	1.423	1.389	1.422	1.372	20.8
TIIP	1.392	1.403	1.395	1.425	1.375	1.425	1.395	1.403	1.392	20.8
isoTIIP	1.383	1.409	1.390	1.448	1.382	1.464	1.383	1.408	1.382	20.8

[a] Molecular length comes from the distance between sulfur atoms in anchoring groups at both ends.

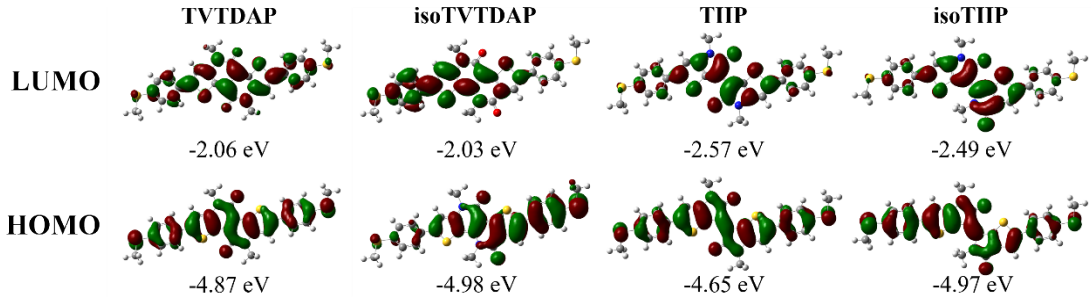


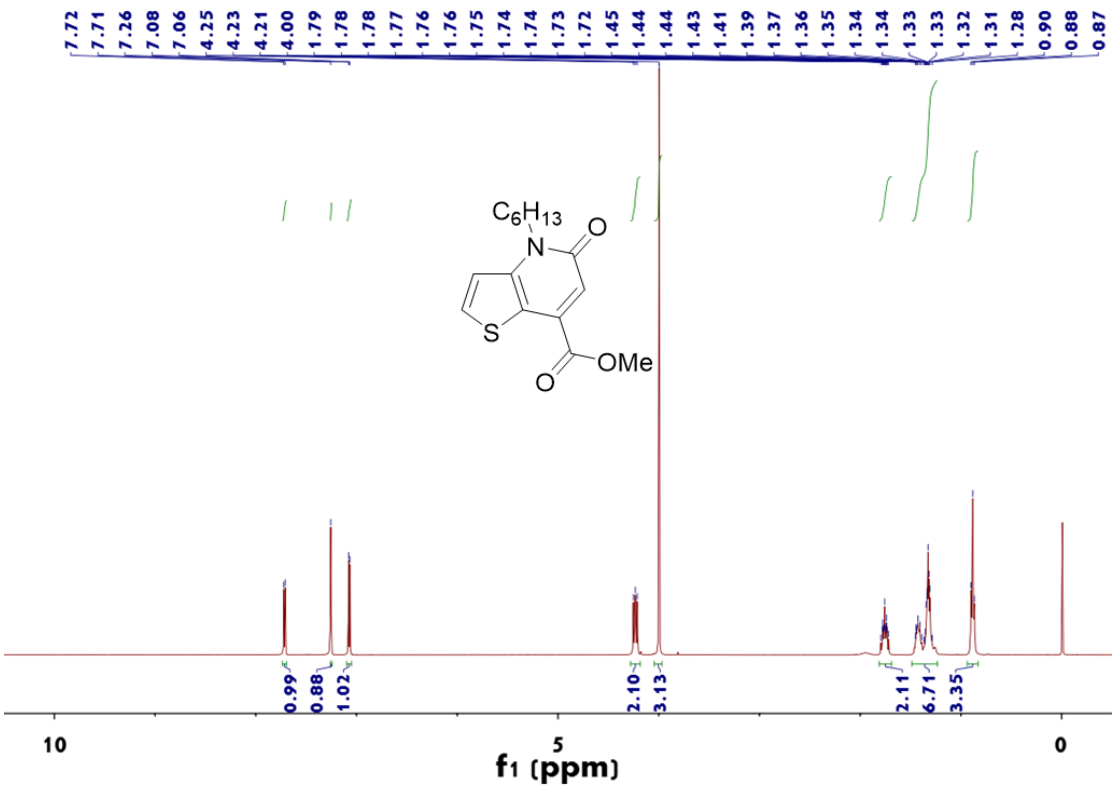
Figure S9. Molecular orbital diagrams of of TVTDAP, isoTVTDAP, TIIP and isoTIIP.

(1) Wang, H. C.; Tao, J. W.; Bai, W. Y.; Xie, Z. Y.; Li, H. X.; Ren, X. C.; Xu, Y. X. Synthesis of a Thiophene Analogue of Isoindigo by C-H Activation/Oxidative Cyclization and Application of Its Copolymeric Materials to Organic Transistors. *Eur. J. Org. Chem.* **2018,** *2018*, 1218-1223.

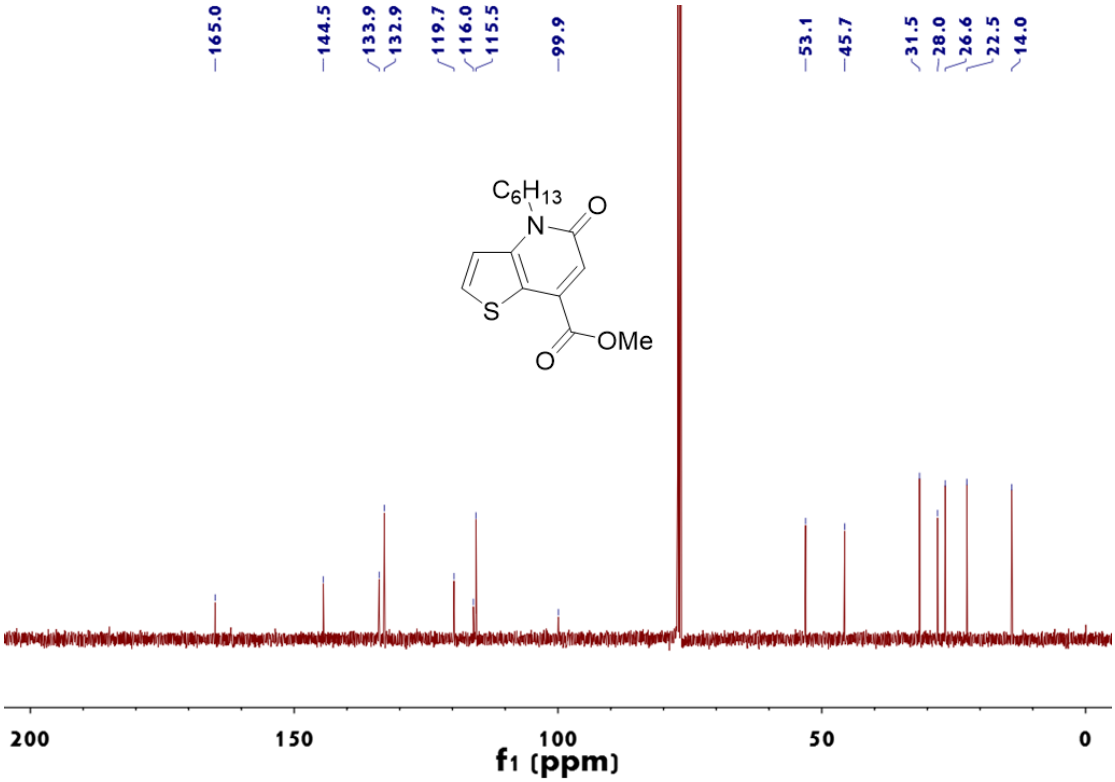
(2) Yoo, D.; Hasegawa, T.; Ashizawa, M.; Kawamoto, T.; Masunaga, H.; Hikima, T.; Matsumoto, H.; Mori, T. N-Unsubstituted thienoisoindigos: preparation, molecular packing and ambipolar organic field-effect transistors. *J. Mater. Chem. C* **2017,** *5*, 2509-2512.

(3) Ogawa, K.; Radke, K. R.; Rothstein, S. D.; Rasmussen, S. C. Synthesis of Secondary and Tertiary Aminothiophenes via Palladium-Catalyzed Amination. *J. Org. Chem.* **2001,** *66*, 9067-9070.

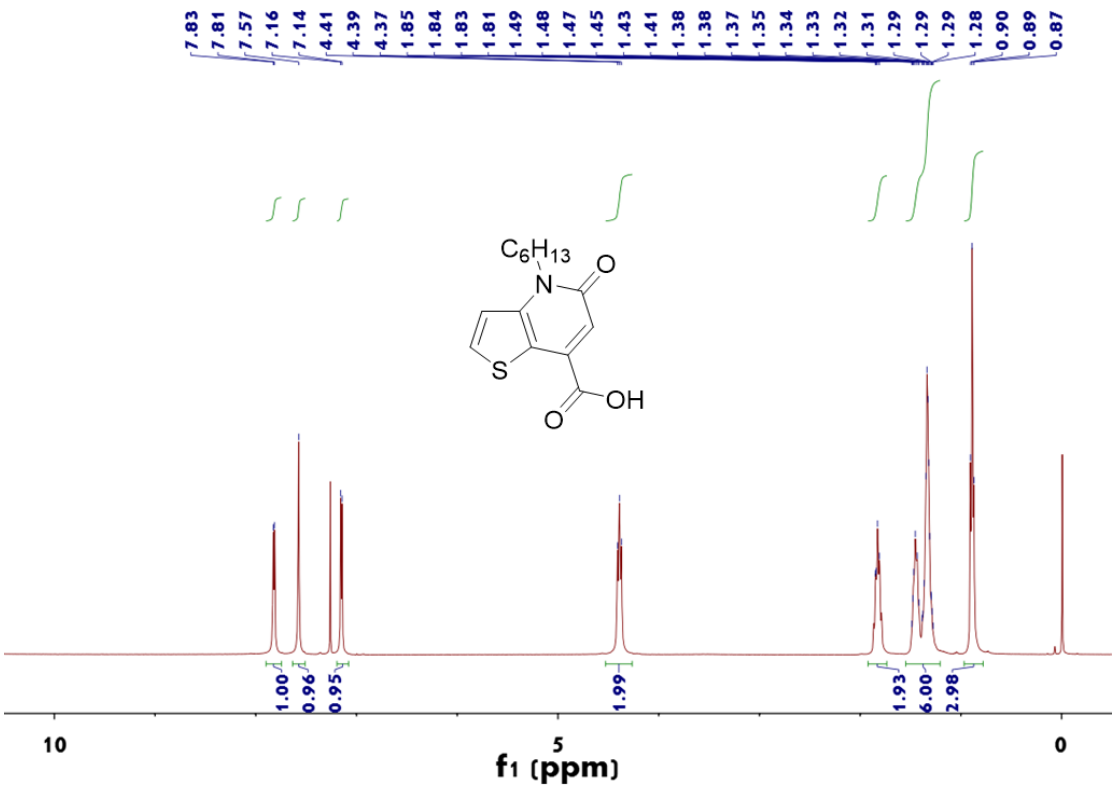
(4) Capozzi, B.; Xia, J.; Adak, O.; Dell, E. J.; Liu, Z. F.; Taylor, J. C.; Neaton, J. B.; Campos, L. M.; Venkataraman, L. Single-molecule diodes with high rectification ratios through environmental control. *Nat. Nanotechnol.* **2015,** *10*, 522-527.



