

Electronic Supplementary Information

Tetraphenylethylene-bridged double-branched sensitizers featuring hetero donors for dye-sensitized solar cells

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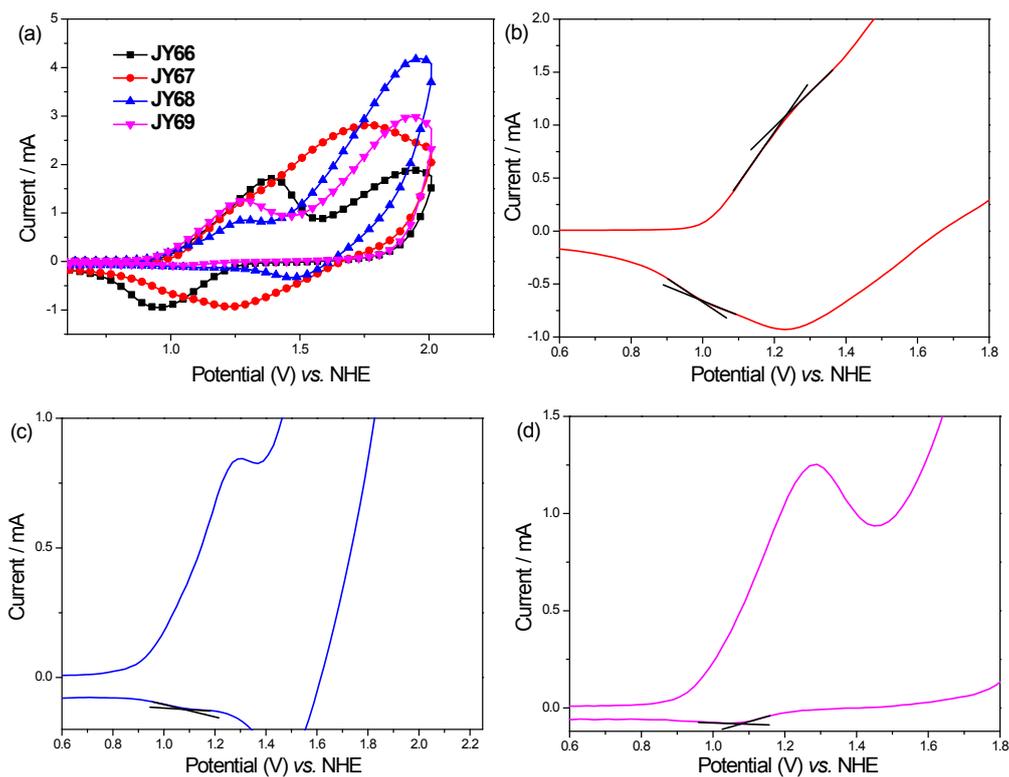


Fig. S1 CV of (a) **JY66-69**-sensitized films, (b) **JY67**-sensitized film, (c) **JY68**-sensitized film and (d) **JY69**-sensitized film in MeCN with 0.1 M TBAPF₆ as the supporting electrolyte.

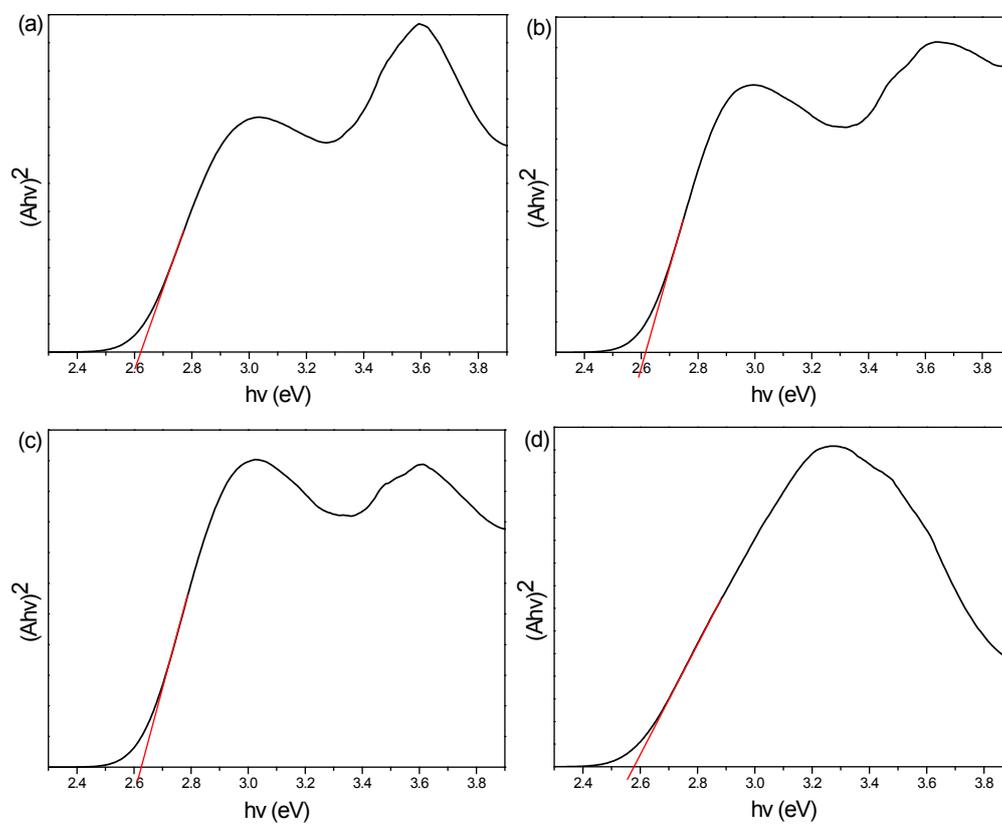


Fig S2 The Tauc plot of dye (a) **JY66**, (b) **JY67**, (c) **JY68** and (d) **JY69**

Table S1Calculated TD-DFT of dye **JY66-69**^a

Dye	Composition	Wavelength (nm)	Oscillator strength
JY66	91% H → L 8% H-1 → L+1	418	0.8393
JY67	47% H → L 46% H → L+1 4% H-1 → L 2% H-1 → L+1	408	0.8546
JY68	62% H → L 17% H → L+1 12% H-1 → L 8% H-1 → L+1	411	0.7725
JY69	83% H → L 13% H-1 → L 3% H → L+1	425	0.8440

^a H=HOMO, L=LUMO, H-1=HOMO-1, L+1=LUMO+1**Table S2**Photovoltaic performance of **JY66-69**^a

Dye	V_{oc}/mV	$J_{sc}/mA\ cm^{-2}$	FF/%	PCE/%
JY66	694 ± 5	8.20 ± 0.21	67.5 ± 0.8	3.89 ± 0.06
JY66+CDCA	691 ± 5	8.15 ± 0.16	67.2 ± 1.4	3.78 ± 0.04
JY67	712 ± 0	9.14 ± 0.13	66.2 ± 0.3	4.35 ± 0.05
JY67+CDCA	712 ± 5	8.93 ± 0.19	65.8 ± 0.6	4.19 ± 0.02
JY68	710 ± 5	8.64 ± 0.14	65.4 ± 1.1	4.05 ± 0.04
JY68+CDCA	707 ± 0	8.31 ± 0.13	66.9 ± 1.2	3.93 ± 0.07
JY69	610 ± 5	7.97 ± 0.19	70.5 ± 0.5	3.48 ± 0.05
JY69+CDCA	610 ± 5	7.78 ± 0.12	70.2 ± 1.1	3.34 ± 0.05

^a An average value was attained from three devices; CDCA was used in 10 mM.

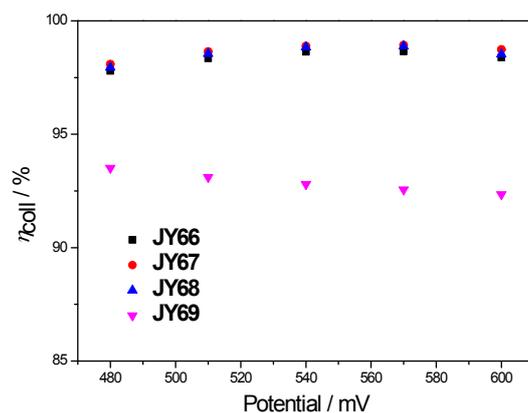


Fig. S3 The η_{collect} calculated from EIS analysis of dye **JY66-69**.

Synthesis

The precursors **I**, **II**, **III**, **IV** and **1** were synthesized according to the previous literatures [1], [2], [3], [4] and [5], respectively.

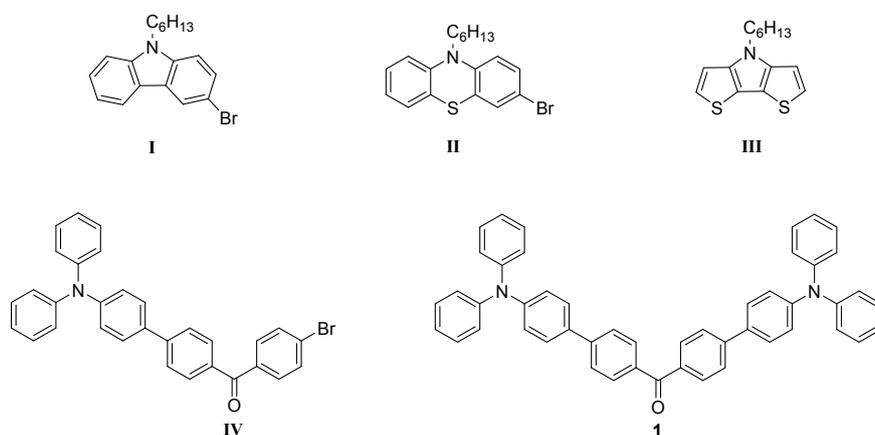
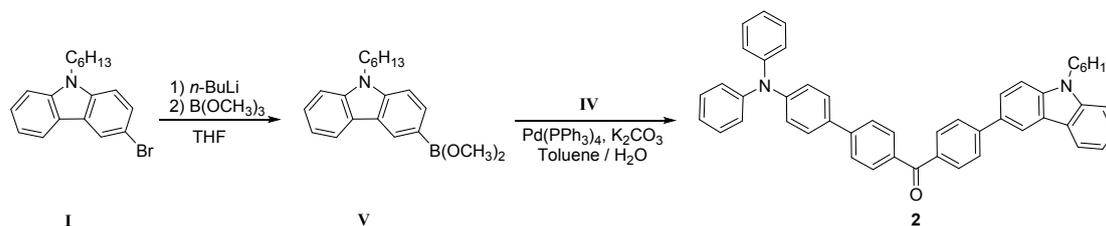


Fig. S4 The molecular structure of precursors **I**, **II**, **III**, **IV** and **1**

Synthesis of compound **2**

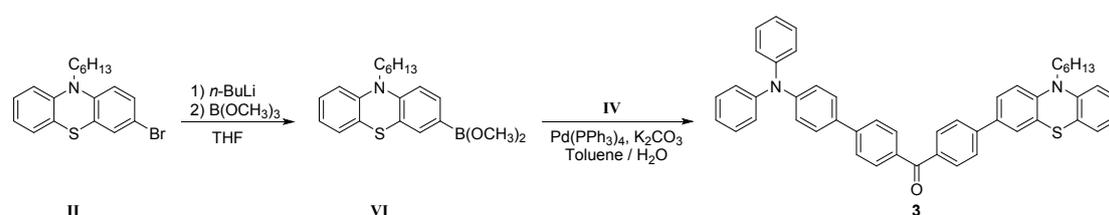


To an oven-dried two-neck flask, compound **I** (1.45 g, 4.4 mmol) was added, and the flask was recharged with argon, then 20 mL dry THF was syringed. The flask was cooled to $-78\text{ }^{\circ}\text{C}$ and 2.5 M *n*-BuLi solution in hexane (2.64 mL, 6.6 mmol) was added by dropwise. After that, the mixture was stirred for 60 min. Then, $\text{B}(\text{OCH}_3)_3$ (0.74 mL, 6.6 mmol) was slowly added at $-78\text{ }^{\circ}\text{C}$, and the reaction mixture was

stirred for 12 h at room temperature. The reaction was quenched with saturated aqueous NH_4Cl solution and extracted with dichloromethane. Next, the organic layer was dried by anhydrous MgSO_4 , filtered, and evaporated under reduced pressure to obtain the solid crude compound **V**.

Compound **IV** (605 mg, 1.2 mmol), K_2CO_3 (498 mg, 3.6 mmol), $\text{Pd}(\text{PPh}_3)_4$ (42 mg, 0.04 mmol) and crude compound **V** just afforded were added into a two-neck flask and charged with argon, then 32 mL THF and 8 mL H_2O were syringed. The reaction mixture was heated to 60 °C and stirred for 12 h. After cooling down, the mixture was extracted with dichloromethane, the collected organic phase was dried by anhydrous MgSO_4 . After removal of the solvent, the crude product was purified by silica-gel column chromatography using petroleum ether/dichloromethane (1 : 1) as the eluent to give compound **2** as a yellow solid (776 mg, 96% yield), m.p. 95-97 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.41 (d, $J = 1.8$ Hz, 1H), 8.18 (d, $J = 7.7$ Hz, 1H), 8.00 – 7.92 (m, 4H), 7.86 (d, $J = 8.2$ Hz, 2H), 7.79 (dd, $J = 8.5, 1.8$ Hz, 1H), 7.71 (d, $J = 8.2$ Hz, 2H), 7.58 – 7.48 (m, 4H), 7.45 (d, $J = 8.1$ Hz, 1H), 7.35 – 7.27 (m, 5H), 7.22 – 7.13 (m, 6H), 7.07 (t, $J = 7.4$ Hz, 2H), 4.34 (t, $J = 7.2$ Hz, 2H), 1.91 (p, $J = 7.3$ Hz, 2H), 1.46 – 1.39 (m, 2H), 1.33 (tt, $J = 9.2, 4.4$ Hz, 4H), 0.88 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 196.02, 148.09, 147.45, 146.19, 144.53, 140.96, 140.45, 136.03, 135.55, 133.36, 130.81, 129.39, 127.97, 126.89, 126.28, 126.04, 125.14, 124.77, 123.48, 123.37, 123.33, 122.88, 120.48, 119.16, 109.14, 108.98, 43.28, 31.61, 29.01, 27.02, 22.58, 14.06. HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{49}\text{H}_{43}\text{N}_2\text{O}$, 675.3375, found, 675.3373.

