Supporting Information for:

All Thiophene-Based Double Helix: Synthesis, Crystal Structure, Chiroptical Property and Arylation

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Table of Contents:

NMR, HRMS and IR Spectra of DH-1

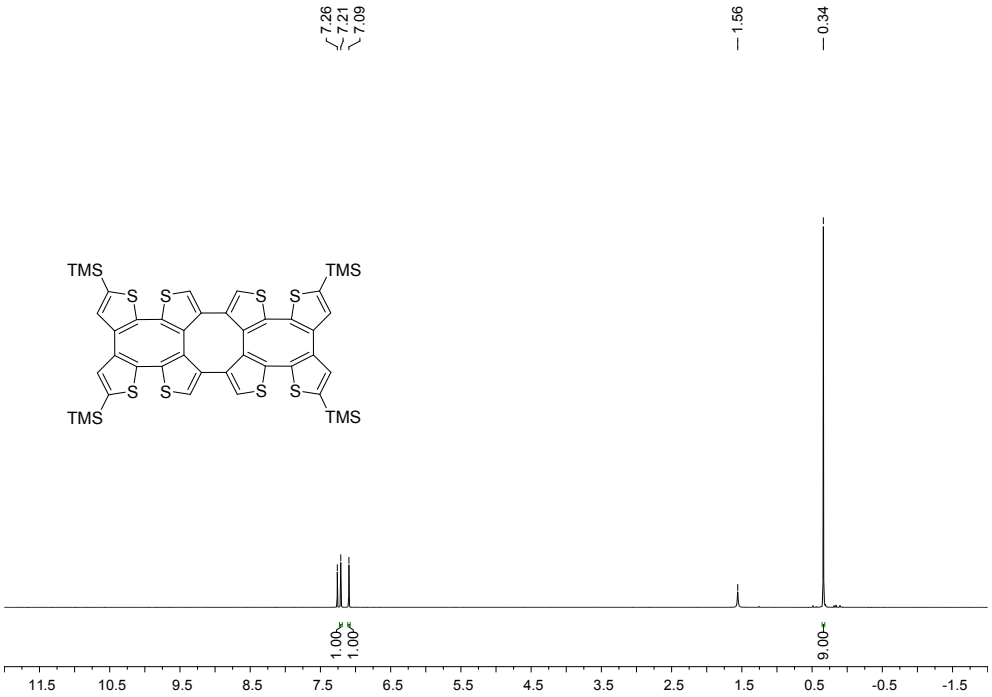

Figure S1. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **DH-1**

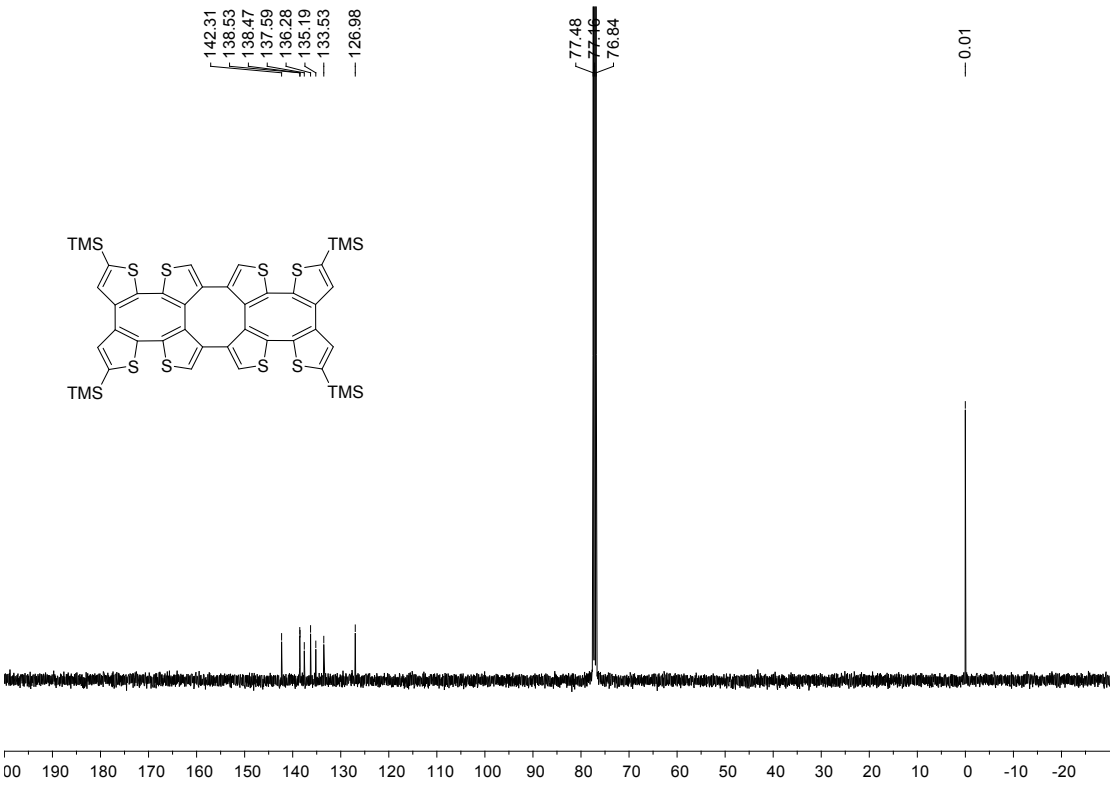

Figure S2. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **DH-1**

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 2069

Sample Serial Number: zs-3-187-col-pp

Operator : HuaQin Date: 2013/10/16

Operation Mode: MALDI/DHB

Elemental Composition Search Report:

Target Mass:
Target m/z = 940.0261 ± 0.004
Charge = +1

Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
Si	27.976927	0	5
S	31.972071	0	9

