Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Novel organoboron compounds derived from thieno[3,2-*b*]thiophene and triphenylamine units for OLED devices†

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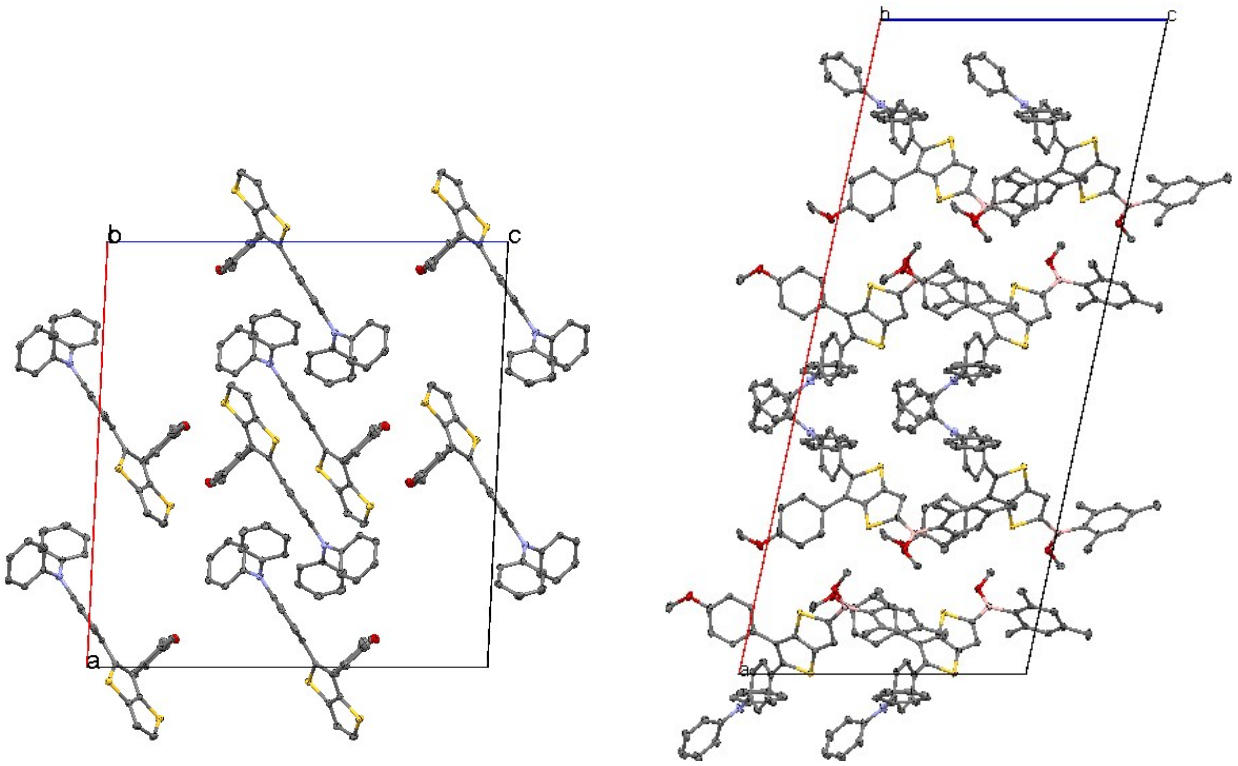
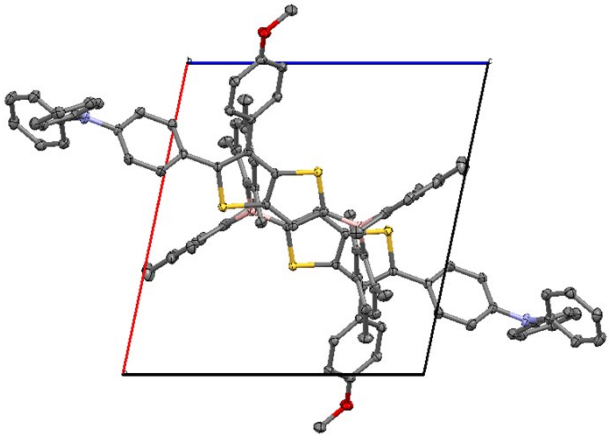
Supporting Information

X-Ray Analysis



4 **6**



7

Figure S1. Crystal packing of compounds **4**, **6** and **7**. Thermal ellipsoids are shown at the 50% probability level, and H atoms are omitted for clarity. For the compounds **4**, **6** and **7** (CCDC 1059468 1059475 and 1059578, respectively) crystallographic data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif. [Fax: int code +44(1223) 336-033; e-mail: deposit@ccdc.cam.ac.uk].

Table S1. Summary of crystal data and structure refinement details for compounds **4**, **6** and **7**.

	4	**6**	**7**
Empirical formula	$C_{31}H_{23}NOS_2$	$C_{41}H_{36}BNO_2S_2$	$C_{49}H_{44}BNOS_2$
Formula weight (g/mol)	489.62	649.67	737.78
T(K)	100	100	100
λ(Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	P 1 21/c 1	C 1 c 1	P -1
a [Å]	23.4920(15)	37.895(11)	12.7147(6)
b [Å],	9.2655(5)	11.540(3)	13.4286(6)
c [Å]	22.1072(12)	16.393(5)	13.6609(6)
α [deg, º]	90	90	118.723(2)
β [deg,º]	92.766(4)	102.316(9)	97.870(2)
γ [deg,º]	90	90	94.810(2)
V [$Å^3$]	4806.4(5)	7004.(3)	1995.91(16)
Z	8	4	2
μ (mm^{-1})	0.247	0.188	0.172
ρ (g cm^{-3})	1.353	1.232	1.228
F (000)	2048	2736	780
Crystal size (mm)	0.07x0.24x0.3	0.05x0.1x0.2	0.08x0.2x0.4
θ range for data collection (º)	2.36 to 25.09	2.31 to 26.40	2.36 to 29.64
Index ranges	-27≤h≤27	-47≤h≤47	-17≤h≤17
	-11≤k≤11	-14≤k≤14	-18≤k≤18
	-26≤l≤26	-20≤l≤20	-18≤l≤18
Reflections collected	33365	106067	67373
Independent reflections	4231	14161	11217
Coverage of independent ref.	99.2%	99.8%	99.5%
Data/parameters	4231/318	14161/857	11217/494
Max. and min. transmission	0.983/0.929	1/0.933	1/0.954
R1, wR2 [$I \geq 2\sigma(I)$]	0.0323	0.0354	0.0407
	0.0840	0.0792	0.1062
R1, wR2 (all data)	0.0360	0.0410	0.0524
	0.0878	0.0817	0.1158
GOF on F^2	1.026	0.999	1.001
Δρmax, Δρmin (e $Å^{-3}$)	0.260/-0.211	0.762/-0.192	0.461/-0.281

UV-Vis and Fluorescence Spectra

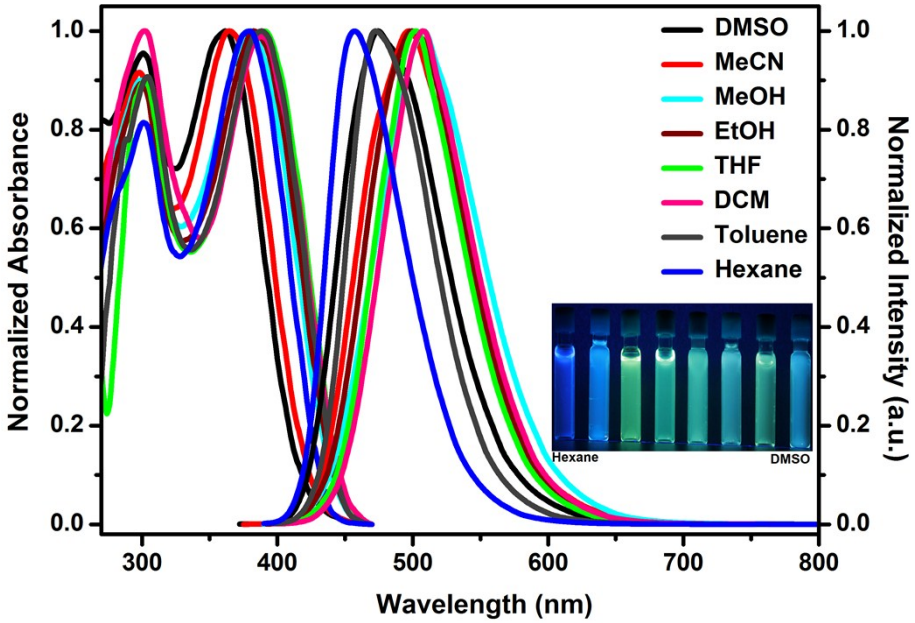


Figure S2. UV-Vis absorption and emission spectra of **6** in different solvents. Inset: Photograph of **6** in solvents exposed to a UV lamp (λ_{ex} = 365 nm).

