Radical-to-radical push-pull effect enhances single-molecule conductance in asymmetric diradicals

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1. General Methods

All reactions were carried out under nitrogen atmosphere using standard Schlenk techniques. All reagents and starting materials were commercially available and used without further purification. Flash column chromatography separation was performed with silica gel (200-300 mesh) as the stationary phase. Thin layer chromatography (TLC) was done on silica gel coated glass plates (HSGF 254, 2.5 x 8 cm) and visualized under UV irradiation at 254 nm and 365 nm. Solution nuclear magnetic resonance (NMR) spectra were recorded using a Bruker AV II-400 MHz spectrometer. Matrix-assisted laser desorption/ionization-time of flight (MALDI-TOF) mass spectra (MS) were measured using a Shimadzu AXIMA Confidence using 7,7,8,8-tetracyanoquinodimethane (TCNQ) in dichloromethane (DCM) as supporting matrix. High-resolution mass (HR MS) determinations were carried out on a Waters-Q-TOF-Premier. UV-vis absorption spectra were recorded on a Shimadzu UV-2600 UV-VIS spectrophotometer in spectroscopy grade DCM at 298K. ESR spectroscopy measurement was conducted by a Bruker EMX plus X-band spectrometer with 9.8 GHz microwave frequency. The sample for ESR measurement with a concentration of 0.1 mmol/L in anhydrous toluene or solid solution. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation.

2 Synthetic Details

2.1 Synthesis of compound **M1**

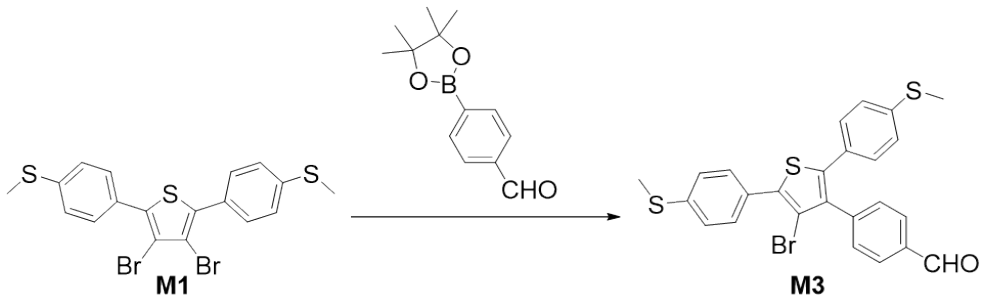
A two-neck round-bottom flask fitted with a condenser was charged with tetrabromothiophene (4.00 g, 10.0 mmol, 1.0 equiv.), 4-(methylthio)phenylboronic acid (4.03 g, 24.0 mmol, 2.4 equiv.), and K_2CO_3 (4.83 g, 35.0 mmol, 4.0 equiv.). Under nitrogen protection, bis(triphenylphosphine)palladium(II) chloride (0.49 g, 0.7 mmol, 0.07 equiv.), DMF (40 mL), and EtOH (10 mL) were added and then the reaction vessel heated at 65 °C for 12 h in an oil bath. The mixture was cooled down to room temperature and poured into 40 mL DCM. Then, the mixture was extracted with DCM (120 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 4:1 (v/v) hexane/DCM). The product compound **M1** was obtained white solid (3.29 g, 68%). ^{1}H NMR (400 MHz, DMSO-d_6,

298K) δ 7.61 (d, J = 8.4 Hz, 4H), 7.40 (d, J = 8.4 Hz, 4H), 2.53 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 138.94, 136.40, 129.82, 128.21, 125.09, 111.11, 14.38; MALDI-TOF MS: m/z: $[M+H]^+$ calcd for $C_{18}H_{14}Br_2S_3$ 484.86, found 484.87.

2.2 Synthesis of compound **M2**

Under nitrogen protection, an oven-dried 100 mL Schlenk bottle was charged with compound **M1** (1.00 g, 2.07 mmol, 1.0 equiv.) and 20 mL tetrahydrofuran. 2.5 M *n*-BuLi (0.83 mL, 2.17 mmol, 1.05 equiv.) was added at -78 °C slowly. The pale yellow solution was stirred at -78 °C for 1 hour. DMF (2 mL) was added dropwise over 5 min. Continue stirring the mixture at -78 °C for 1 hour and then the mixture was gradually warmed to room temperature. After the reaction, the obtained reaction solution was quenched with 10 mL HCl/EtOH mixture (4:1 (v/v)). Then the solution was extracted three times by saturated salt water and methylene chloride. The organic phase was dehydrated with Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 2:1 (v/v) hexane/DCM). The product compound **M2** was obtained yellow solid (0.77 g, 86%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 9.85 (s, 1H), 7.57 (dd, J = 16.2, 8.4 Hz, 4H), 7.40 (dd, J = 8.4, 4.4 Hz, 4H), 2.54 (d, J = 2.4 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 184.70, 153.07, 140.64, 139.27, 136.98, 131.31, 129.12, 128.74, 127.06, 126.22, 124.96, 114.89, 107.04, 14.25, 13.11; MALDI-TOF MS: m/z: $[M+H]^+$ calcd for $C_{19}H_{15}BrOS_3$ 434.95, found 434.93.

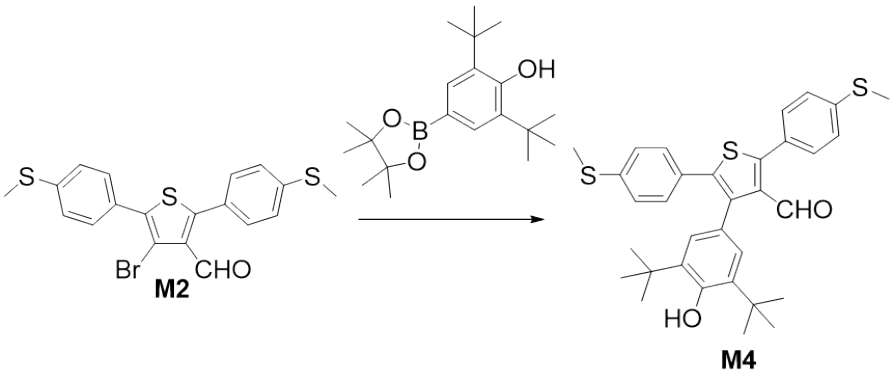
2.3 Synthesis of compound **M3**



A two-neck round-bottom flask fitted with a condenser was charged with Compound **M1** (1.20 g, 2.48 mmol, 1 equiv.), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (0.69 g, 2.98 mmol, 1.2 equiv.), and Cs_2CO_3 (1.62 g, 4.96 mmol, 2 equiv.). Under nitrogen protection, $Pd(dppf)Cl_2$ (0.088 g, 0.12 mmol, 0.05 equiv.), THF (40 mL), and H_2O (8 mL) were added and then the reaction vessel heated at 70 °C for 18 h in an oil bath. The mixture was cooled down to room temperature and poured into

40 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 2:1 (v/v) hexane/DCM). The product compound **M3** was obtained white solid (0.65 g, 64%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 10.05 (s, 1H), 7.96 (d, J = 8.1 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.1 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.14 (dd, J = 22.8, 8.5 Hz, 4H), 2.54 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 190.87, 141.19, 138.55, 138.11, 136.23, 134.43, 130.56, 130.03, 128.75, 128.47, 128.02, 125.06, 108.97, 14.32; MALDI-TOF MS: m/z: $[M+H]^+$ calcd for $C_{25}H_{19}BrOS_3$ 510.98, found 511.02.

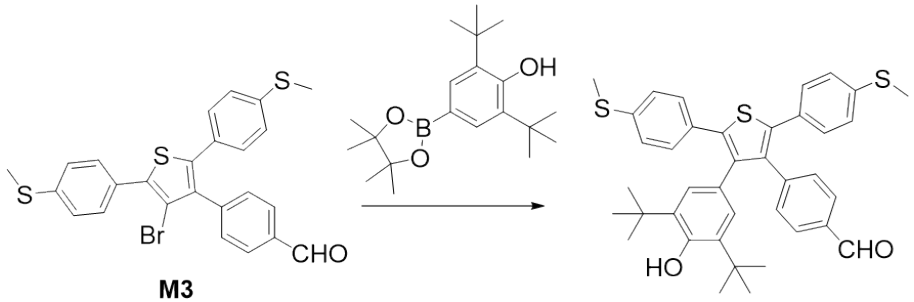
2.4 Synthesis of **M4**



A two-neck round-bottom flask fitted with a condenser was charged with Compound **M2** (0.70 g, 1.61 mmol, 1 equiv.), 2,6-di-tert-butyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (0.65 g, 1.94 mmol, 1.2 equiv.), and Cs_2CO_3 (1.05 g, 3.22 mmol, 2 equiv.). Under nitrogen protection, $Pd(dppf)Cl_2$ (0.059 g, 0.081 mmol, 0.05 equiv.), THF (30 mL), and H_2O (6 mL) were added and then the reaction vessel heated at 70 °C for 18 h in an oil bath. The mixture was cooled down to room temperature and poured into 40 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 2:1 (v/v) hexane/DCM). The product compound **M4** was obtained white solid (0.80 g, 89%). ^{1}H NMR (400 MHz, $CDCl_3$, 298K) δ 9.78 (s, 1H), 7.58 (d, J = 8.3 Hz, 2H), 7.32 (d, J = 8.3 Hz, 2H), 7.12 (d, J = 8.4 Hz, 2H), 7.06 (d, J = 8.4 Hz, 2H), 7.03 (s, 2H), 5.25 (s, 1H), 2.54 (s, 3H), 2.45 (s, 3H), 1.36 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 186.28, 152.47, 150.60, 140.18, 139.42, 137.14, 134.61, 133.13, 129.28, 128.53, 127.81, 126.72, 125.23, 124.75, 123.61, 33.27, 29.25, 28.67, 14.74, 14.35; MALDI-TOF MS: m/z: $[M]^+$ calcd for $C_{33}H_{36}O_2S_3$ 560.18, found

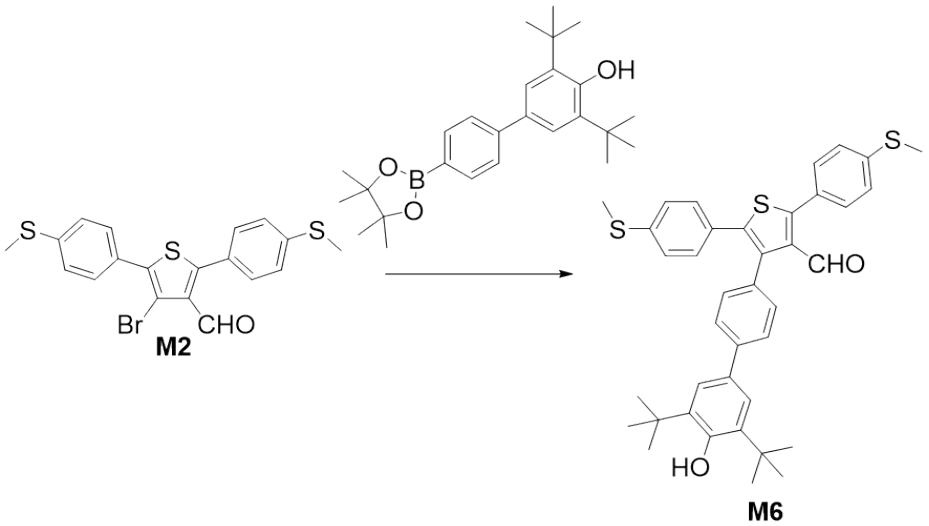
560.58.