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

Search Results:
Number of Hits = 5

m/z	Delta m/z	DBE	Formula
940.02602	0.00008	55.0	$C_{64}H_{20}Si_2S_3^{+1}$
940.02466	0.00144	28.0	$C_{47}H_{40}Si_4S_7^{+1}$
940.02803	-0.00193	23.0	$C_{44}H_{44}Si_4S_8^{+1}$
940.02939	-0.00329	50.0	$C_{61}H_{24}Si_2S_4^{+1}$
940.02265	0.00345	60.0	$C_{67}H_{16}Si_2S_2^{+1}$

Figure S3. HRMS data of **DH-1**

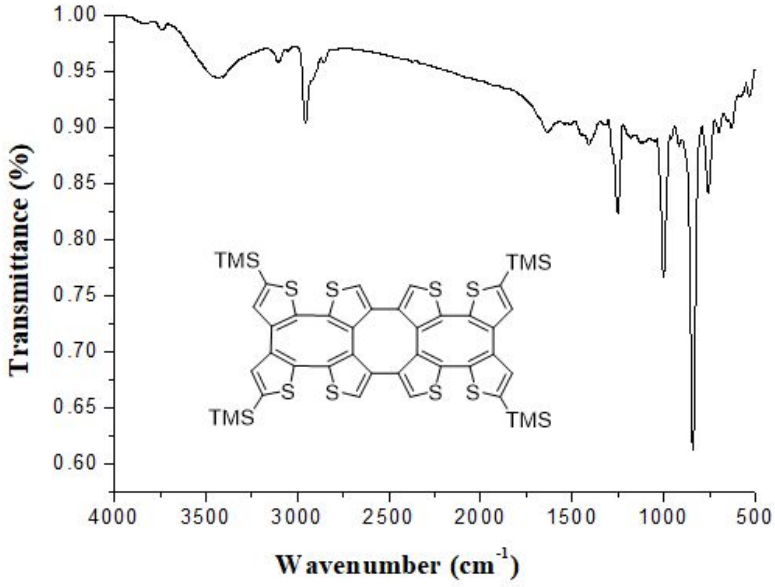

Figure S4. IR spectrum of **DH-1**

NMR, HRMS and IR Spectra of DH-1-Br

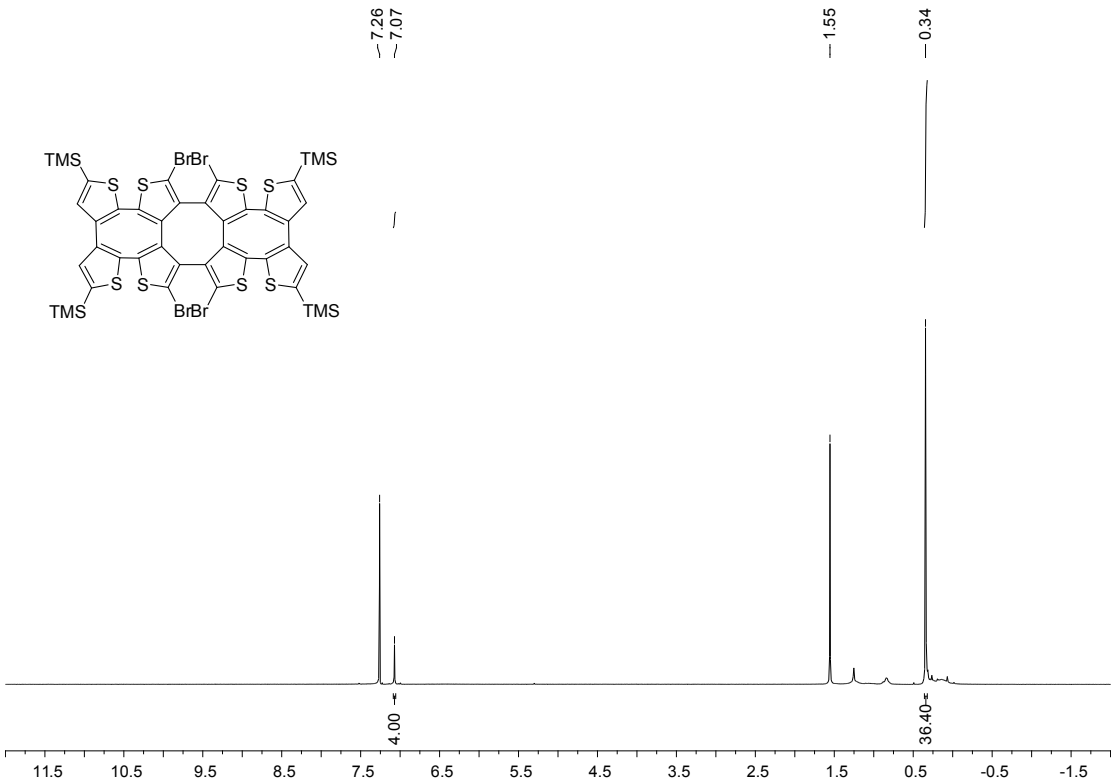

Figure S5. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **DH-1-Br**

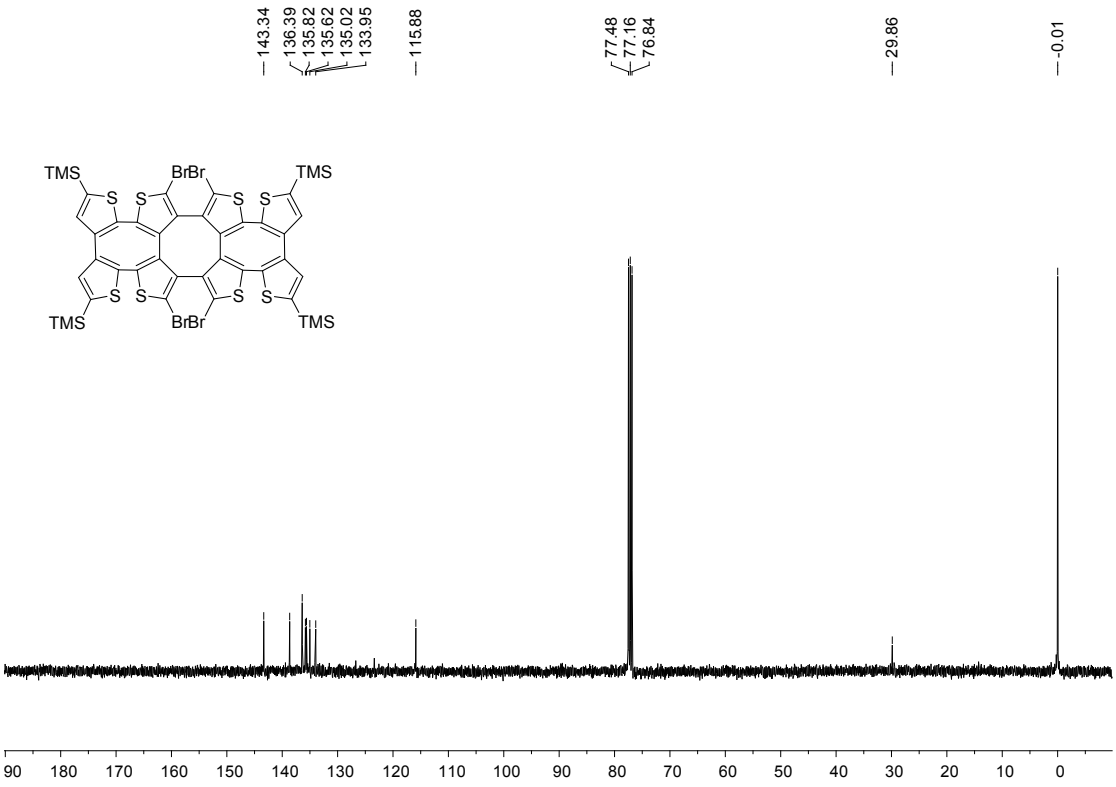

Figure S6. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **DH-1-Br**

LBB-4BrOH: HRMS (ESI) m/z calcd for $C_{44}H_{41}Br_4S_8Si_4^+$ $(M+H)^+$ 1252.67790, found 1252.68481.