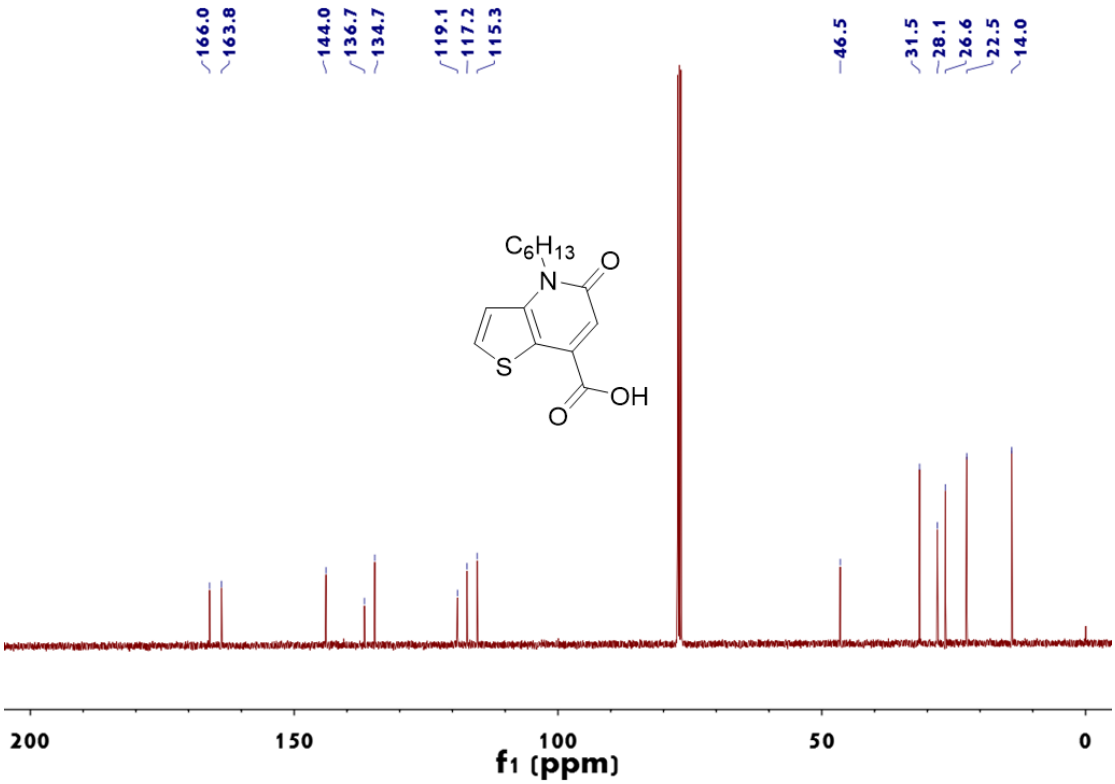
^{1}H NMR of compound TAE



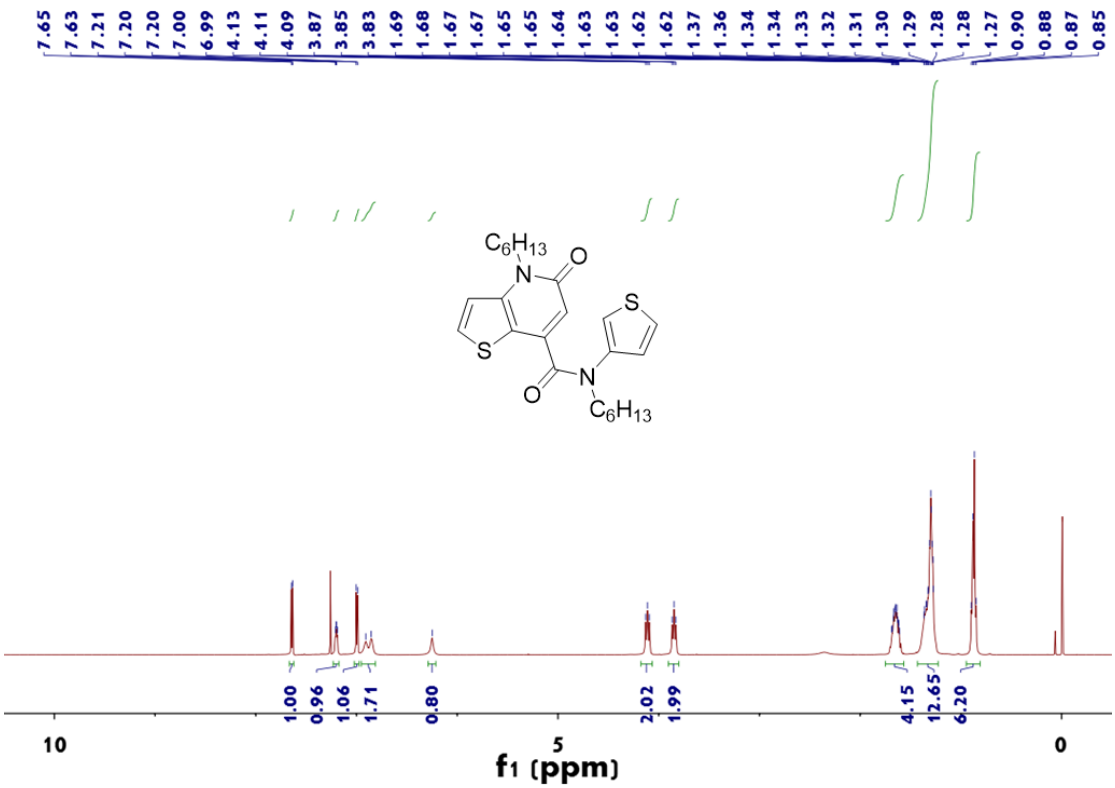
^{13}C NMR of compound TAE



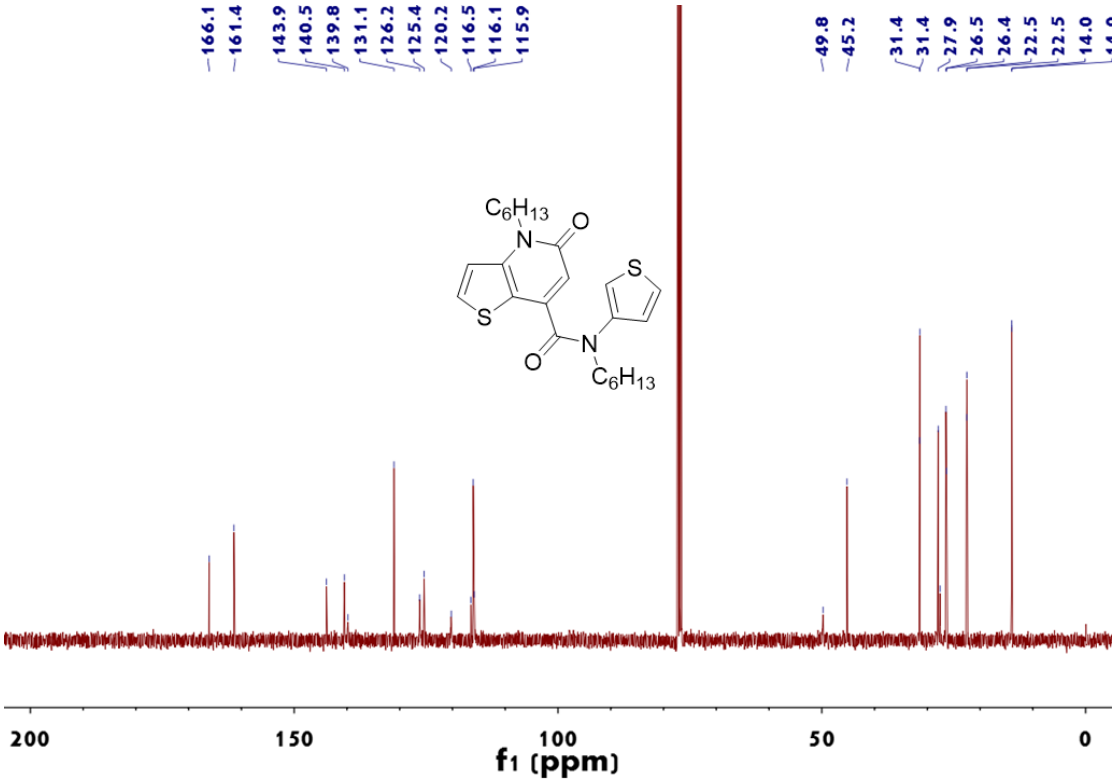
^{1}H NMR of compound TAAc



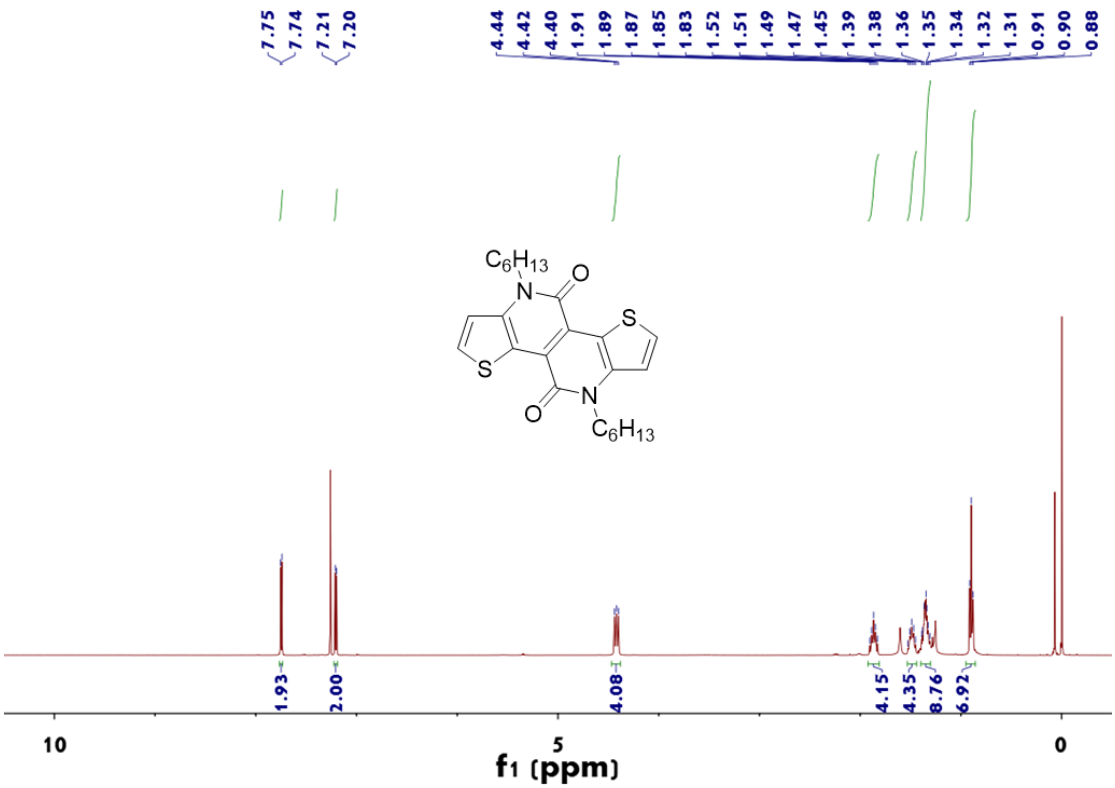
^{13}C NMR of compound TAAc



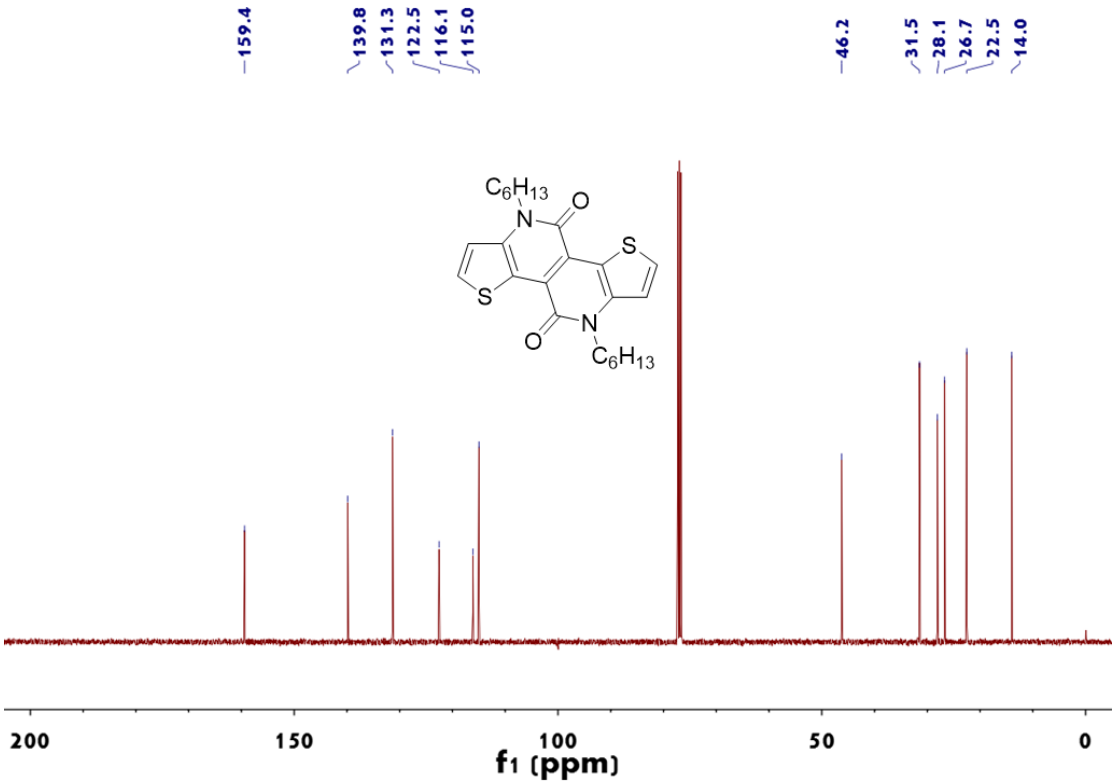
^{1}H NMR of compound TAA



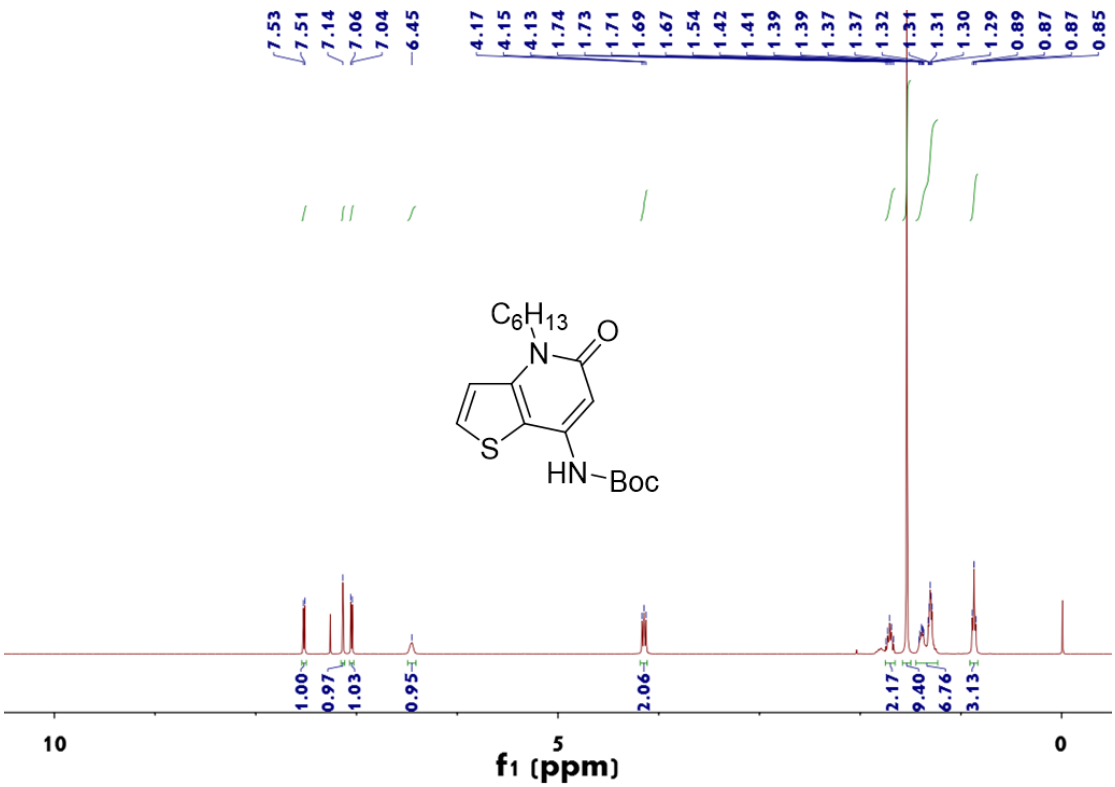
^{13}C NMR of compound TAA



