

## Supporting Information

### Computational-Assisted Molecular Design, Synthesis and Application of Benzobisthiadiazole-Based Near-Infrared Dye in Electrowetting Display

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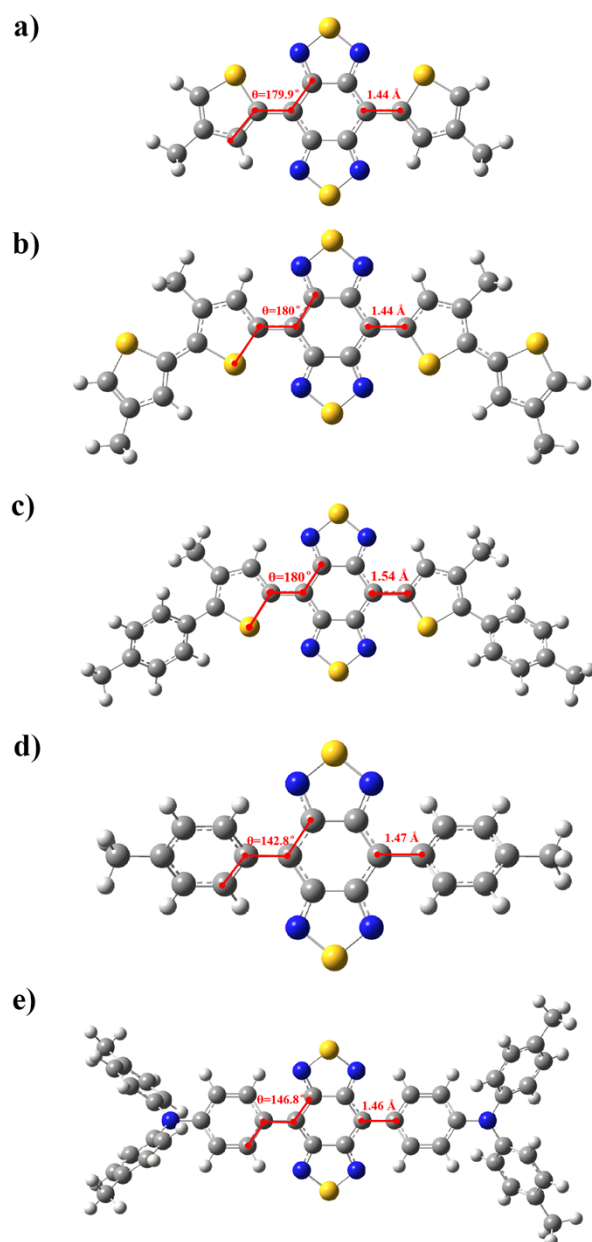
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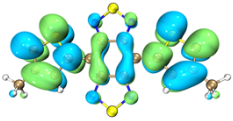
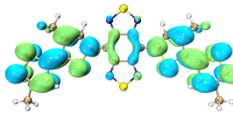
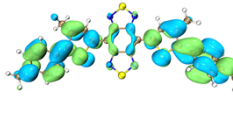
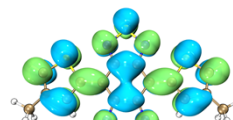
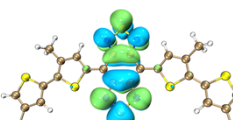
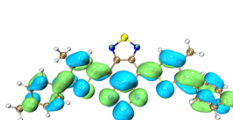
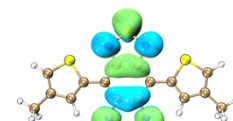
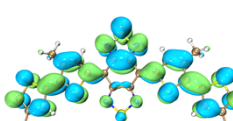
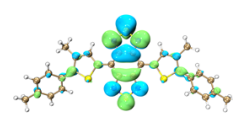
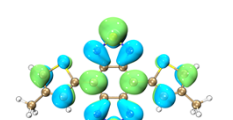
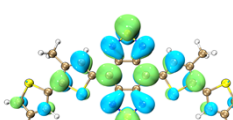
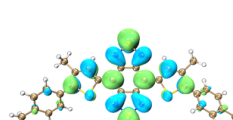
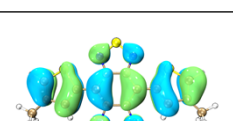
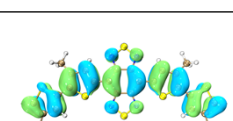
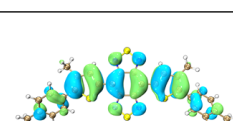

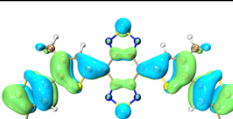
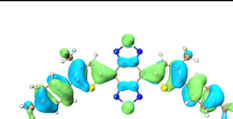
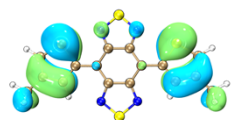
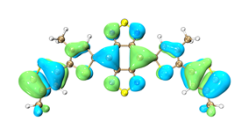
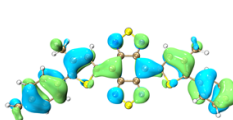
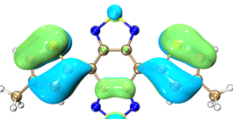
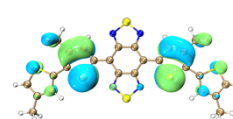
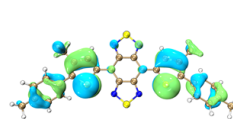
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## DFT and TDDFT calculations

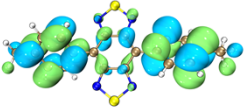
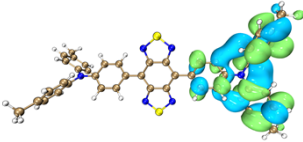
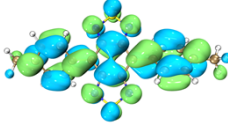
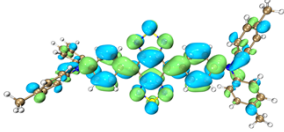
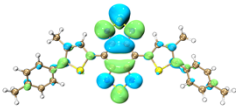
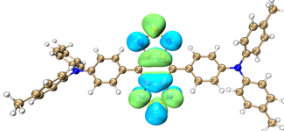
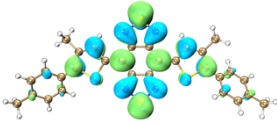
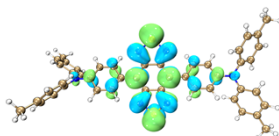
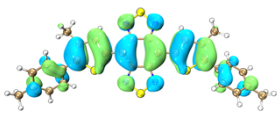
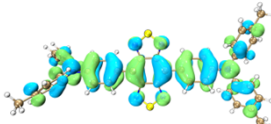
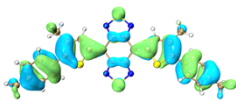
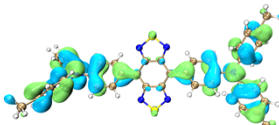
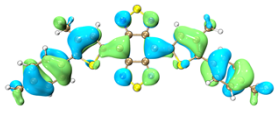
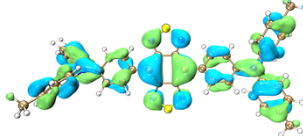
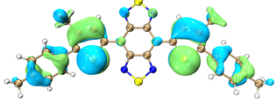
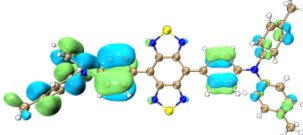


**Figure S1.** Calculated global minima point conformations of the five molecules BBT-Th-1 – BBT-Th-3 and BBT-Ph, BBT-TPA (ordered from top to bottom), in the global minima conformations, the presence of dihedral angles  $\theta$  and C-C bond lengths between the benzobisthiadiazole receptor and the neighboring donor moiety.

**Figure S2.** The molecular orbital diagrams of BBT-Th-1 – BBT-Th-3.

	<b>BBT-Th-1</b>	<b>BBT-Th-2</b>	<b>BBT-Th-3</b>
<b>LUMO+3</b>			
<b>LUMO+2</b>			
<b>LUMO+1</b>			
<b>LUMO</b>			
<b>HOMO</b>			
<b>HOMO-1</b>			
<b>HOMO-2</b>			
<b>HOMO-3</b>			

**Figure S3.**The molecular orbital diagrams of BBT-Ph and BBT-TPA.

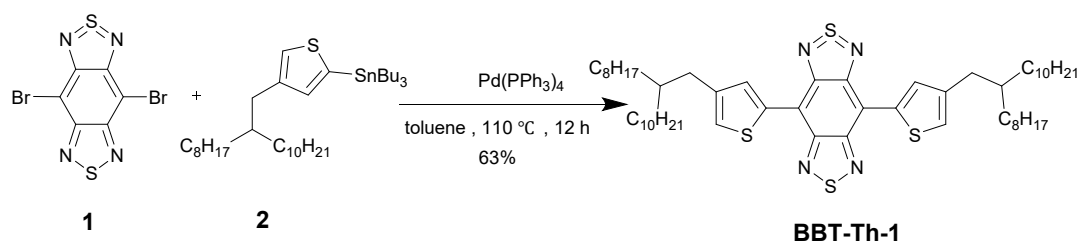
	<b>BBT-Ph</b>	<b>BBT-TPA</b>
<b>LUMO+3</b>		
<b>LUMO+2</b>		
<b>LUMO+1</b>		
<b>LUMO</b>		
<b>HOMO</b>		
<b>HOMO-1</b>		
<b>HOMO-2</b>		
<b>HOMO-3</b>		

## Experimental Section

### General methods

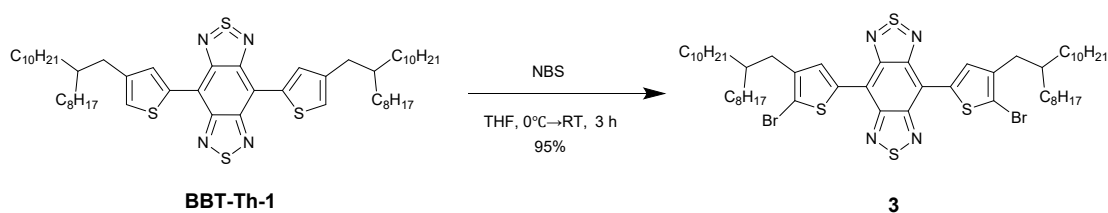
All the chemicals were used as received unless otherwise indicated. All oxygen or moisture-sensitive reactions were performed under an inert atmosphere. All the chemicals were purchased from commercial sources and used without further purification.  $^1\text{H}$  NMR was measured in a Bruker Avance (III) 600 MHz spectrometer, and  $^{13}\text{C}$  NMR spectra were measured in 151 MHz using  $\text{CDCl}_3$  as the internal solvent. The  $^1\text{H}$  NMR chemical shifts were recorded in parts per million (ppm) relative to the solvent residual peak ( $\text{CDCl}_3$ , 7.26 ppm). The  $^{13}\text{C}$  NMR shifts are reported relative to the solvent residual peak ( $\text{CDCl}_3$ , 77.00 ppm). The multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet), and the coupling constant values (J) are reported in Hz. The UV-visible absorption spectra of all the compounds were recorded in n-hexane at room temperature on a UV755B UV-visible spectrophotometer from Shanghai Youke Instrumentation Co. with a scanning range of 300 nm to 1100 nm and a scanning accuracy of 1 nm. High resolution mass spectrometry (HRMS) was recorded on Agilent 1290 Infinity II Bio LC and 6545XT AdvanceBio LC/Q-TOF. The cyclic voltammogram (CVs) and differential pulse voltammograms were recorded on an electrochemical analyzer using glassy carbon as the working electrode, Pt wire as the counter electrode, and Ag/AgCl as the reference electrode.