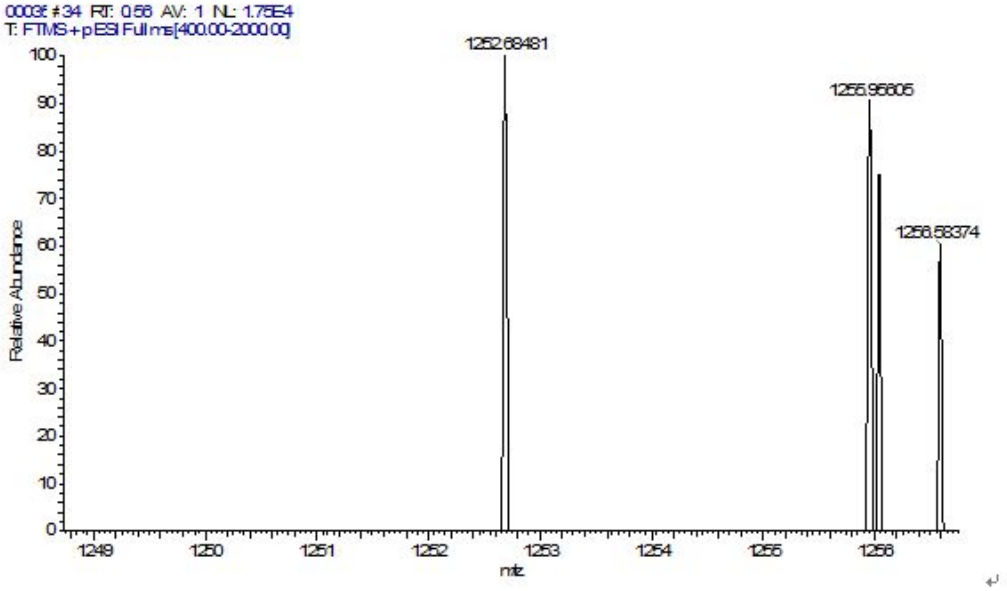

Figure S7. HRMS spectrum of **DH-1-Br**

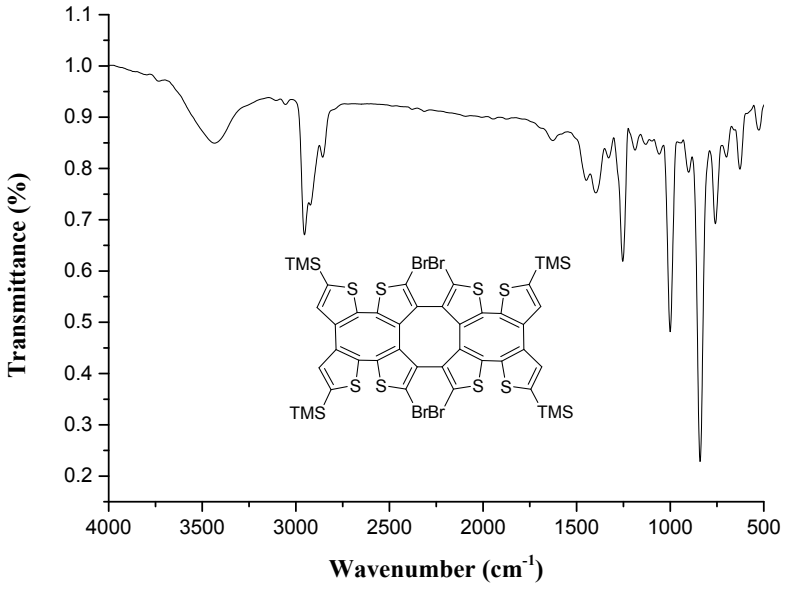

Figure S8. IR spectrum of **DH-1-Br**

NMR, HRMS and IR Spectra of DH-1-Ph

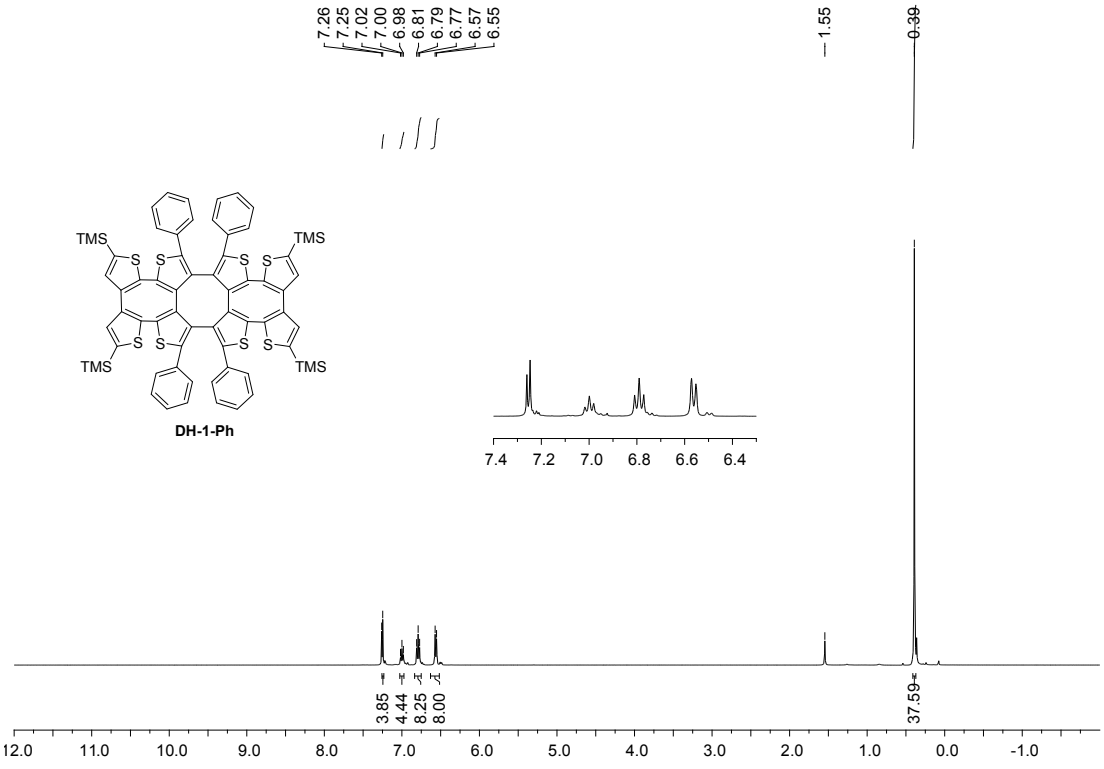