2.5 Synthesis of compound **M5**



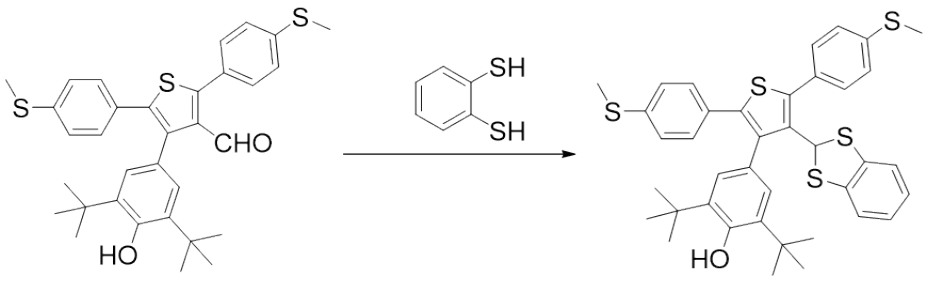
A two-neck round-bottom flask fitted with a condenser was charged with Compound **M3** (0.60 g, 1.18 mmol, 1 equiv.), 2,6-di-tert-butyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (0.47 g, 1.41 mmol, 1.2 equiv.), and Cs_2CO_3 (0.77 g, 2.36 mmol, 2 equiv.). Under nitrogen protection, $Pd(dppf)Cl_2$ (0.043 g, 0.059 mmol, 0.05 equiv.), THF (30 mL), and H_2O (5 mL) were added and then the reaction vessel heated at 70 °C for 18 h in an oil bath. The mixture was cooled down to room temperature and poured into 40 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 2:1 (v/v) hexane/DCM). The product compound **M5** was obtained white solid (0.69 g, 92%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 9.97 (s, 1H), 7.76 (d, J = 8.0 Hz, 2H), 7.25-7.10 (m, 10H), 6.87 (s, 1H), 6.57 (s, 2H), 2.44 (d, J = 5.7 Hz, 6H), 1.06 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 190.91, 151.62, 142.93, 138.86, 137.76, 137.20, 136.69, 136.29, 134.13, 133.43, 130.77, 130.19, 129.35, 128.60, 128.25, 126.91, 125.34, 125.05, 124.64, 33.04, 29.06, 14.88, 14.35; MALDI-TOF MS: m/z: $[M]^+$ calcd for $C_{39}H_{40}O_2S_3$ 636.21, found 636.21.

2.6 Synthesis of **M6**



A two-neck round-bottom flask fitted with a condenser was charged with Compound **M2** (0.65 g, 1.50 mmol, 1 equiv.), 3,5-di-*tert*-butyl-4'-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1'-biphenyl]-4-ol (0.73 g, 1.80 mmol, 1.2 equiv.), and Cs_2CO_3 (0.98 g, 3.0 mmol, 2 equiv.). Under nitrogen protection, $Pd(dppf)Cl_2$ (0.055 g, 0.075 mmol, 0.05 equiv.), THF (40 mL), and H_2O (5 mL) were added and then the reaction vessel heated at 70 °C for 18 h in an oil bath. The mixture was cooled down to room temperature and poured into 40 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 2:1 (v/v) hexane/DCM). The product compound **M6** was obtained white solid (0.81 g, 85%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 9.68 (s, 1H), 7.60 (t, J = 7.7 Hz, 4H), 7.40 (d, J = 7.9 Hz, 4H), 7.30 (d, J = 8.1 Hz, 2H), 7.17 (s, 4H), 7.11 (s, 1H), 2.55 (s, 3H), 2.43 (s, 3H), 1.44 (d, J = 4.1 Hz, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 185.74, 152.65, 151.72, 140.11, 139.73, 138.02, 137.55, 135.23, 134.13, 133.71, 131.57, 130.56, 129.79, 129.37, 128.42, 127.33, 125.56, 125.23, 124.91, 123.05, 122.76, 82.67, 33.44, 30.54, 29.31, 28.62, 23.84, 21.62, 14.26, 13.10; MALDI-TOF MS: m/z: $[M]^+$ calcd for $C_{39}H_{40}O_2S_3$ 636.21, found 636.07.

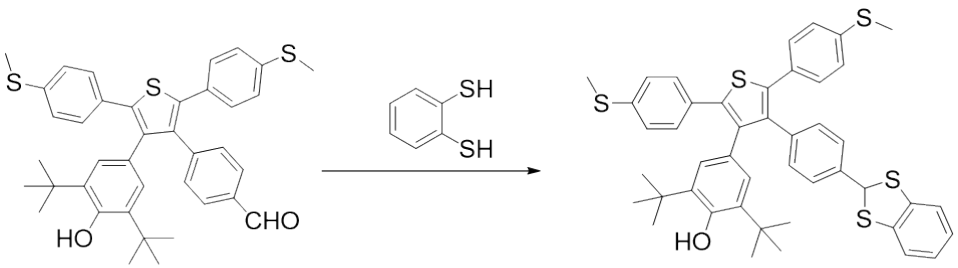
2.7 Synthesis of **Di-T1**



M4 **Di-T1**

Under nitrogen protection, a two-neck round-bottom flask was charged with 1,2-benzenedithiol (0.15 g, 1.07 mmol, 1.0 equiv.), *p*-toluenesulfonic acid monohydrate (0.21 g, 1.07 mmol, 1.1 equiv.) and 30 mL toluene. The mixture solution was stirred at 105 °C for 2 hours. Then compound **M4** (0.6 g, 1.07 mmol, 1.0 equiv.) was added at 105 °C slowly. Continue stirring the mixture at 105 °C for 20 hours. The mixture was cooled down to room temperature and poured into 50 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 4:1 (v/v) hexane/DCM). The product **Di-T1** was obtained white solid (0.56 g, 76%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 7.43 (d, J = 8.3 Hz, 2H), 7.11 (dd, J = 13.9, 8.4 Hz, 4H), 7.06-7.02 (m, 3H), 6.99-6.93 (m, 5H), 6.26 (s, 1H), 5.76 (s, 1H), 2.46 (s, 3H), 2.43 (s, 3H), 1.29 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K)δ 152.24, 140.87, 139.03, 137.41, 137.19, 136.81, 136.34, 134.81, 134.47, 130.07, 129.70, 129.25, 128.23, 126.96, 125.12, 124.06, 123.80, 119.99, 47.80, 33.34, 29.31, 14.79, 14.41; MALDI-TOF MS: m/z: $[M]^+$ calcd for $C_{39}H_{40}OS_5$ 684.16, found 684.70.

2.8 Synthesis of **Di-T2**

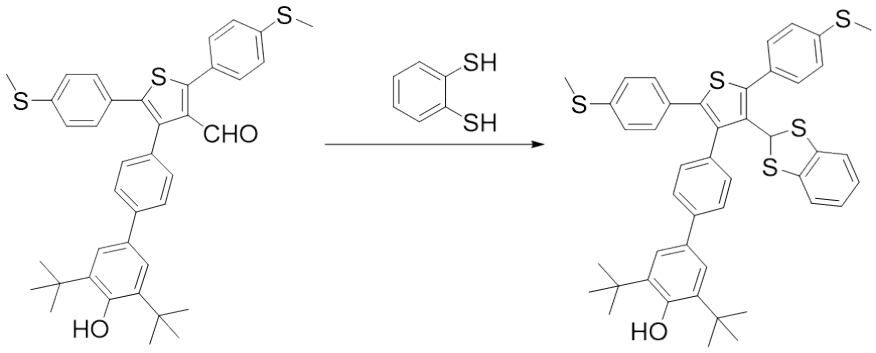


M5 **Di-T2**

Under nitrogen protection, a two-neck round-bottom flask was charged with 1,2-benzenedithiol (0.15 g, 1.07 mmol, 1.0 equiv.), *p*-toluenesulfonic acid monohydrate (0.21 g, 1.07 mmol, 1.1 equiv.) and 35 mL toluene. The mixture solution was stirred at 105 °C for 2 hours. Then compound **M5** (0.68 g, 1.07 mmol, 1.0 equiv.) was added at 105 °C slowly. Continue stirring the mixture at 105 °C for 20 hours. The mixture was

cooled down to room temperature and poured into 50 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 4:1 (v/v) hexane/DCM). The product **Di-T2** was obtained white solid (0.59 g, 72%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 7.43 (dd, J = 14.9, 8.2 Hz, 6H), 7.30 (d, J = 3.7 Hz, 4H), 7.27 (d, J = 8.1 Hz, 4H), 7.11 (s, 4H), 7.08 (s, 1H), 6.27 (s, 1H), 2.41 (s, 6H), 1.44 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 151.43, 139.05, 137.44, 136.84, 136.63, 136.35, 135.74, 133.82, 130.60, 130.33, 129.80, 128.80, 128.52, 127.07, 125.77, 125.42, 125.06, 124.69, 120.82, 55.43, 33.06, 29.13, 14.98, 14.44; MALDI-TOF MS: m/z: $[M]^+$ calcd for $C_{45}H_{44}OS_5$ 760.19, found 760.28.

2.9 Synthesis of **Di-T3**

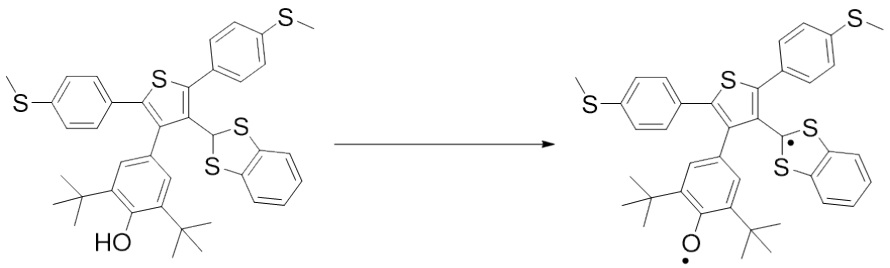


M6 **Di-T3**

Under nitrogen protection, a two-neck round-bottom flask was charged with 1,2-benzenedithiol (0.15 g, 1.07 mmol, 1.0 equiv.), *p*-toluenesulfonic acid monohydrate (0.21 g, 1.07 mmol, 1.1 equiv.) and 35 mL toluene. The mixture solution was stirred at 105 °C for 2 hours. Then compound **M6** (0.68 g, 1.07 mmol, 1.0 equiv.) was added at 105 °C slowly. Continue stirring the mixture at 105 °C for 20 hours. The mixture was cooled down to room temperature and poured into 50 mL DCM. Then, the mixture was extracted with DCM (100 mL) three times, and the combined organic phase was washed with water three times and dried over Na_2SO_4. Evaporate the solvent under reduced pressure and purified by column chromatography on silica gel (eluent: 4:1 (v/v) hexane/DCM). The product **Di-T3** was obtained white solid (0.55 g, 68%). ^{1}H NMR (400 MHz, DMSO-d_6, 298K) δ 7.46-7.40 (m, 6H), 7.30 (s, 4H), 7.27 (d, J = 7.9 Hz, 4H), 7.11 (s, 4H), 7.08 (s, 1H), 6.27 (s, 1H), 2.41 (s, 6H), 1.44 (s, 18H); ^{13}C NMR (101 MHz, $CDCl_3$, 298K) δ 152.56, 139.62, 138.18, 137.77, 137.13, 135.17, 134.96, 130.59, 130.30, 129.73, 129.52, 128.93, 128.17, 125.01, 124.64, 123.67, 122.71, 119.93, 47.13, 33.50, 30.49, 29.51, 28.76, 28.50, 28.23, 28.06, 14.38, 13.10 (s); MALDI-TOF MS:

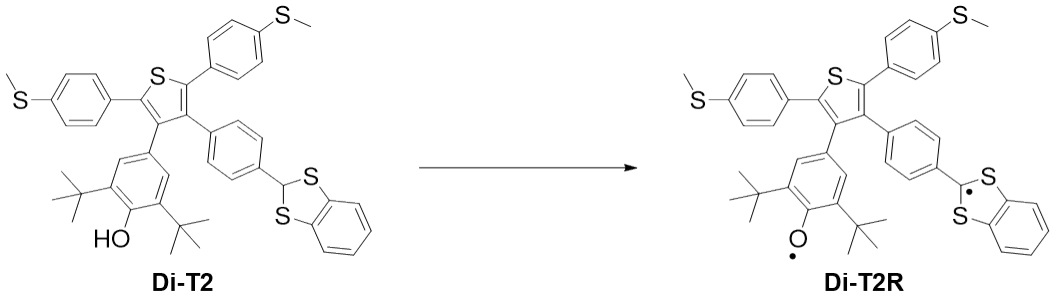
m/z: $[M]^+$ calcd for $C_{45}H_{44}OS_5$ 760.19, found 760.76.

2.10 Synthesis of **Di-T1R**



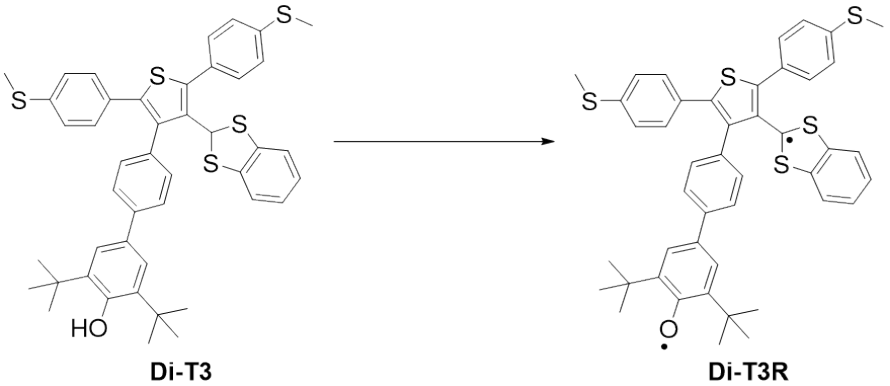
Lead (IV) oxide (0.14 g, 40.0 eq) and **T-1** (10 mg, 1.0 eq) were suspended in DCM (10 mL). After stirring the reaction mixture at room temperature for 40 minutes, the excess lead(IV) oxide was filtered off and the solvent was removed under reduced pressure to yield **Di-T1R** as a dark green solid. Yield: 98 %. HRMS (ESI^+): calcd for $C_{39}H_{38}OS_5$ 682.1526, found $[M+H]^+$ 683.1604.