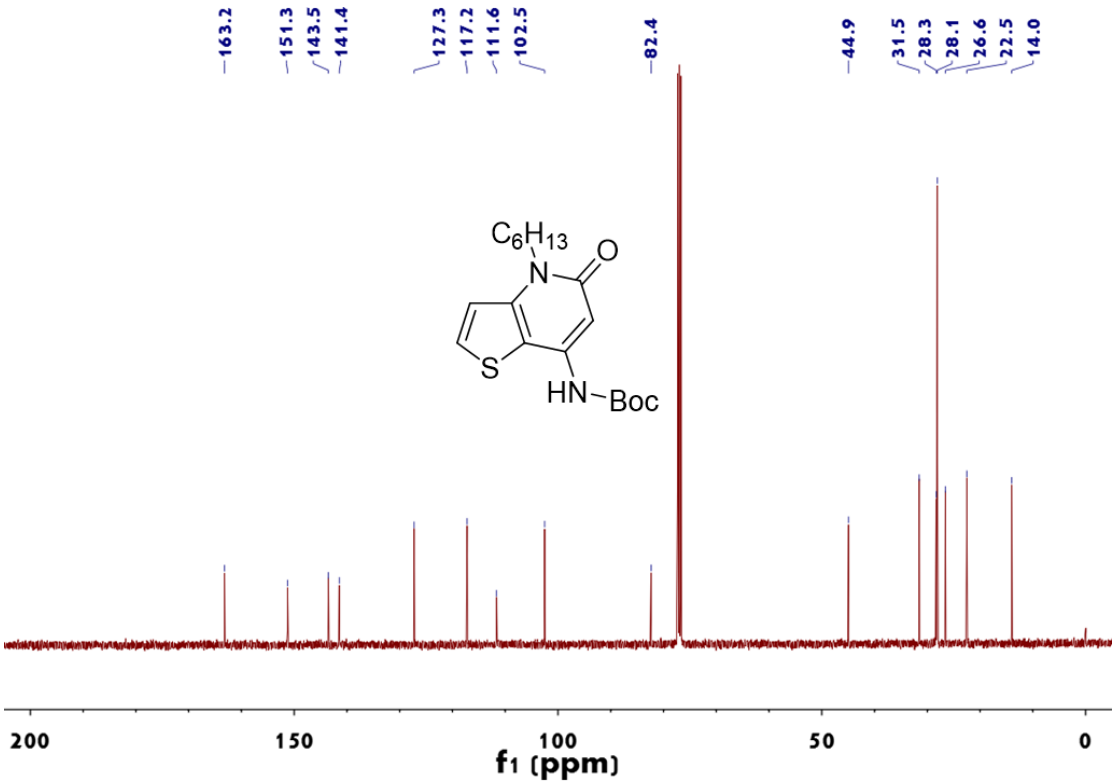
^{1}H NMR of compound TVTDA



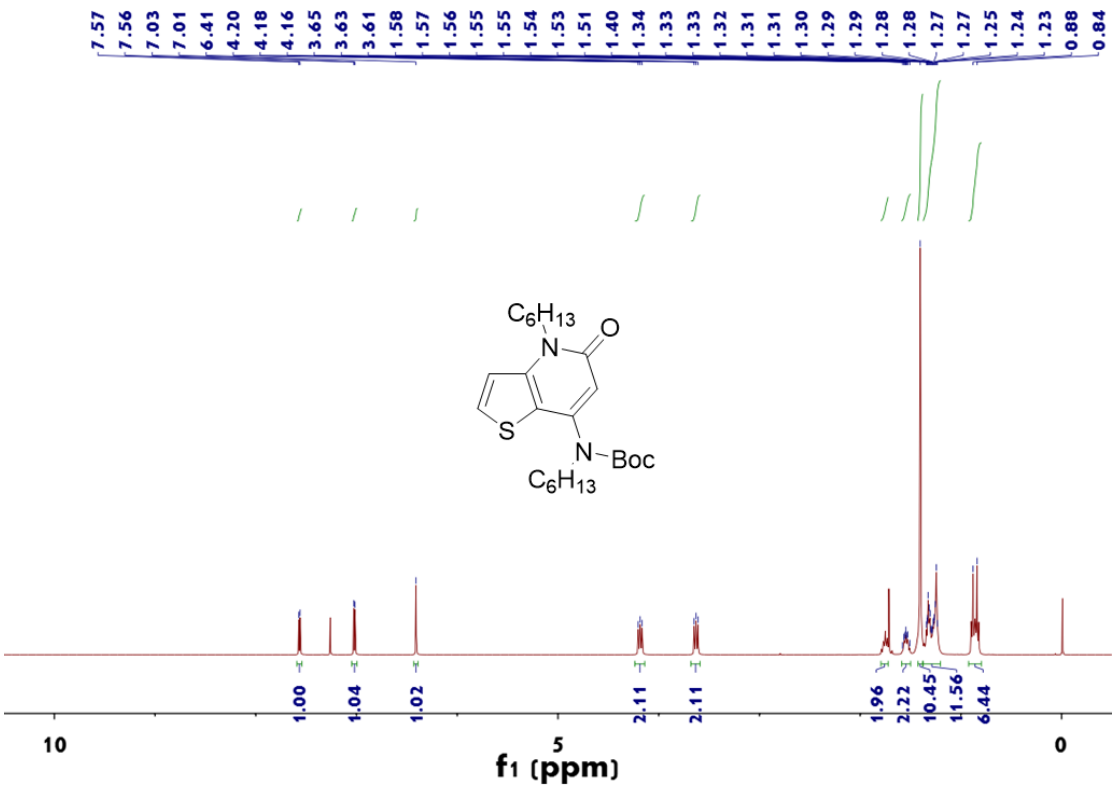
^{13}C NMR of compound TVTDA



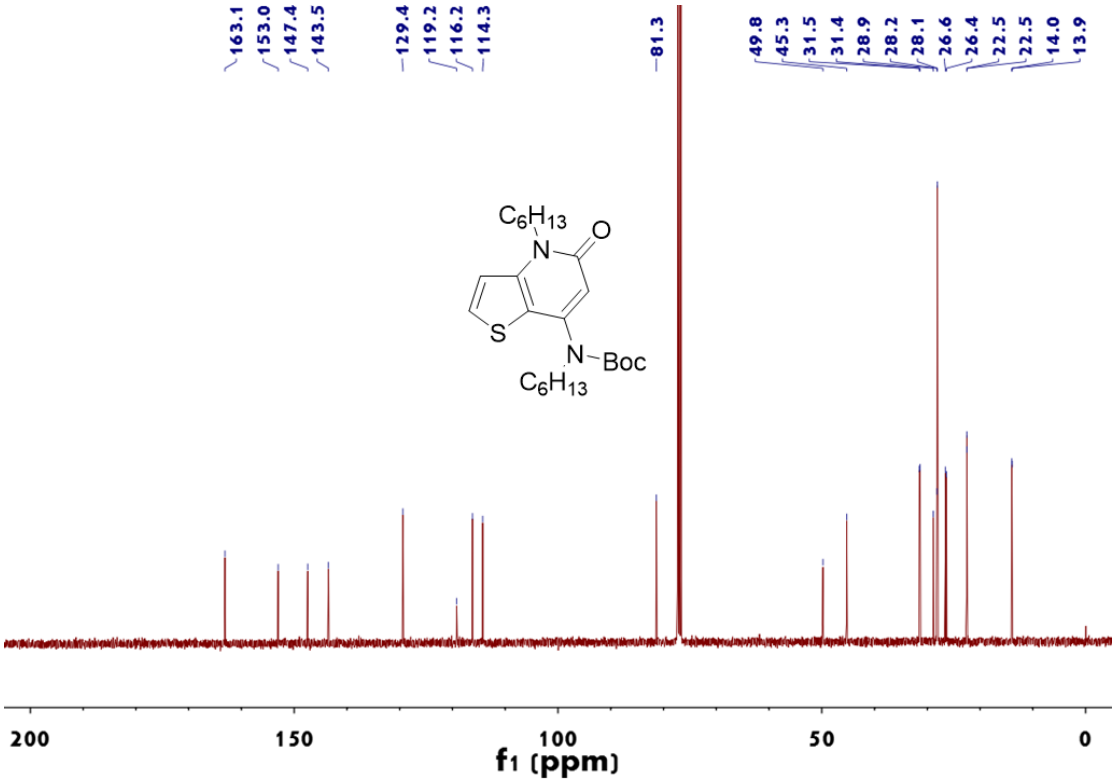
^{1}H NMR of compound TA-Boc



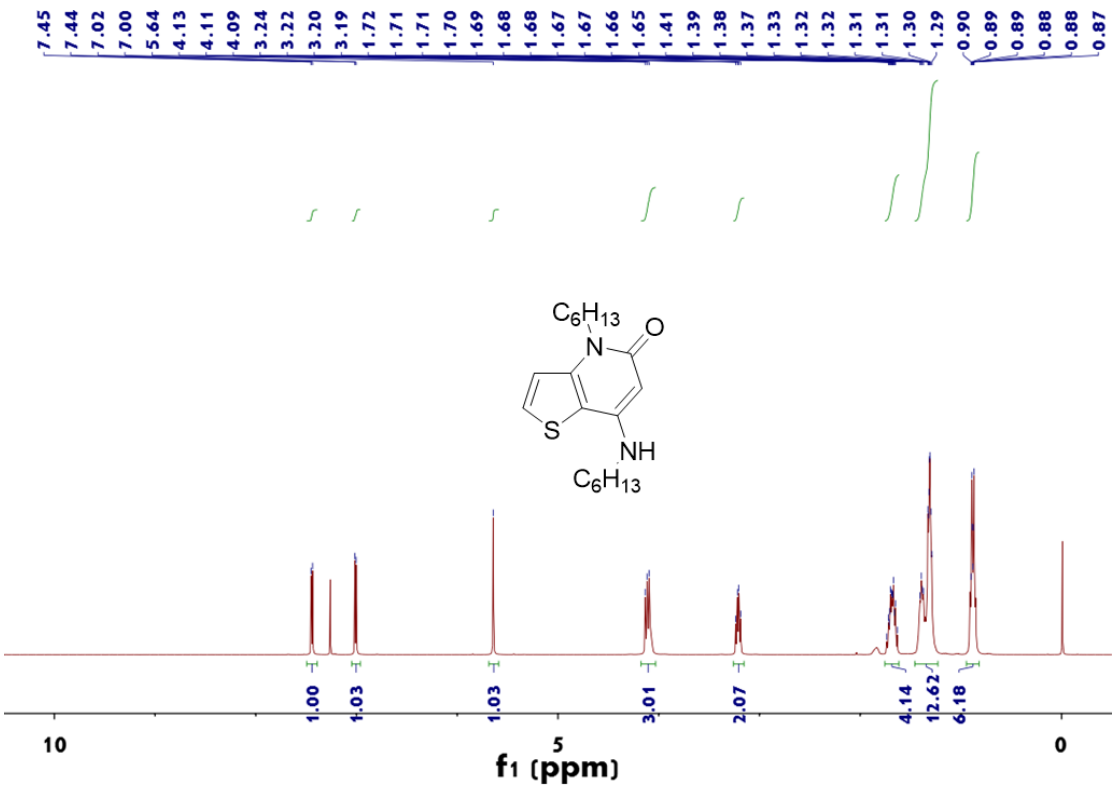
^{13}C NMR of compound TA-Boc



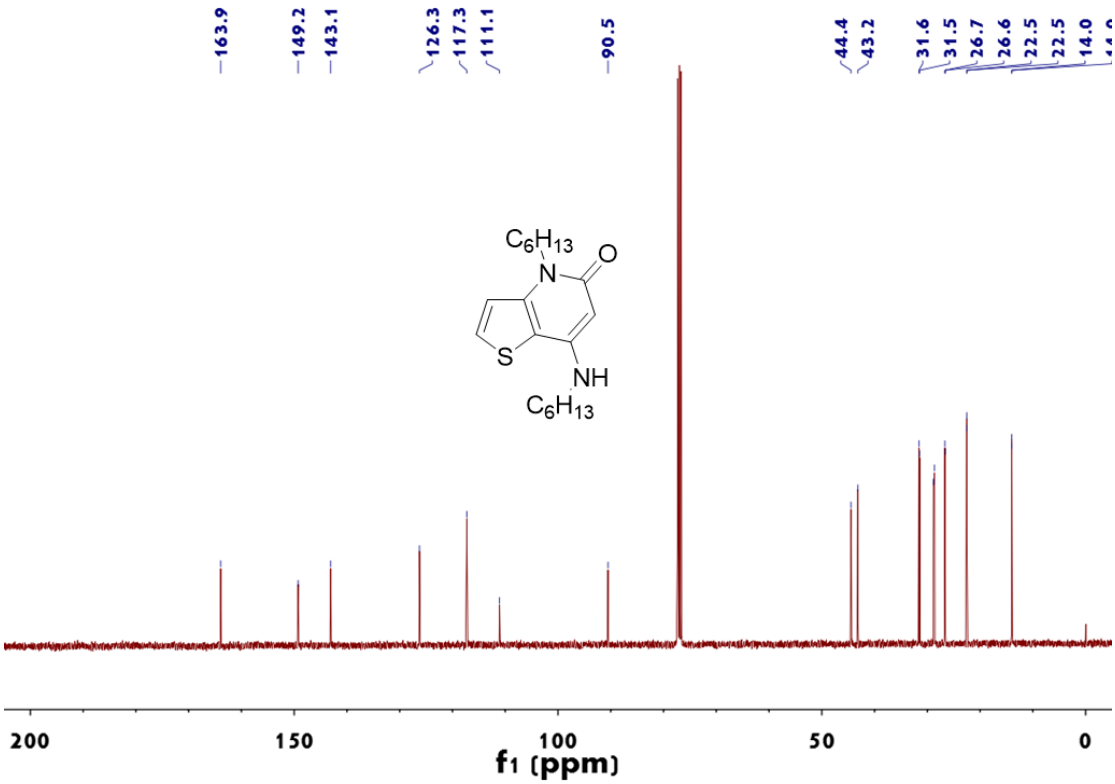
^{1}H NMR of compound TA-H-Boc



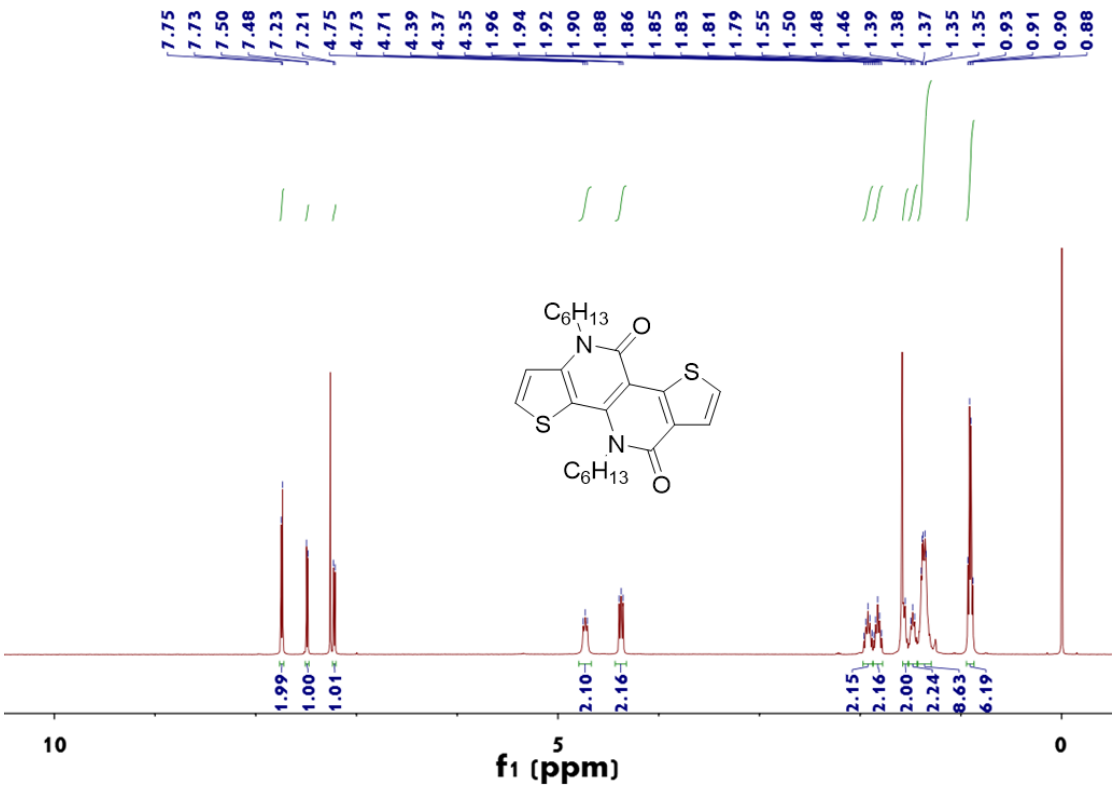