Figure S9. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **DH-1-Ph**

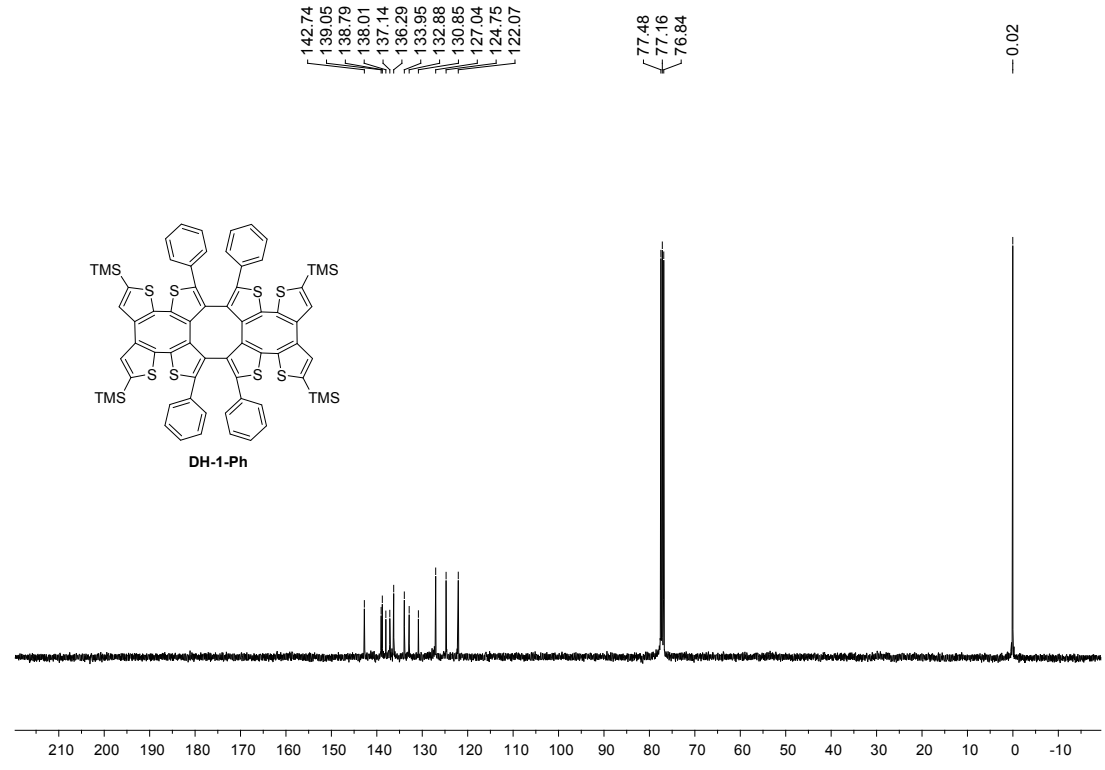

Figure S10. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **DH-1-Ph**

LBB-5-11: HRMS (ESI) m/z calcd for $C_{68}H_{61}S_8Si_4^+$ $(M+H)^+$ 1245.16105, found 1245.16152.

