BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Thiophene/selenophene-based S-shaped double helicenes: regioselective synthesis and structures

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Spectral and computational data

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1. NMR and HRMS spectra

NMR spectra and HRMS data of compound 5a

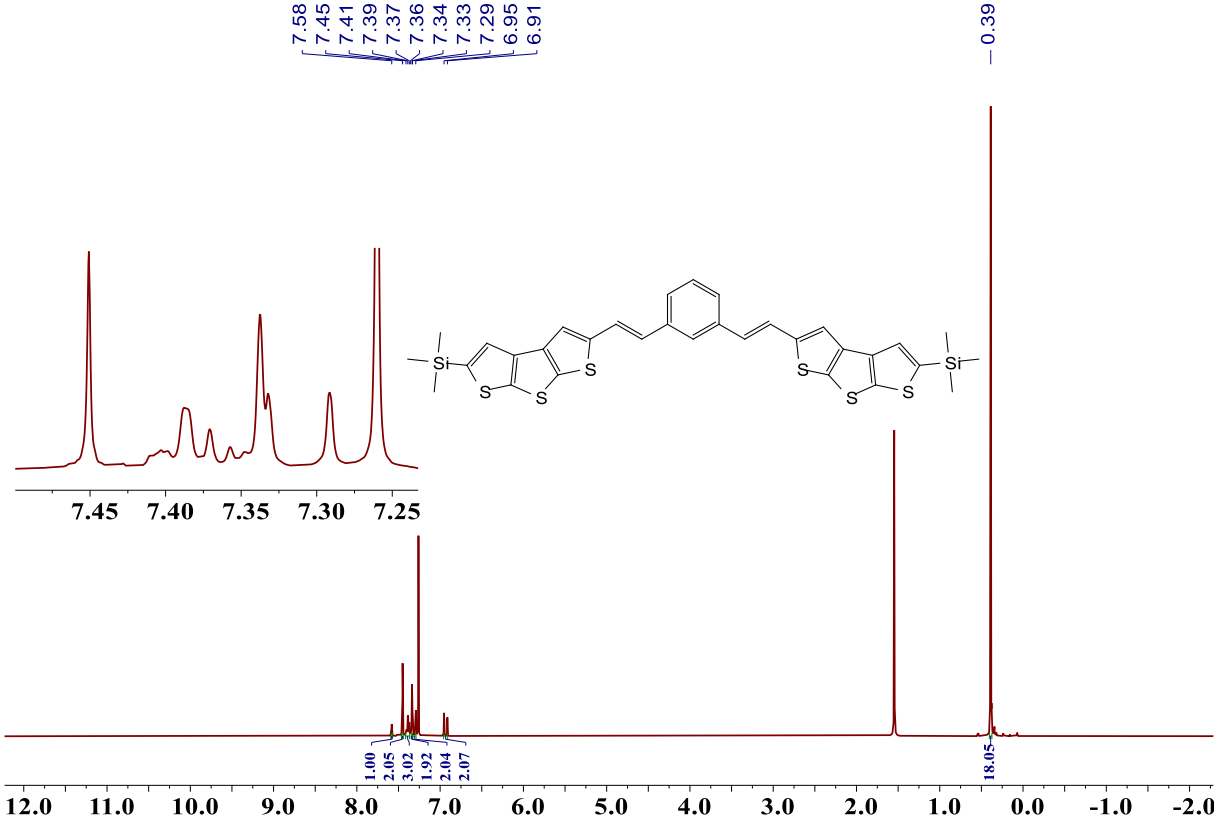


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5a**

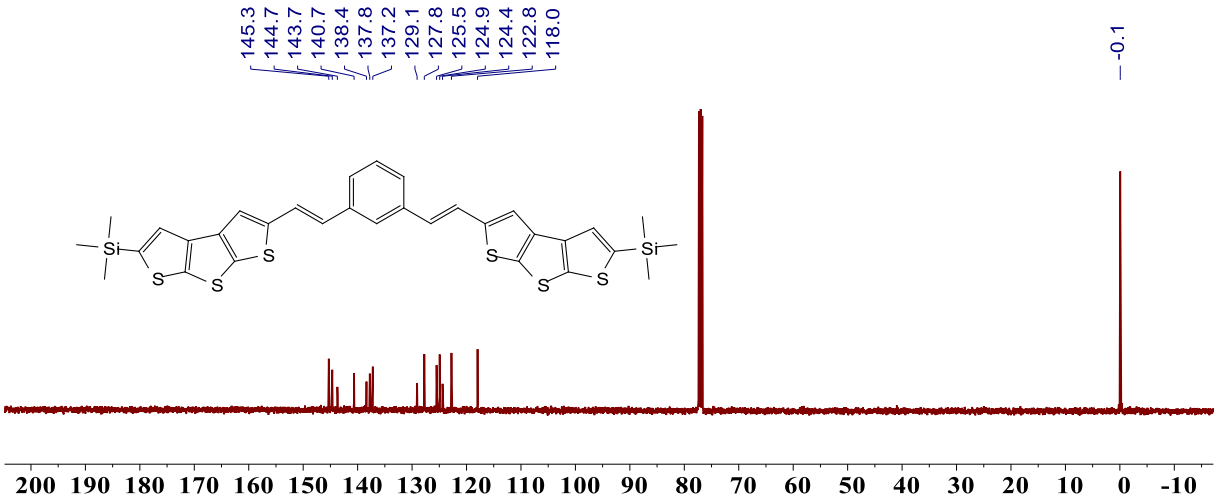


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **5a**

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
662.02162 ± 0.00331	5.0 ppm	Odd/Even	+1	-0.5 - 200.0	100

Elements

C	H	N	Si	S	Na
0 - 32	0 - 150	0 - 4	0 - 2	0 - 6	0 - 1

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C28 H27 N4 Na Si S6	662.02214	18.0	0.00052	-0.00052	-0.78
2	C32 H30 Si2 S6	662.02048	20.0	0.00114	0.00114	1.73
3	C31 H23 N4 Na Si S5	662.01877	23.0	0.00285	0.00285	4.31
4	C30 H26 N4 Si S6	662.02455	21.0	0.00292	-0.00292	-4.42

