Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Syntheses, structures, one- and two-photon excited fluorescence of dimesitylboryl-ended quadrupolar hybrid-oligothiophenes

Senhao Zhou,[§a] Shiqian Zhang, [§a] Jinsong Li,[a] Zhiqiang Liu,[a,b]* Xiaoqiang Yu[a]*

[a]State Key Laboratory of Crystal Materials, Shandong University, Jinan 250100, China

[b]Shenzhen Research Institute of Shandong University, Shenzhen 518057, China

[§]These authors contribute equally.

E-mail: zqliu@sdu.edu.cn; yuxq@sdu.edu.cn

Table of contents

Table S-1. Crystallographic parameters for compounds **1** and **2**

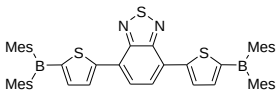
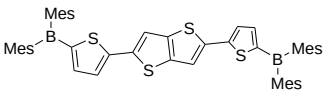
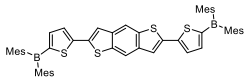
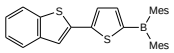
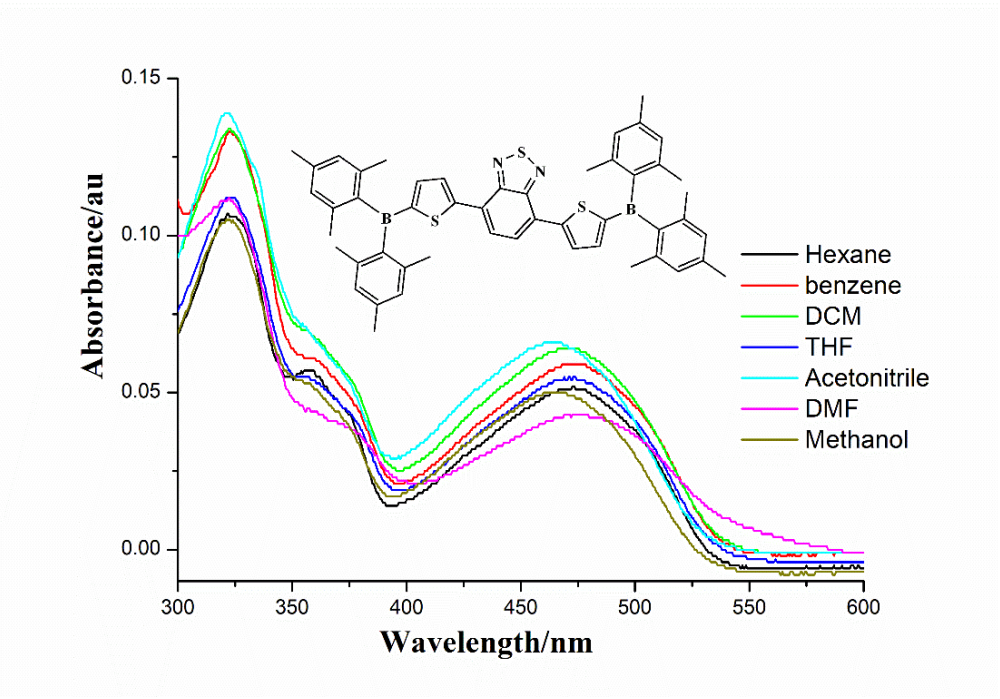
		
	1	**2**
CCDC Number	2062056	2062057
Empirical formula	$C_{50}H_{48}B_2N_2S_3$	$C_{50}H_{50}B_2S_4$
Formula weight	794.70	892.89
Temperature/K	296(2)	296.15
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	8.2837(10)	17.1329(4)
b/Å	16.1677(3)	8.2168(2)
c/Å	16.6633(3)	19.5322(4)
α/°	90	90
β/°	93.001(10)	113.3421(13)
γ/°	90	90
Volume/Å^3	2228.63(6)	2524.65(10)
Z	2	2
ρ_{calc}g/cm^3	1.184	1.175
μ/mm^{-1}	0.202	0.224
F(000)	840.0	948.0
Crystal size/mm^3	0.4 × 0.38 × 0.3	0.4 × 0.2 × 0.04
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.512 to 55.016	4.064 to 54.952
Index ranges	-10 ≤ h ≤ 10, -18 ≤ k ≤ 21, -19 ≤ l ≤ 21	-22 ≤ h ≤ 22, -10 ≤ k ≤ 10, -25 ≤ l ≤ 25
Reflections collected	19664	42323
Independent reflections	5112 [R_{int} = 0.0256, R_{sigma} = 0.0287]	5782 [R_{int} = 0.0576, R_{sigma} = 0.0378]
Data/restraints/parameters	5114/0/277	5782/87/311
Goodness-of-fit on F^2	1.020	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0570, wR_2 = 0.1579	R_1 = 0.0482, wR_2 = 0.1272
Final R indexes [all data]	R_1 = 0.0793, wR_2 = 0.1707	R_1 = 0.0867, wR_2 = 0.1511
Largest diff. peak/hole / e Å^{-3}	0.28/-0.24	0.21/-0.31

Table S-2. Crystallographic parameters for compounds **3** and **5**

		
	3	**5**
CCDC Number	2062059	2062058
Empirical formula	$C_{54}H_{52}B_2S_4$	$C_{30}H_{29}BS_2$
Formula weight	850.81	464.46
Temperature/K	297	297(2)
Crystal system	monoclinic	triclinic
Space group	C2/c	P-1
a/Å	42.4881(14)	7.99790(10)
b/Å	15.1359(5)	11.7834(2)
c/Å	8.0769(2)	13.5026(2)
α/°	90	96.2150(10)
β/°	92.305(3)	93.8950(10)
γ/°	90	100.2200(10)
Volume/$Å^3$	5190.0(3)	1240.02(3)
Z	4	2
$\rho_{calc}g/cm^3$	1.089	1.244
μ/mm^{-1}	1.915	0.231
F(000)	1800.0	492.0
Crystal size/mm^3	0.13 × 0.11 × 0.08	0.99 × 0.16 × 0.08
Radiation	Cu Kα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.33 to 153.472	3.046 to 54.584
Index ranges	-52 ≤ h ≤ 53, -19 ≤ k ≤ 19, -6 ≤ l ≤ 10	-10 ≤ h ≤ 10, -15 ≤ k ≤ 14, -17 ≤ l ≤ 16
Reflections collected	16352	19365
Independent reflections	5105 [R_{int} = 0.0488, R_{sigma} = 0.0500]	5465 [R_{int} = 0.0193, R_{sigma} = 0.0179]
Data/restraints/parameters	5105/291/320	5465/0/324
Goodness-of-fit on F^2	1.1175	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0839, wR_2 = 0.1935	R_1 = 0.0347, wR_2 = 0.0949
Final R indexes [all data]	R_1 = 0.0947, wR_2 = 0.1977	R_1 = 0.0375, wR_2 = 0.0977
Largest diff. peak/hole / e $Å^{-3}$	0.24/-0.26	0.34/-0.27

(a)



(b)

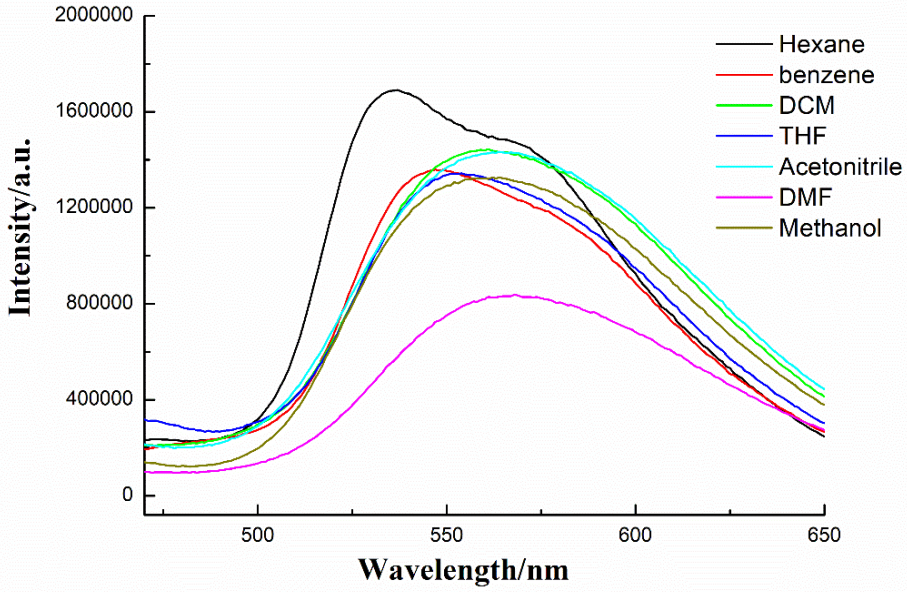
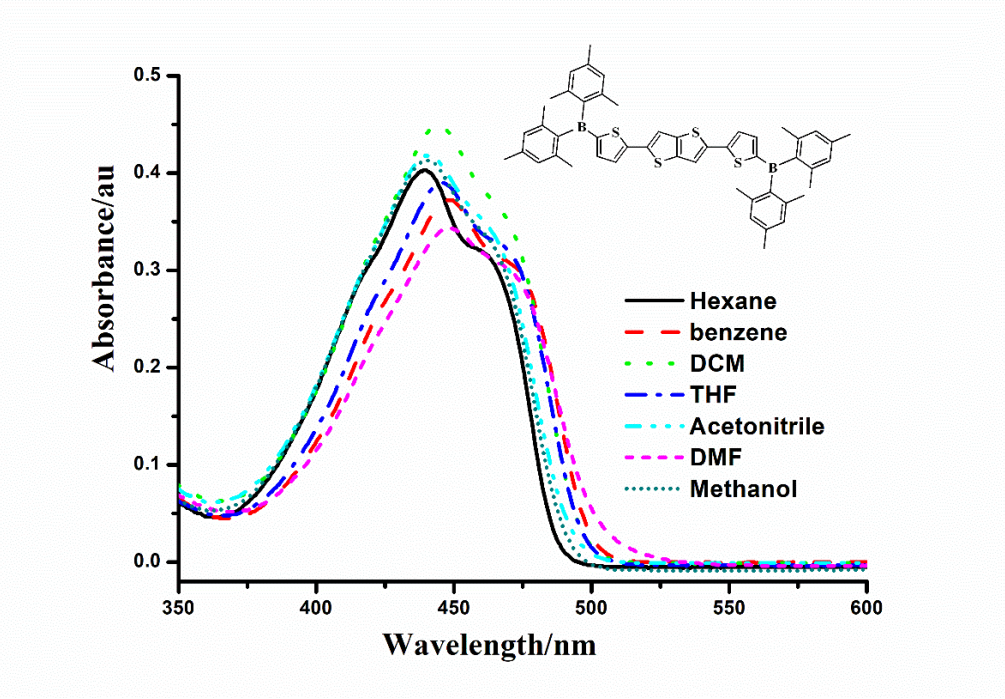