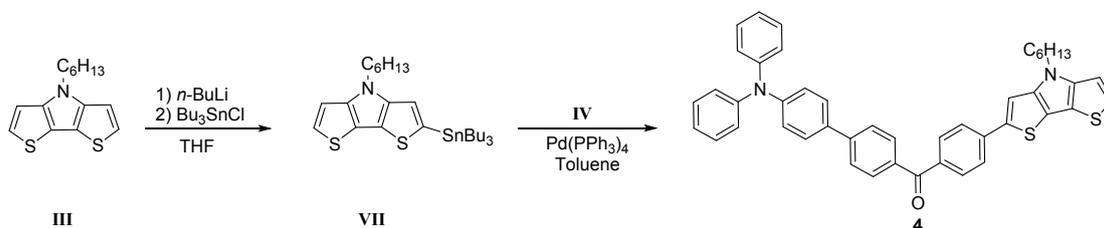
Synthesis of compound **3**



Compound **3** was synthesized using the same procedure employed for compound **2**, while replacing compound **I** with compound **II**. The residue was purified by column chromatography to afford compound **3** (95% yield), an orange solid, m.p. 73-75 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.89 (dd, $J = 8.2, 3.7$ Hz, 4H), 7.67 (dd, $J = 16.0, 8.0$ Hz, 4H), 7.54 (d, $J = 8.3$ Hz, 2H), 7.45 (d, $J = 8.1$ Hz, 2H), 7.30 (t, $J = 7.7$ Hz, 4H), 7.16 (d, $J = 8.0$ Hz, 8H), 7.07 (t, $J = 7.4$ Hz, 2H), 6.96 – 6.86 (m, 3H), 3.88 (t, $J = 7.3$ Hz, 2H), 1.84 (p, $J = 7.5$ Hz, 2H), 1.46 (q, $J = 6.1, 4.8$ Hz, 2H), 1.33 (p, $J = 3.6$ Hz, 4H), 0.92 – 0.86 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.84, 148.13, 147.45, 145.41, 144.83, 144.62, 143.91, 136.09, 135.85, 133.96, 133.30, 130.76, 129.40, 127.96, 127.51, 127.38, 126.28, 126.14, 125.91, 125.46, 124.79, 124.23, 123.35, 122.63, 115.58, 115.47, 47.60, 31.50, 26.88, 26.69, 22.64, 14.04. HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{49}\text{H}_{43}\text{N}_2\text{OS}$, 707.3096, found, 707.3095.

Synthesis of compound 4



Compound **III** (1.32 g, 5 mmol) was set into an oven-dried two-neck flask, and the flask was recharged with argon, then 20 mL dry THF was syringed. The flask was cooled to -78 °C and 2.5 M *n*-BuLi solution in hexane (2.4 mL, 6 mmol) was added by dropwise. After that, the mixture was stirred for 60 min. Then, Bu_3SnCl (1.63 mL, 6 mmol) was slowly added at -78 °C, and the reaction mixture was stirred for 12 h at room temperature. The reaction was quenched with saturated aqueous NH_4Cl solution and extracted with dichloromethane. The organic layer was dried by anhydrous MgSO_4 , filtered, and evaporated under reduced pressure to obtain the oil crude compound **VII**.

Compound **IV** (1.2 g, 2.5 mmol), $\text{Pd}(\text{PPh}_3)_4$ (139 mg, 0.12 mmol) and crude compound **VII** just obtained were added into a two-neck flask and flushed with argon, then 40 mL toluene were added. The reaction mixture was heated to 110 °C and stirred for 12 h. After cooling down, the mixture was extracted with dichloromethane, the collected organic phase was dried by anhydrous MgSO_4 . After removal of the solvent, the crude product was purified by silica-gel column chromatography using petroleum ether/dichloromethane (1 : 1) as the eluent to give compound **4** as a red

solid (1.6 g, 94% yield), m.p. 102-104 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.91 (t, *J* = 7.9 Hz, 4H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.42 (s, 1H), 7.32 (t, *J* = 7.7 Hz, 4H), 7.19 (dd, *J* = 8.4, 6.6 Hz, 7H), 7.09 (t, *J* = 7.3 Hz, 2H), 7.04 (d, *J* = 5.3 Hz, 1H), 4.25 (t, *J* = 7.1 Hz, 2H), 1.37 – 1.28 (m, 6H), 0.90 (d, *J* = 3.3 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 195.36, 148.09, 147.43, 145.47, 145.25, 144.55, 139.78, 139.59, 135.88, 135.74, 133.28, 130.97, 130.67, 129.36, 127.93, 126.25, 124.76, 124.61, 124.20, 123.33, 115.67, 114.93, 110.90, 108.36, 47.46, 31.42, 30.36, 26.69, 22.52, 14.01. HRMS (ESI): *m/z* [M+H]⁺ calcd for C₄₅H₃₉N₂OS₂, 687.2504, found, 687.2499.

Synthesis of compound 9

Compound **1** (669 mg, 1 mmol), zinc (523 mg, 8 mmol) and bis(4-bromophenyl)methanone (1.02 g, 3 mmol) was placed into an oven-dried two-neck flask, and the flask was recharged with argon, then 20 mL dry THF was added by syringe. The flask was cooled to -78 °C and TiCl₄ (0.5 mL, 4 mmol) was added dropwise, after that, the mixture was stirred for 30 min. Afterwards, the reaction mixture was heated to 60 °C and stirred for 12 h. After cooling down room temperature, the reaction was treated with saturated aqueous K₂CO₃ solution, and the organic layer was extracted with dichloromethane then dried over with anhydrous MgSO₄. After removal of the solvent, the crude product was purified by silica-gel column chromatography using petroleum ether/dichloromethane (5 : 1) as the eluent to give crude compound **5** as a yellow solid.

In a two-neck flask, (5-formylthiophen-2-yl)boronic acid (187 mg, 1.2 mmol), K₂CO₃ (276 mg, 2 mmol), Pd(dppf)Cl₂ (15 mg, 0.02 mmol) and crude compound **5** just obtained were dissolved in 15 mL of toluene and 30 mL of methanol. The mixture was heated at 75 °C for 12 h under nitrogen atmosphere. Afterwards, it was cooled to room temperature, diluted with dichloromethane and washed with water and brine. The organic layer was dried over anhydrous MgSO₄ and concentrated in vacuum. The residue was purified by column chromatography using petroleum ether/dichloromethane (1 : 2) as the eluent to obtain compound **9** (367 mg, 51% yield), an orange solid, m.p. 143-145 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.90 (s, 2H), 7.74 (d,

$J = 4.0$ Hz, 2H), 7.49 (dd, $J = 8.4, 4.8$ Hz, 8H), 7.44 – 7.37 (m, 6H), 7.29 (dd, $J = 9.1, 6.5$ Hz, 8H), 7.21 – 7.11 (m, 20H), 7.06 (t, $J = 7.3$ Hz, 4H). ^{13}C NMR (100 MHz, CDCl_3) δ 182.68, 153.94, 147.57, 147.29, 144.95, 142.35, 142.20, 141.61, 138.97, 138.85, 137.39, 134.11, 132.25, 131.88, 131.17, 129.26, 127.46, 125.89, 125.86, 124.40, 123.96, 123.83, 122.97. HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{72}\text{H}_{51}\text{N}_2\text{O}_2\text{S}_2$, 1039.3392, found, 1039.3389.

Synthesis of compound 10

Compound **10** was synthesized using the same procedure employed for compound **9**, while replacing compound **1** with compound **2**. The residue was purified by column chromatography to obtain compound **10** (47% yield), an orange solid, m.p. 131-133 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.89 (d, $J = 4.5$ Hz, 2H), 7.75 – 7.70 (m, 3H), 7.59 – 7.55 (m, 2H), 7.50 (ddt, $J = 8.4, 6.9, 2.1$ Hz, 7H), 7.46 – 7.41 (m, 4H), 7.38 (d, $J = 3.9$ Hz, 2H), 7.31 – 7.17 (m, 14H), 7.16 – 7.11 (m, 5H), 7.08 – 7.03 (m, 2H), 4.33 (t, $J = 7.2$ Hz, 2H), 1.90 (p, $J = 7.3$ Hz, 2H), 1.46 – 1.39 (m, 2H), 1.36 – 1.30 (m, 4H), 0.89 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 182.74, 154.03, 147.59, 147.29, 145.11, 142.49, 142.17, 141.78, 141.12, 140.87, 140.60, 140.03, 138.95, 138.72, 137.46, 134.18, 132.31, 131.96, 131.31, 131.14, 129.29, 127.50, 126.71, 126.52, 125.92, 125.88, 125.82, 124.88, 124.41, 123.98, 123.87, 123.33, 122.98, 122.92, 120.40, 118.93, 118.63, 108.92, 108.87, 43.22, 31.60, 28.98, 26.99, 22.56, 14.05. HRMS (ESI): m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{72}\text{H}_{57}\text{N}_2\text{O}_2\text{S}_2$, 1045.3861, found, 1045.3865.

Synthesis of compound 11

Compound **11** was synthesized using the same procedure employed for compound **9**, while replacing compound **1** with compound **3**. The residue was purified by column chromatography to obtain compound **11** (57% yield), an orange solid, m.p. 122-124 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.89 (s, 2H), 7.72 (d, $J = 4.0$ Hz, 2H), 7.48 (dd, $J = 8.4, 3.2$ Hz, 6H), 7.41 (d, $J = 8.0$ Hz, 2H), 7.39 – 7.33 (m, 6H), 7.29 (d, $J = 7.8$ Hz, 4H), 7.19 – 7.11 (m, 17H), 7.05 (t, $J = 7.3$ Hz, 2H), 6.91 (dd, $J = 22.1, 7.8$ Hz, 3H), 3.87 (s, 2H), 1.83 (p, $J = 7.4$ Hz, 2H), 1.45 (q, $J = 5.7, 5.0$ Hz, 2H), 1.35 – 1.31 (m, 4H), 0.92 – 0.88 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3) δ 183.40, 154.65, 148.29,

148.01, 145.66, 145.28, 143.00, 142.91, 142.43, 142.32, 139.69, 139.62, 139.12, 138.10, 135.18, 134.83, 132.96, 132.60, 131.93, 131.90, 129.98, 128.18, 128.13, 127.97, 126.62, 126.59, 126.47, 126.28, 126.23, 125.89, 125.12, 125.02, 124.72, 124.68, 124.55, 123.69, 123.11, 116.14, 116.03, 48.22, 32.17, 27.55, 27.36, 23.31, 14.71. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{72}H_{57}N_2O_2S_3$, 1077.3582, found, 1077.3580.

Synthesis of compound 12

Compound **12** was synthesized using the same procedure employed for compound **9**, while replacing compound **1** with compound **4**. The residue was purified by column chromatography to obtain compound **12** (58% yield), an orange solid, m.p. 157-158 °C. 1H NMR (400 MHz, $CDCl_3$) δ 9.85 (d, $J = 2.2$ Hz, 2H), 7.70 (dd, $J = 4.0, 1.5$ Hz, 2H), 7.50 – 7.42 (m, 8H), 7.37 (m, 5H), 7.27 (s, 1H), 7.21 (s, 3H), 7.18 – 7.08 (m, 15H), 7.06 – 7.01 (m, 2H), 7.01 – 6.96 (m, 1H), 4.16 (t, $J = 7.0$ Hz, 2H), 1.84 (p, $J = 7.1$ Hz, 2H), 1.33 – 1.25 (m, 6H), 0.84 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.76, 153.96, 147.58, 147.32, 145.16, 144.91, 142.19, 141.84, 141.54, 140.92, 139.04, 138.91, 137.47, 134.30, 134.09, 132.28, 132.05, 131.94, 131.27, 131.19, 129.29, 127.49, 125.97, 125.87, 124.58, 124.41, 124.04, 123.84, 123.40, 122.99, 114.91, 114.37, 110.91, 107.06, 99.98, 47.40, 31.44, 30.36, 26.68, 22.52, 14.04. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{68}H_{53}N_2O_2S_4$, 1057.2990, found, 1057.2988.

Synthesis of dye JY66

To compound **9** (208 mg, 0.2 mmol) and cyanoacetic acid (205 mg, 2.4 mmol) in a dry two-neck flask, 10 mL chloroform, 10 mL acetonitrile, and 0.4 mL piperidine were added, then the resultant solution was heated to 75 °C for 12 h under nitrogen. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane and washed with aqueous HCl (1 M) and water, and then dried by anhydrous $MgSO_4$. Solvent was removed and the crude product was purified by silica-gel column using dichloromethane/methanol (20 : 1) as the eluent and recrystallized from THF/methanol to give dye **JY66** as a dark red solid (140 mg, 69%), m.p. 223-225 °C. 1H NMR (400 MHz, $DMSO-d_6$) δ 8.45 (s, 2H), 7.95 (d, $J =$

3.9 Hz, 2H), 7.66 (d, $J = 4.1$ Hz, 2H), 7.56 (d, $J = 7.9$ Hz, 4H), 7.49 (d, $J = 8.3$ Hz, 4H), 7.42 (d, $J = 7.9$ Hz, 4H), 7.27 (t, $J = 7.7$ Hz, 8H), 7.02 (m, 24H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 164.00, 152.45, 147.39, 147.19, 146.62, 144.84, 142.06, 141.80, 141.41, 139.36, 138.36, 135.13, 133.47, 132.41, 131.95, 131.04, 130.01, 127.83, 126.21, 125.98, 125.63, 124.59, 123.69, 123.55, 117.03, 99.46. HRMS (ESI): m/z $[\text{M}-2\text{H}]^{-2}$ calcd for $\text{C}_{78}\text{H}_{50}\text{N}_4\text{O}_4\text{S}_2$, 585.1642, found, 585.1640.

