Supporting Information

Synthesis of Tetraphenylethene-based D-A Conjugated Molecules with Near-Infrared AIE Features, and Application in Photodynamic Therapy

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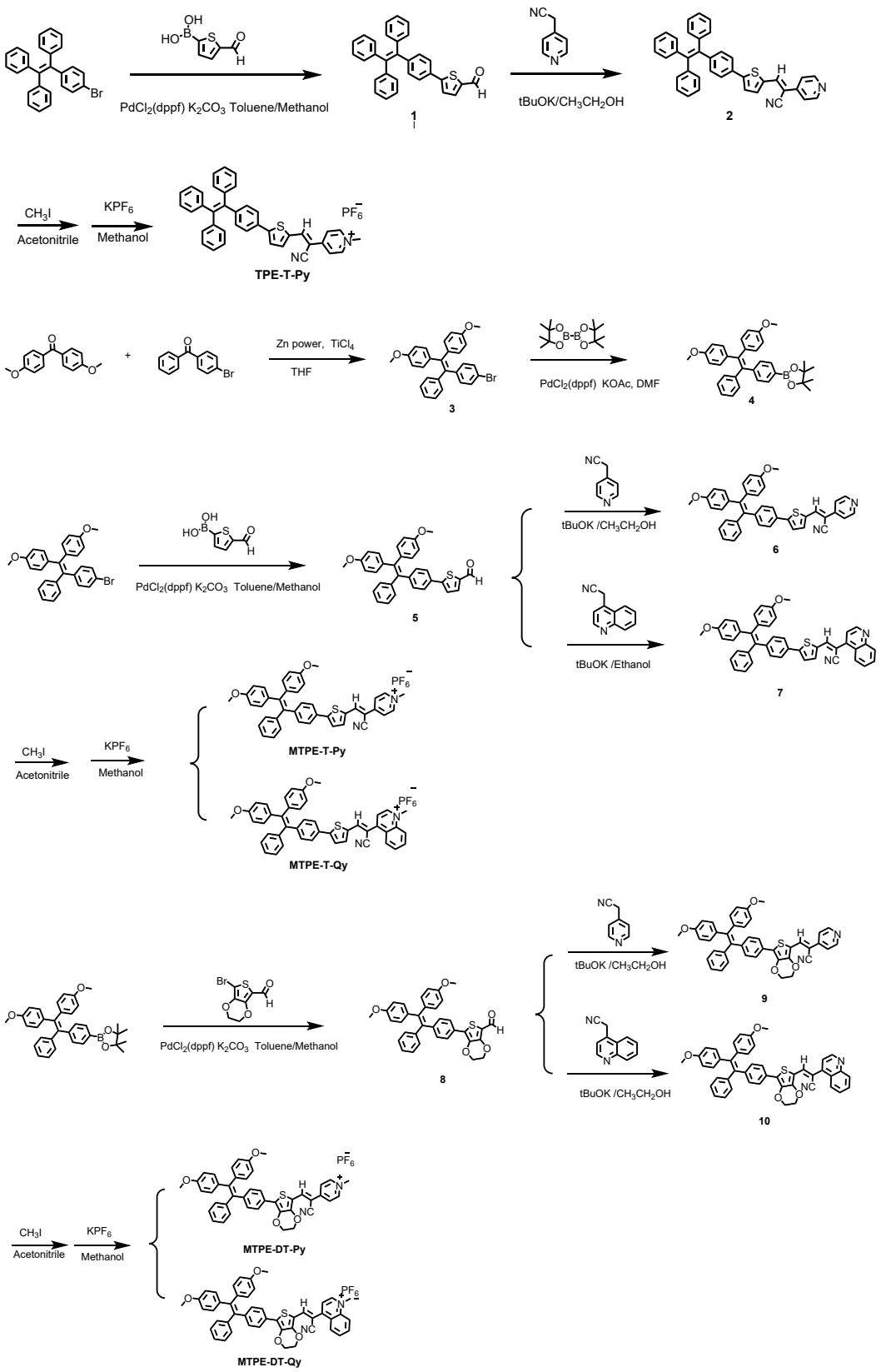


Scheme S1. The structures and synthetic routes of **TPE-T-Py, MTPE-T-Py**, **MTPE-T-Qy**, **MTPE-DT-Py** and **MTPE-DT-Qy**.

Synthesis of Compound 1. 1-(4-bromophenyl)-1,2,2-triphenylethylene (1.025 g, 2.5 mmol) and Pd(dppf)Cl_2 (183 mg, 0.25 mmol) was dissolved in 24 mL anhydrous toluene under nitrogen, then 5-formyl-2-thiopheneboronic acid (780 mg, 5 mmol), K_2CO_3 (1.38 g, 7.5 mmol) in anhydrous methanol was added. The mixture was heated to reflux for 16 h under nitrogen. After cooling to room temperature, the reaction is quenched by water. The organic layer was extracted by dichloromethane, washed with brine, dried over anhydrous Na_2SO_4 and evaporated to dryness under reduced pressure. The crude product was purified by silica gel with column to give compound **1** as yellow powder (770 mg, yield: 70%). ^{1}HNMR (500 MHz, Chloroform-d) δ 9.90 (s, 1H), 7.74 (d, J = 4.0 Hz, 1H), 7.46 (d, J = 8.1 Hz, 2H), 7.38 (d, J = 4.0 Hz, 1H), 7.21 – 7.02 (m, 17H). HRMS (ESI$^+$): calcd. for $C_{31}H_{22}OS^+[M+H]^+$ 443.1464, found 443.1459.

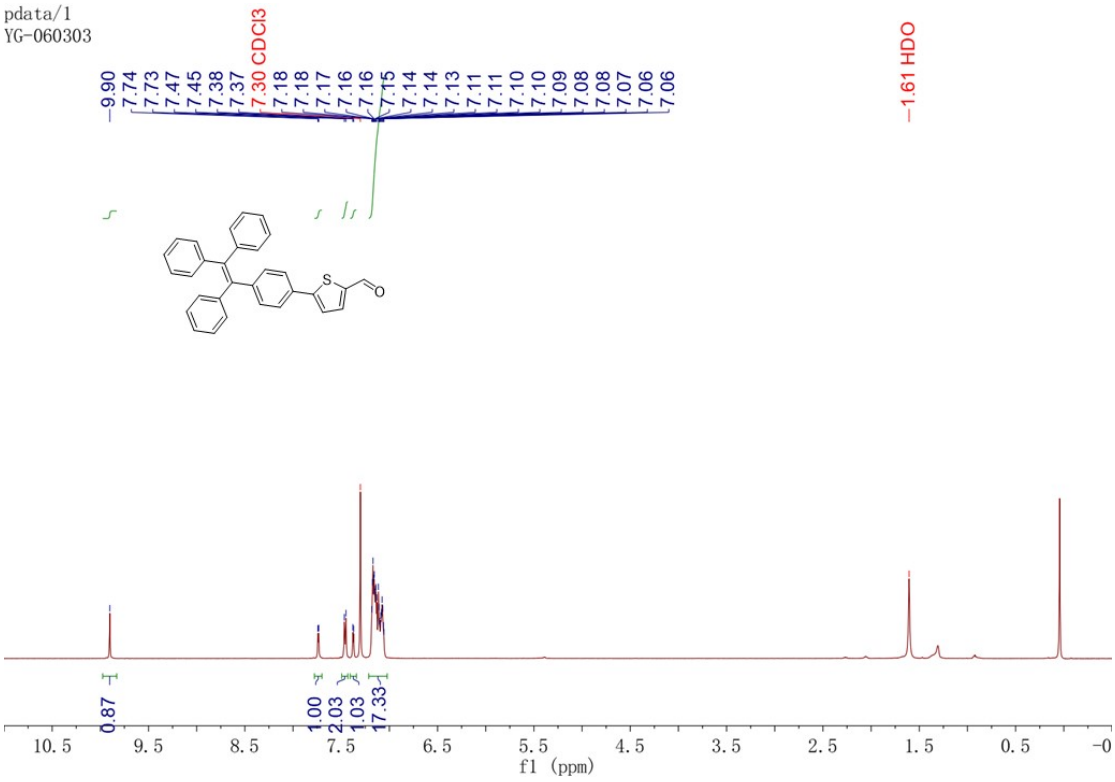


Figure S1. ^{1}H NMR spectrum of compound 1

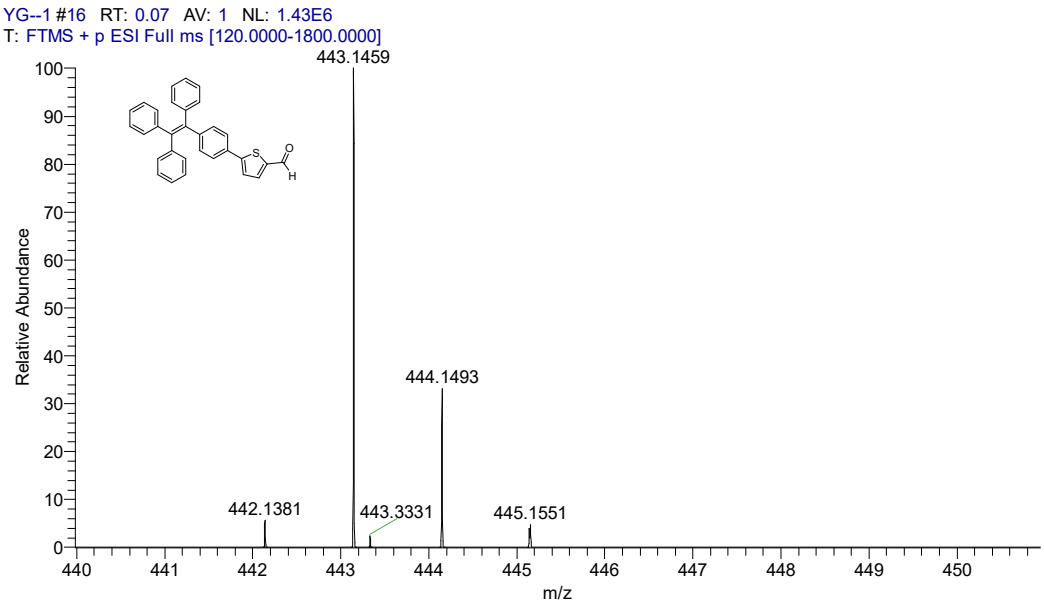


Figure S2. HRMS spectrum of compound **1**

Synthesis of Compound 2. 4-pyridineacetonitrile (56.68 mg, 0.48 mmol) and *t*-BuOK (67 mg, 0.6 mmol) were successively added to anhydrous EtOH (15 mL) in a round bottomed flask, which was stirred at room temperature for 10 min. Then compound **1** (176 mg, 0.4 mmol) was added to the solution, and the mixture was further stirred at room temperature for 36 h. Then the solid was filtered off, washed with 30 mL EtOH and dried under vacuum. The obtained solid was purified by silica gel chromatography using petroleum ether/CH_2Cl_2 mixture as an orange yellow powder (195 mg, yield: 90%). ^{1}HNMR (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 6.1 Hz, 2H), 7.80 (s, 1H), 7.63 (d, *J* = 4.0 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.32 (d, *J* = 4.0 Hz, 1H), 7.16 – 7.03 (m, 17H). ^{13}C NMR (100 MHz, Chloroform-d) δ 151.47, 150.21, 145.05, 143.45, 141.98, 140.00, 137.01, 136.24, 136.00, 132.16, 131.38, 131.32, 127.93, 127.84, 127.70, 126.84, 126.71, 126.66, 125.53, 123.83, 119.56, 117.26, 104.20. HRMS (ESI$^+$): calcd. for $C_{38}H_{27}N_2S^+[M+H]^+$ 543.1889, found 543.1879.

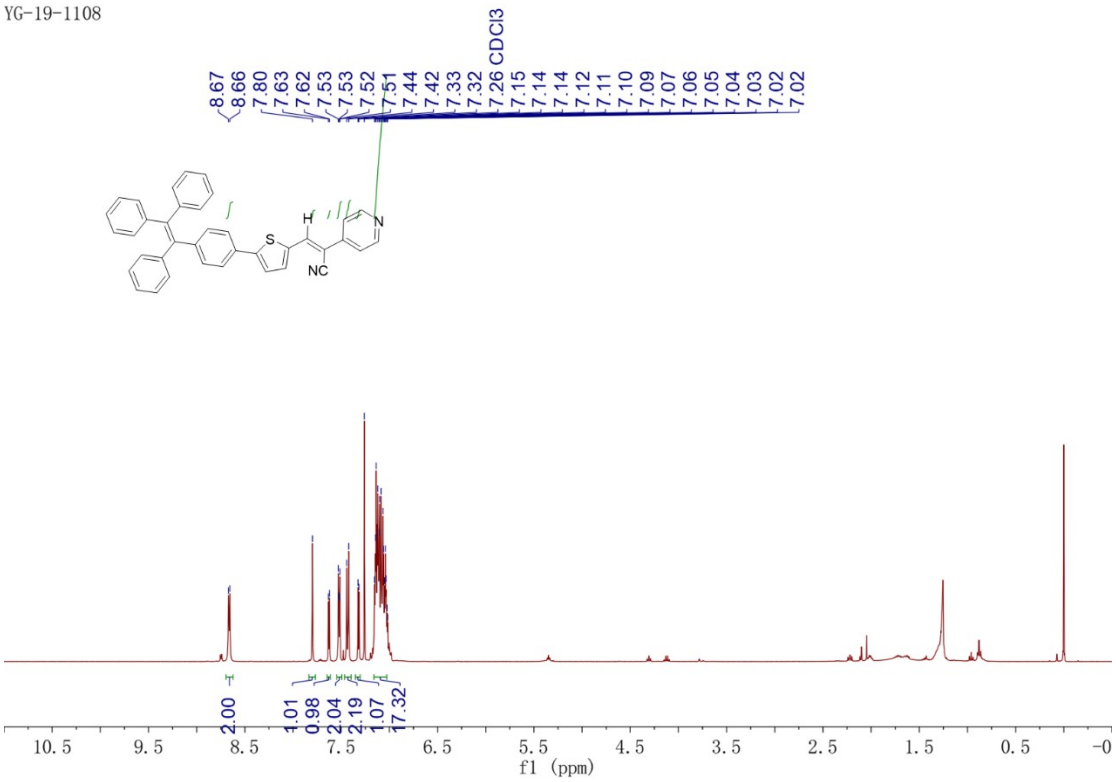


Figure S3. ^{1}H NMR spectrum of compound **2**

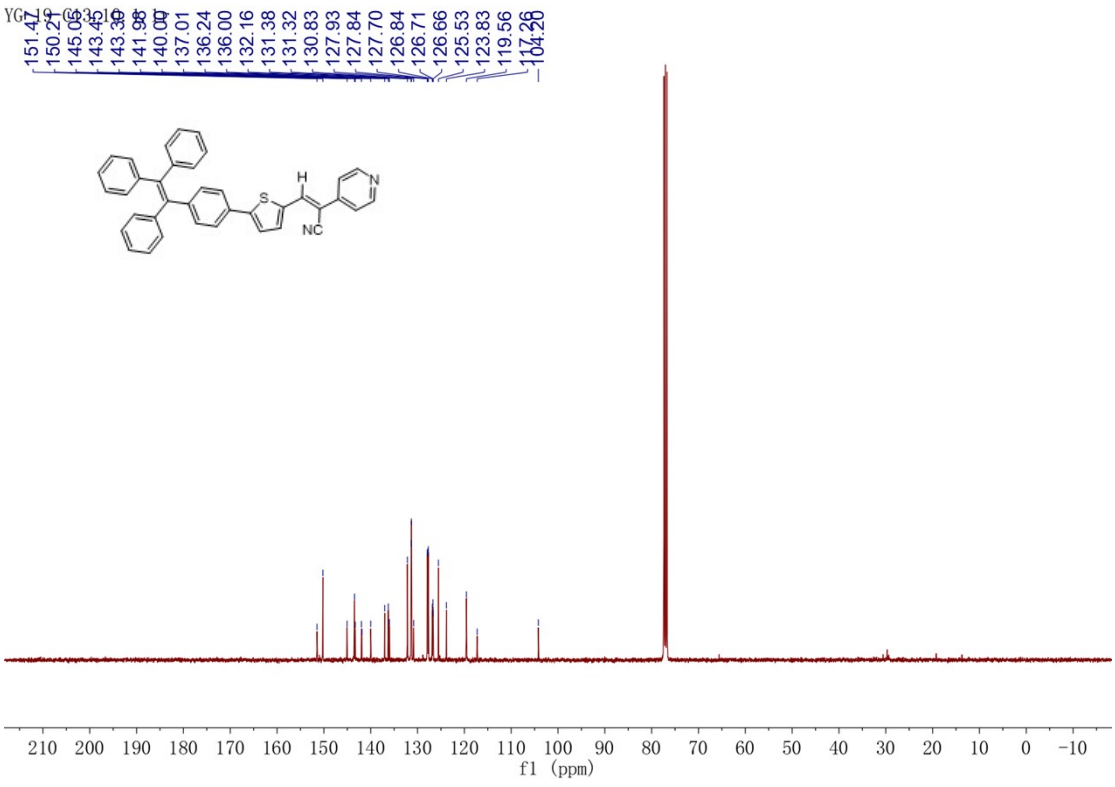


Figure S4. ^{13}C NMR spectrum of compound **2**

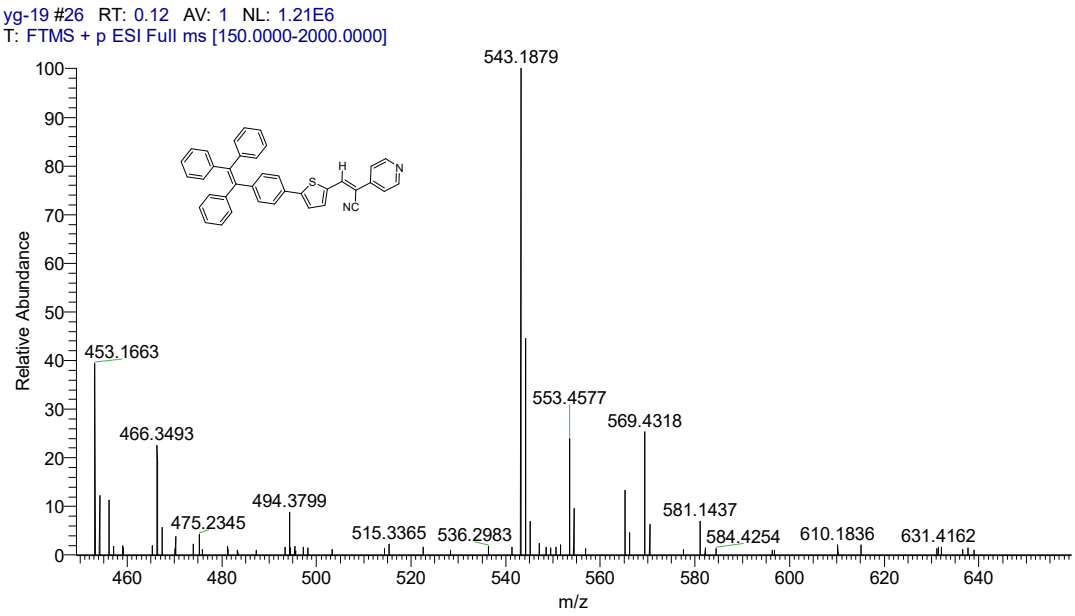


Figure S5. HRMS spectrum of compound **2**

Synthesis of 1,1'-[1-(4-bromophenyl)-1,2-ethenediylidene] bis[methoxybenzene] (3). 4-Bromobenzophenone (2.6 g, 10 mmol), 4, 4'-dimethoxybenzophenone (3.1 g, 12 mmol) and zinc powder (6.5 g, 100 mmol) were mixed in anhydrous THF (150 mL) and stirred at ice water bath. Titanium tetrachloride (6.7 mL, 60 mmol) was then injected dropwise for 30 min. After recovering to room temperature, the mixture was heated at 80 °C for 24 h. The reaction was quenched with 10% K_2CO_3 aqueous solution and filtrated with silica gel powder. The residue was washed with ethyl acetate (50 mL × 3). The organic phase was dried with Na_2SO_4 and the solvent was removed under reduced pressure. The obtained residue was purified with chromatography (hexane/dichloromethane = 4/1, v/v) to give compound **3** as a white powder (2.05 g, yield: 43%). ^{1}HNMR (400 MHz, Chloroform-d) δ 7.25–6.83 (m, 13H), 6.70–6.57 (m, 4H), 3.84–3.69 (m, 6H). HRMS (ESI+): calcd. For $C_{28}H_{23}BrO_2Na^+$[M+Na]$^+$ 493.0774, found 493.0761.

