Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Synthesis and Properties of [7]Helicene and [7]Helicene-like Compounds with a Cyclopenta[1,2-*b*:4,3-*b*']dithiophene or Dithieno[2,3-*b*:3',2'-*d*]heterole skeleton

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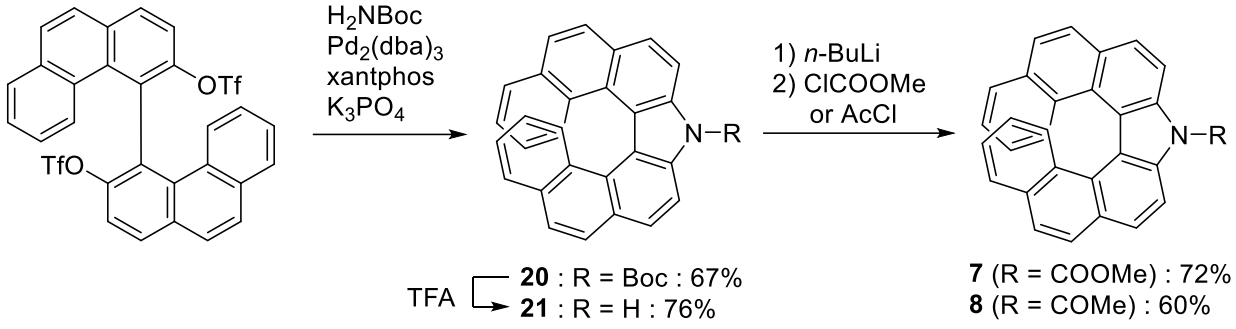
Synthetic Procedures for 7 and 8



Synthesis of *tert*-butyl 9*H*-dinaphtho[2,1-*c*:1',2'-*g*]carbazole-9-carboxylate (20)

A mixture of *rac*-[4,4′-biphenanthrene]-3,3′-diyl bis(trifluoromethanesulfonate) (0.14 g, 0.20 mmol), *tert*-butyl carbamate (31 mg, 0.26 mmol), $Pd_2(dba)_3$(16 mg, 0.015 mmol), xantphos (15 mg, 0.026 mmol), anhydrous K_3PO_4 (0.15 g, 0.71 mmol), and xylene (15 mL) in a Schlenk tube was stirred at 100 °C for 49 h. The resulting mixture was washed with 1 M aqueous HCl, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude residue was purified by silica-gel column chromatography with CH_2Cl_2/hexane (3/2) as an eluent to give **20** as a colorless solid (65 mg, 67%): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, J = 8.7 Hz, 2H), 8.11 (d, J =8.7 Hz, 2H), 7.97 (d, J = 8.7 Hz, 2H), 7.85 (d, J = 8.7 Hz, 2H), 7.78 (d, J = 7.3 Hz, 2H), 7.46 (d, J =8.2 Hz, 2H), 7.20-7.16 (m, 2H), 6.32-6.28 (m, 2H), 1.93 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ151.1, 138.3, 131.4, 130.4, 128.7, 127.8, 127.6, 126.51, 126.45, 126.3, 125.9, 123.2, 120.5, 115.3, 85.0, 28.6; HRMS-APCI (*m/z*) calcd for $C_{29}H_{18}NO_2$ ([M-C_4H_9+2H]$^+$), 412.1332; found, 412.1346.

Synthesis of 9*H*-dinaphtho[2,1-*c*:1',2'-*g*]carbazole (21)

To the solution of **20** (0.13 g, 0.28 mmol) in CH_2Cl_2 (2 mL) was added trifluoroacetic acid (0.64 mL, 8.3 mmol) at 0 ℃. The resulting mixture was stirred at room temperature for 13 h. The reaction was quenched with saturated aqueous $NaHCO_3$, and the resulting mixture was extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude residue was purified by silica-gel column chromatography with EtOAc/hexane (1/2) as an eluent to give **21** as a brownish solid (78 mg, 76% yield): ^{1}H NMR (400 MHz, acetone-d_6) δ 11.71 (s, 1H), 8.15-8.06 (m, 6H), 7.86 (d, J = 8.4 Hz, 4H), 7.50 (d, J =8.8 Hz, 2H), 7.18-7.14 (m, 2H), 6.22-6.18 (t, 2H); ^{13}C NMR (101 MHz, acetone-d_6) δ 140.1, 140.0, 132.4, 131.3, 128.7, 127.9, 127.8, 127.3, 126.7, 124.9, 123.3, 117.5, 117.4, 113.2, 113.1; HRMS-APCI (*m/z*) [M+H]$^+$ calcd for $C_{28}H_{18}N$, 368.1434; found, 368.1457.

Synthesis of methyl 9*H*-dinaphtho[2,1-*c*:1',2'-*g*]carbazole-9-carboxylate (7)

n-BuLi (2.6 M in hexane, 0.045 mL, 0.12 mmol) was added dropwise to the solution of **21** (0.037 g, 0.10 mmol) in THF (1.5 mL) at 0 °C. After stirring at room temperature for 30 min, methyl chloroformate (0.011 mL, 0.14 mmol) was added to the reaction mixture at room temperature. The resulting mixture was stirred for overnight, and the reaction was quenched with water (20 mL).