Figure S-1. Absorption (a) and emission (b) spectra of compound **1**.
(C = 2.5 μM, λ_{ex} = 460 nm)

(a)



(b)

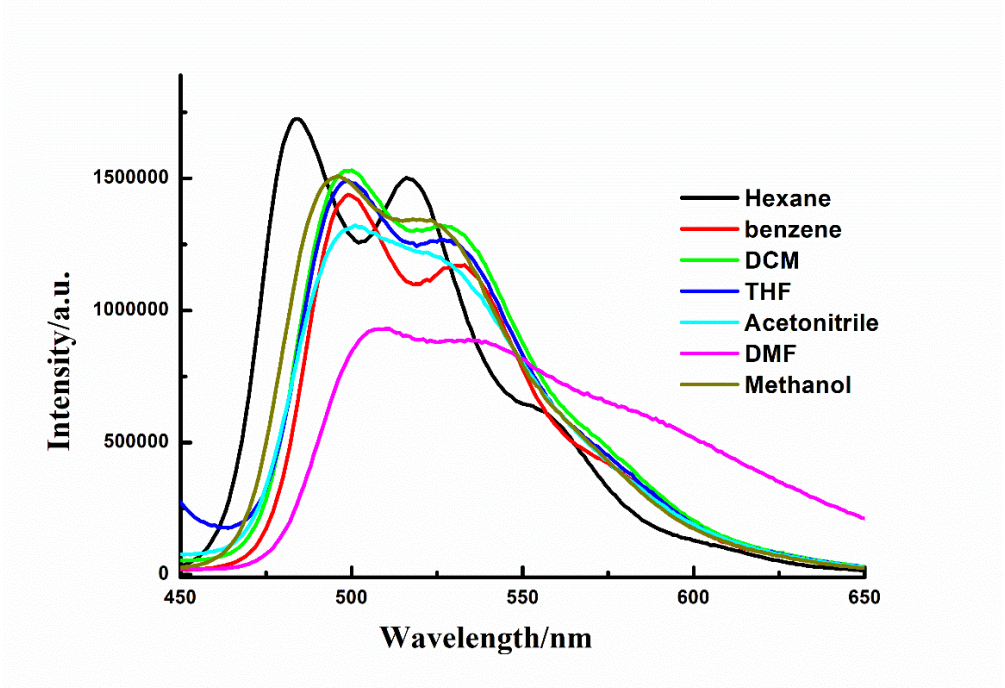
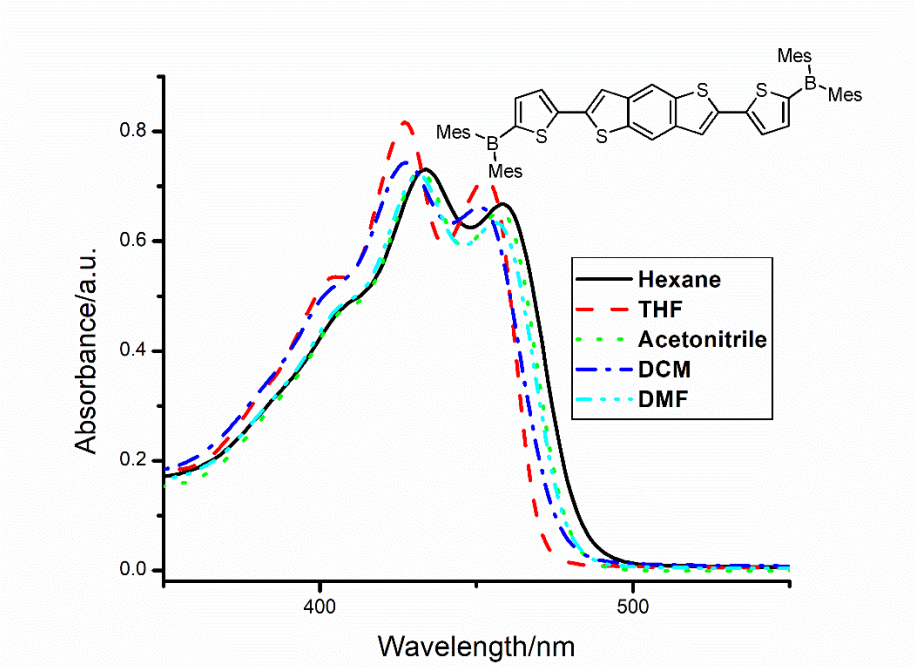


Figure S-2. Absorption (a) and emission (b) spectra of compound **2**.
(C = 4.7 μM, λ_{ex} = 440 nm)

(a)



(b)

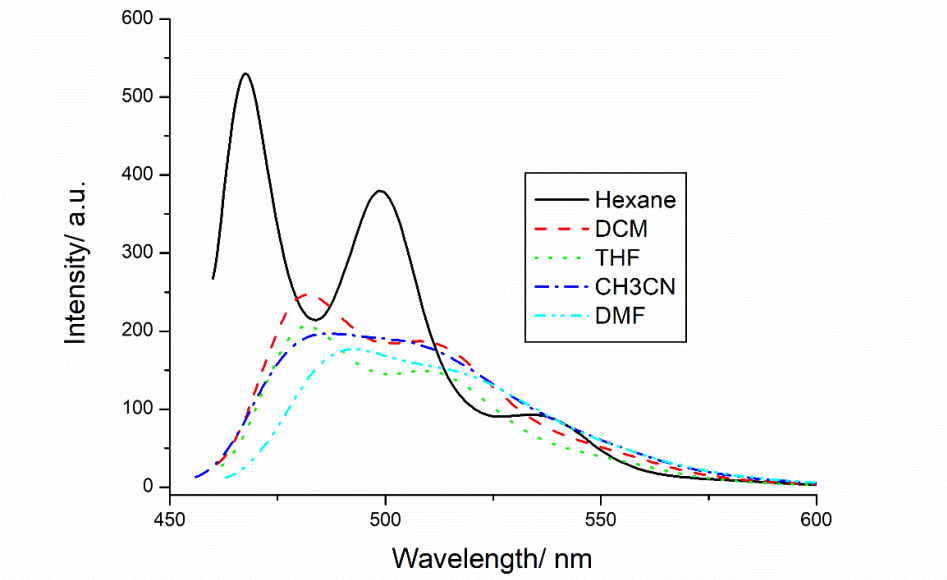


Figure S-3. Absorption (a) and emission (b) spectra of compound **3**.
(C = 10.0 μM, λ_{ex} = 440 nm)

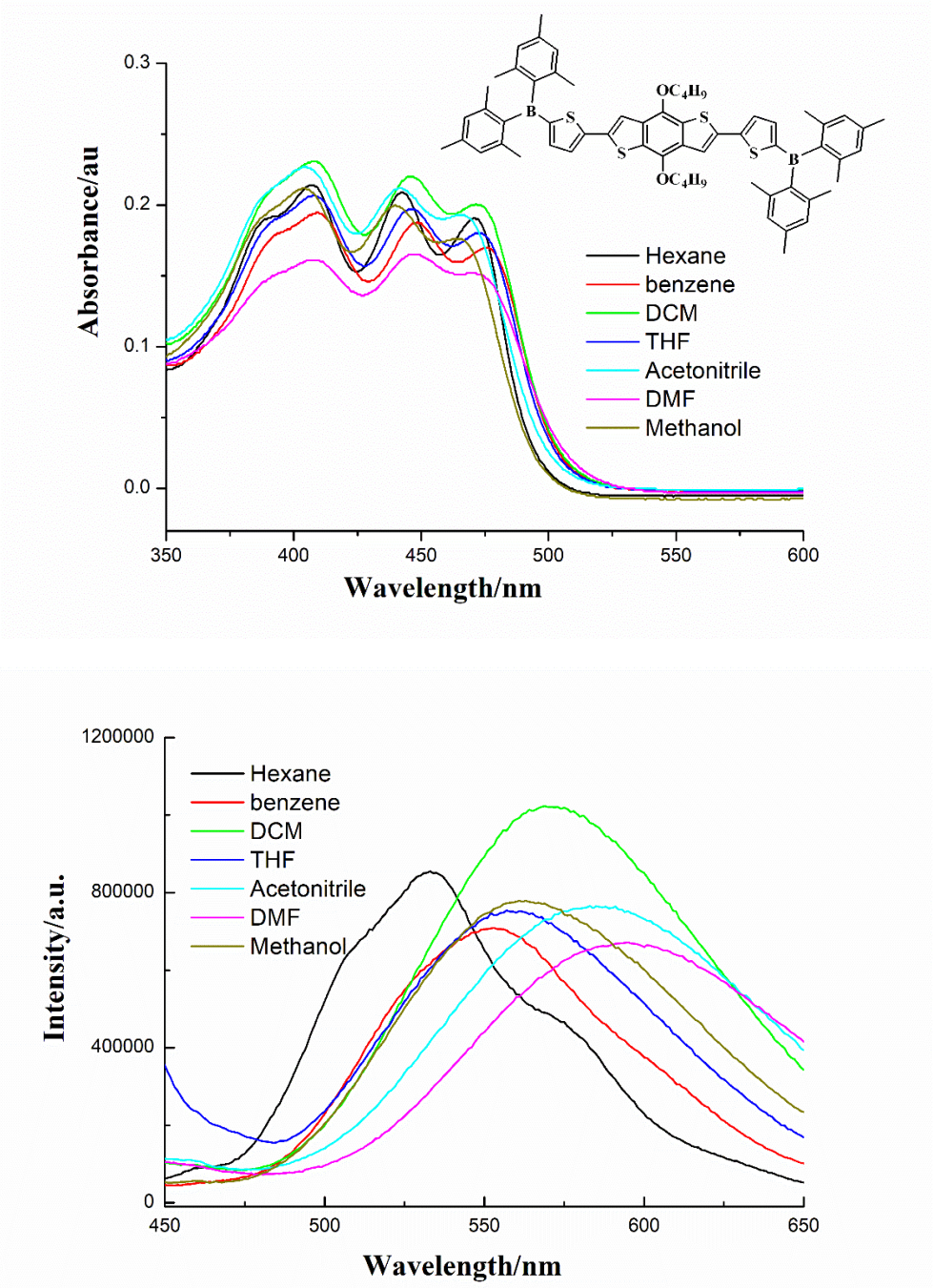
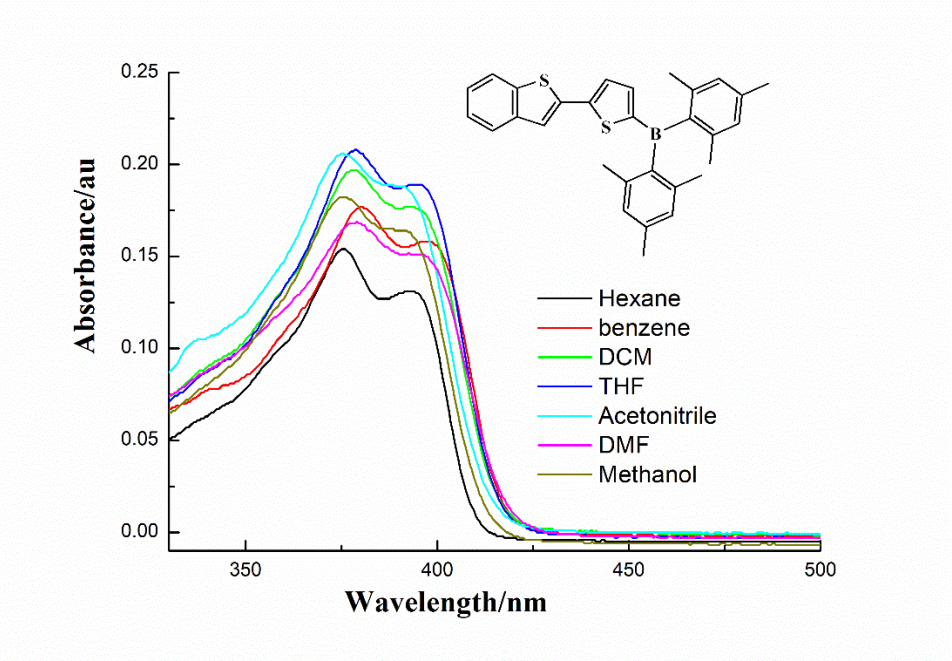