### Synthetic procedures and characterization data



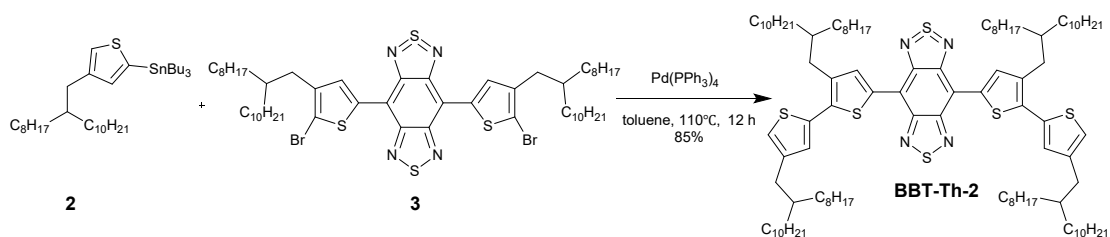
**Synthesis and Characterization of BBT-Th-1.** Under an argon atmosphere, 4,8-Dibromobenzo[1,2-c:4,5-c']bis([1,2,5]thiadiazole) **1** (0.2 g, 0.57 mmol),

tributyl(4-(2-octyldodecyl)thiophen-2-yl)stannane **2** (0.8 g, 1.22 mmol), and Pd(PPh<sub>3</sub>)<sub>4</sub> (0.066 g, 0.057 mmol) were added to a 100 ml two-necked round bottom flask containing 40 ml of dry toluene. The resulting mixture was bubbled with argon for 10 min and then refluxed at 110°C for 12 hours. After the reaction was completed, the solvent was removed under reduced pressure. The crude product was purified by column chromatography using a mixture of dichloromethane and n-hexane (1:1, v/v) as the eluent. After removal of the solvent under reduced pressure, the teal-colored product **BBT-Th-1** was obtained (330 mg, 63% yield). <sup>1</sup>H NMR (Chloroform-*d*) δ: 8.73 (s, 2H), 7.24 (s, 2H), 2.70 (d, *J* = 6.9 Hz, 4H), 1.79–1.74 (m, 2H), 1.41–1.20 (m, 64H), 0.86 (t, *J* = 6.9 Hz, 12H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ: 150.63, 142.25, 137.01, 134.05, 117.93, 112.47, 38.56, 34.15, 33.42, 33.40, 31.93, 30.11, 30.09, 29.73, 29.69, 29.67, 29.40, 29.36, 26.59, 22.68, 14.11. HRMS (ESI) *m/z*(%): 919.58 [M+H]<sup>+</sup>. Calcd for C<sub>54</sub>H<sub>87</sub>N<sub>4</sub>S<sub>4</sub> (*m/z*) 919.57.

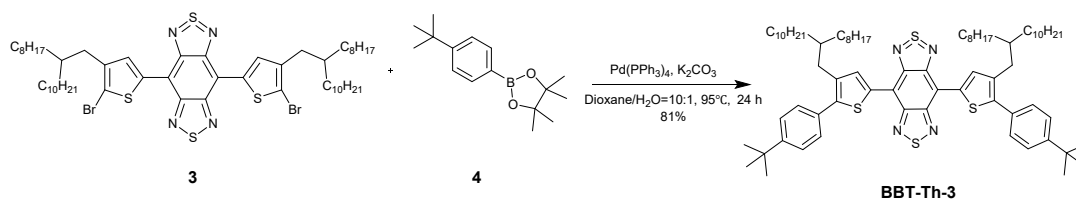


**Synthesis and Characterization of 3.** Compound **BBT-Th-1** (0.8 g, 0.87 mmol) and NBS (0.31 g, 1.76 mmol) were dissolved in 40 mL of THF, and the reaction mixture was stirred at room temperature under ambient pressure for 12 hours. After removing the solvent, the solid was dissolved in a small amount of DCM, and the solution was added dropwise to a large volume of methanol. The teal-colored precipitate was then collected, followed by column chromatography using petroleum ether as the eluent. After concentration and drying under vacuum, the teal-colored product **6** was obtained in 95% yield. <sup>1</sup>H NMR (Chloroform-*d*) δ: 8.59 (s, 2H), 2.63 (d, *J* = 7.2 Hz, 4H), 1.83–1.81 (m, 2H), 1.41–1.19 (m, 64H), 0.85 (td, *J* = 7.1, 3.0 Hz, 12H).



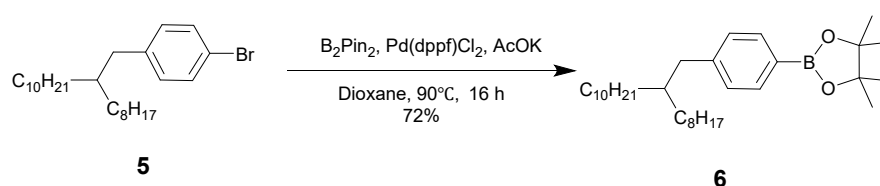


**Synthesis and Characterization of BBT-Th-2.** In a 100 mL two-necked round bottom flask, compound **3** (200 mg, 0.18 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (13 mg, 0.018mmol), and compound **2** (304 mg, 0.465 mmol, 2.5 eq.) were added to 10 mL of freshly distilled toluene. The resulting mixture was bubbled with argon for 10 min and then refluxed for 20 hours. After the reaction was completed, the solvent was removed under reduced pressure. Finally, the crude product was purified by column chromatography to remove unreacted tin compounds, using petroleum ether as the eluent. The yellow-green solid compound **BBT-Th-2** was isolated with a yield of 85.2%. <sup>1</sup>H NMR (Chloroform-*d*) δ: 8.78 (s, 2H), 7.15 (d, *J* = 1.4 Hz, 2H), 6.94 (s, 2H), 2.85 (d, *J* = 7.3 Hz, 4H), 2.59 (d, *J* = 6.9 Hz, 4H), 1.89–1.86 (m, 2H), 1.70–1.68 (m, 2H), 1.40–1.15 (m, 128H), 0.87 (dq, *J* = 13.3, 6.7 Hz, 24H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ: 151.11, 142.56, 139.36, 137.92, 136.75, 135.78, 135.23, 128.21, 121.57, 112.69, 38.97, 38.63, 35.08, 34.00, 33.47, 33.41, 31.95, 31.94, 31.50, 30.19, 30.12, 29.78, 29.76, 29.74, 29.71, 29.44, 29.39, 26.69, 26.48, 22.71, 22.69, 14.11. HRMS (ESI) *m/z*(%):1645.14 [M+H]<sup>+</sup>. Calcd for C<sub>102</sub>H<sub>171</sub>N<sub>4</sub>S<sub>6</sub> (*m/z*) 1645.18.

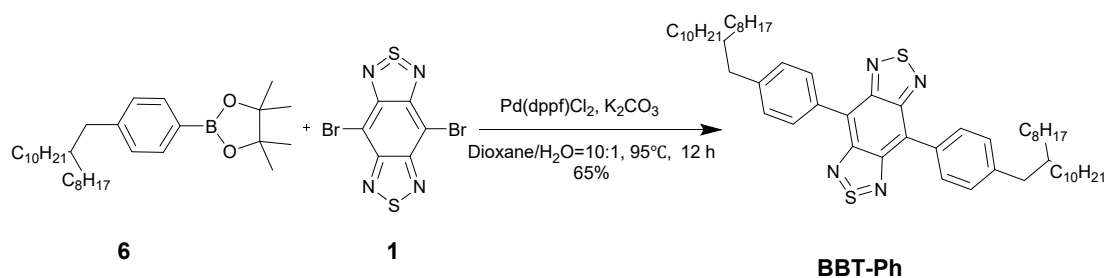


**Synthesis and Characterization of BBT-Th-3.** Under an argon atmosphere, compound **3** (100 mg, 0.09 mmol), 4-tert-butylphenylboronic acid pinacol ester **4** (58.53 mg, 0.225 mmol, 2.5 eq.), and Pd(PPh<sub>3</sub>)<sub>4</sub> (10 mg, 0.009 mmol) were placed in a 100 ml two-necked round bottom flask. Toluene (20 ml) and 2 M potassium carbonate solution (2 ml) were then added, and the mixture was heated to 90°C and stirred for 20 hours. After completion of the reaction, the temperature was slowly cooled to room temperature. The mixture was poured into water and extracted twice with dichloromethane. The organic layer was collected, dried over magnesium sulfate,