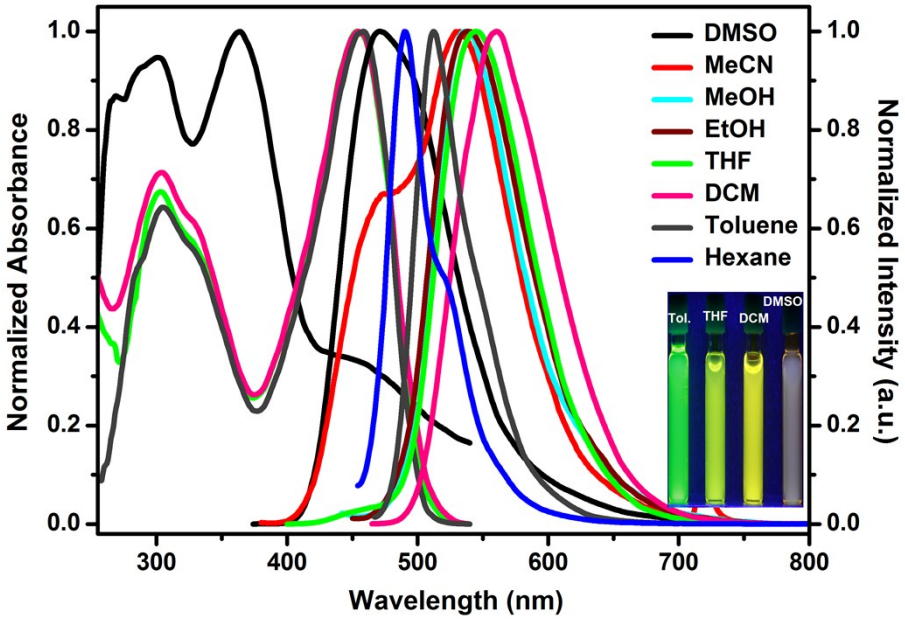
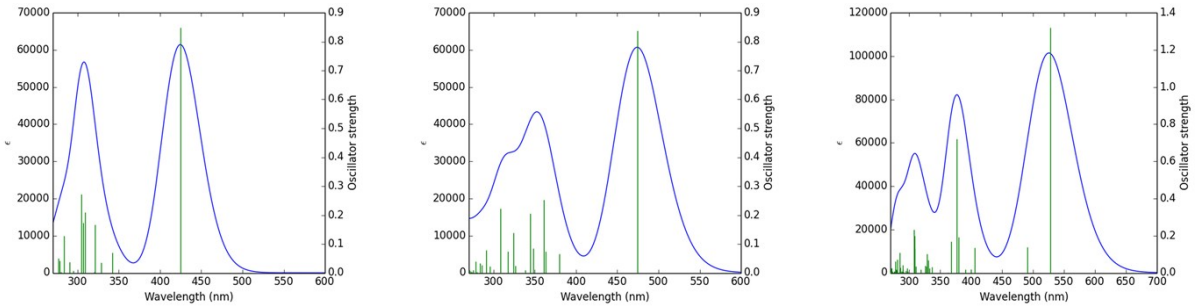


Figure S3. UV-Vis absorption and emission spectra of 8 in different solvents. Inset: Photograph of **8** in solvents exposed to a UV lamp (λ_{ex} = 365 nm).

Table S2. UV-Vis absorption and emission λ_{max} values of **6** − **8** in a variety of solvents.

Solvents	λ_{abs} (nm)			λ_{em} (nm)		
	6	**7**	**8**	**6**	**7**	**8**
DMSO	361	412	364	474	562	472
ACN	364	404	-	497	556	531
MeOH	381	404	-	498	534	536
EtOH	383	404	444	507	517	537
THF	391	411	454	502	520	545
DCM	388	411	455	508	528	560
Toluene	388	414	459	473	493	512
n-Hexane	380	404	-	456	467	490

Computation

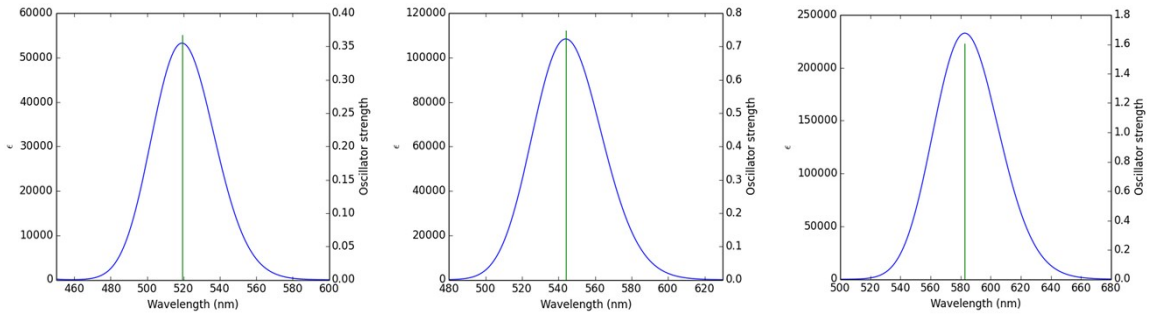


6 **7** **8**

Figure S4. Predicted UV-Vis absorption spectra of **6** − **8** at TD-B3LYP/6-31G(d)/(PCM:THF) level.

Table S3. Excited state electronic transitions derived from TD-B3LYP/6-31G(d)/(PCM:THF) level computations (H: HOMO, L: LUMO).

Comp.	States	Absorption (nm)	Energy (eV)	Oscillator strength (*F*)	Major contribution (%)	Exp. (nm)
	S_1	425	2.92	0.847	H → L (98%)	390
6	S_6	309	4.01	0.209	H → L+3 (95%)	301
	S_8	304	4.07	0.272	H-4 → L (52%), H-3 → L (38%)	292
	S_1	474	2.61	0.838	H → L (98%)	411
7	S_4	361	3.43	0.252	H-2 → L (90%)	332
	S_{11}	309	4.02	0.223	H → L+3 (95%)	305
	S_1	528	2.35	1.321	H → L (97%)	454
8	S_7	376	3.29	0.722	H-4 → L (78%)	328
	S_{20}	308	4.03	0.231	H-3 → L+1 (82%)	303



6 **7** **8**

Figure S5. Predicted emission spectra of **6** − **8** at TD-B3LYP/6-31G(d)/(PCM:THF) level.

Device Results

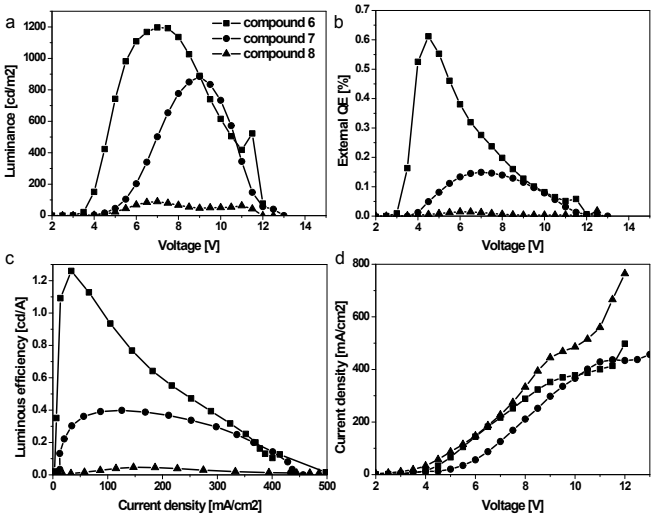


Figure S6. a) Luminance–voltage b) external quantum efficiency (EQE)–current density c) luminous efficiency–current density and d) current density–voltage characteristics of the OLEDs fabricated from compound **6**–**8**.

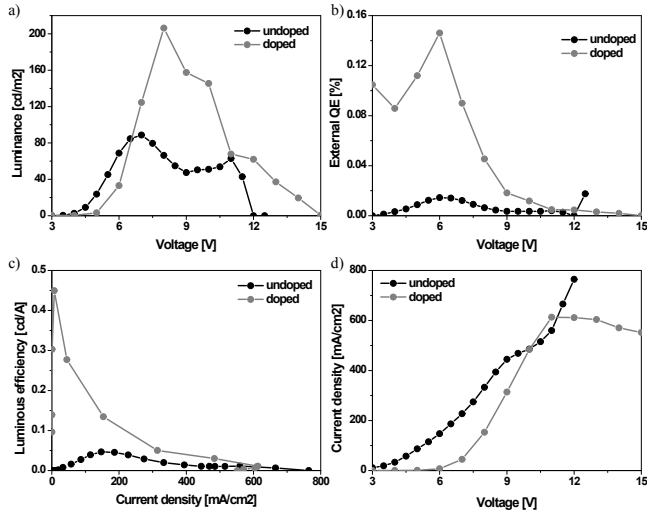


Figure S7. a) Luminance–voltage b) external quantum efficiency (EQE)–current density c) luminous efficiency–current density and d) current density–voltage characteristics of the OLED fabricated from compound **8** doped with compound **7**.