Synthesis of dye JY67

Dye **JY67** was synthesized using the same procedure employed for dye **JY66**, while replacing compound **9** with compound **10**. The residue was purified by column chromatography and recrystallized to obtain dye **JY67** (60% yield), a dark red solid, m.p. 201-203 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.46 (d, $J = 8.4$ Hz, 2H), 8.43 (s, 1H), 8.17 (d, $J = 7.7$ Hz, 1H), 7.96 (dd, $J = 9.2, 4.1$ Hz, 2H), 7.69 – 7.52 (m, 11H), 7.50 – 7.39 (m, 5H), 7.28 (t, $J = 7.8$ Hz, 4H), 7.14 (s, 1H), 7.11 – 6.98 (m, 14H), 6.94 (d, $J = 8.3$ Hz, 2H), 4.35 (d, $J = 8.2$ Hz, 2H), 1.70 (q, $J = 7.2$ Hz, 2H), 1.25 – 1.14 (m, 6H), 0.75 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.47, 152.17, 146.83, 146.60, 146.41, 144.42, 141.62, 141.36, 141.12, 140.67, 140.32, 139.49, 139.32, 138.58, 137.73, 134.44, 132.92, 131.84, 131.41, 130.39, 130.35, 129.95, 129.44, 127.23, 125.85, 125.69, 125.36, 125.05, 124.34, 124.01, 123.12, 123.00, 122.56, 122.14, 120.45, 118.70, 118.10, 116.31, 109.44, 109.26, 98.22, 42.21, 30.85, 28.39, 26.03, 21.88, 13.72. HRMS (ESI): m/z $[\text{M}-2\text{H}]^{-2}$ calcd for $\text{C}_{78}\text{H}_{56}\text{N}_4\text{O}_4\text{S}_2$, 588.1877, found, 588.1875.

Synthesis of dye JY68

Dye **JY68** was synthesized using the same procedure employed for dye **JY66**, while replacing compound **9** with compound **11**. The residue was purified by column chromatography and recrystallized to obtain dye **JY68** (64% yield), a dark red solid, m.p. 210-212 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.46 (s, 2H), 7.96 (s, 2H), 7.64 (s, 2H), 7.55 (d, $J = 8.0$ Hz, 3H), 7.48 (d, $J = 8.2$ Hz, 2H), 7.40 (t, $J = 8.9$ Hz, 4H), 7.33 (s, 1H), 7.27 (t, $J = 7.7$ Hz, 4H), 7.17 – 6.91 (m, 23H), 3.82 (t, $J = 6.9$ Hz, 2H), 1.62 (q, $J = 7.4$ Hz, 2H), 1.33 (t, $J = 7.7$ Hz, 2H), 1.20 (t, $J = 7.6$ Hz, 4H), 0.78 (m, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.53, 152.20, 146.89, 146.68, 146.44, 144.41,

144.34, 144.29, 143.99, 141.53, 141.40, 141.33, 141.14, 138.83, 137.83, 137.07, 134.53, 133.18, 132.96, 131.89, 131.43, 130.50, 129.49, 127.55, 127.30, 127.04, 125.73, 125.46, 125.28, 125.13, 124.55, 124.08, 124.01, 123.19, 123.05, 122.41, 116.38, 115.82, 115.67, 98.35, 46.47, 30.77, 26.10, 25.77, 22.01, 13.77. HRMS (ESI): m/z $[M-2H]^{-2}$ calcd for $C_{78}H_{56}N_4O_4S_3$, 604.1737, found, 604.1735.

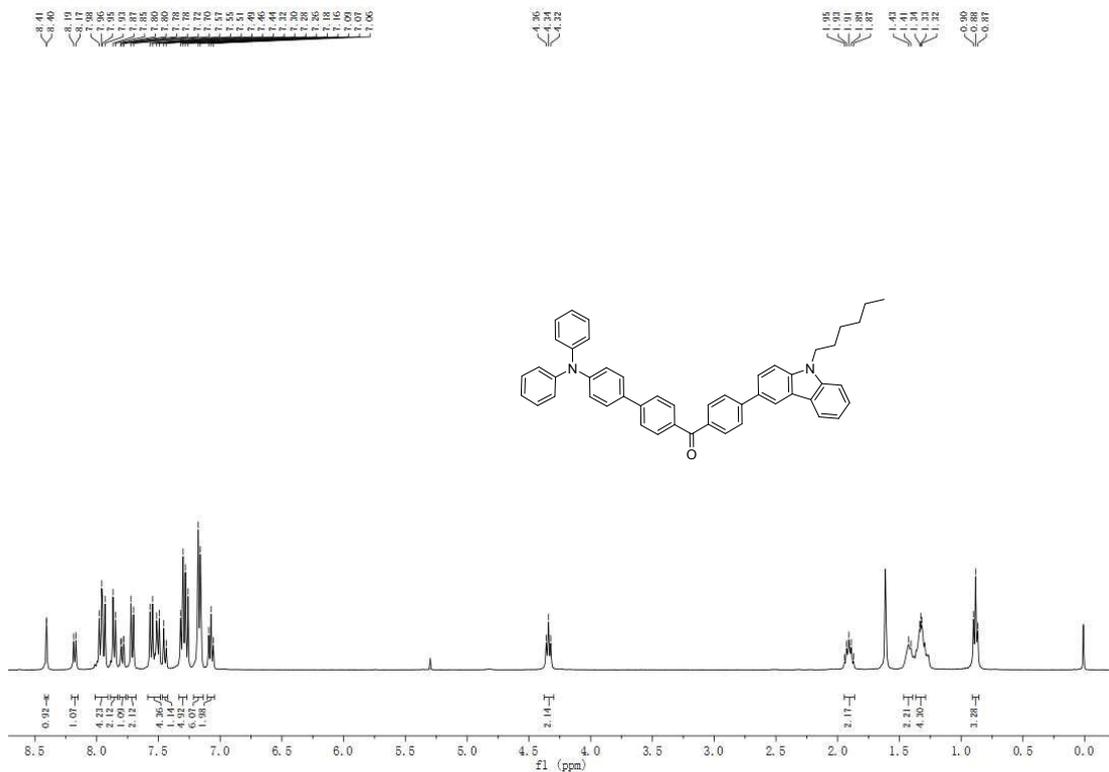
Synthesis of dye JY 69

Dye **JY69** was synthesized using the same procedure employed for dye **JY66**, while replacing compound **9** with compound **12**. The residue was purified by column chromatography and recrystallized to obtain dye **JY69** (75% yield), a dark red solid, m.p. 272-274 °C. 1H NMR (400 MHz, DMSO- d_6) δ 8.47 (d, $J = 4.9$ Hz, 2H), 8.00 – 7.94 (m, 2H), 7.73 (s, 1H), 7.69 (s, 2H), 7.63 – 7.56 (m, 4H), 7.56 – 7.50 (m, 4H), 7.47 (d, $J = 8.1$ Hz, 2H), 7.36 (d, $J = 5.2$ Hz, 1H), 7.30 (t, $J = 7.7$ Hz, 4H), 7.25 (d, $J = 5.2$ Hz, 1H), 7.13 (d, $J = 12.0$ Hz, 3H), 7.06 (d, $J = 7.3$ Hz, 6H), 7.02 (d, $J = 8.1$ Hz, 5H), 6.97 (d, $J = 8.4$ Hz, 2H), 4.30 – 4.16 (m, 2H), 1.78 – 1.70 (m, 2H), 1.23 – 1.20 (m, 6H), 0.77 (t, $J = 6.5$ Hz, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.46, 152.15, 146.83, 146.61, 146.38, 144.95, 144.91, 144.28, 141.33, 141.11, 141.05, 139.47, 138.78, 137.80, 134.44, 133.63, 132.91, 131.81, 131.53, 131.43, 130.40, 129.43, 127.23, 125.65, 125.61, 125.37, 125.02, 124.01, 123.11, 123.00, 116.30, 113.70, 112.98, 111.80, 108.65, 99.41, 98.24, 46.39, 30.66, 29.64, 25.77, 21.88, 13.71. HRMS (ESI): m/z $[M-2H]^{-2}$ calcd for $C_{74}H_{52}N_4O_4S_4$, 594.1441, found, 594.1440.

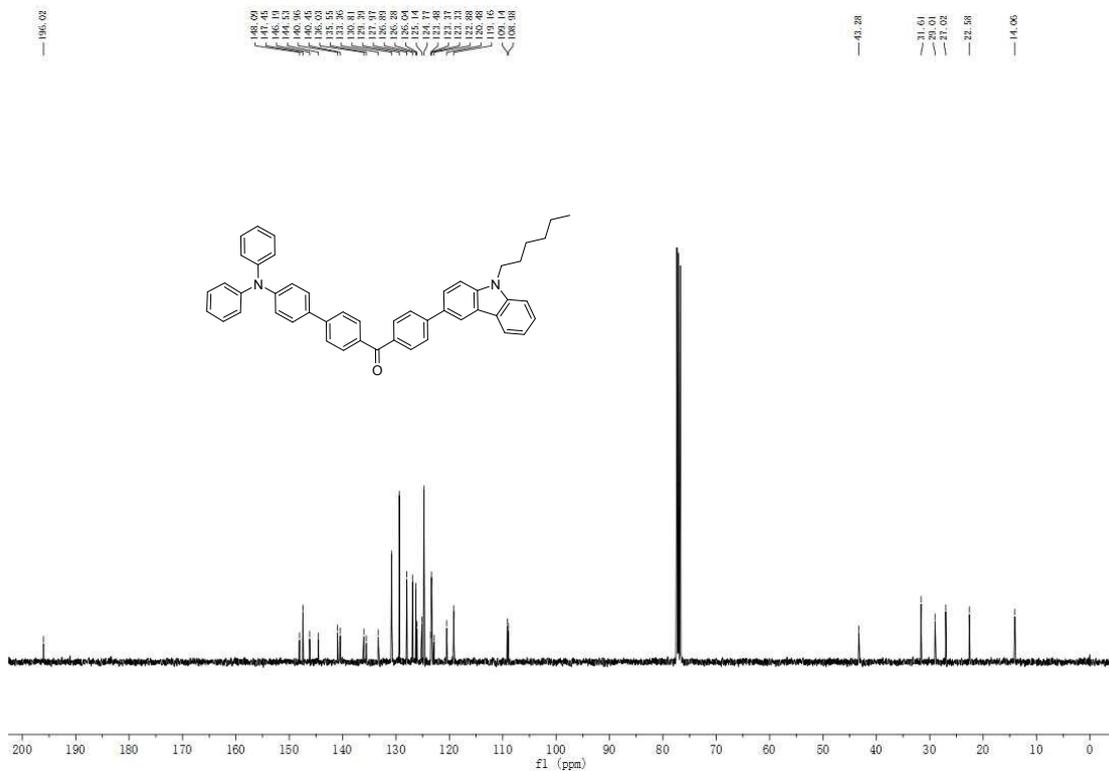
Reference

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- [3] Förtsch S, Bäuerle P. Synthesis and characterization of two isomeric dithienopyrrole series and the corresponding electropolymers. *Polym Chem* 2017;8:3586–95.
- [4] Kim Y-H, Zhao Q, Kwon S-K. *J. Polym. Sci.*, Synthesis and characterization of poly(fluorene)-based copolymer containing triphenylamine group. Part A: *Polym Chem* 2006;44:172–82.
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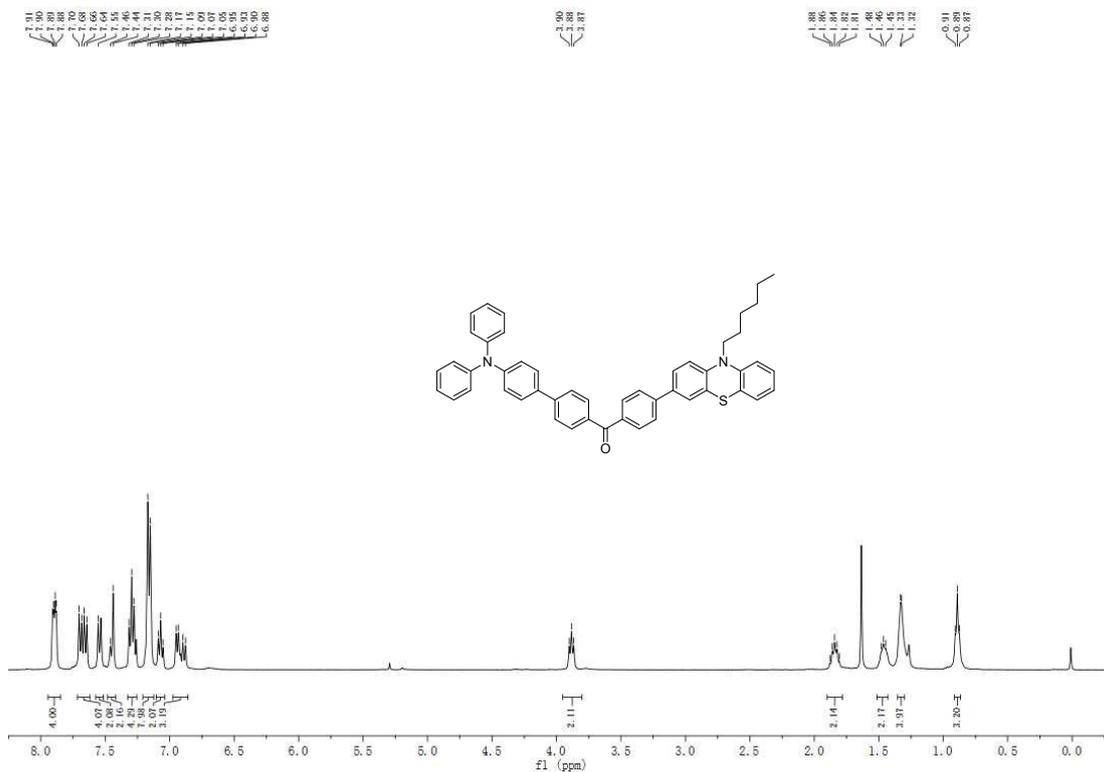
writable properties by electrochemical treatments. *Electrochim Acta* 2014;116:69–77.