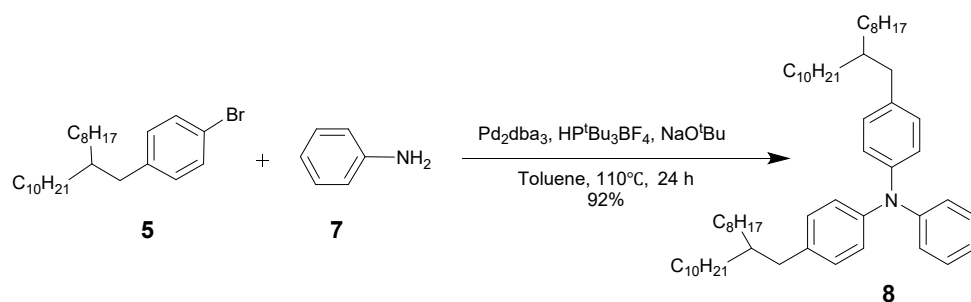
and concentrated under reduced pressure. The crude product was purified by column chromatography on silica using n-hexane/DCM (1:1, v/v) as the eluent, affording the yellow-green solid compound **BBT-Th-3** (88 mg) in 81.1% yield.  $^1\text{H}$  NMR (Chloroform-*d*)  $\delta$ : 7.46 (s, 2H), 7.54 (d,  $J = 8.4$  Hz, 4H), 7.47 (d,  $J = 8.4$  Hz, 4H), 2.78 (d,  $J = 7.1$  Hz, 4H), 1.80–1.76 (m, 2H), 1.39 (s, 18H), 1.32–1.16 (m, 64H), 0.85 (q,  $J = 7.1$  Hz, 12H).  $^{13}\text{C}$  NMR (151 MHz, Chloroform-*d*)  $\delta$ : 151.32, 150.73, 144.91, 138.91, 136.07, 135.50, 131.74, 129.00, 125.43, 113.22, 39.09, 34.67, 33.44, 33.05, 31.92, 31.37, 31.33, 30.06, 29.73, 29.71, 29.67, 29.39, 29.36, 26.48, 22.68, 14.11. HRMS (ESI)  $m/z$ (%):1182.76 . Calcd for  $\text{C}_{74}\text{H}_{110}\text{N}_4\text{S}_4$  ( $m/z$ ) 1182.76.



**Synthesis and Characterization of compound 6.** Under an argon atmosphere, compound **5** (500 mg, 1.14 mmol) was added to a 100 mL Schlenk flask that had been previously dried. Subsequently, pinacol diborane (376 mg, 1.482 mmol, 1.3 eq) and potassium acetate (336 mg, 3.42 mmol, 3 eq) were added, followed by the addition of 10 mL of anhydrous 1,4-dioxane. The mixture was subjected to three cycles of vacuum and nitrogen purging. Bis(diphenylphosphino)ferrocene palladium(II) dichloride (0.228 mmol, 167 mg, 20 mol%) was added to the mixture, which was then heated to 95°C and stirred for 24 hours. After cooling to room temperature, the mixture was poured into water and extracted with petroleum ether. The organic layer was washed with water and brine, dried over magnesium sulfate, and filtered through Celite. The solvent was removed under reduced pressure. Purification by column chromatography using petroleum ether:dichloromethane = 4:1 (v/v) as the eluent afforded compound **6** as a brown viscous liquid (398 mg, 0.822 mmol, 72% yield).  $^1\text{H}$  NMR (Chloroform-*d*)  $\delta$ : 7.71 (d,  $J = 7.9$  Hz, 2H), 7.15 (d,  $J = 7.8$  Hz, 2H), 2.53 (d,  $J = 7.0$  Hz, 2H), 1.63–1.59 (m, 1H), 1.34 (s, 12H), 1.32–1.19 (m, 32H), 0.93–0.83 (m, 6H).

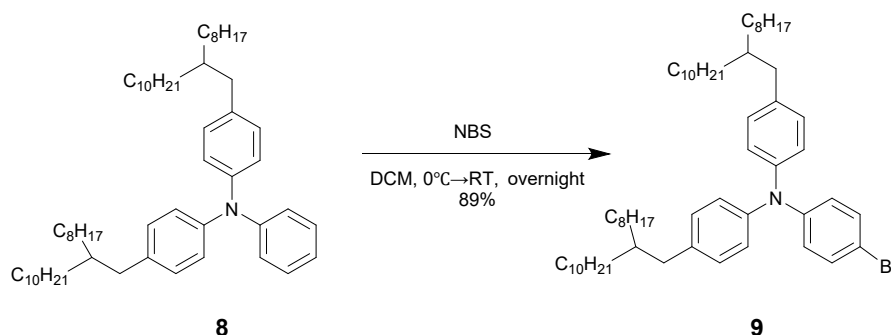


**Synthesis and Characterization of BBT-Ph.** In a 100 mL Schlenk round-bottom flask, 4,7-dibromo-benzo[1,2-c:4,5-c']bis([1,2,5]thiadiazole) **1** (0.66 g, 1.88 mmol), compound **6** (1.8 g, 4.11 mmol, 2.2 eq), potassium carbonate (1.3 g, 9.38 mmol, 5 equiv), and 1,1'-bis(diphenylphosphino)ferrocene palladium(II) dichloride (137 mg, 0.187 mmol, 10 mol%) were added. The resulting mixture was purged with argon for 10 min. Then, 20 mL of 1,4-dioxane and 10 mL of deionized water were added under a nitrogen atmosphere, and the mixture was stirred at 95 °C for 12 hours. After cooling to room temperature, the solvent was removed under reduced pressure. The mixture was filtered through Celite and washed with petroleum ether, followed by concentration under reduced pressure. The crude product was purified by column chromatography using petroleum ether:dichloromethane = 1:1 (v/v) as the eluent. Purification yielded **BBT-Ph** as a purple viscous liquid (1.1 g, 1.21 mmol, 65% yield). <sup>1</sup>H NMR (Chloroform-*d*) δ: 8.16 (d, *J* = 8.2 Hz, 4H), 7.44 (d, *J* = 8.0 Hz, 4H), 2.67 (d, *J* = 7.0 Hz, 4H), 1.80–1.76 (m, 2H), 1.38–1.22 (m, 64H), 0.93–0.88 (m, 12H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ = 152.80, 137.75, 134.58, 131.47, 129.30, 128.69, 39.61, 33.68, 33.23, 31.92, 31.89, 30.05, 29.98, 29.73, 29.69, 29.66, 29.61, 29.37, 29.35, 29.31, 26.60, 26.51, 24.86, 22.69, 14.12. HRMS (ESI) *m/z*(%):907.66 [*M*+*H*]<sup>+</sup>. Calcd for C<sub>58</sub>H<sub>91</sub>N<sub>4</sub>S<sub>2</sub> (*m/z*) 907.66.

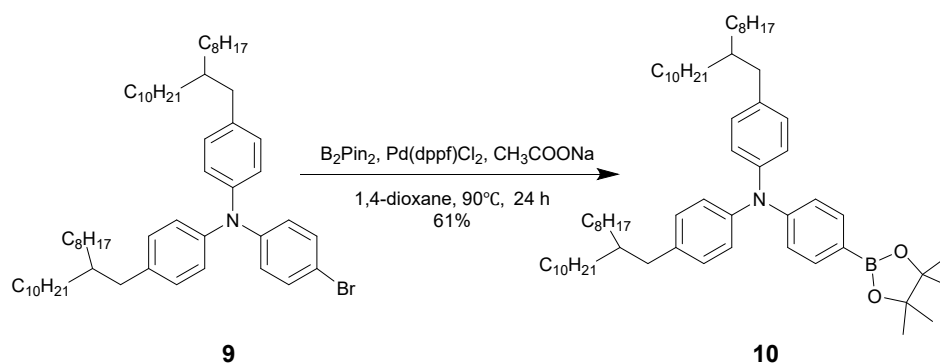


**Synthesis and Characterization of compound 8.** Distilled aniline **7** (0.532 g, 5.715 mmol), compound **5** (6 g, 13.716 mmol, 2.4 eq), Pd<sub>2</sub>dba<sub>3</sub> (0.261 g, 0.285 mmol, 5 mol%), and HP<sup>t</sup>Bu<sub>3</sub>BF<sub>4</sub> (0.23 g, 0.472 mmol, 10 mol%) were dissolved in 30 mL of freshly distilled anhydrous toluene under argon and stirred for 5 min. Subsequently,

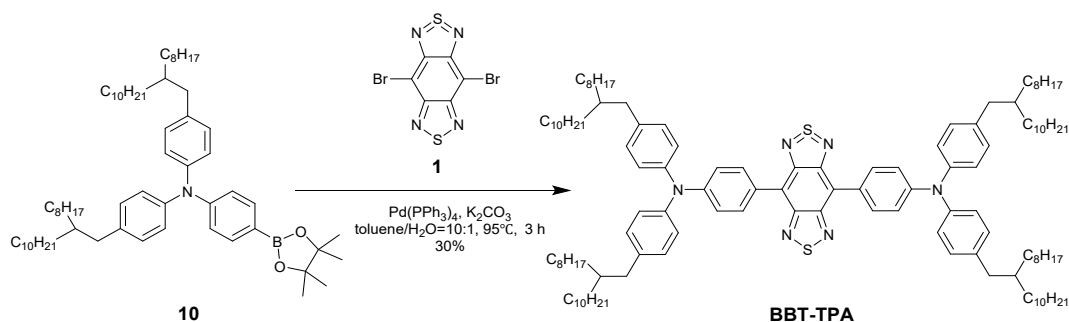
sodium tert-butoxide (1.65 g, 17.15 mmol, 3 eq) was added, and the mixture was stirred under reflux at 110 °C for 24 h. After cooling, the reaction mixture was filtered through Celite and washed with aqueous hydrochloric acid solution, water, and brine. The organic layer was then dried over anhydrous magnesium sulfate, filtered, and concentrated to yield a dark-colored oil. Finally, the crude product was purified by silica gel column chromatography using a mixture of petroleum ether and dichloromethane (volume ratio of 3:1) as the eluent, affording a viscous yellow oil **8** (4.24 g, 5.258 mmol, 92%). <sup>1</sup>H NMR (Chloroform-*d*) δ: 7.23–7.19 (m, 2H), 7.05 (d, *J* = 7.3 Hz, 2H), 7.03–6.97 (m, 8H), 6.94 (t, *J* = 7.3 Hz, 1H), 2.48 (d, *J* = 7.0 Hz, 4H), 1.64–1.54 (m, 2H), 1.34–1.20 (m, 64H), 0.93–0.85 (m, 12H).