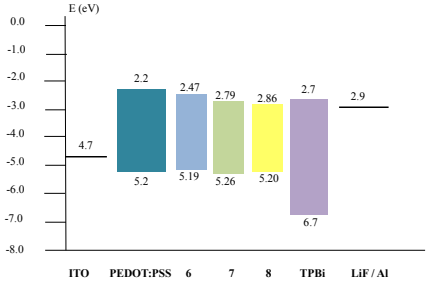


Figure S8. Energy levels of the OLED device layers.

MS and HRMS Spectra

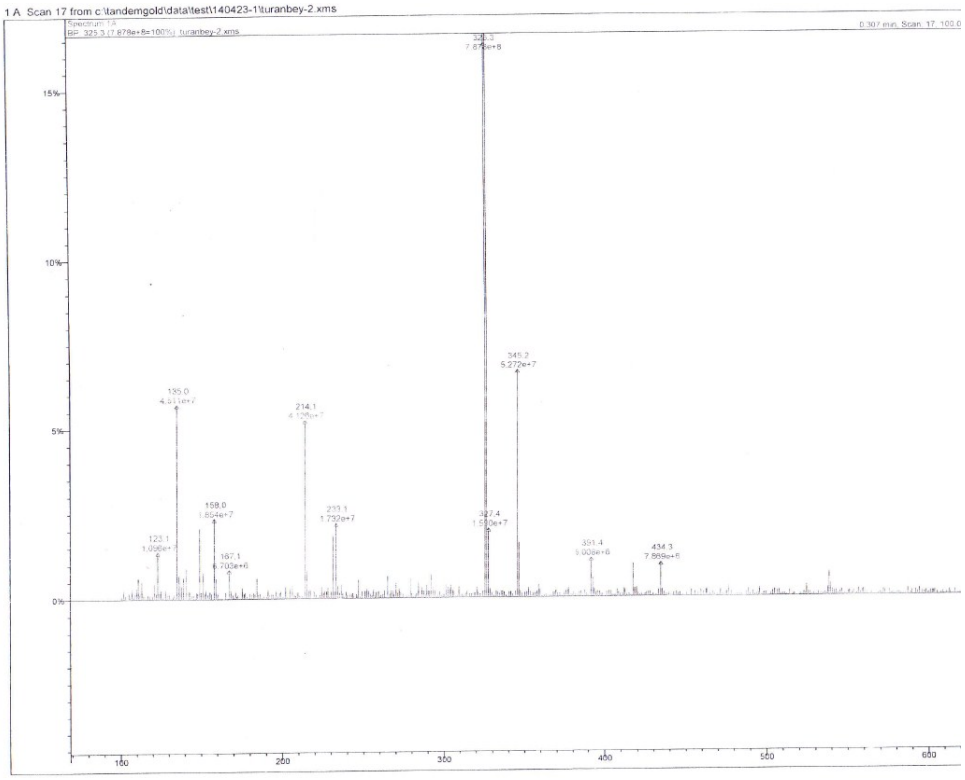


Figure S9. MS spectrum of compound **2**.

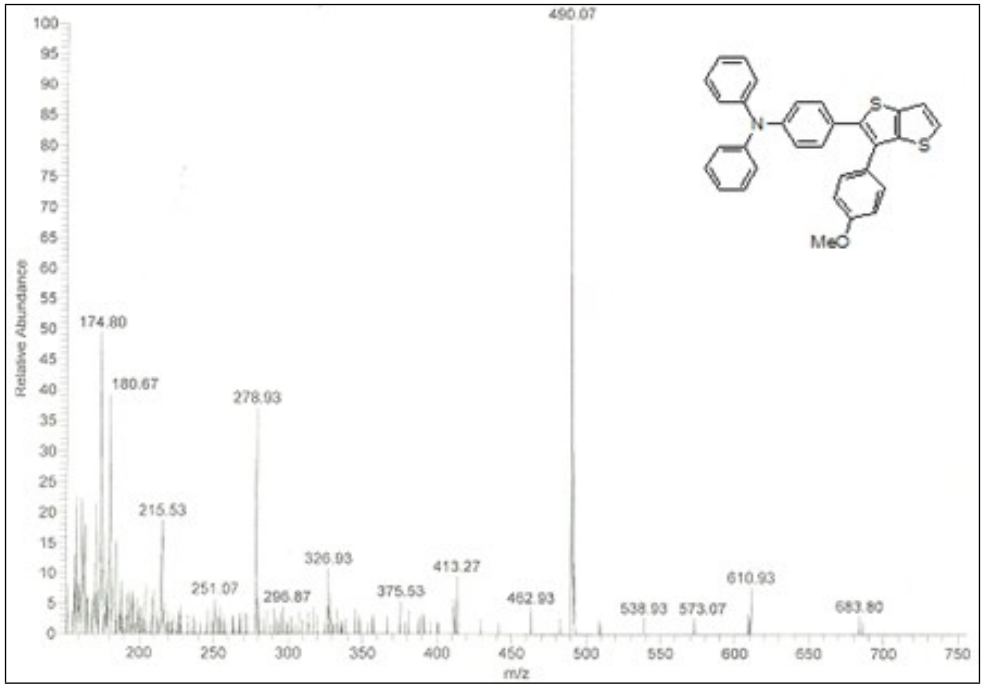


Figure S10. MS spectrum of compound **4**.

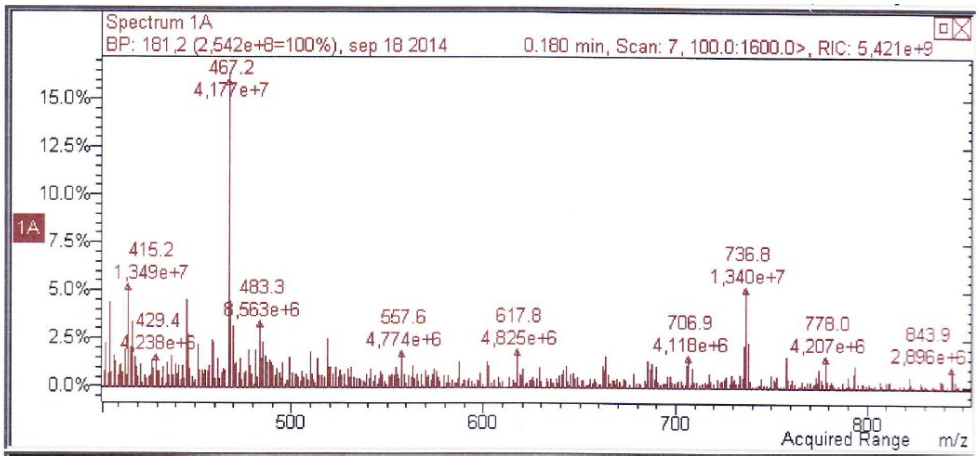


Figure S11. MS spectrum of compound **6**.

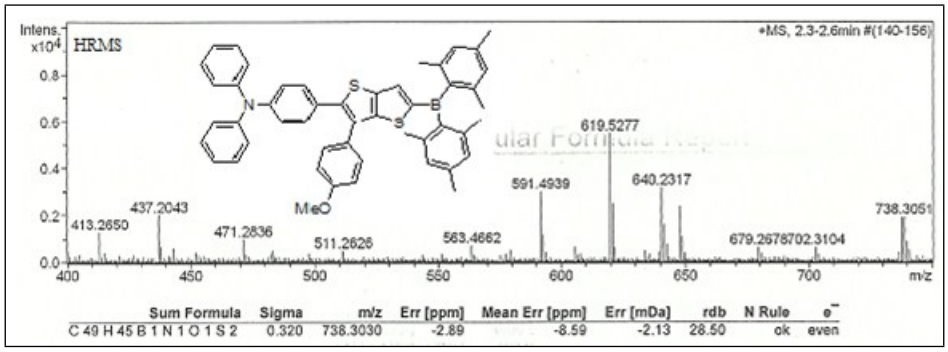


Figure S12. HRMS spectrum of compound **7**.