2.11 Synthesis of **Di-T2R**



Lead (IV) oxide (0.13 g, 30.0 eq) and **T-2** (10 mg, 1.0 eq) were suspended in DCM (10 mL). After stirring the reaction mixture at room temperature for 40 minutes, the excess lead(IV) oxide was filtered off and the solvent was removed under reduced pressure to yield **Di-T2R** as a dark green solid. Yield: 98 %. HRMS (ESI^+): calcd for $C_{45}H_{42}OS_5$ 758.1839, found $[M+H]^+$ 759.1908.

2.11 Synthesis of **Di-T3R**



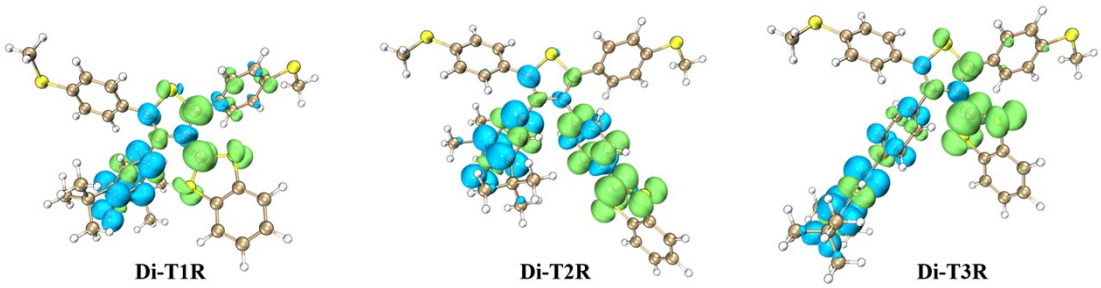
Lead (IV) oxide (0.13 g, 30.0 eq) and **T-3** (10 mg, 1.0 eq) were suspended in DCM (10

mL). After stirring the reaction mixture at room temperature for 40 minutes, the excess lead(IV) oxide was filtered off and the solvent was removed under reduced pressure to yield **Di-T3R** as a dark purple solid. Yield: 98 %. HRMS (ESI^+): calcd for $C_{45}H_{42}OS_5$ 758.1839, found $[M+H]^+$ 759.1907.

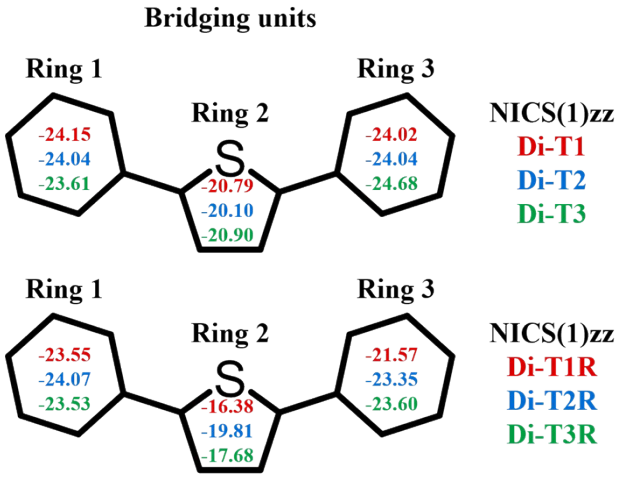
3. DFT calculations

Theoretical calculations were performed on the all compounds with the Gaussian 16 program suite using the density functional theory (DFT) with the long-range-corrected hybrid exchange-correlation functional CAM-B3LYP employing the 6-311+g(d,p) basis set for all atoms (Ref. *Chem. Phys. Lett.* **2004**, *393*, 51-57). And the obtained stationary points were characterized by frequency calculations.

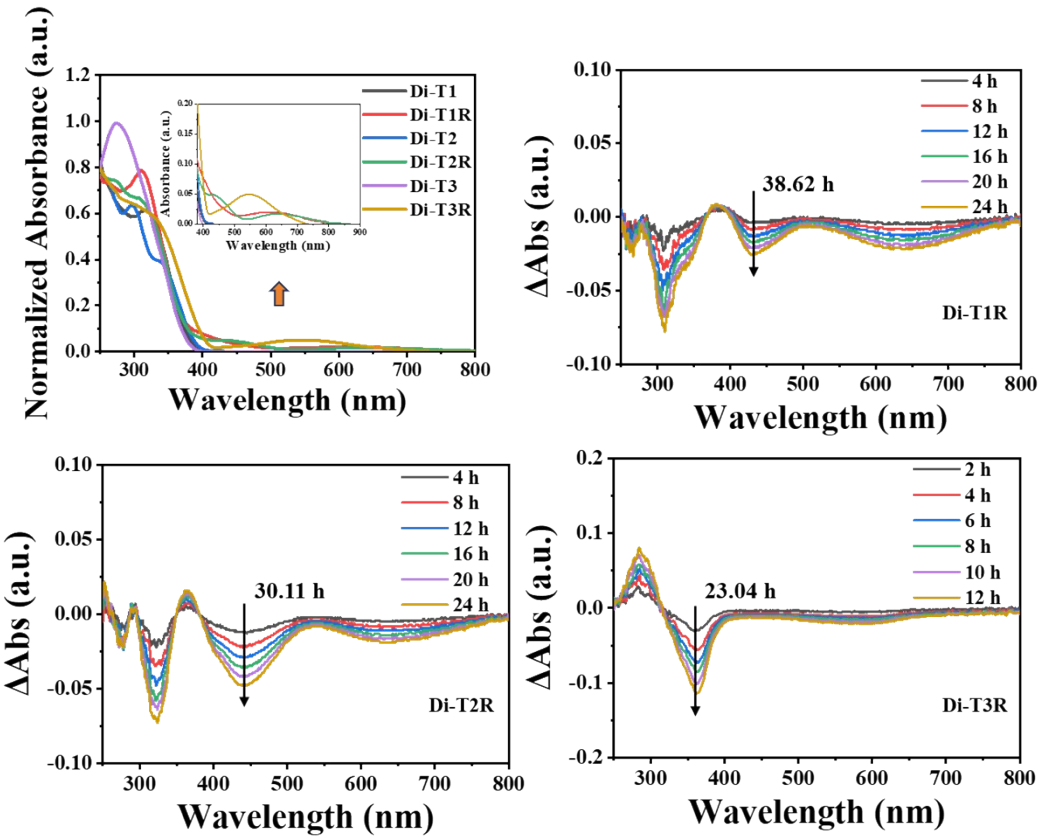
To have a deep insight into the conductance trend during the reaction process, theoretical simulations using a combination of DFT and nonequilibrium Green's functions (NEGF) in the Quantum ATK package (Quantum ATK, 2022.12 U version) were carried out. Two gold electrodes (111) consist of 6×6 unit cells to ensure no intermolecular interactions within the device, with an extension region thickness of three gold layers. The electrode tips adopt a two-layer pyramidal cluster structure, providing stable contact with the sulphur-methyl anchor points on both sides. The generalized gradient approximation (GGA) Perdew Burke-Ernzerhof (PBE) formulation is adopted for the molecules as the exchange correlation function, except for polarized GGA for the radical ones. The double-zeta plus polarization (DZP) basis set is for all the atoms, except for Au atoms with a double-zeta (DZ) basis set, to save computational time. A mesh cutoff energy is set to be 200 Ry and the optimization force tolerance of the molecular device is 0.02 eV/Å. The transmission probability through the molecular junction can be obtained from the Landauer-like Equation. The k point with a grid of (5×5×201) was used in the calculation of the transmission spectrum. (Ref. *Sci. Adv.* **2024**, *10*, eadp7307; *J. Am. Chem. Soc.* **2024**, *146*, 35347)



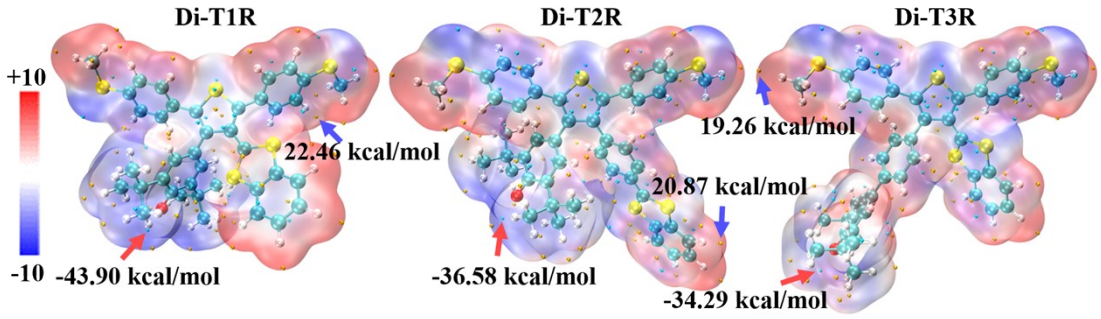
Supplementary Fig. 1. The spin density distribution maps for the asymmetric diradical Di-T1R, Di-T2R, and Di-T3R in their ground spin state.



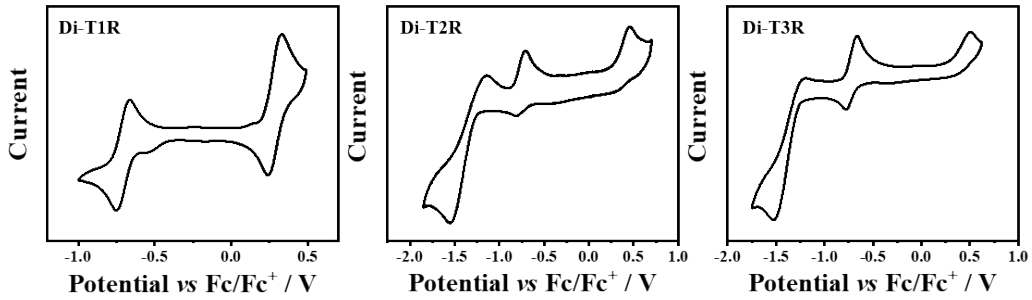
Supplementary Fig. 2. Calculated NICS(1)zz values for Di-T1, Di-T2, Di-T3, Di-T1R, Di-T2R and Di-T3R.



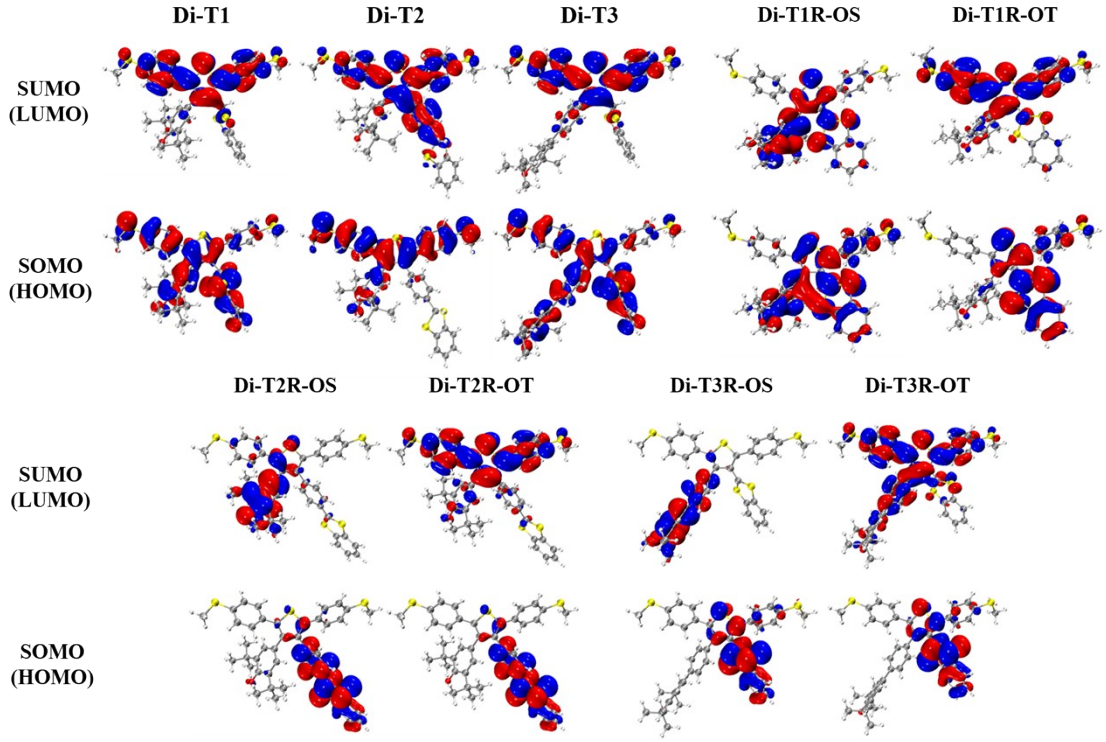
Supplementary Fig. 3. The UV-*vis*-NIR absorption spectra of Di-T1R, Di-T1, Di-T2R, Di-T2, Di-T3R and Di-T3 in air at room temperature. The difference spectra obtained by subtracting the initial absorption spectrum (0 h) from those recorded at different time intervals. The half-lives (τ) of the radicals were determined by the equation $I(t)=I_0\ (1/2)^{(t/\tau)}$.