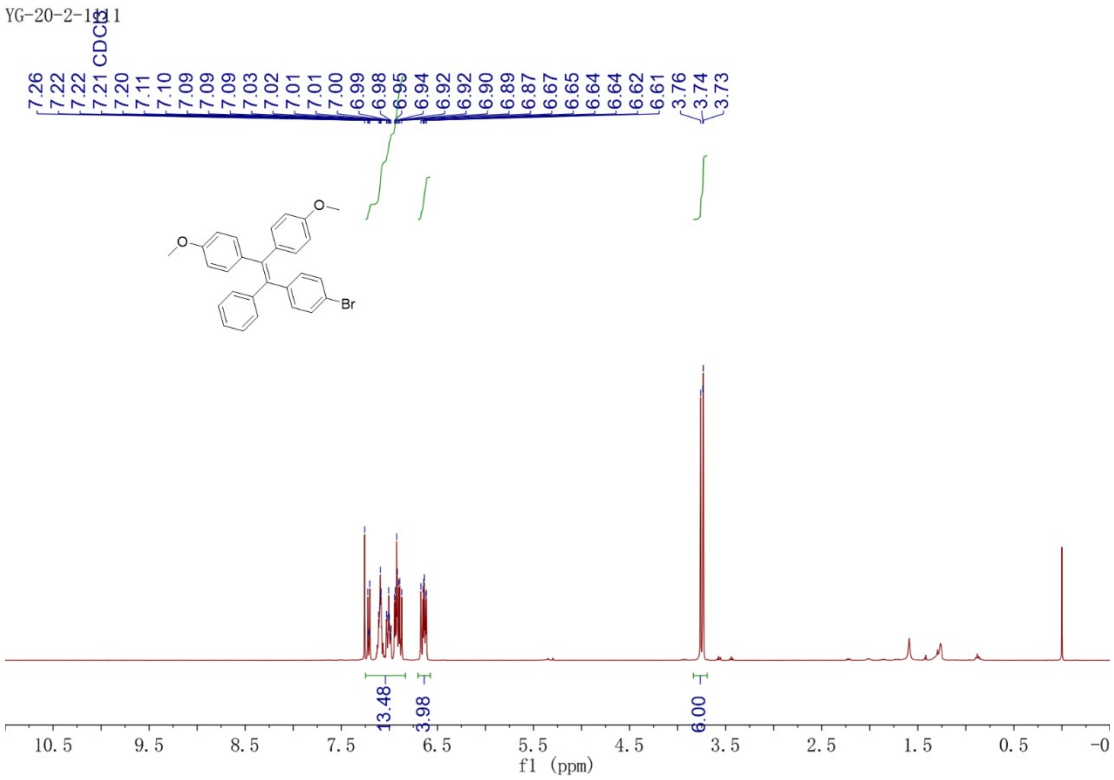


Figure S6. [1]H NMR spectrum of compound **3**

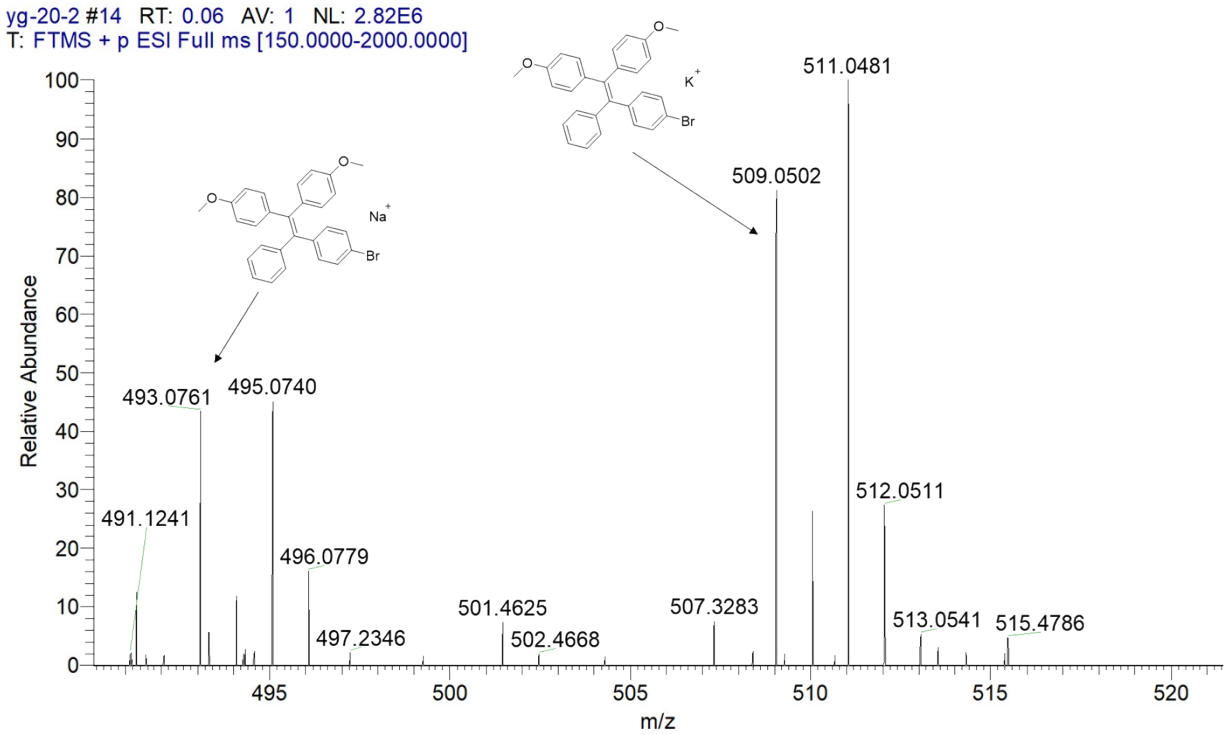


Figure S7. HRMS spectrum of compound **3**

Synthesis of 2-[4-[1,2-bis(4-methoxyphenyl)-2-phenylethenyl]phenyl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4). A mixture of Compound 3 (705 mg, 1.5 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (457 mg, 1.8 mmol), potassium acetate (588 mg, 6 mmol), and Pd(dppf)Cl_2 (54 mg, 0.074 mmol) in anhydrous dimethyl sulfoxide (15 mL) was stirred at 100 °C under Nitrogen for 24 h and then water added. The crude product was extracted into ethyl acetate, washed with brine, and dried over anhydrous sodium sulfate. After removing solvent under reduced pressure, the residue was purified by column chromatography (CH_2Cl_2/petroleum ether, 1/2, v/v) on silica gel to yield a white powder (650 mg, yield: 83.6%). ^{1}HNMR (400 MHz, DMSO-d6) δ 7.43 (d, J = 8.2 Hz, 2H), 7.19 – 7.04 (m, 3H), 7.00 – 6.90 (m, 4H), 6.86 (dd, J = 8.8, 5.6 Hz, 4H), 6.74 – 6.66 (m, 4H), 3.68 (d, J = 2.7 Hz, 6H), 1.26 (s, 12H). ^{13}CNMR (100 MHz, DMSO-d_6) δ 158.27, 147.54, 144.09, 140.90, 138.97, 135.93, 134.44, 132.52, 131.22, 130.74, 128.34, 126.80, 113.65, 81.82, 55.39, 25.30

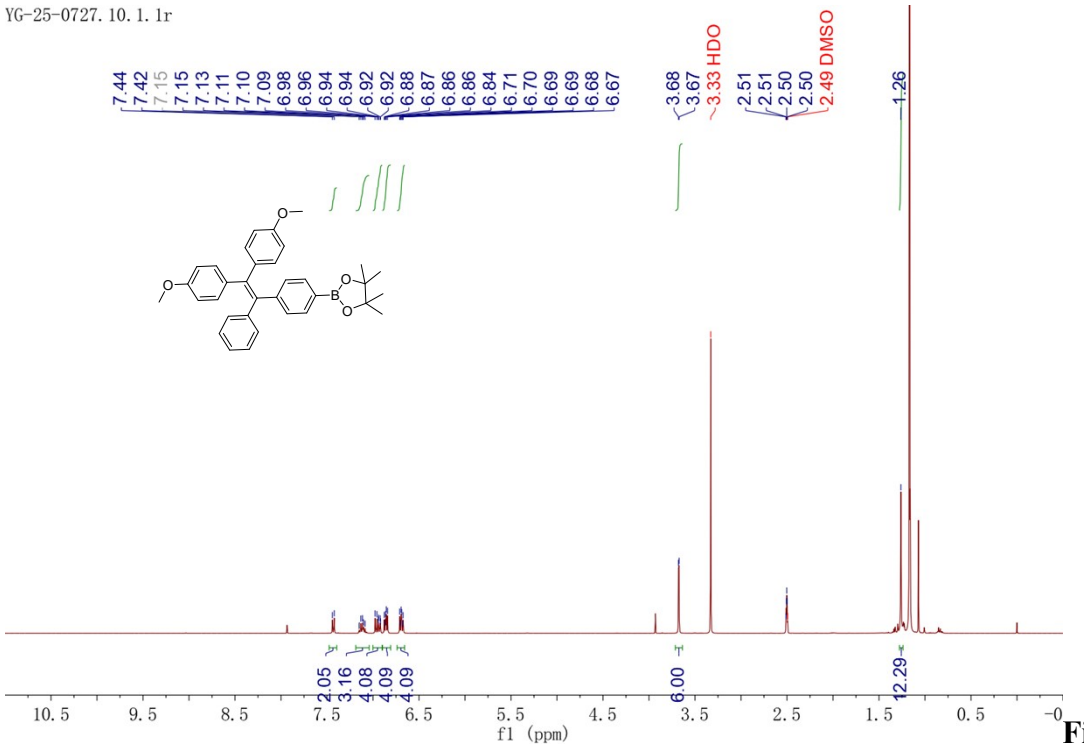
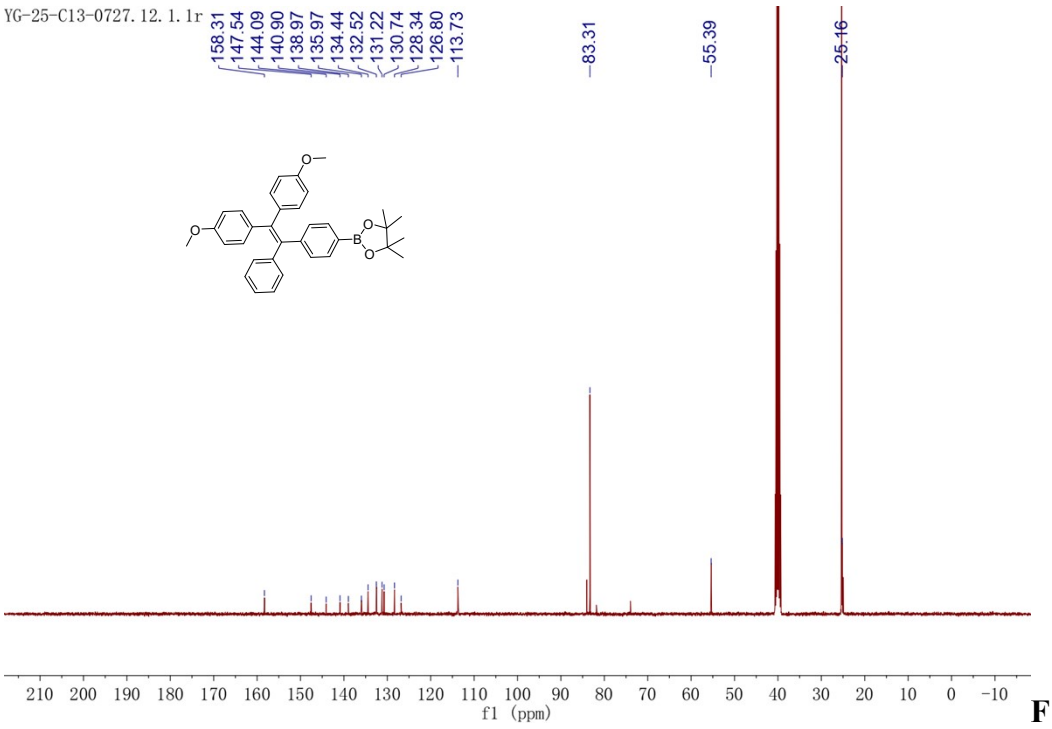


Figure S8. ^{1}H NMR spectrum of compound **4**



F igure S9. ^{13}C NMR spectrum of compound **4**

Synthesis of Compound 5. The same synthetic procedure as described compound **1** for using compound **3** (345 mg, 0.8 mmol), affording the product as an orange yellow powder (321 mg, yield: 64%). ^{1}HNMR (400 MHz, Chloroform-d) δ 9.86 (s, 1H), 7.70 (d, J = 3.9 Hz, 1H), 7.42 (d, J = 8.3 Hz, 2H), 7.34 (d, J = 4.0 Hz, 1H), 7.18 – 6.88 (m, 11H), 6.65 (dd, J = 12.4, 8.8 Hz, 4H), 3.75 (d, J = 3.7 Hz, 6H). HRMS (ESI+): calcd. for $C_{33}H_{26}O_3S^+[M+H]^+$ 503.1675, found 503.1665. HRMS (ESI+): calcd. for $C_{33}H_{26}O_3S^+[M+Na]^+$ 525.1495, found 525.1489.

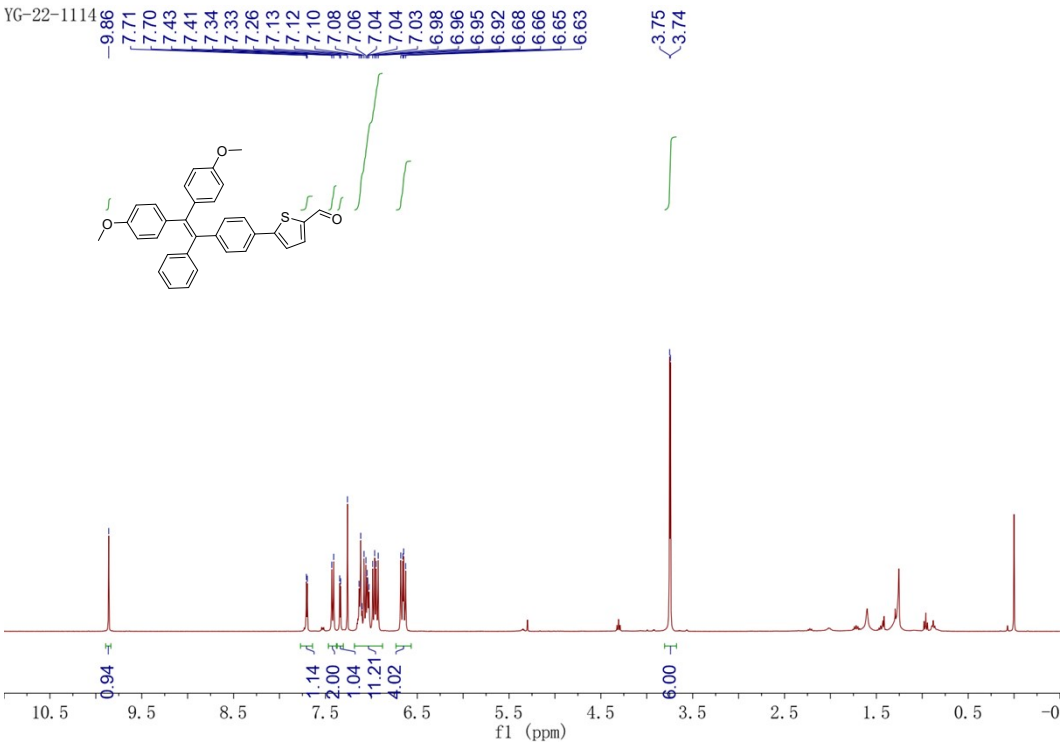


Figure S10. ^{1}H NMR spectrum of compound **5**

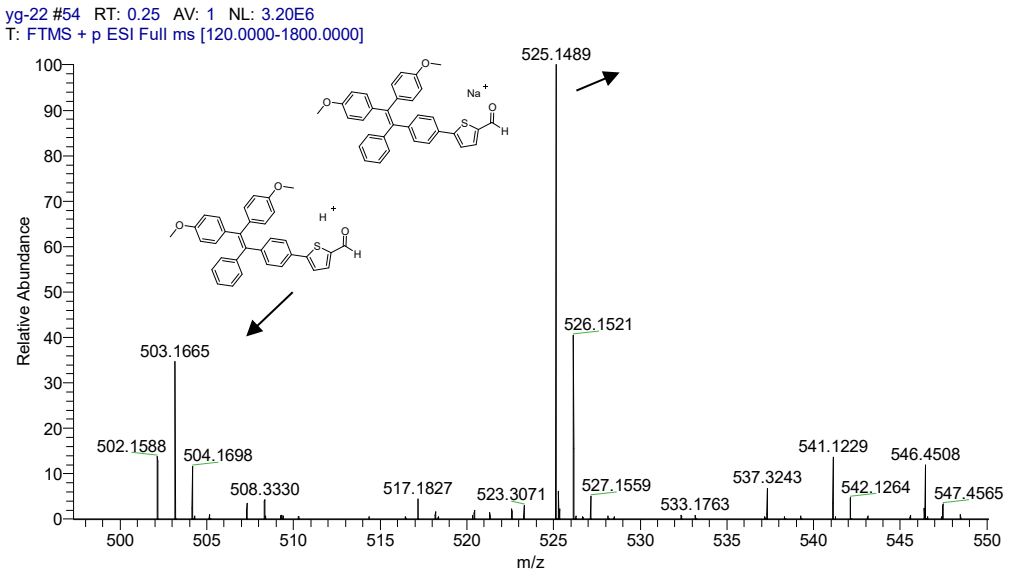


Figure S11. HRMS spectrum of compound **5**

Synthesis of Compound 6. The same synthetic procedure as described compound **2** for using compound **5** (345 mg, 0.8 mmol), affording the product as an orange yellow powder (90 mg, yield: 75%).[1]HNMR (400 MHz, Chloroform-d) δ 8.66 (d, J = 6.3 Hz, 2H), 7.83 – 7.60 (m, 2H), 7.52 (dd, J = 4.7, 1.5 Hz, 2H), 7.44 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 4.0 Hz, 1H), 7.13 (d, J = 7.2 Hz, 3H), 7.08 – 7.03 (m, 4H), 7.00 – 6.92 (m, 4H), 6.66 (dd, J = 14.6, 8.8 Hz, 4H), 3.75 (d, J = 6.8 Hz, 6H). [13]C NMR (100 MHz, Chloroform-d) δ 158.39, 158.24, 151.52, 150.39, 145.69, 143.87, 141.68, 141.19, 138.24, 136.91, 136.18, 136.05, 135.89, 132.61, 132.18, 131.43, 130.44, 127.86, 126.36, 125.53, 123.68, 119.49, 117.31, 113.25, 113.03, 104.15, 55.12. HRMS (ESI+): calcd. for $C_{40}H_{32}N_2O_2S^+$ $[M+H]^+$603.2101, found 603.2098.