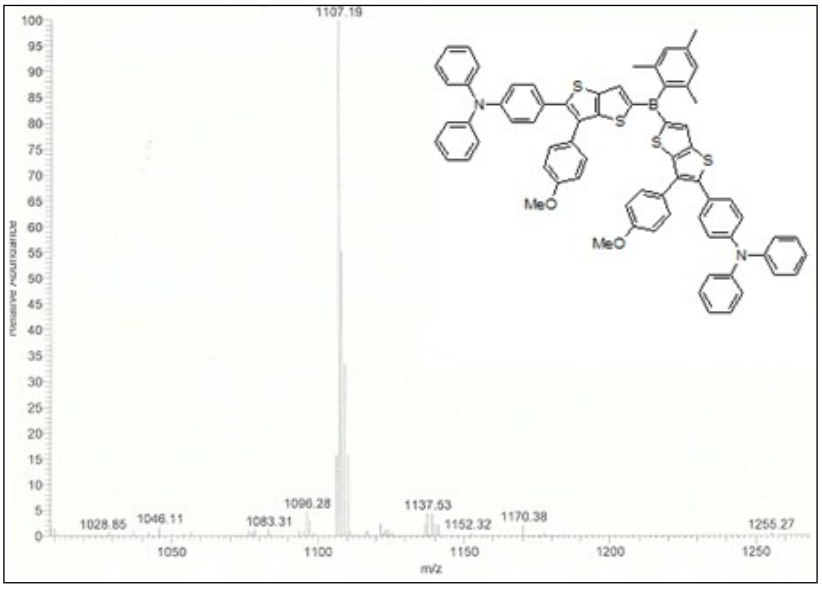


Figure S13. MS spectrum of compound **8**.

NMR Spectra

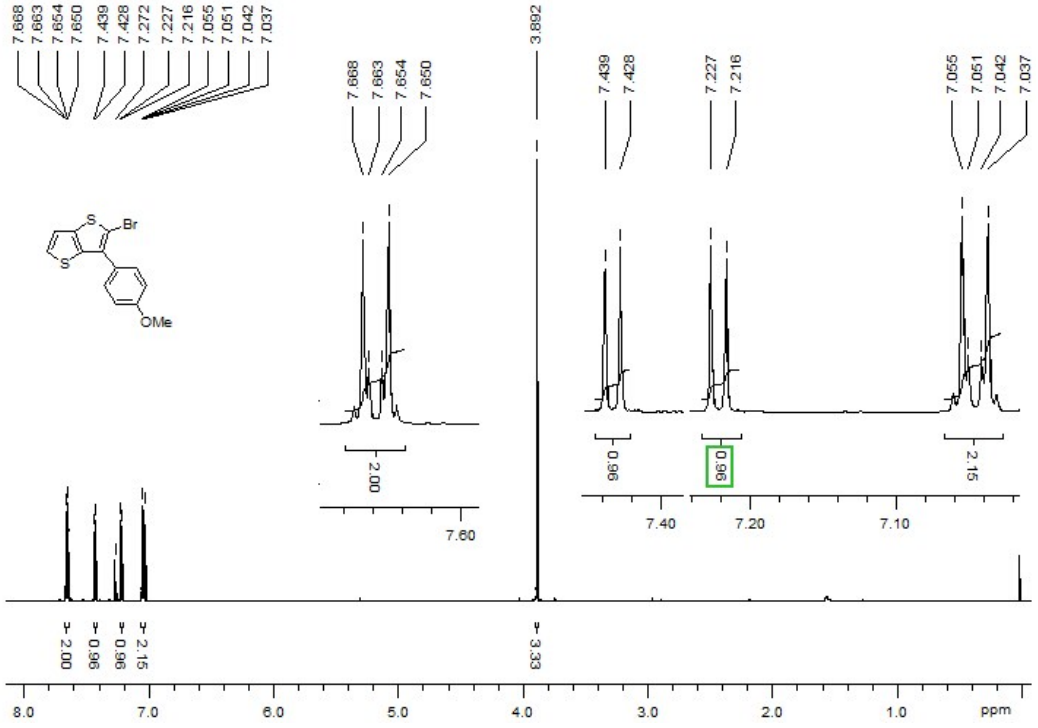


Figure S14. ^{1}H-NMR spectrum of compound **2** in $CDCl_3$ at 500 MHz.

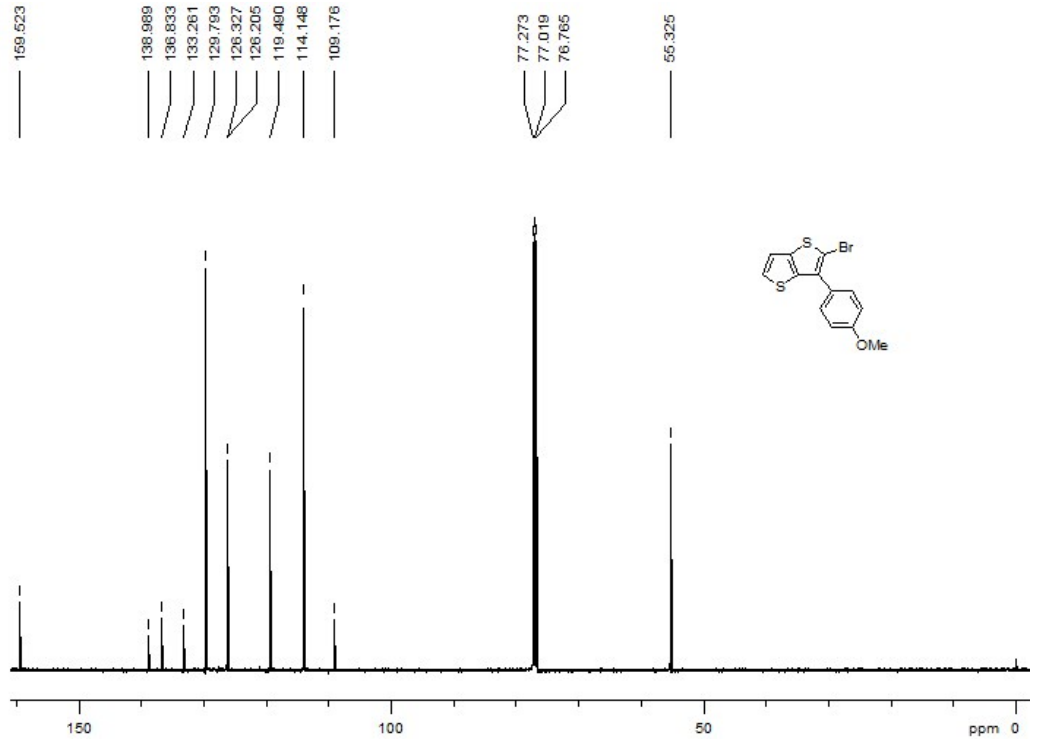


Figure S15. ^{13}C-NMR spectrum of compound **2** in $CDCl_3$ at 125 MHz.

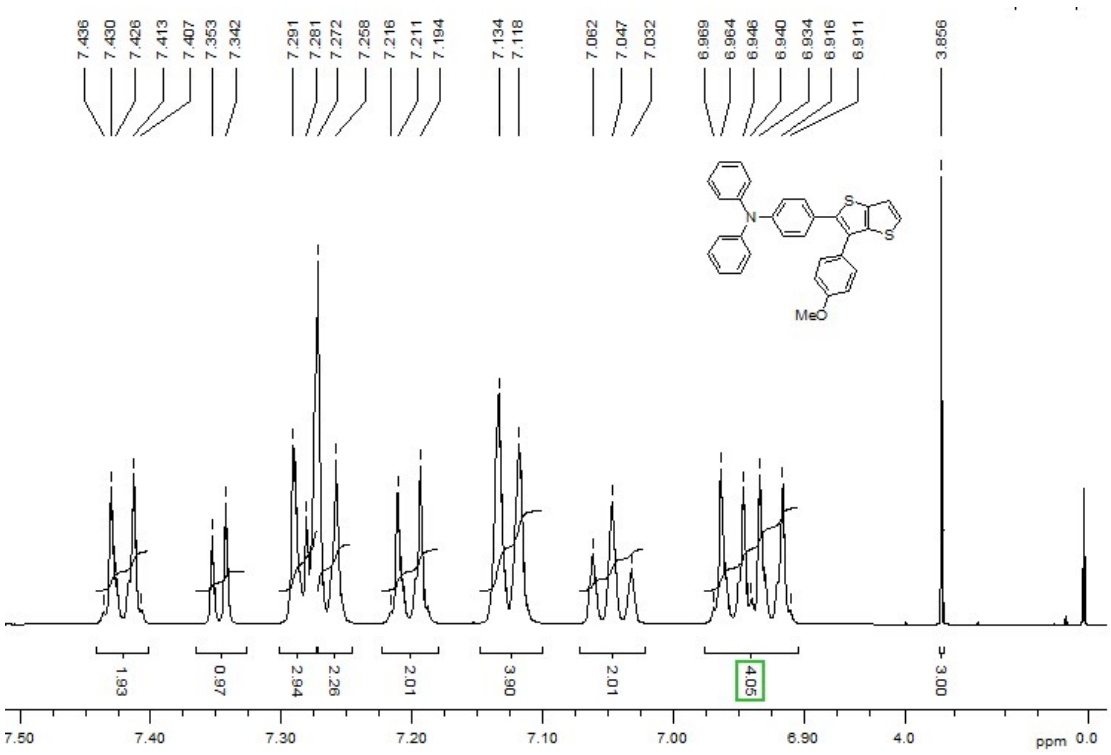


Figure S16. ^{1}H-NMR spectrum of compound **4** in $CDCl_3$ at 500 MHz.