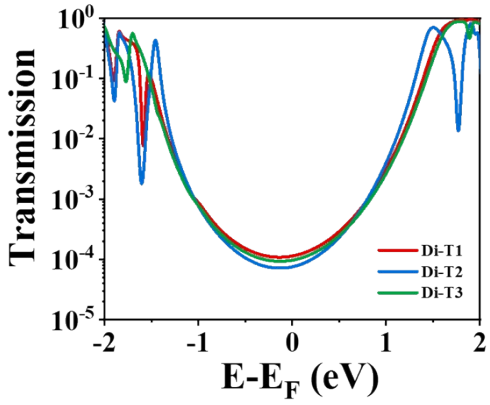
Supplementary Fig. 4. The surface electrostatic potential analysis of Di-T1R, Di-T2R, and Di-T3R.



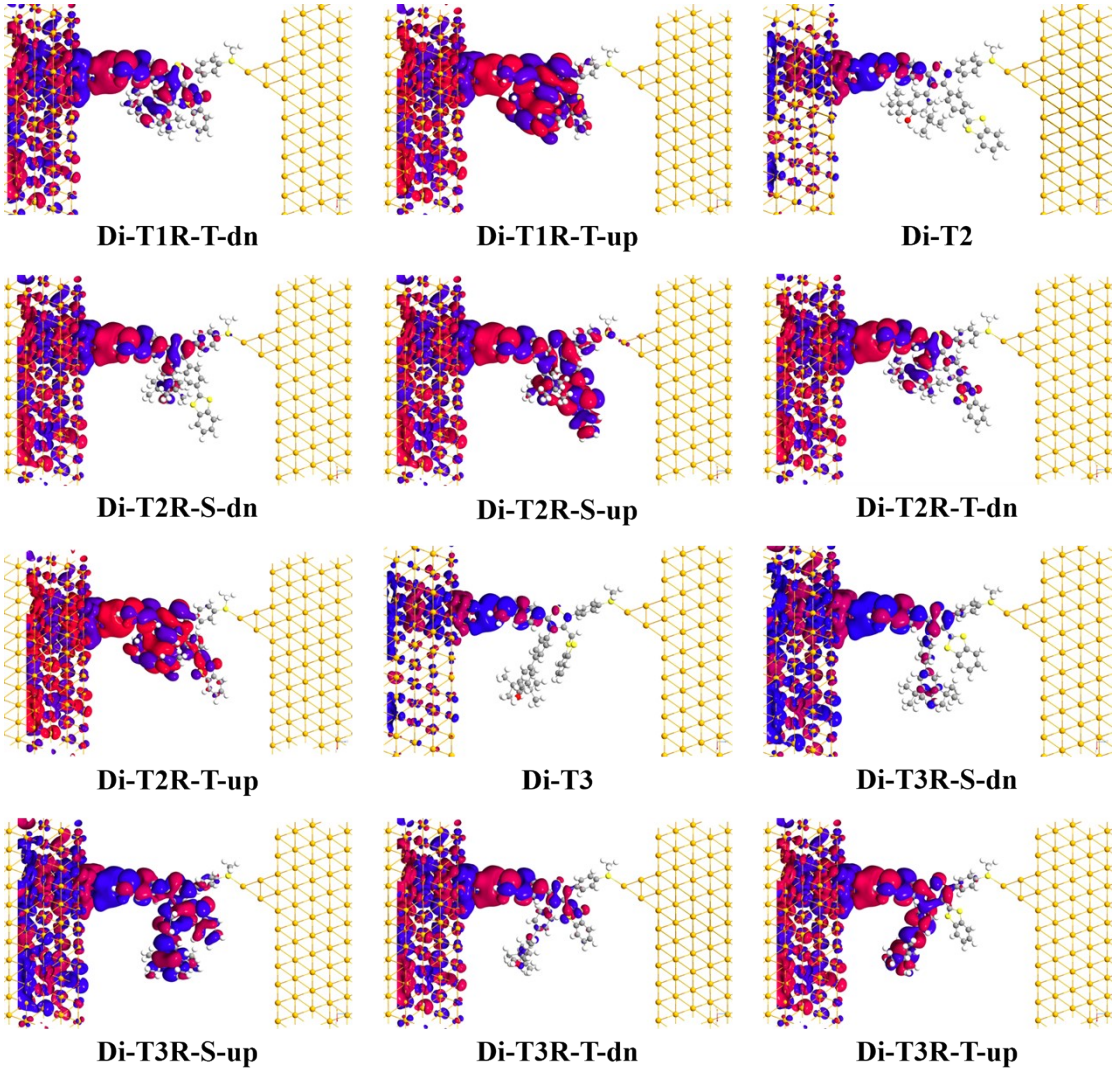
Supplementary Fig. 5. Cyclic voltammetry test curves of Di-T1R, Di-T2R, and Di-T3R in air at room temperature.



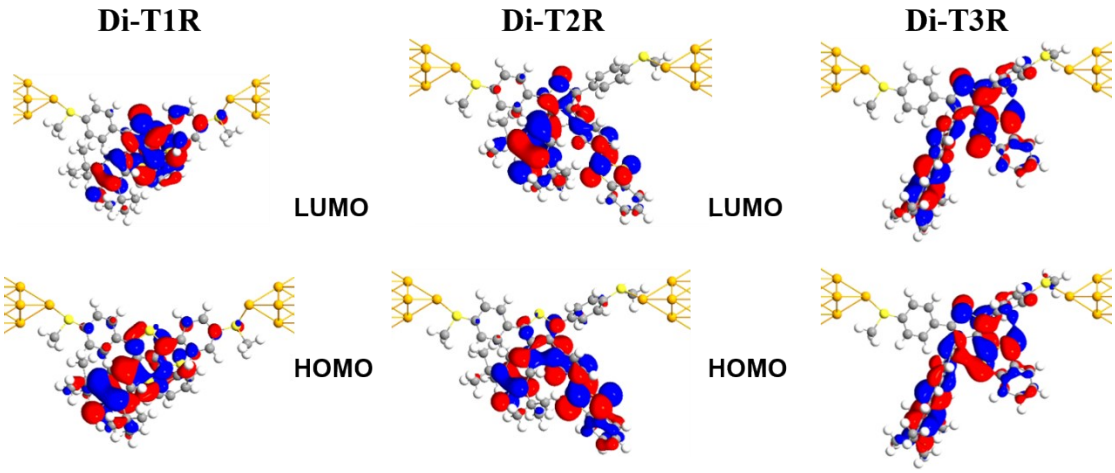
Supplementary Fig. 6. The molecular frontier orbital of thiophene derivatives.



Supplementary Fig. 7. Transmission spectra plotted semi-logarithmically (against energy relative to the Fermi energy) for Di-T1, Di-T2, and Di-T3.



Supplementary Fig. 8. The calculated transmission eigenstate near the 0 V the Fermi level. The iso value is uniformly set at 0.03 for better comparison.

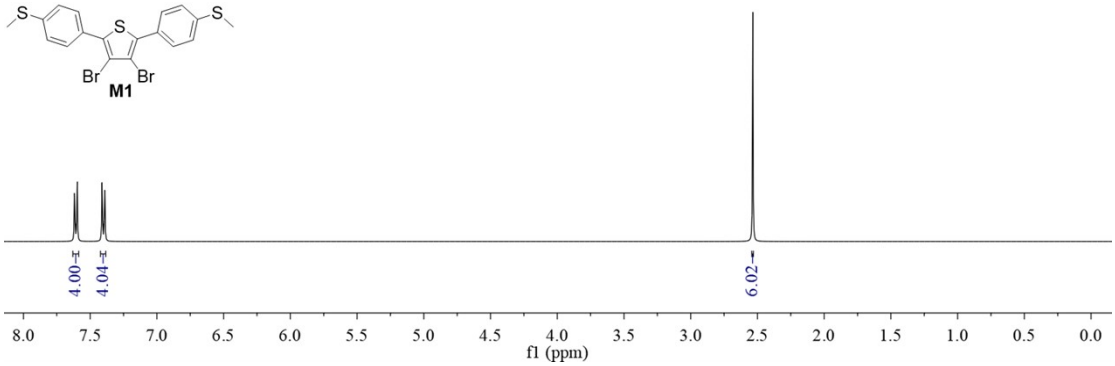


Supplementary Fig. 9. The calculated Molecular Projection Self-Consistent Hamid (MPSH) for radical molecules. The iso value is uniformly set at 0.05 for better comparison.

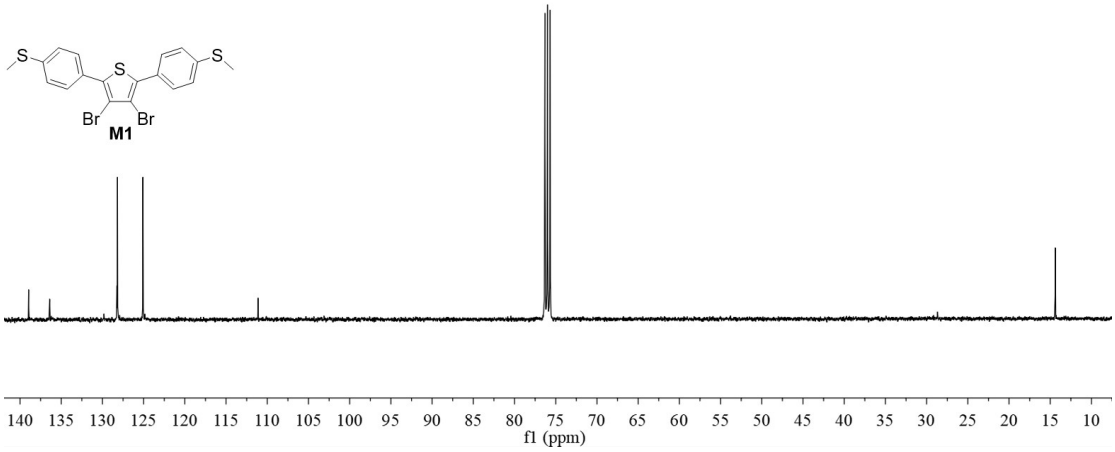
4. NMR and Mass Spectra

4.1 NMR Spectra

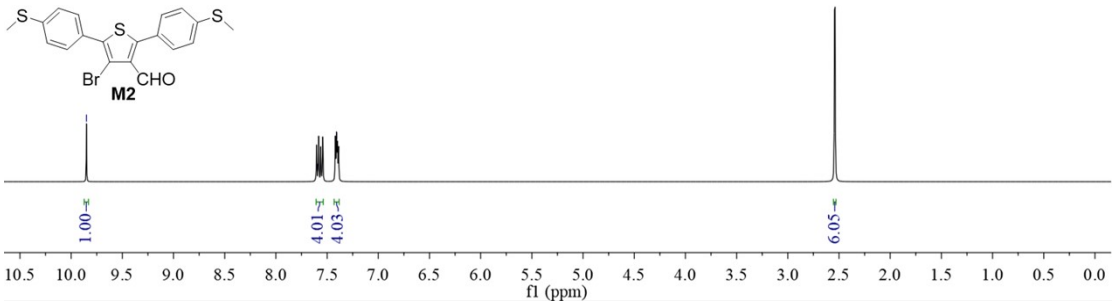
^{1}H-NMR of **M1** (400 MHz, $CDCl_3$, 298K)