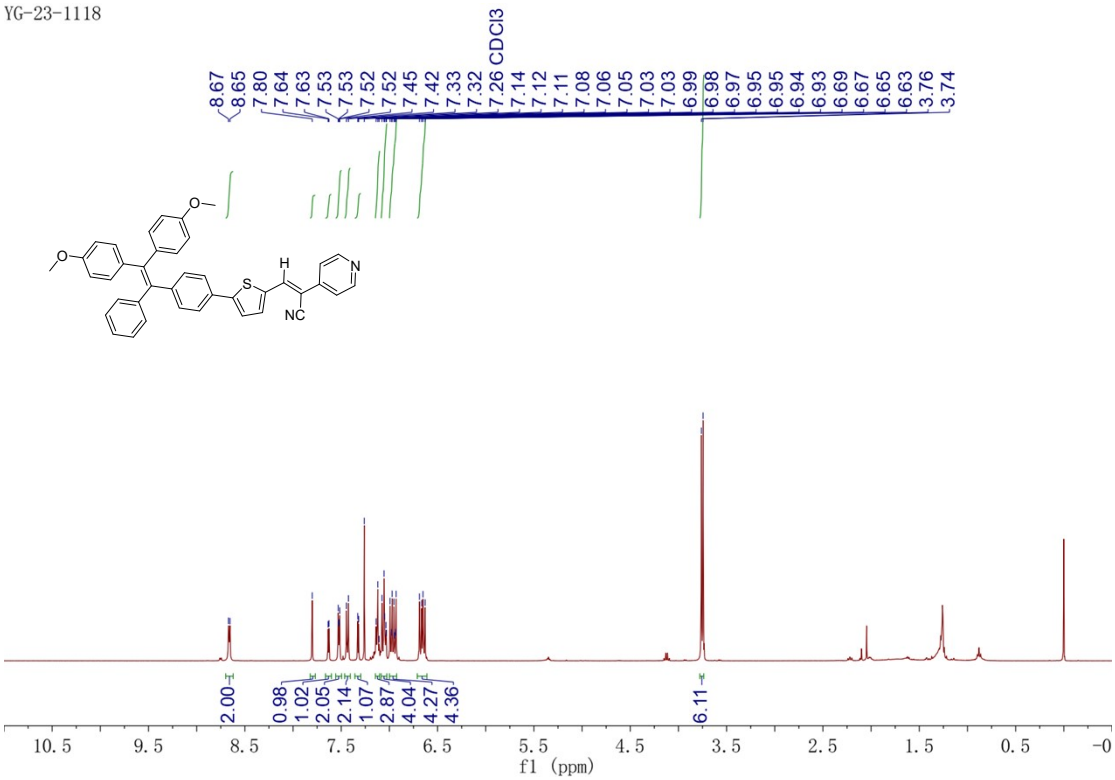


Figure S12. [1]H NMR spectrum of compound **6**

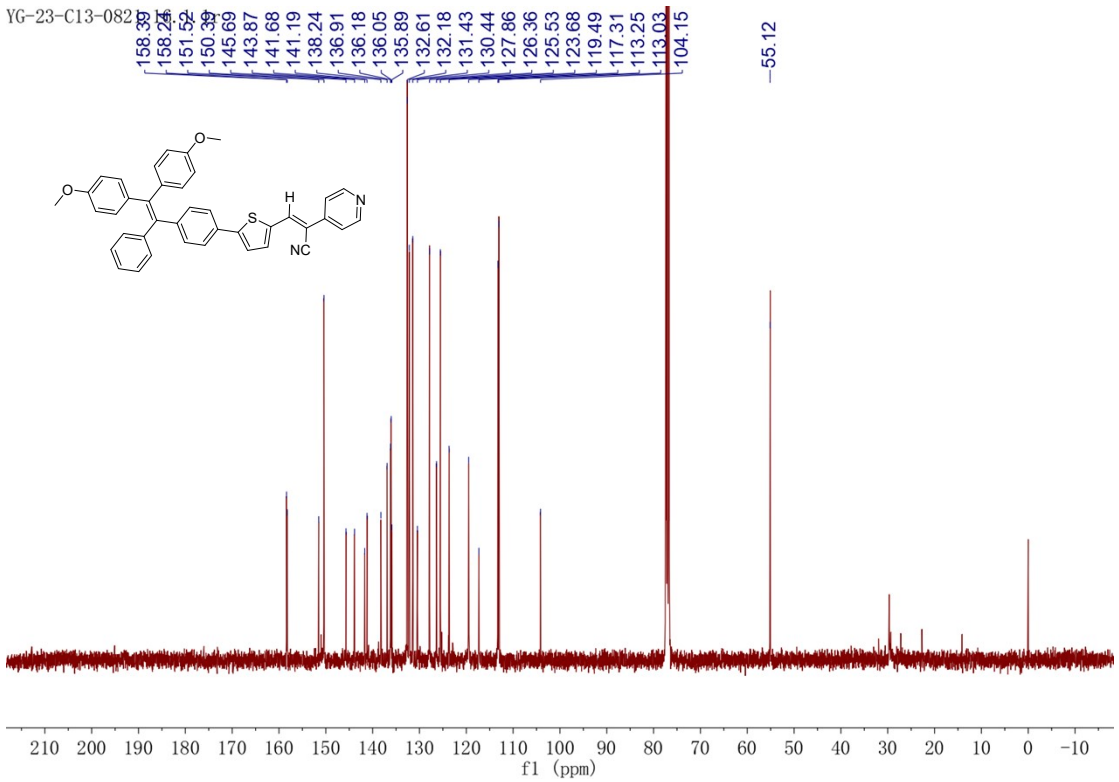


Figure S13. ^{13}C NMR spectrum of compound **6**

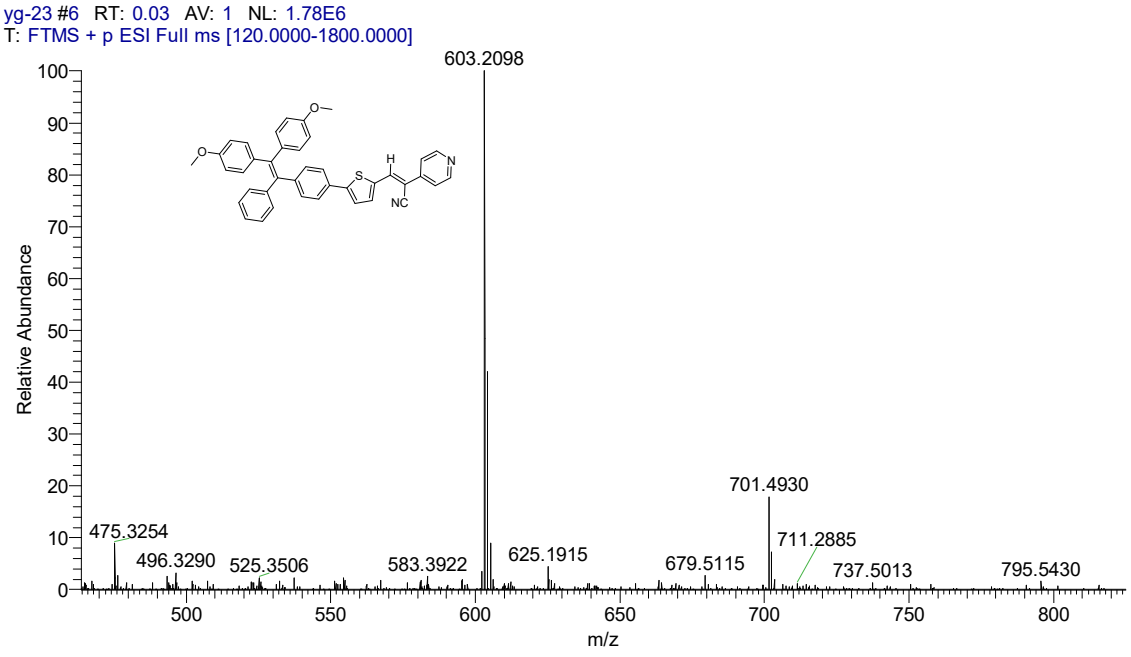


Figure S14. HRMS spectrum of compound **6**

Synthesis of Compound 7. The same synthetic procedure as described compound **2** for using compound **5** (200 mg, 0.4 mmol) and 2-(quinolin-4-yl)acetonitrile (84 mg, 0.5 mmol), affording the product as an orange red powder (90 mg, yield: 35%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.94 (d, *J* = 4.5 Hz, 1H), 8.22 (dd, *J* = 21.1, 8.2 Hz, 2H), 7.78 (dd, *J* = 16.7, 8.3 Hz, 1H), 7.70 – 7.62 (m, 1H), 7.60 (d, *J* = 4.4 Hz, 1H), 7.52 (d, *J* = 6.8 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.33 (d, *J* = 4.0 Hz, 1H), 7.17 – 7.04 (m, 6H), 7.01 – 6.84 (m, 6H), 6.72 – 6.57 (m, 4H), 3.76 (s, 6H). ^{13}C NMR (100MHz, Chloroform-d) δ 158.38, 158.20, 150.85, 149.99, 148.79, 143.89, 141.60, 141.43, 141.15, 138.26, 136.06, 135.79, 135.56, 132.63, 132.55, 131.43, 131.32, 130.54, 130.36, 130.04, 127.86, 127.55, 126.35, 125.53, 123.51,120.80, 113.24, 113.03, 55.10. HRMS (ESI+): calcd. For $C_{44}H_{33}N_2O_2S^+$ $[M+H]^+$ 653.2257, found 653.2222.

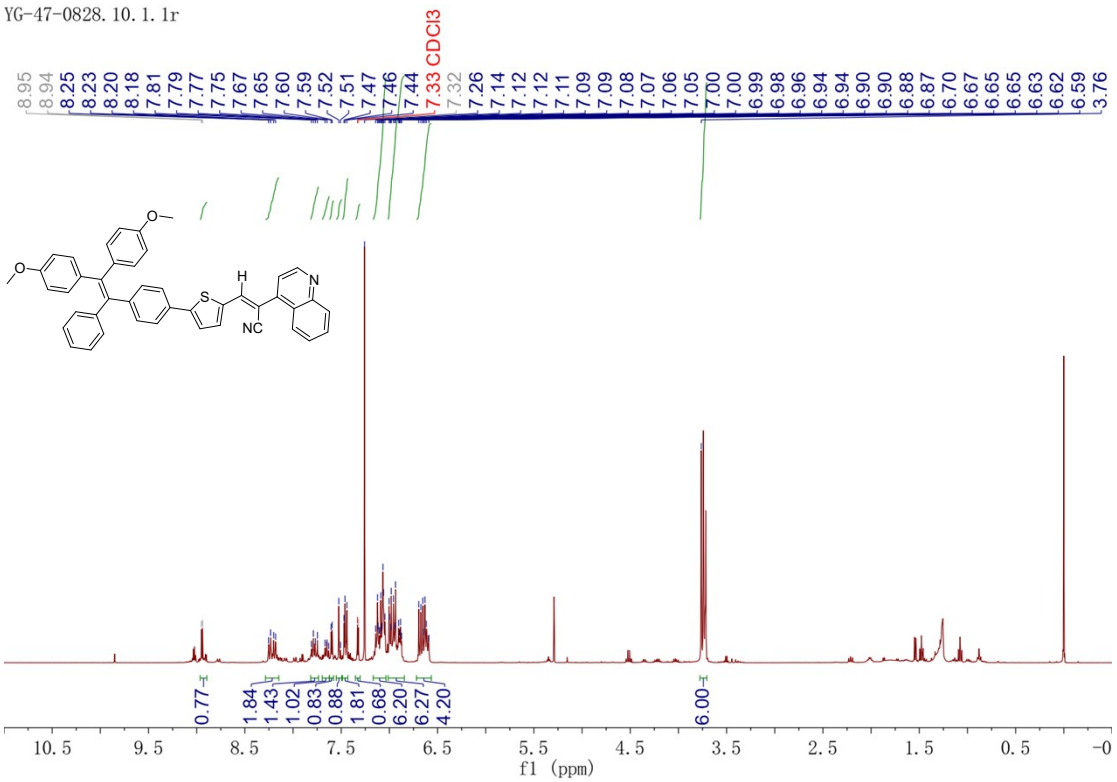


Figure S15. ^{1}H NMR spectrum of compound **7**

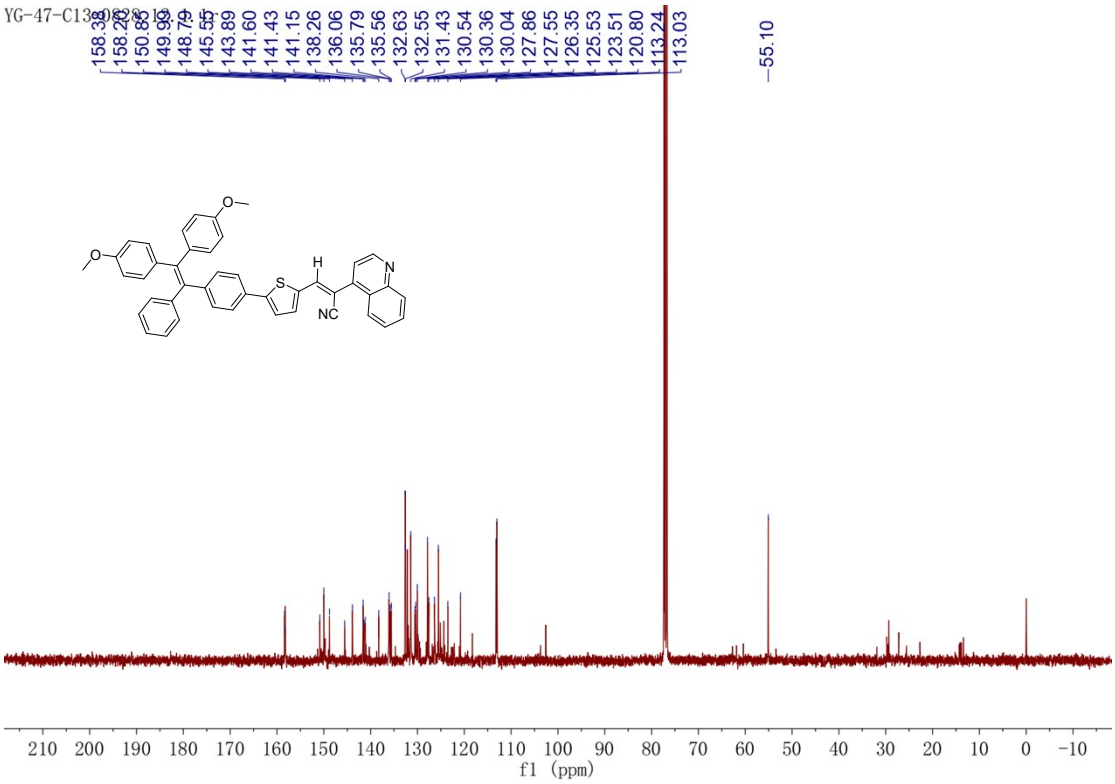


Figure S16. ^{13}C NMR spectrum of compound **7**

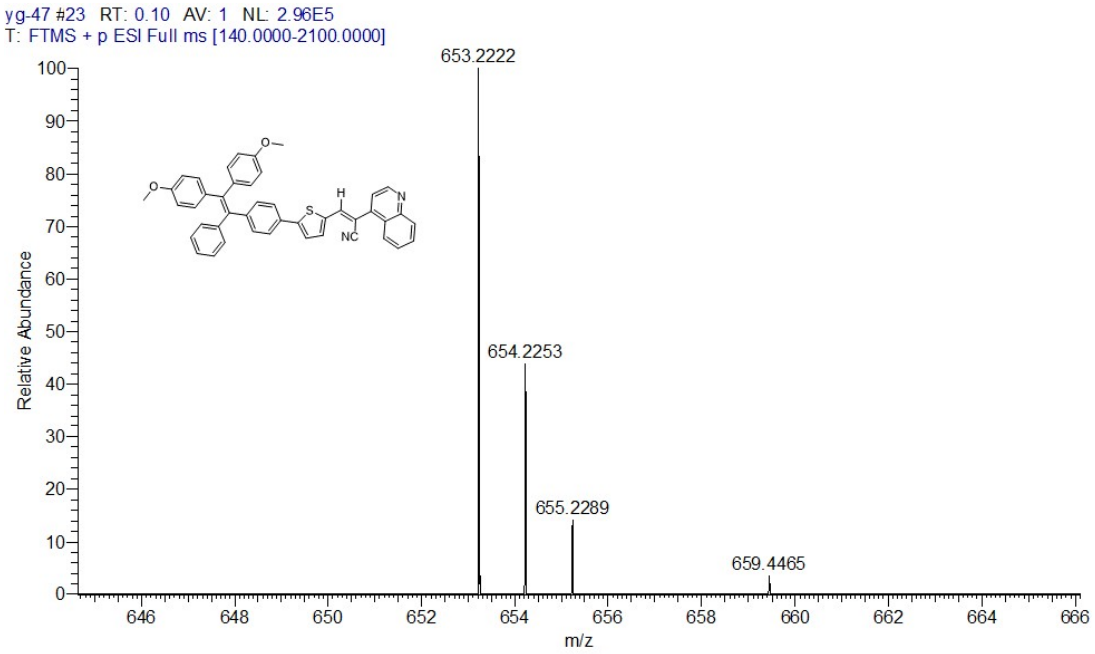


Figure S17. HRMS spectrum of compound **7**

Synthesis of Compound 8. The same synthetic procedure as described compound **1** for using compound **4** (414 mg, 0.8 mmol) and 7-bromo-2,3-dihydrothieno[3,4-b][1,4]dioxine-5-carbaldehyde (98 mg, 0.4 mmol) affording the product as an orange powder (190 mg, yield: 85%). ^{1}H NMR (400 MHz, Chloroform-d) δ 9.90 (s, 1H), 7.55 (d, J = 8.5 Hz, 2H), 7.15 – 6.89 (m, 11H), 6.64 (dd, J = 12.2, 8.8 Hz, 4H), 4.40 – 4.32 (m, 4H), 3.74 (d, J = 4.8 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-d) δ 179.59 , 158.30 , 158.19 , 145.14 , 143.95 , 140.98 , 138.40 , 137.69 , 136.12 , 132.63 , 131.82 , 131.43 , 129.31 , 127.80 , 126.28 , 126.08 , 115.38 , 113.21 , 113.00 , 65.09 , 64.49 , 55.12 .

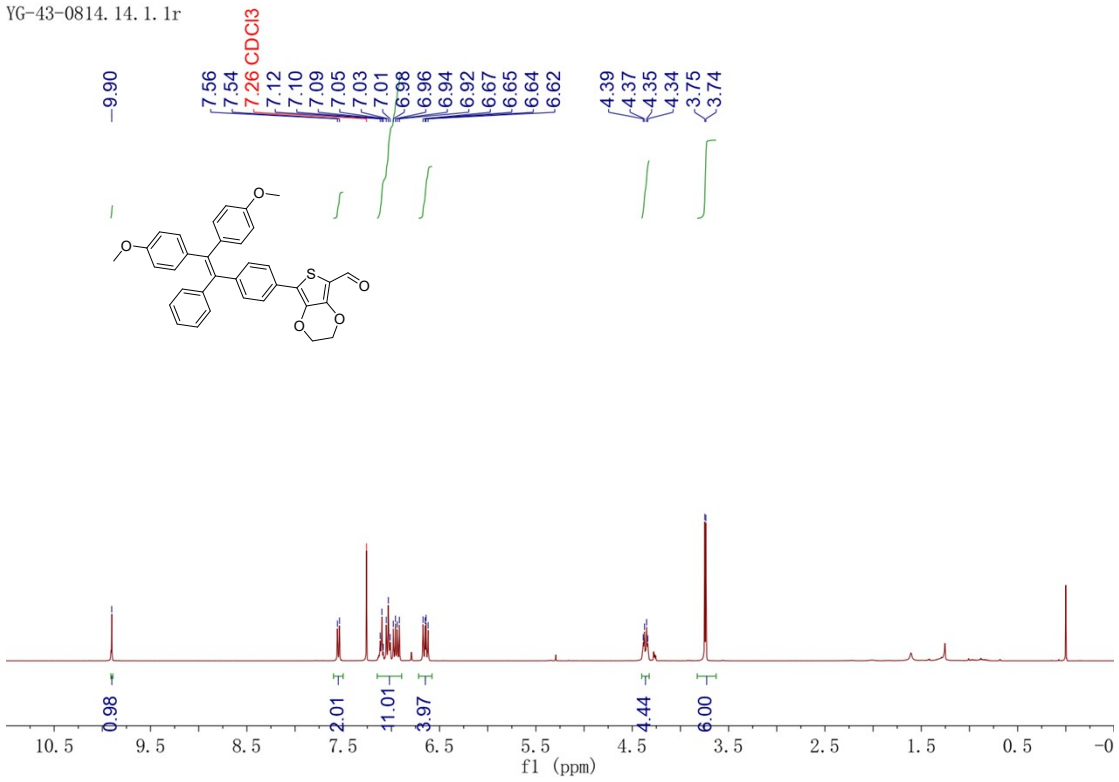


Figure S18. ^{1}H NMR spectrum of compound **8**

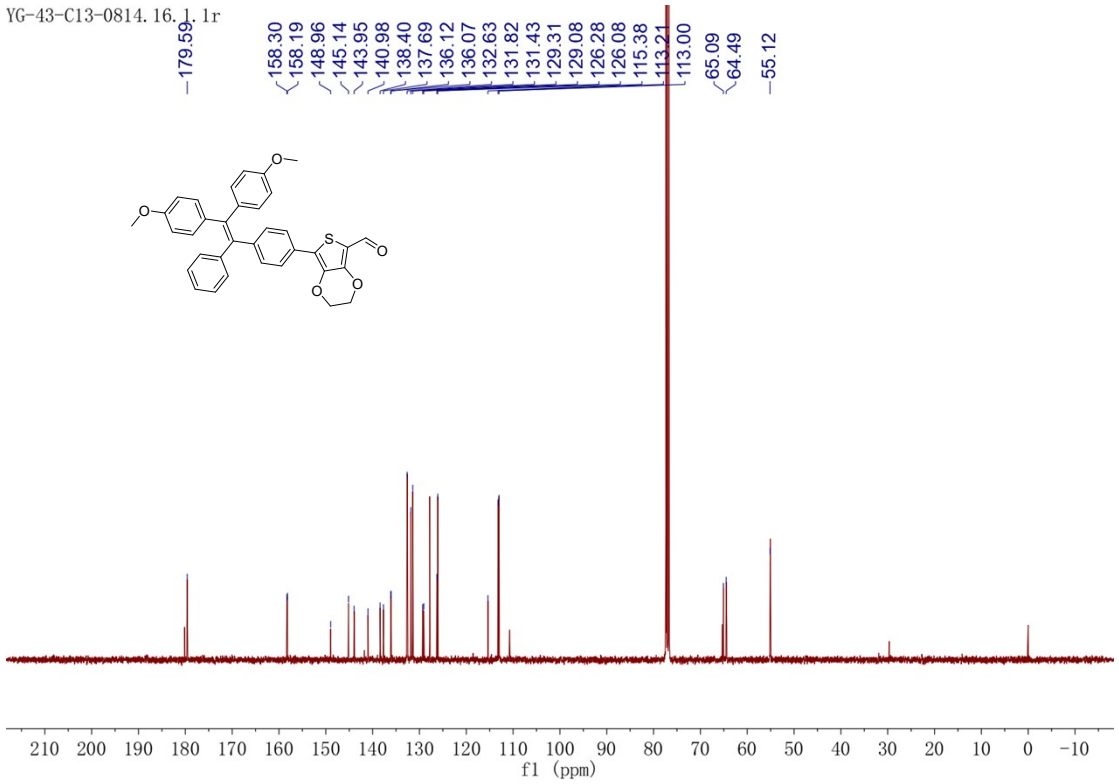


Figure S19. ^{13}C NMR spectrum of compound **8**

Synthesis of Compound 9. The same synthetic procedure as described compound **2** for using compound **8** (200 mg, 0.36 mmol), affording the product as an orange red powder (163 mg, yield: 69%).^{1}H NMR (400 MHz, Chloroform-d) δ 8.61 (d, J = 6.2 Hz, 2H), 7.95 (s, 1H), 7.59 (s, 2H), 7.49 (d, J = 6.3 Hz, 2H), 7.11 (d, J = 9.1 Hz, 3H), 7.06 – 7.02 (m, 4H), 6.96 (dd, J = 15.8, 8.8 Hz, 4H), 6.70 – 6.59 (m, 4H), 4.36 (dd, J = 15.0, 5.2 Hz, 4H), 3.75 (d, J = 8.3 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-d) δ 158.33, 158.18, 150.19, 146.60, 144.87, 143.94, 142.22, 141.00, 138.45, 137.65, 136.16, 136.11, 132.62, 132.00, 131.85, 131.46, 129.30, 127.80, 126.28, 126.08, 119.19, 117.90, 113.23, 113.00, 111.17, 100.26, 65.20, 64.59, 55.12. HRMS (ESI^+): calcd. for $C_{42}H_{33}N_2O_4S^+[M+H]^+$661.2156, found 661.2147.