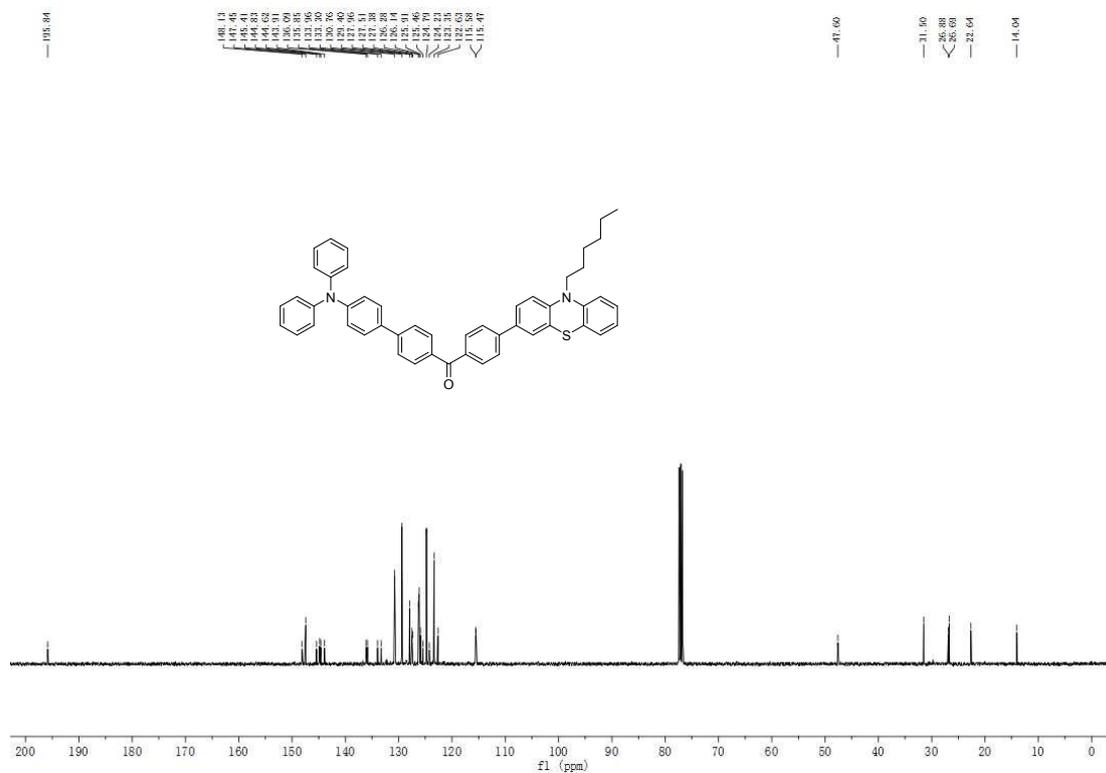
¹H NMR spectrum of compound 2 in CDCl₃



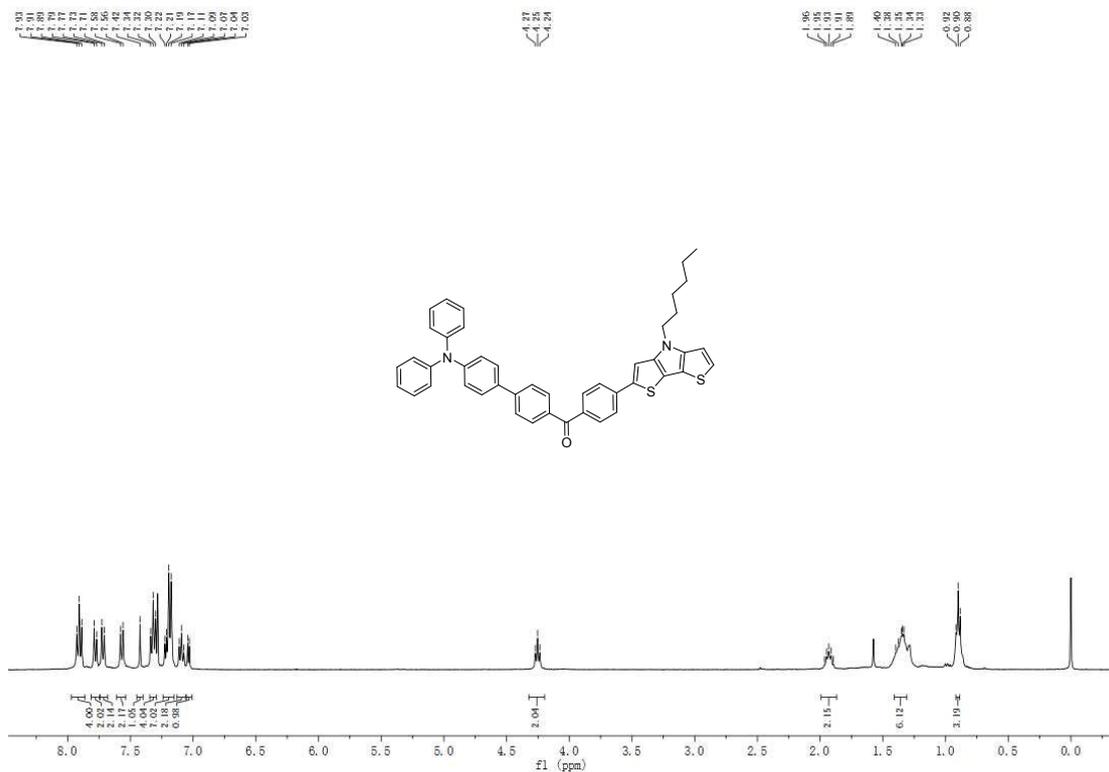
¹³C NMR spectrum of compound 2 in CDCl₃



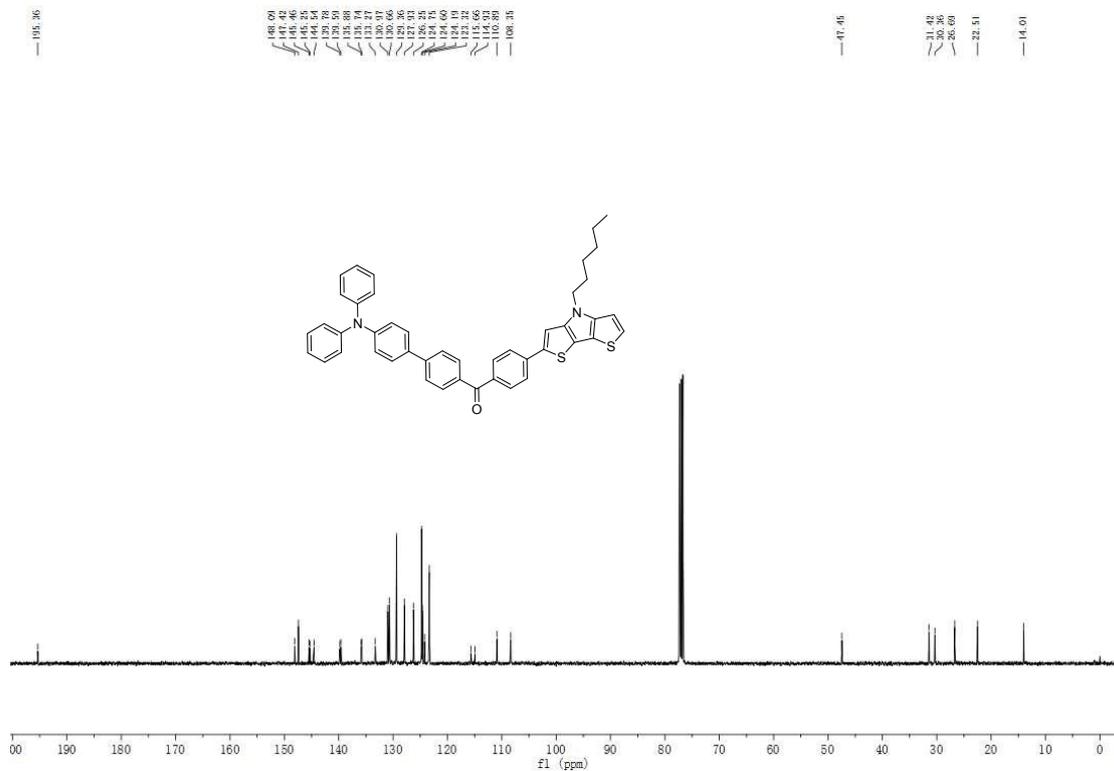
¹H NMR spectrum of compound 3 in CDCl₃



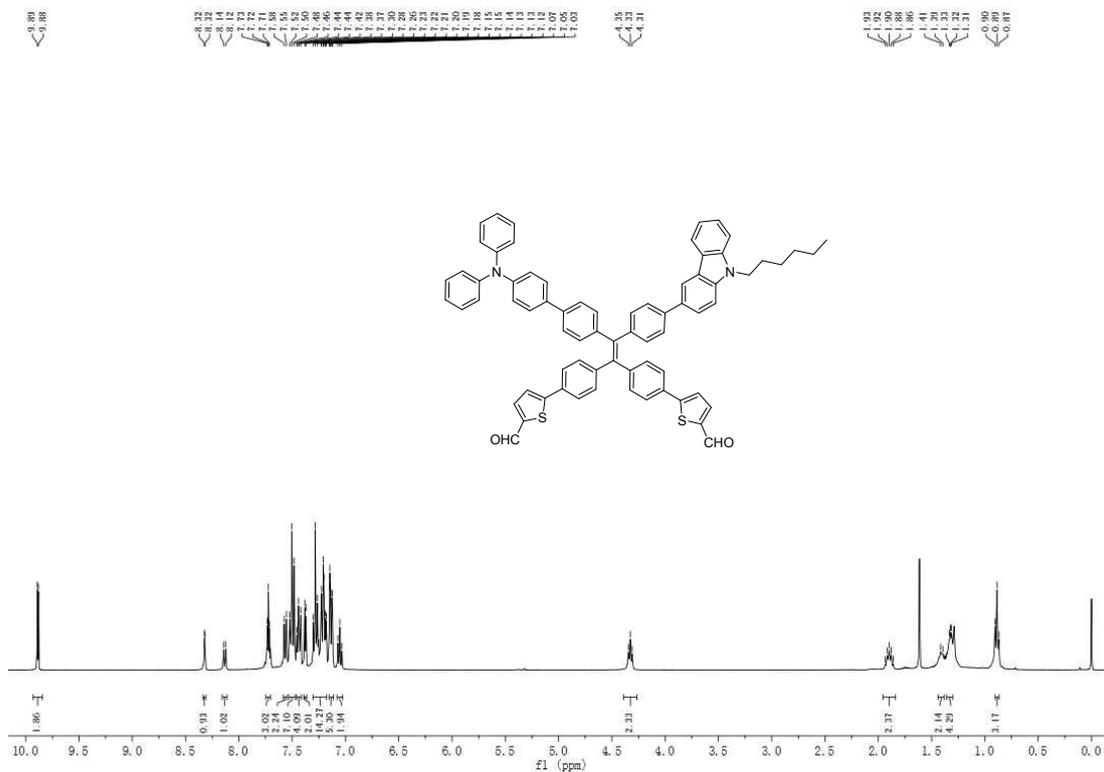
¹³C NMR spectrum of compound 3 in CDCl₃



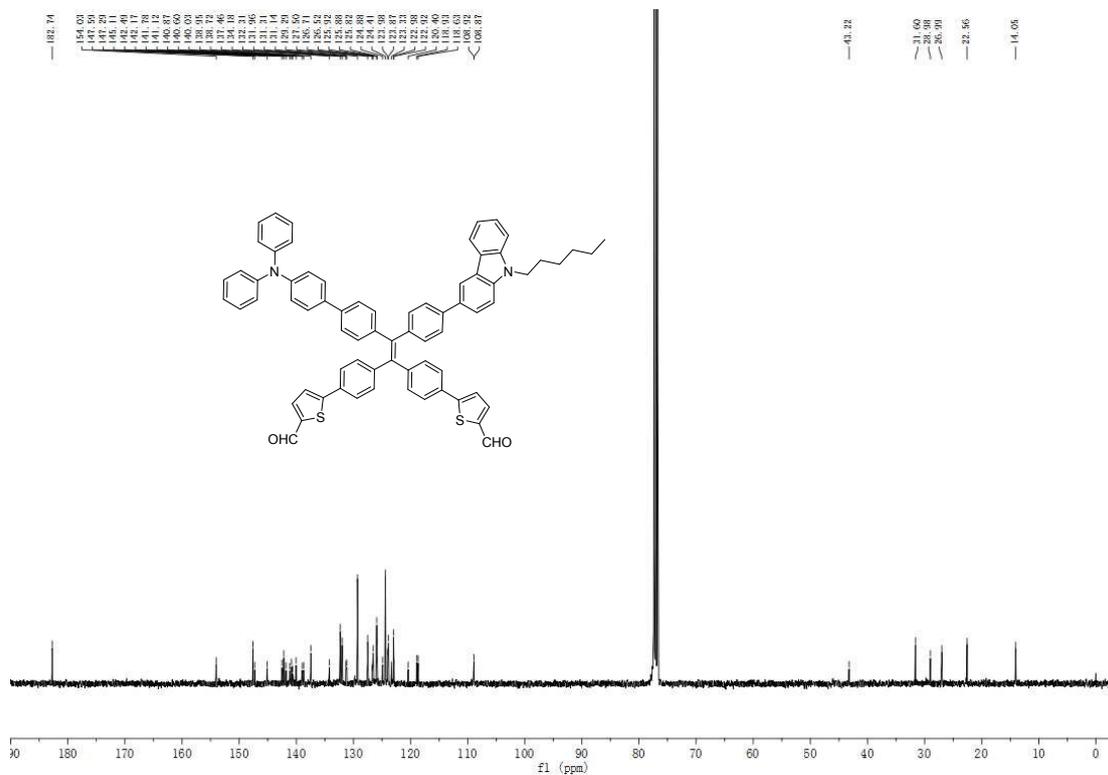
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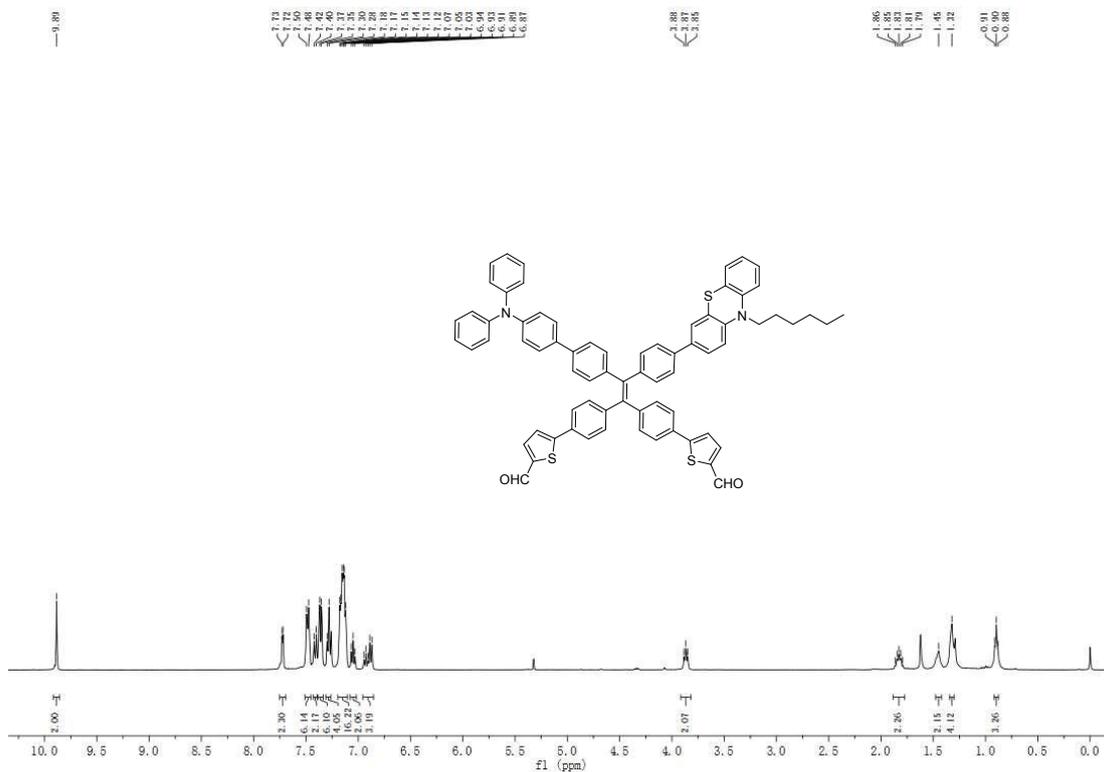