Figure S-4. Absorption (a) and emission (b) spectra of compound **4**.
(C = 3.0 μM, λ_{ex} = 440 nm)

(a)



(b)

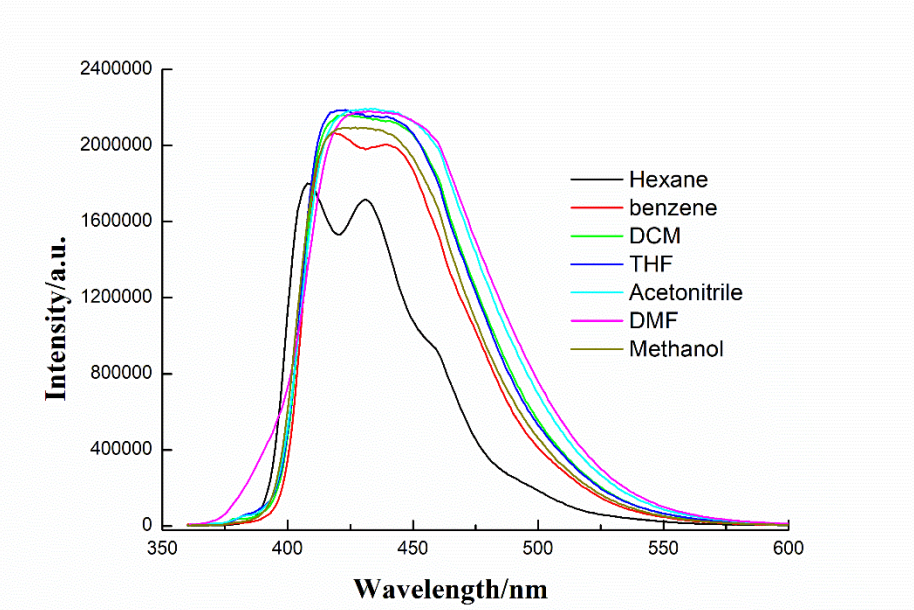


Figure S-5. Absorption (a) and emission (b) spectra of compound **5**.
(C = 7.0 μM, λ_{ex} = 330 nm)

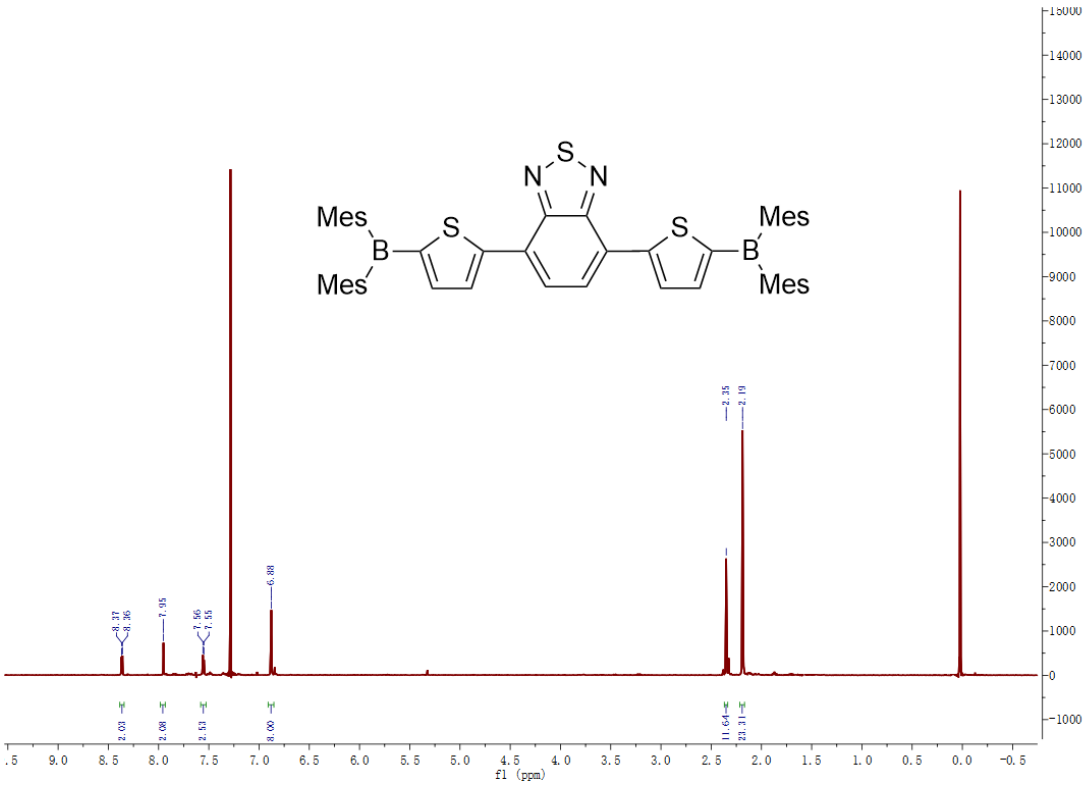


Figure S-6. ^{1}H NMR spectrum of compound **1** (400 MHz, $CDCl_3$).

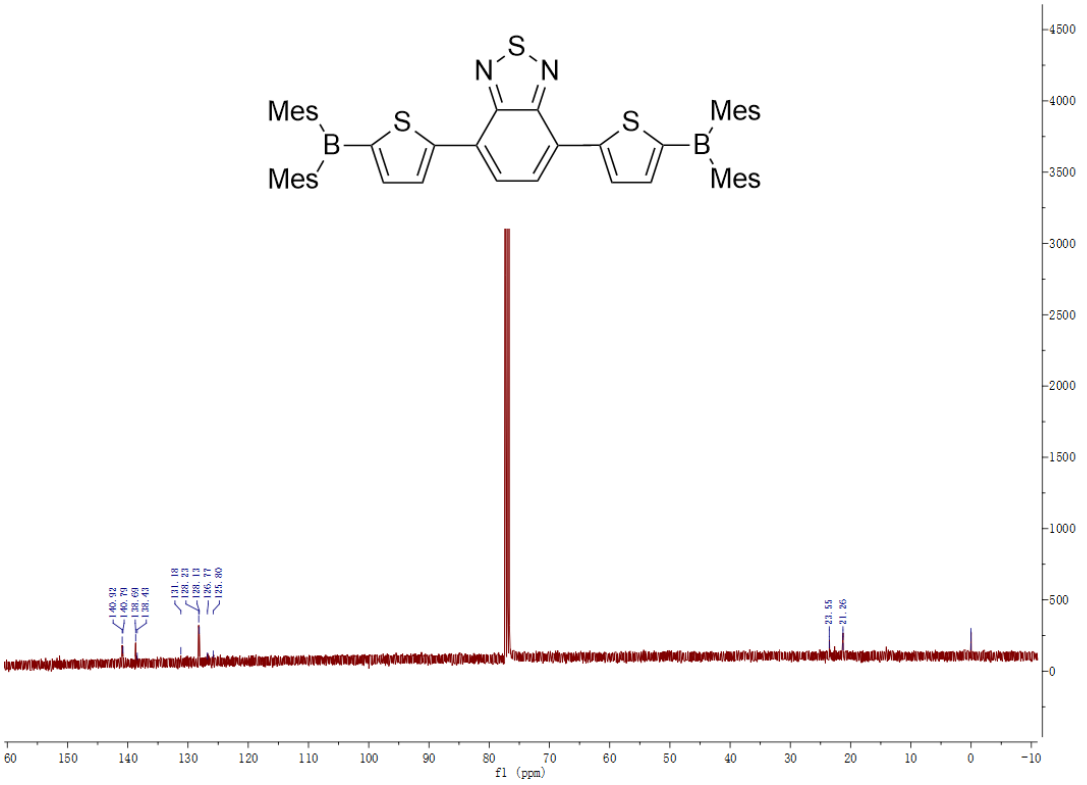


Figure S-7. ^{13}C NMR spectrum of compound **1** (100 MHz, $CDCl_3$).