**Synthesis and Characterization of compound 9.** Compound **8** (4.24 g, 5.258 mmol) was dissolved in 20 mL of dry dichloromethane and cooled to 0 °C in an ice-water bath. N-Bromosuccinimide (0.842 g, 4.72 mmol, 0.9 eq) was added in two portions, and the solution was stirred overnight in the dark, slowly warming to room temperature. The mixture was filtered through Celite and concentrated to yield a brown oily residue with precipitates. The mixture was purified by column chromatography using petroleum ether:dichloromethane = 2:1 (v/v) as the eluent, affording **compound 9** as a pale yellow oil (4.143 g, 4.680 mmol, 89% yield). <sup>1</sup>H NMR (Chloroform-*d*) δ: 7.28 (d, *J* = 8.9 Hz, 2H), 7.02 (d, *J* = 8.3 Hz, 4H), 6.97 (d, *J* = 8.3 Hz, 4H), 6.90 (d, *J* = 8.8 Hz, 2H), 2.47 (d, *J* = 7.0 Hz, 4H), 1.61–1.55 (m, 2H), 1.36–1.18 (m, 64H), 0.88 (td, *J* = 7.0, 1.6 Hz, 12H).



**Synthesis and Characterization of compound 10.** To a 100 mL Schlenk flask containing 15 mL of freshly distilled anhydrous 1,4-dioxane, **compound 9** (4 g, 4.518 mmol), pinacol diborane (1.49 g, 5.873 mmol, 1.3 eq), and potassium acetate (1.33 g, 13.554 mmol, 3 eq) were added. The flask was evacuated and purged with nitrogen three times, and then the catalyst 1,1'-bis(diphenylphosphino)ferrocene palladium(II) dichloride (0.33 g, 0.4518 mmol, 10 mol%) was added. The mixture was heated to 90 °C and stirred for 24 hours. After cooling to room temperature, the mixture was poured into water and extracted with petroleum ether. The organic layer was washed with water and brine, dried over magnesium sulfate, filtered through Celite, and concentrated under reduced pressure. The mixture was purified by column chromatography using petroleum ether:dichloromethane = 2:1 (v/v) as the eluent, affording **compound 10** as a colorless viscous liquid (2.530 g, 2.756 mmol, 61% yield). <sup>1</sup>H NMR (Chloroform-*d*) δ: 7.63 (d, *J* = 8.4 Hz, 2H), 7.04–6.95 (m, 10H), 2.48 (d, *J* = 7.0 Hz, 4H), 1.65–1.54 (m, 2H), 1.32 (s, 12H), 1.31–1.21 (m, 64H), 0.88 (td, *J* = 7.0, 2.5 Hz, 12H).



**Synthesis and Characterization of BBT-TPA.** In a 100 mL single-neck round-bottom flask, 4,7-dibromo-benzo[1,2-c:4,5-c']bis([1,2,5]thiadiazole) **1** (352 mg, 1.0 mmol), **compound 10** (2.8 g, 3 mmol), and Pd(PPh<sub>3</sub>)<sub>4</sub> (115.5 mg, 0.1 mmol) were added. The flask was evacuated and purged with argon three times. Toluene:water = 20 mL:2 mL was added sequentially using a syringe. The reaction mixture was stirred

at 95 °C for 3 h. After cooling to room temperature, the solvent was removed under reduced pressure, and the residue was added to methanol. The solid was filtered and dissolved in 1,2-dichloromethane, followed by concentration under reduced pressure. The crude product was purified by column chromatography using a mixture of petroleum ether and dichloromethane (volume ratio of 4:1) as the eluent, affording compound BBT-TPA as a cyan solid (580 mg, 0.3 mmol, 30% yield). <sup>1</sup>H NMR (Chloroform-*d*) δ: 8.17 (d, *J* = 8.4 Hz, 4H), 7.22 (d, *J* = 8.5 Hz, 4H), 7.16 (d, *J* = 8.0 Hz, 8H), 7.09 (d, *J* = 8.0 Hz, 8H), 2.51 (d, *J* = 7.0 Hz, 8H), 1.65–1.59 (m, 4H), 1.36–1.20 (m, 128H), 0.87 (q, *J* = 6.8 Hz, 24H). <sup>13</sup>C NMR (151 MHz, Chloroform-*d*) δ: 152.75, 148.77, 144.66, 137.56, 132.58, 130.10, 129.94, 125.41, 120.47, 120.07, 40.12, 39.65, 37.09, 33.26, 31.92, 30.05, 30.03, 30.00, 29.97, 29.72, 29.70, 29.66, 29.62, 29.40, 29.36, 29.33, 29.31, 27.97, 26.60, 26.57, 24.83, 22.69, 14.12. HRMS (APCI) *m/z*(%): 1803.44 [M+H]<sup>+</sup>. Calcd for C<sub>122</sub>H<sub>189</sub>N<sub>6</sub>S<sub>2</sub> (*m/z*) 1803.44.

# $^1\text{H}/^{13}\text{C}$ NMR and HR mass spectra

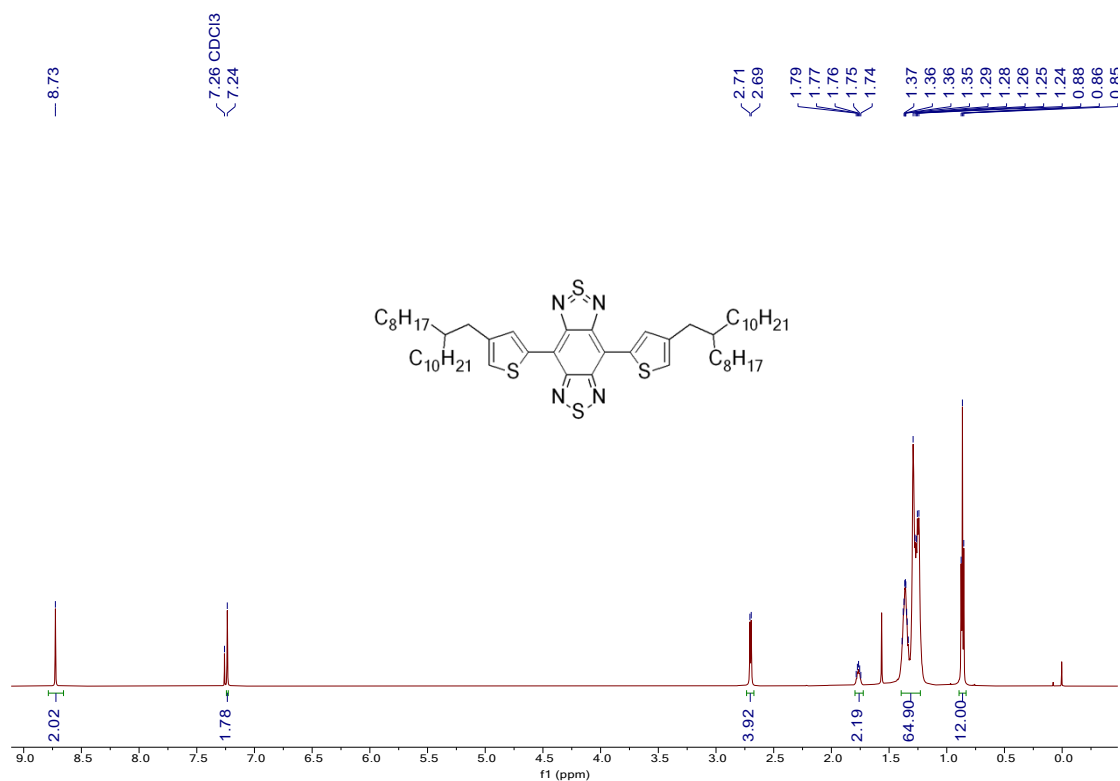


Figure S4.  $^1\text{H}$  NMR spectrum of BBT-Th-1.

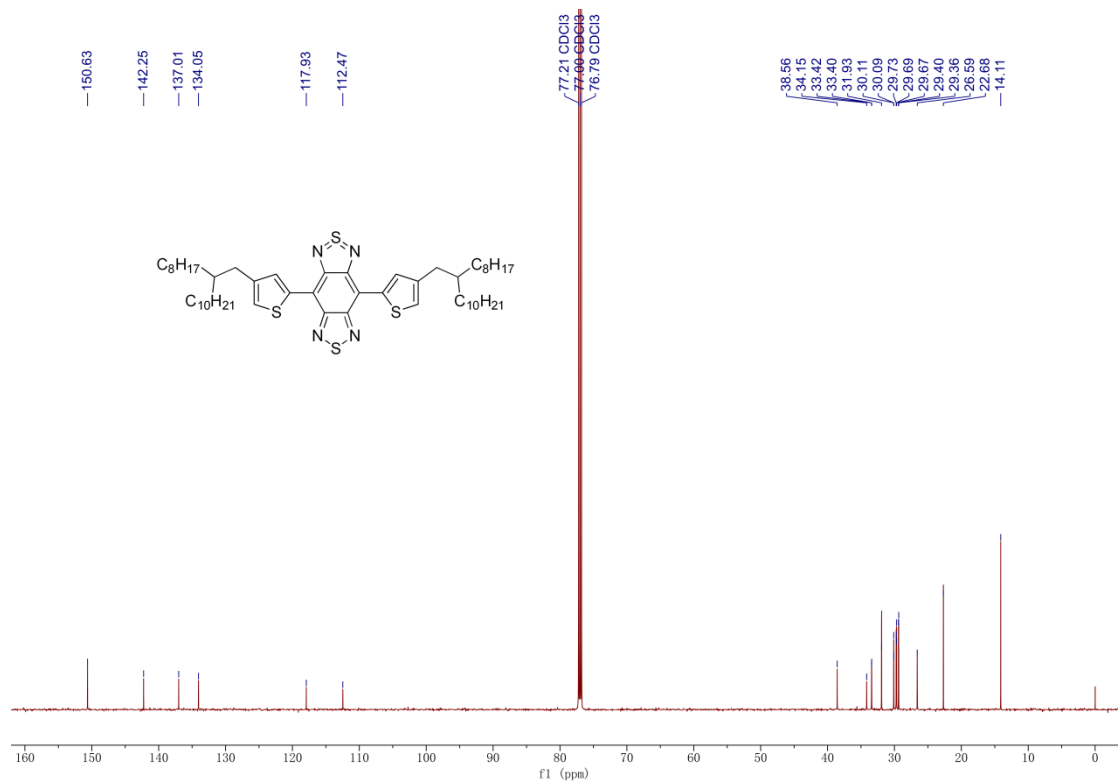


Figure S5.  $^{13}\text{C}$  NMR spectrum of BBT-Th-1.