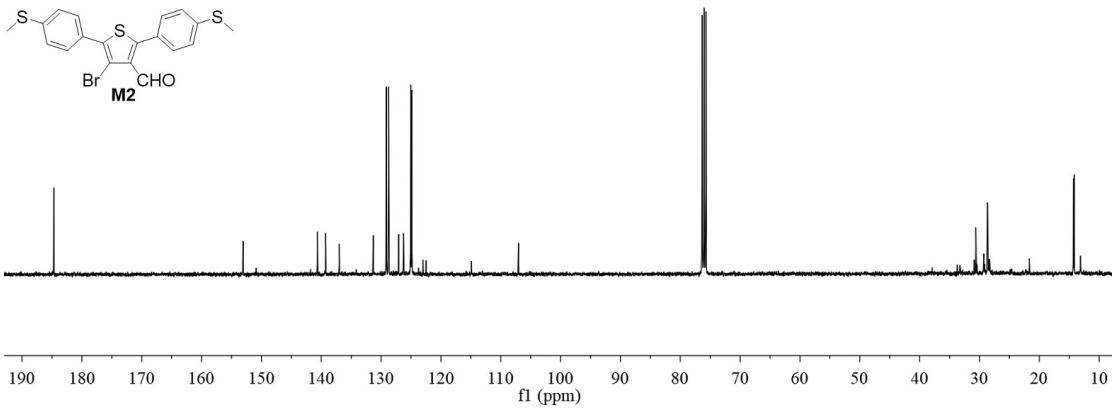
^{13}C-NMR of **M1** (101 MHz, $CDCl_3$, 298K)



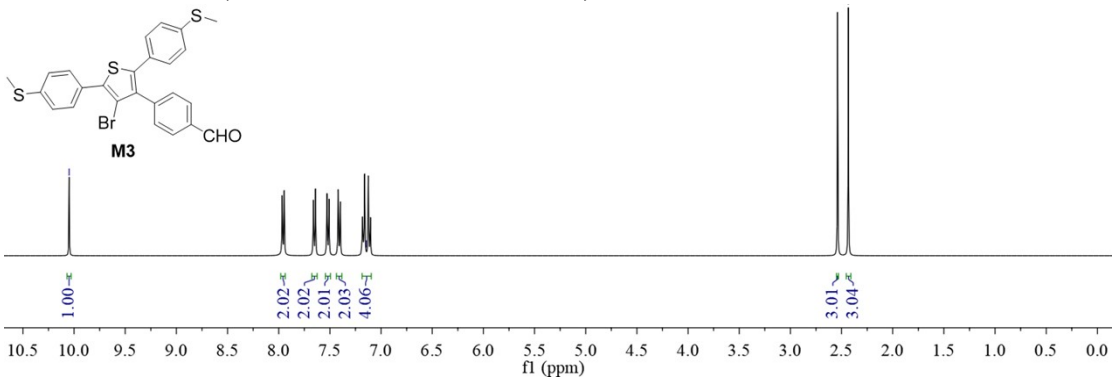
^{1}H-NMR of **M2** (400 MHz, DMSO-d_6, 298K)



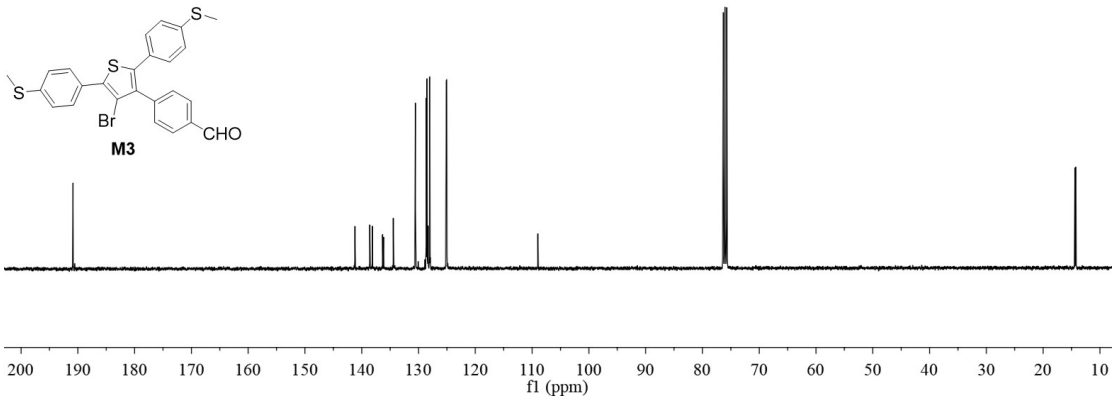
^{13}C-NMR of **M2** (101 MHz, $CDCl_3$, 298K)



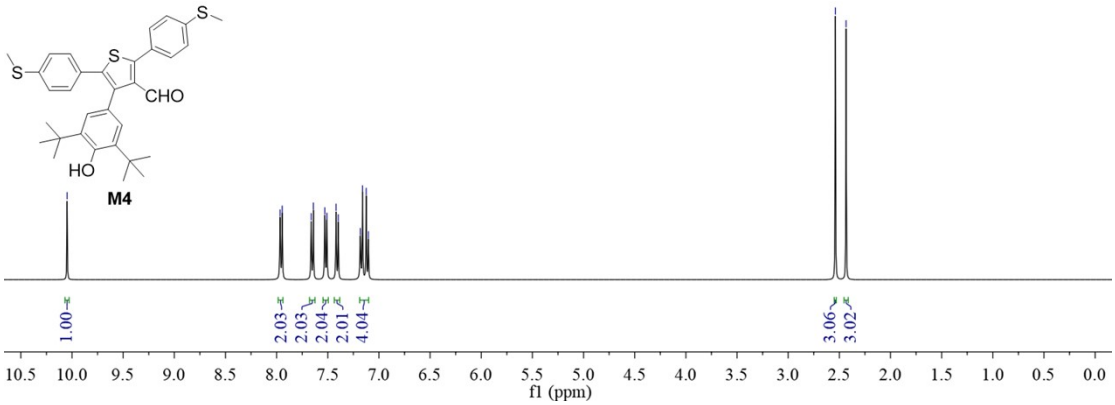
^{1}H-NMR of **M3** (400 MHz, DMSO-d_6, 298K)



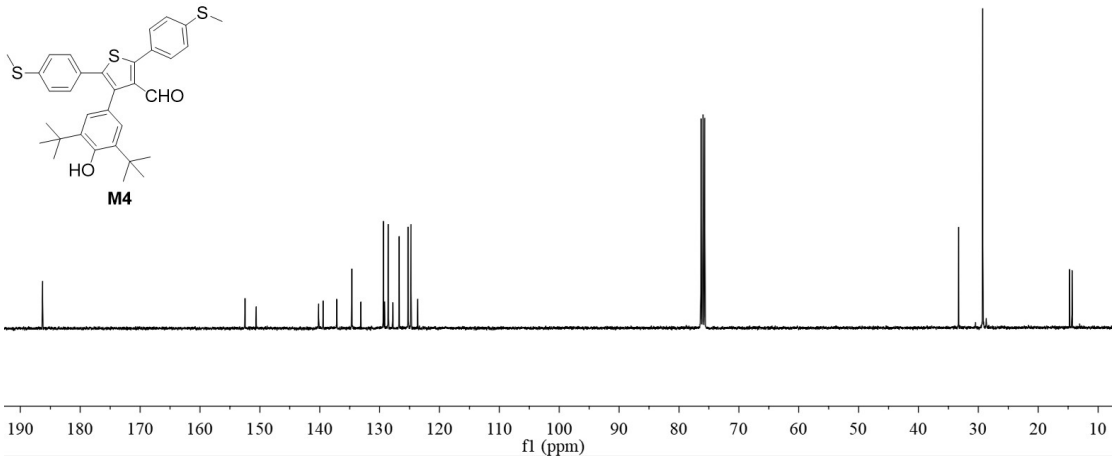
^{13}C-NMR of **M3** (101 MHz, $CDCl_3$, 298K)



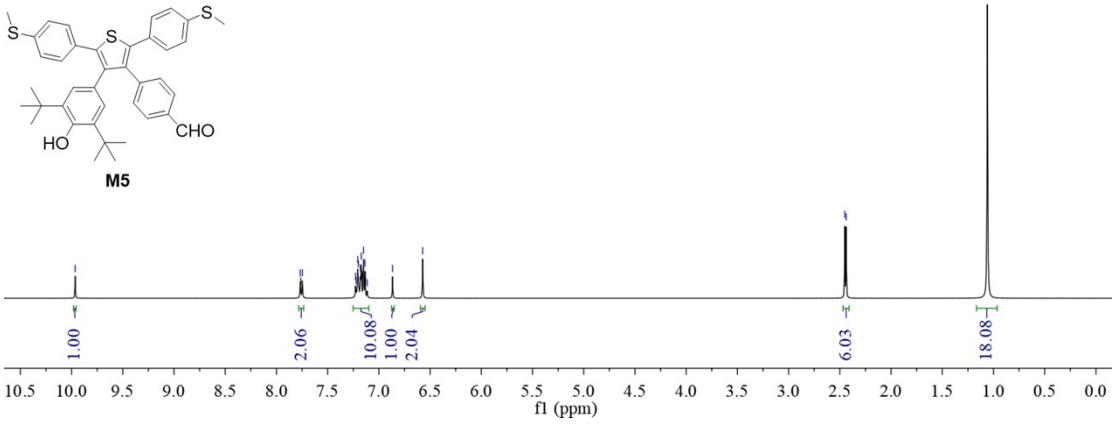
^{1}H-NMR of **M4** (400 MHz, DMSO-d_6, 298K)



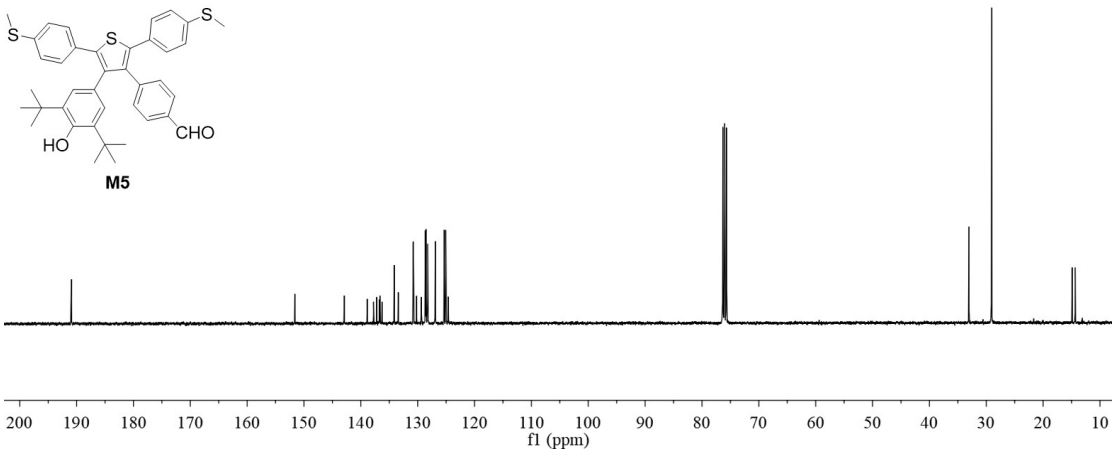
^{13}C-NMR of **M4** (101 MHz, $CDCl_3$, 298K)



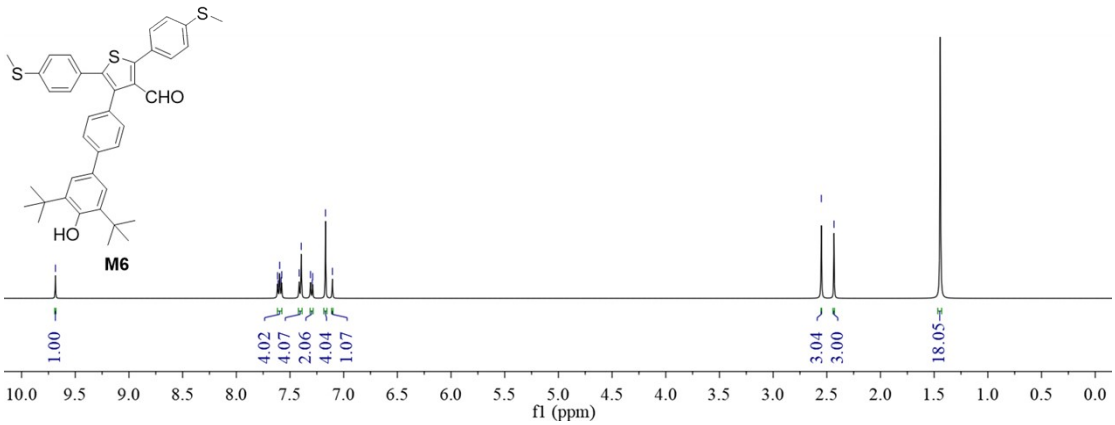
^{1}H-NMR of **M5** (400 MHz, DMSO-d_6, 298K)