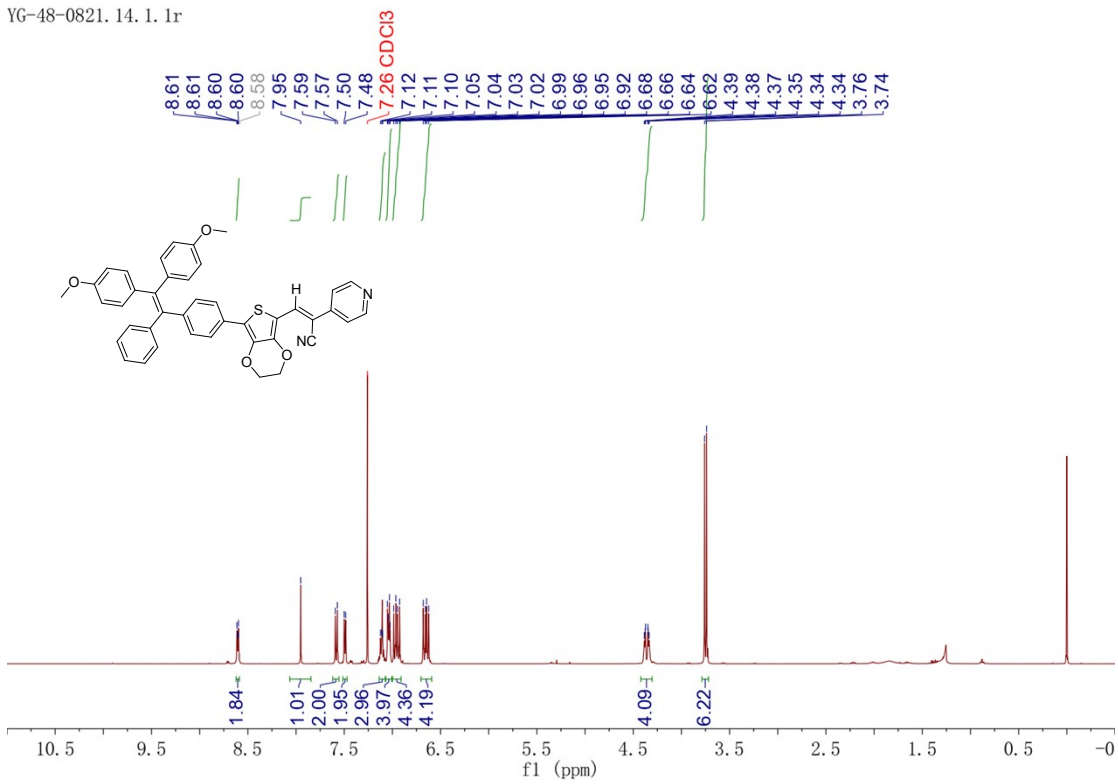


Figure S20. ^{1}H NMR spectrum of compound **9**

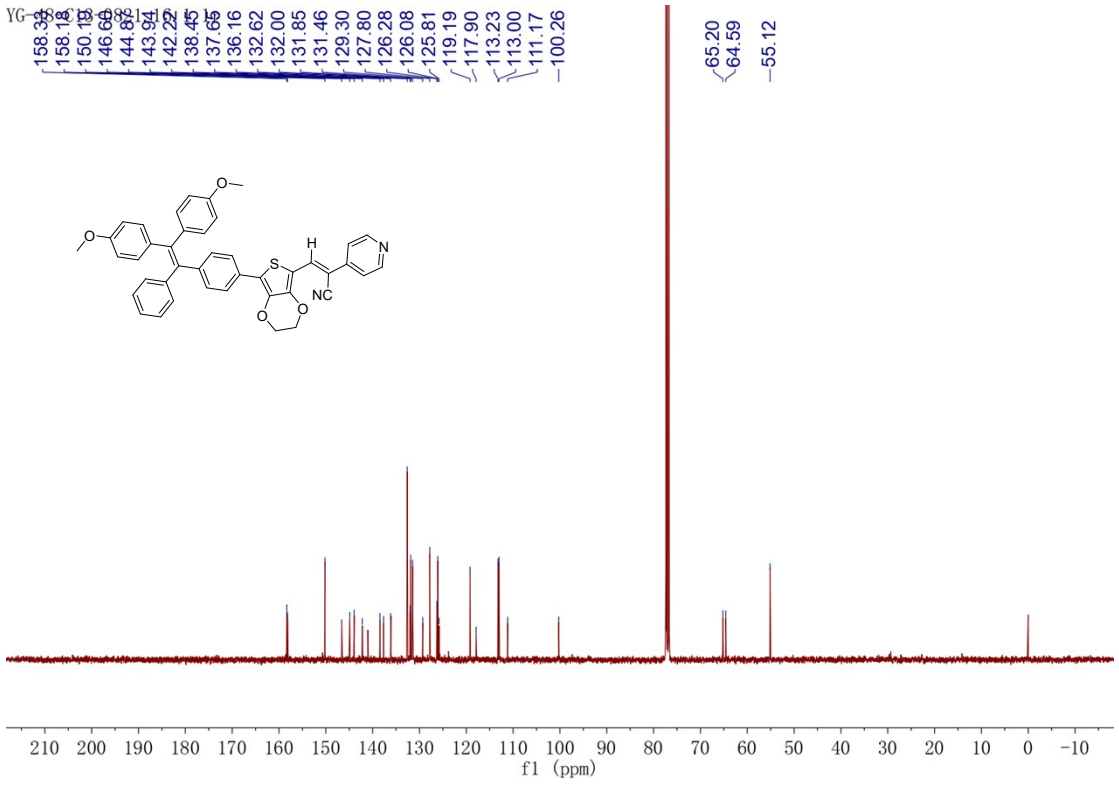


Figure S21. ^{13}C NMR spectrum of compound **9**

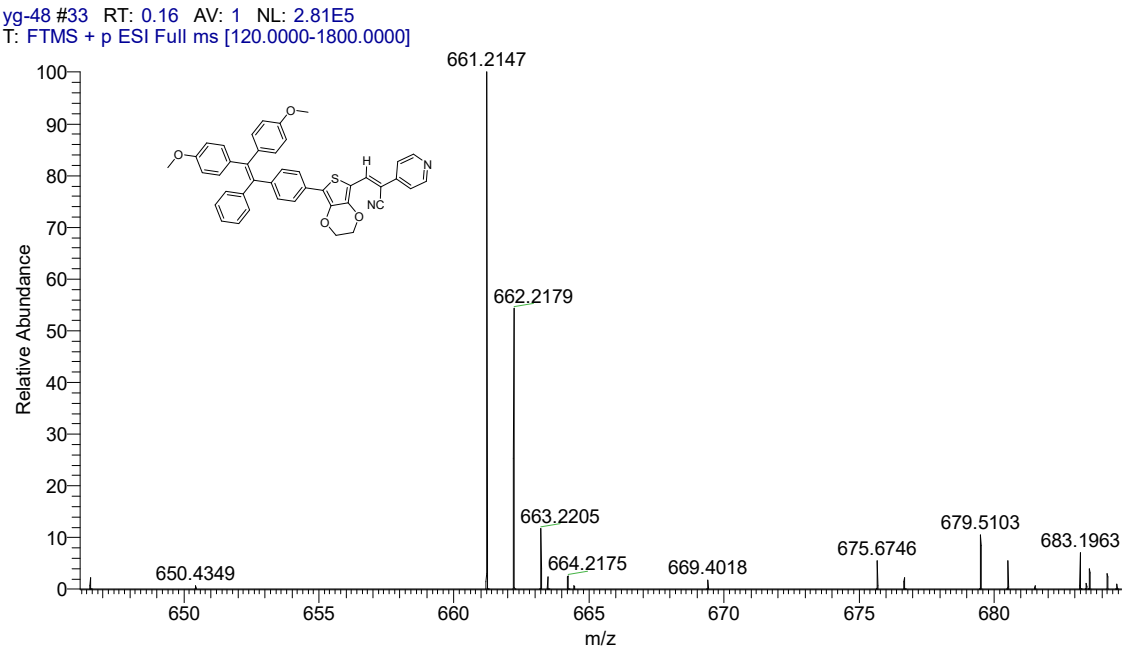


Figure S22. HRMS spectrum of compound **9**

Synthesis of Compound 10. The same synthetic procedure as described compound **2** for using compound **8** (200 mg, 0.36 mmol) and 2-(quinolin-4-yl)acetonitrile (84 mg, 0.5 mmol) affording the product as an orange red powder (165 mg, yield: 66%).^{1}H NMR (400 MHz, Chloroform-d) δ 8.91 (d, J = 4.5 Hz, 1H), 8.29 (d, J = 8.3 Hz, 1H), 8.19 (d, J = 8.3 Hz, 1H), 7.78 (t, J = 8.1 Hz, 1H), 7.72 – 7.57 (m, 4H), 7.46 (d, J = 4.5 Hz, 1H), 7.11 (t, J = 6.7 Hz, 3H), 7.05 (s, 4H), 6.97 (dd, J = 17.4, 8.7 Hz, 4H), 6.66 (dd, J = 16.3, 8.7 Hz, 4H), 4.33 (s, 4H), 3.75 (d, J = 10.8 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-d) δ 158.36 , 158.20 , 149.73 , 146.27, 140.98 , 138.50 , 137.60, 137.05 , 136.20 , 136.14 , 132.64 , 131.87 , 131.49 , 130.02 , 129.40 , 127.82 , 127.43 , 126.29 , 126.08 , 125.61 , 124.57 , 120.69 , 113.25 , 113.03 , 110.91 , 98.79 , 65.14, 64.60, 55.11. HRMS (ESI^{+}): calcd. for $C_{46}H_{35}N_2O_4S^{+}$[M+H]$^{+}$ 711.2312, found 711.2300.

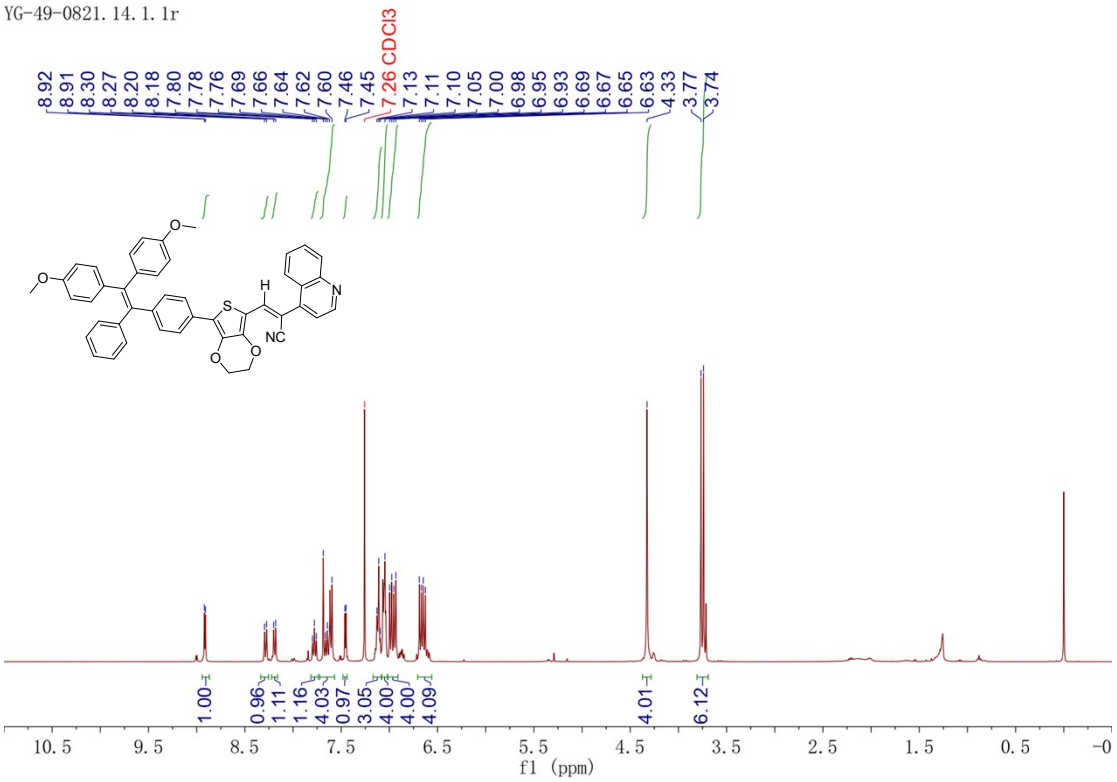


Figure S23. ^{1}H NMR spectrum of compound **10**

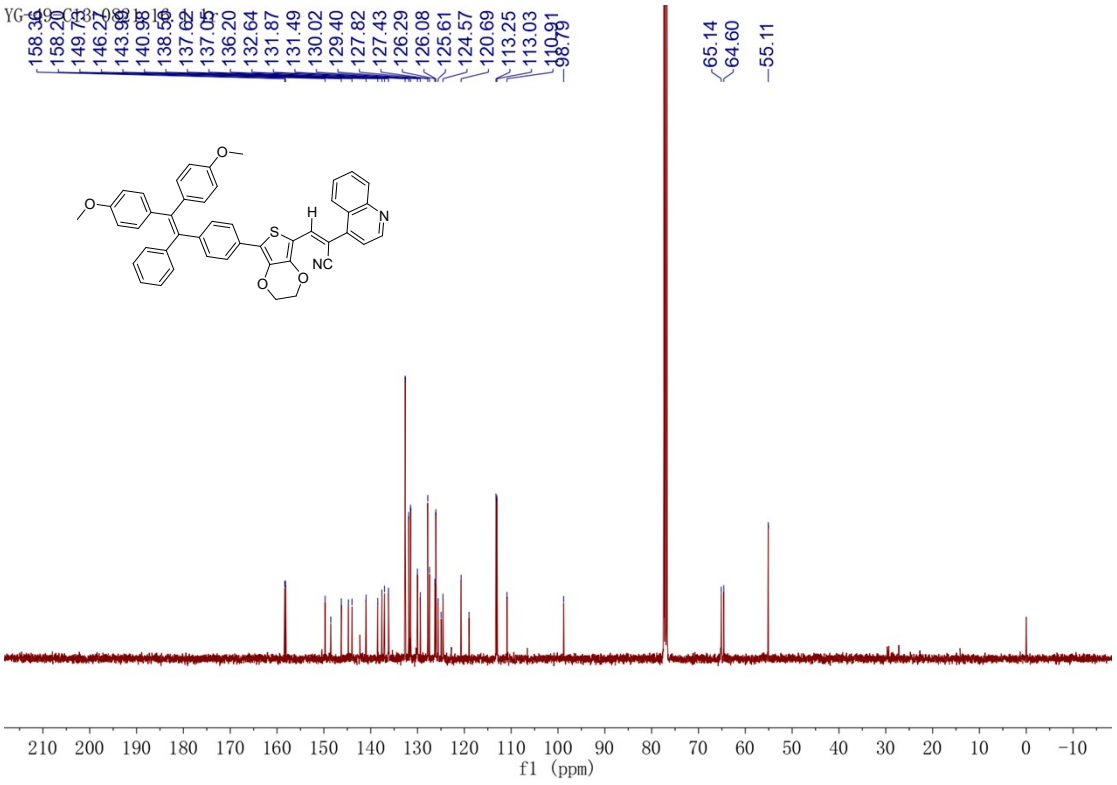


Figure S24. ^{13}C NMR spectrum of compound **10**

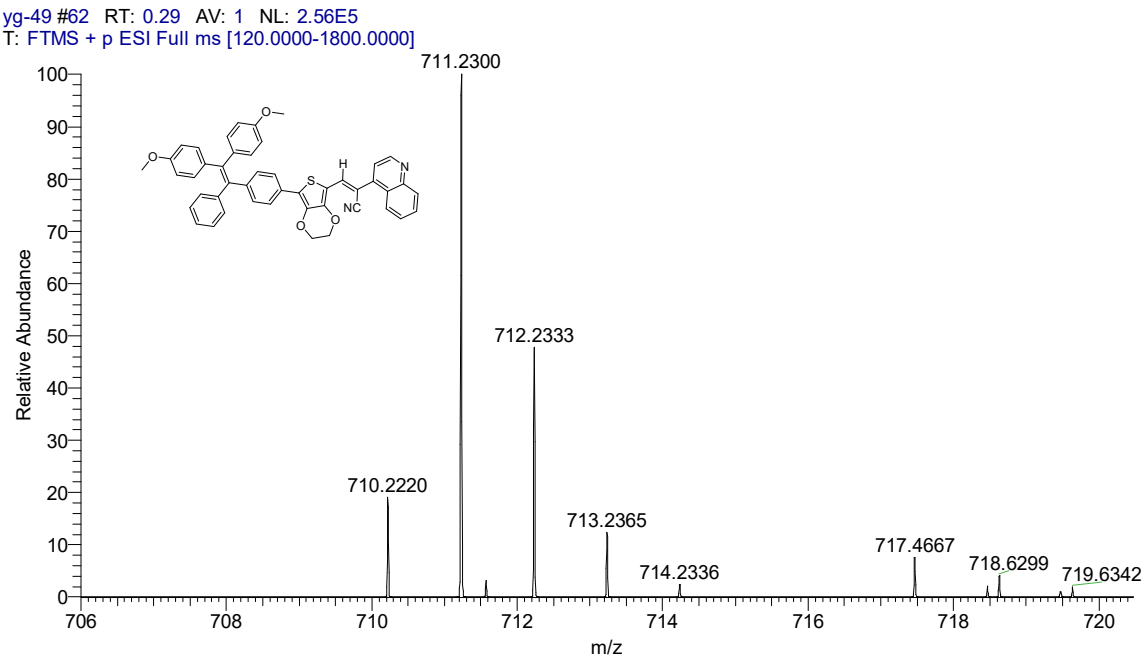


Figure S25. HRMS spectrum of compound **10**

Synthesis of TPE-T-Py. To a stirred solution of compound **2** (60 mg, 0.12 mmol) in acetonitrile, iodomethane (1.92 mmol, 16 equiv) was added and the mixture was heated to reflux for 24 h under nitrogen. After cooling to room temperature, the mixture was poured into diethyl ether. The precipitates were filtered and re-dissolved in 20 mL methanol, followed by adding saturated KPF_6 solution (15 mL). After stirring for 1 h, the solvent was evaporated and the residue was filtered again, washed with water and dried under reduced pressure to give target compound as an orange red powder (60mg, yield: 71%).^{1}H NMR (400 MHz, DMSO-d_6) δ 8.96 (d, J = 7.1 Hz, 3H), 8.30 (d, J = 7.1 Hz, 2H), 7.97 (d, J = 4.2 Hz, 1H), 7.80 (d, J = 4.1 Hz, 1H), 7.63 (d, J = 8.4 Hz, 2H), 7.21 – 6.96 (m, 17H), 4.30 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 153.54, 149.39, 145.98, 145.49, 144.18, 143.40, 143.20, 142.07, 141.86, 140.15, 136.11, 132.30, 131.22, 131.17, 131.10, 130.64, 128.52, 128.47, 128.33, 127.42, 127.28, 127.23, 126.21, 126.12, 122.74, 116.95, 100.61, 47.59. HRMS (ESI+): calcd. for $C_{39}H_{29}N_2S^+$ $[M\text{-}PF_6]^+$557.2046, found 557.2025.