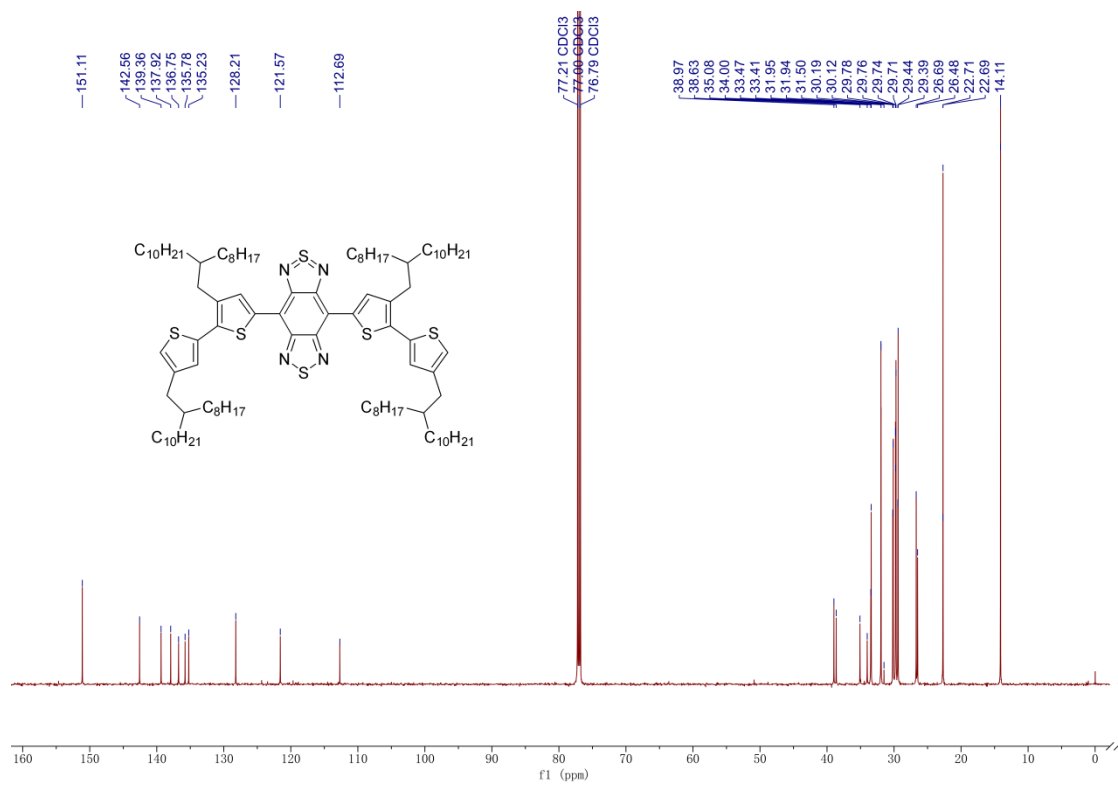


Figure S8. <sup>13</sup>C NMR spectrum of BBT-Th-2.

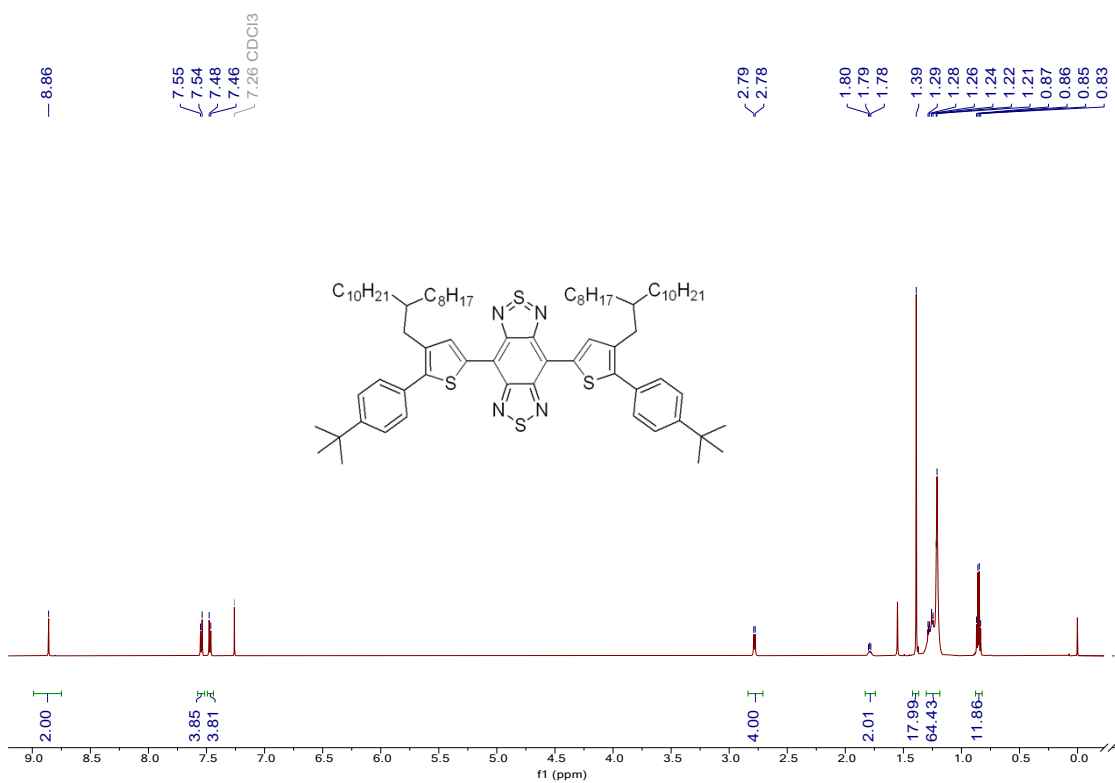


Figure S9. <sup>1</sup>H NMR spectrum of BBT-Th-3.

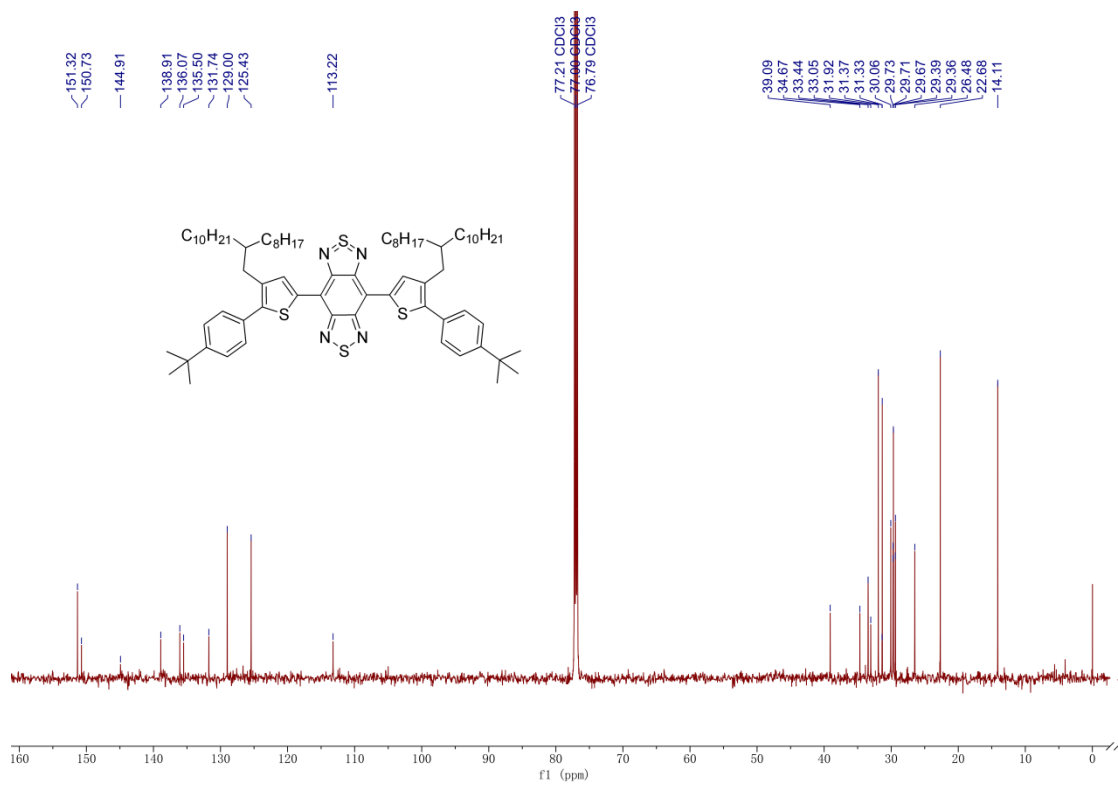


Figure S10.  $^{13}C$  NMR spectrum of BBT-Th-3.