^{13}C NMR of compound TA-H-Boc



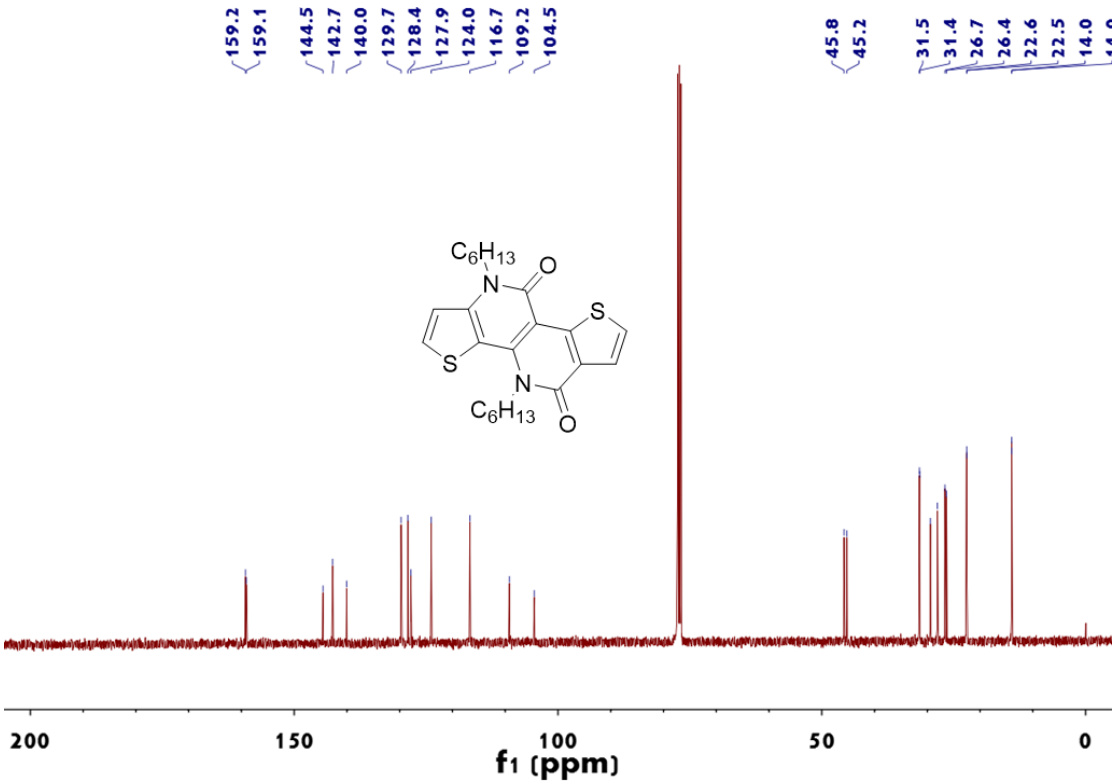
^{1}H NMR of compound TA-H



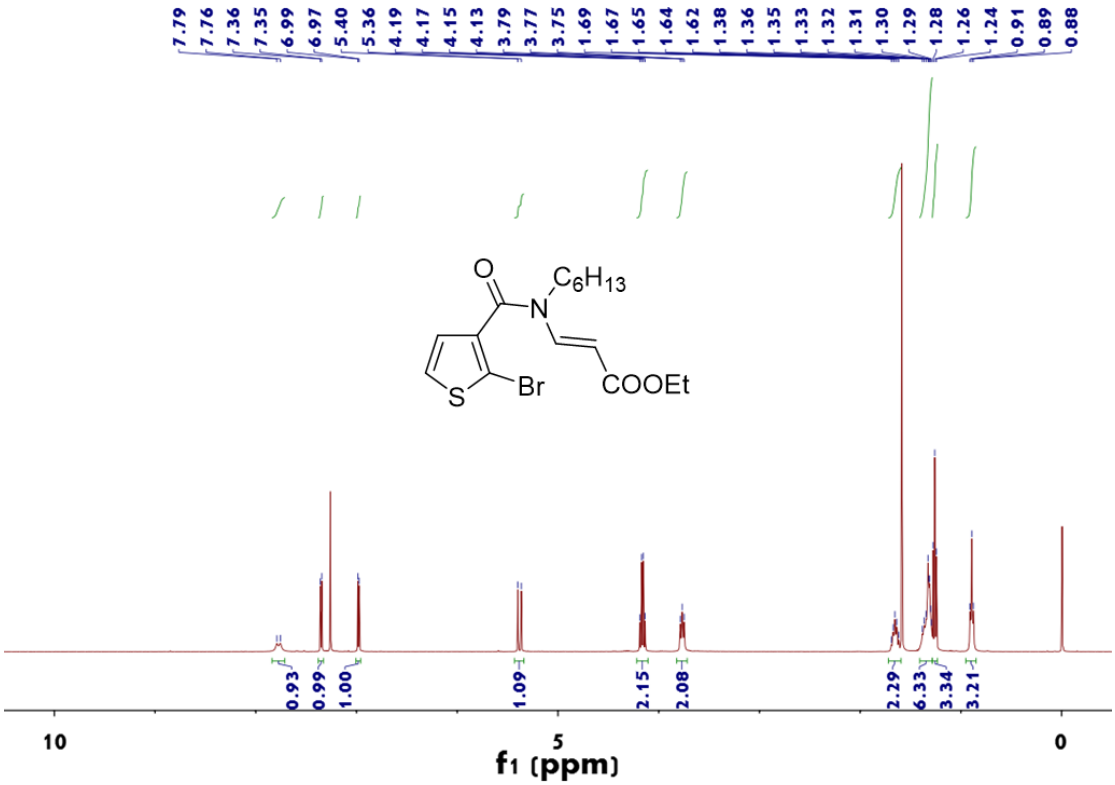
^{13}C NMR of compound TA-H



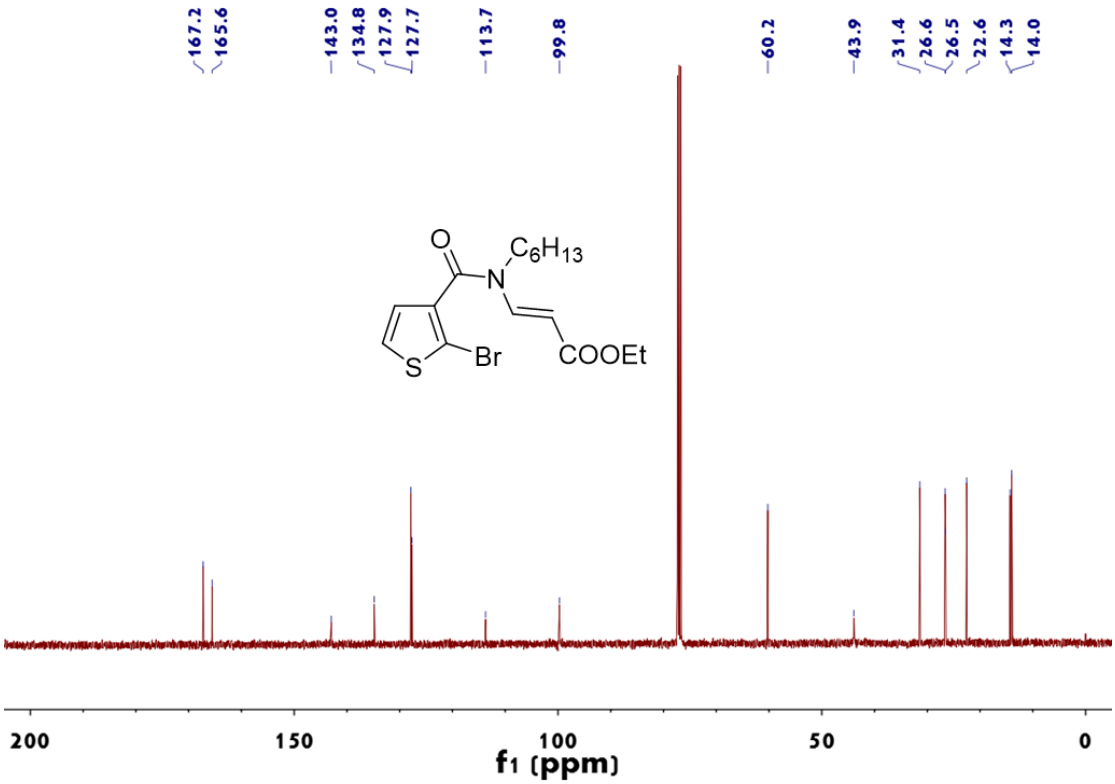
^{1}H NMR of compound isoTVTDA



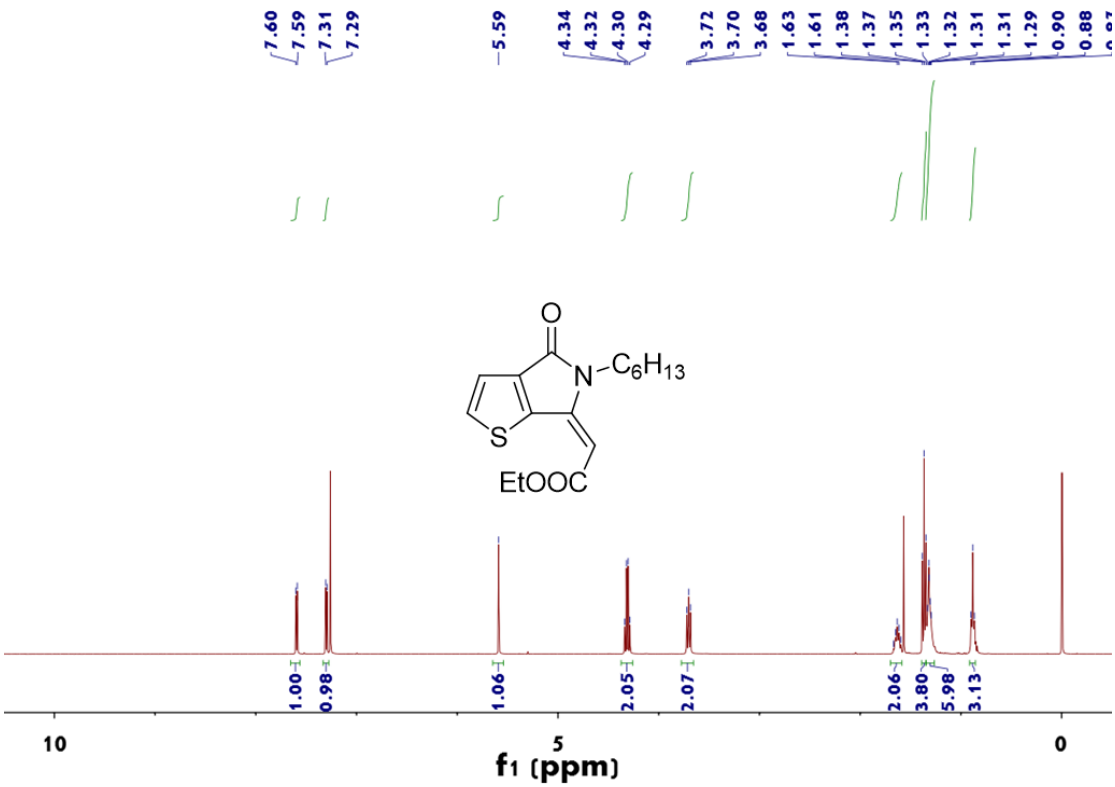
^{13}C NMR of compound isoTVTDA



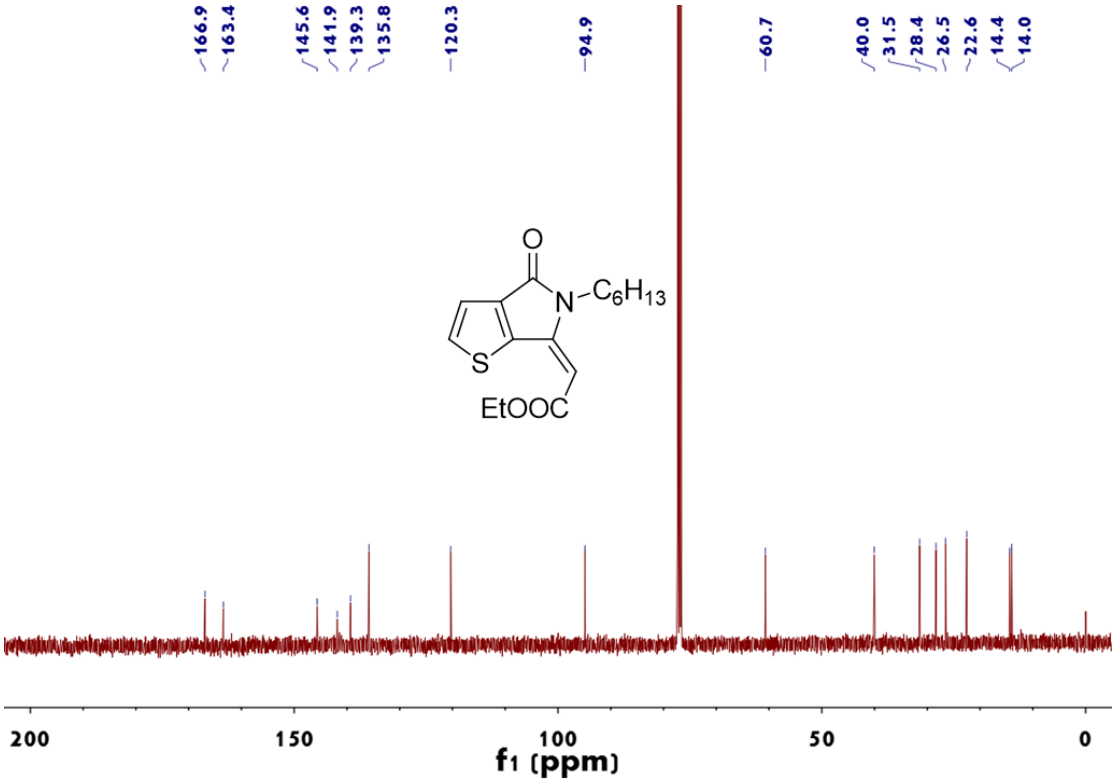
^{1}H NMR of compound T-AE



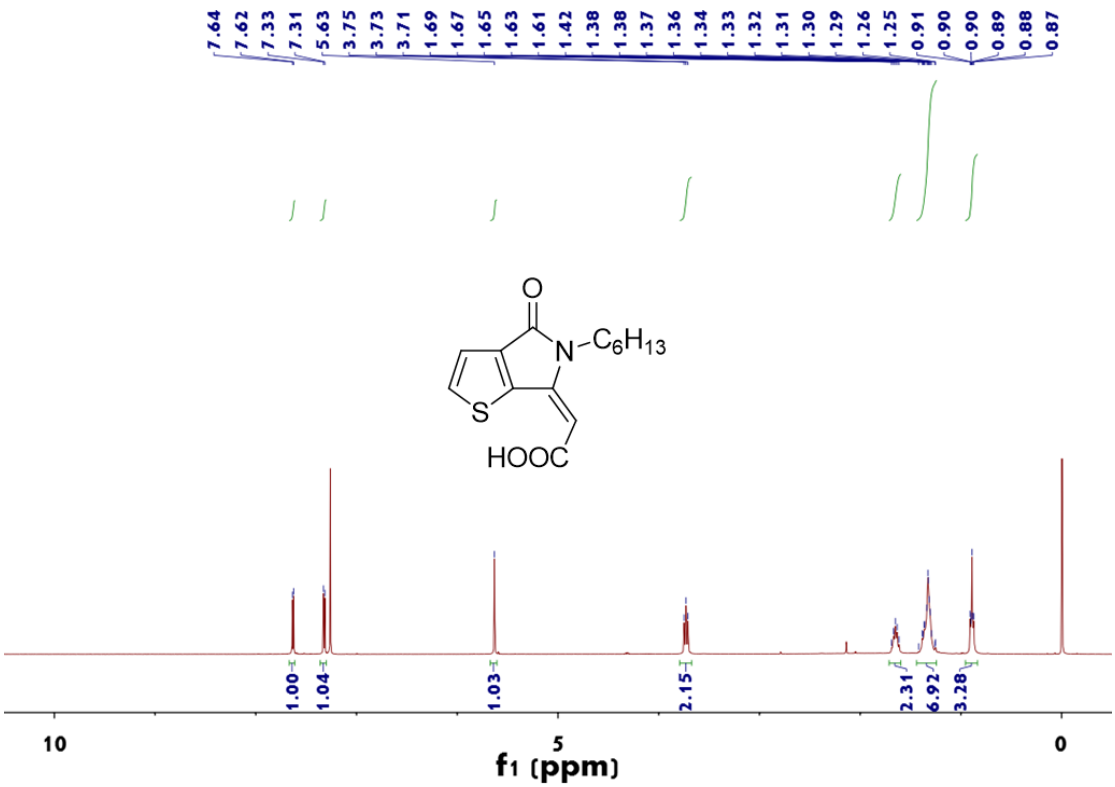