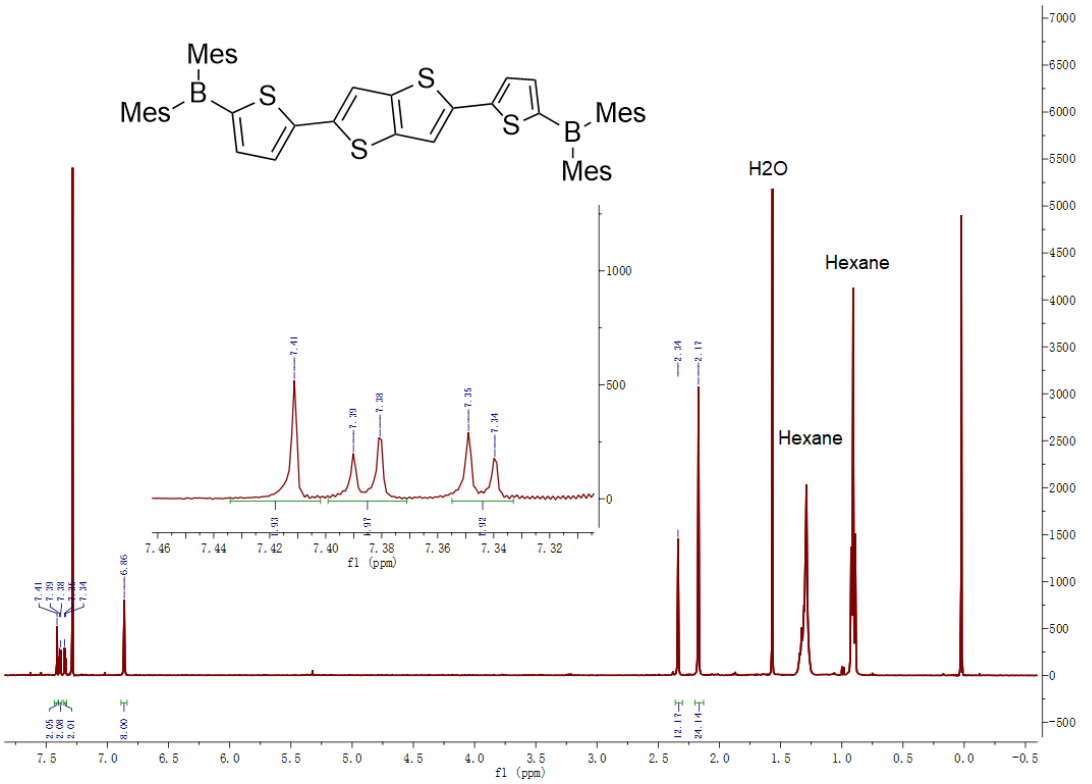


Figure S-8. ^{1}H NMR spectrum of compound **2** (400 MHz, $CDCl_3$).

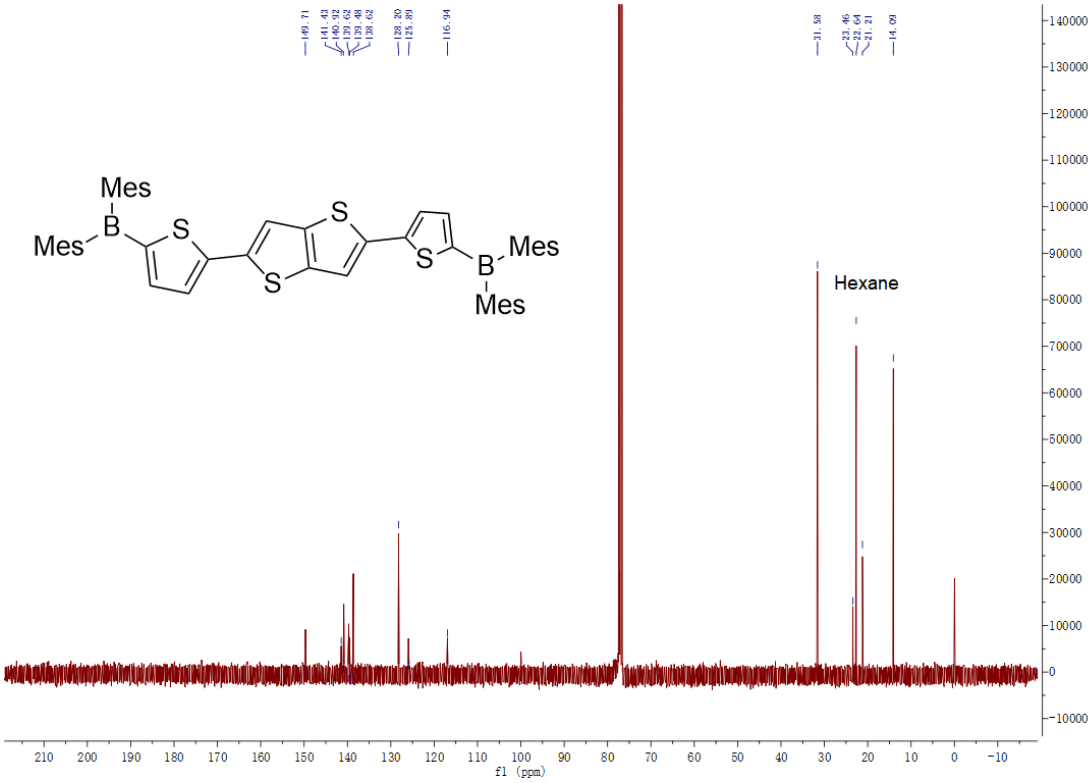


Figure S-9. ^{13}C NMR spectrum of compound **2** (100 MHz, $CDCl_3$).

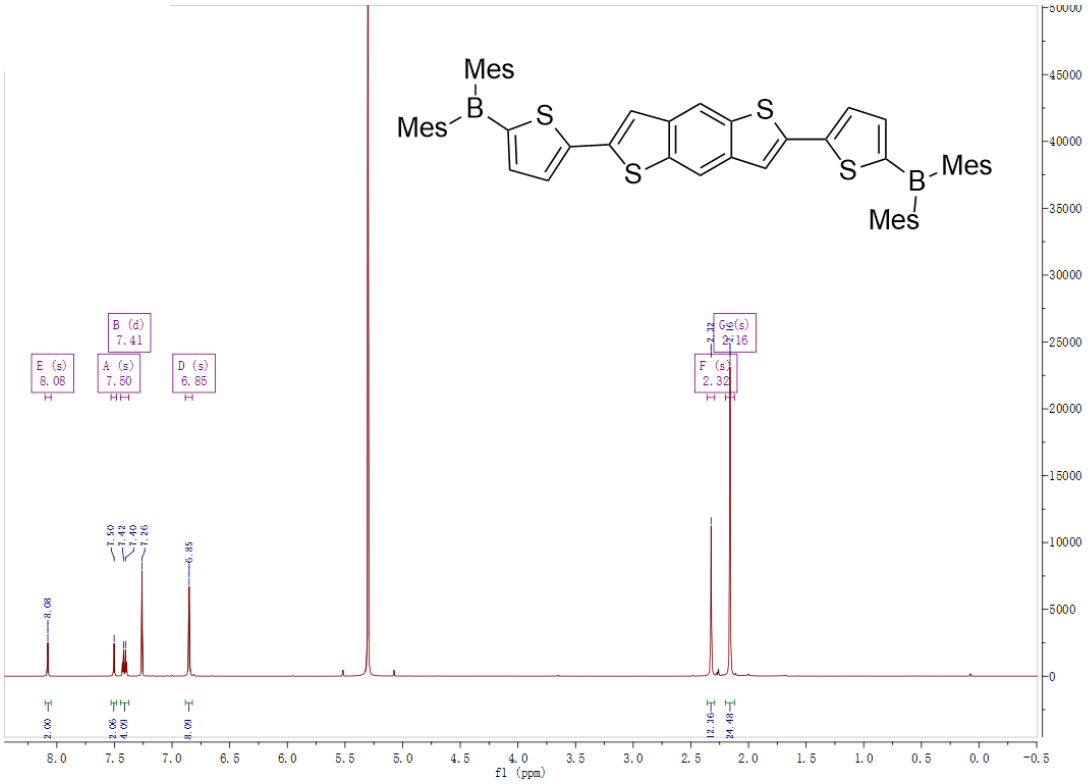


Figure S-10. ^{1}H NMR spectrum of compound **3** (400 MHz, $CDCl_3$).

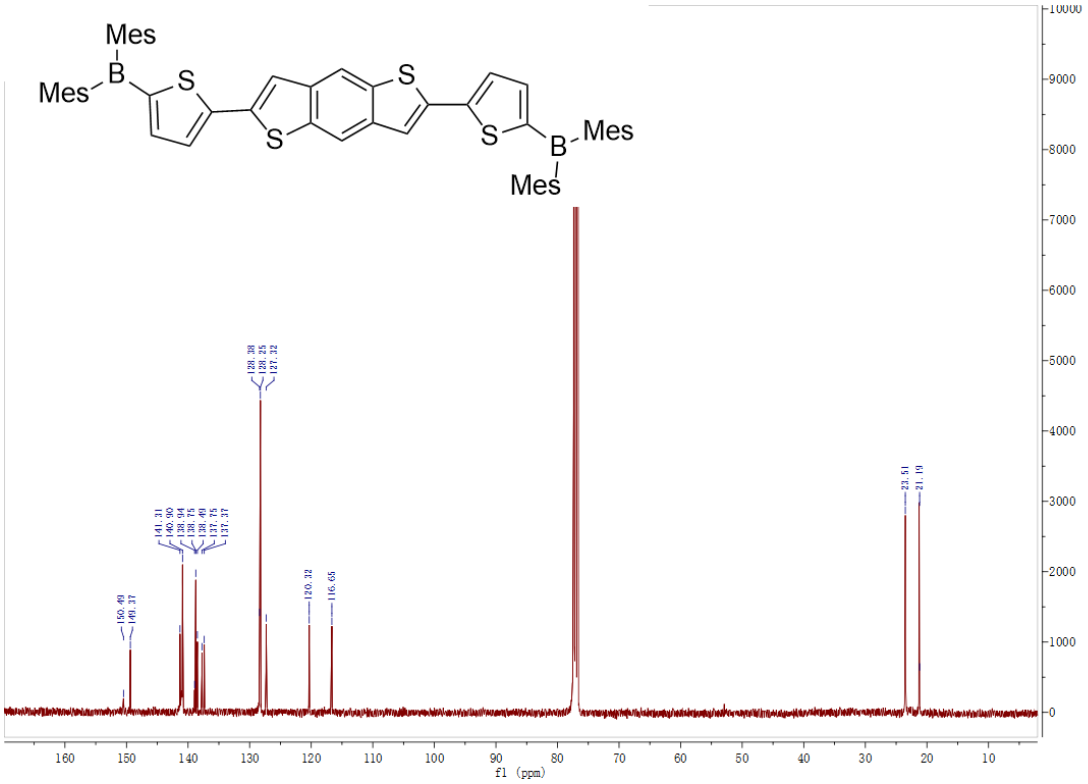


Figure S-11. ^{13}C NMR spectrum of compound **3** (100 MHz, $CDCl_3$).