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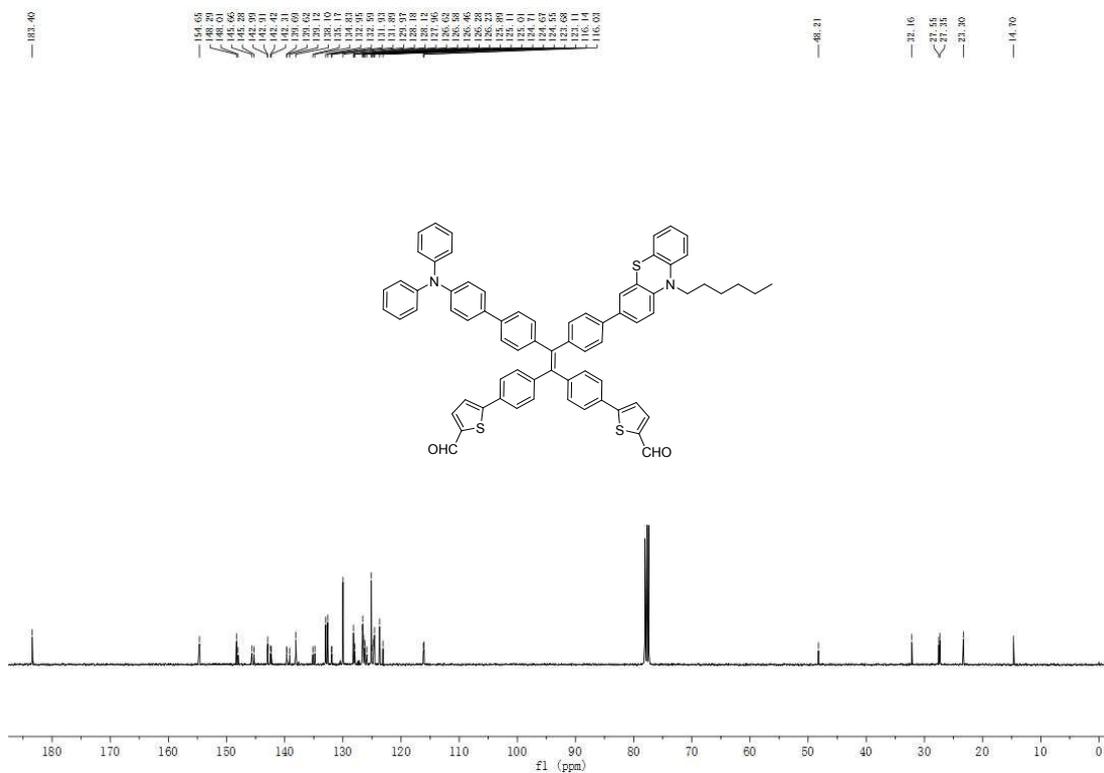
¹H NMR spectrum of compound 10 in CDCl₃



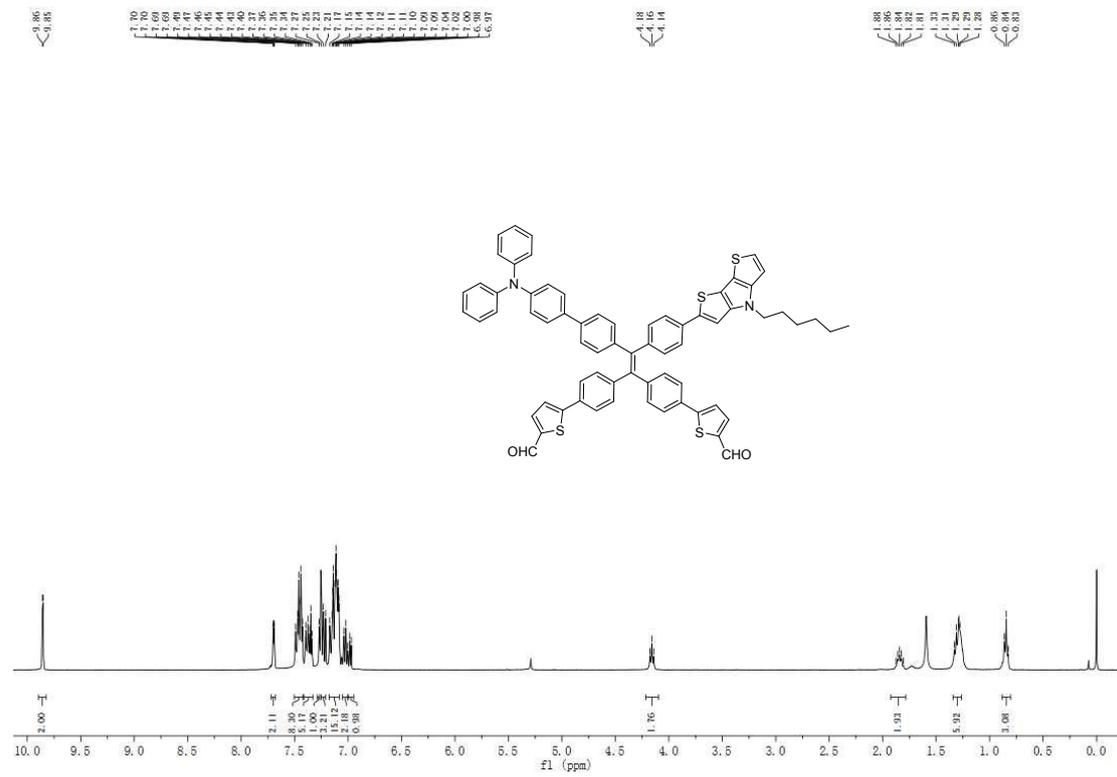
¹³C NMR spectrum of compound 10 in CDCl₃



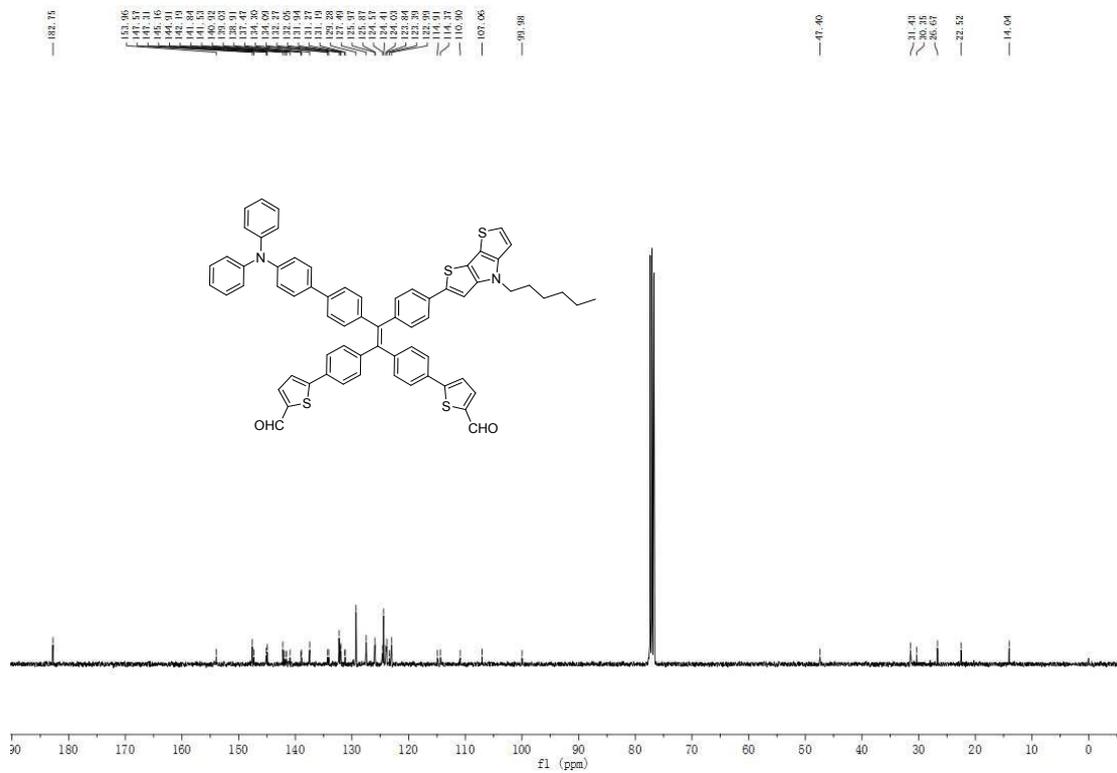
^1H NMR spectrum of compound **11** in CDCl_3



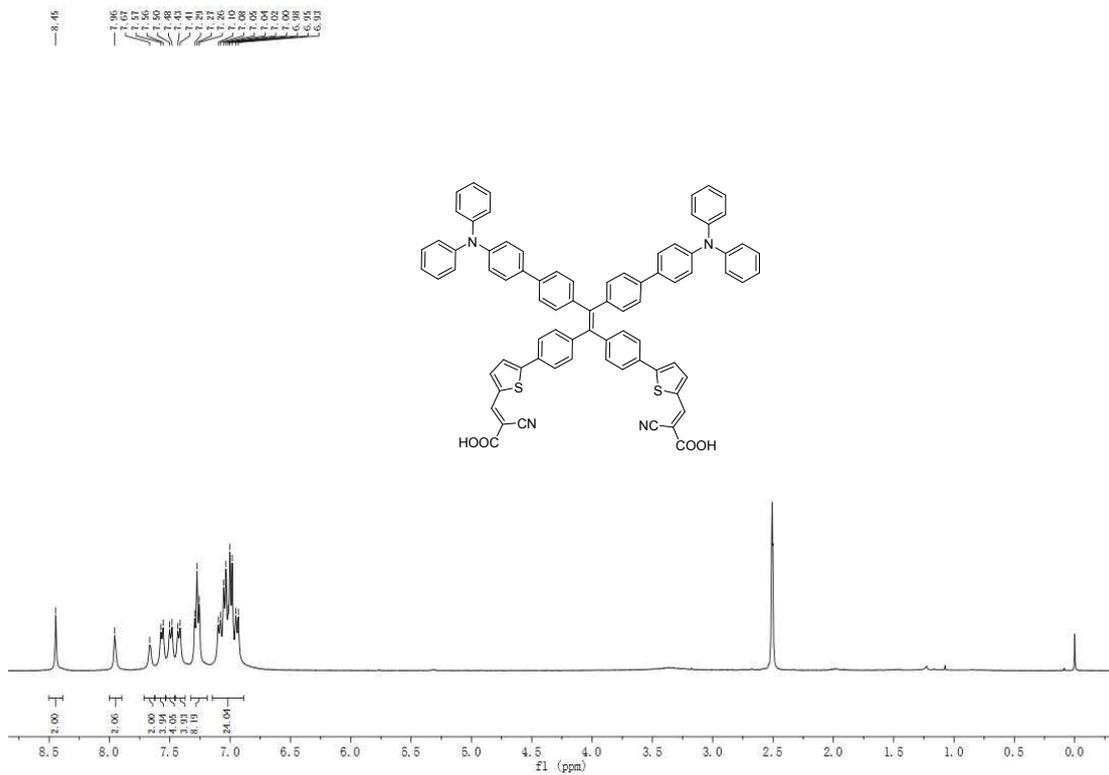
^{13}C NMR spectrum of compound **11** in CDCl_3