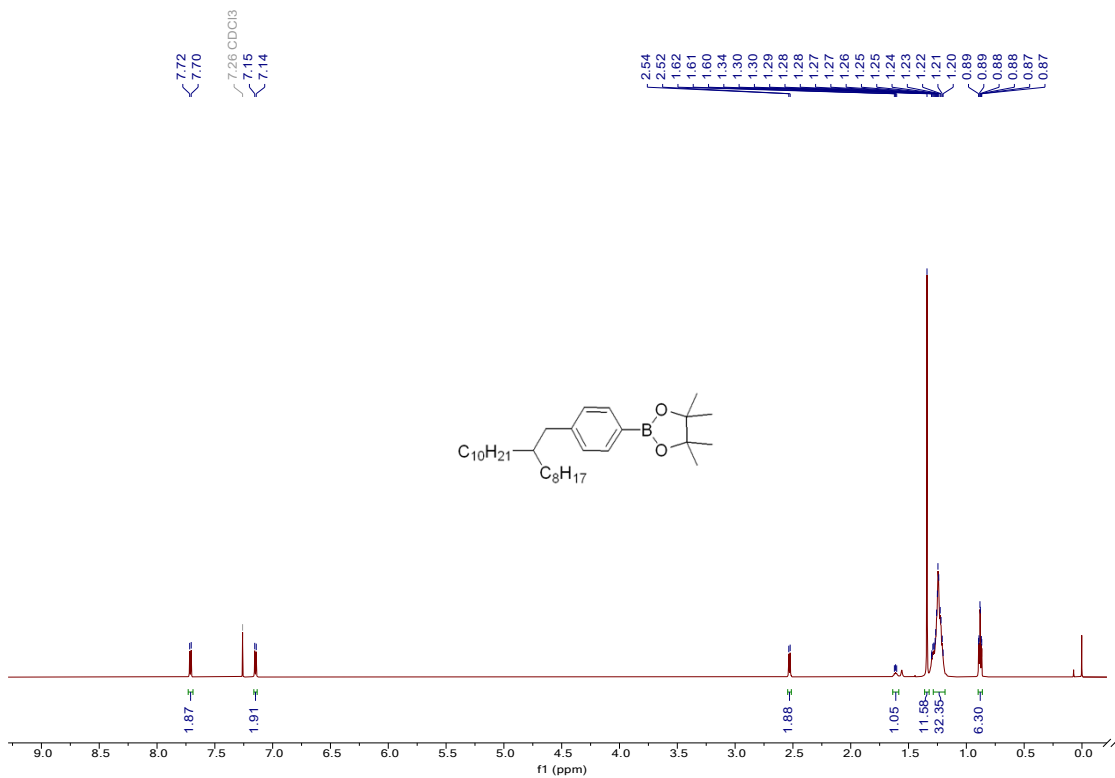


Figure S11.  $^1H$  NMR spectrum of compound 6.

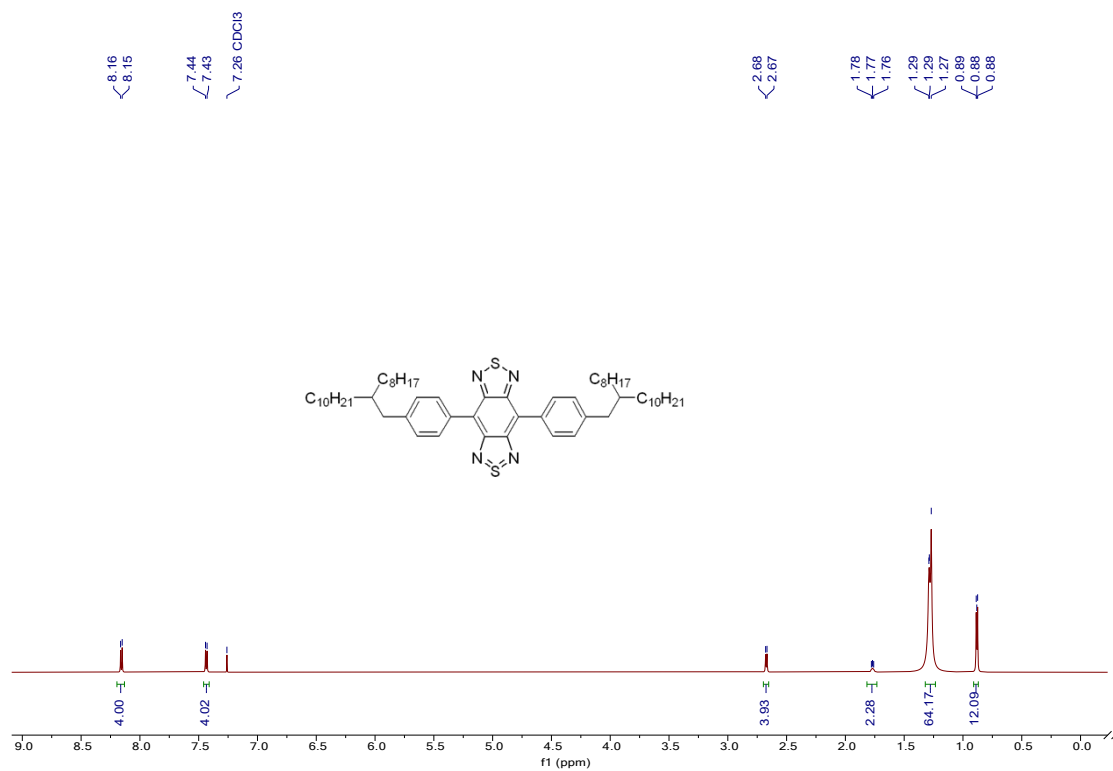


Figure S12. <sup>1</sup>H NMR spectrum of BBT-Ph.

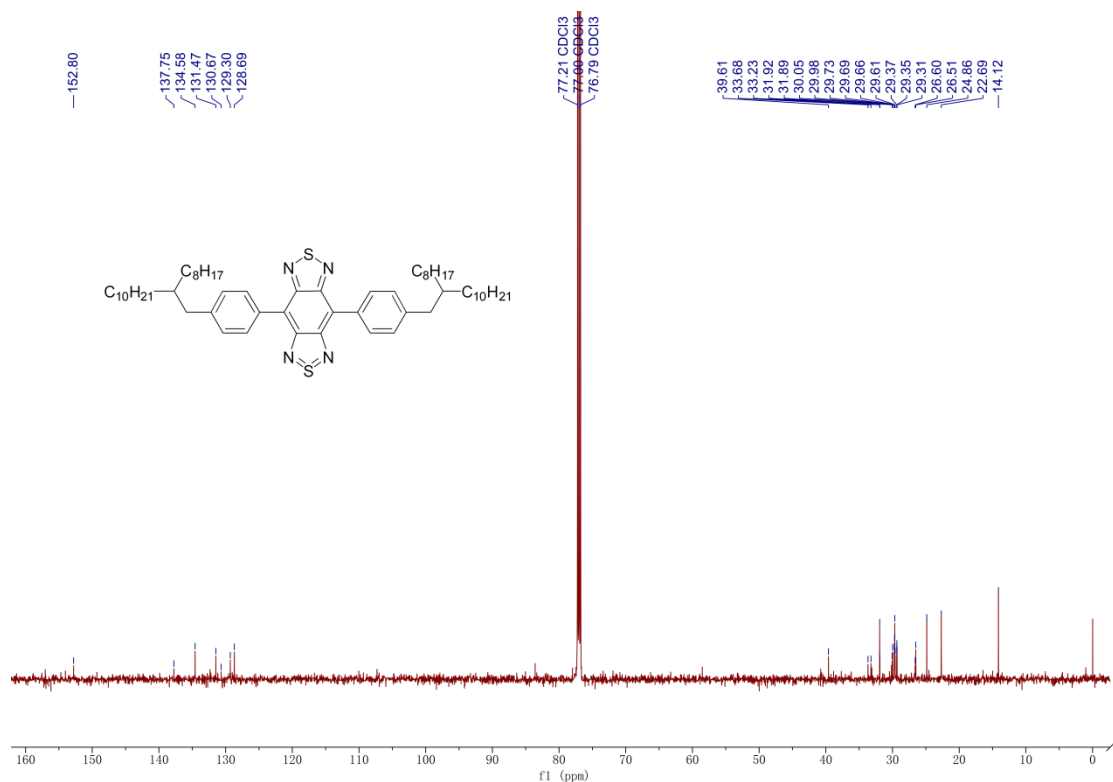


Figure S13. <sup>13</sup>C NMR spectrum of BBT-Ph.



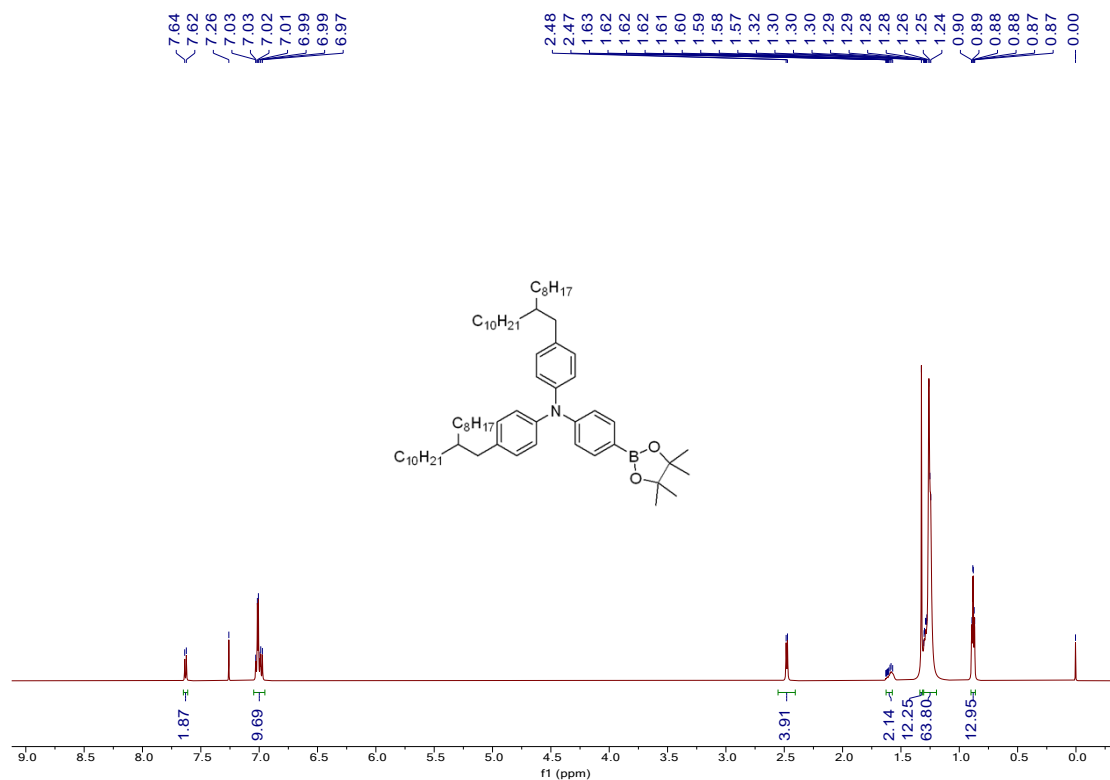


Figure S16. <sup>1</sup>H NMR spectrum of compound 10.