^{13}C NMR of compound T-AE



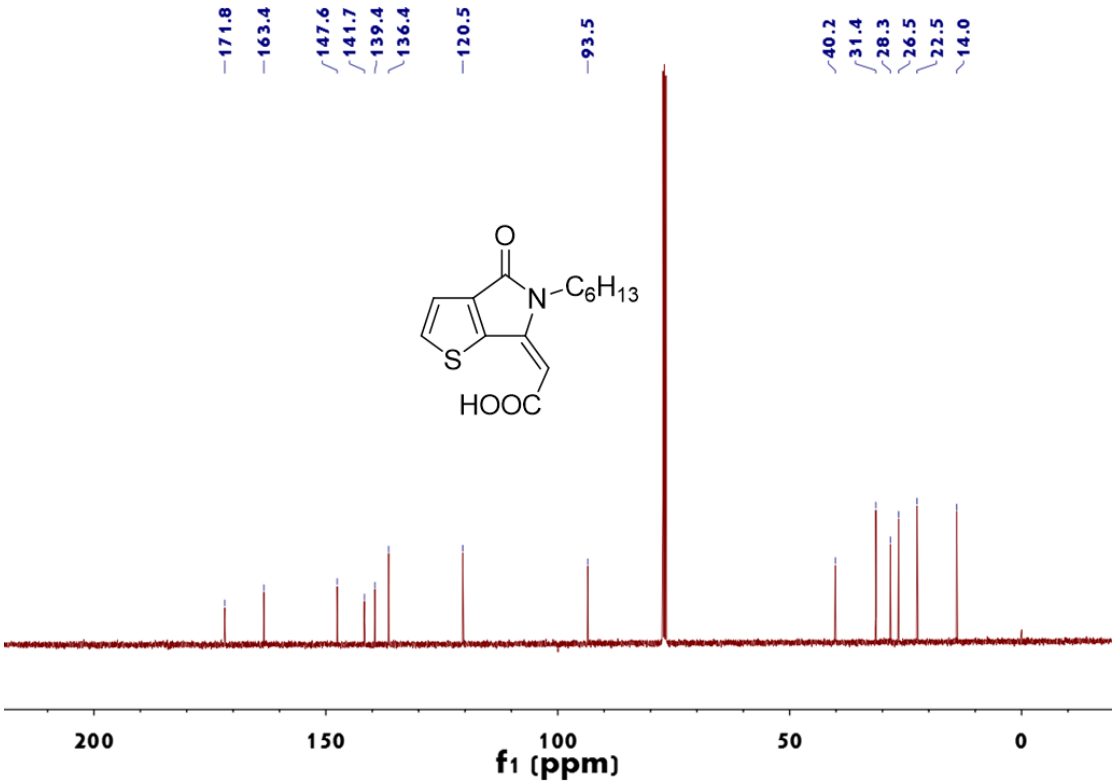
^{1}H NMR of compound TPYE



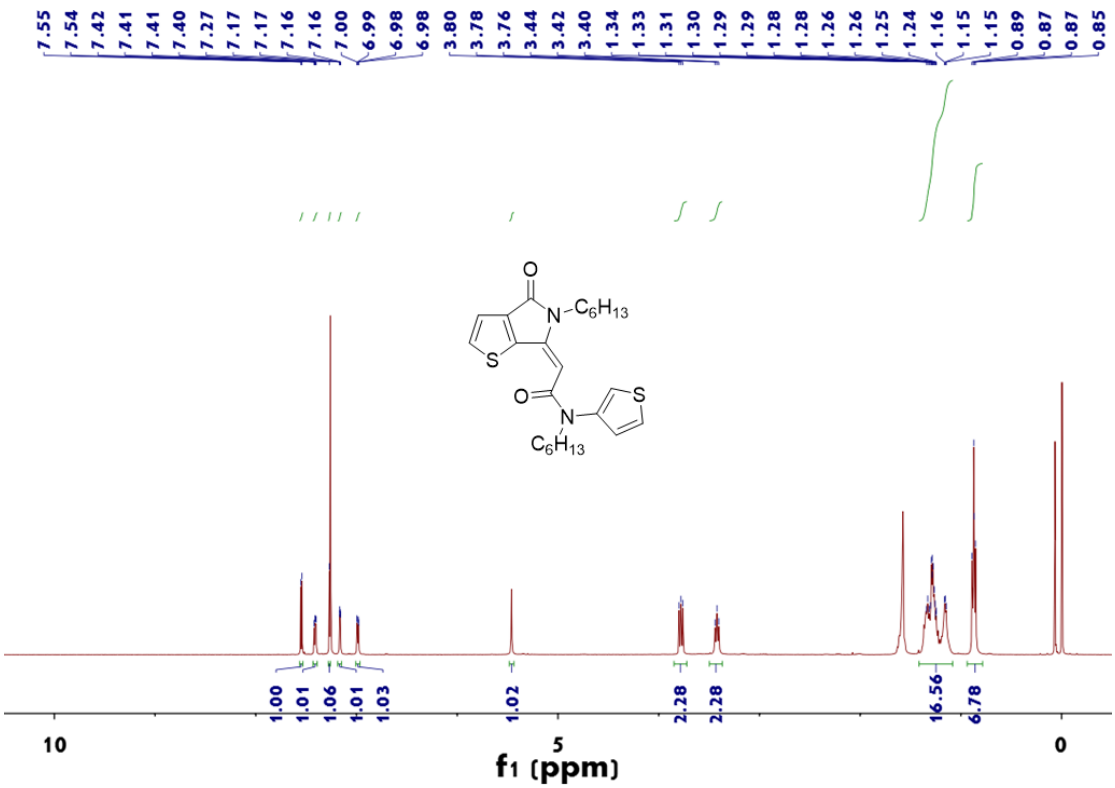
^{13}C NMR of compound TPYE



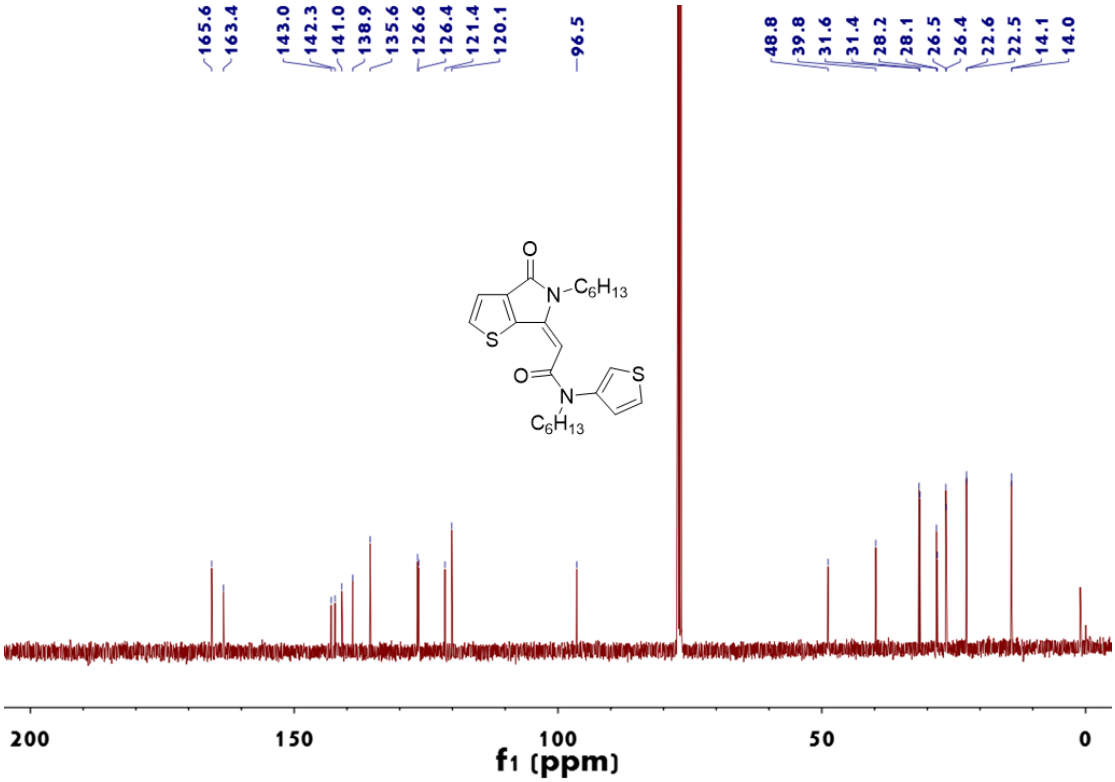
^{1}H NMR of compound TPYAc



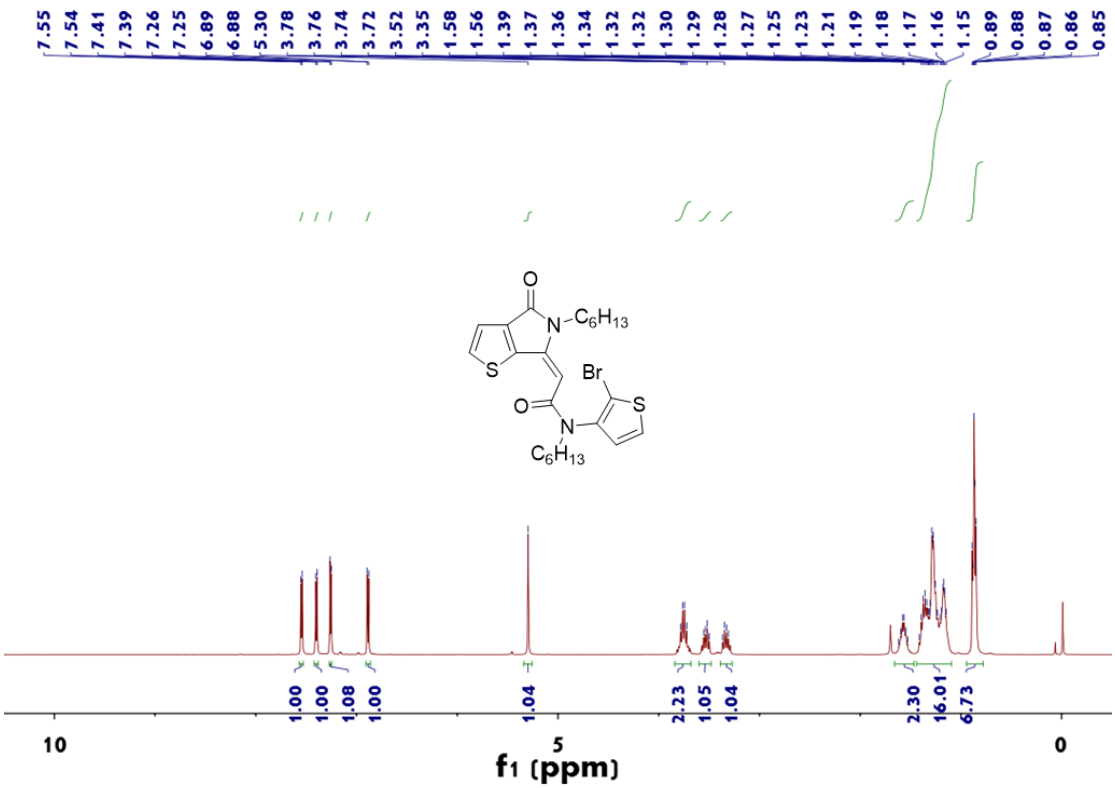
^{13}C NMR of compound TPYAc



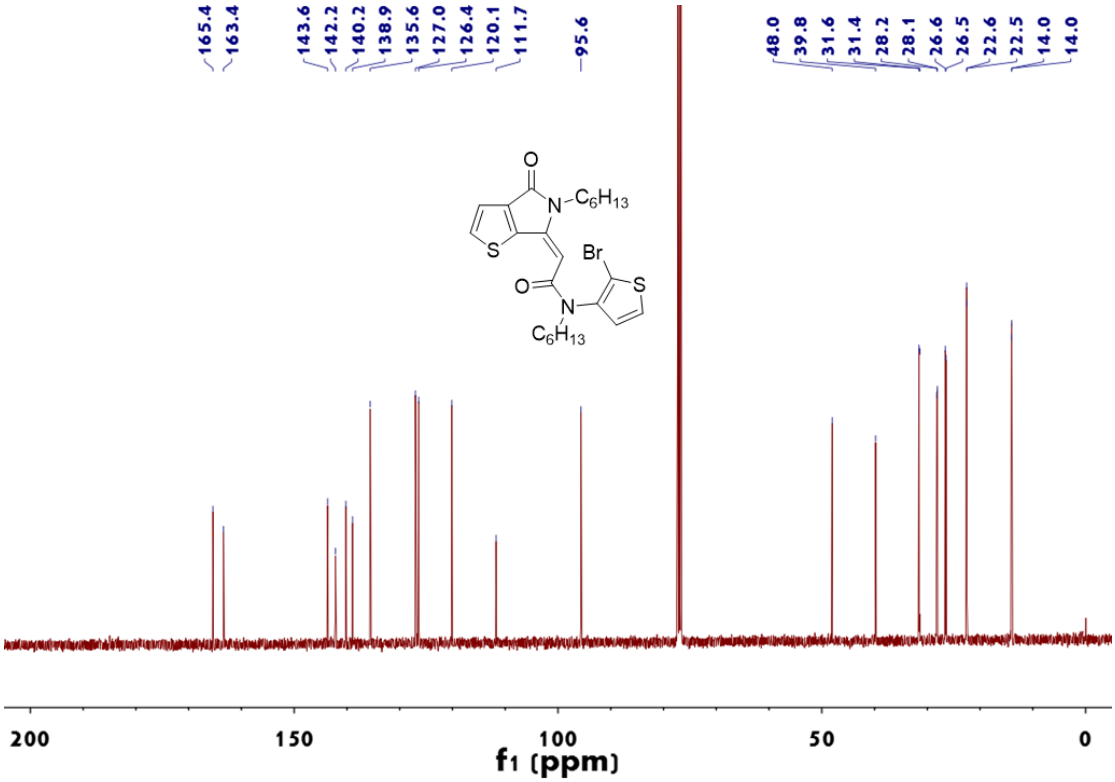
^{1}H NMR of compound TPYA



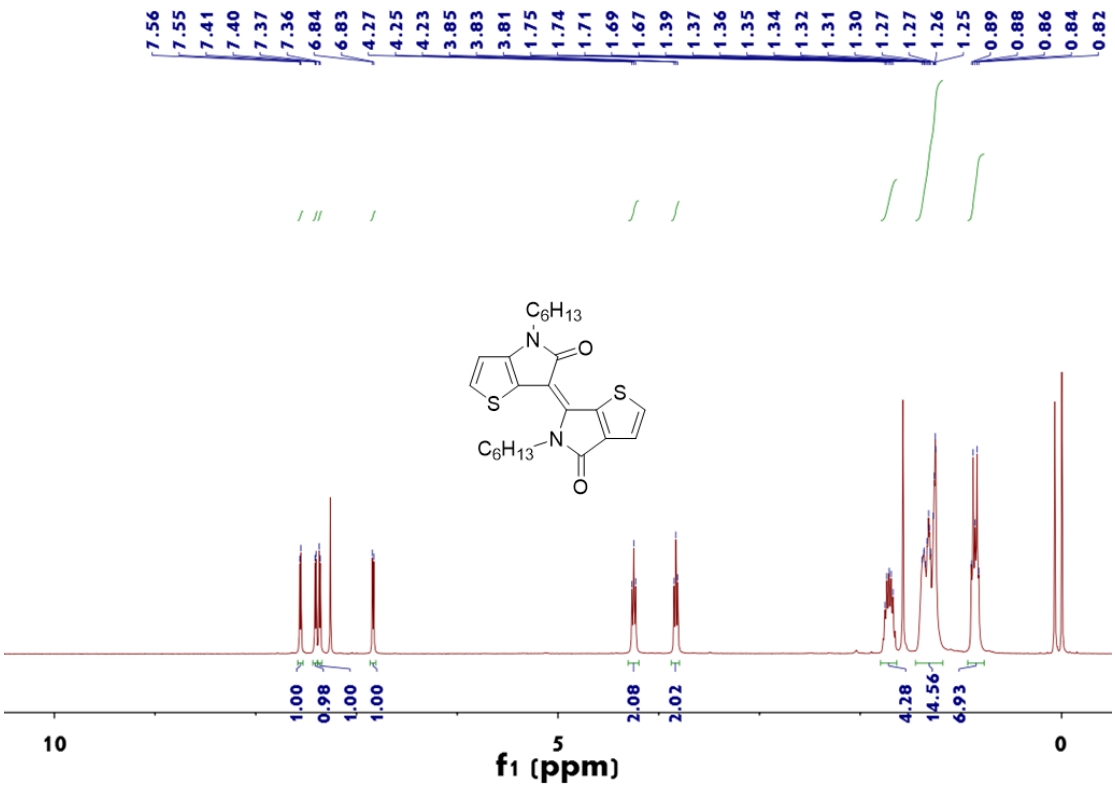