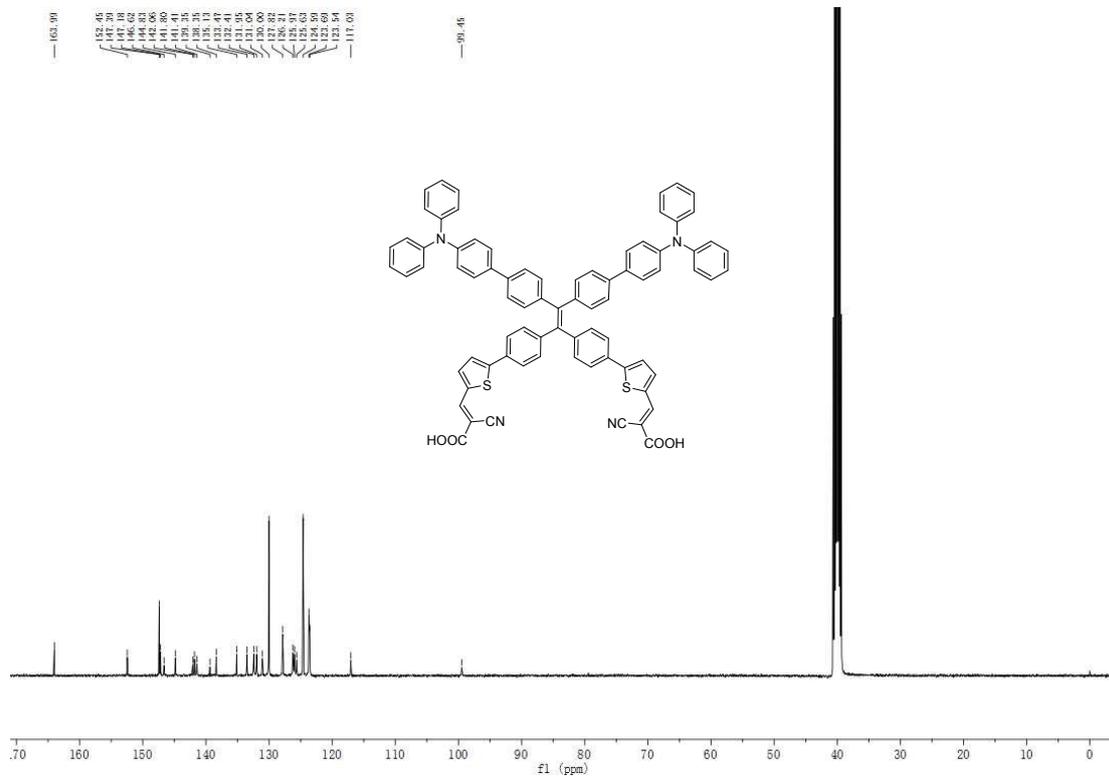
¹H NMR spectrum of compound **12** in CDCl₃



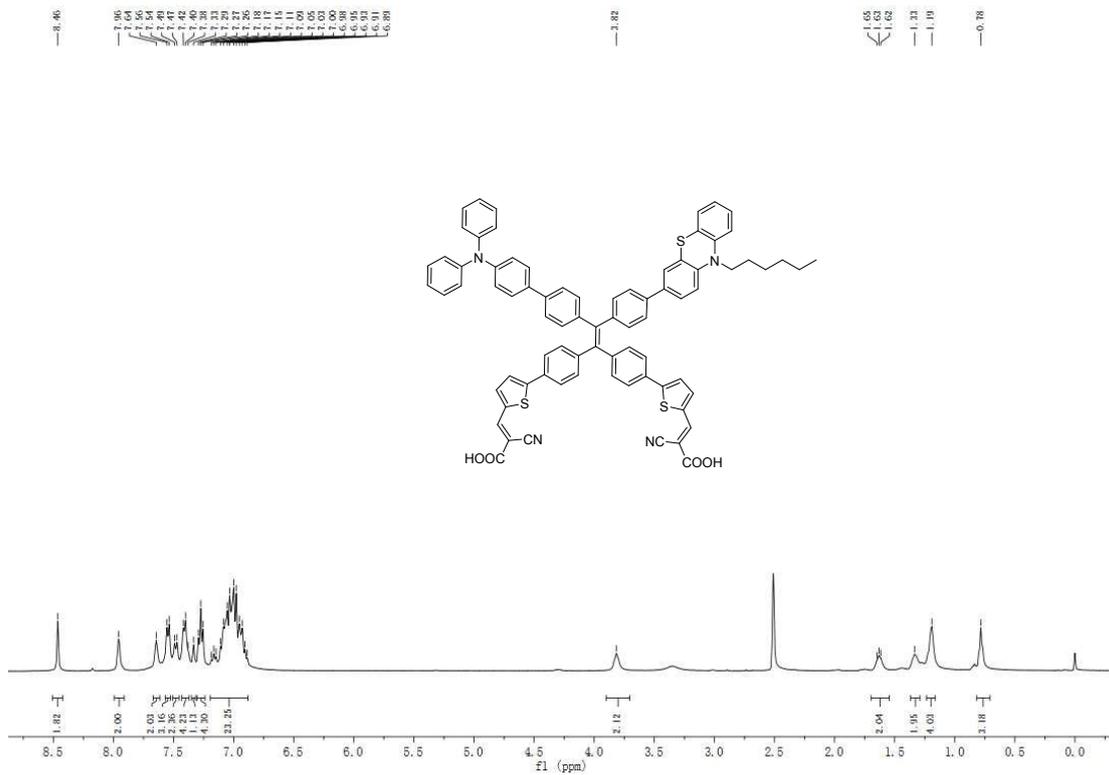
¹³C NMR spectrum of compound **12** in CDCl₃



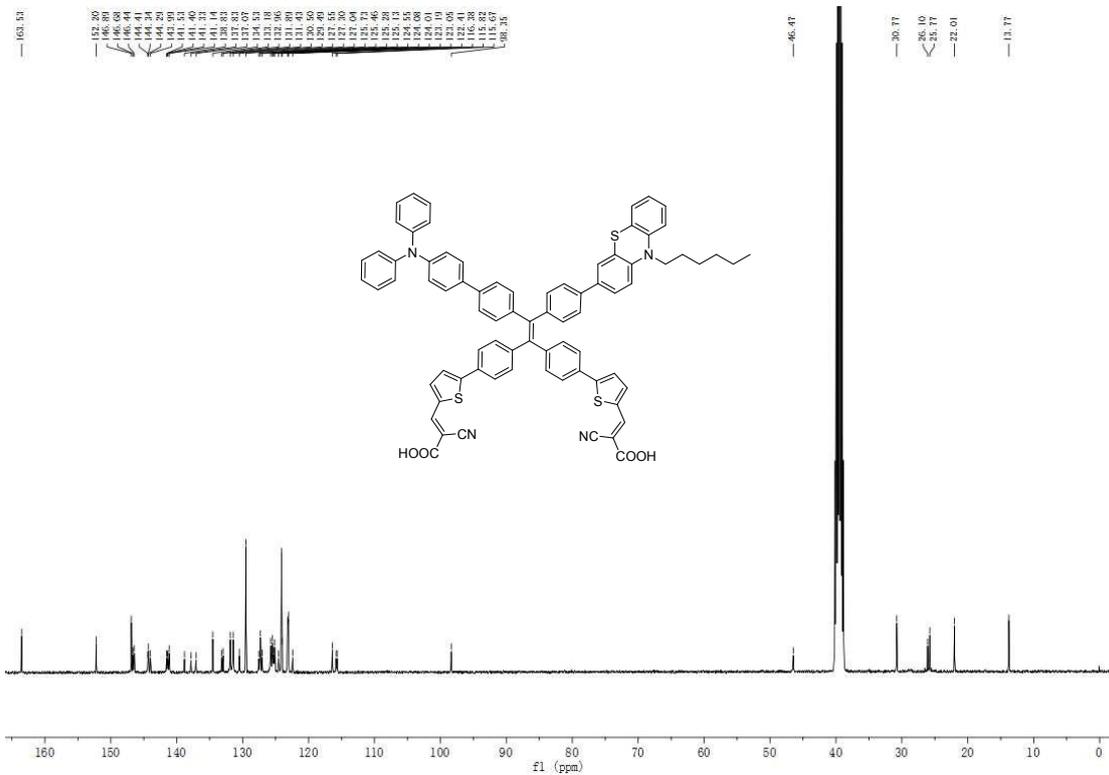
¹H NMR spectrum of dye JY66 in DMSO-*d*₆



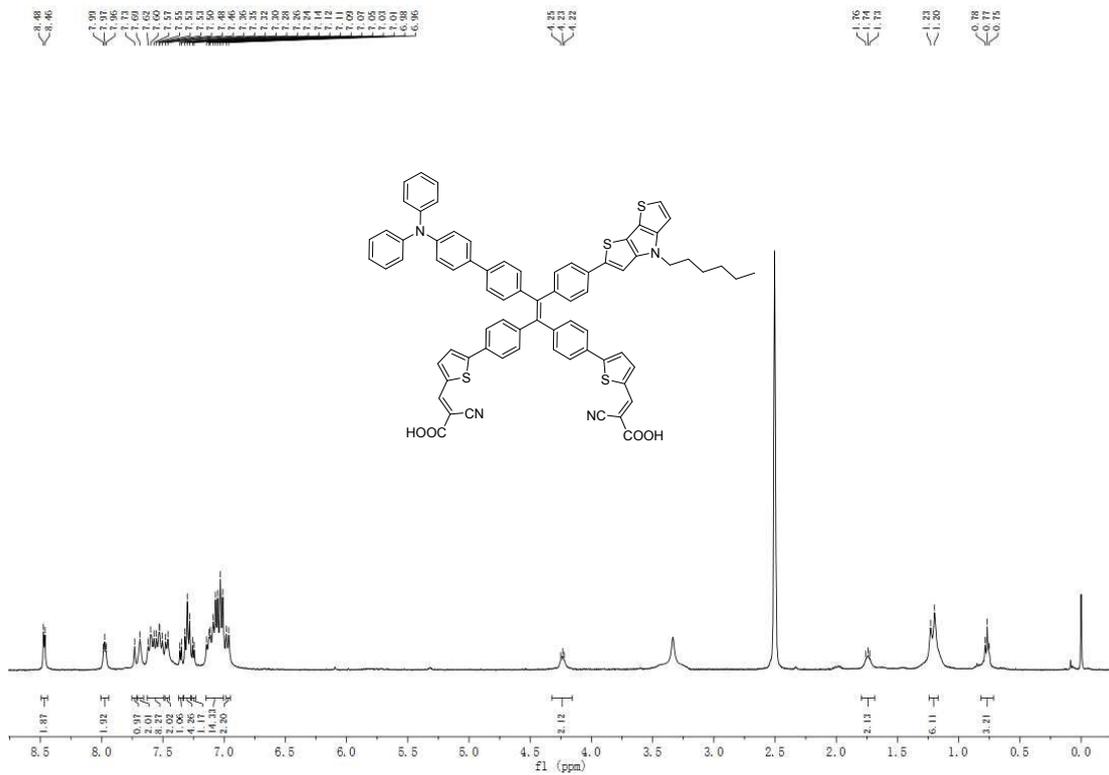
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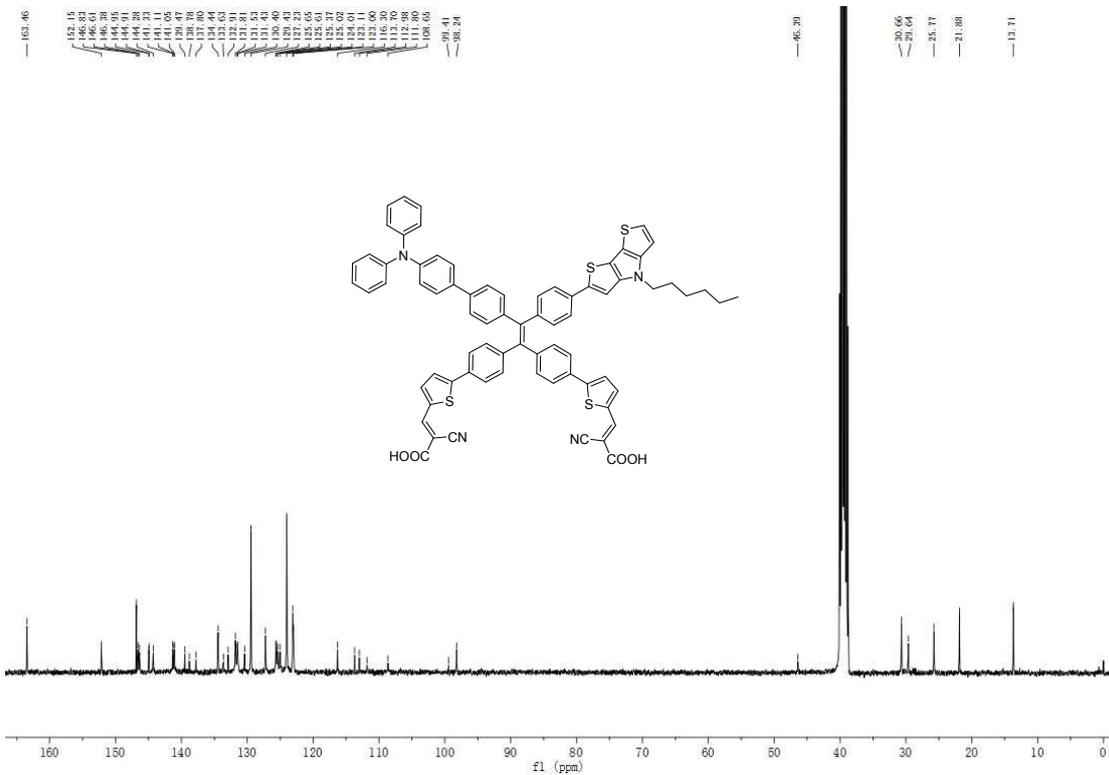
¹H NMR spectrum of dye JY68 in DMSO-*d*₆