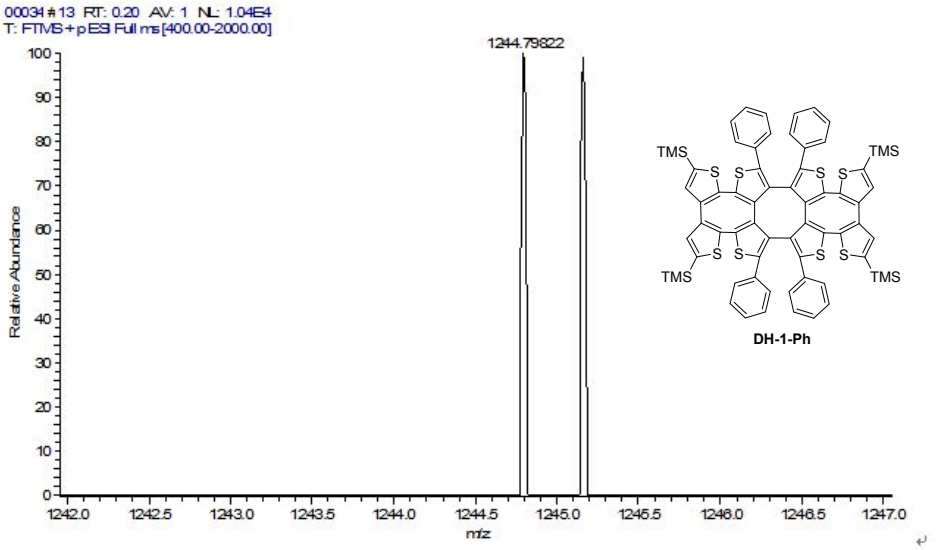

Figure S11. HRMS spectrum of **DH-1-Ph**

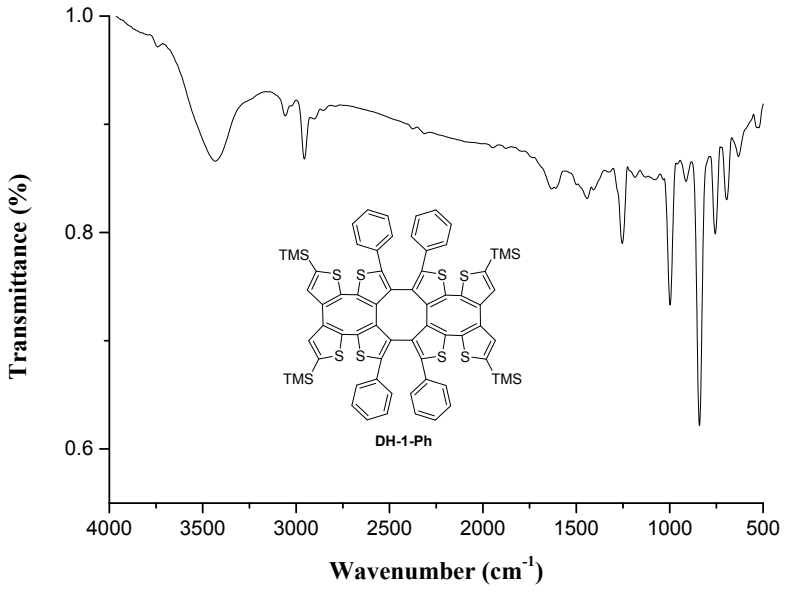

Figure S12. IR spectrum of **DH-1-Ph**

NMR, HRMS and IR Spectra of DH-1-Th

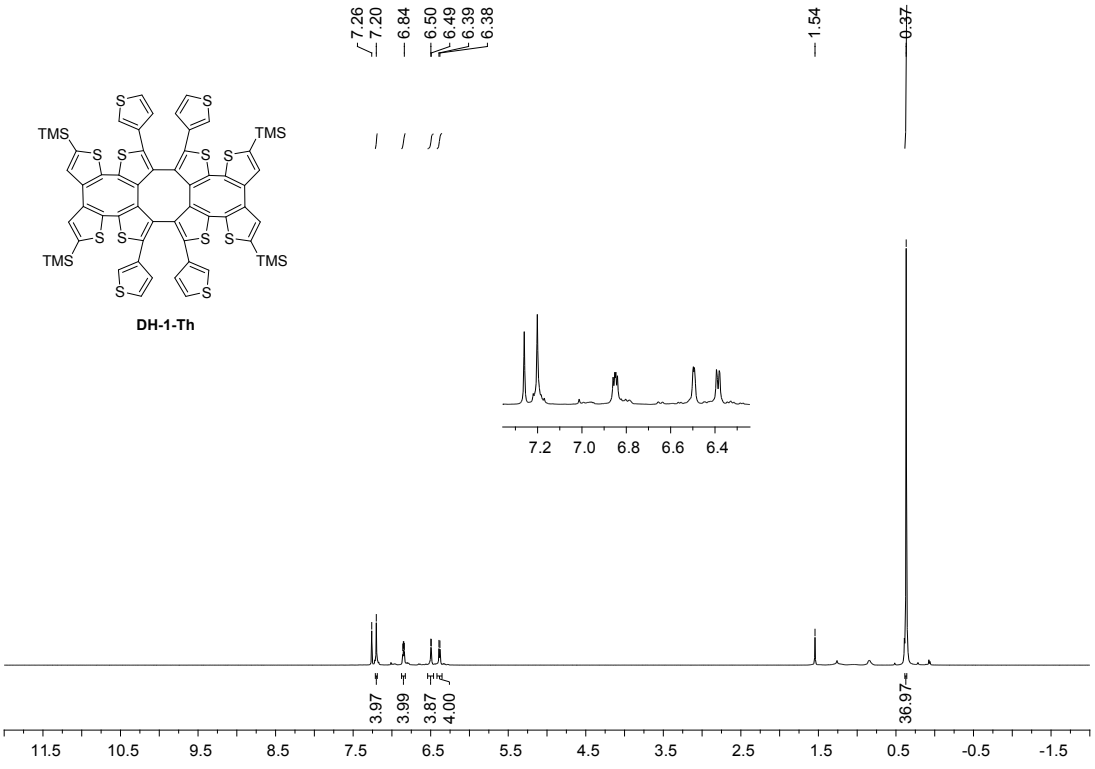