Figure S3. HRMS data of **5a**

NMR and HRMS spectra of 5b

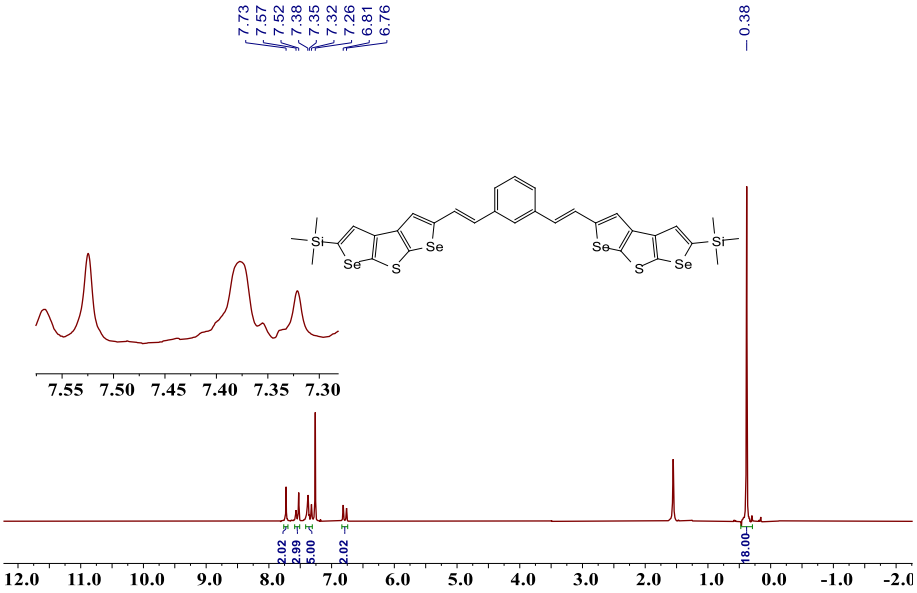


Figure S4. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **5b**

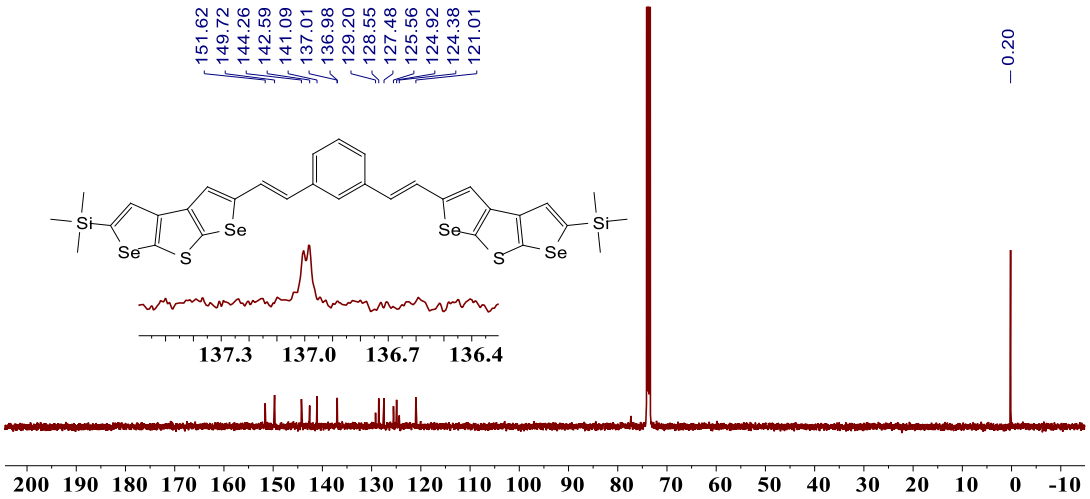


Figure S5. ^{13}C NMR (150 MHz, $C_2D_2Cl_4$) spectrum of **5b**

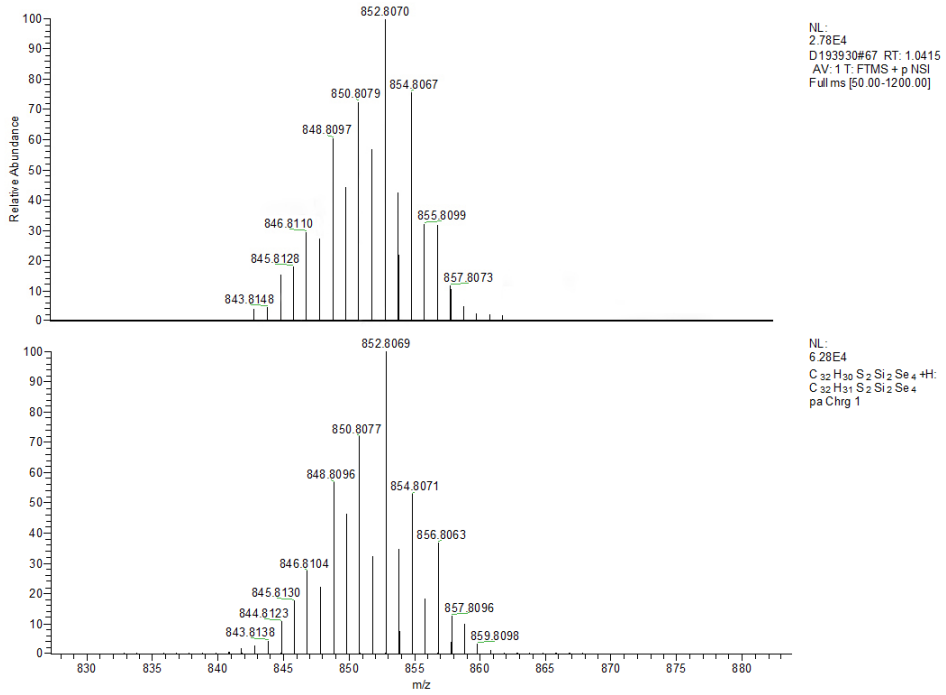