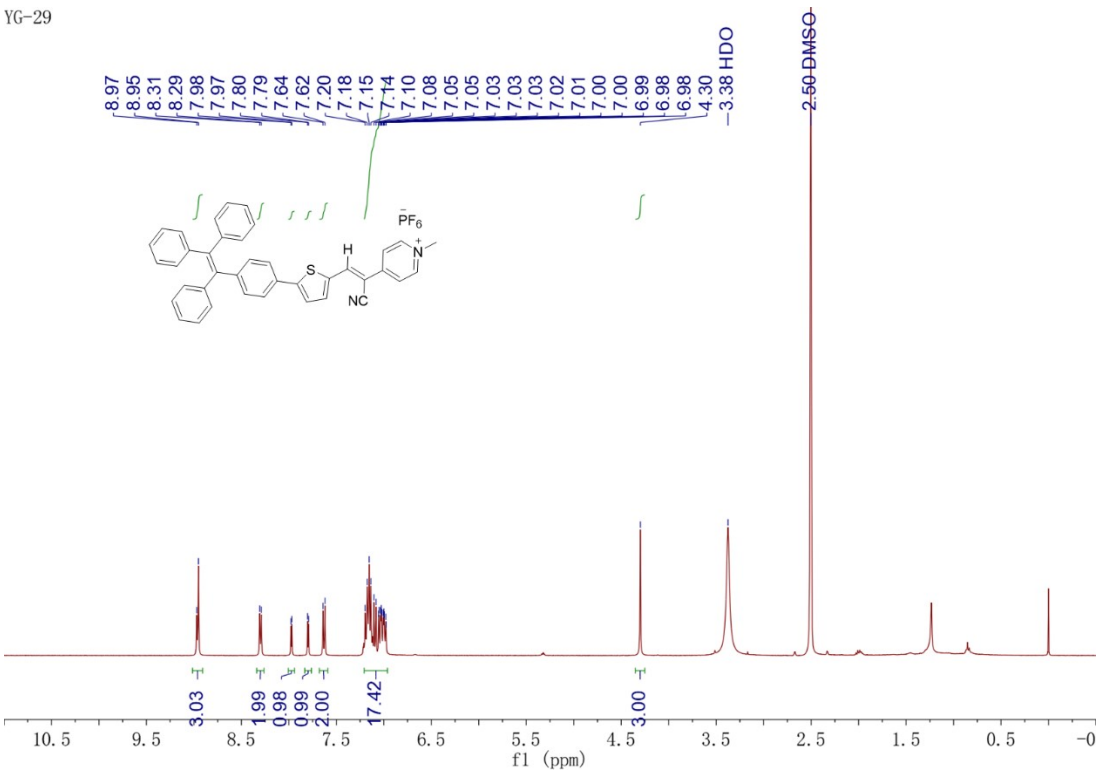


Figure S26. ^{1}H NMR spectrum of **TPE-T-Py**

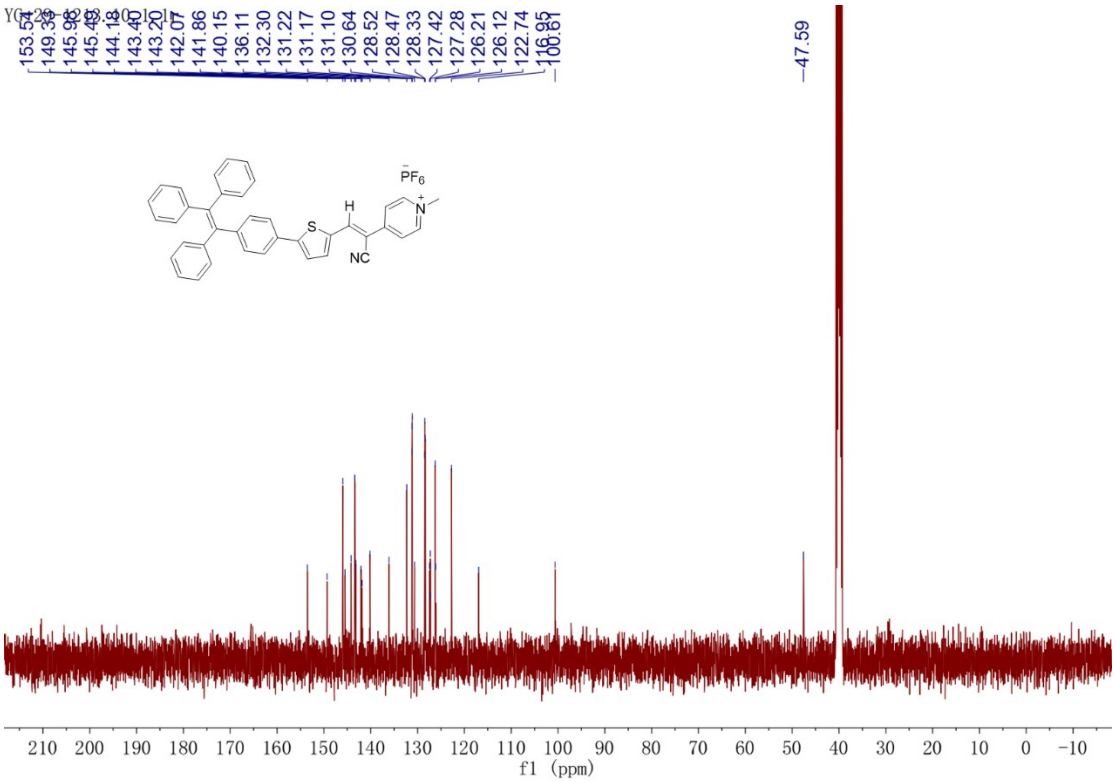


Figure S27. ^{13}C NMR spectrum of **TPE-T-Py**

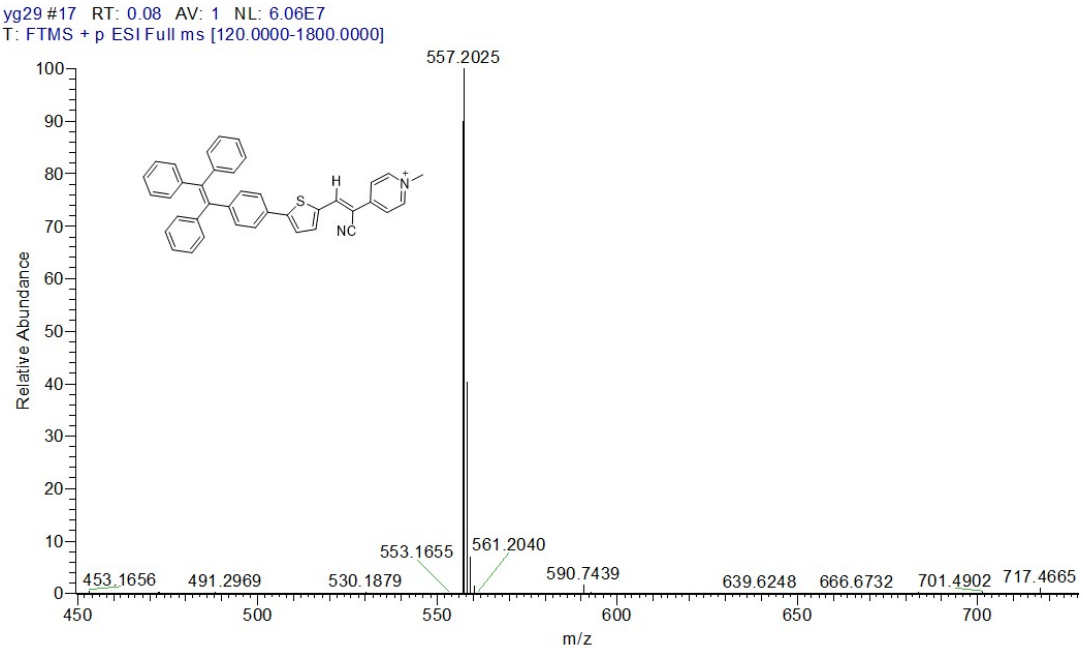


Figure S28. HRMS spectrum of **TPE-T-Py**

Synthesis of MTPE-T-Py. The same synthetic procedure as described **TPE-T-Py** for using compound **6** (90 mg, 0.15 mmol), affording the product as a red powder (80 mg, yield: 70%).^{1}H NMR (400 MHz, DMSO-d_6) δ 8.96 (d, J = 7.2 Hz, 3H), 8.30 (d, J = 7.0 Hz, 2H), 7.97 (d, J = 4.2 Hz, 1H), 7.80 (d, J = 4.1 Hz, 1H), 7.63 (d, J = 8.4 Hz, 2H), 7.24–7.04 (m, 5H), 7.03–6.97 (m, 2H), 6.93 (d, J = 8.7 Hz, 2H), 6.87 (d, J = 8.7 Hz, 2H), 6.72 (dd, J = 18.5, 8.8 Hz, 4H), 4.30 (s, 3H), 3.69 (d, J = 2.4 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.50, 158.35, 153.77, 149.36, 146.27, 145.98, 144.17, 143.89, 141.89, 141.46, 138.29, 136.00, 135.87, 132.63, 132.56, 132.38, 131.33, 130.28, 128.50, 126.99, 126.24, 126.01, 122.71, 113.87, 113.67, 100.49, 55.41, 47.58. HRMS (ESI+): calcd. for $C_{41}H_{33}N_2O_2S^+$ $[M\text{-}PF_6]^+$ 617.2257, found 617.2231.

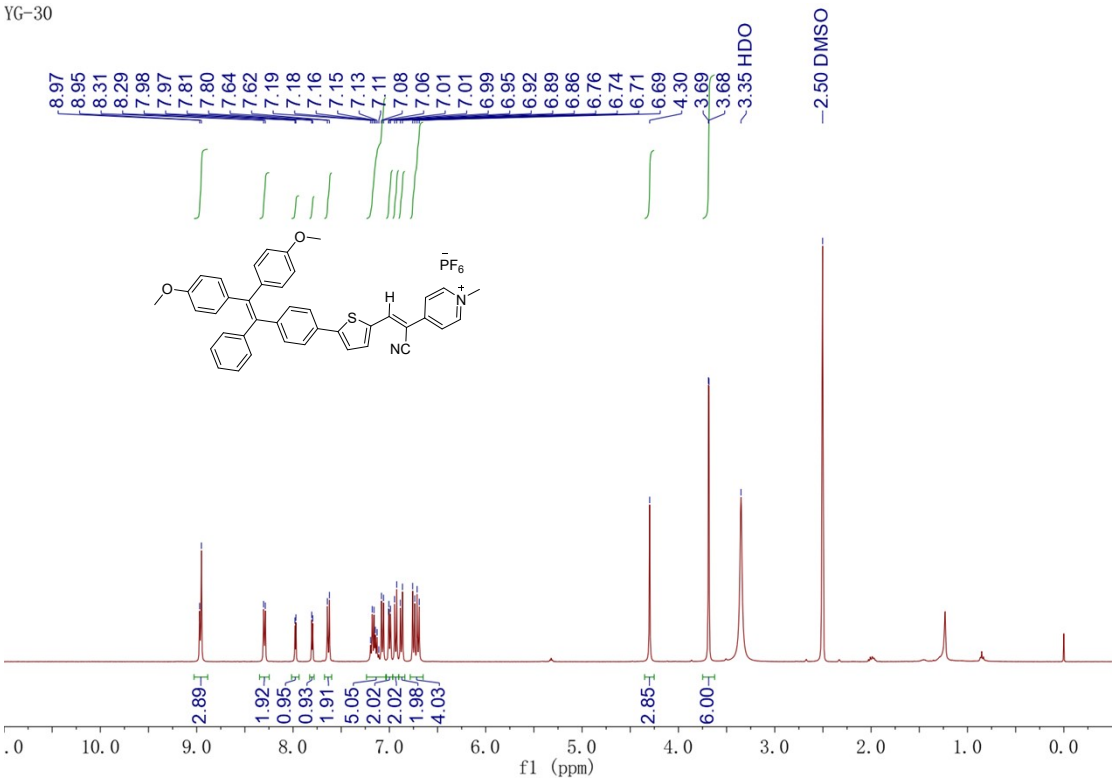


Figure S29. ^{1}H NMR spectrum of **MTPE-T-Py**

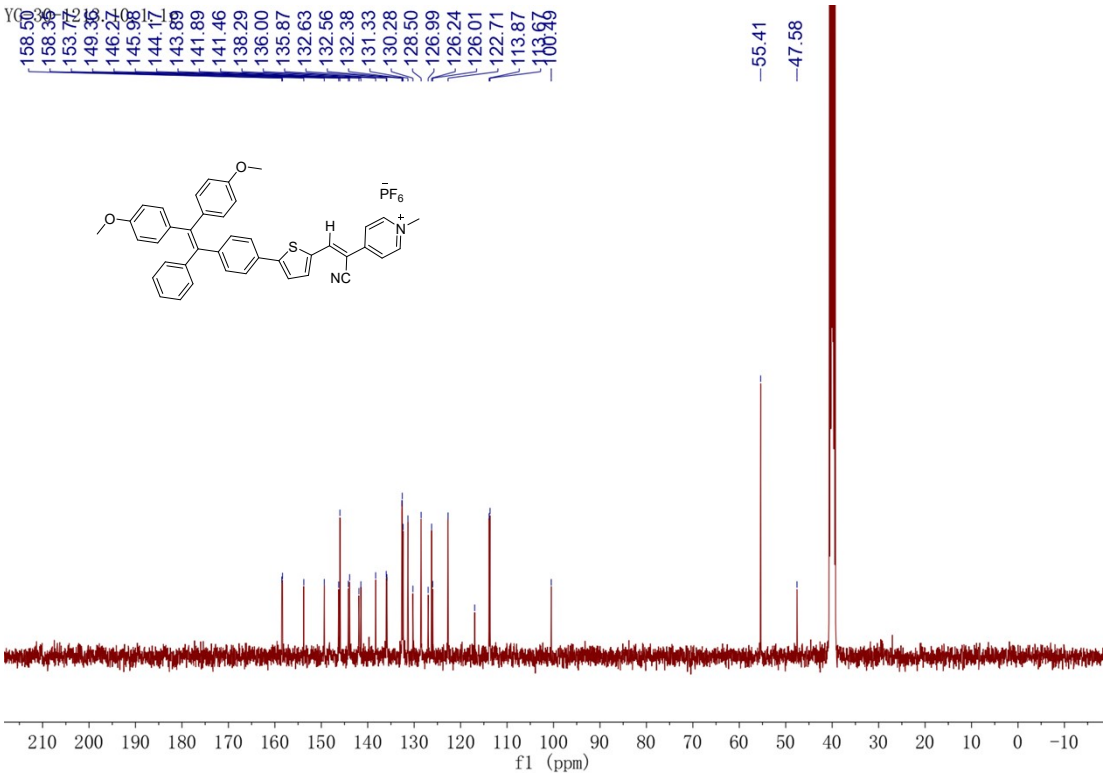


Figure S30. ^{13}C NMR spectrum of **MTPE-T-Py**

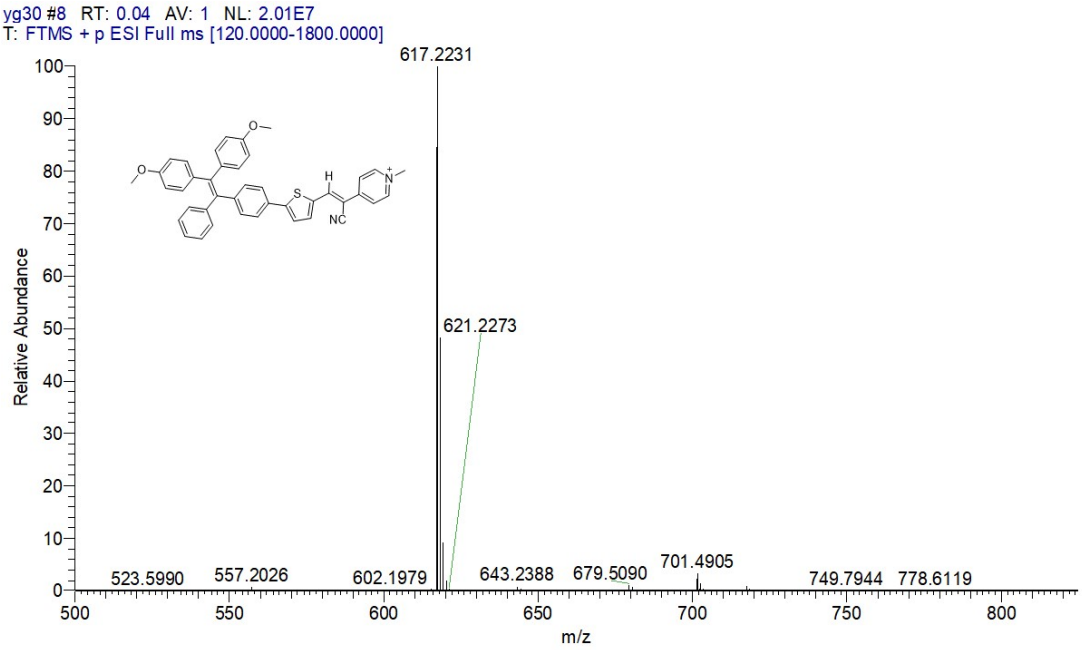


Figure S31. HRMS spectrum of MTPE-T-Py

Synthesis of MTPE-T-Qy. The same synthetic procedure as described **TPE-T-Py** for using compound **7** (90 mg, 0.15 mmol), affording the product as a black red powder (40 mg, yield: 55%).^{1}H NMR (400 MHz, DMSO-d_6) δ 9.58 (d, J = 6.4 Hz, 1H), 8.69 (d, J = 8.4 Hz, 1H), 8.59 (d, J = 9.0 Hz, 1H), 8.42 (s, 1H), 8.39 – 8.32 (m, 2H), 8.20 – 8.11 (m, 1H), 7.99 (d, J = 4.1 Hz, 1H), 7.78 (d, J = 4.0 Hz, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.16 (dd, J = 13.3, 7.2 Hz, 3H), 7.09 (d, J = 8.4 Hz, 2H), 7.01 (d, J = 8.1 Hz, 2H), 6.95 (d, J = 6.9 Hz, 2H), 6.89 (d, J = 8.7 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 6.72 – 6.69 (m, 2H), 4.66 (s, 3H), 3.69 (d, J = 5.3 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.51 , 158.36 , 152.16 , 150.98 , 149.91 , 146.93 , 145.97 , 143.94 , 141.39 , 140.90 , 139.28, 138.35 , 135.98 , 132.62 , 132.36 , 131.33 , 130.91 , 130.45 , 128.50 , 127.35 , 126.97 , 126.47 , 126.14 , 125.56 , 118.16 , 113.89 , 99.43 , 55.42 , 45.94 . HRMS (ESI+): calcd. for $C_{45}H_{35}N_2O_2S^+[M\text{-}PF_6]^+$ 667.2414, found 667.2409.