^{13}C NMR of compound TPYA



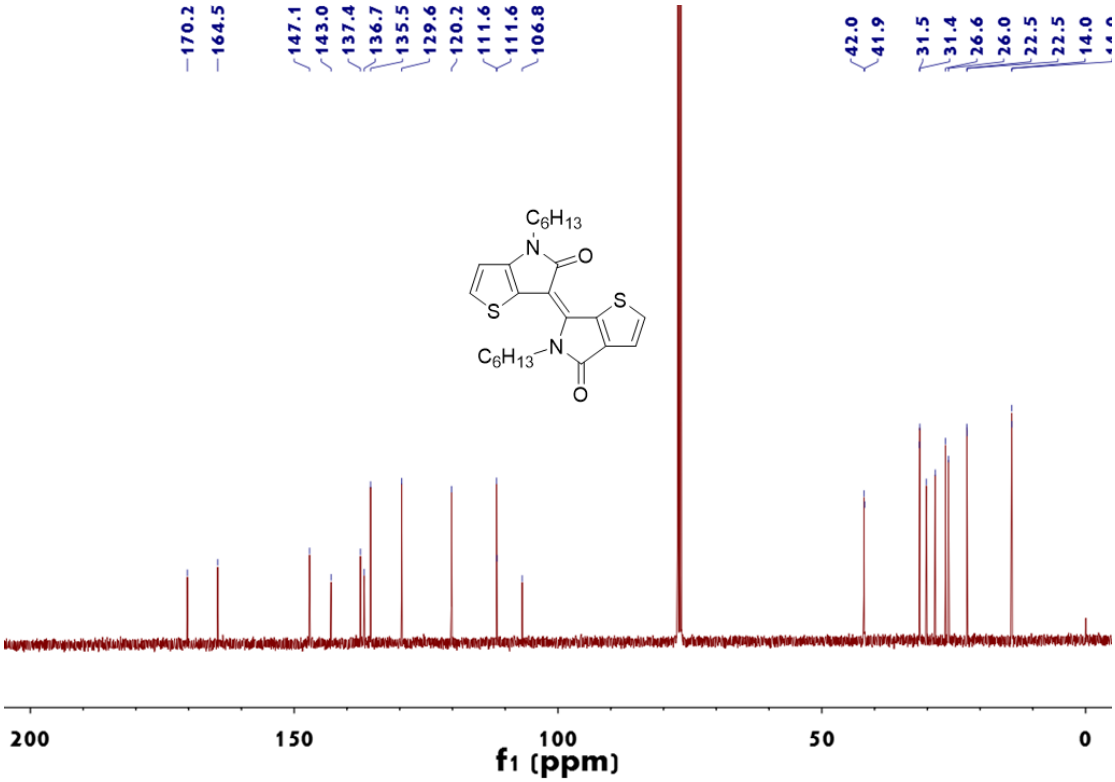
^{1}H NMR of compound TPYA-Br



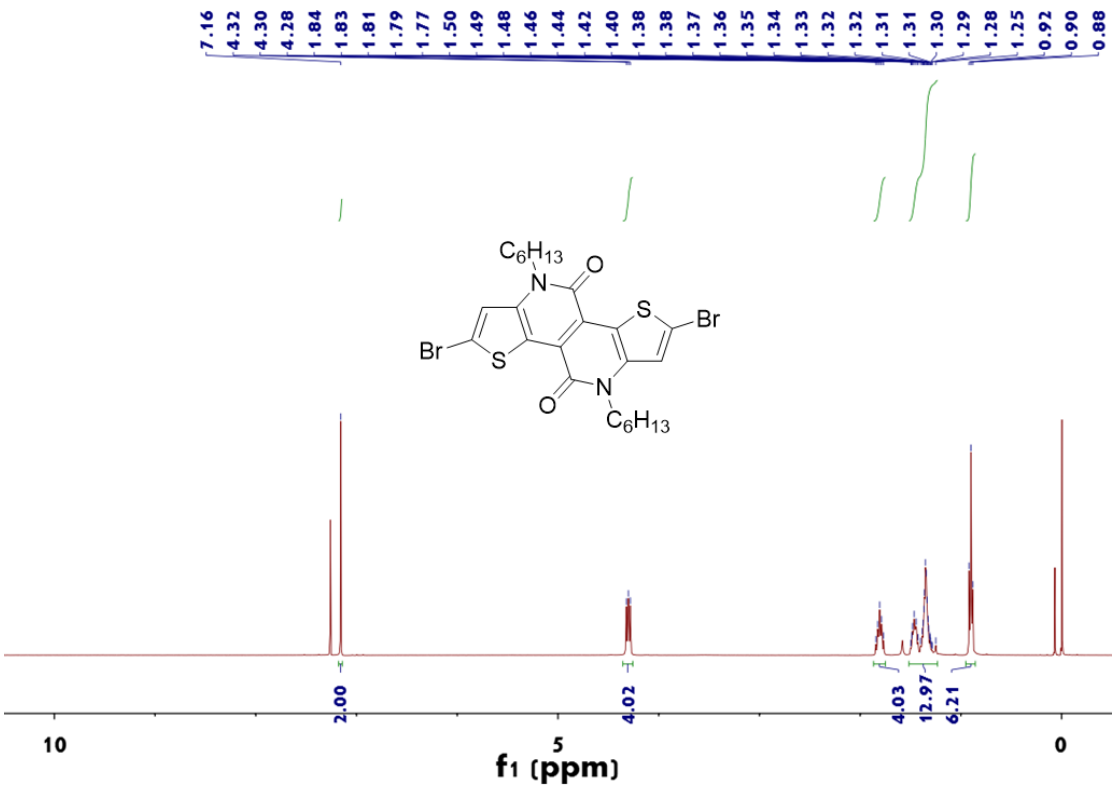
^{13}C NMR of compound TPYA-Br



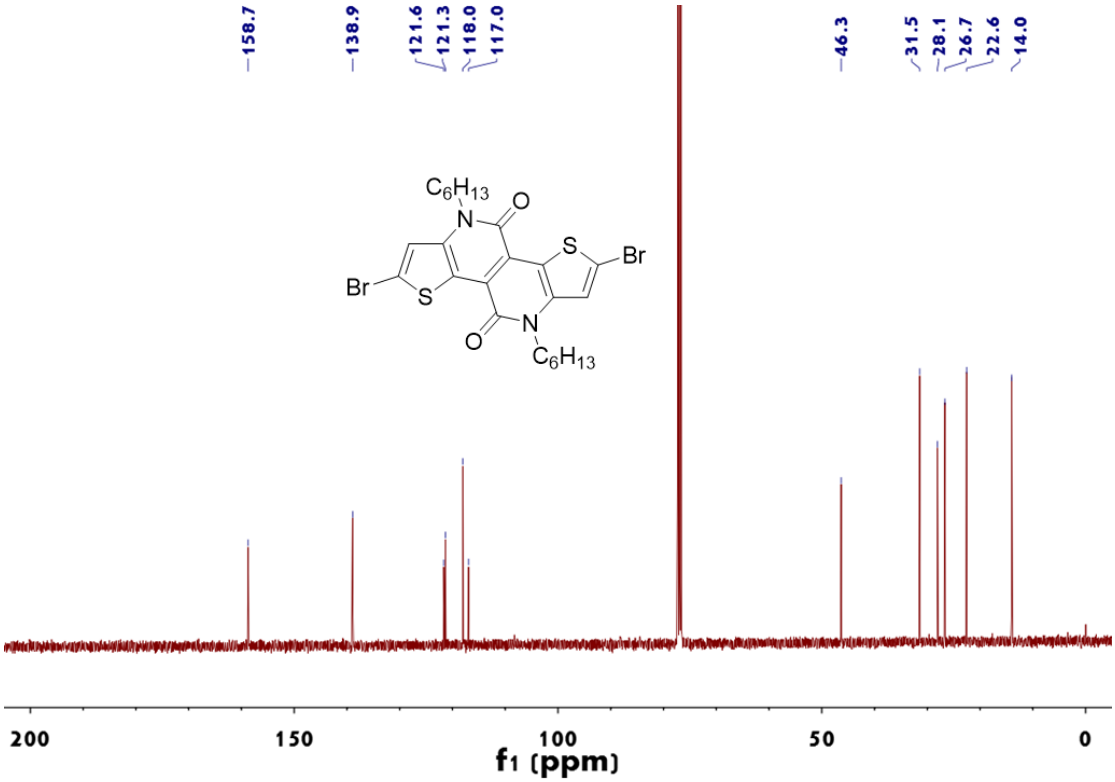
^{1}H NMR of compound isoTII



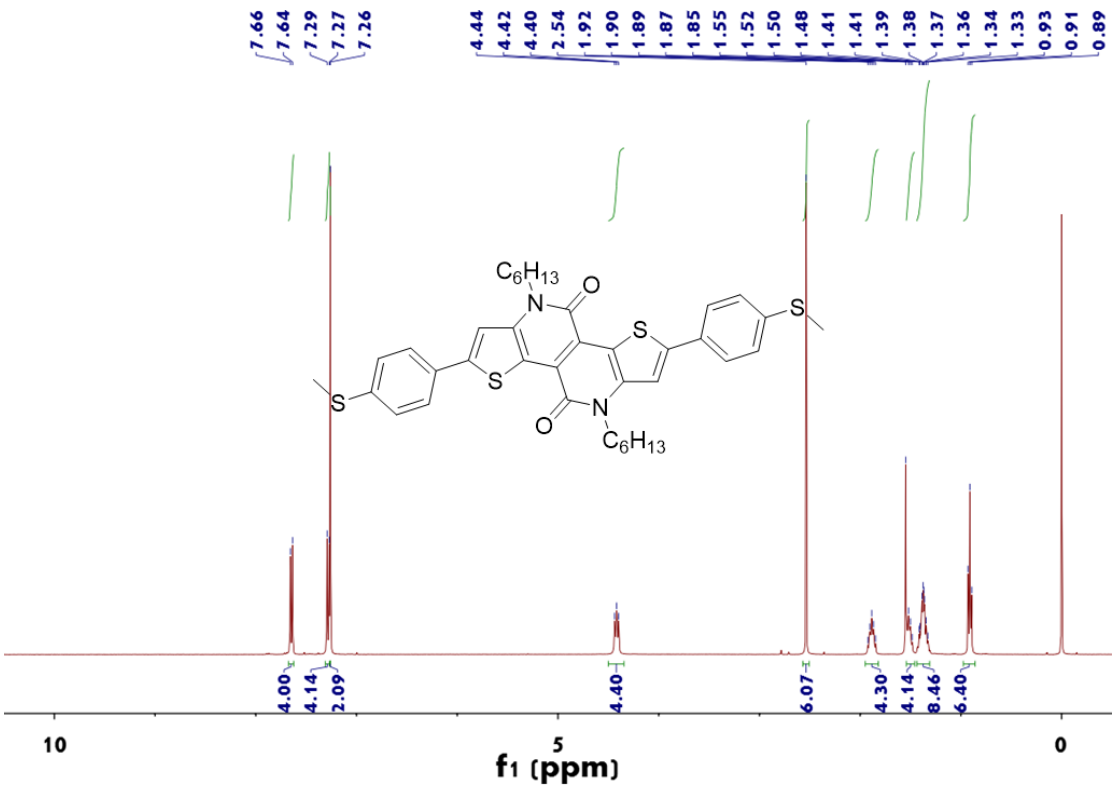
^{13}C NMR of compound isoTII



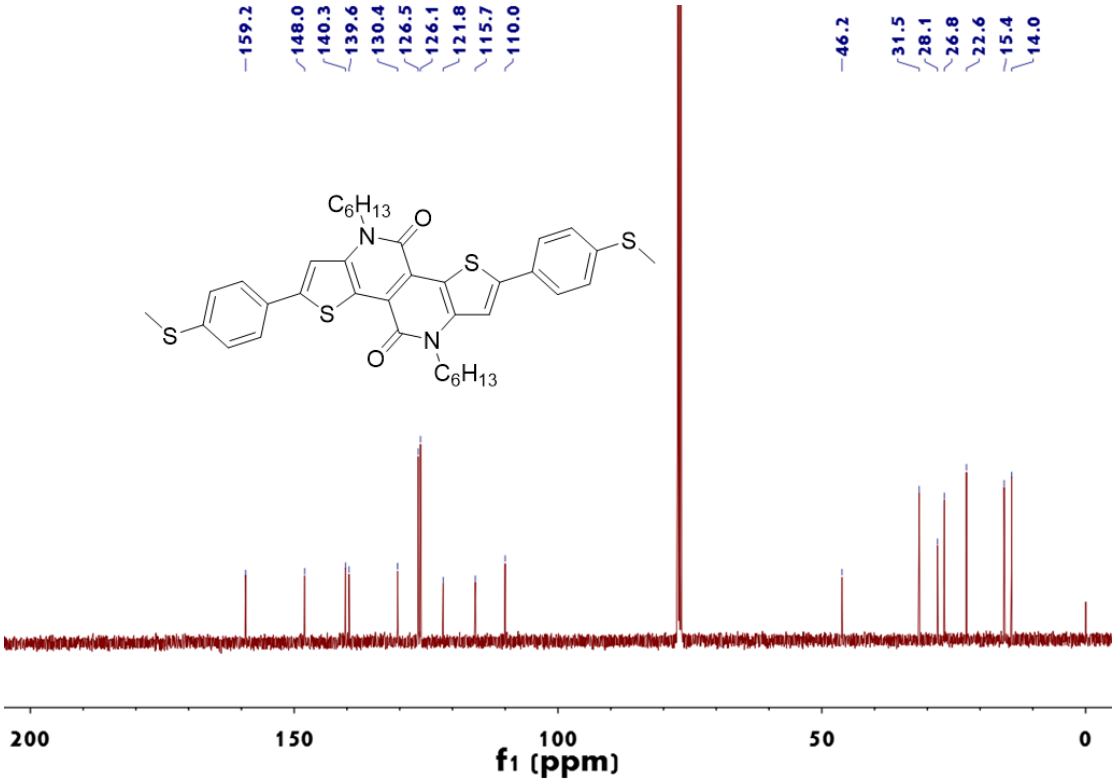
^{1}H NMR of compound TVTDA-diBr