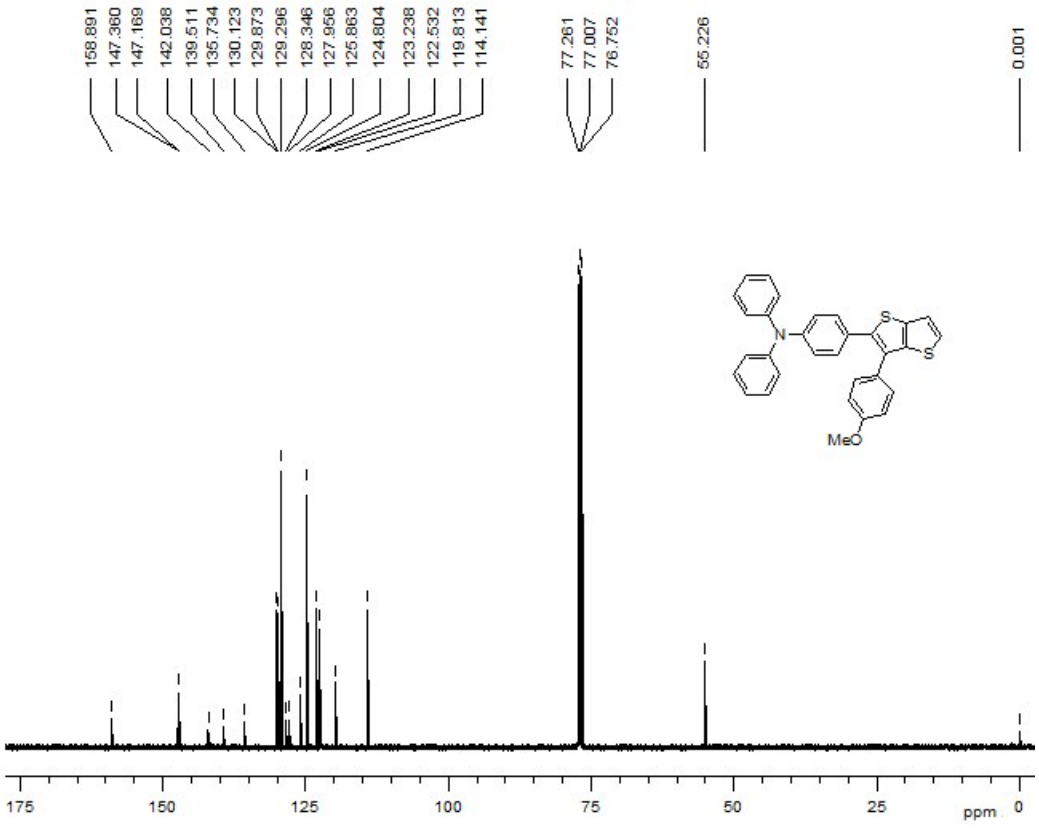


Figure S17. ^{13}C-NMR spectrum of compound **4** in $CDCl_3$ at 125 MHz.

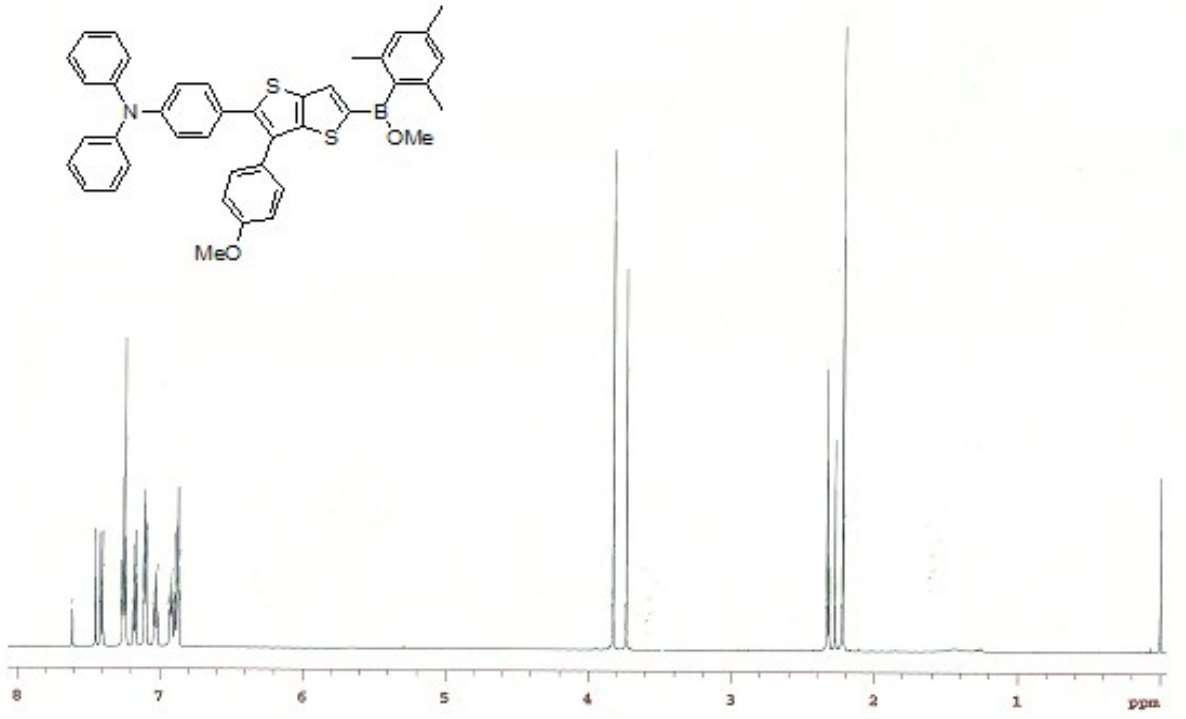


Figure S18. ^{1}H-NMR spectrum of compound **6** in $CDCl_3$ at 600 MHz.

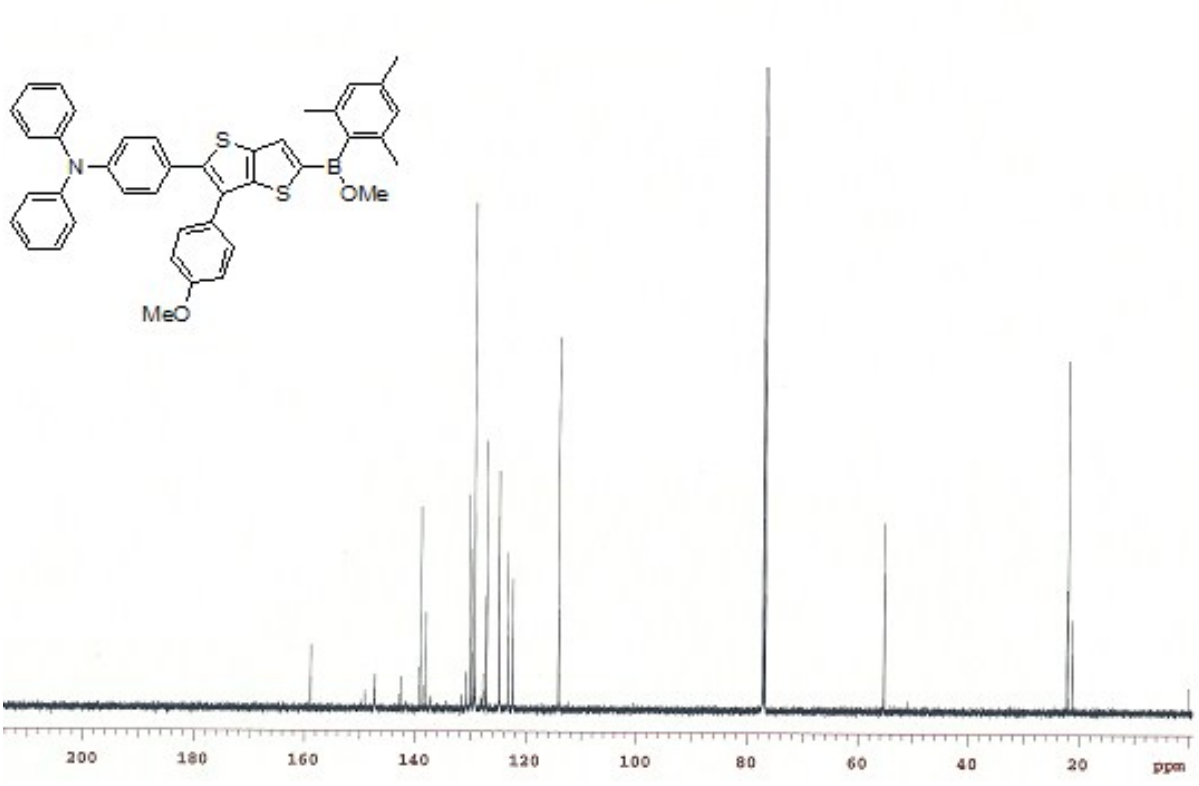


Figure S19. ^{13}C-NMR spectrum of compound **6** in $CDCl_3$ at 150 MHz.