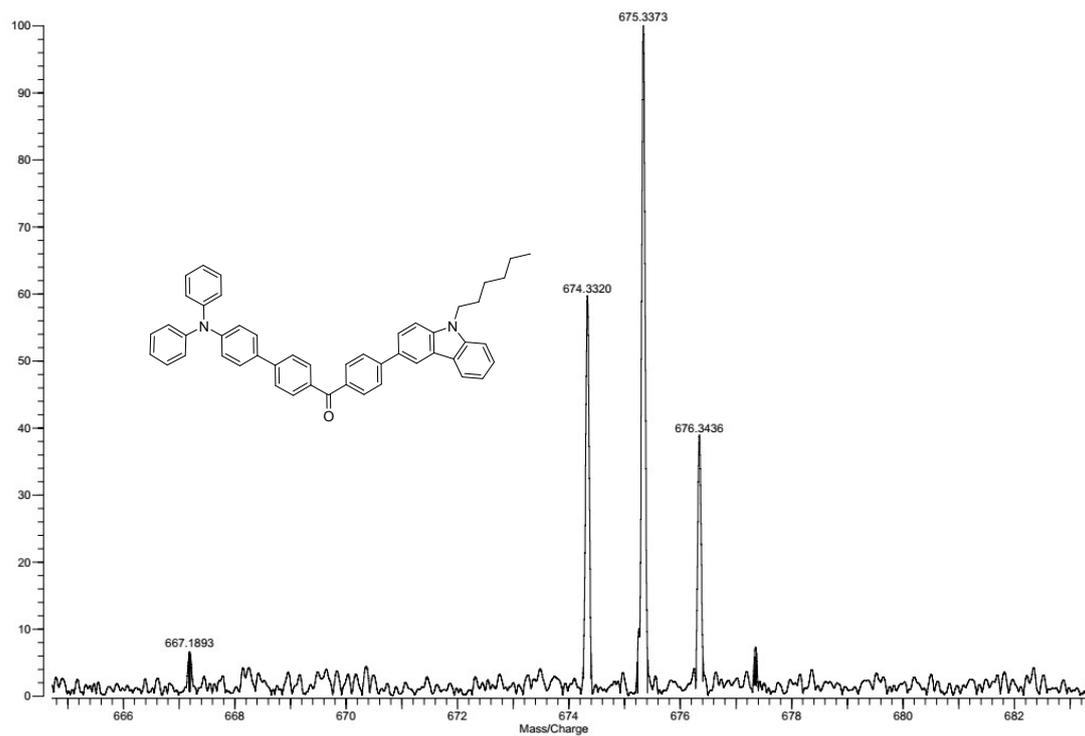
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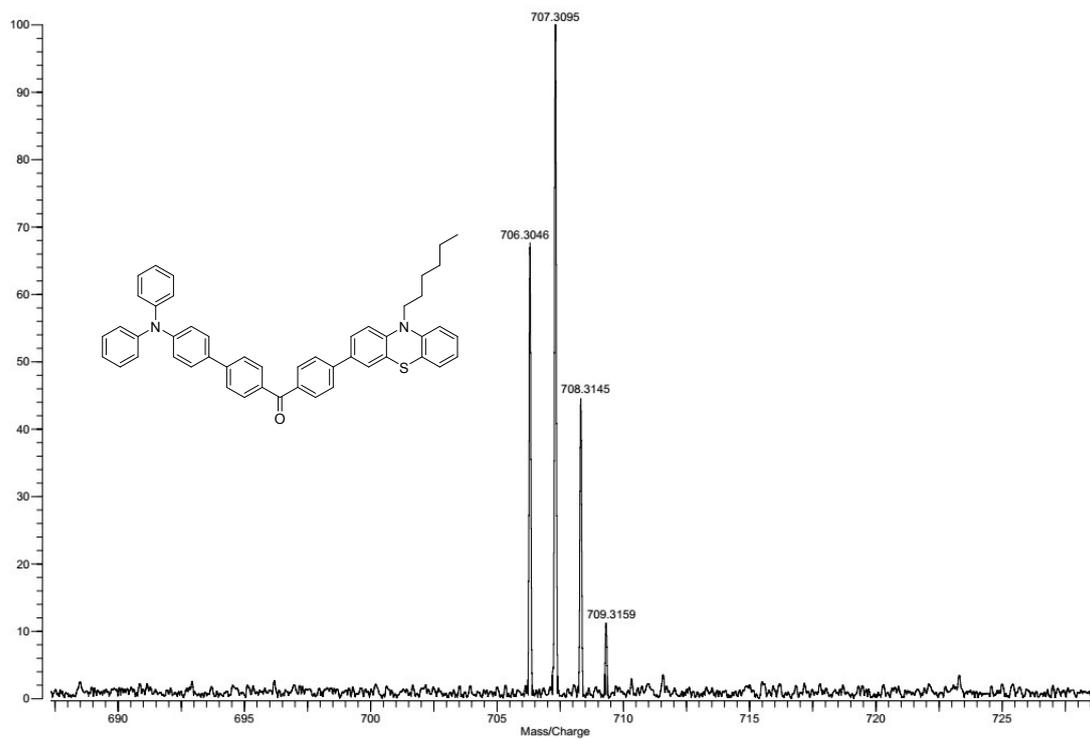
¹H NMR spectrum of dye JY69 in DMSO-*d*₆



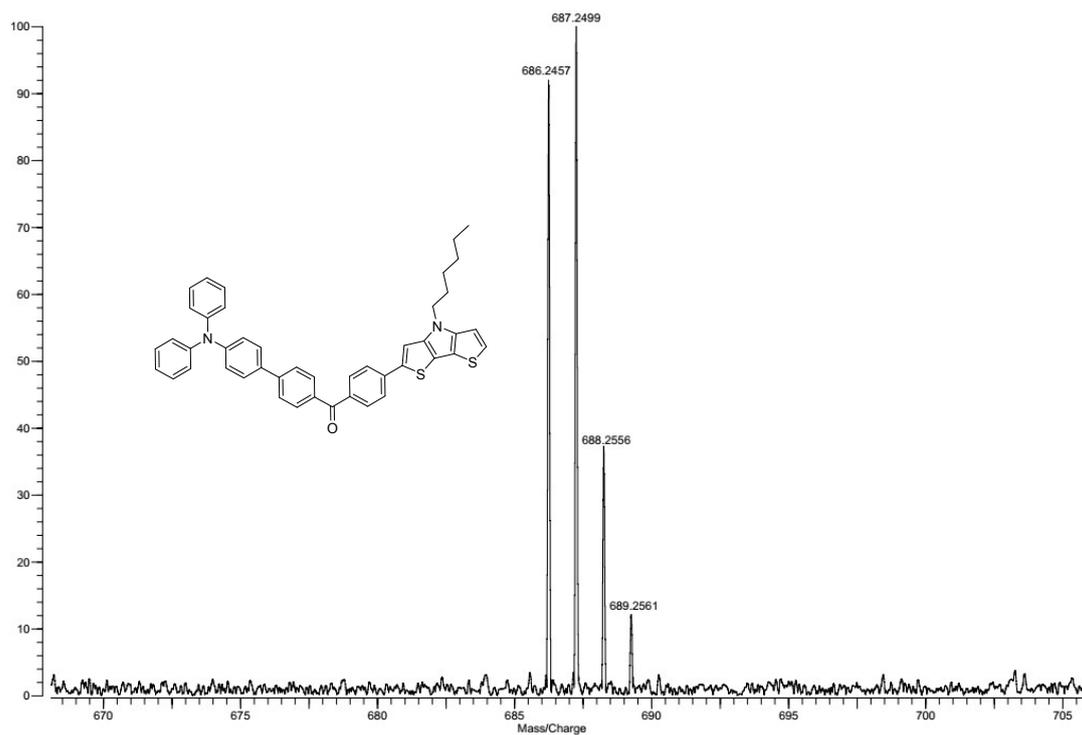
¹³C NMR spectrum of dye JY69 in DMSO-*d*₆