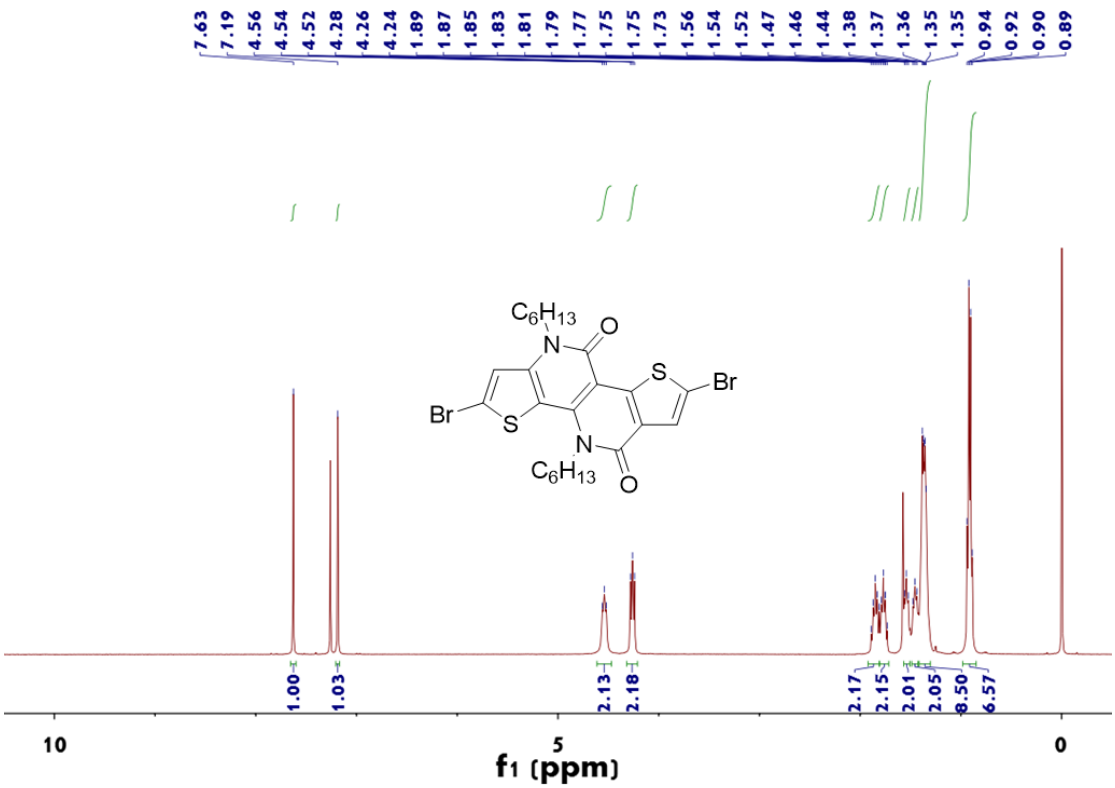
^{13}C NMR of compound TVTDA-diBr



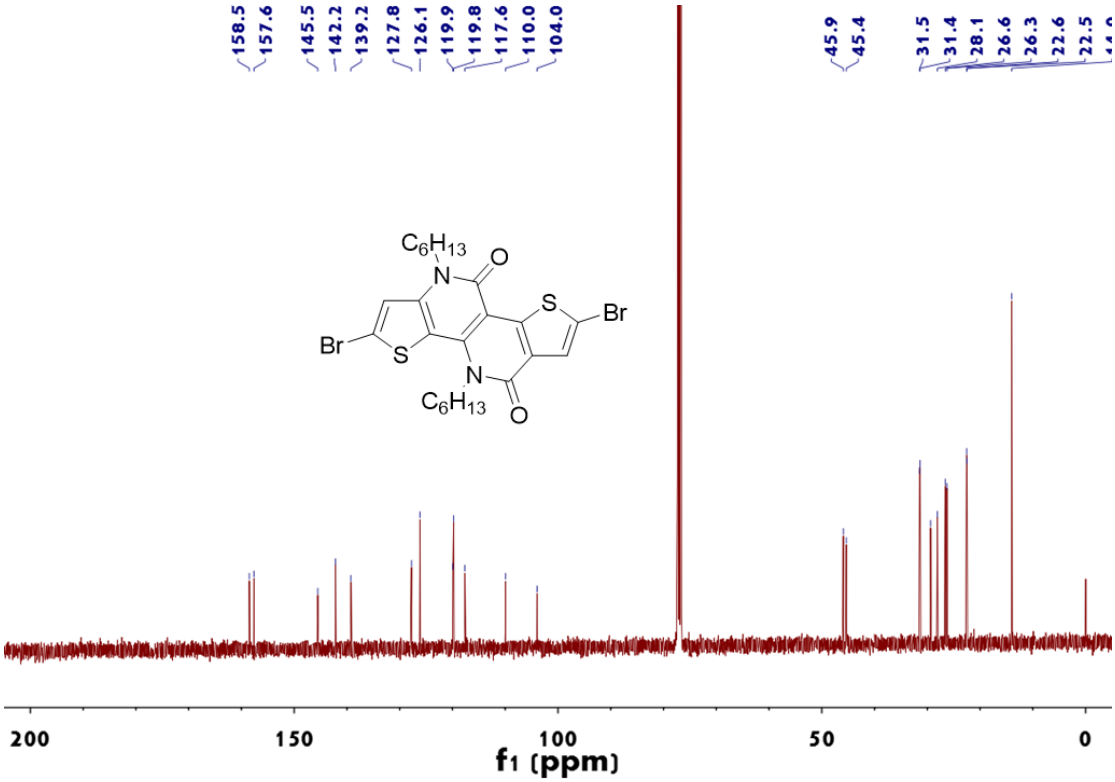
^{1}H NMR of compound TVTDAP



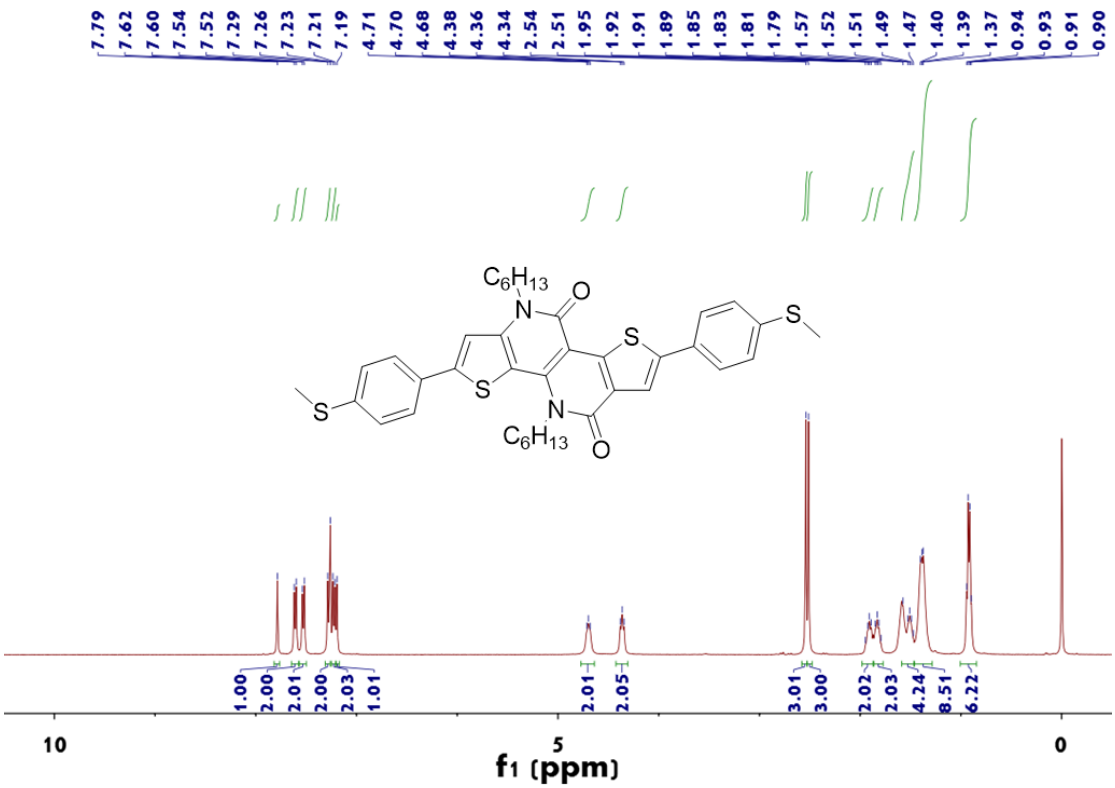
^{13}C NMR of compound TVTDAP



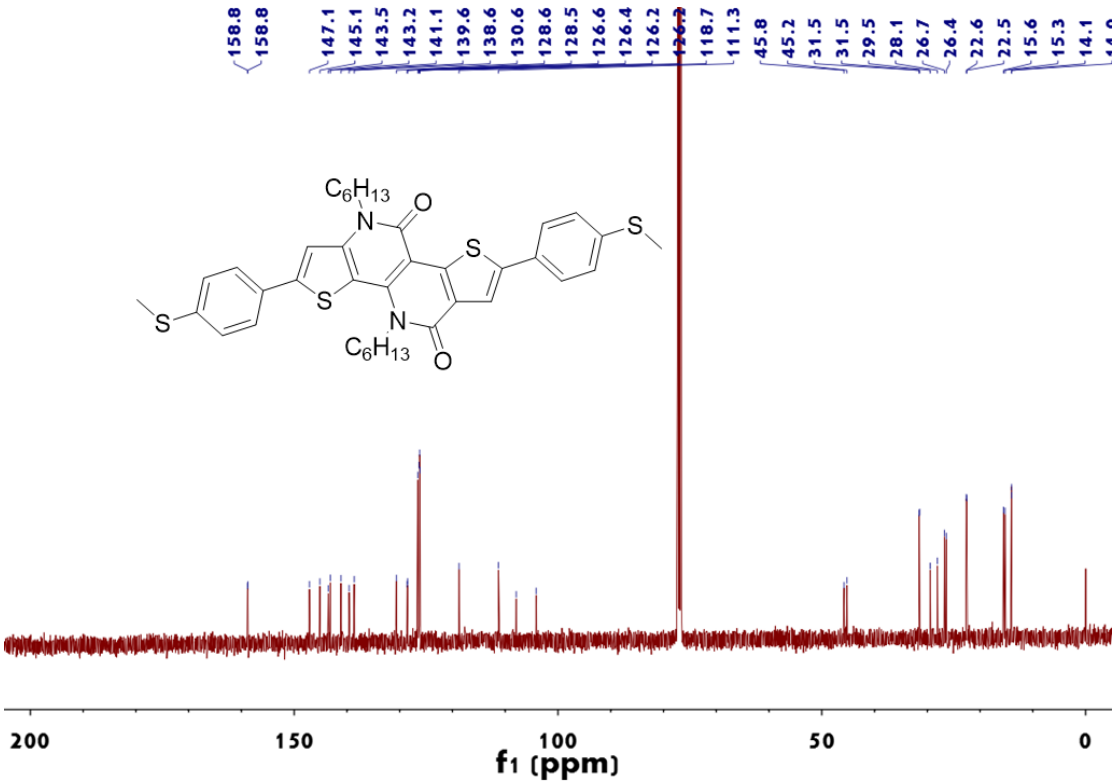
^{1}H NMR of compound isoTVTDA-diBr



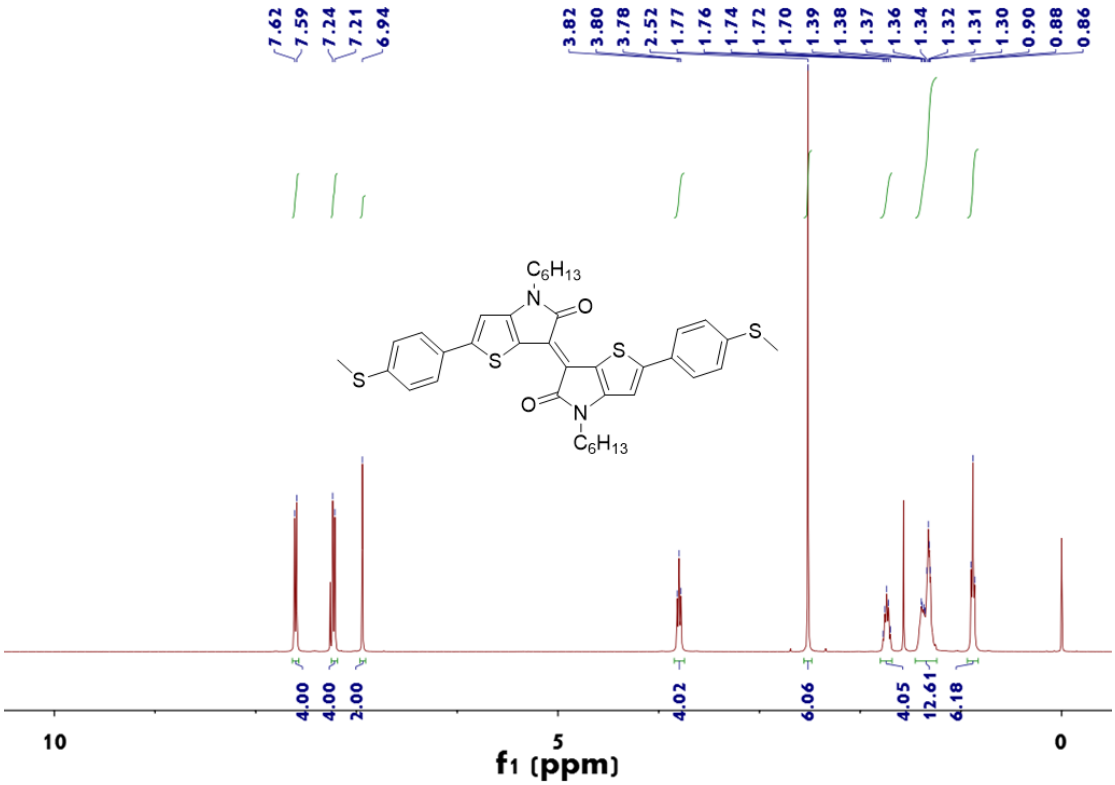
^{13}C NMR of compound isoTVTDA-diBr



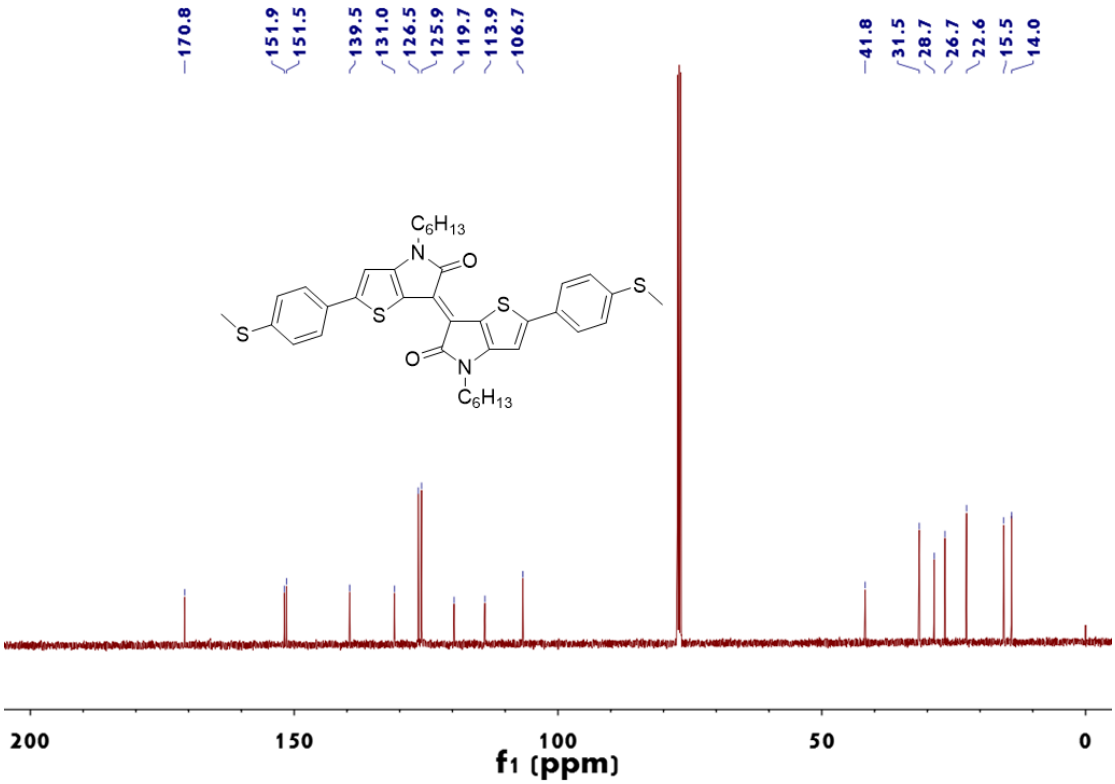