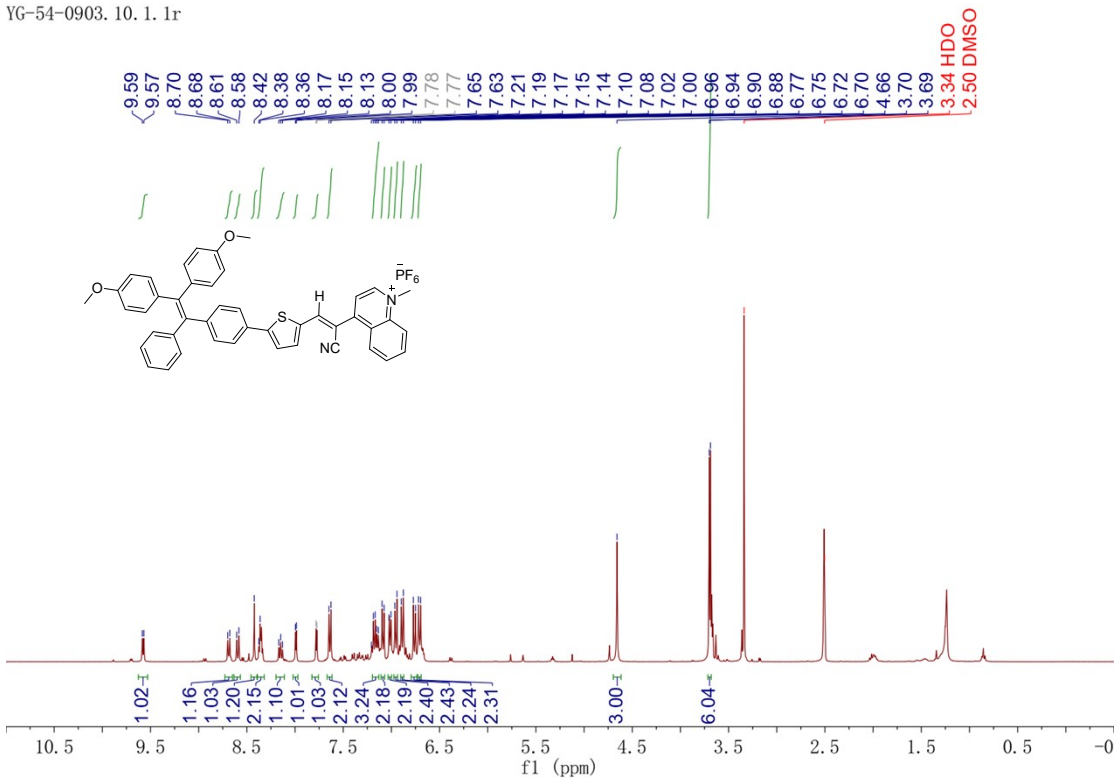


Figure S32. ^{1}H NMR spectrum of **MTPE-T-Qy**

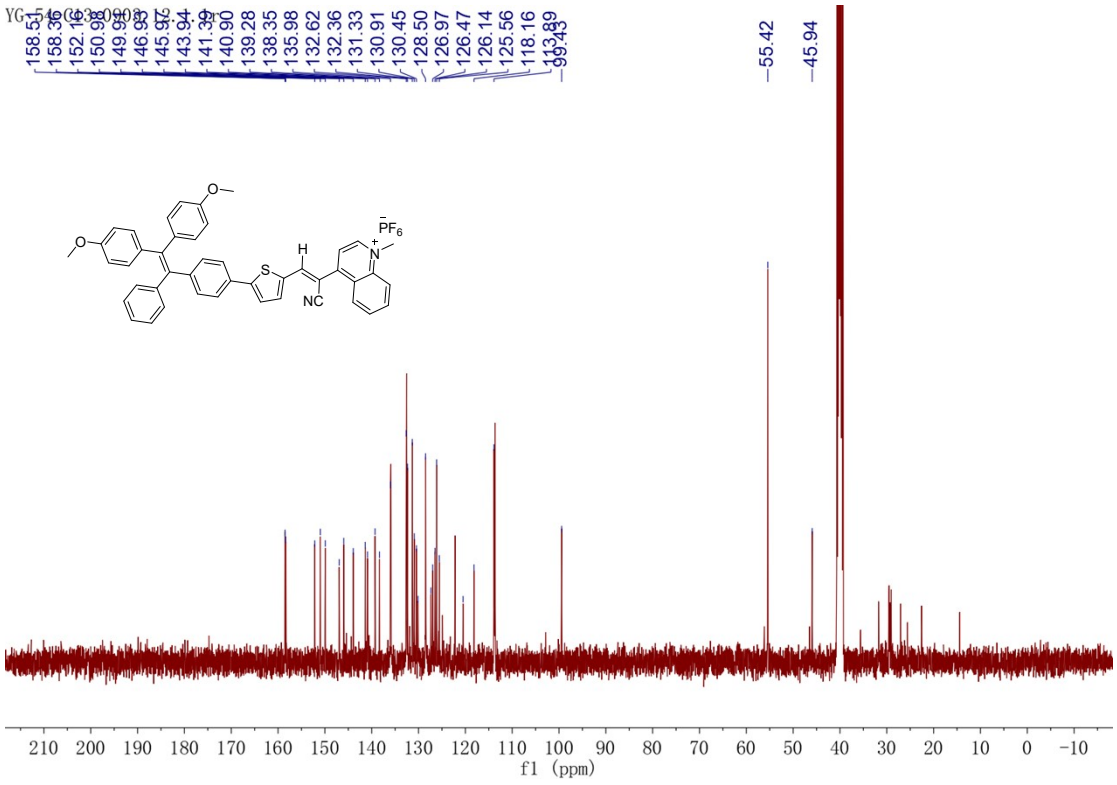


Figure S33. ^{13}C NMR spectrum of **MTPE-T-Qy**

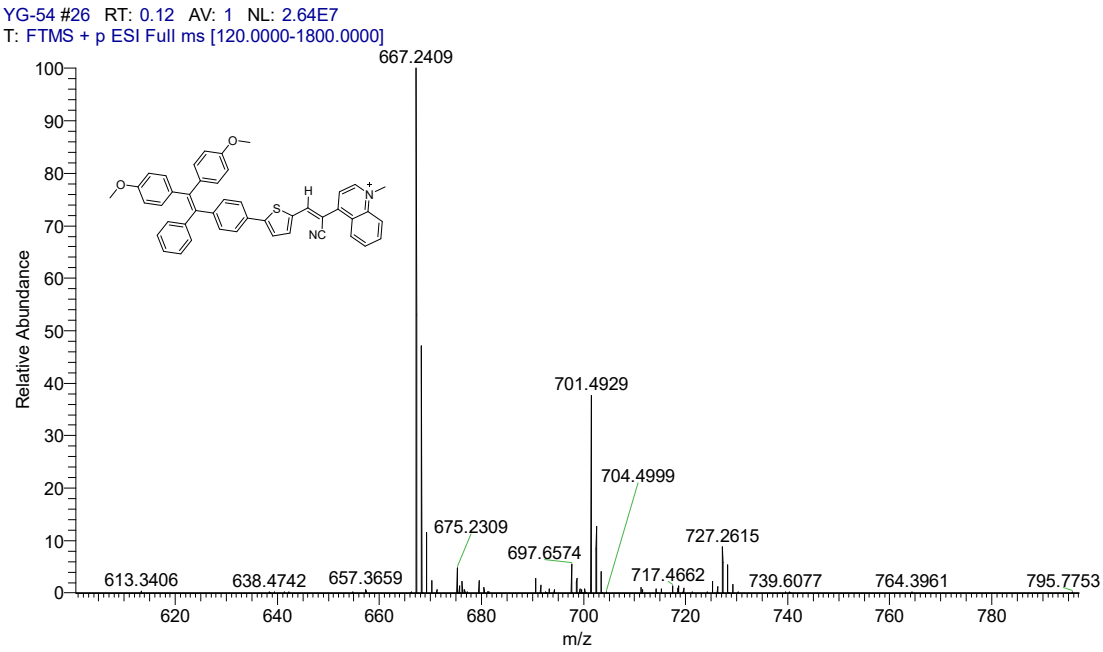


Figure S34. HRMS spectrum of **MTPE-T-Qy**

Synthesis of MTPE-DT-Py. The same synthetic procedure as described **TPE-T-Py** for using compound **9** (120 mg, 0.18 mmol), affording the product as an orange red powder (110 mg, yield: 75%).^{1}H NMR (400 MHz, DMSO-d_6) δ 8.84 (d, J = 7.0 Hz, 2H), 8.47 (s, 1H), 8.27 (d, J = 7.0 Hz, 2H), 7.61 (d, J = 8.5 Hz, 2H), 7.21 – 7.05 (m, 5H), 7.02 – 6.97 (m, 2H), 6.90 (dd, J = 20.4, 8.7 Hz, 4H), 6.72 (dd, J = 17.4, 8.8 Hz, 4H), 4.63 – 4.40 (m, 4H), 4.27 (s, 3H), 3.69 (d, J = 3.6 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.48, 158.38, 150.75, 149.56, 145.75, 145.61, 143.85, 141.48 ,139.06, 138.37, 137.72, 135.88, 132.63, 132.55, 132.15, 131.32, 129.11, 128.48, 127.95, 126.98, 126.58, 122.31, 113.86, 113.68, 111.04, 96.68, 66.18, 65.18, 55.42, 47.34. HRMS (ESI+): calcd. for $C_{43}H_{35}N_2O_4S^+[M\text{-}PF_6]^+$ 675.2312, found 675.2307.

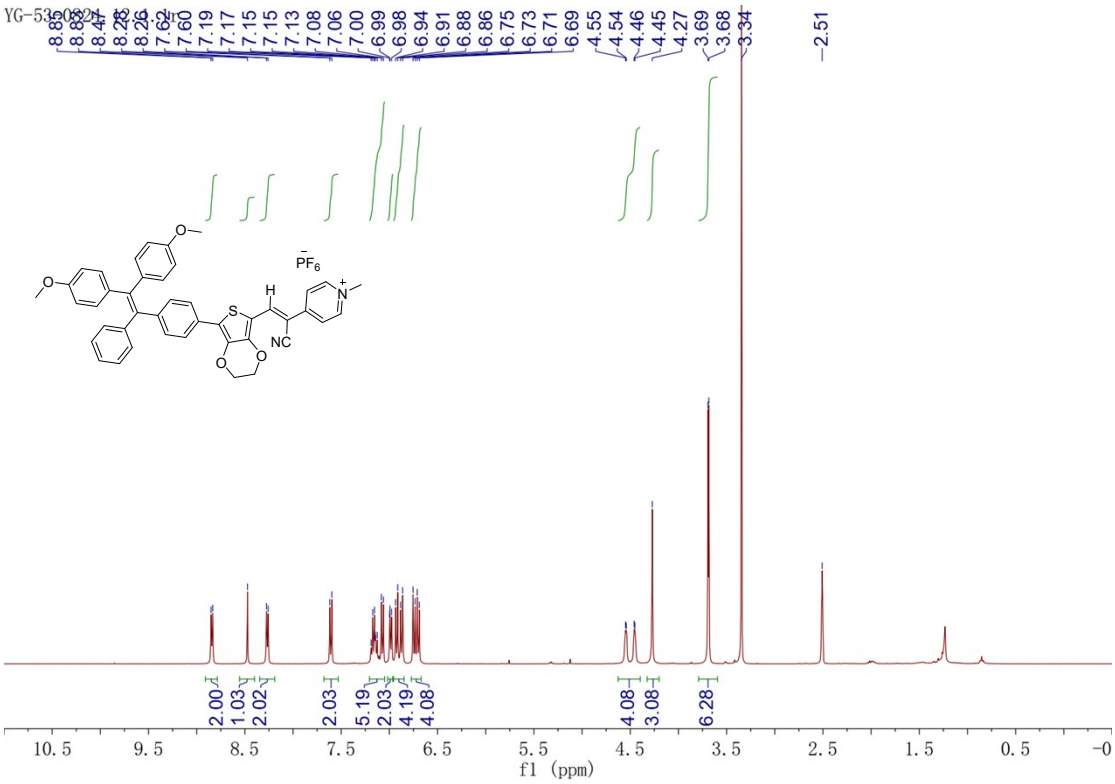


Figure S35. ^{1}H NMR spectrum of **MTPE-DT-Py**

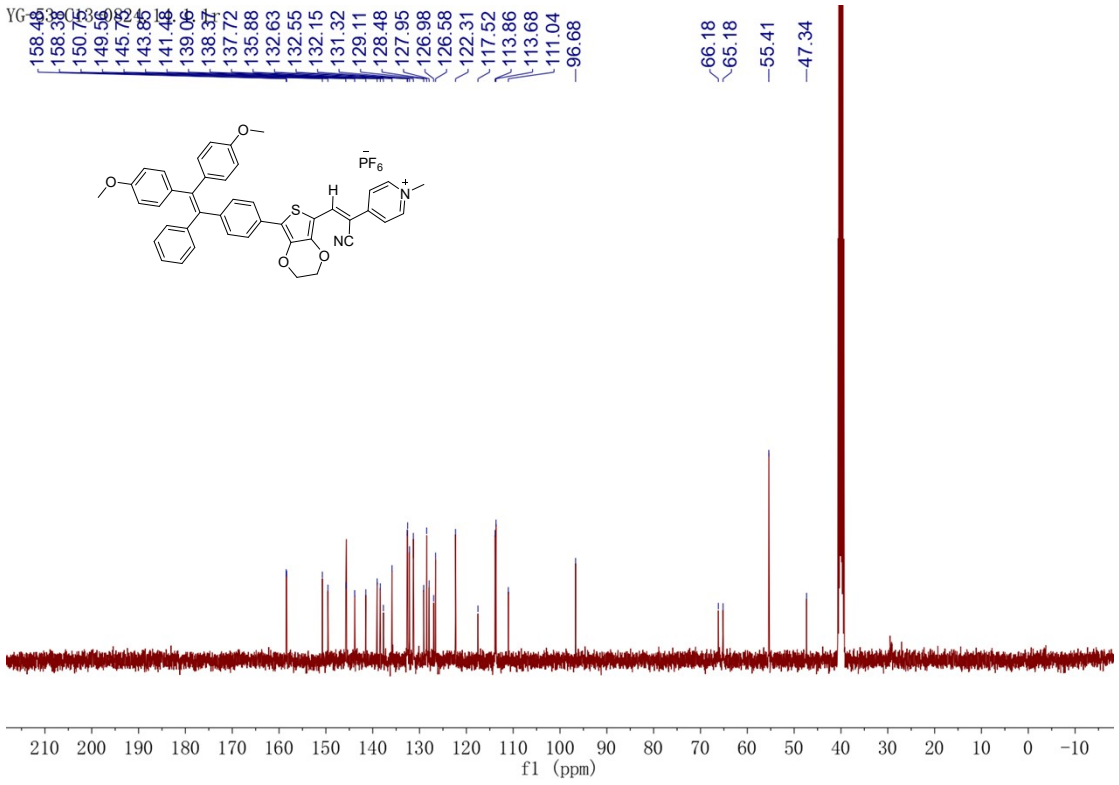


Figure S36. ^{13}C NMR spectrum of **MTPE-DT-Py**

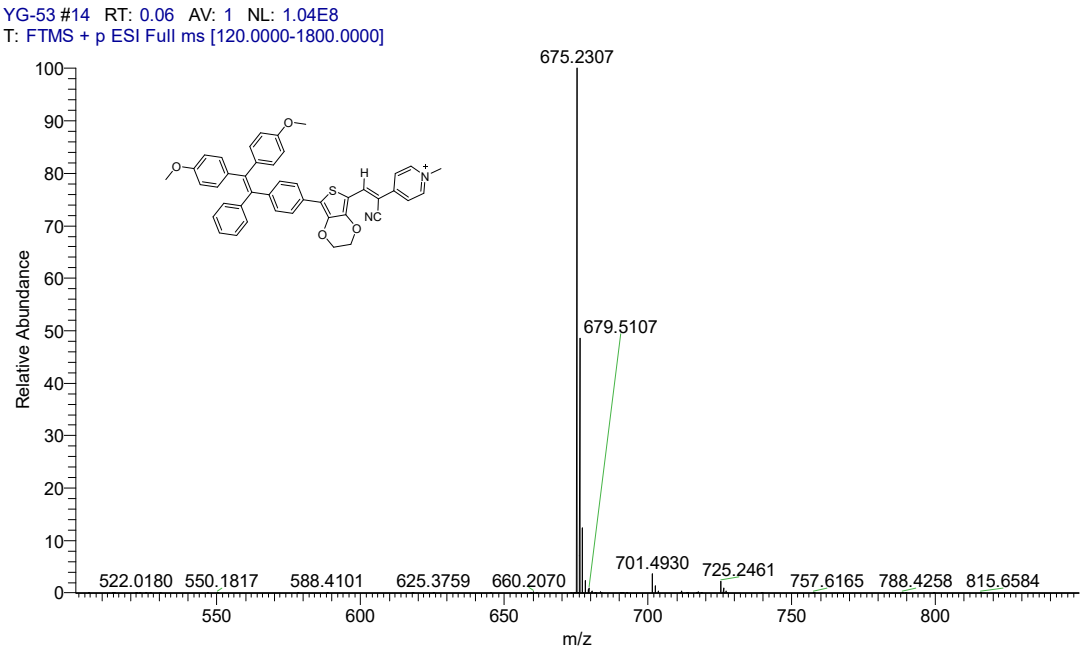


Figure S37. HRMS spectrum of **MTPE-DT-Py**

Synthesis of MTPE-DT-Qy. The same synthetic procedure as described **TPE-T-Py** for using compound **10** (110 mg, 0.15 mmol), affording the product as an orange red powder (70 mg, yield: 54%).^{1}H NMR (400 MHz, DMSO-d_6) δ 9.47 (d, J = 6.5 Hz, 1H), 8.64 (d, J = 8.5 Hz, 1H), 8.56 (d, J = 9.0 Hz, 1H), 8.33 (dd, J = 10.4, 6.8 Hz, 2H), 8.17–8.09 (m, 1H), 8.04 (s, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.16 (dt, J = 12.0, 6.8 Hz, 3H), 7.09 (d, J = 8.4 Hz, 2H), 7.03 – 6.98 (m, 2H), 6.94 (d, J = 8.7 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 6.76 (d, J = 8.8 Hz, 2H), 6.70 (d, J = 8.8 Hz, 2H), 4.63 (s, 3H), 4.46 (dd, J = 19.3, 4.5 Hz, 4H), 3.69 (d, J = 7.5 Hz, 6H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.47, 158.36, 151.44, 149.67, 149.62, 145.42, 143.90, 141.38, 139.25, 138.89, 138.41, 135.91, 132.63, 132.55, 132.14, 131.32, 130.70, 130.12, 129.25, 128.48, 126.46, 126.04, 121.89, 113.87, 113.68, 110.68, 95.78, 66.08, 65.24, 55.44, 55.41, 45.71. HRMS (ESI+): calcd. for $C_{47}H_{37}N_2O_4S^+$[M-PF_6]$^+$ 725.2469, found 725.2460