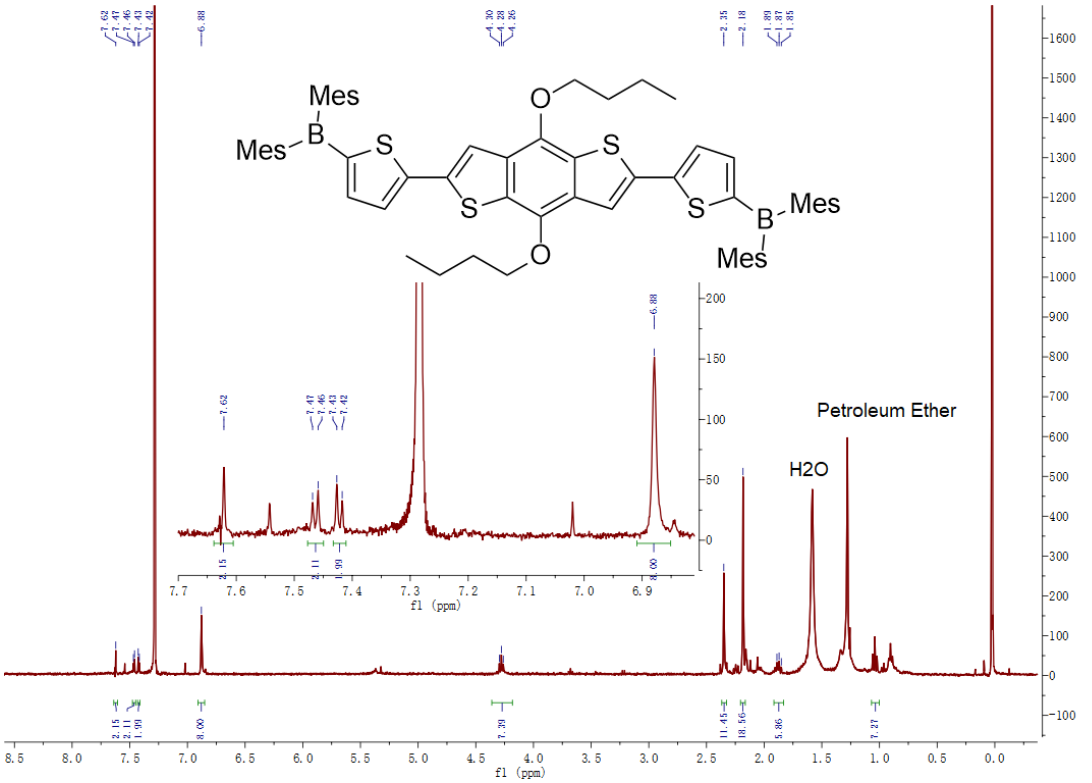


Figure S-12. ^{1}H NMR spectrum of compound **4** (400 MHz, $CDCl_3$).

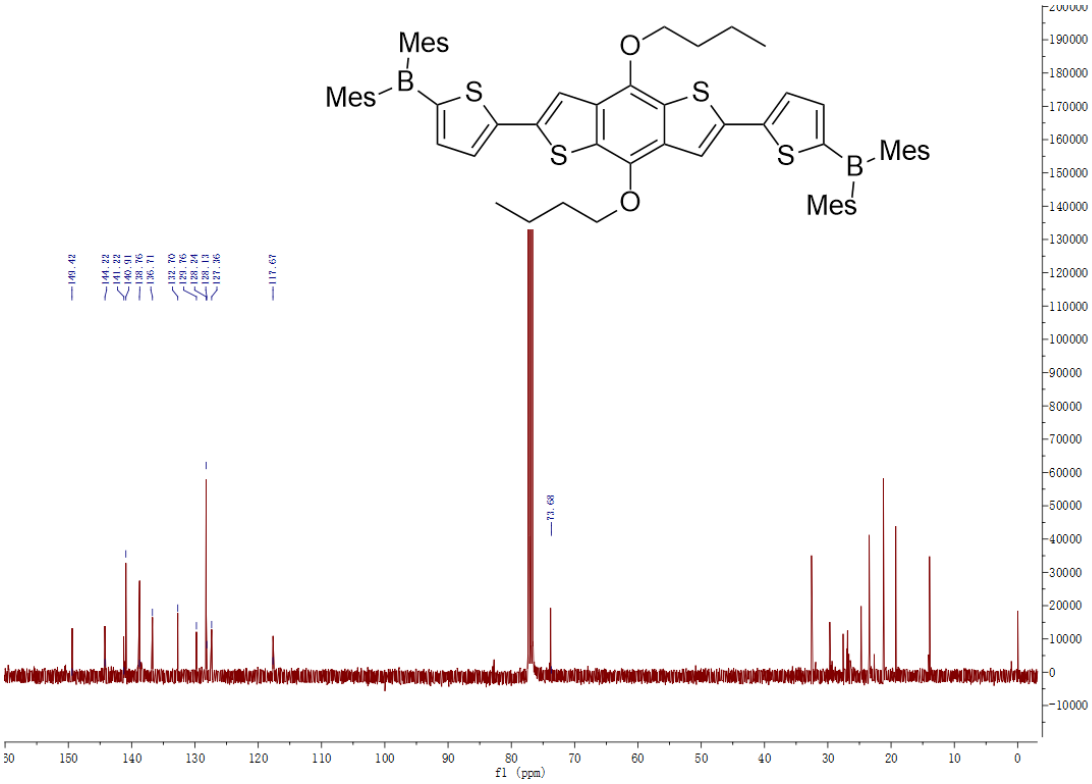


Figure S-13. ^{13}C NMR spectrum of compound **4** (100 MHz, $CDCl_3$).

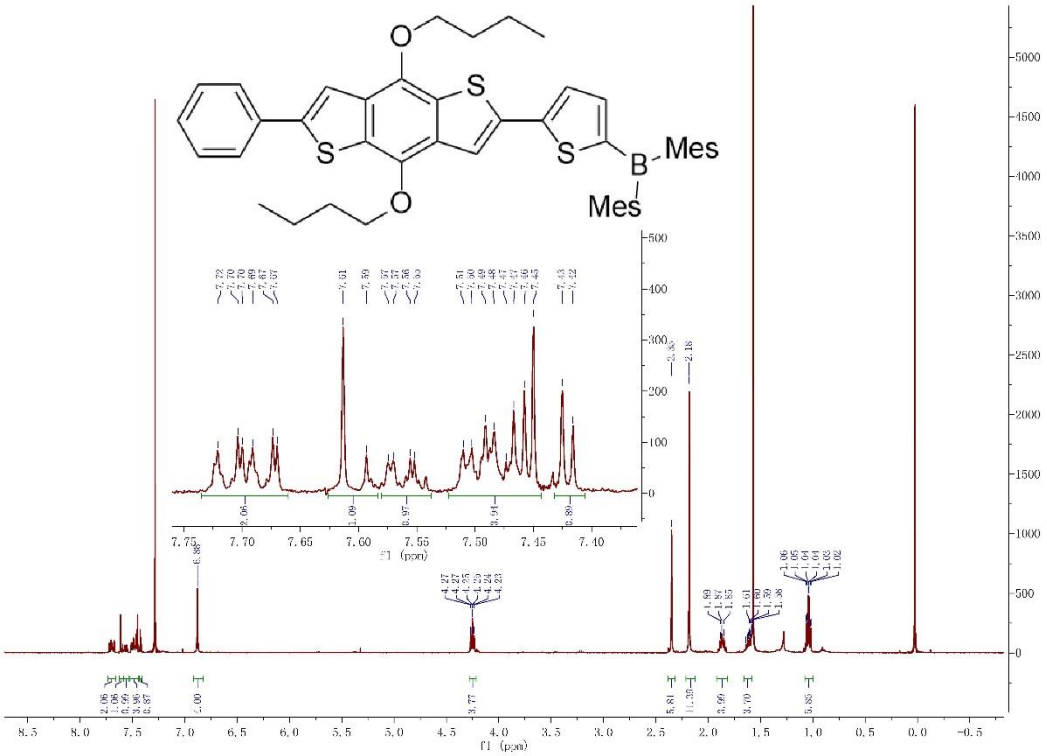


Figure S-14. ^{1}H NMR spectrum of compound **4'** (400 MHz, $CDCl_3$).

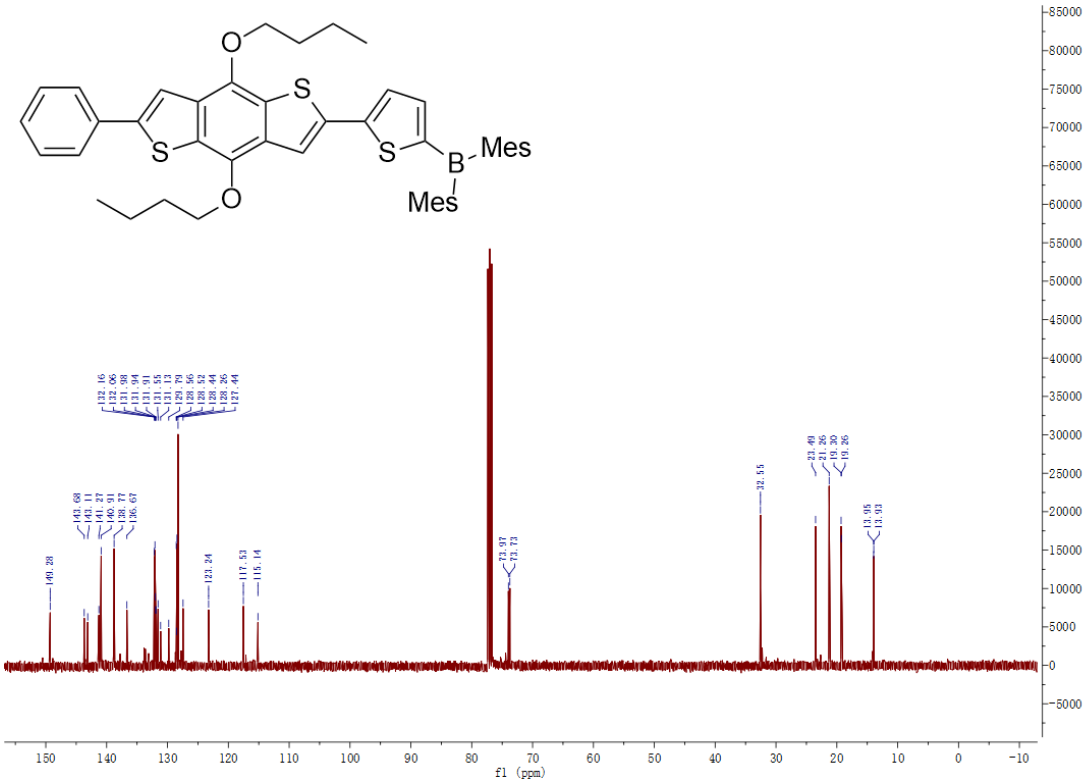


Figure S-15. ^{13}C NMR spectrum of compound **4'** (100 MHz, $CDCl_3$).