Figure S13. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **DH-1-Th**

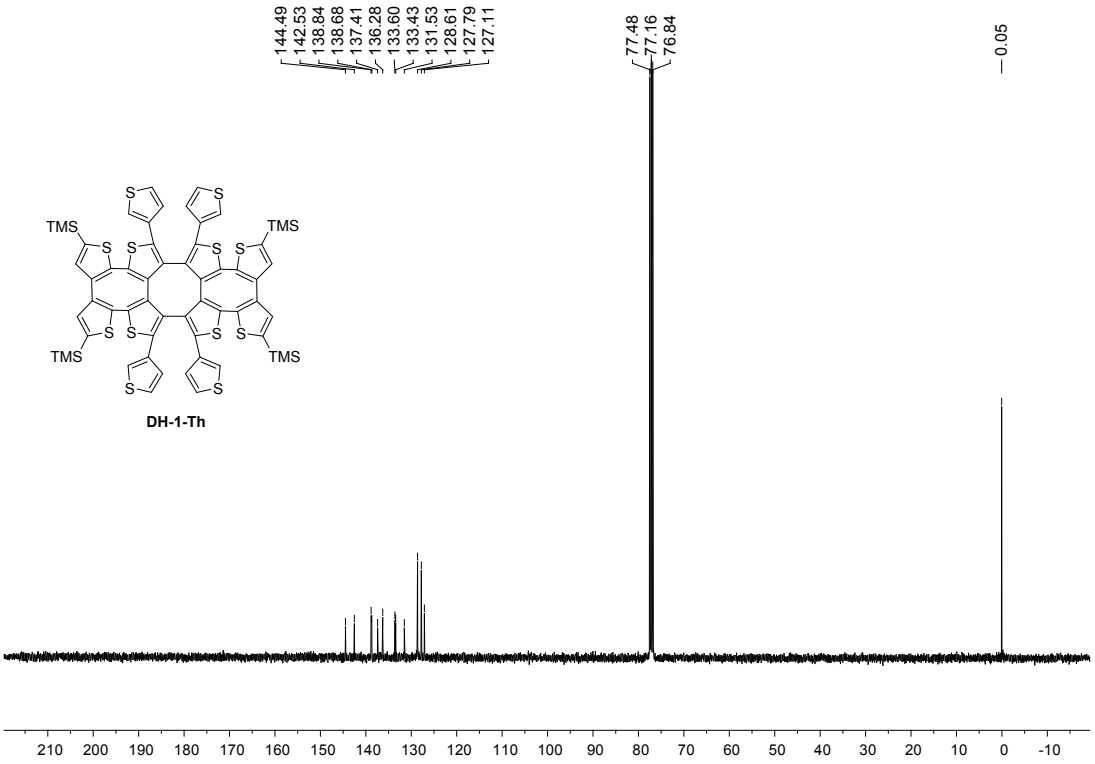

Figure S14. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of **DH-1-Th**

LBB-5-13: HRMS (ESI) m/z calcd for $C_{60}H_{53}S_{12}Si_4^+$ $(M+H)^+$ 1268.98673, found 1268.98865.