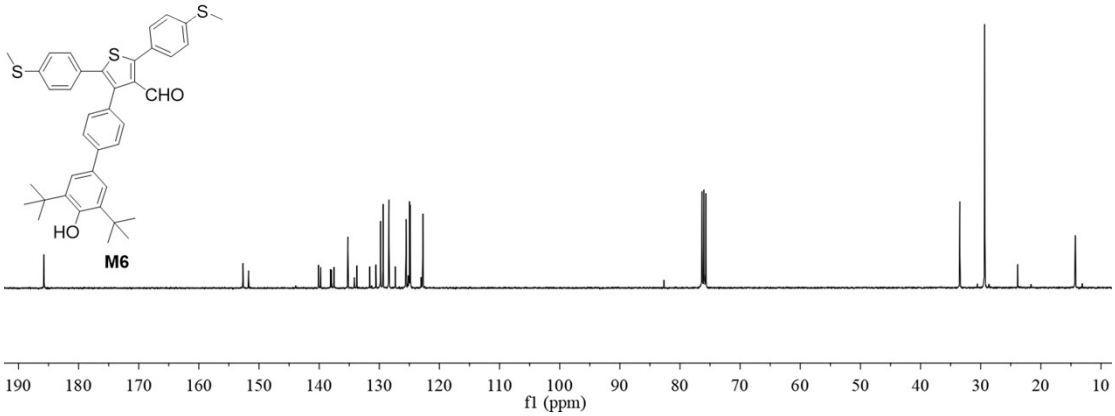
^{13}C-NMR of **M5** (101 MHz, $CDCl_3$, 298K)



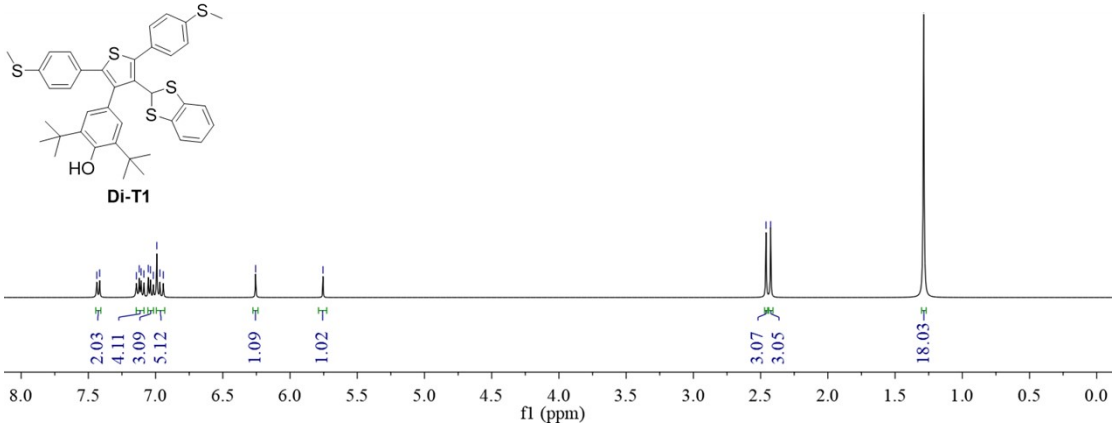
^{1}H-NMR of **M6** (400 MHz, DMSO-d_6, 298K)



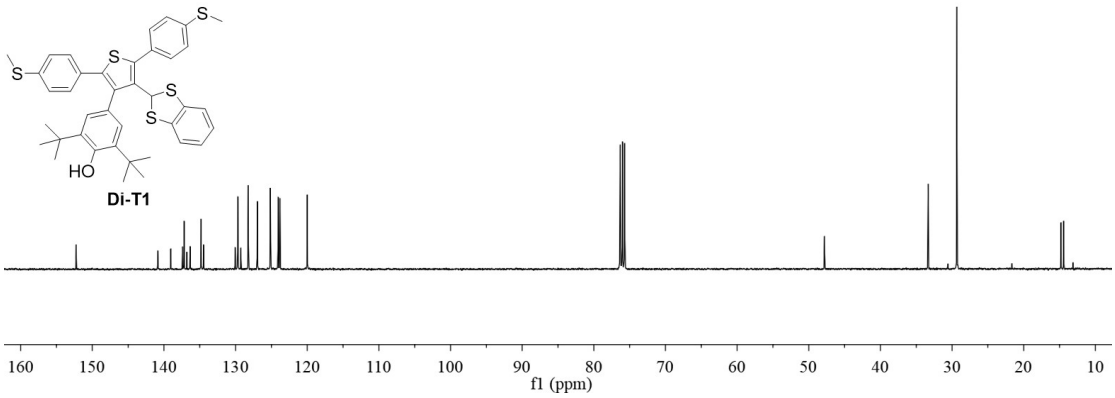
^{13}C-NMR of **M6** (101 MHz, $CDCl_3$, 298K)



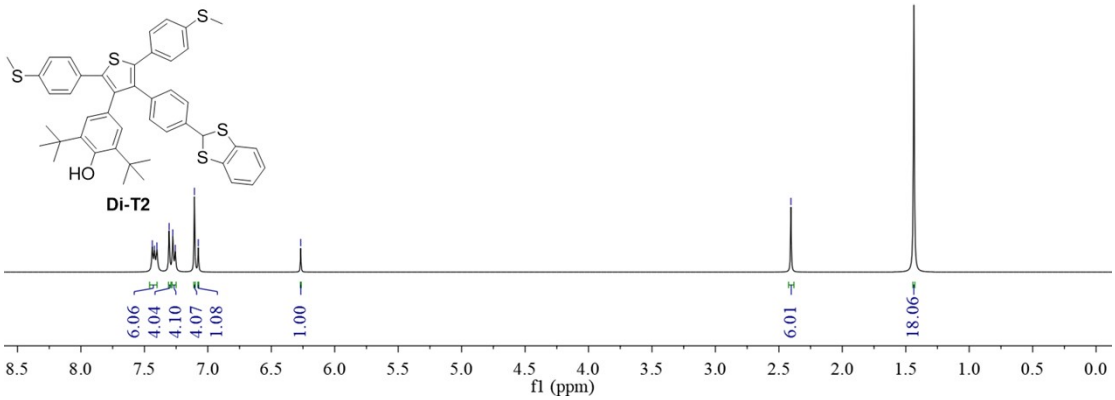
^{1}H-NMR of **Di-T1** (400 MHz, DMSO-d_6, 298K)



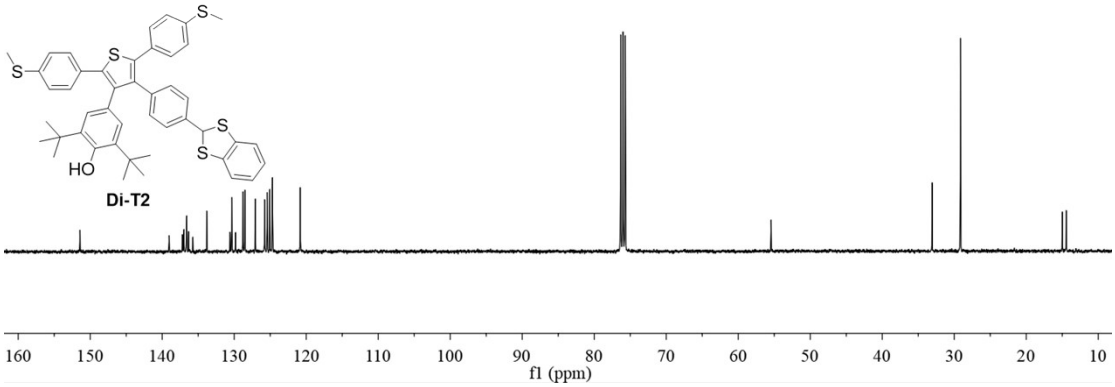
^{13}C-NMR of **Di-T1** (101 MHz, $CDCl_3$, 298K)



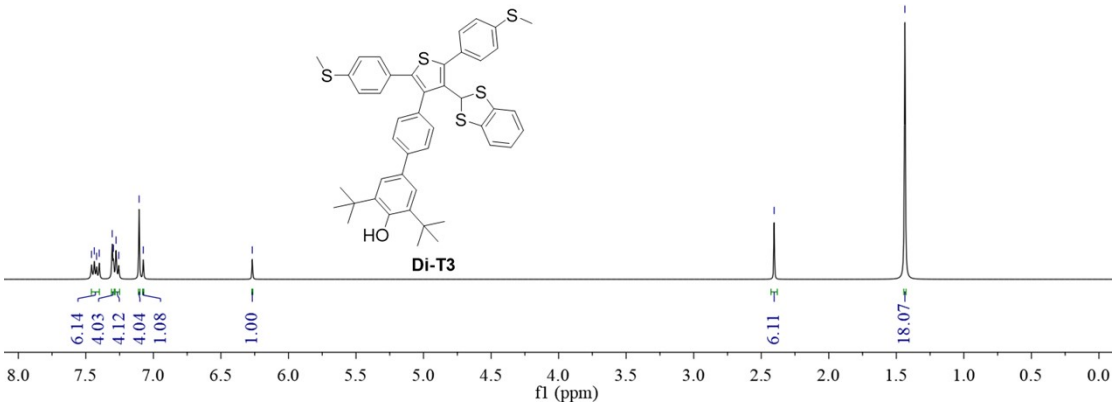
^{1}H-NMR of **Di-T2** (400 MHz, DMSO-d_6, 298K)



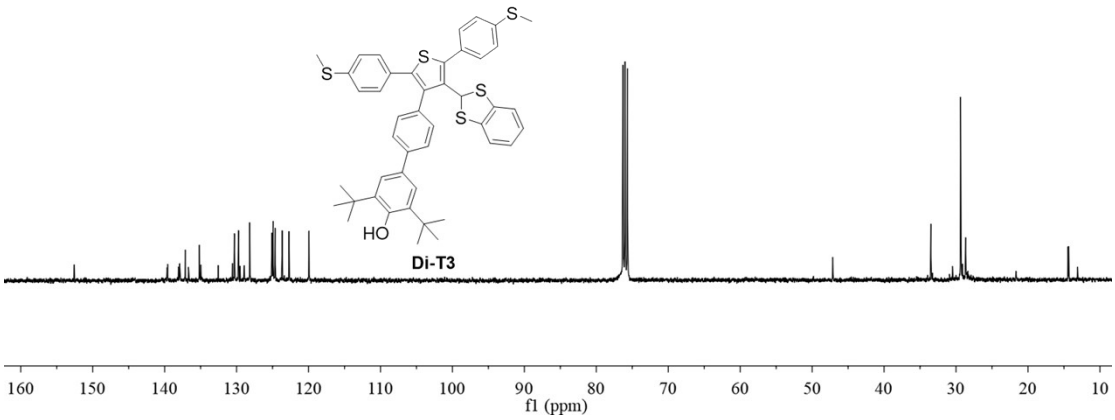
^{13}C-NMR of **Di-T2** (101 MHz, $CDCl_3$, 298K)



^{1}H-NMR of **Di-T3** (400 MHz, DMSO-d_6, 298K)