.

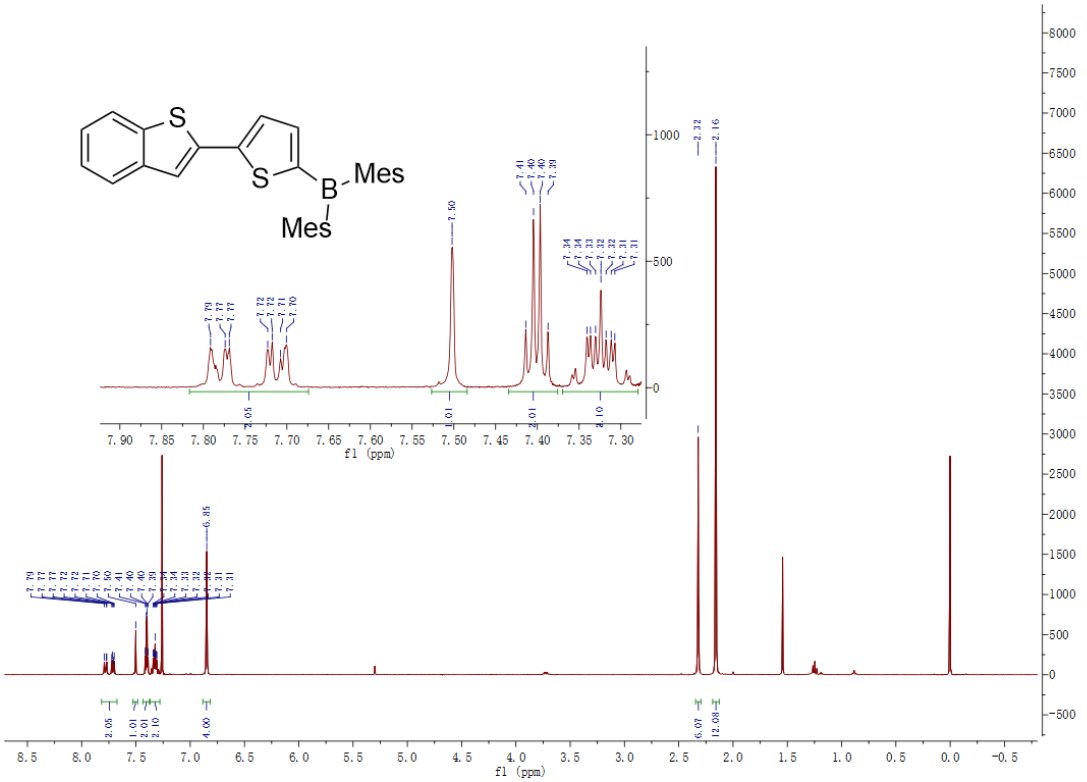


Figure S-16. ^{1}H NMR spectrum of compound **5** (400 MHz, $CDCl_3$).

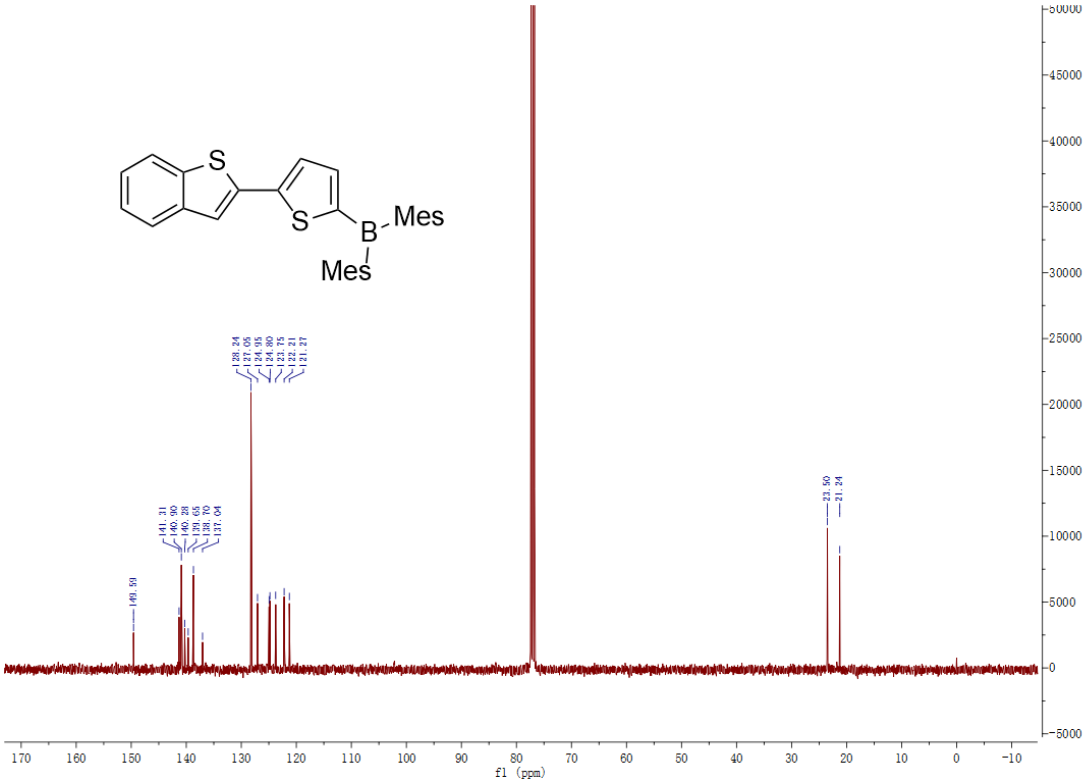


Figure S-17. ^{13}C NMR spectrum of compound **5** (100 MHz, $CDCl_3$).

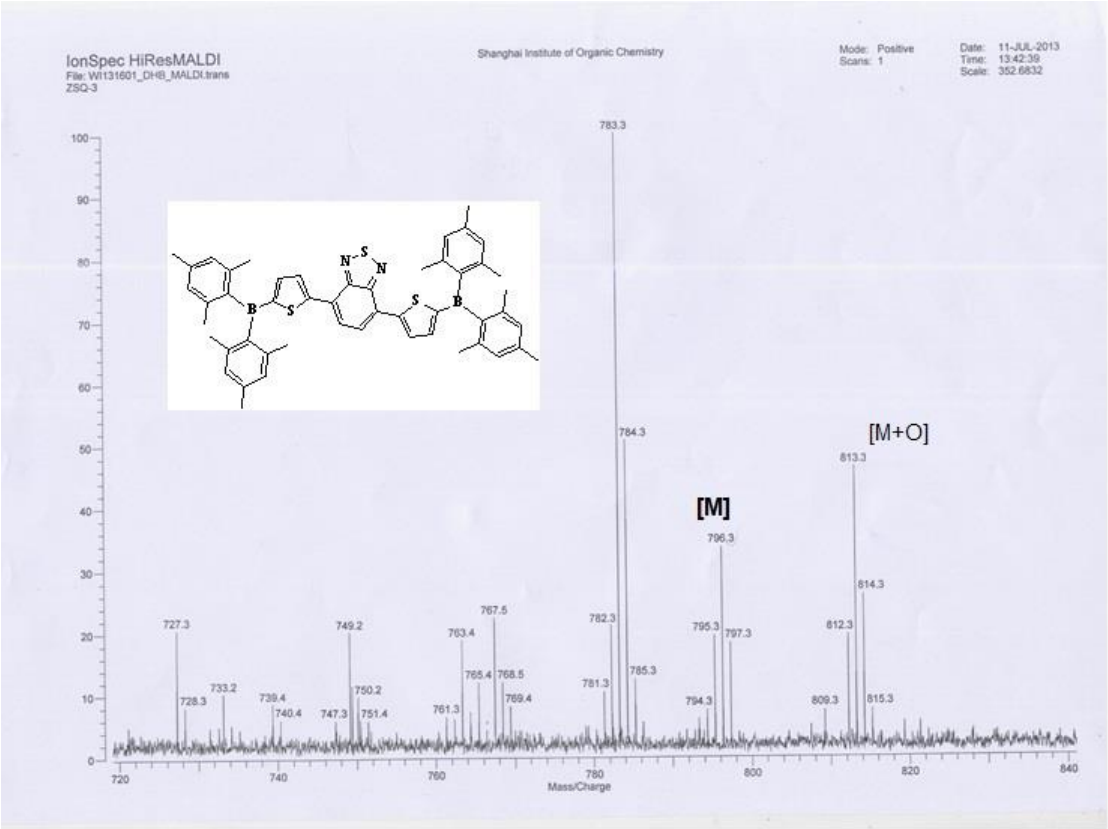


Figure S-18. MS spectra of compound **1**.

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

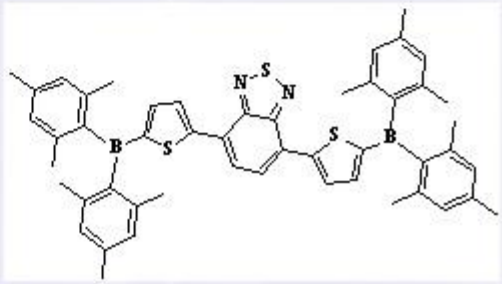
Card Serial Number : WI13 1602

Sample Serial Number: ZSQ-3

Operator : HuaQin Date: 2013/07/11

Operation Mode: MALDI/DHB

Elemental Composition Search Report:



Target Mass:
Target m/z = 794.3408 ± 0.003
Charge = +1

Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
10B	10.012937	0	2
N	14.003074	0	5
S	31.972071	0	5

Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 9

m/z	Delta m/z	DBE	Formula
794.34040	0.00040	40.0	$C_{58}H_{42}N_4^{+1}$
794.34131	-0.00051	20.5	$C_{45}H_{56}N_5S_4^{+1}$
794.34140	-0.00060	41.5	$C_{60}H_{40}{}^{10}B_2N^{+1}$
794.34224	-0.00144	18.0	$C_{47}H_{60}{}^{10}BS_5^{+1}$
794.34231	-0.00151	22.0	$C_{47}H_{54}{}^{10}B_2N_2S_4^{+1}$
794.33894	0.00186	27.0	$C_{50}H_{50}{}^{10}B_2N_2S_3^{+1}$
794.33887	0.00193	23.0	$C_{50}H_{56}{}^{10}BS_4^{+1}$
794.33793	0.00287	25.5	$C_{48}H_{52}N_5S_3^{+1}$
794.34377	-0.00297	35.0	$C_{55}H_{46}N_4S^{+1}$

Figure S-19. HR-MS data report of compound **1**.