Figure S6. HRMS spectrum of **5b**

NMR and HRMS spectra of 5c

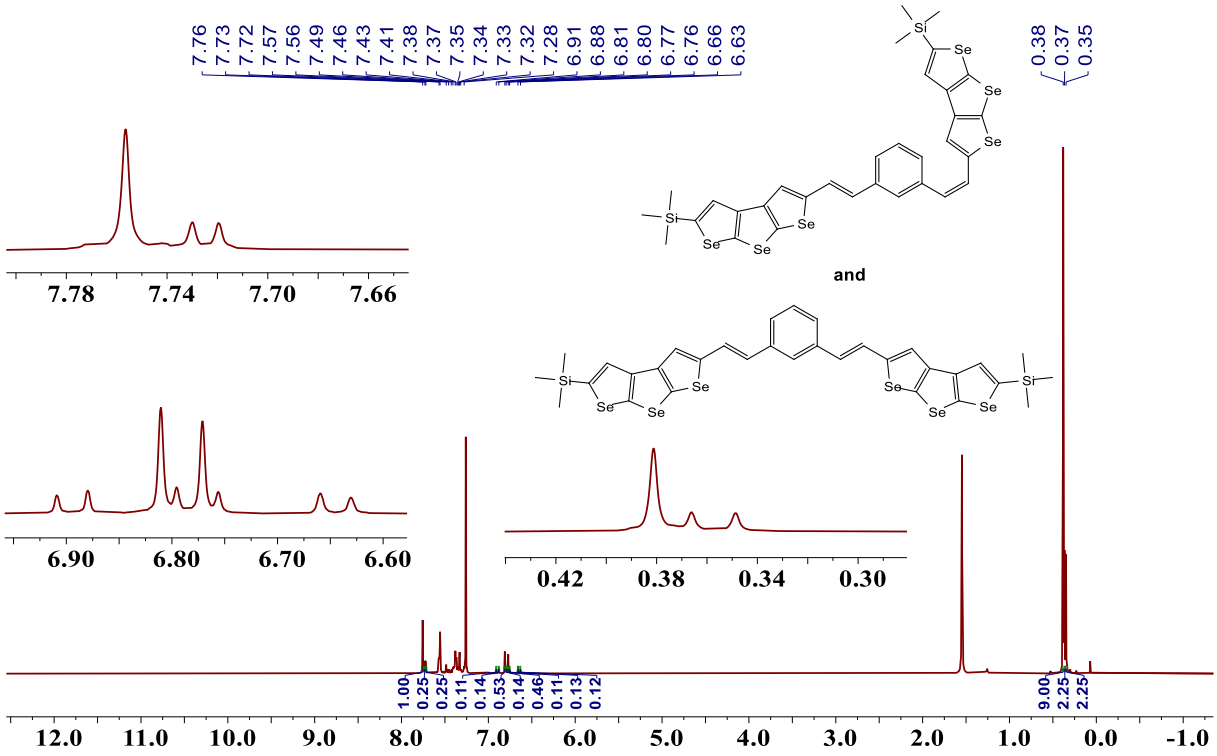


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of mixture of *cis*- and *trans*-**5c**

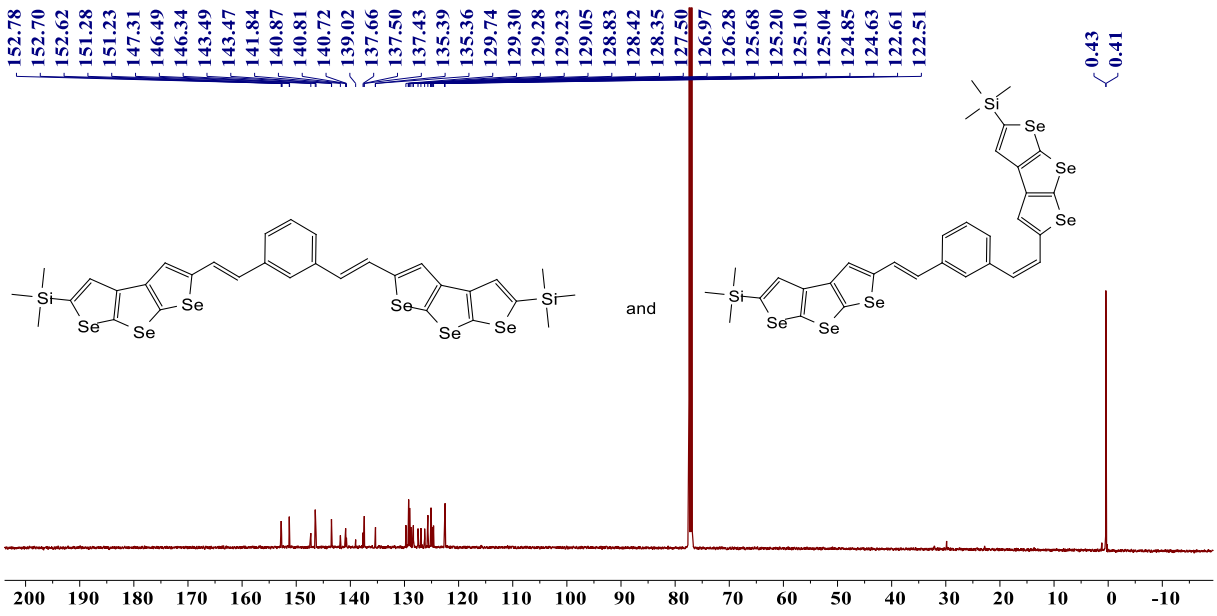


Figure S8. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of mixture of *cis*- and *trans*-**5c**