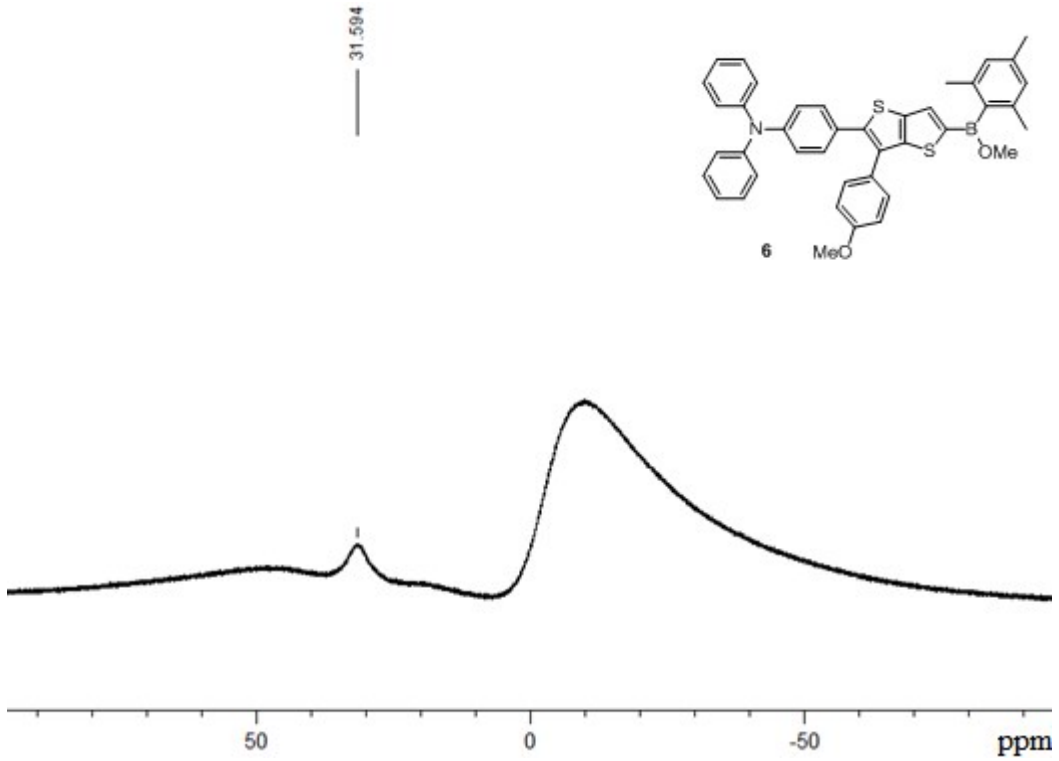


Figure S20. ^{11}B-NMR spectrum of compound **6** in $CDCl_3$ at 160 MHz.

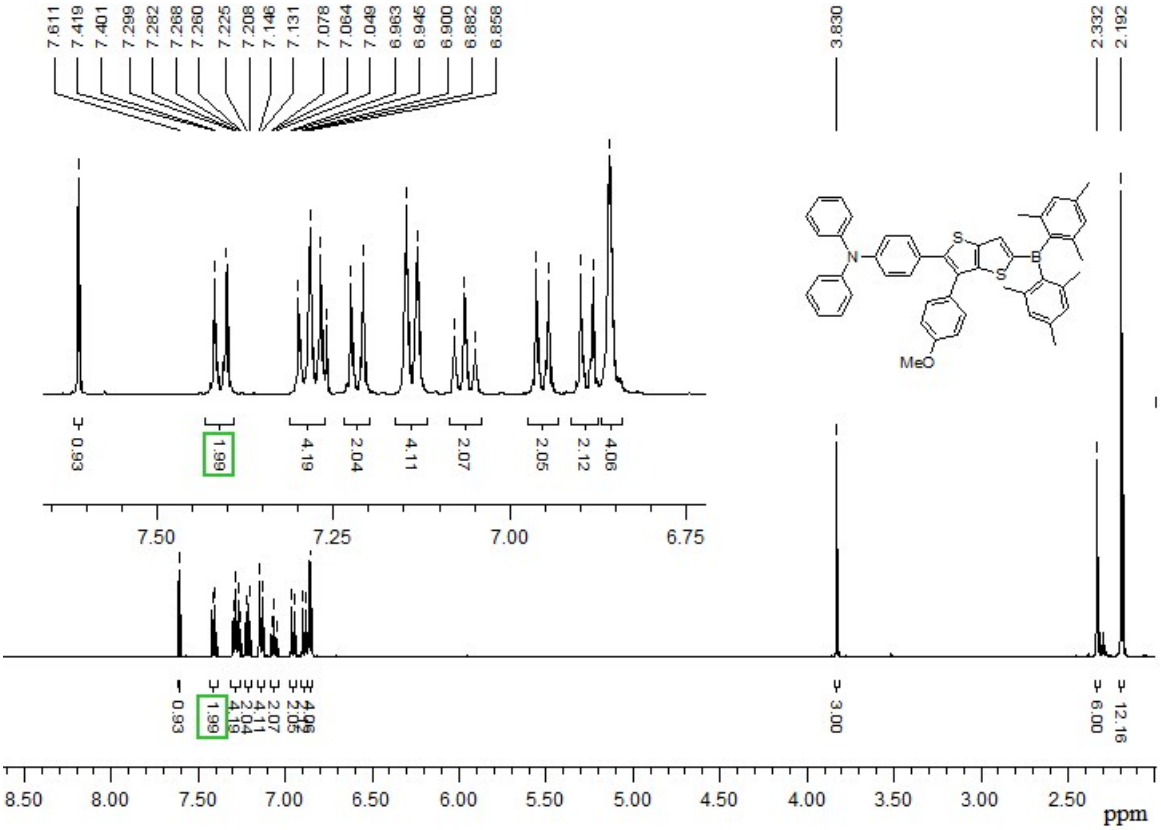


Figure S21. ^{1}H-NMR spectrum of compound **7** in $CDCl_3$ at 500 MHz.

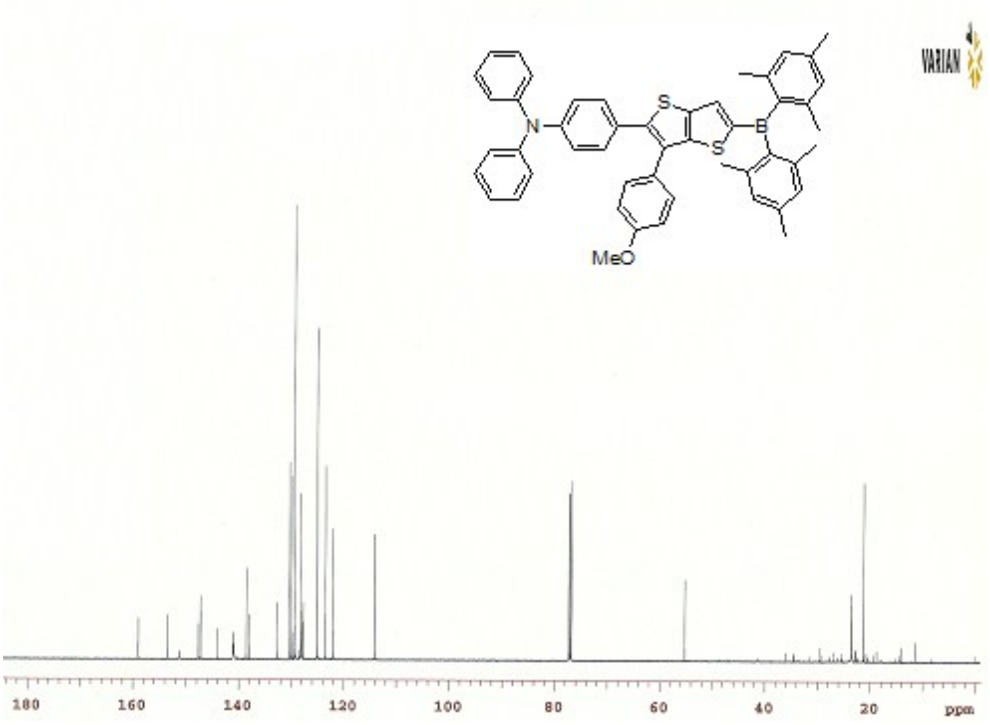


Figure S22. ^{13}C NMR spectrum of compound **7** in $CDCl_3$ at 125 MHz.