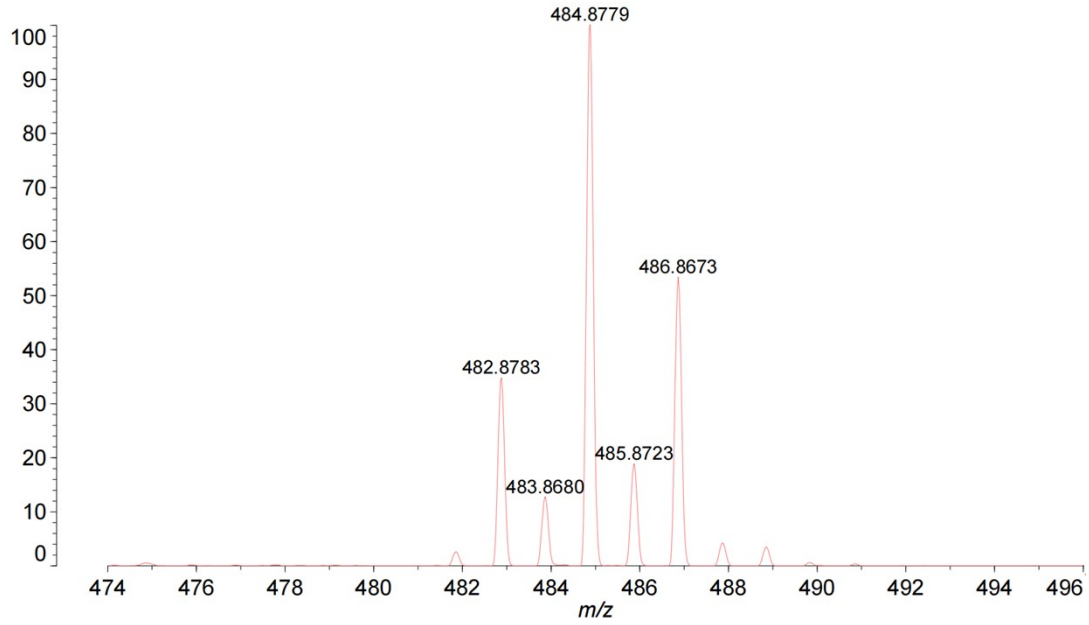


^{13}C-NMR of **Di-T3** (101 MHz, $CDCl_3$, 298K)