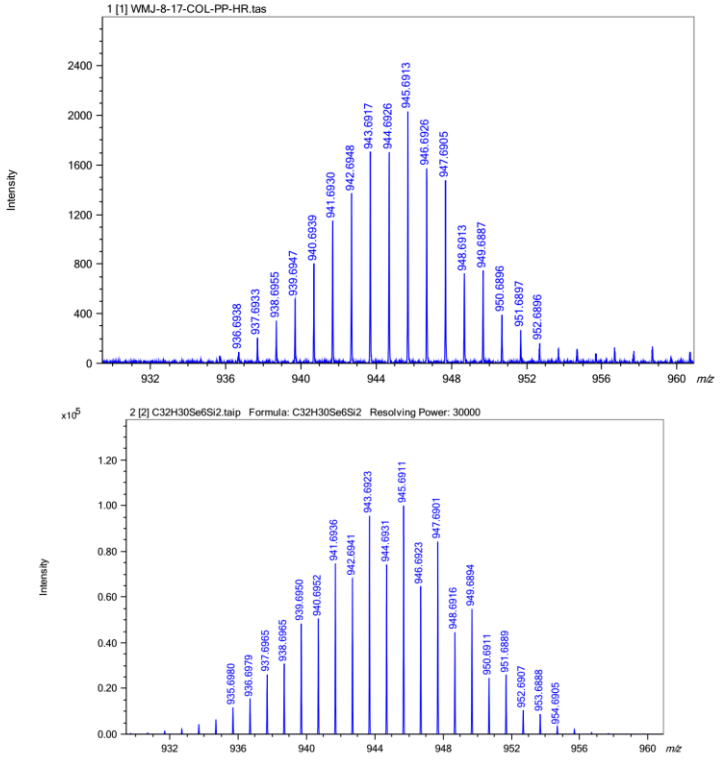


Figure S9. HRMS spectrum and data of **5c**

NMR spectra and HRMS data of DH-1

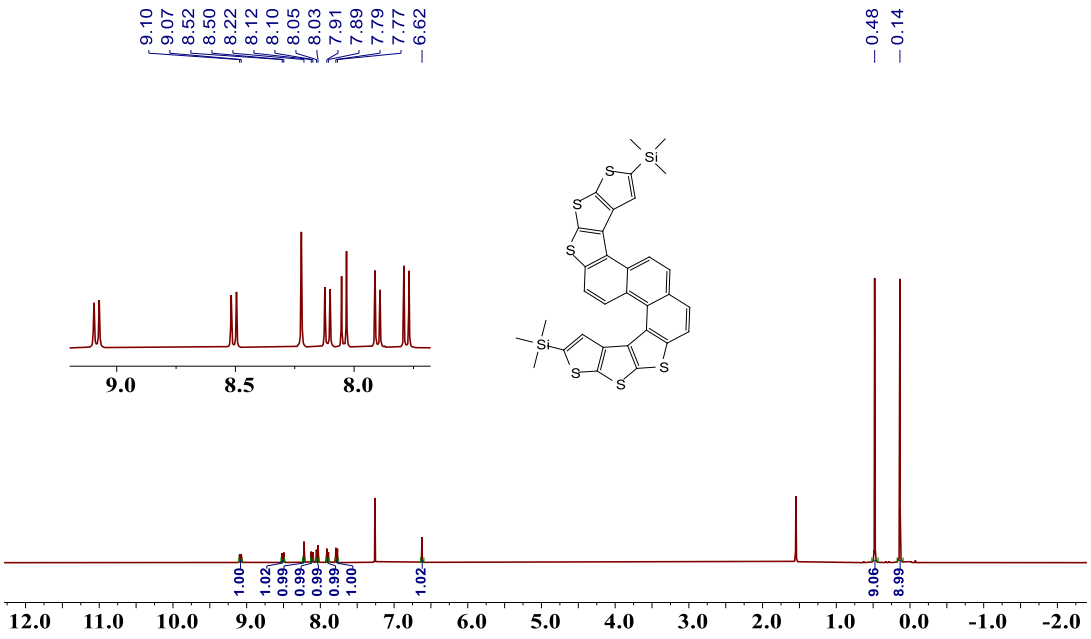


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **DH-1**

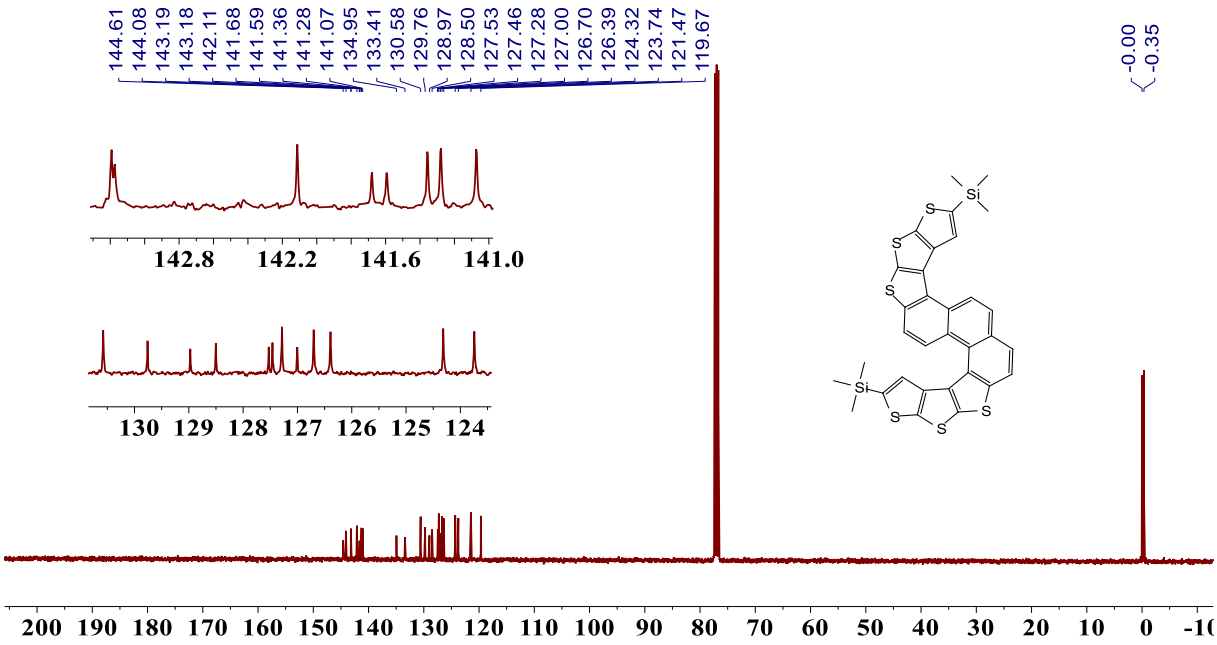


Figure S11. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **DH-1**

Parameters:

Mass	Tolerance	Electron Mode	Charge	DBE Range	Max Results
657.98961 ± 0.00329	5.0 ppm	Odd/Even	+1	-0.5 - 200.0	100

Elements

C 0 - 32 H 0 - 150 N 0 - 4 Si 0 - 2 S 0 - 6 Na 0 - 1

Results:

#	Formula	Mass	DBE	Abs. Error (u)	Error (u)	Error (ppm)
1	C32 H26 Si2 S6	657.98918	22.0	0.00043	0.00043	0.65
2	C28 H23 N4 Na Si S6	657.99084	20.0	0.00123	-0.00123	-1.87
3	C31 H19 N4 Na Si S5	657.98747	25.0	0.00214	0.00214	3.25
4	C30 H27 Na Si2 S6	657.98677	19.0	0.00284	0.00284	4.31

Figure S12. HRMS data of **DH-1**

NMR and HRMS spectra of DH-2

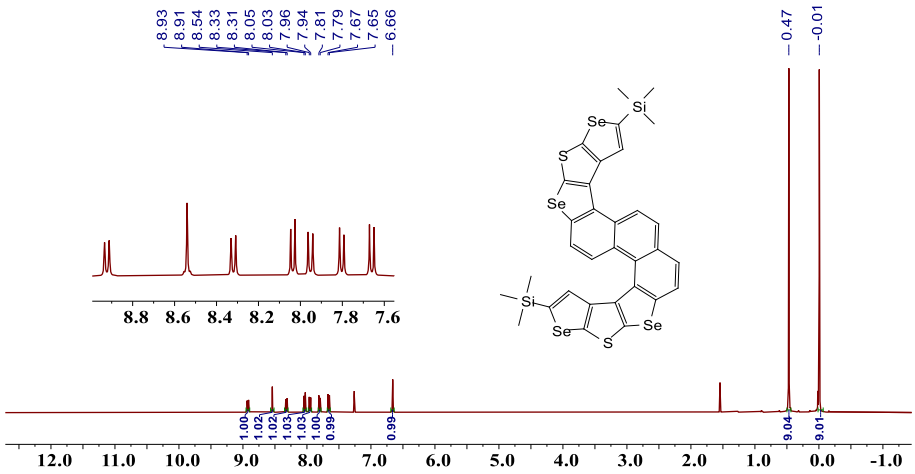


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **DH-2**

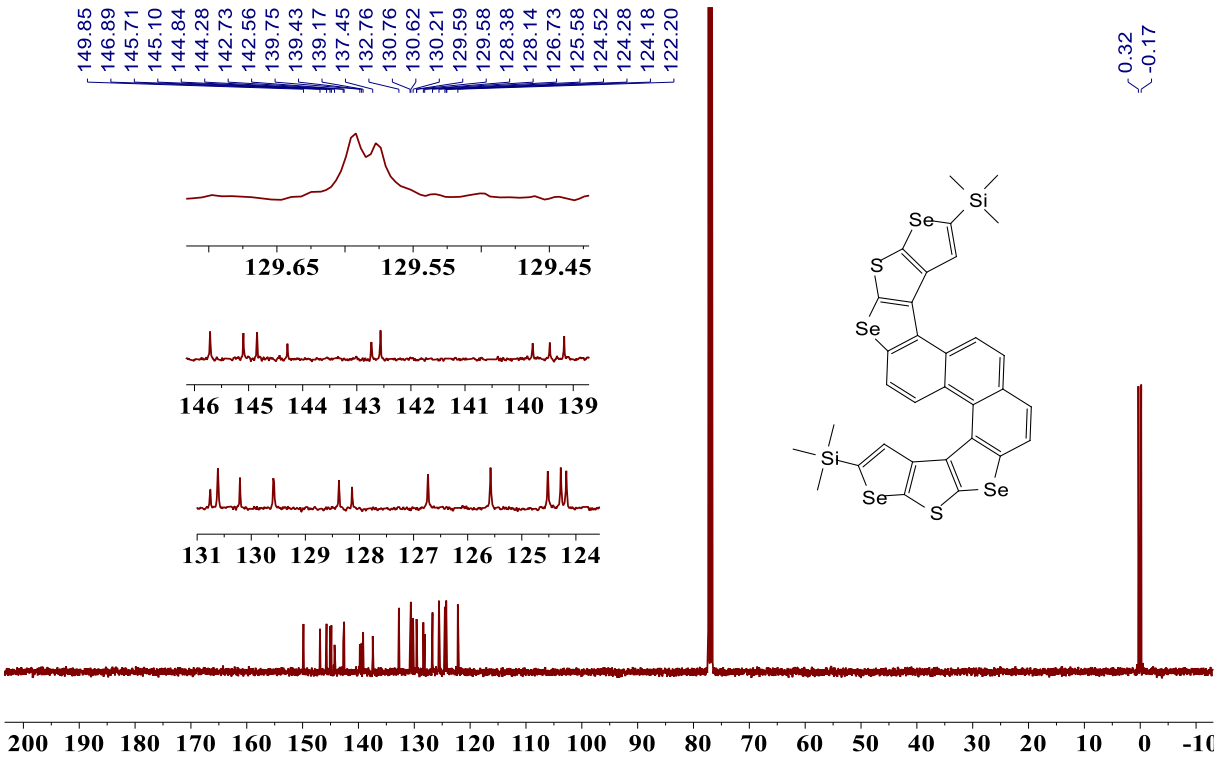


Figure S14. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **DH-2**

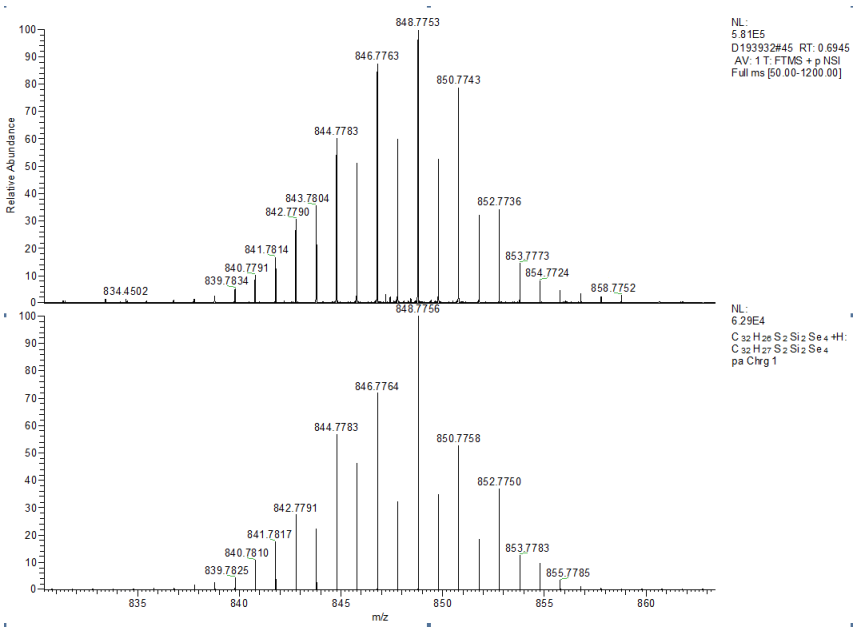


Figure S15. HRMS spectrum of **DH-2**

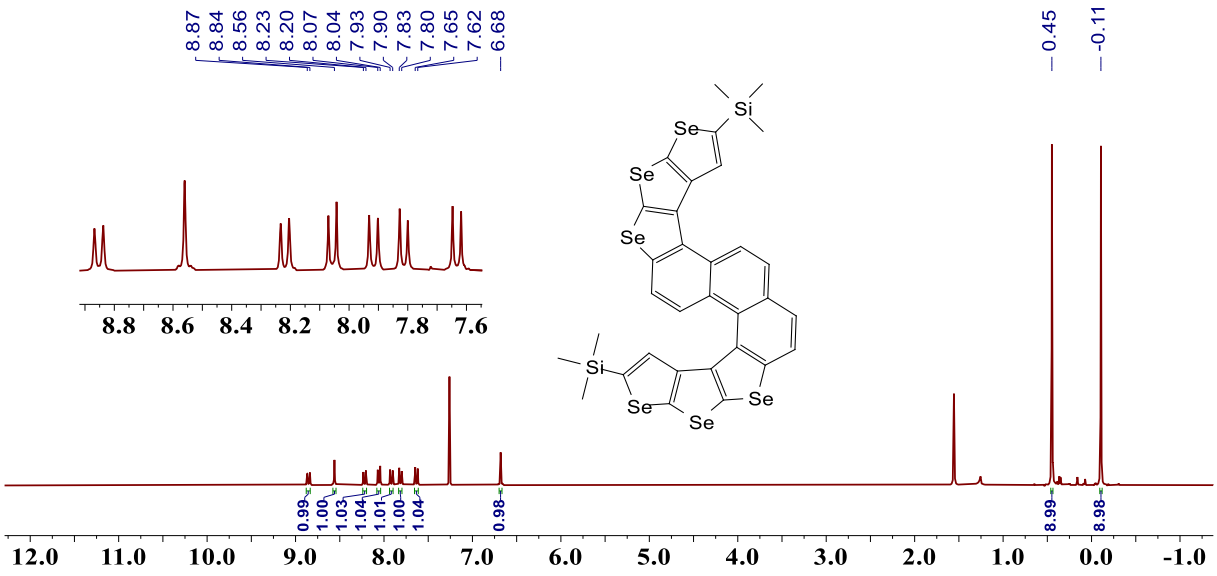


Figure S16. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **DH-3**

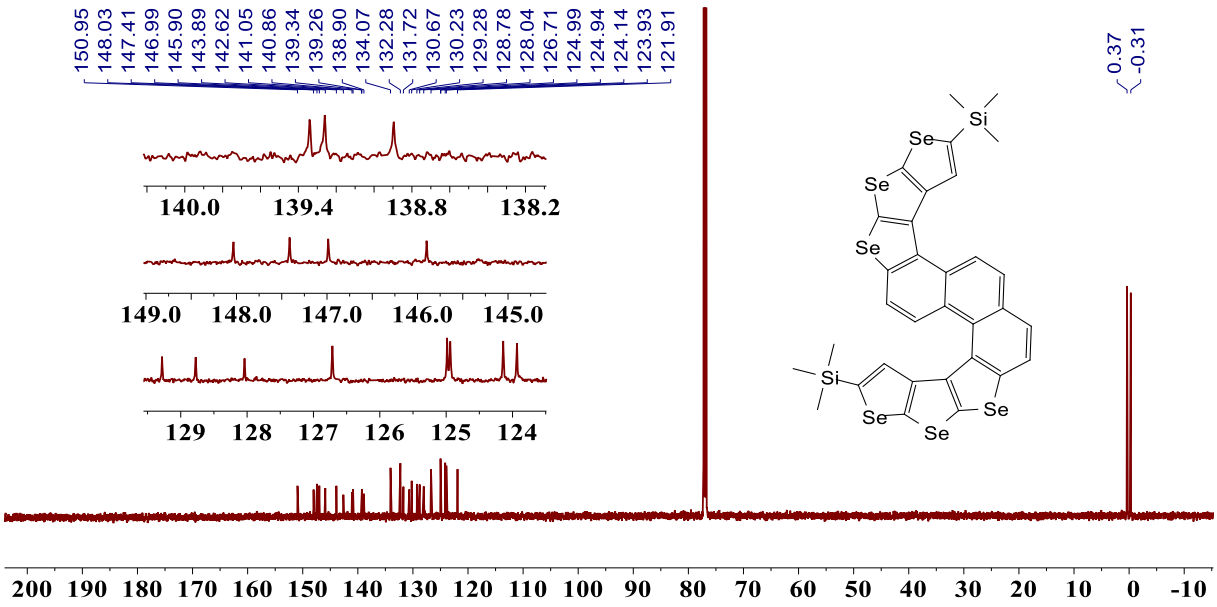


Figure S17. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **DH-3**