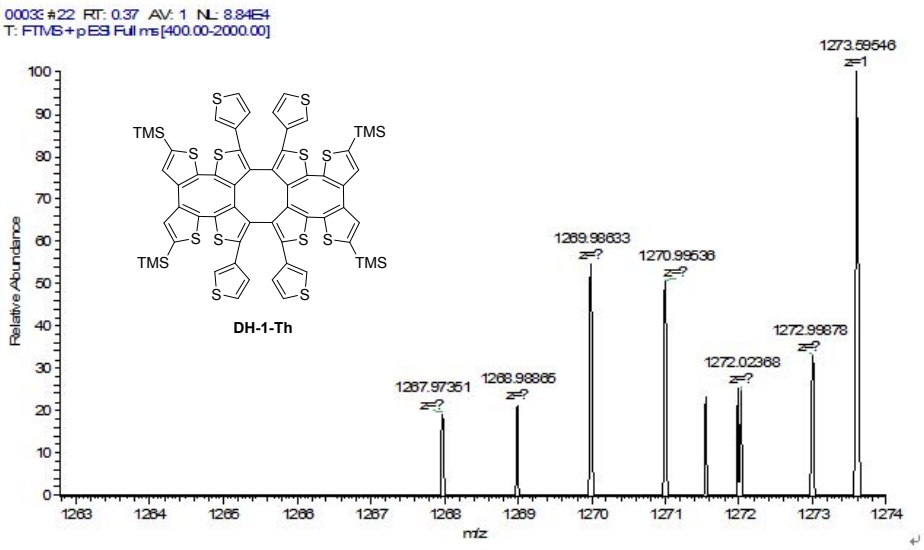

Figure S15. HRMS spectrum of **DH-1-Th**

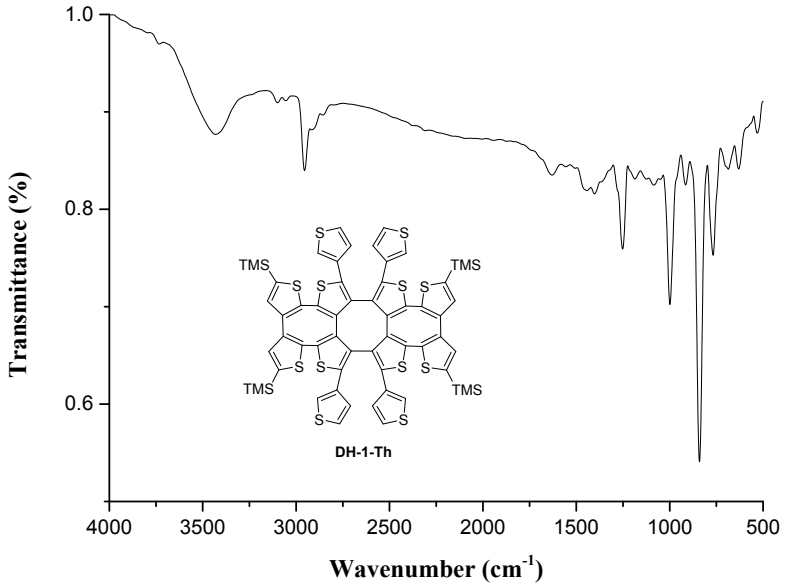

Figure S16. IR spectrum of **DH-1-Th**

Resolution of *rac*-DH-1

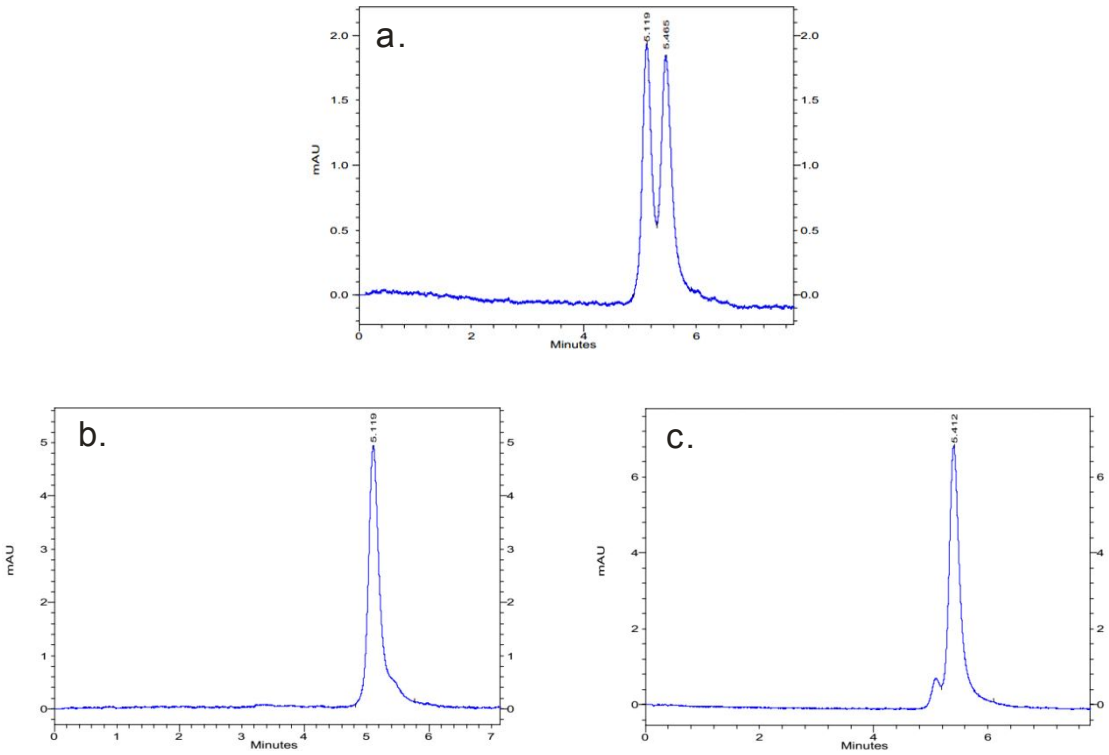

Figure S17. HPLC spectra of (a) *rac*-**DH-1**, (b) (-)-**DH-1** and (c) (+)-**DH-1** (*n*-hexane/isopropanol (99.5:0.5, v/v), flow rate: 1.0 mL/min).

Table S1. X-ray crystallographic data of DH-1

Identification code	**DH-1**
Empirical formula	$C_{46}H_{46}C_{l6}S_8Si_4$
Formula weight	1180.37
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a= 11.9267(15) Å α = 108.373(2) °.
	b = 15.095(2) Å β = 105.652(2) °.
	c = 17.872(2) Å γ = 101.258(2) °.
Volume	2798.7(6) Å ^{3}
Z, Calculated density	2, 1.401 Mg/m^3
Absorption coefficient	0.723 mm^{-1}
F(000)	1216
Crystal size	0.33 × 0.21 × 0.17 mm
Theta range for data collection	1.54 to 25.00 °.
Limiting indices	-13<=h<=14, -17<=k<=17, -21<=l<=21
Reflections collected / unique	14179 / 9774 [R(int) = 0.0263]

Completeness to theta = 25.00	99.20%
Max. and min. transmission	0.8869 and 0.7963
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9774 / 36 / 577
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R1 = 0.0658, wR2 = 0.1598
R indices (all data)	R1 = 0.0855, wR2 = 0.1708
Largest diff. peak and hole	1.806 and -1.899 e. Å $^{-3}$