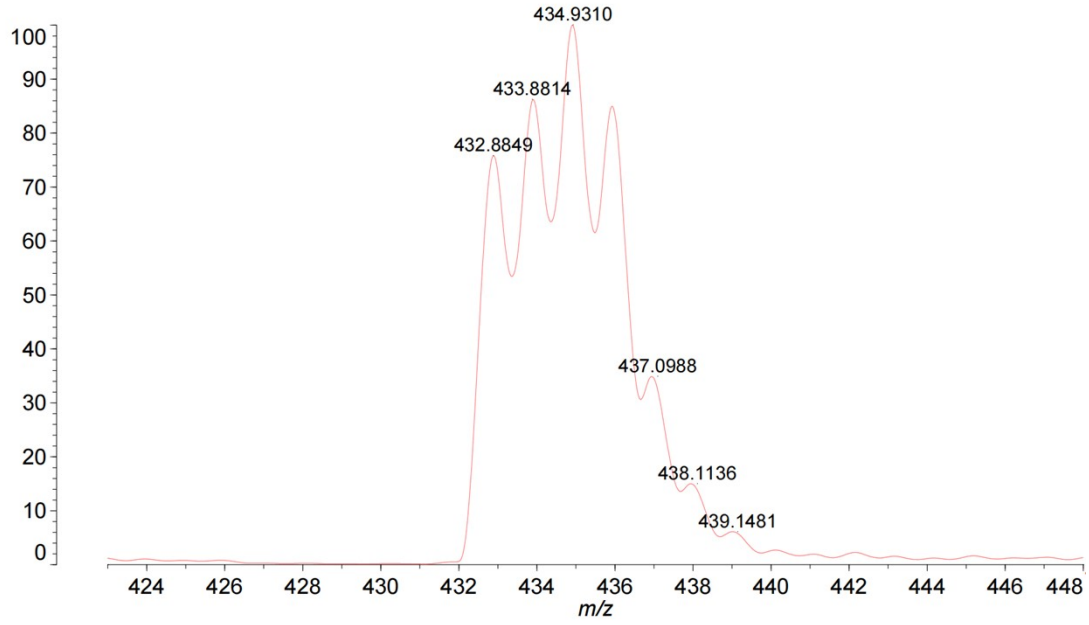


4.2 Mass Spectra

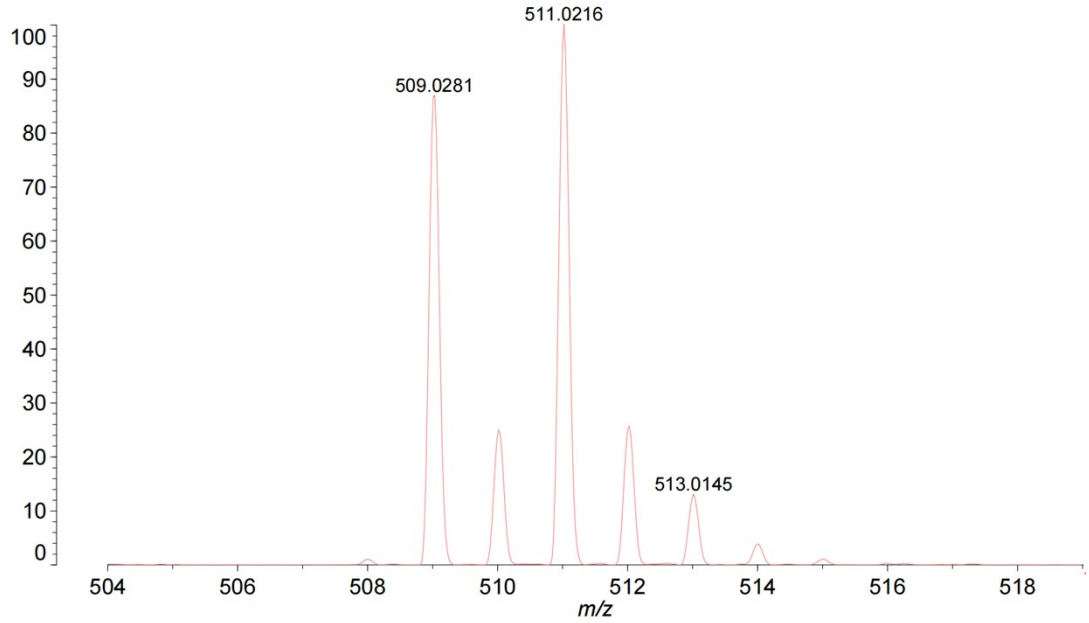
Maldi-Tof mass spectra of **M1**



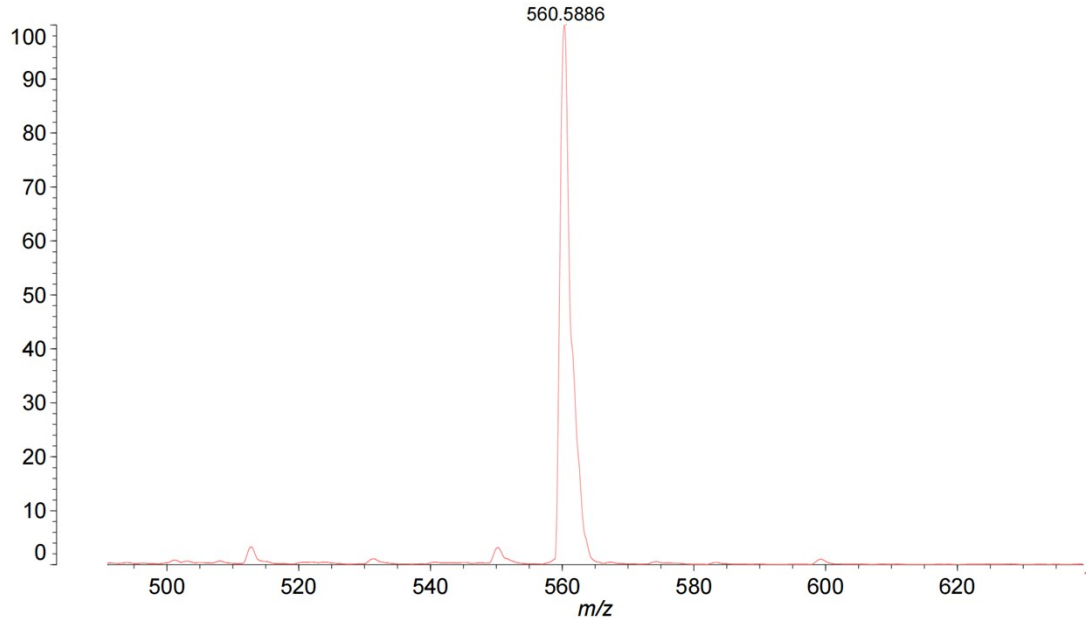
Maldi-Tof mass spectra of **M2**



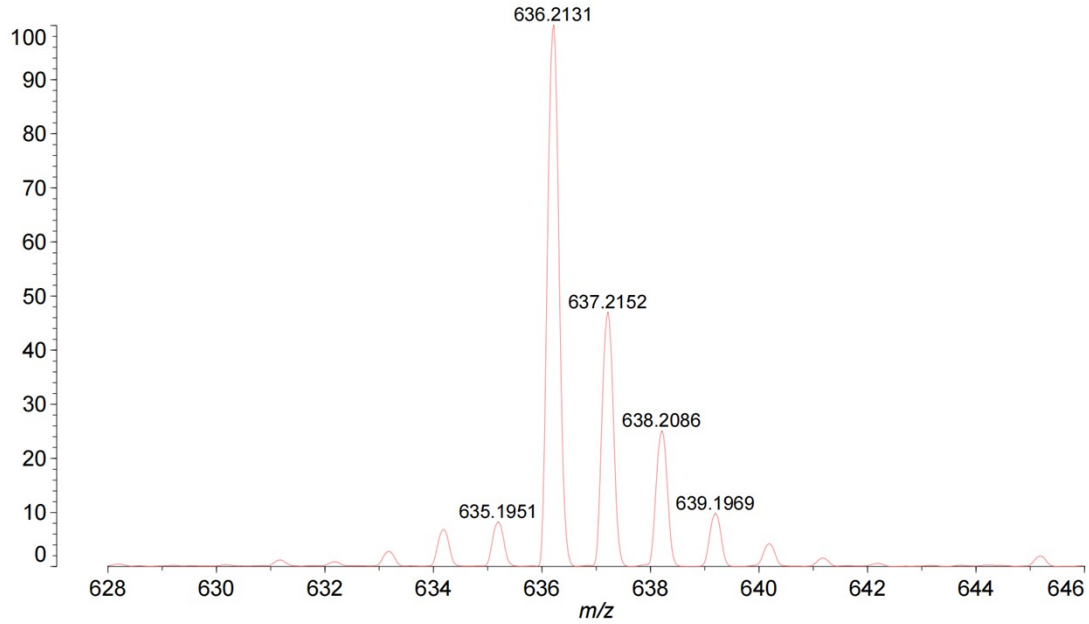
Maldi-Tof mass spectra of **M3**



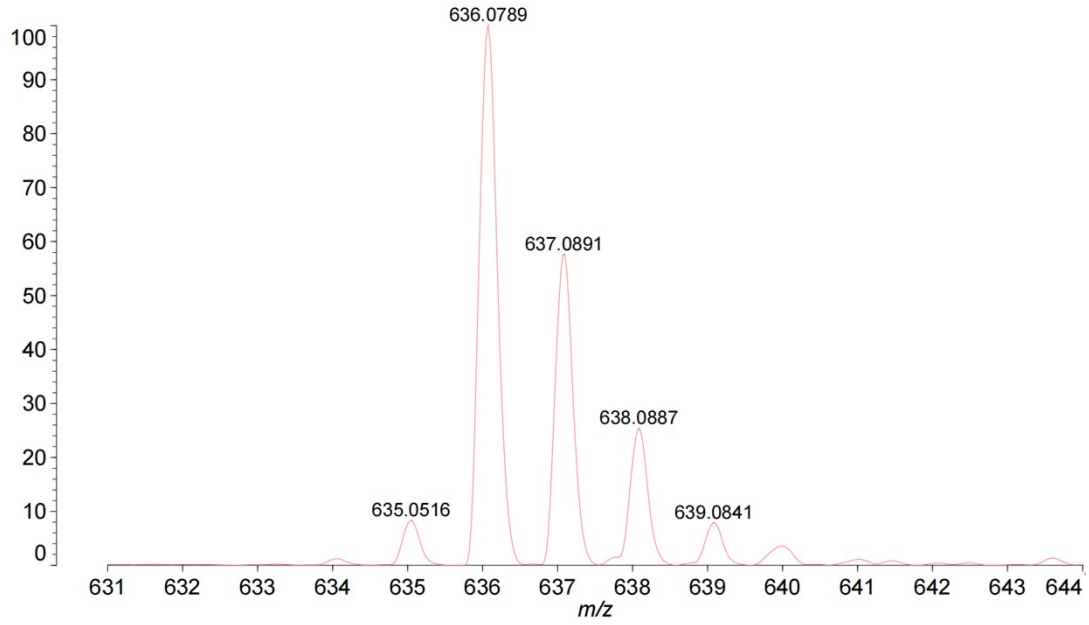
Maldi-Tof mass spectra of **M4**



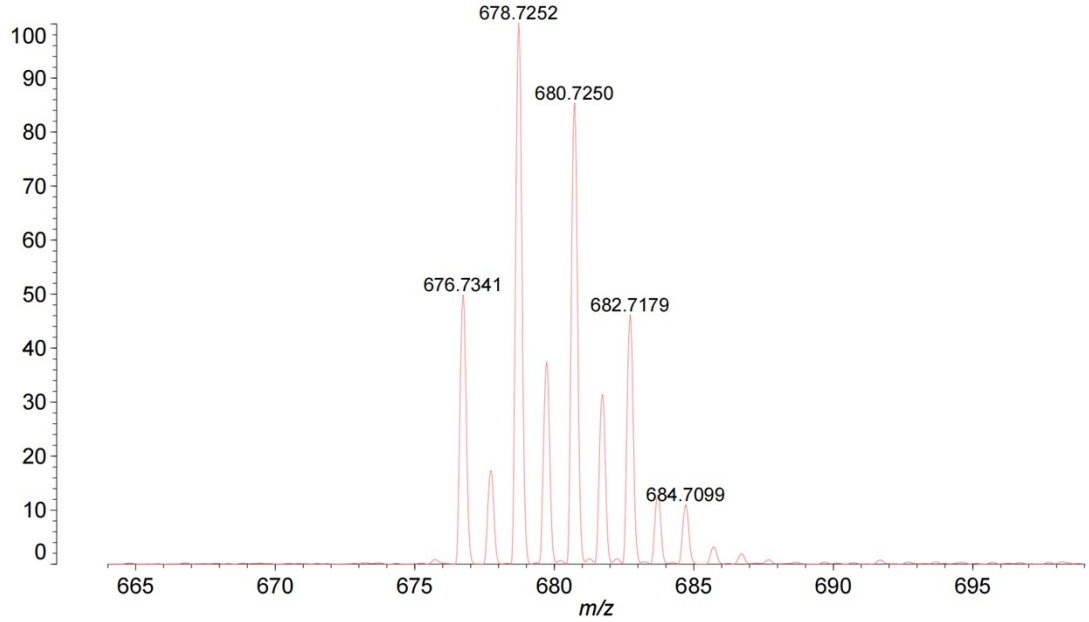
Maldi-Tof mass spectra of **M5**



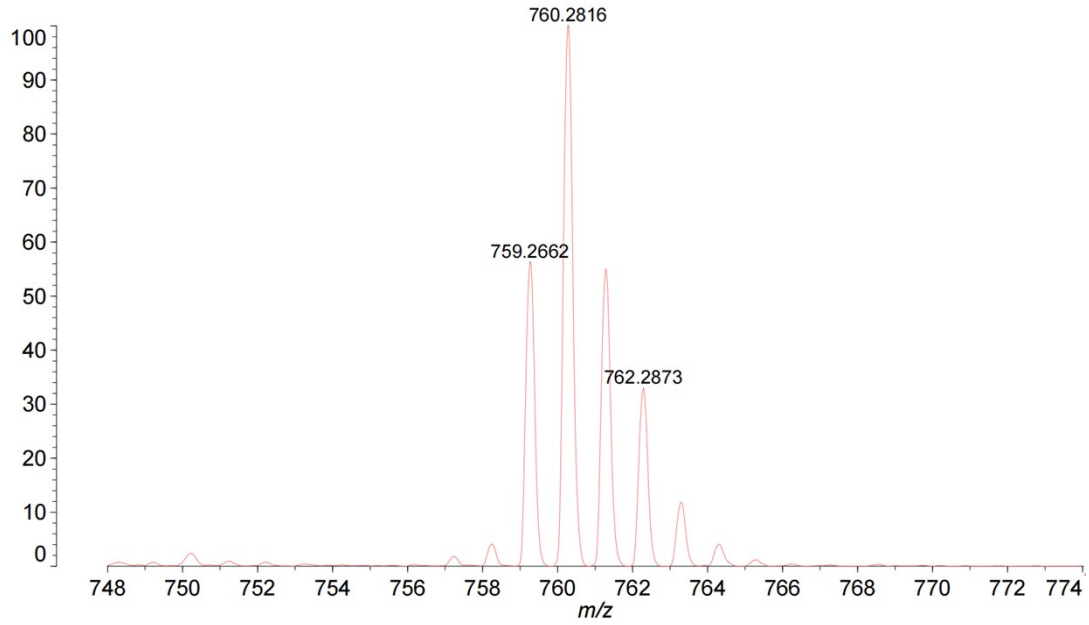
Maldi-Tof mass spectra of **M6**



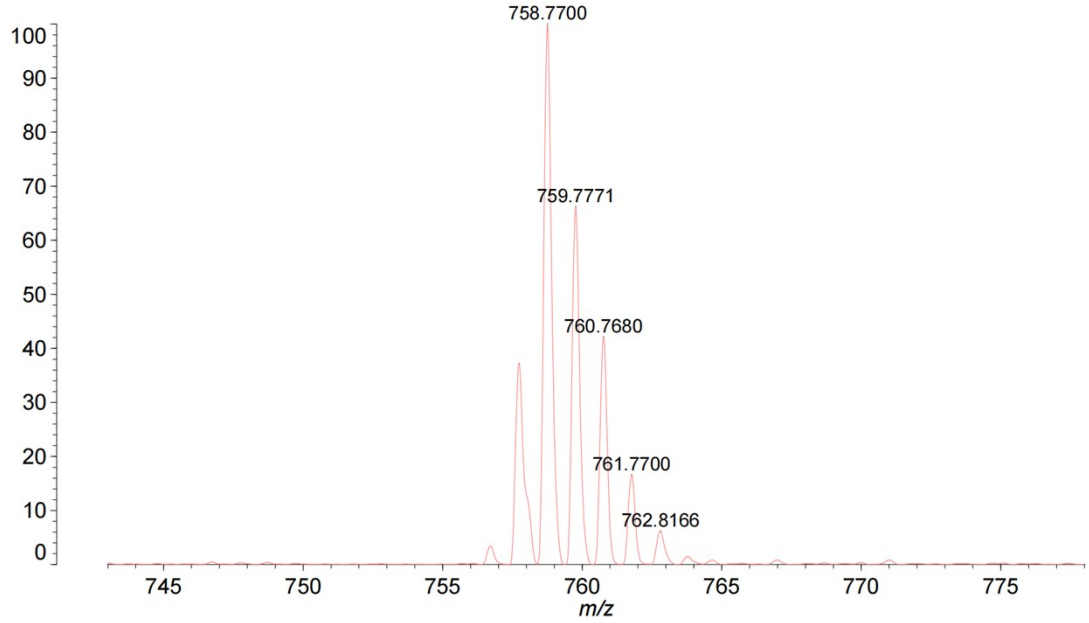
Maldi-Tof mass spectra of **Di-T1**



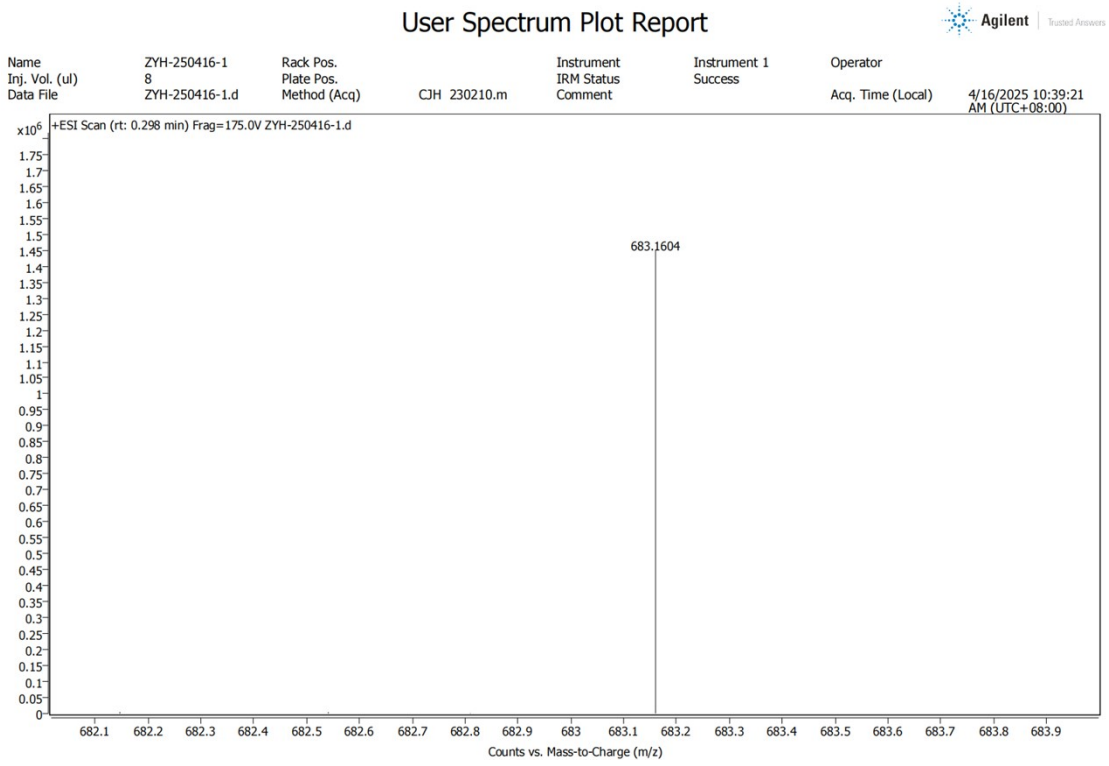
Maldi-Tof mass spectra of **Di-T2**



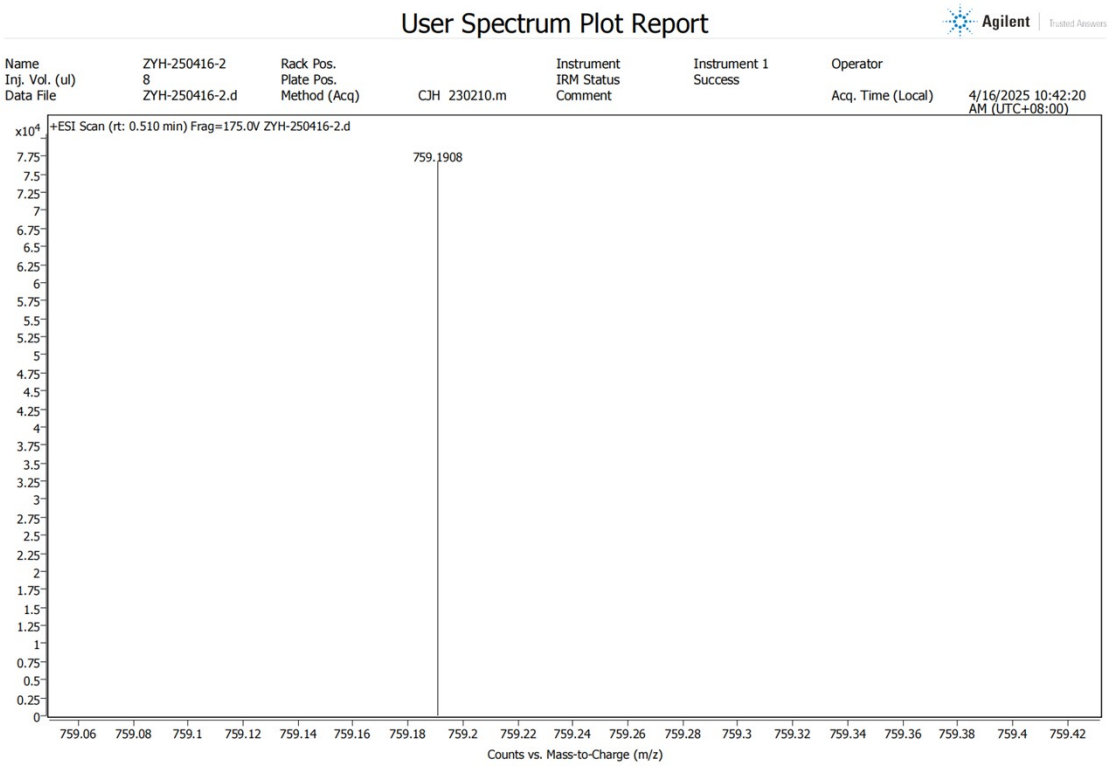
Maldi-Tof mass spectra of **Di-T3**



HRMS spectra of **Di-T1R**



HRMS spectra of **Di-T2R**



HRMS spectra of **Di-T3R**