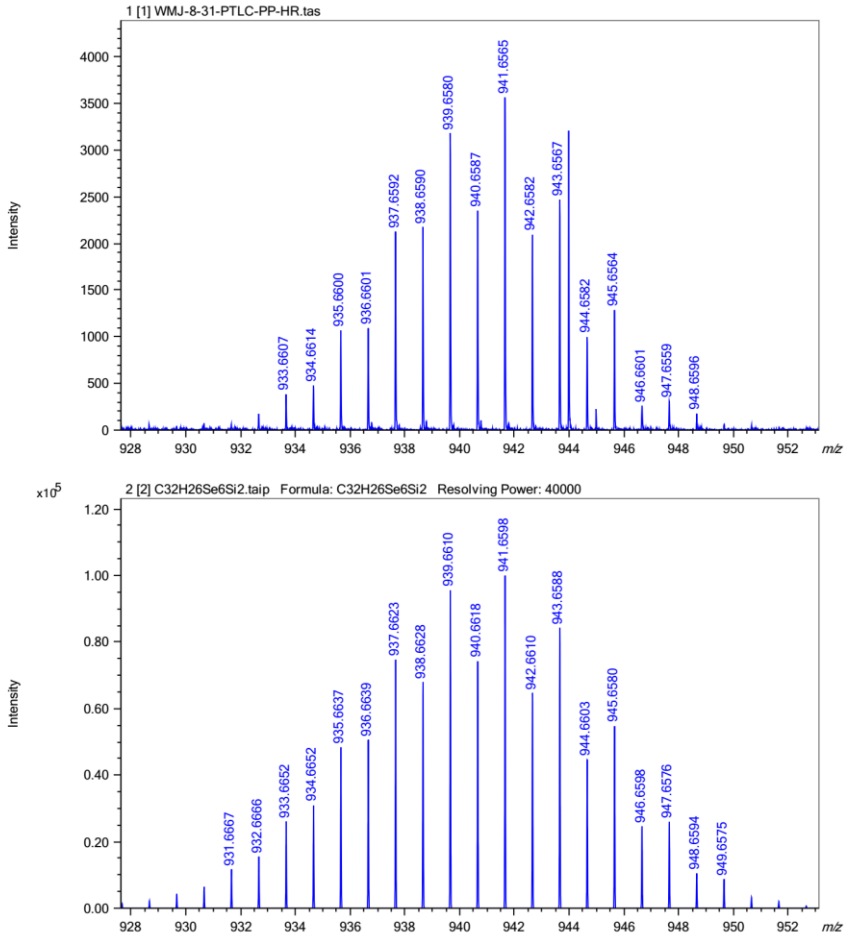


Figure S18. HRMS spectrum and data of **DH-3**

2. Fluorescence spectra and fluorescence quantum yield

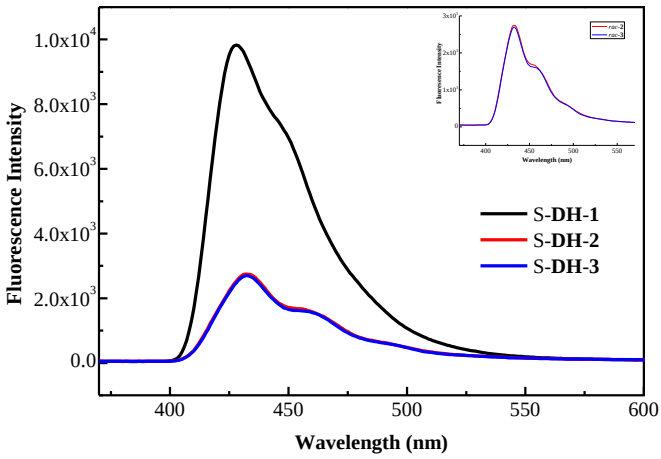


Figure S19. Fluorescence spectra of **DH-1–3** at room temperature in dichloromethane ([C] = 1 × 10^{-5} M, λ_{ex} = 350 nm, slit: 1/1 nm).

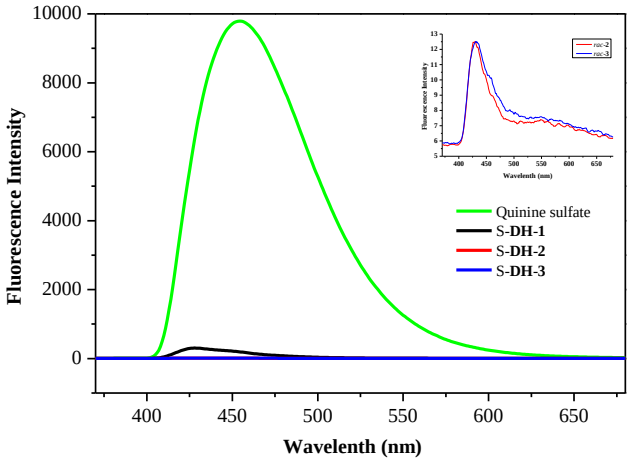


Figure S20. Excitation spectra of compound **DH-1**–**3** in dichloromethane and quinine sulfate dehydrate in 0.1N H_2SO_4. (λ_{ex} = 350 nm, [C] = 1 × 10^{-5} M).