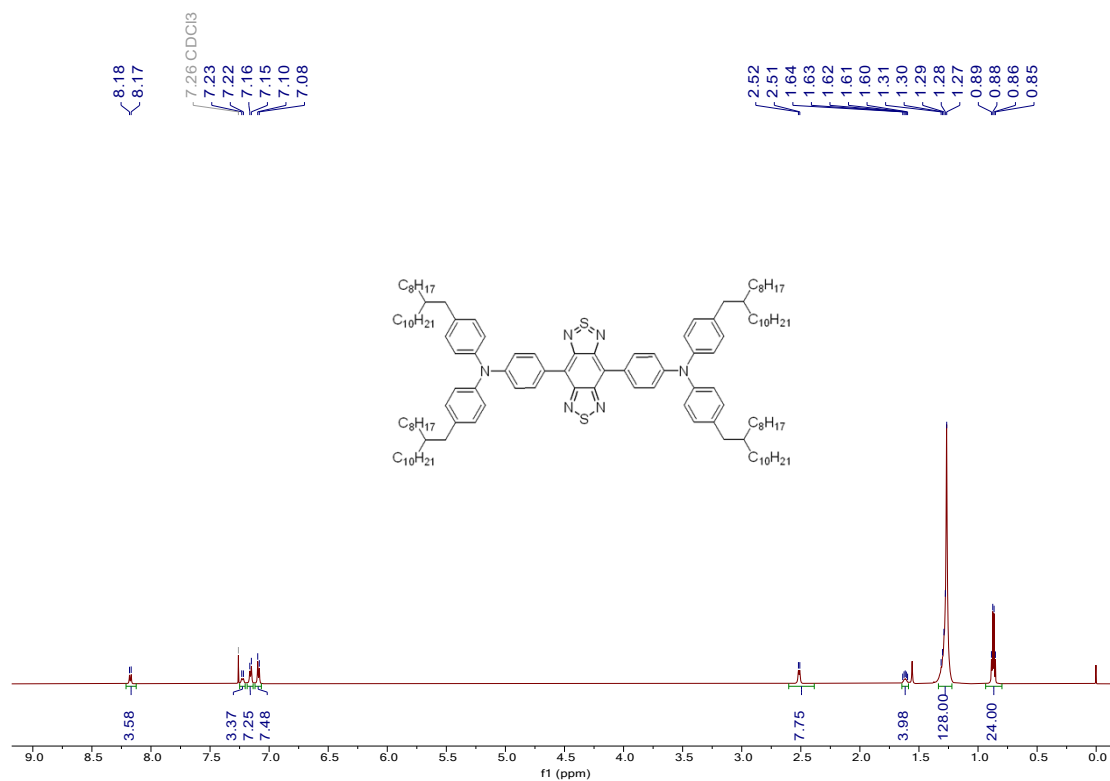


Figure S17. <sup>1</sup>H NMR spectrum of BBT-TPA.

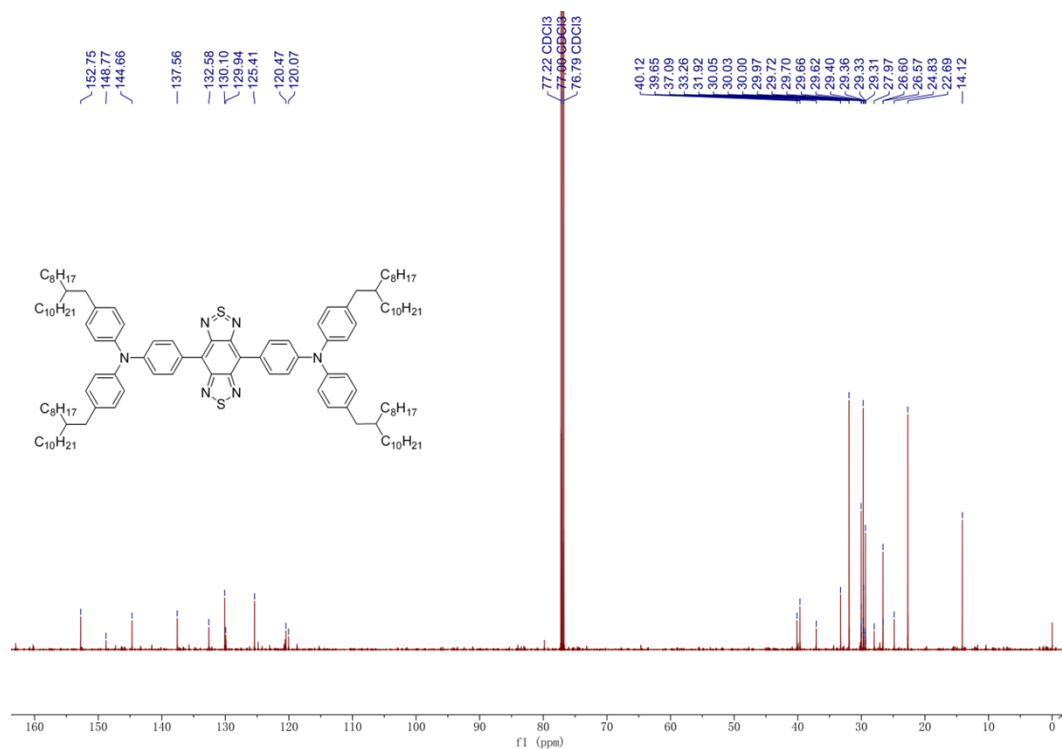


Figure S18. <sup>13</sup>C NMR spectrum of BBT-TPA.

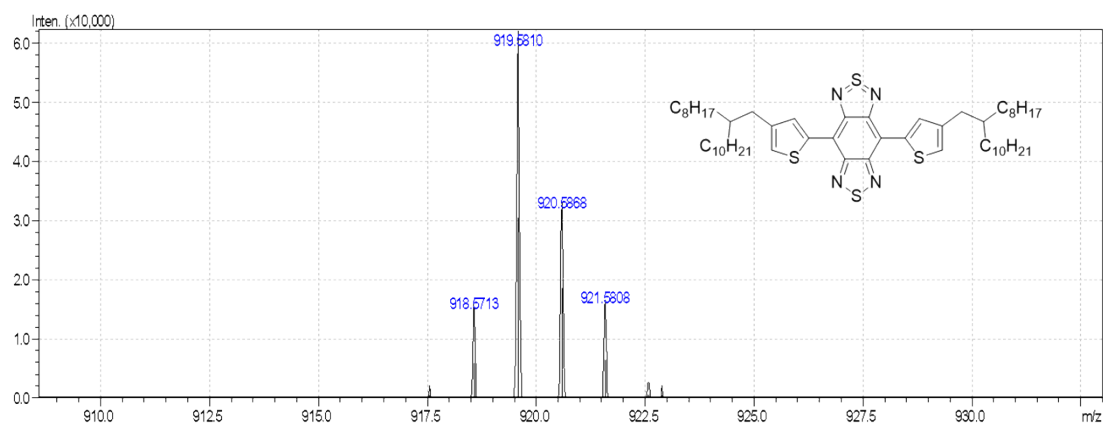


Figure S19. HRMS spectrum of BBT-Th-1.

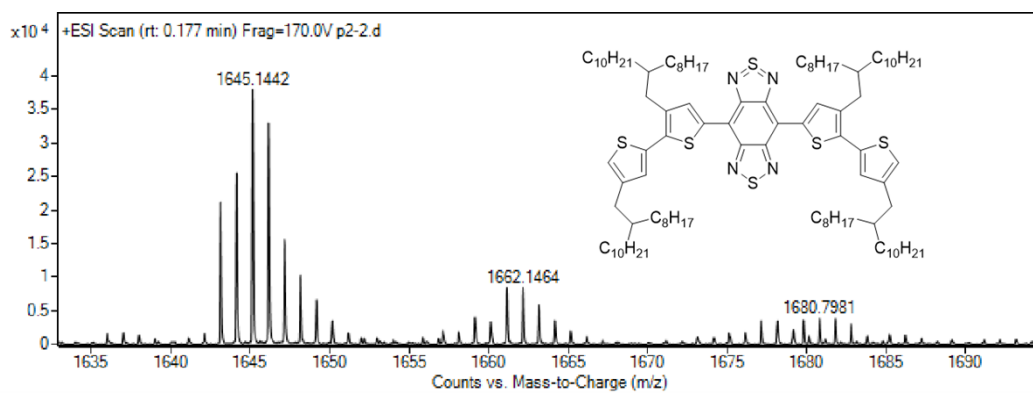
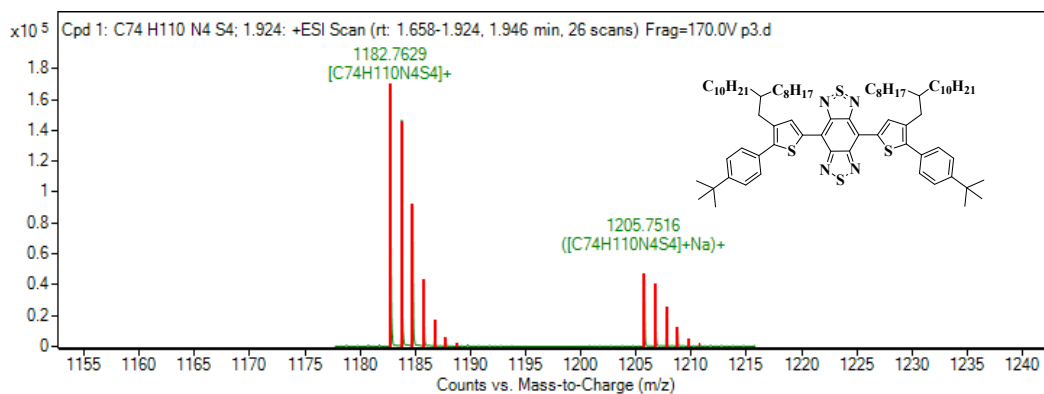
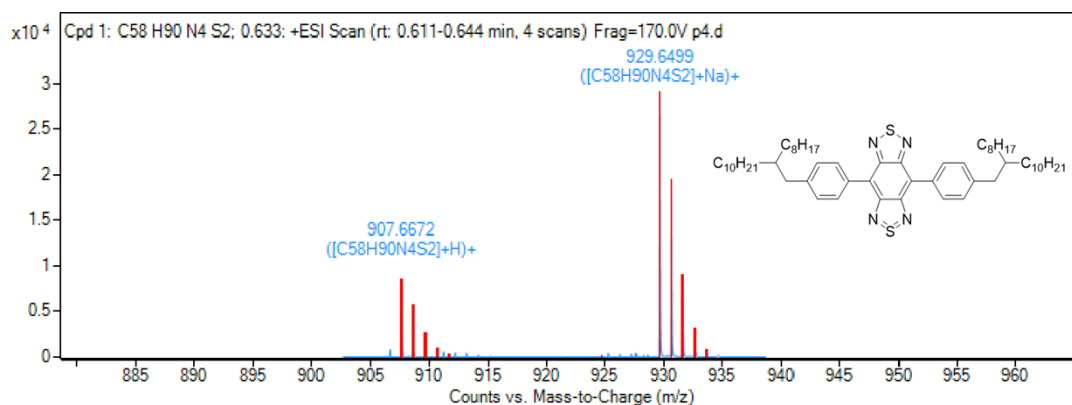