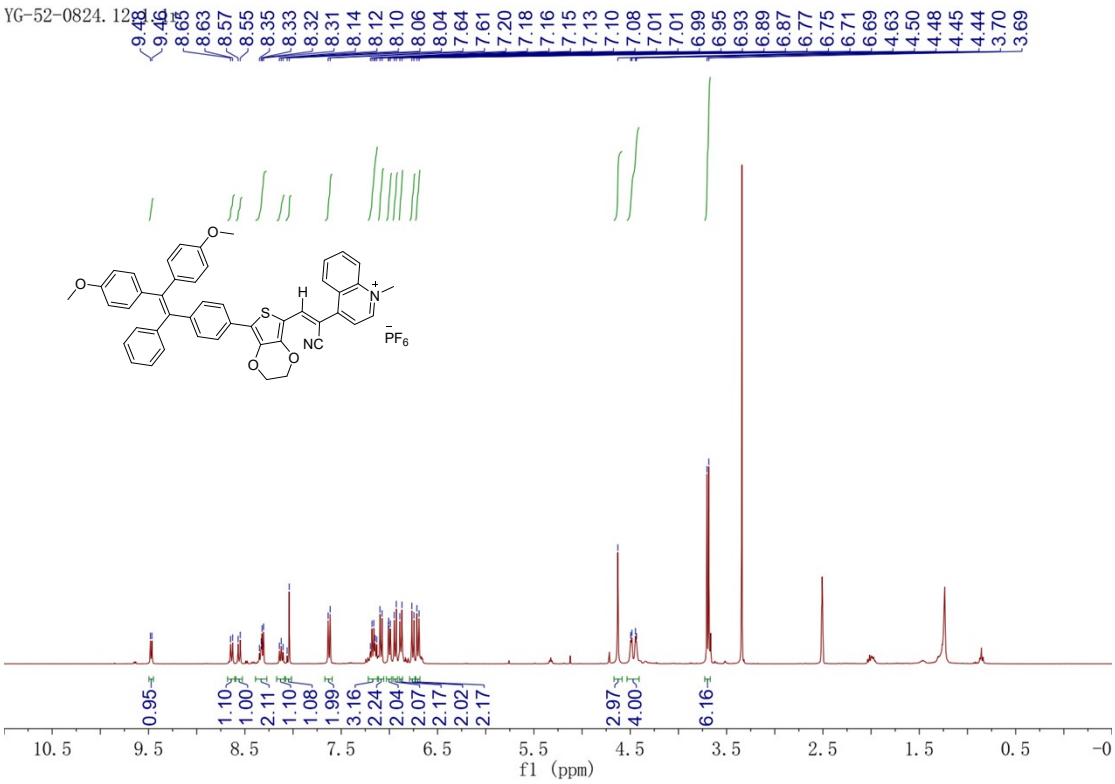


Figure S38. ^{1}H NMR spectrum of **MTPE-DT-Qy**

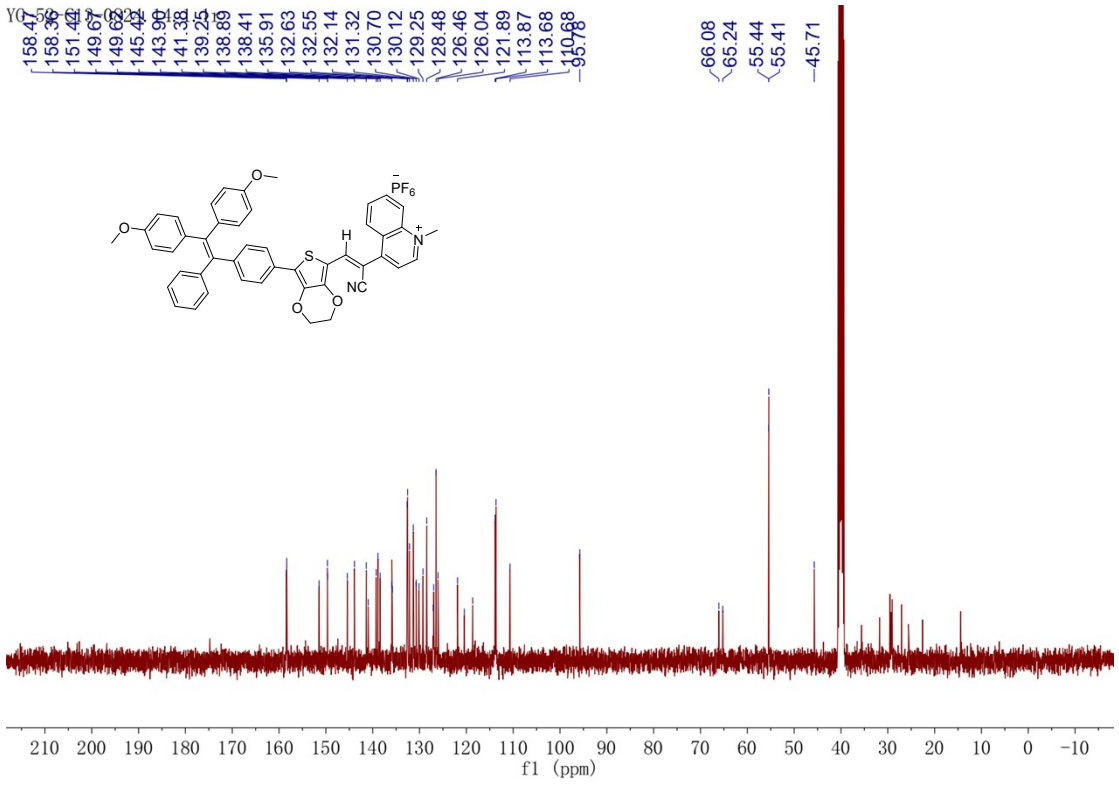


Figure S39. ^{13}C NMR spectrum of **MTPE-DT-Qy**

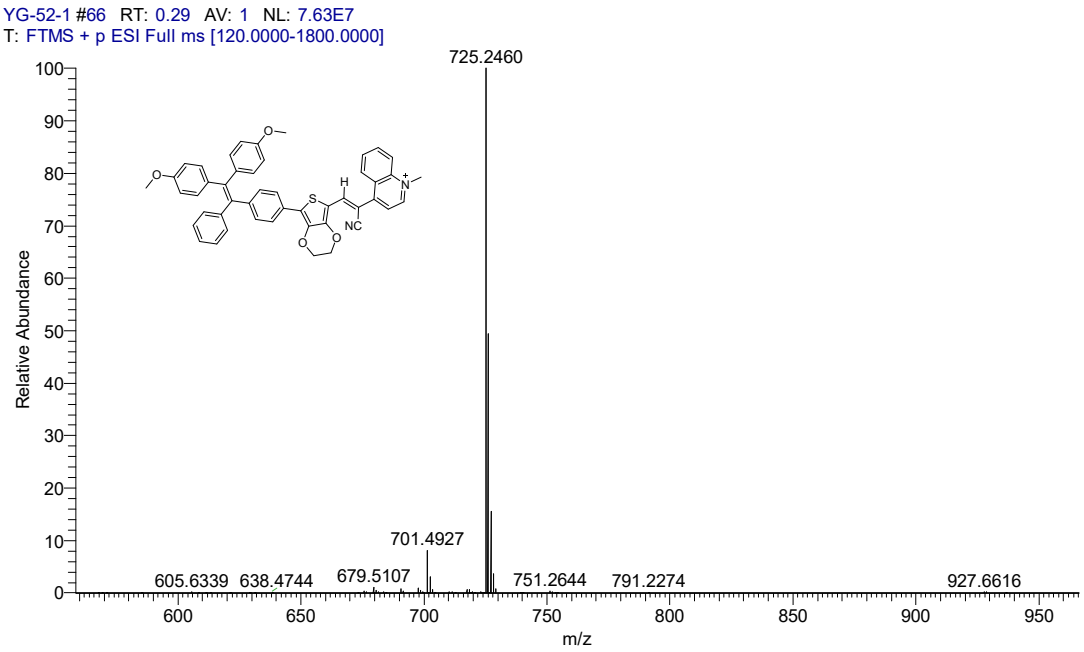


Figure S40. ^{1}H NMR spectrum of **MTPE-DT-Qy**

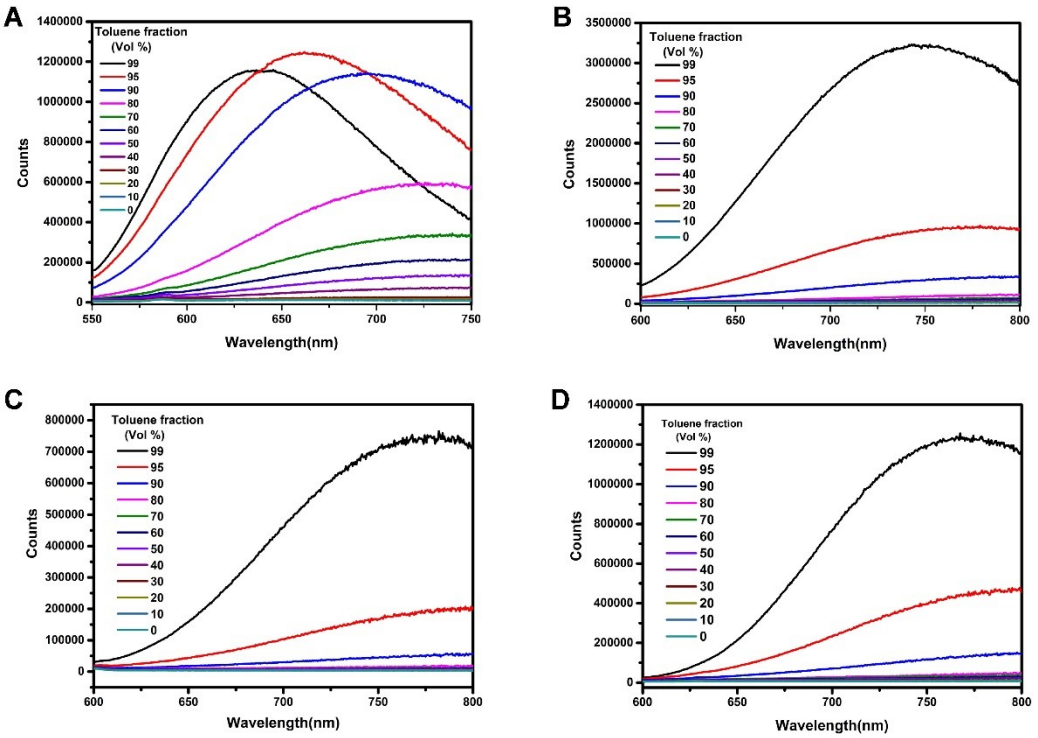


Figure S41. PL spectra of (A) TPE-T-Py (B) MTPE-T-Py (C) MTPE-T-Qy (D) MTPE- DT-Qy in DMSO/toluene mixtures with different toluene fractions. [AIE-PSs]=10^{-5} M.

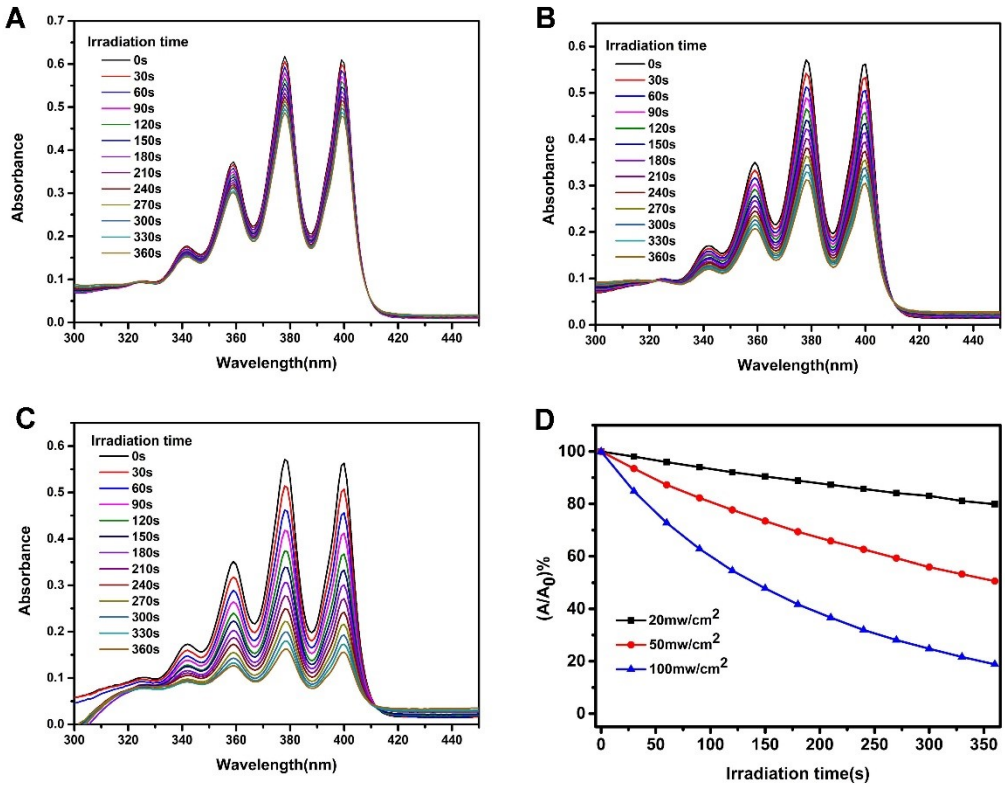


Figure S42. Absorption spectra of ABDA in the presence of Rose Bengal under (A) 20 mW cm^{-2} , (B) 50 mW cm^{-2} , and (C) 100 mW cm^{-2} white light irradiation. (D) Decomposition rates of ABDA in the presence of Rose Bengal under different light intensities, where A_0 and A are the absorbance of ABDA at 378 nm.

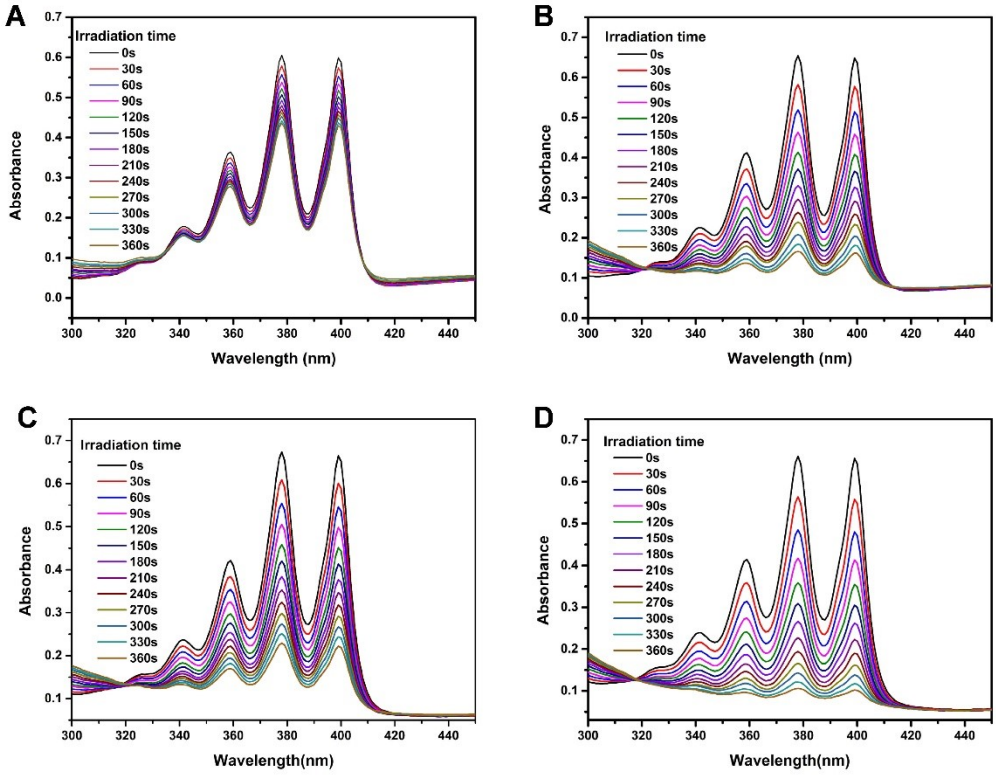


Figure S43. Absorption spectra of ABDA (50×10^{-6} M) in (A) TPE-T-Py and (B) MTPE-T-Py (C) MTPE-T-Qy (D) MTPE-DT-Qy solutions (5×10^{-6} M) irradiated for different durations with white light irradiation (20 mW cm^{-2})

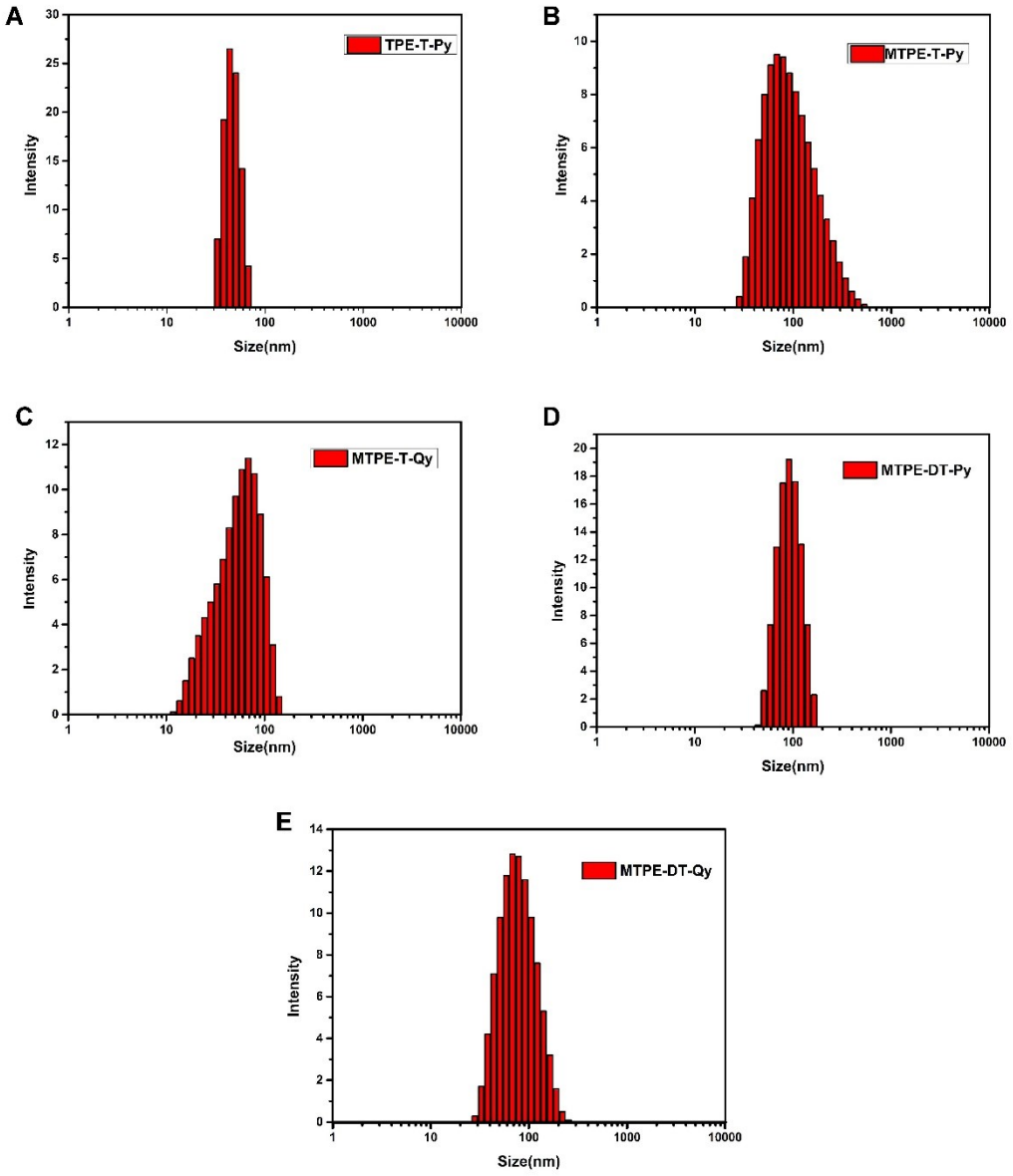


Figure S44. Particle size distributions of (A) TPE-T-Py. (B) MTPE-T-Py. (C) MTPE-T-Qy. (D) MTPE-DT-Py. (E) MTPE-DT-Qy aggregates in DMSO/H_2O mixture with 99% H_2O fraction

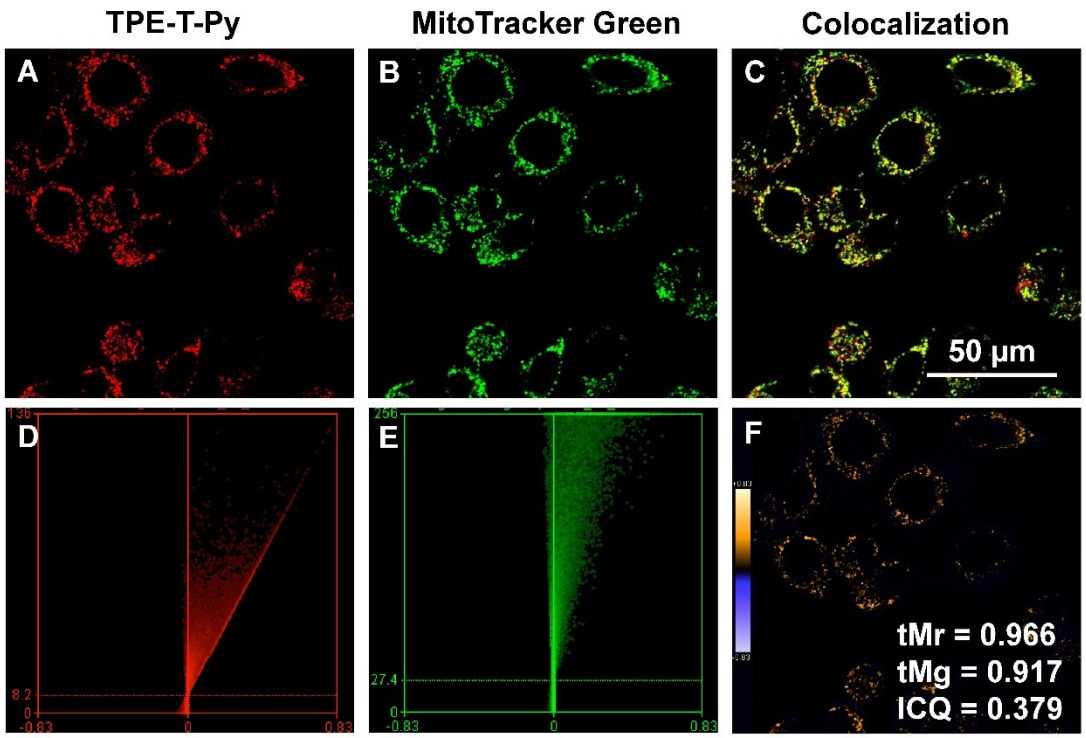


Figure S45. Confocal images of MCF-7 **c**ells incubated with (A) TPE -T-Py and (B) MitoTracker Green, and (C) their merged images. (D, E) Intensity correlation plots (ICP) of red and green signals in the (A) and (B), respectively. (F) PDM image for visualizing the extent of colocalization. Scale bar: 50 μm. The value of tMr (tMg) indicates the percentage of the red (green) signals colocalized with green (red) signals in the corresponding thresholded image. ICQ value indicated the correlation intensity of two channels and ranged from -0.5 to 0.5 (+0.1 to +0.5 implies a strong covariance).