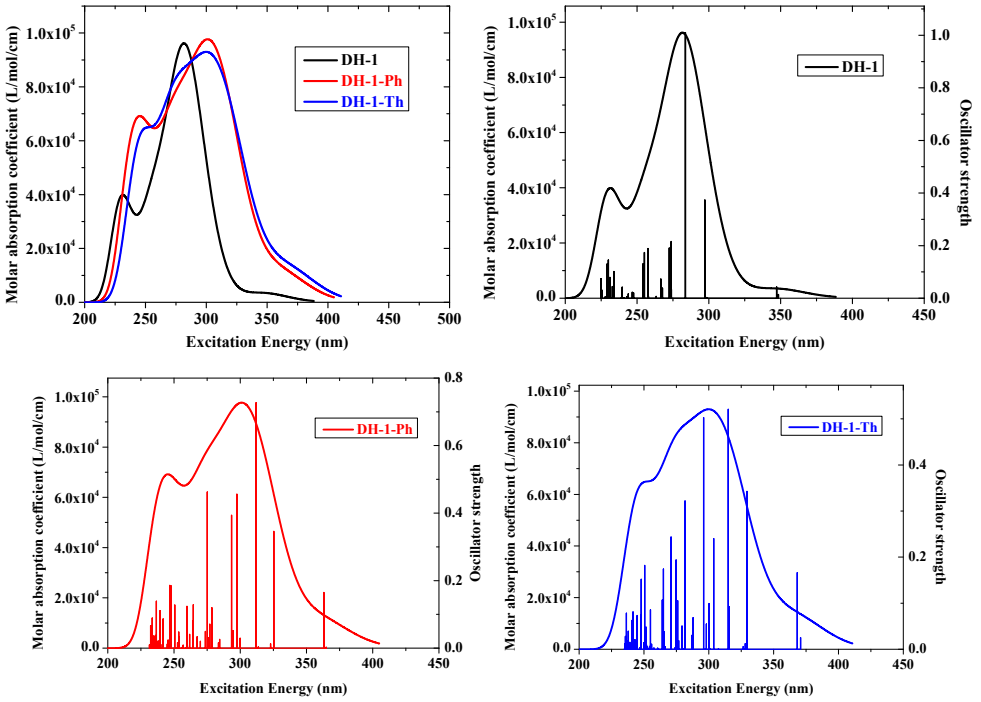

Figure S18. Calculated absorption spectra of **DH-1**, **DH-1-Ph** and **DH-1-Th** in dichloromethane solution using TDDFT/PCM approaches.

Table S2. The peaks position (nm, experimental values in parentheses) of the predicted UV-vis spectra and computational absorption energies (λ, nm), oscillator strength (*f*), and transition nature and the square of transition dipole moment between the excited-state and ground-state(μ_{eg}^2).

	Peaks position	states	λ (nm)	f	Transition contributions	μ_{eg}^2
DH-1	231 (231)	$S_0 \rightarrow S_{37}$	233.7	0.1013	HOMO-6→LUMO+3(10%) HOMO-4→LUMO+3(36%) HOMO-1→LUMO+6(21%)	0.7798
	282 (281)	$S_0 \rightarrow S_7$	283.5	1.0098	HOMO-1→LUMO+3(37%) HOMO→LUMO+2(58%)	9.4248
	347 (344)	$S_0 \rightarrow S_2$	346.9	0.0424	HOMO-1→LUMO+1(45%) HOMO→LUMO(53%)	0.4842
DH-1-Ph	245 (239)	$S_0 \rightarrow S_{47}$	247.6	0.1845	HOMO-15→LUMO(14%)	1.5042

					HOMO-11→LUMO(26%) HOMO-1→LUMO+8(17%)	
		$S_0 \rightarrow S_{48}$	246.6	0.1856	HOMO-11→LUMO+1(18%) HOMO→LUMO+8(18%)	1.5065
		$S_0 \rightarrow S_{59}$	239.3	0.111	HOMO-11→LUMO+2(23%) HOMO-11→LUMO+3(33%) HOMO-9→LUMO+5(15%)	0.8747
	300 (286)	$S_0 \rightarrow S_8$	311.8	0.7275	HOMO-4→LUMO+2(65%) HOMO-4→LUMO+3(30%)	7.4681
		$S_0 \rightarrow S_{11}$	297.2	0.4558	HOMO-5→LUMO+2(94%)	4.4600
		$S_0 \rightarrow S_{14}$	293.2	0.3934	HOMO-5→LUMO+1(80%)	3.7968
		$S_0 \rightarrow S_2$	362.8	0.1648	HOMO-2→LUMO (53%) HOMO-2→LUMO+1(42%)	1.9686
DH-1-Th	250 (239)	$S_0 \rightarrow S_{48}$	250.3	0.1818	HOMO-9→LUMO+6(41%) HOMO-8→LUMO+7(27%)	1.4978
		$S_0 \rightarrow -S_{51}$	247.7	0.1519	HOMO-9→LUMO+6(14%) HOMO-10→LUMO+8(13%) HOMO-10→LUMO+9(19%)	1.2389
	300 (286)	$S_0 \rightarrow S_8$	314.8	0.5206	HOMO-4→LUMO+2(25%) HOMO-5→LUMO+3(48%) HOMO-3→LUMO+2(23%)	5.3948
		$S_0 \rightarrow S_{10}$	303.6	0.2401	HOMO-5→LUMO+1(45%) HOMO-5→LUMO+3(15%) HOMO-3→LUMO+2(16%)	2.3998
		$S_0 \rightarrow S_{14}$	295.8	0.5026	HOMO-5→LUMO+2(93%)	4.8947
		$S_0 \rightarrow S_2$	368.0	0.1663	HOMO-2→LUMO(24%) HOMO-3→LUMO+1(49%) HOMO-1→LUMO (22%)	2.0142