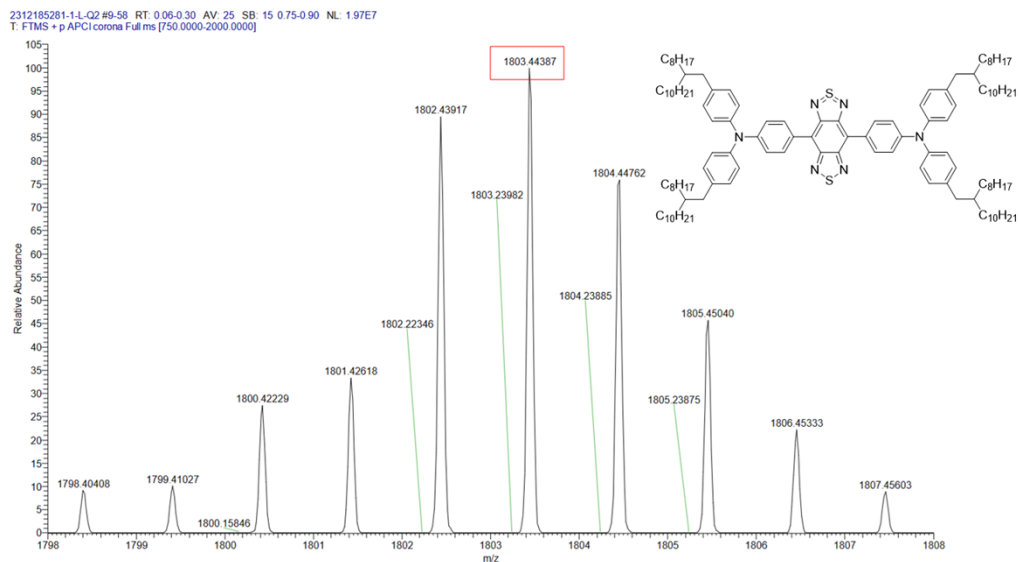
Figure S20. HRMS spectrum of BBT-Th-2.



**Figure S21. HRMS spectrum of BBT-Th-3.**



**Figure S22. HRMS spectrum of BBT-Ph.**



**Figure S23. HRMS spectrum of BBT-TPA.**

**Table S1. Calculated absorption wavelength  $\lambda$  (nm), main configuration and oscillator strength (f) for the studied compounds at the SMD-TD-M06-2X/ 6-31G(d) level.**

Molecules	State	$\lambda$ (nm)	$f_a$	Major contribs
BBT-Th-1	$S_0>S_1$	762	0.425	HOMO->LUMO (1.00)
	$S_0>S_2$	391	0	H-1->LUMO (0.98)
	$S_0>S_3$	377	0.002	H-2->LUMO (0.98)
	$S_0>S_4$	361	0	H-3->LUMO (0.97)
	$S_0>S_5$	342	0.002	HOMO->L+1 (0.97)
	$S_0>S_6$	318	0.437	H-5->LUMO (0.91)
	$S_0>S_7$	312	0.115	H-4->LUMO (0.95)
	$S_0>S_8$	303	0	H-6 -> L (0.75)
	$S_0>S_9$	297	0.642	HOMO->L+2 (0.94)
BBT-Th-2	$S_0>S_1$	873	0.655	HOMO->LUMO (1.00)
	$S_0>S_2$	485	0.021	H-1->LUMO (0.97)
	$S_0>S_3$	383	0.271	H-2->LUMO (0.86)
	$S_0>S_4$	372	0.068	H-3->LUMO (0.72)
	$S_0>S_5$	369	0.000	H-4->LUMO (0.88)
	$S_0>S_6$	364	0.192	HOMO->L+1 (0.37)
				HOMO->L+2 (0.31)
	$S_0>S_7$	358	0.607	HOMO->L+2 (0.54)
			HOMO->L+1 (0.38)	
BBT-Th-3	$S_0>S_1$	810	0.586	HOMO->LUMO (1.00)
	$S_0>S_2$	437	0.014	H-1->LUMO (0.95)
	$S_0>S_3$	376	0.017	H-3->LUMO (0.64)
				H-2->LUMO (0.31)
	$S_0>S_4$	373	0.000	H-4->LUMO (0.97)
$S_0>S_5$	355	0.135	H-2->LUMO (0.52)	



				H-3->LUMO (0.19)
	S <sub>0</sub> >S <sub>6</sub>	355	0.105	HOMO->L+1 (0.75)
	S <sub>0</sub> >S <sub>7</sub>	328	0.973	HOMO->L+2 (0.85)
BBT-Ph	S <sub>0</sub> >S <sub>1</sub>	606	0.401	HOMO->LUMO (1.00)
	S <sub>0</sub> >S <sub>2</sub>	354	0.000	H-1->LUMO (0.93)
	S <sub>0</sub> >S <sub>3</sub>	332	0.000	H-2->LUMO (0.90)
	S <sub>0</sub> >S <sub>4</sub>	324	0.003	H-3->LUMO (0.94)
	S <sub>0</sub> >S <sub>5</sub>	316	316	H-5->LUMO (0.93)
	S <sub>0</sub> >S <sub>6</sub>	314	0.001	HOMO->L+1 (0.93)
	S <sub>0</sub> >S <sub>7</sub>	313	0.074	H-4->LUMO (0.96)
	S <sub>0</sub> >S <sub>8</sub>	288	0	H-6 -> L (0.66)
				H-8 -> L+1 (0.14)
	S <sub>0</sub> >S <sub>9</sub>	283	0.006	H-8 ->L (0.67)
				H-6 ->L+1 (0.13)
	S <sub>0</sub> >S <sub>10</sub>	271	0.727	HOMO->L+2(0.96)
BBT-TPA	S <sub>0</sub> >S <sub>1</sub>	763	0.7221	HOMO->LUMO (0.95)
	S <sub>0</sub> >S <sub>2</sub>	516	0.000	H-1->LUMO (0.97)
	S <sub>0</sub> >S <sub>3</sub>	425	0.039	H-2->LUMO (0.91)
	S <sub>0</sub> >S <sub>4</sub>	341	0.000	HOMO->L+1 (0.79)
	S <sub>0</sub> >S <sub>5</sub>	324	0.000	H-3->LUMO (0.38)
				H-7 ->L (0.25)
	S <sub>0</sub> >S <sub>6</sub>	319	0.107	H-4->LUMO (0.28)
				H-13->L (0.24)
	S <sub>0</sub> >S <sub>7</sub>	316	1.433	HOMO->L+2 (0.82)

$f_a$  oscillator strength.

**Table S2. Table of calculated and experimental maximum absorption peak wavelengths for the investigated BBT series molecules**

	BBT-Th-1	BBT-Th-2	BBT-Th-3	BBT-Ph	BBT-TPA
$\lambda_{\max}^{\text{cal.}}$ (nm) <sup>a</sup>	762	873	810	606	763
$\lambda_{\max}^{\text{exp.}}$ (nm) <sup>b</sup>	756	852	824	597	745

<sup>a</sup> Excited state spectral data calculated at the TD-M06-2X/6-31G\* level of theory.

<sup>b</sup> UV-vis-NIR spectrum of the studied molecules in n-hexane at  $3 \times 10^{-5}$  mol·L<sup>-1</sup>.

**Table S3. Comparison table of performance between dyes in this study and other dyes.**

Dyes	Anthraquinone <sup>65</sup>	Azo dyes with benzene rings <sup>66</sup>	Azopyrazolones <sup>67</sup>	Metal complex	Perylene <sup>68,69</sup>	This study
Color	Blue, purple, and magenta	Yellow, Red, Magenta, Purple, Blue	yellow	Purple	Yellow, orange, red, magenta, green	Purple, blue, cyan
Molar absorptivity (L·mol <sup>-1</sup> ·cm <sup>-1</sup> )	1.5×10 <sup>4</sup>	1000–9950	1.6×10 <sup>4</sup> –2.7×10 <sup>4</sup>	1×10 <sup>5</sup>	0.4×10 <sup>4</sup> –5×10 <sup>4</sup>	0.66×10 <sup>4</sup> –3×10 <sup>4</sup>
Solubility in decane	0.14–0.22 mol/L	1%–10%	0.06–0.87 mol/L	5%–10%	2.8%–17%	3%–30%
FoM (cm <sup>-1</sup> )	317–3406	100–1000	31320	-	1000–5000	327–3250
Driving voltage (V)	-	32	24	-	24	8
Aperture ratio (%)	-	68.5%–75.0%	68.5%	-	56%–60%	62%–67.4%
Threshold Voltage		DC 40V	DC 40V		DC 30V	DC 18V
Response speed (ms)	-	81	18	200	20	91
Photostability (%)	28.5	1-23.9	3.2-16.3	-	1.4-4.25	5.1-32.8

**Table S4. The table of data related to the solubility, molar absorption coefficient, and photostability of the series of compounds in this study.**

	BBT-Th-1	BBT-Th-2	BBT-Th-3	BBT-Ph	BBT-TPA
Solubility in decane (w/w, %)	3	13.5	27	28	30
$\lambda_{\max}$ (nm)	756	852	824	597	748
$\epsilon$ (L·mol <sup>-1</sup> ·cm <sup>-1</sup> )	22467	31833	22300	6604	26300
Photostability (%)	–	5.1	7.4	32.8	100