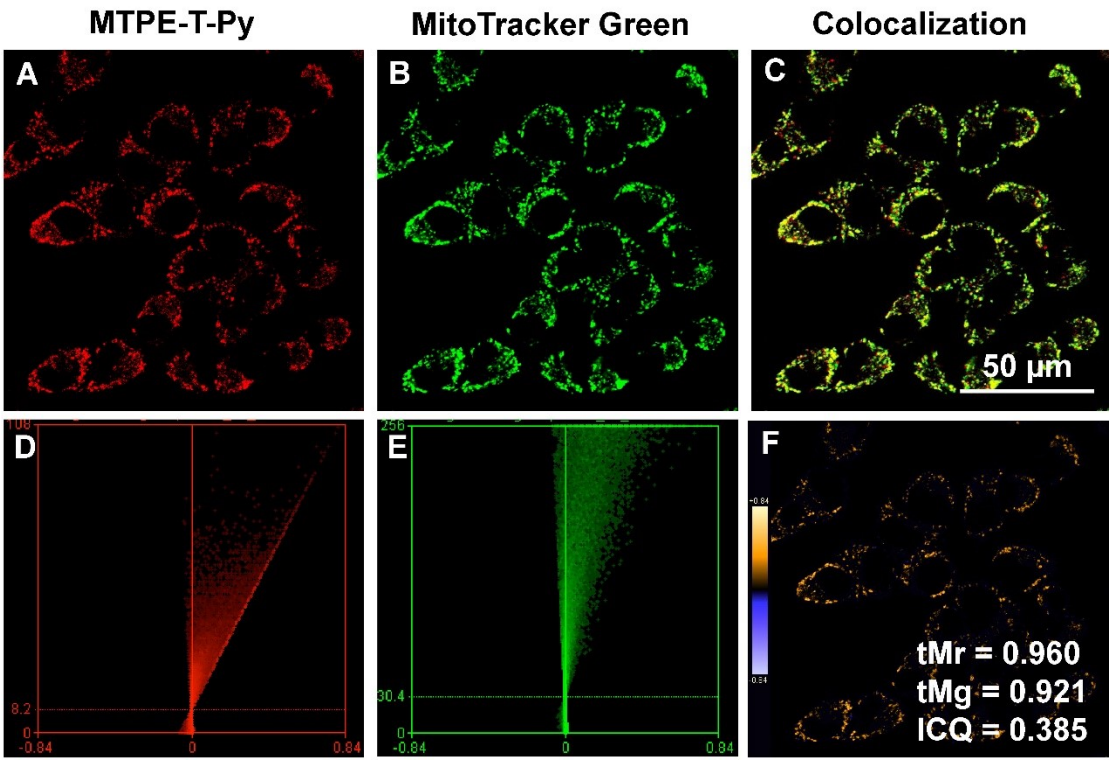


Figure S46. Confocal images of MCF-7 cells incubated with (A) MTPE-T-Py and (B) MitoTracker Green, and (C) their merged images. (D, E) Intensity correlation plots (ICP) of red and green signals in the (A) and (B), respectively. (F) PDM image for visualizing the extent of colocalization. Scale bar: 50 μm. The value of tMr (tMg) indicates the percentage of the red (green) signals colocalized with green (red) signals in the corresponding thresholded image. ICQ value indicated the correlation intensity of two channels and ranged from -0.5 to 0.5 (+0.1 to +0.5 implies a strong covariance).

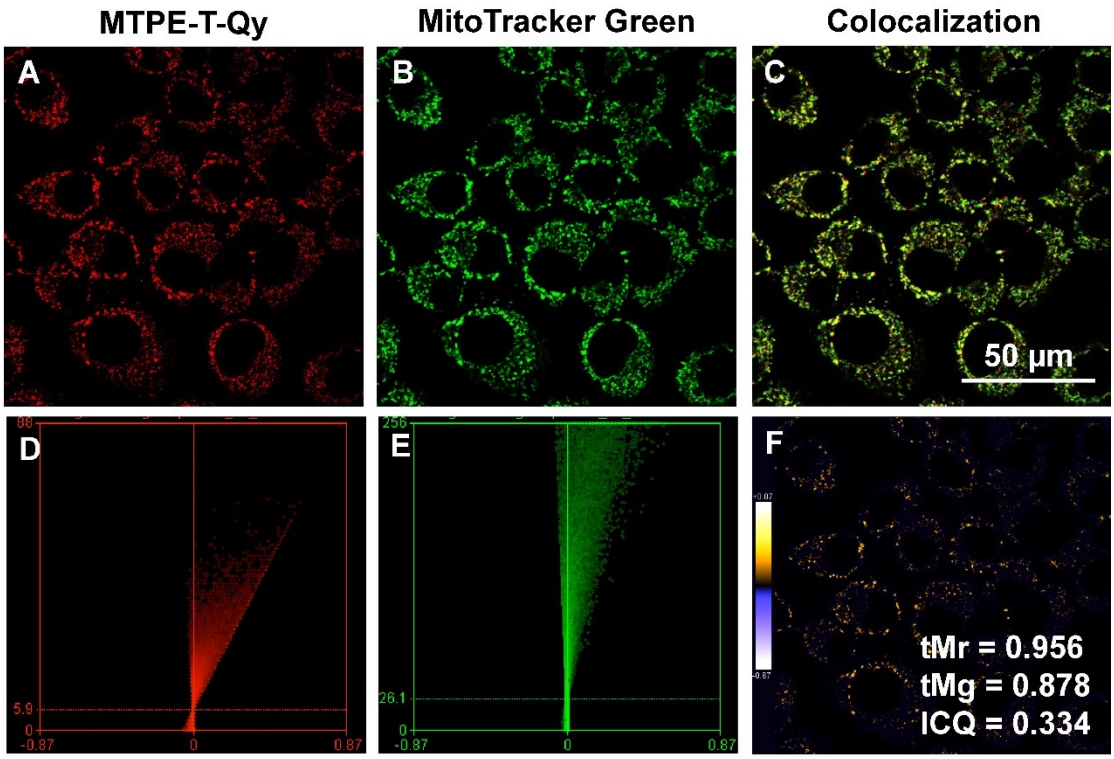


Figure S47. Confocal images of MCF-7 cells incubated with (A) MTPE-T-Qy and (B) MitoTracker Green, and (C) their merged images. (D, E) Intensity correlation plots (ICP) of red and green signals in the (A) and (B), respectively. (F) PDM image for visualizing the extent of colocalization. Scale bar: 50 μm. The value of tMr (tMg) indicates the percentage of the red (green) signals colocalized with green (red) signals in the corresponding thresholded image. ICQ value indicated the correlation intensity of two channels and ranged from -0.5 to 0.5 (+0.1 to +0.5 implies a strong covariance).

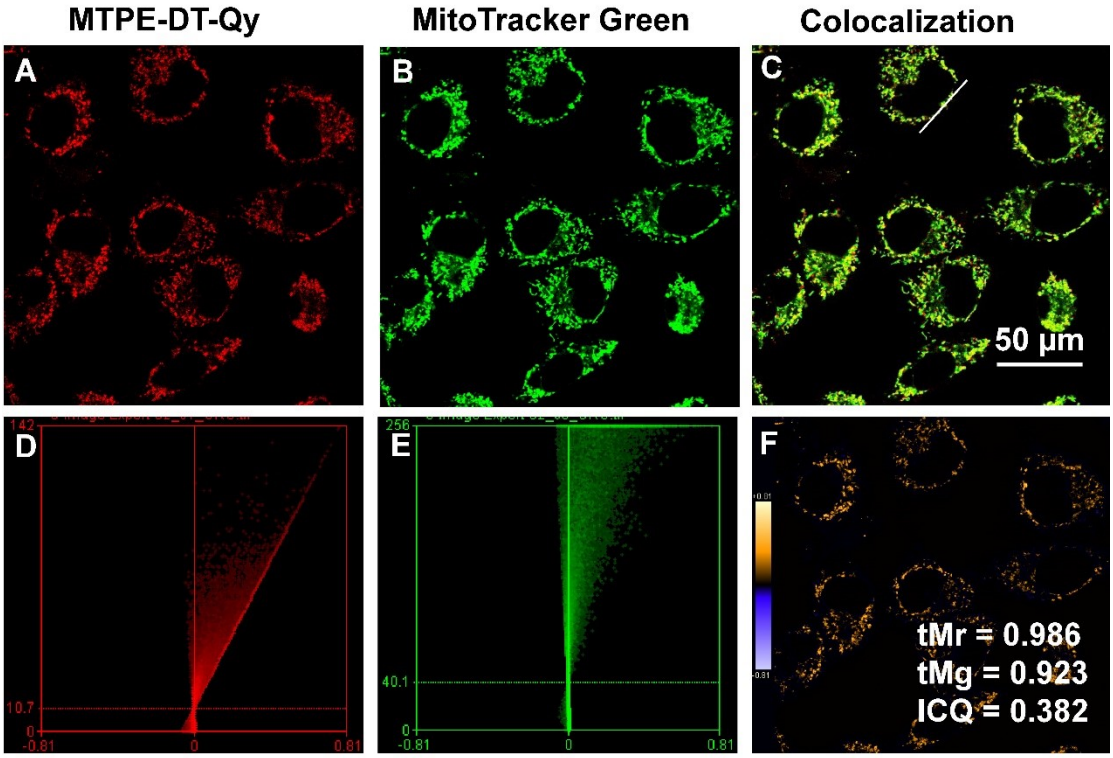


Figure S48. Confocal images of MCF-7 cells incubated with **(**A) MTPE-DT-Qy and (B) MitoTracker Green, and (C) their merged images. (D, E) Intensity correlation plots (ICP) of red and green signals in the (A) and (B), respectively. (F) PDM image for visualizing the extent of colocalization. Scale bar: 50 μm. The value of tMr (tMg) indicates the percentage of the red (green) signals colocalized with green (red) signals in the corresponding thresholded image. ICQ value indicated the correlation intensity of two channels and ranged from -0.5 to 0.5 (+0.1 to +0.5 implies a strong covariance).

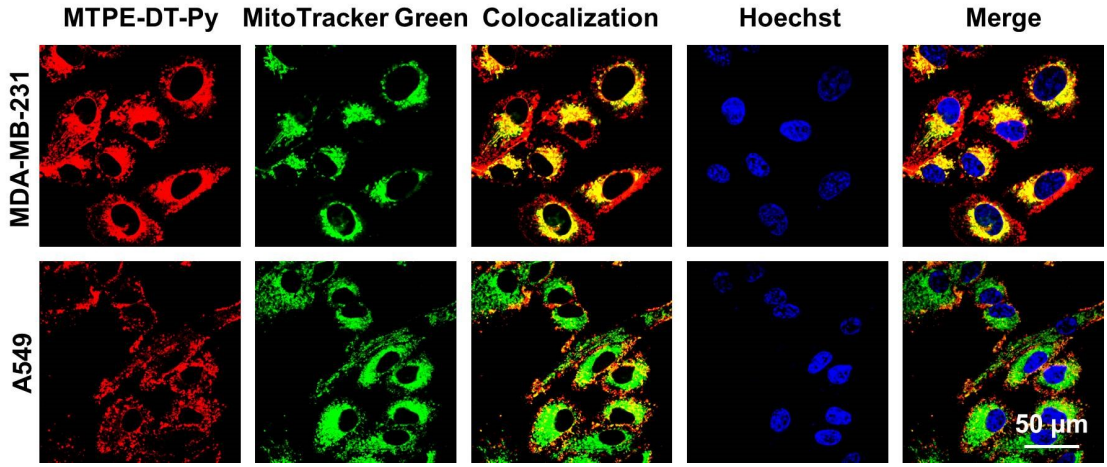


Fig S49. Confocal images of cancer cells (top: MDA-MB-231 cells, bottom: A549 cells) incubated with MTPE-DT-Py (red, 10 μM) and MitoTracker Green (green), and their merged images. Scale bar: 50 μm.

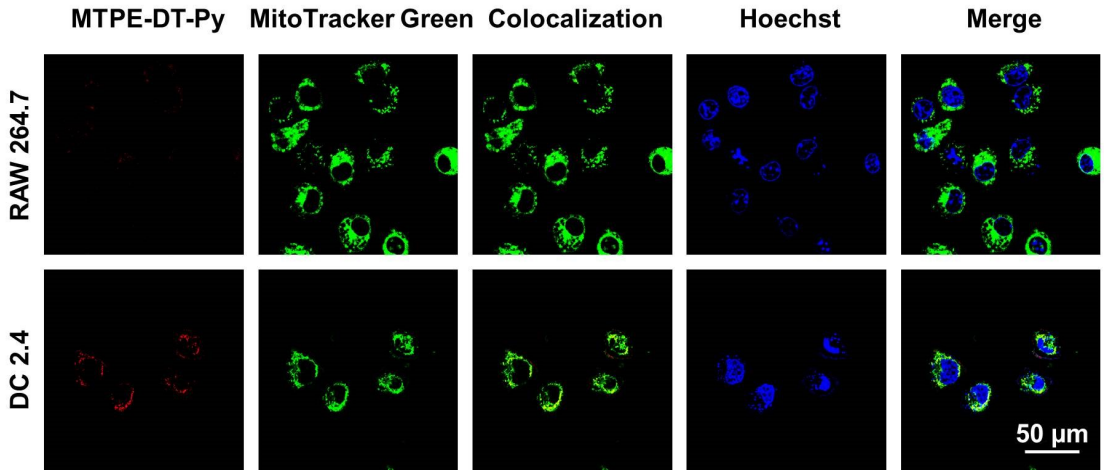


Fig S50. Confocal images of normal cells (top: RAW 264.7 cells, bottom: DC 2.4 cells) incubated with MTPE-DT-Py (red, 10 μM) and MitoTracker Green (green), and their merged images. Scale bar: 50 μm.

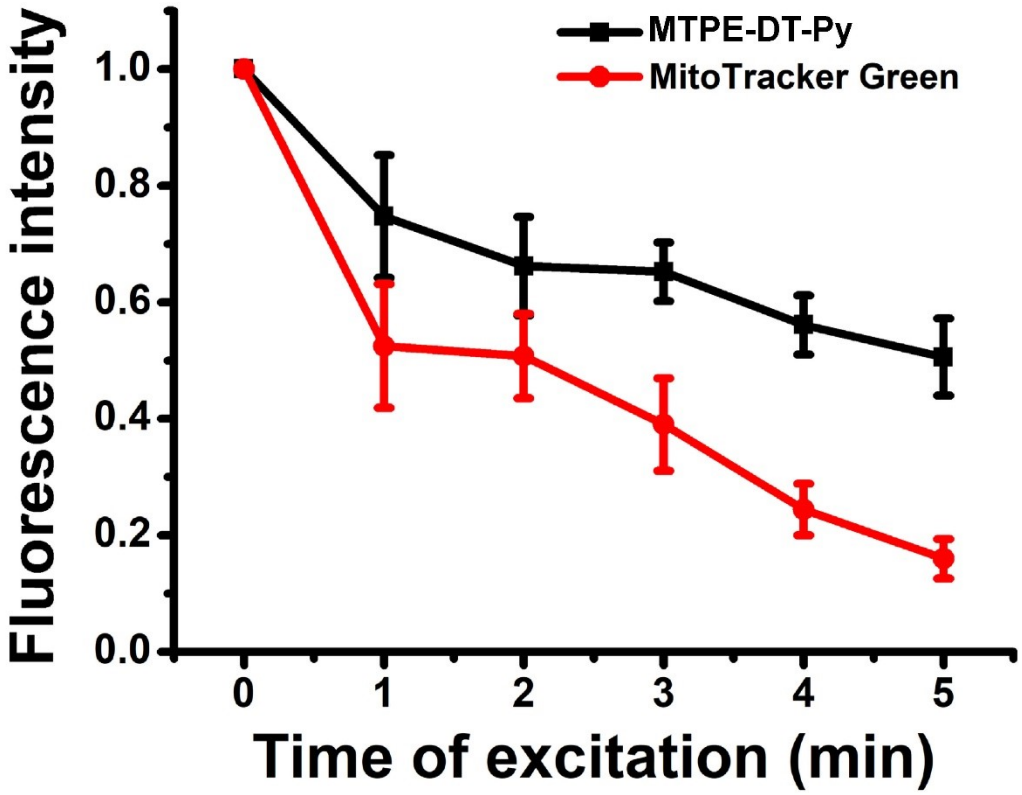


Figure S51. Photostability of MTPE-DT-Py and MitoTracker Green inside MCF-7 cells. The MCF-7 cells were excited sequentially by 488 nm laser and the emission fluorescence intensity was recorded at different time. Emission fluorescence signal intensity was normalized to the maximum intensity at the beginning of irradiation (n=10).

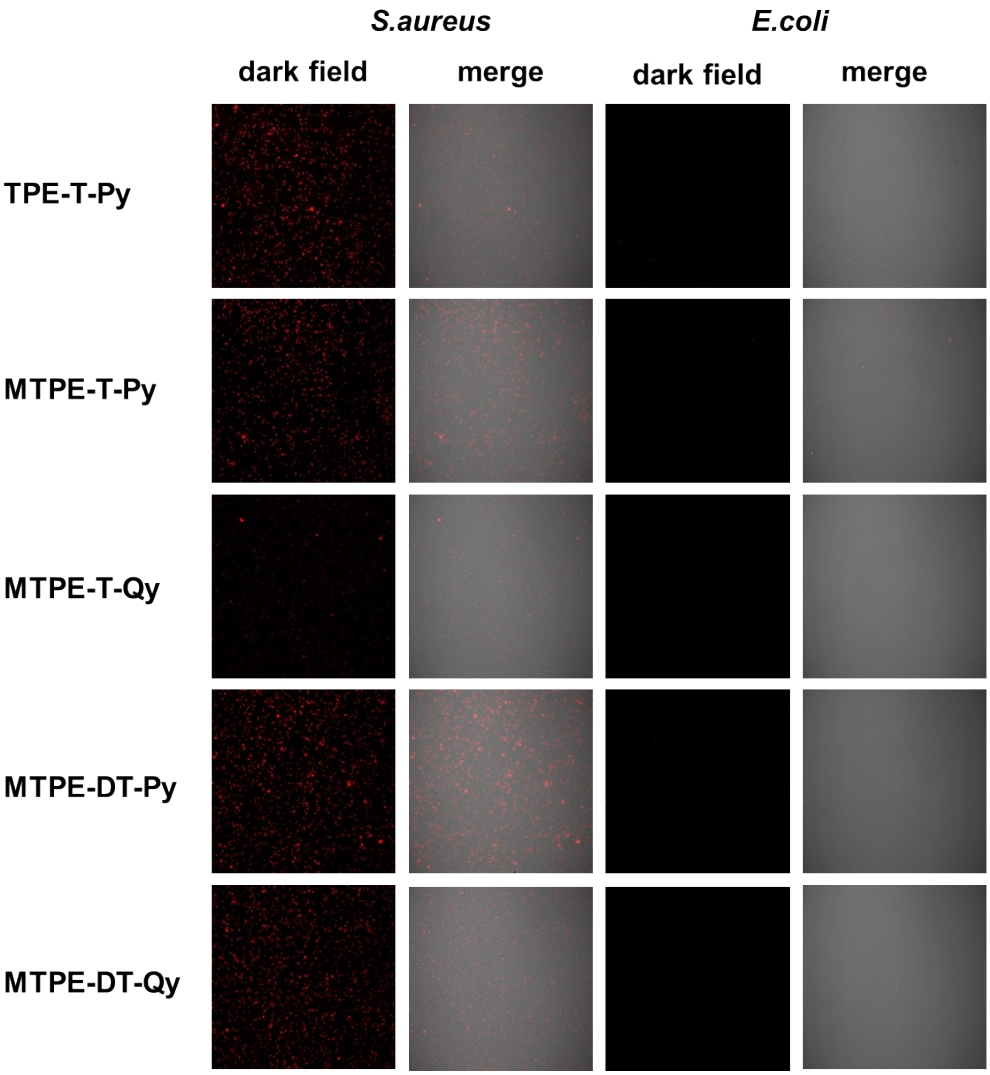


Figure S52. Confocal images and bright-field of *E. coli* and *S. aureus* incubated with 2×10^{-6} M of AIE-PSs for 20 min. λ_{ex}: 488 nm, λ_{em}: 600–740 nm.