Table S1. The fluorescence quantum yield (Φ) of **DH-1**–**3** calculated according to the formula: $\Phi_F = (n_x/n_s)^2 A_s/A_x D_x/D_s \Phi_s$

Compound	Peak Area(D)	Refractive index(n)	Yeild(Φ)
DH-1	1.6×10^4	1.42	0.0123
DH-2	2.3×10^3	1.42	0.0016
DH-3	2.4×10^3	1.42	0.0017
Quinine sulfate	8.4×10^5	1.33	0.54

3. Theoretical study

Orbital-weighted Fukui function of **5a**

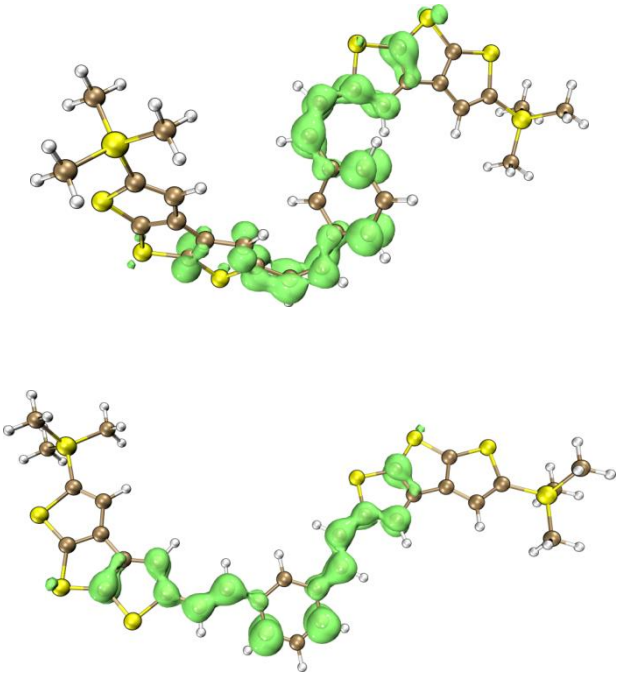


Figure S21. Orbital-weighted Fukui function of **5a**.

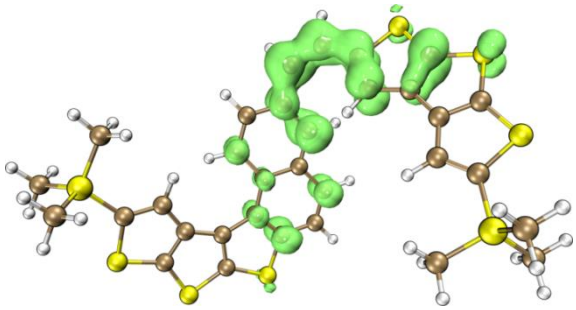
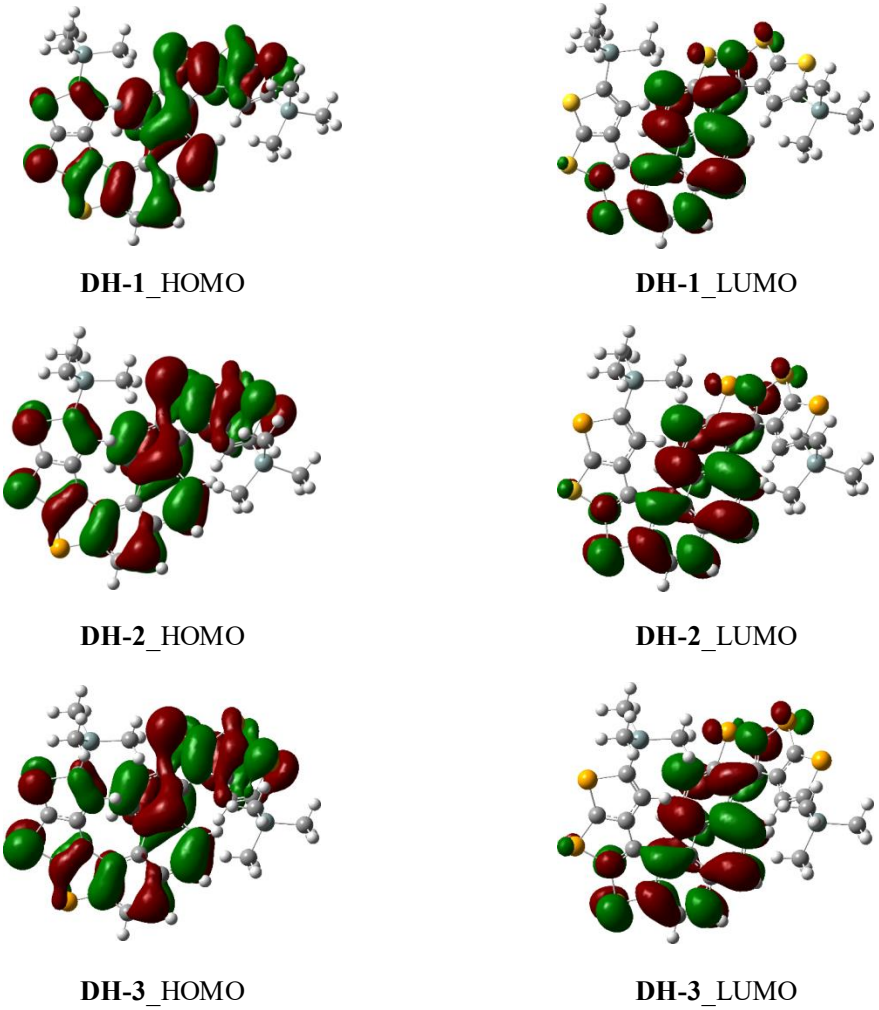


Figure S22. Orbital-weighted Fukui function of closing one benzene compound.

Calculated HOMO and LUMO energy



DH-1_HOMO **DH-1**_LUMO

DH-2_HOMO **DH-2**_LUMO

DH-3_HOMO **DH-3**_LUMO

Figure S23. The contour plots of the HOMOs and LUMOs for **DH-1**, **DH-2**, and **DH-3**.

Table S2. Calculated HOMO and LUMO energy levels and energy gap at B3LYP/6-31G** level of theory and the optical band gaps estimated from the absorption edges.

Compounds	LUMO (eV) theory	HOMO (eV) theory	E_g (eV) theory	λ_{onset} (nm) experimental	E_g^{opt} (eV) experimental
DH-1	-1.42	-5.39	3.97	403	3.08
DH-2	-1.49	-5.32	3.83	412	3.01
DH-3	-1.47	-5.28	3.81	416	2.98