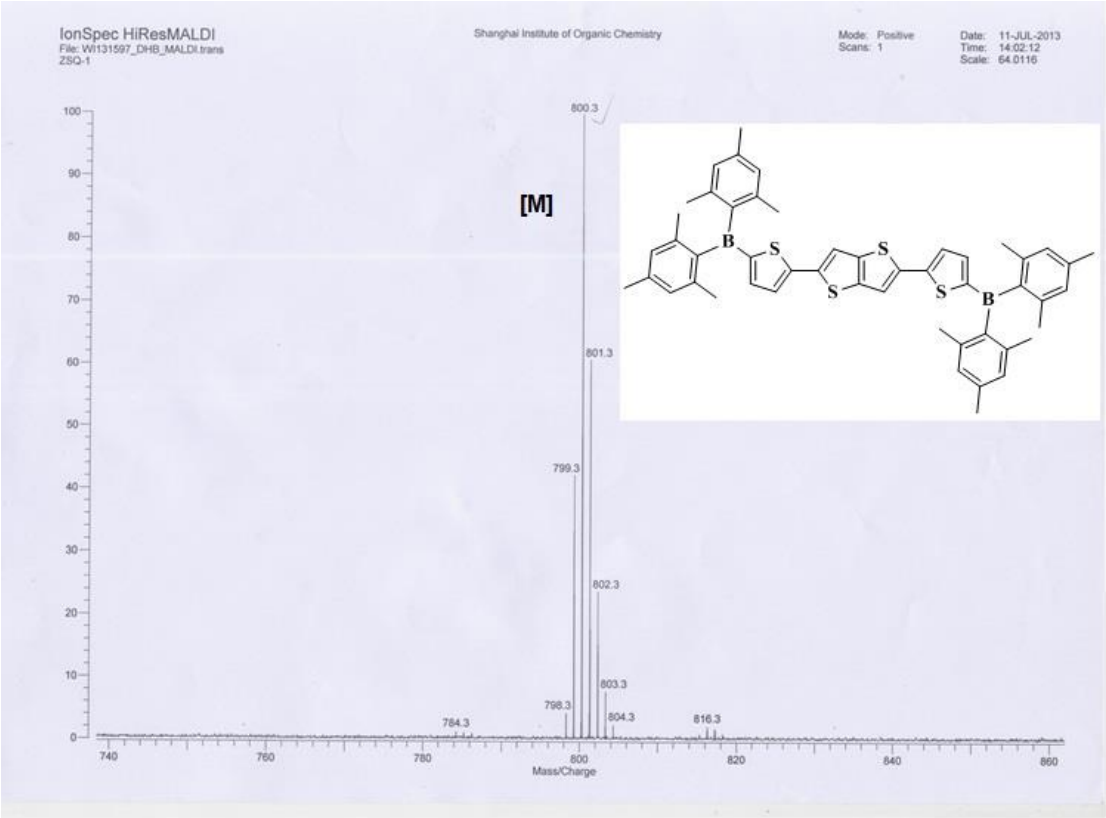


Figure S-20. MS spectra of compound **2**.

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

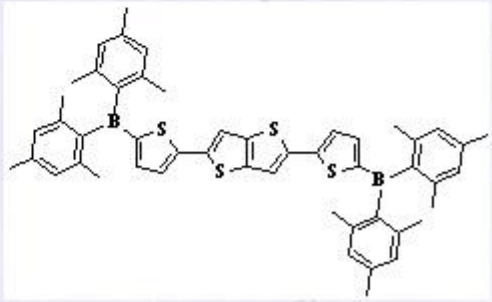
Card Serial Number : WI13 1598

Sample Serial Number: ZSQ-1

Operator : HuaQin Date: 2013/07/11

Operation Mode: MALDI/DHB

Elemental Composition Search Report:



Target Mass:
Target m/z = 798.3060 ± 0.003
Charge = +1

Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
10B	10.012937	0	5
S	31.972071	0	5

Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 2

m/z	Delta m/z	DBE	Formula
798.30486	0.00114	26.0	$C_{50}H_{50}{}^{10}B_2S_4{}^{+1}$
798.30823	-0.00223	21.0	$C_{47}H_{54}{}^{10}B_2S_5{}^{+1}$

Figure S-21. HR-MS data report of compound **2**.

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FTICR-MS
Card Serial Number : D2021629
Sample Serial Number: SD
Operator : DONG Date: 2021/03/18
Operation Mode: DART POSITIVE

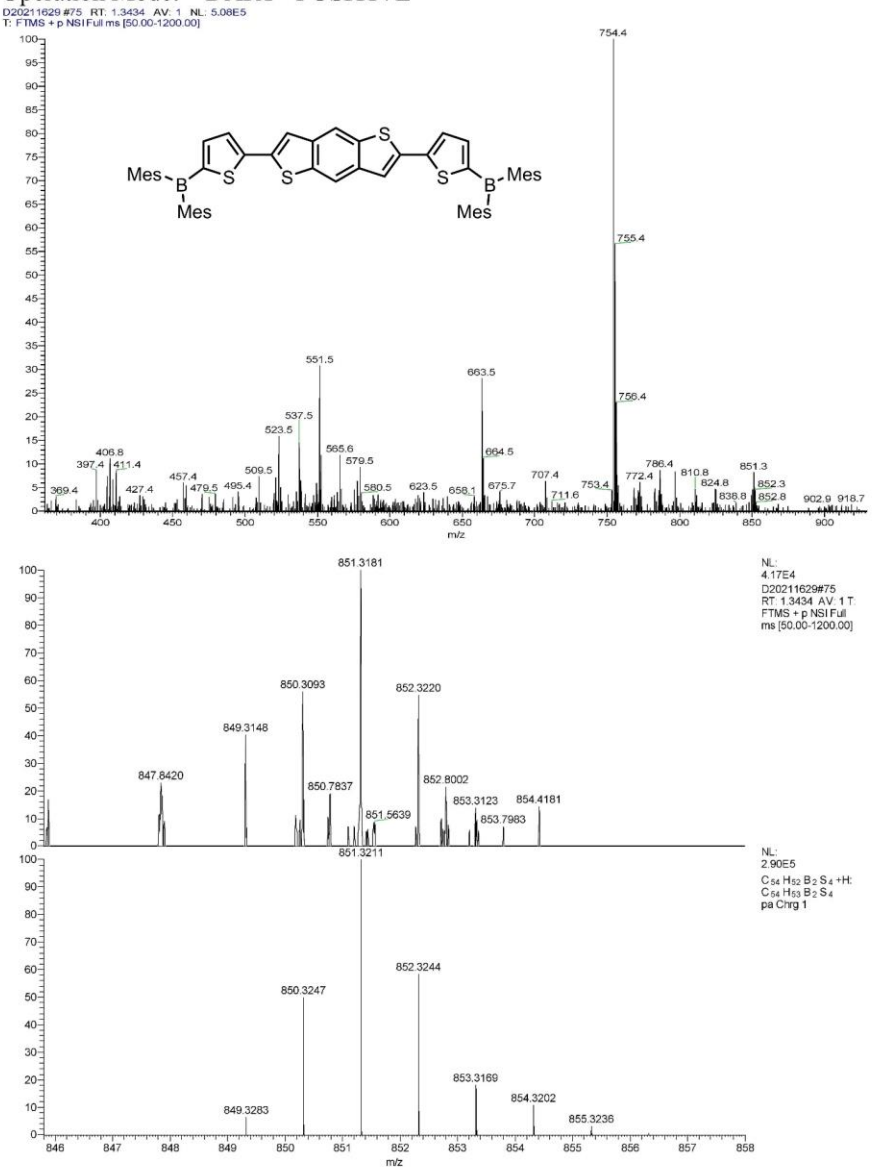


Figure S-22. HR-MS spectra of compound **3**.

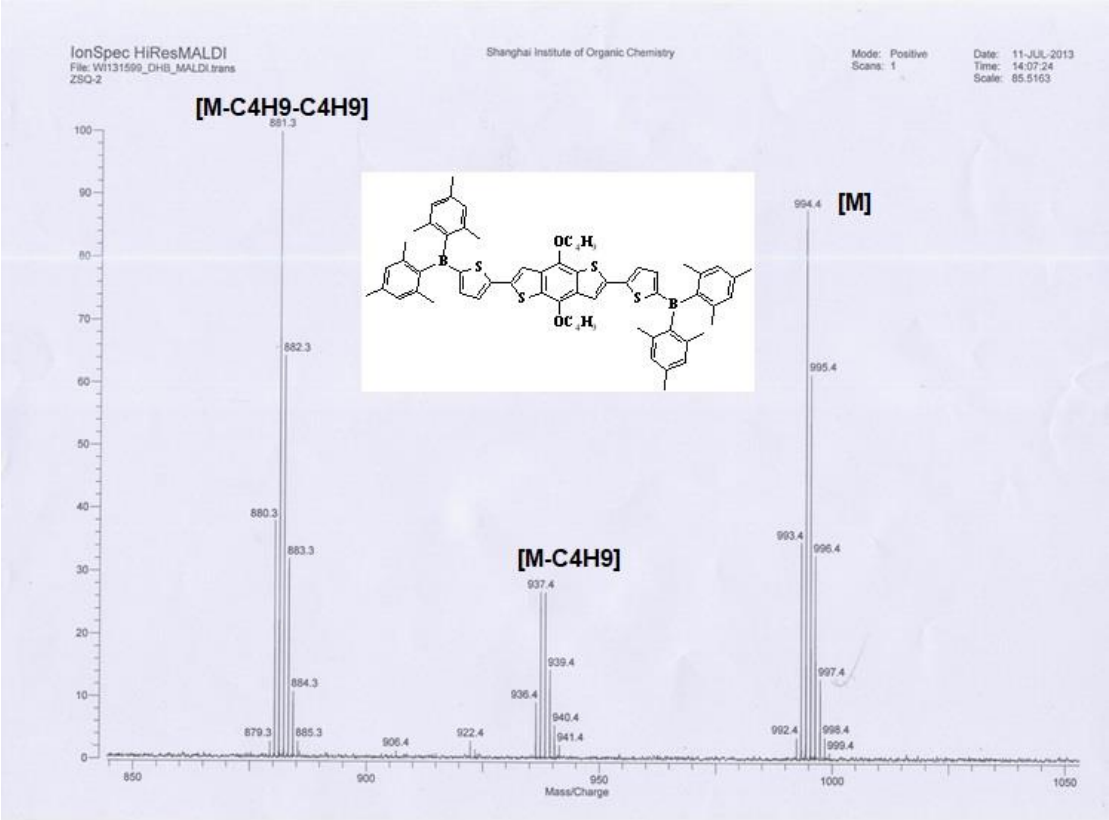


Figure S-23. MS spectra of compound **4**.