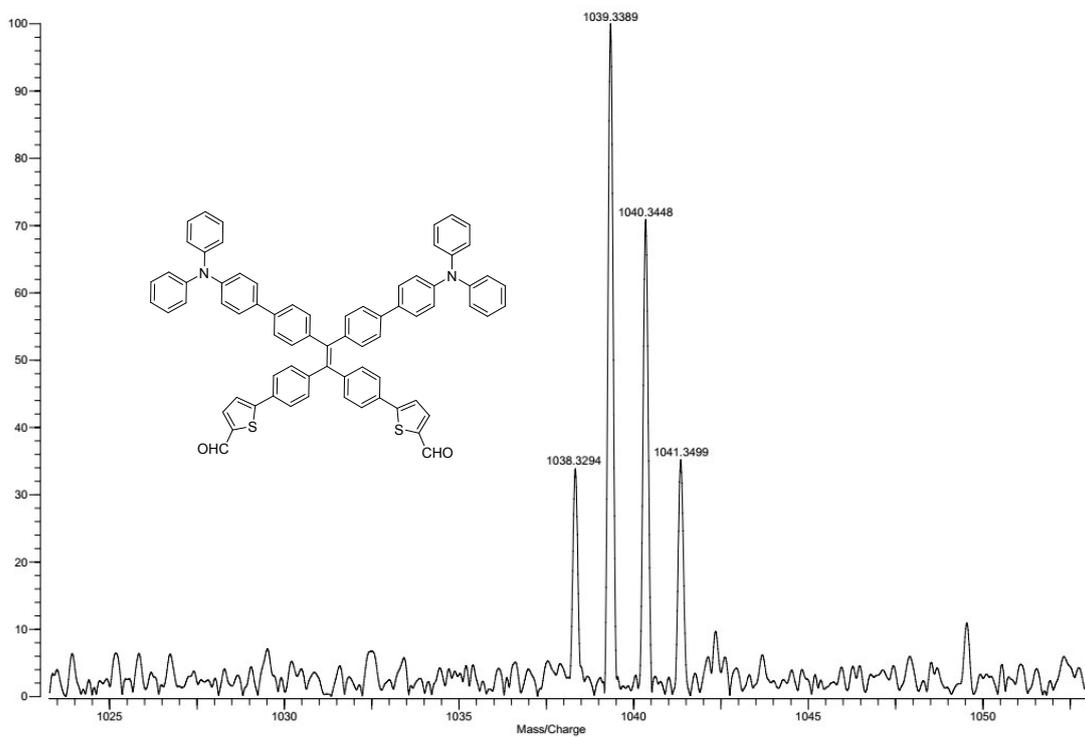
HR-MS spectrum of compound 2



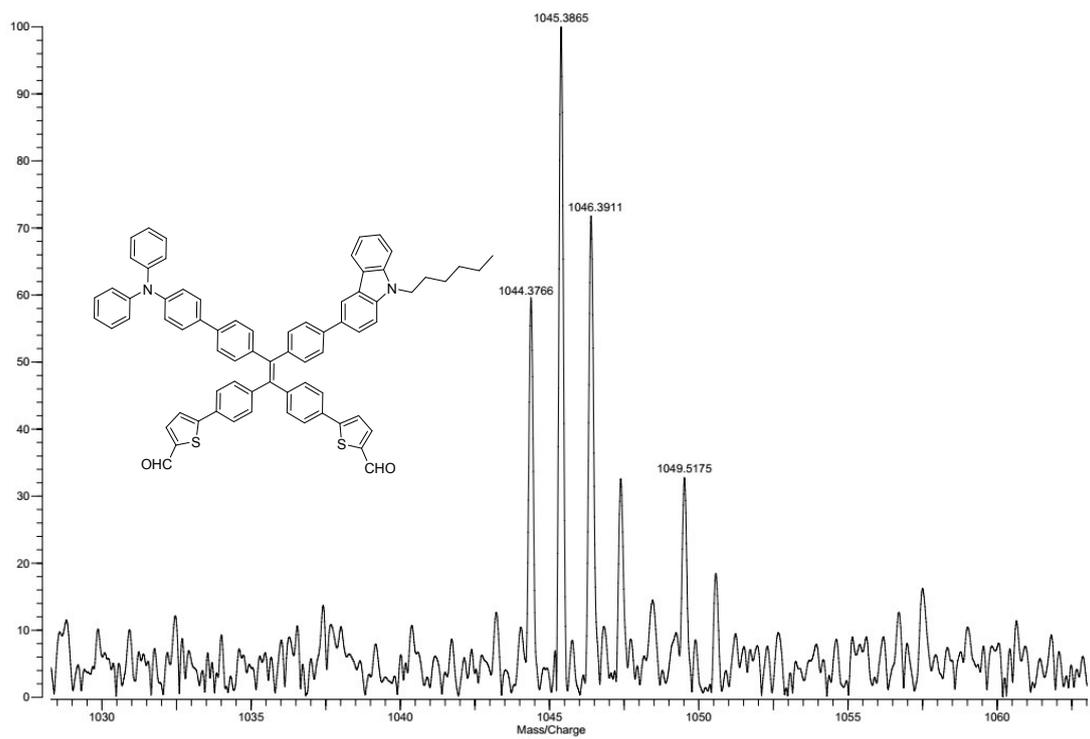
HR-MS spectrum of compound 3



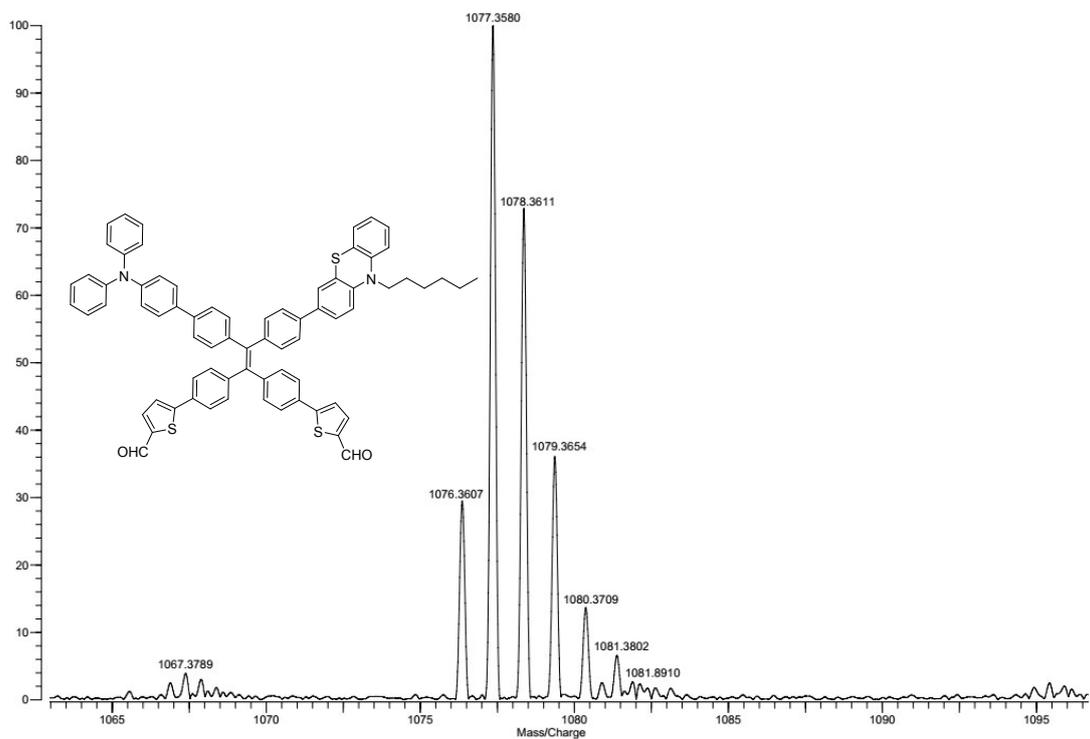
HR-MS spectrum of compound 4



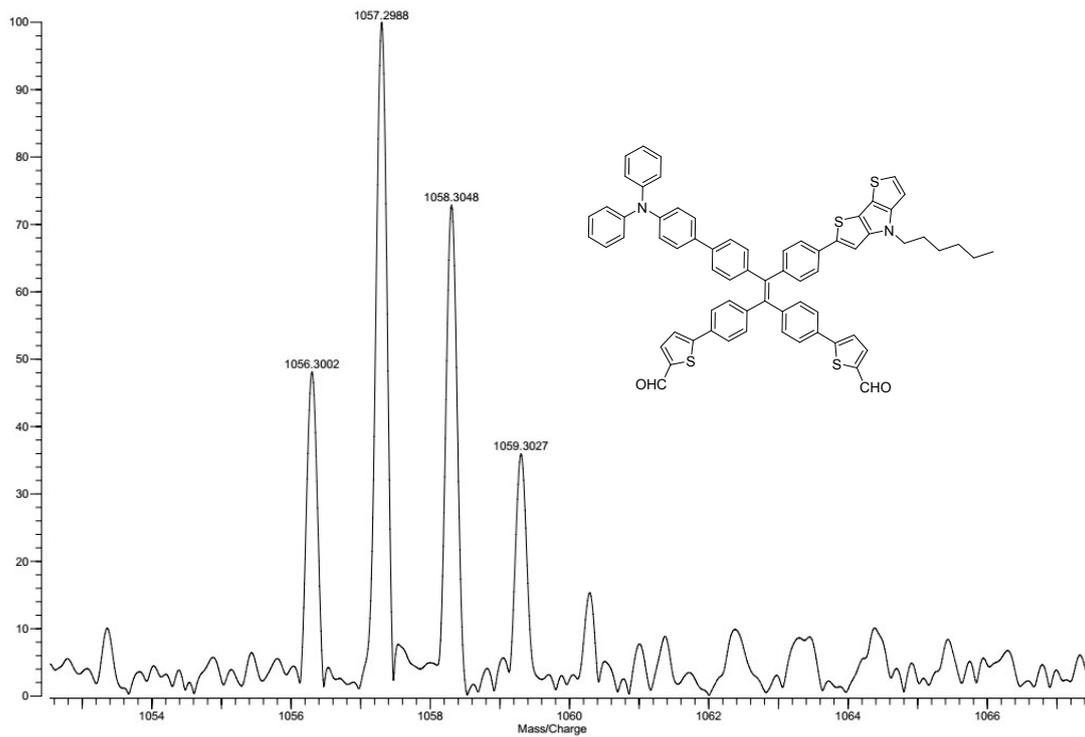
HR-MS spectrum of compound 9



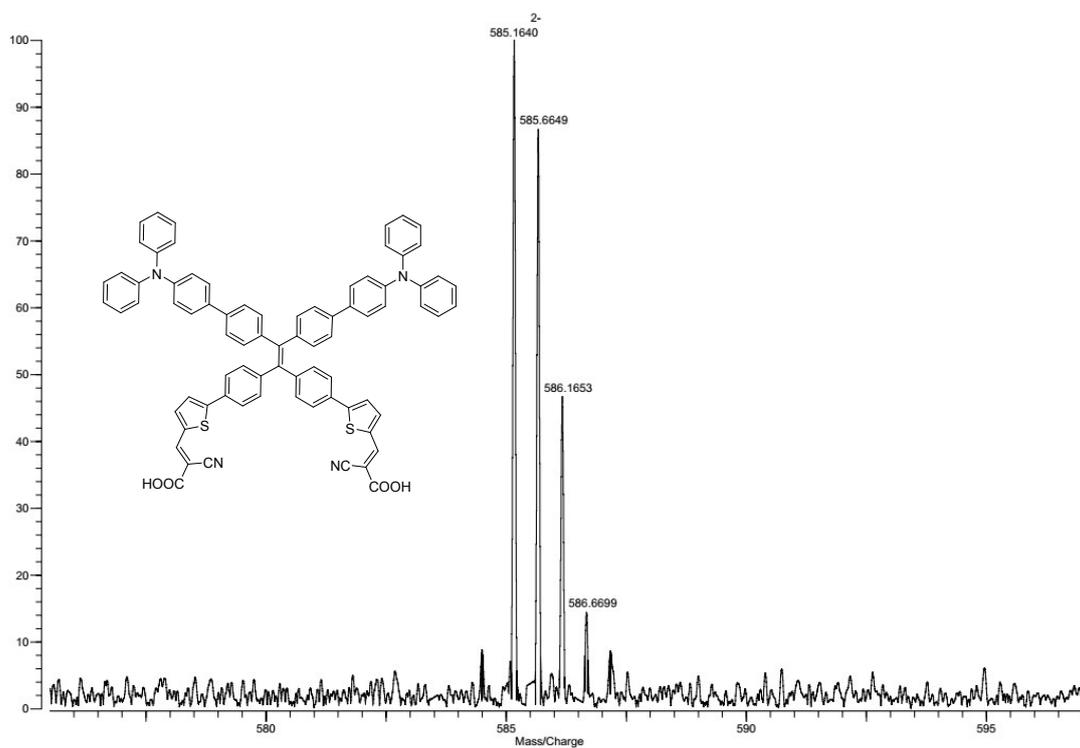
HR-MS spectrum of compound **10**



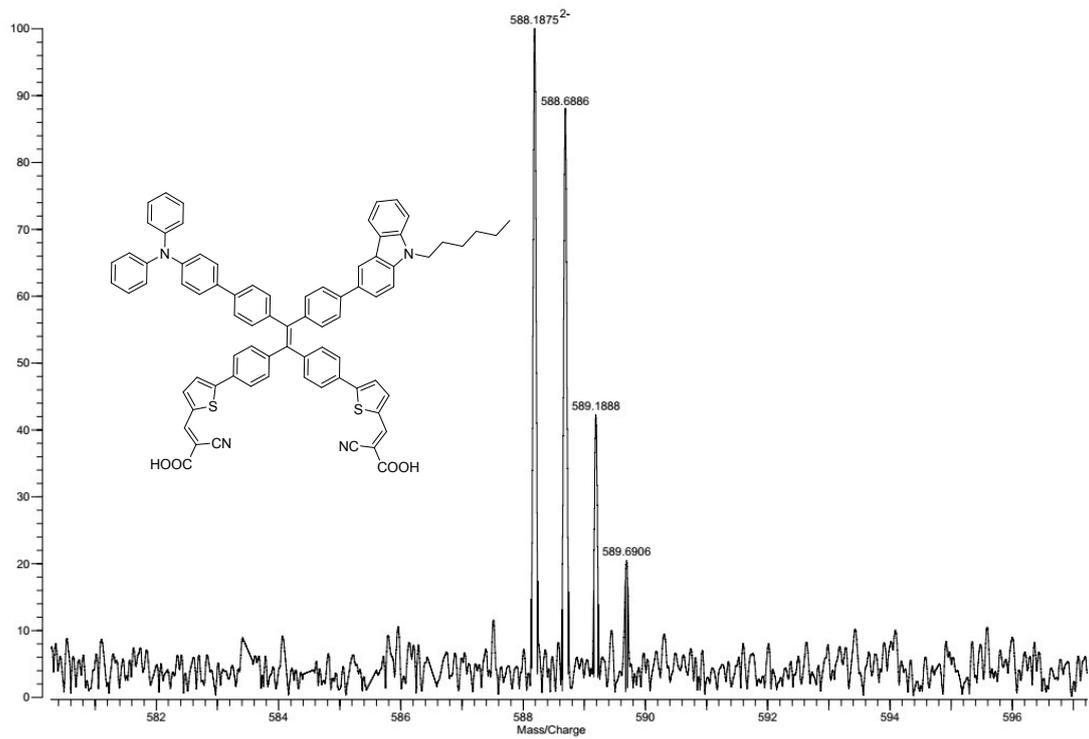
HR-MS spectrum of compound **11**



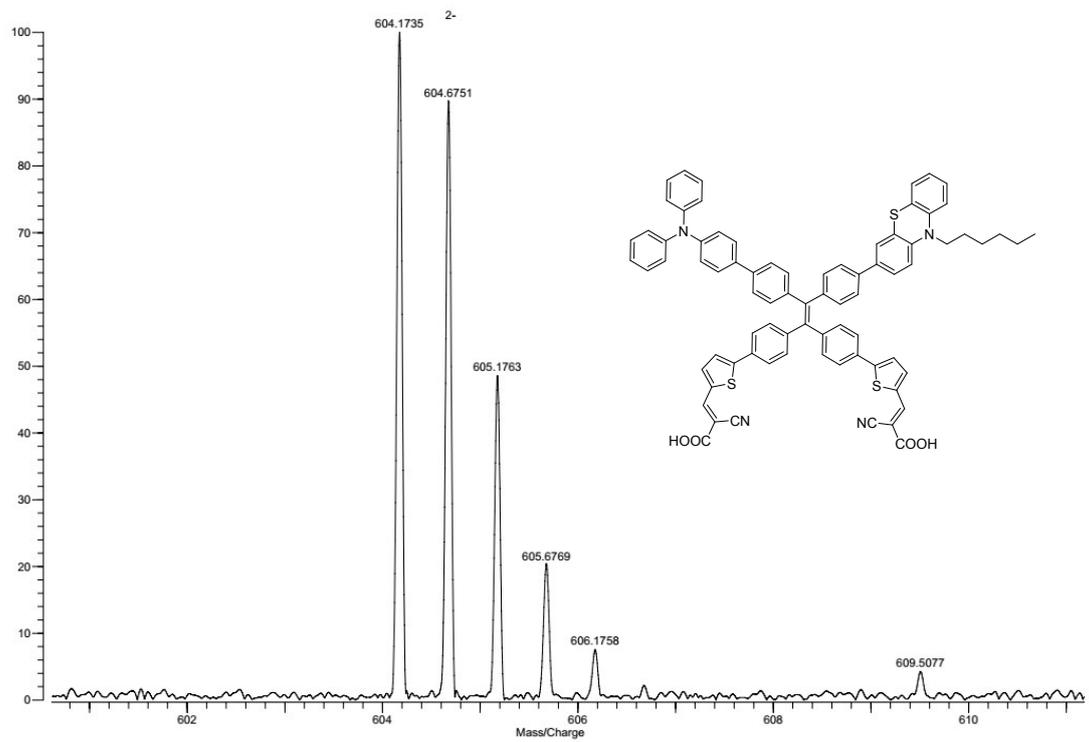
HR-MS spectrum of compound **12**



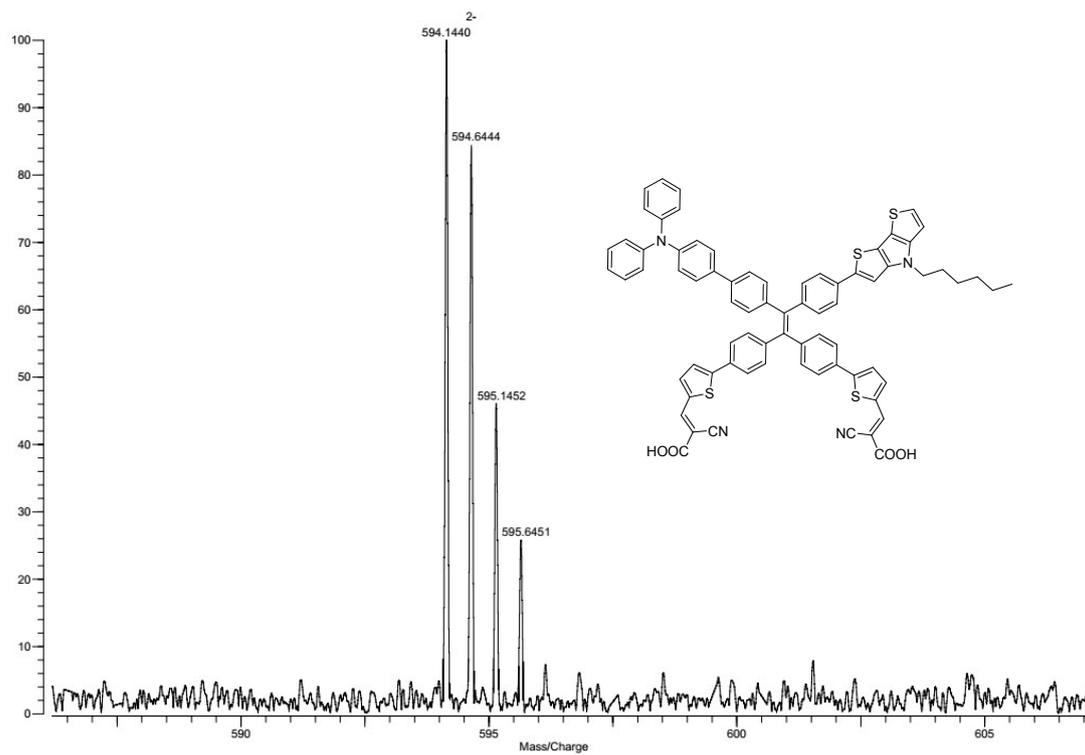
HR-MS spectrum of dye **JY66**



HR-MS spectrum of dye **JY67**



HR-MS spectrum of dye **JY68**



HR-MS spectrum of dye **JY69**