^{1}H NMR of compound isoTVTDAP



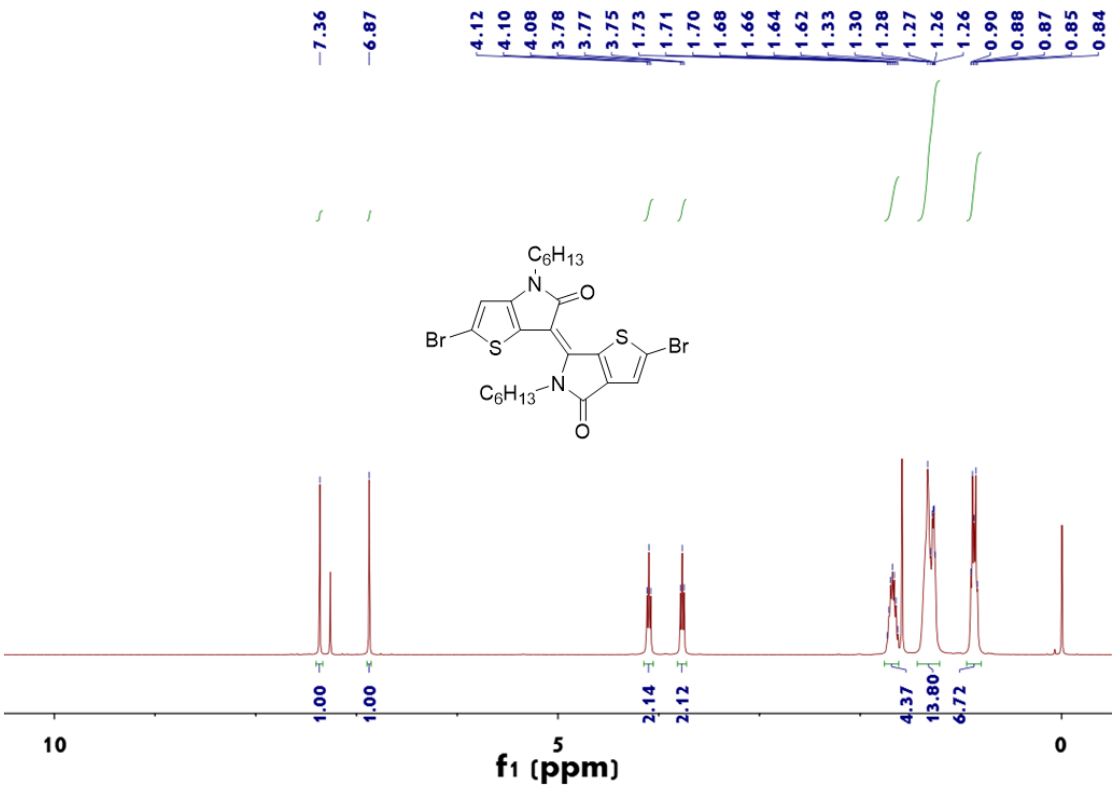
^{13}C NMR of compound isoTVTDAP



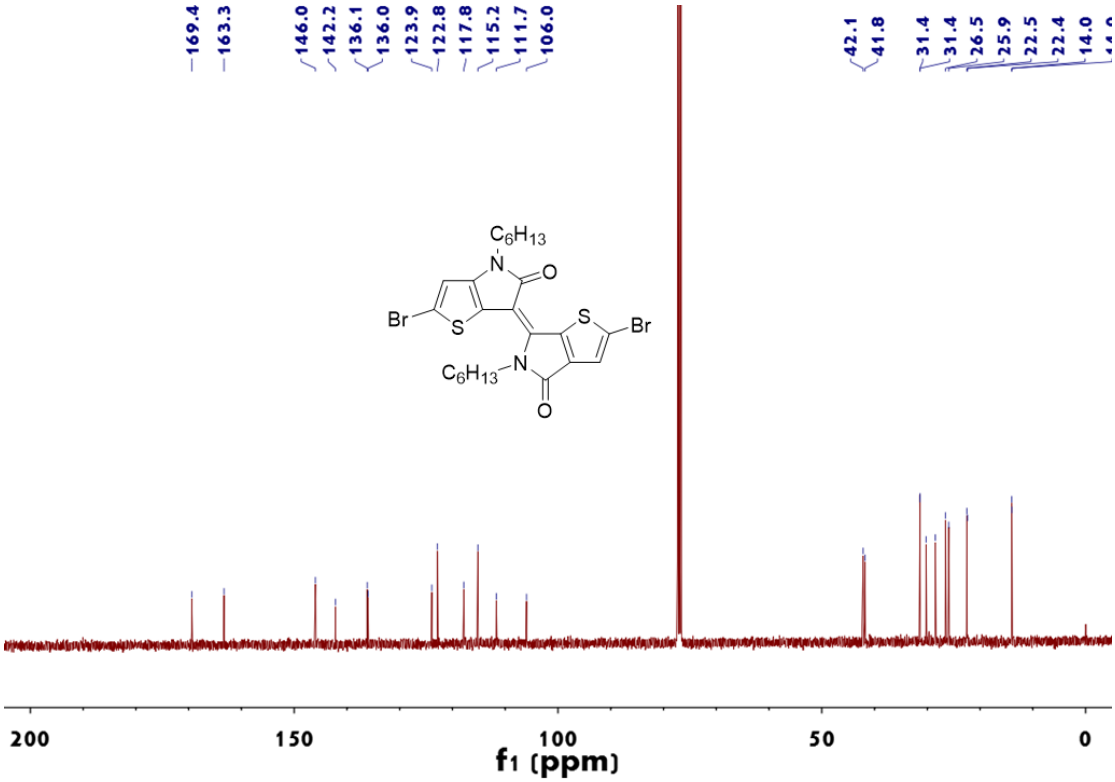
^{1}H NMR of compound TIIP



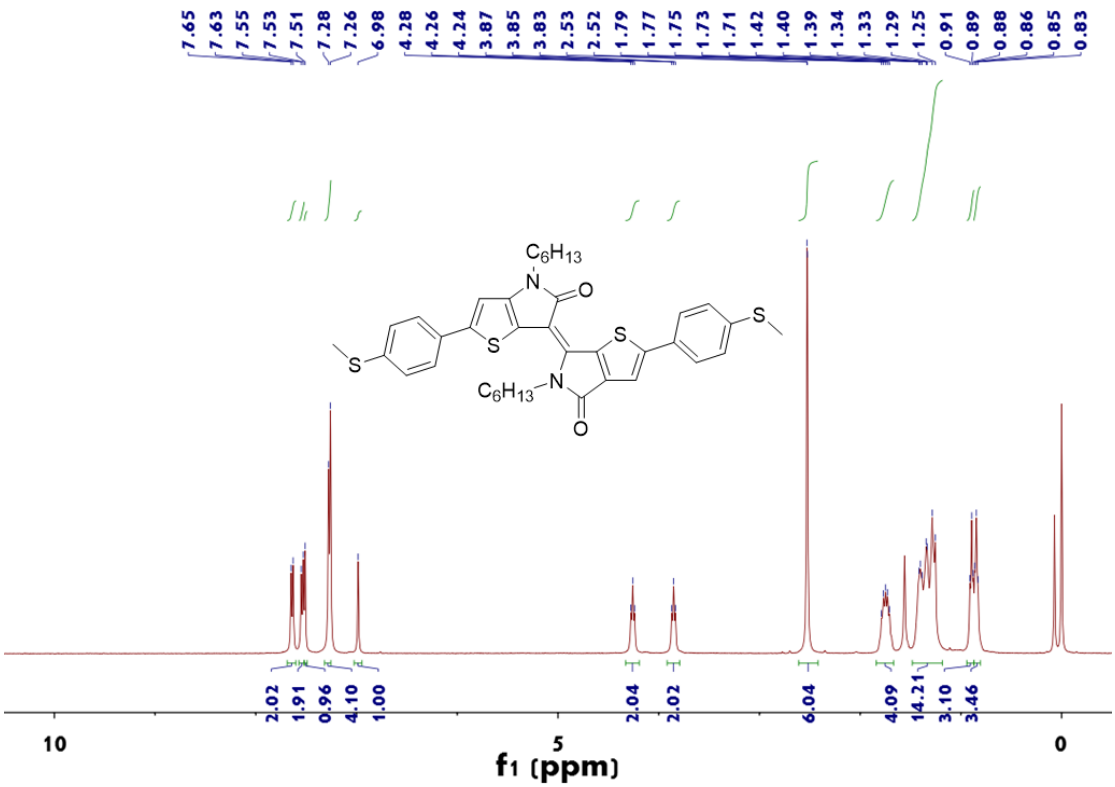
^{13}C NMR of compound TIIP



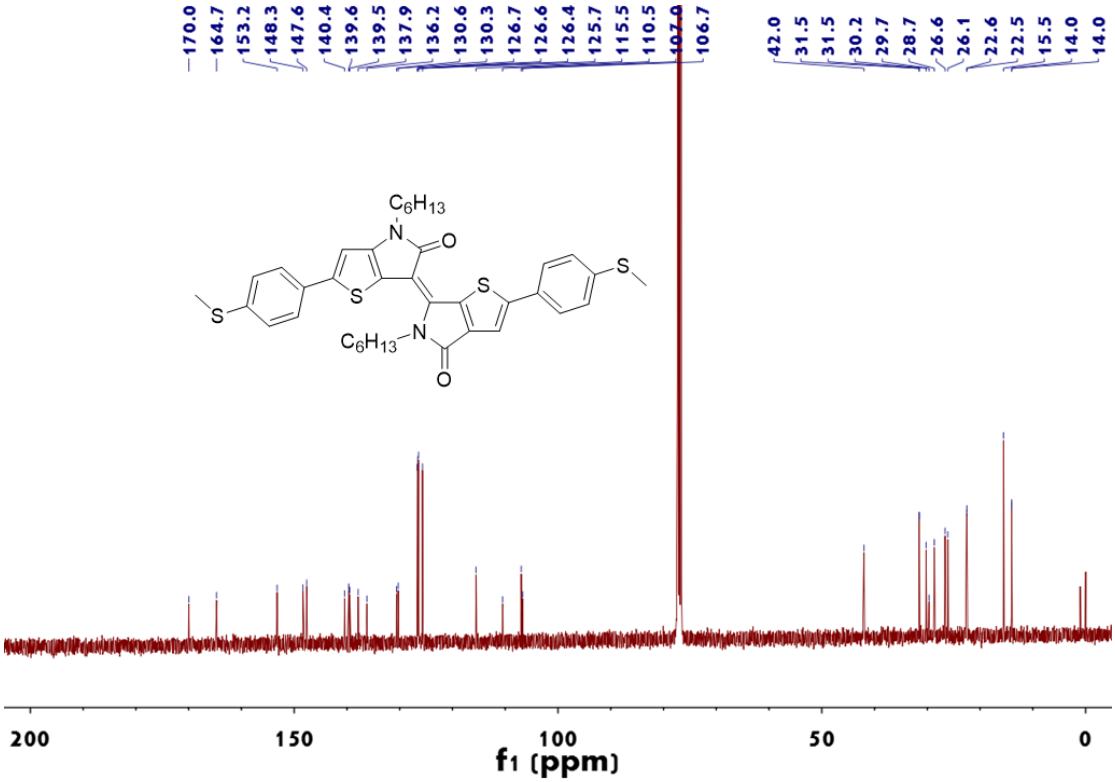
^{1}H NMR of compound isoTII-diBr



^{13}C NMR of compound isoTII-diBr



^{1}H NMR of compound isoTIIP



^{13}C NMR of compound isoTIIP