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

Card Serial Number : WI13 1600

Sample Serial Number: ZSQ-2

Operator : HuaQin Date: 2013/07/11

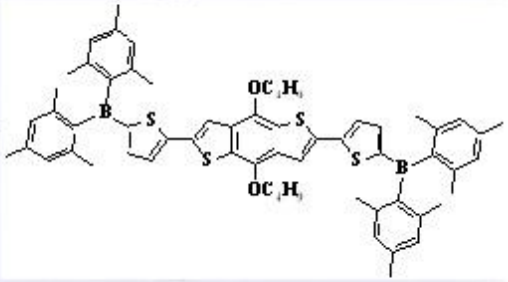
Operation Mode: MALDI/DHB

Elemental Composition Search Report:

Target Mass:
Target m/z = 992.4360 ± 0.003
Charge = +1

Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
10B	10.012937	0	2
O	15.994915	0	5
S	31.972071	0	5

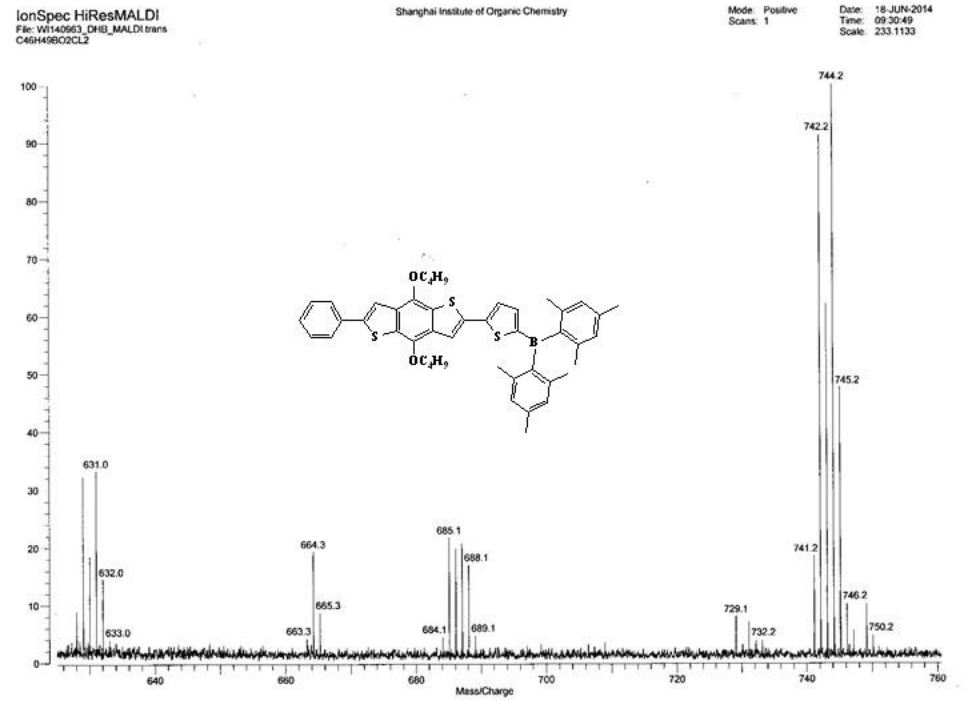


Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 6

m/z	Delta m/z	DBE	Formula
992.43588	0.00012	27.0	$C_{62}H_{72}O_3S_4^{+1}$
992.43554	0.00046	29.0	$C_{62}H_{68}{}^{10}B_2O_2S_4^{+1}$
992.43660	-0.00060	40.0	$C_{70}H_{62}{}^{10}BOS_2^{+1}$
992.43765	-0.00165	51.0	$C_{78}H_{56}^{+1}$
992.43322	0.00278	45.0	$C_{73}H_{58}{}^{10}BOS^{+1}$
992.43891	-0.00291	24.0	$C_{59}H_{72}{}^{10}B_2O_2S_5^{+1}$

Figure S-24. HR-MS data report of compound **4**.



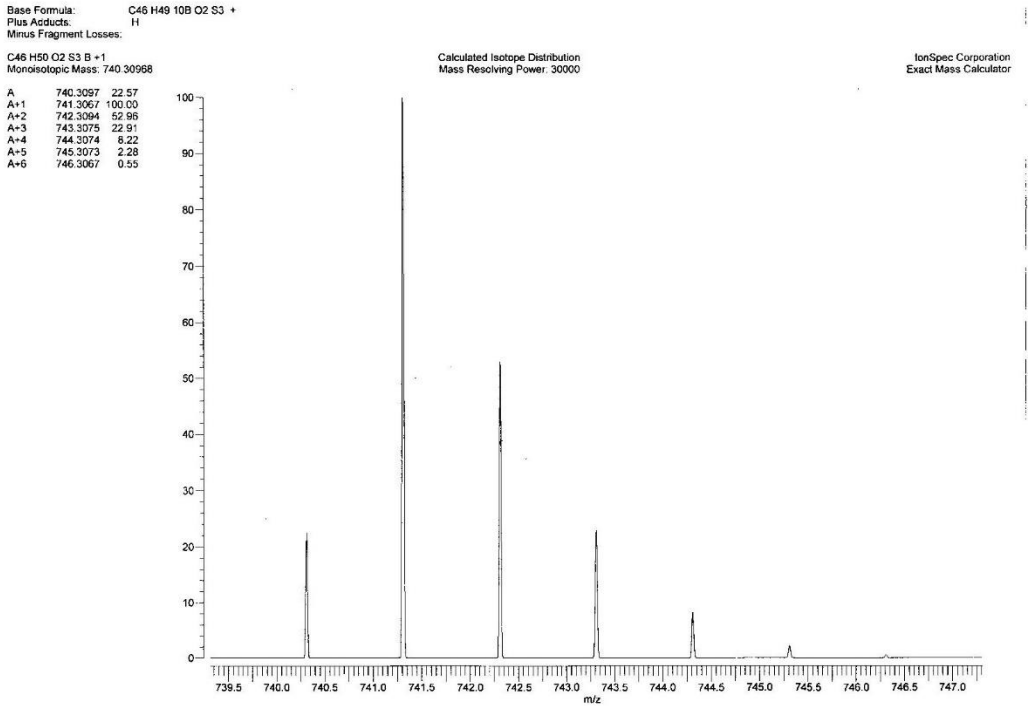


Figure S-25. MS spectra of compound **4'**.

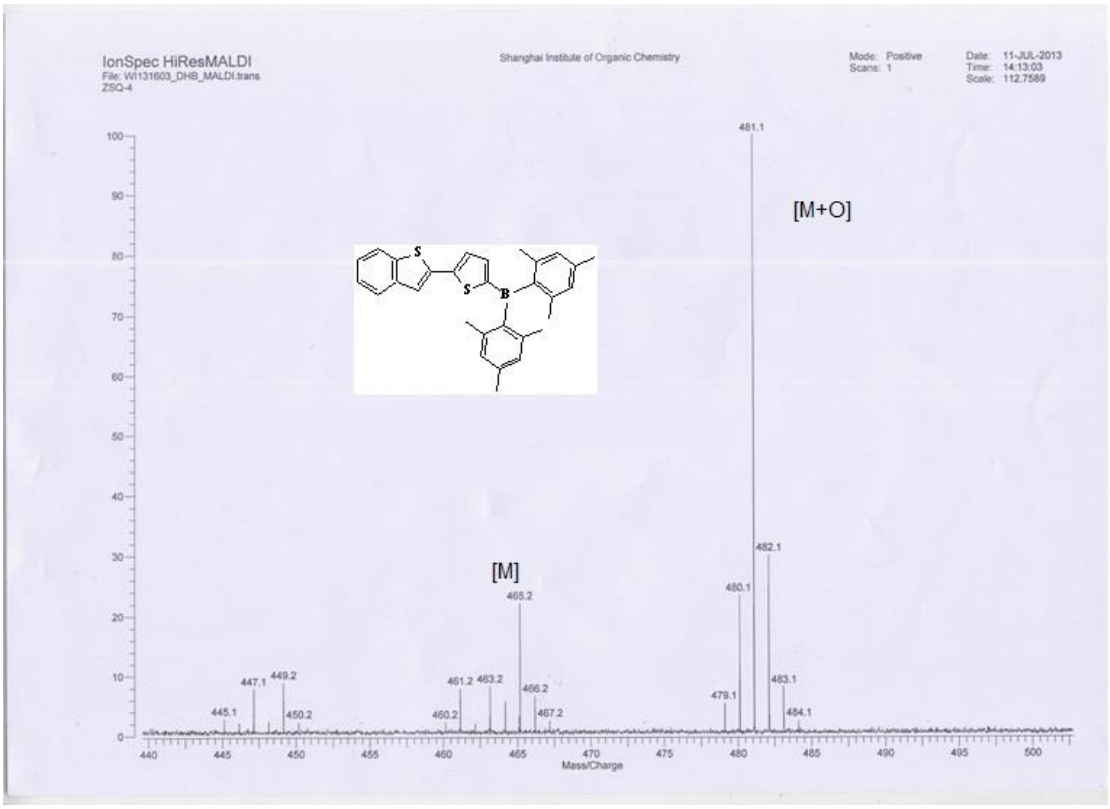


Figure S-26. MS spectra of compound **5**.

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: IonSpec 4.7 Tesla FTMS

Card Serial Number : WI13 1604

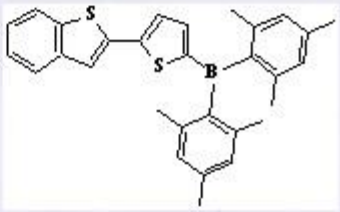
Sample Serial Number: ZSQ-4

Operator : HuaQin Date: 2013/07/11

Operation Mode: MALDI/DHB

Elemental Composition Search Report:

Target Mass:
Target m/z = 464.1915 ± 0.002
Charge = +1



Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
10B	10.012937	0	2
S	31.972071	0	5

Additional Search Restrictions:
DBE Limit Mode = Both Integer and Half-Integer
Minimum DBE = 0

Search Results:
Number of Hits = 1

m/z	Delta m/z	DBE	Formula
464.19128	0.00022	16.0	$C_{30}H_{30}{}^{10}BS_2{}^{+1}$

Figure S-27. HR-MS data report of compound **5**