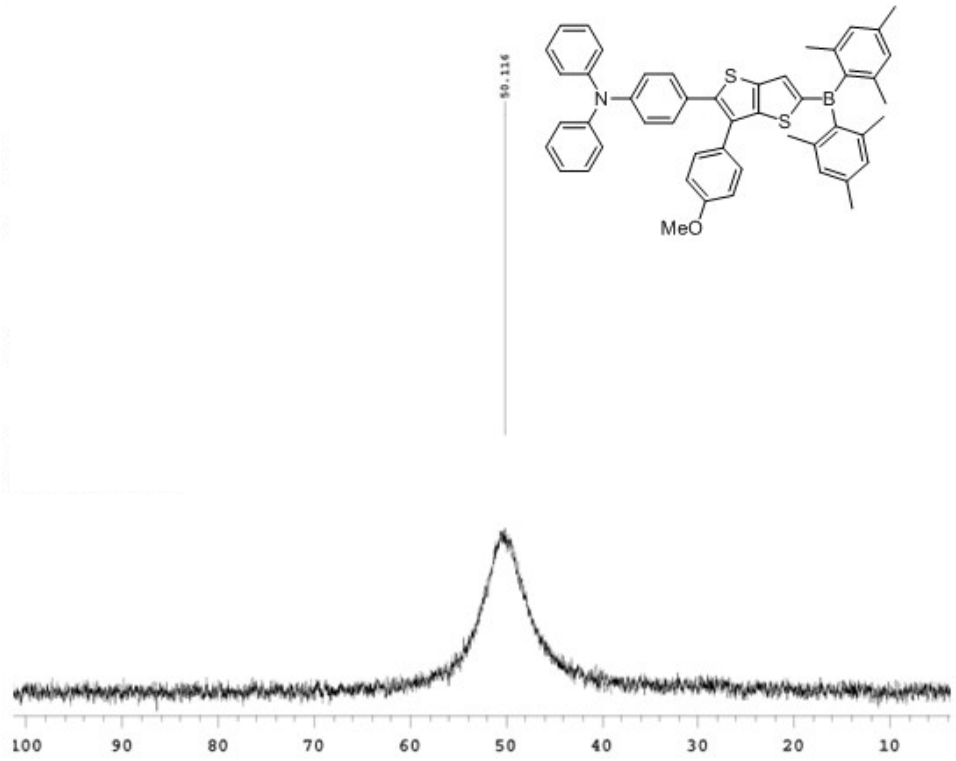


Figure S23. ^{11}B-NMR spectrum of compound **7** in $CDCl_3$ at 160 MHz.

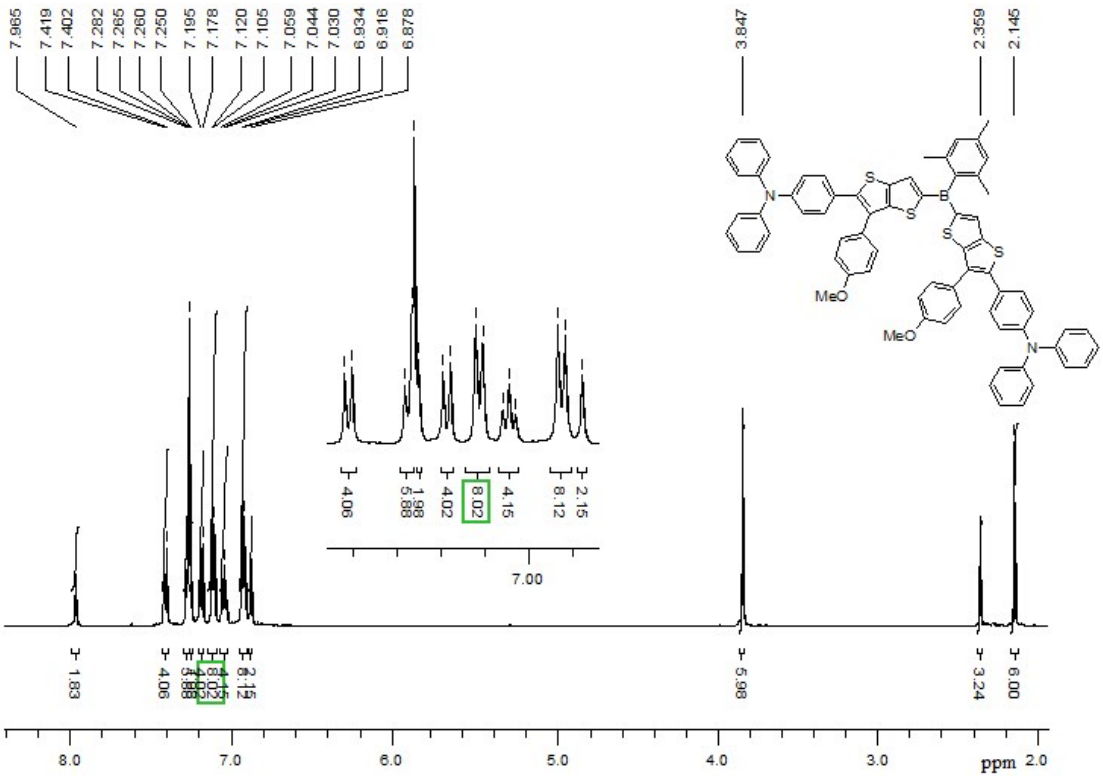


Figure S24. ^{1}H-NMR spectrum of compound **8** in $CDCl_3$ at 500 MHz.

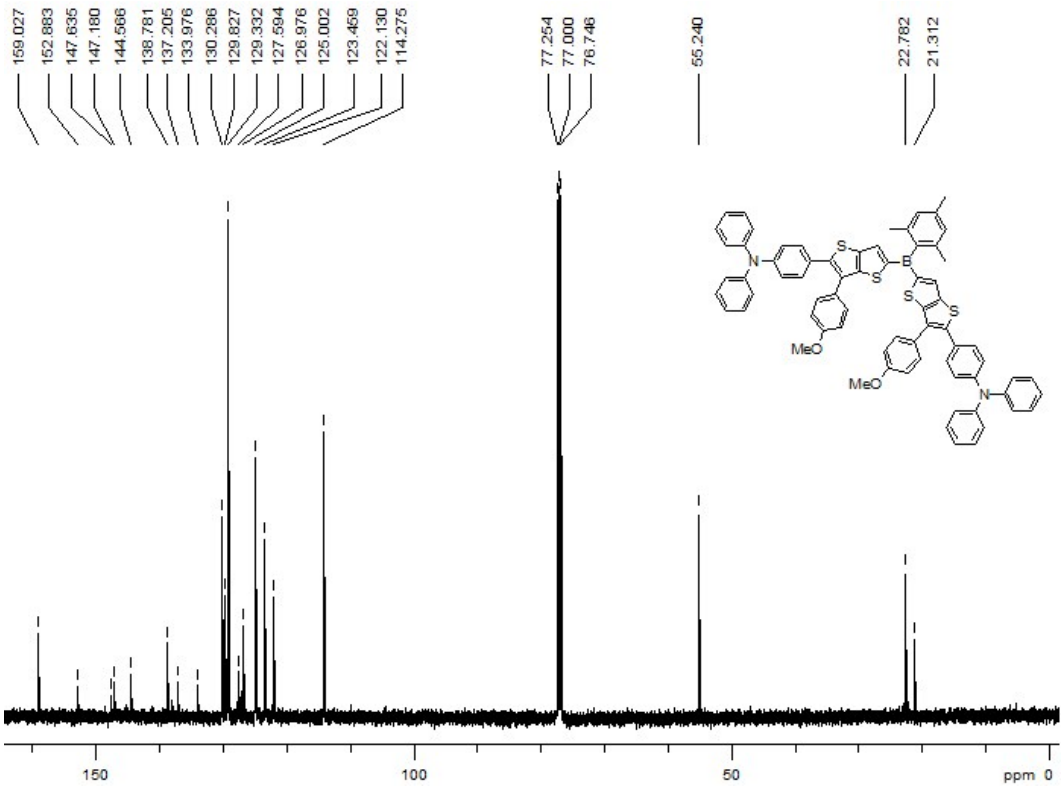


Figure S25. ^{13}C-NMR spectrum of compound **8** in $CDCl_3$ at 125 MHz.

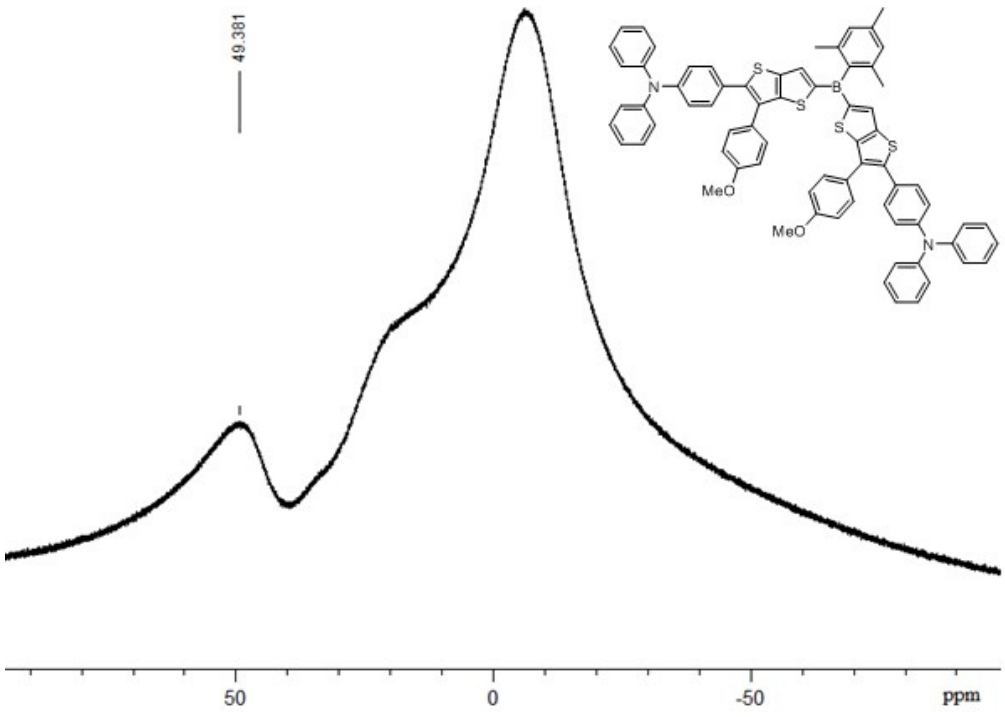
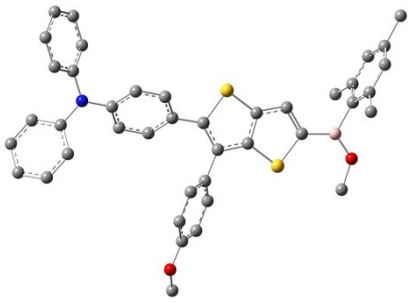


Figure S26. ^{11}B-NMR spectrum of compound **8** in $CDCl_3$ at 160 MHz.

Cartesian Coordinates

6



C	1.9935570	0.7974660	0.0025240
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C	3.7946160	-0.7207270	0.0001670
C	4.5064680	0.4684090	0.0170770
H	4.2905230	-1.6846670	-0.0066450
C	-0.0962520	-0.2022050	-0.0896200
S	1.0067760	-1.5888770	-0.0601700
C	0.5784180	1.0105460	-0.0567210
S	3.3806860	1.8469080	0.0121430
C	-1.5403760	-0.4765500	-0.0783990
C	-2.0867520	-1.5293910	-0.8355370
C	-2.4233200	0.2706300	0.7244530
C	-3.4457650	-1.8178560	-0.8048850
H	-1.4394320	-2.1139640	-1.4837670
C	-3.7806300	-0.0181370	0.7680480
H	-2.0324010	1.0701890	1.3445810
C	-4.3191410	-1.0680200	0.0016030
H	-3.8390950	-2.6238480	-1.4152970
H	-4.4326830	0.5622230	1.4123440
B	6.0636260	0.5320850	0.0364980
N	-5.7013820	-1.3650480	0.0457470
C	-6.1480650	-2.7154590	-0.0326190
C	-5.5182990	-3.7203750	0.7184120
C	-7.2306690	-3.0571670	-0.8579530
C	-5.9582430	-5.0400430	0.6333930
H	-4.6861910	-3.4605800	1.3652280
C	-7.6752010	-4.3765090	-0.9227100
H	-7.7183100	-2.2843850	-1.4438170
C	-7.0403100	-5.3764280	-0.1829690
H	-5.4595680	-5.8062780	1.2211560
H	-8.5147100	-4.6245000	-1.5669310
H	-7.3848180	-6.4049530	-0.2413540
C	-6.6609110	-0.3201390	0.1665660
C	-6.5388290	0.8545180	-0.5925210
C	-7.7493090	-0.4557610	1.0426600
C	-7.4810230	1.8736050	-0.4655880
H	-5.7043370	0.9619680	-1.2782260
C	-8.6965730	0.5608760	1.1490200
H	-7.8466320	-1.3598240	1.6353800
C	-8.5670090	1.7330360	0.4010820
H	-7.3711850	2.7767440	-1.0601910
H	-9.5332350	0.4394040	1.8320640
H	-9.3032600	2.5265620	0.4917030
C	6.8836850	-0.8249550	0.0538100
C	7.3175600	-1.4129720	-1.1538130
C	7.2100080	-1.4574050	1.2729620
C	8.0443050	-2.6079200	-1.1269030
C	7.9391290	-2.6511000	1.2663790
C	8.3619100	-3.2471520	0.0747140
H	8.3724440	-3.0491510	-2.0668770
H	8.1854580	-3.1259060	2.2150040
O	6.8265010	1.6624360	0.0320010
C	-0.0373750	2.3570240	-0.1402300
C	-0.9790680	2.6718230	-1.1386980
C	0.3310710	3.3713600	0.7527550
C	-1.5313320	3.9403250	-1.2303750
H	-1.2708850	1.9090830	-1.8538670
C	-0.2169790	4.6542880	0.6723200
H	1.0501310	3.1571360	1.5387160
C	-1.1555910	4.9439010	-0.3236550
H	-2.2526100	4.1849380	-2.0039500
H	0.0918480	5.4081450	1.3874750
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C	-1.4088410	7.2117390	0.3828100
H	-1.9940080	8.0753580	0.0616610
H	-1.6628780	6.9686080	1.4231160
H	-0.3398030	7.4547260	0.3206750
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H	7.2655580	0.1348540	2.7458830
H	5.7079500	-0.6858360	2.6413500
H	7.0740180	-1.4825190	3.4373540
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H	5.9368830	-0.5936900	-2.6190490
H	7.4936220	0.2329760	-2.5550070
H	7.3707070	-1.3578710	-3.3214800
C	9.1181680	-4.5556590	0.0848580
H	8.4327370	-5.4142340	0.0731680
H	9.7689960	-4.6494160	-0.7912720
H	9.7408530	-4.6524100	0.9811110
C	6.3549490	3.0031030	0.0065000
H	5.7578170	3.1997530	-0.8912590
H	5.7534300	3.2312870	0.8938900
H	7.2316090	3.6567580	-0.0025690

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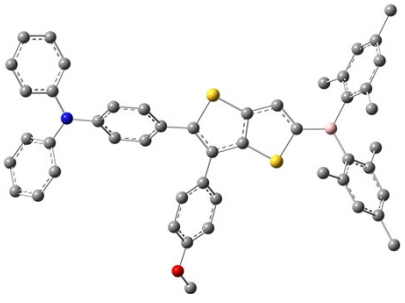

C	-1.0913130	0.1189820	0.0249220
C	-1.2976540	-1.2521650	0.1877990
C	-2.6553900	-1.6321430	0.2034880
C	-3.5244870	-0.5577110	0.0608630
H	-3.0143450	-2.6485680	0.3219020
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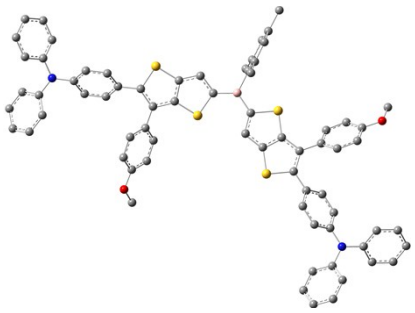

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