The resulting mixture was extracted with CH_2Cl_2 (10 mL × 3), and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude residue was purified by silica-gel column chromatography with CH_2Cl_2/hexane (1/1) as an eluent to give **7** as a colorless solid (31 mg, 72% yield): 235-236 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 9.2 Hz, 2H), 8.05 (d, *J* = 9.2 Hz, 2H), 7.91 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.13 (dt, *J* = 6.8, 1.2 Hz, 2H), 6.24 (dt, *J* = 7.2, 1.2 Hz, 2H), 4.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.1, 138.0, 131.4, 130.4, 129.0, 128.0, 127.6, 126.6, 126.44 (two carbons), 126.40, 126.1, 123.3, 120.9, 115.2, 54.2; HRMS-APCI (*m/z*) calcd for $C_{30}H_{20}NO_2$ ($[M+H]^+$) 426.1489, found 426.1494.

Synthesis of 1-(9*H*-dinaphtho[2,1-*c*:1',2'-*g*]carbazol-9-yl)ethan-1-one (8)

n-BuLi (2.6 M in hexane, 0.045 mL, 0.12 mmol) was added dropwise to the solution of **21** (0.037 g, 0.10 mmol) in THF (1.5 mL) at 0 °C. After stirring at room temperature for 30 min, acetyl chloride (0.011 mL, 0.16 mmol) was added to the reaction mixture at room temperature. The resulting mixture was stirred for overnight, and the reaction was quenched with water (20 mL). The resulting mixture was extracted with CH_2Cl_2 (10 mL × 3), and the combined organic layers were dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude residue was purified by silica-gel column chromatography with CH_2Cl_2/hexane (1/1) as an eluent to give **8** as a colorless solid (23 mg, 60% yield): 236-237 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 8.8 Hz, 2H), 8.07 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.82 (d, *J* = 8.8 Hz, 2H), 7.73 (d, *J* = 6.8 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.14 (dt, *J* = 6.8, 1.6 Hz, 2H), 6.26 (dt, *J* = 7.6, 1.6 Hz, 2H), 3.12 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 138.1, 131.5, 130.4, 129.0, 128.0, 127.6, 126.63, 126.57, 126.5, 126.4, 126.3, 123.4, 121.2, 114.8, 28.6; HRMS-APCI (*m/z*) calcd for $C_{30}H_{20}NO$ ($[M+H]^+$) 410.1539, found 410.1545.

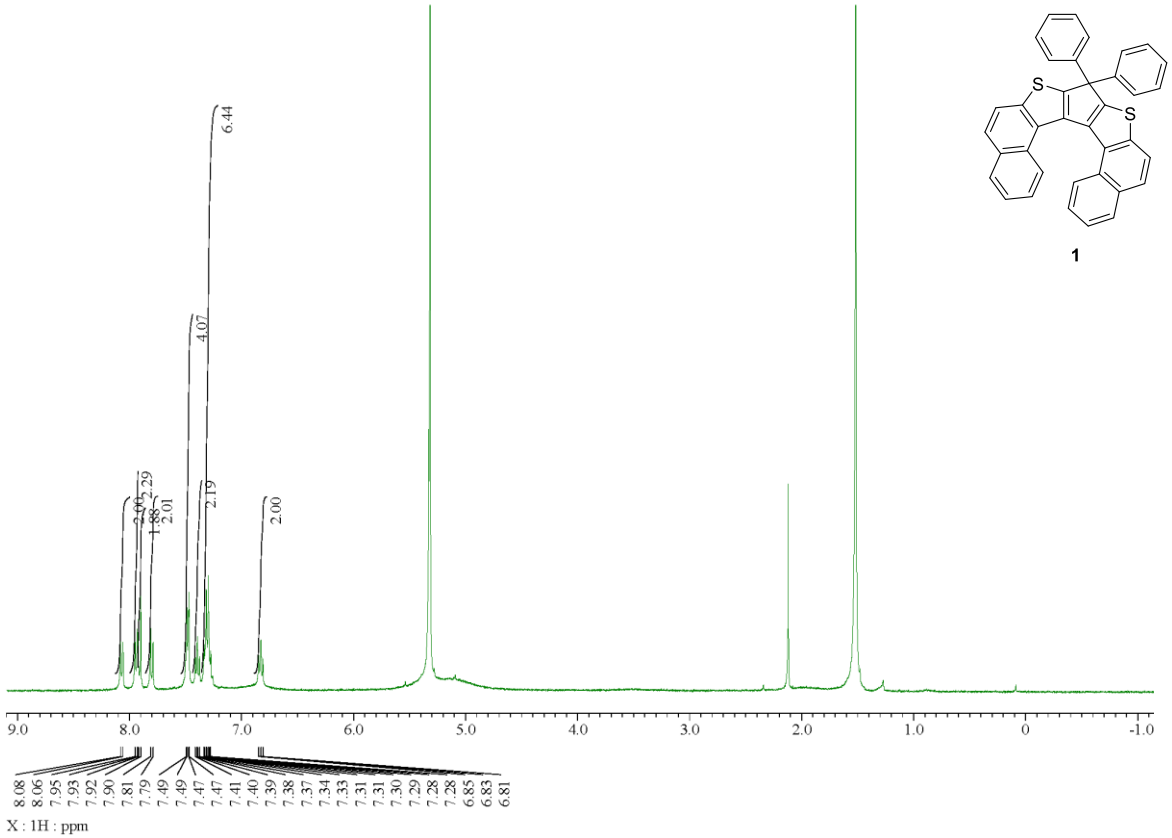


Figure S1. ^{1}H NMR spectrum of **1** (400 MHz, CD_2Cl_2, 35 °C).

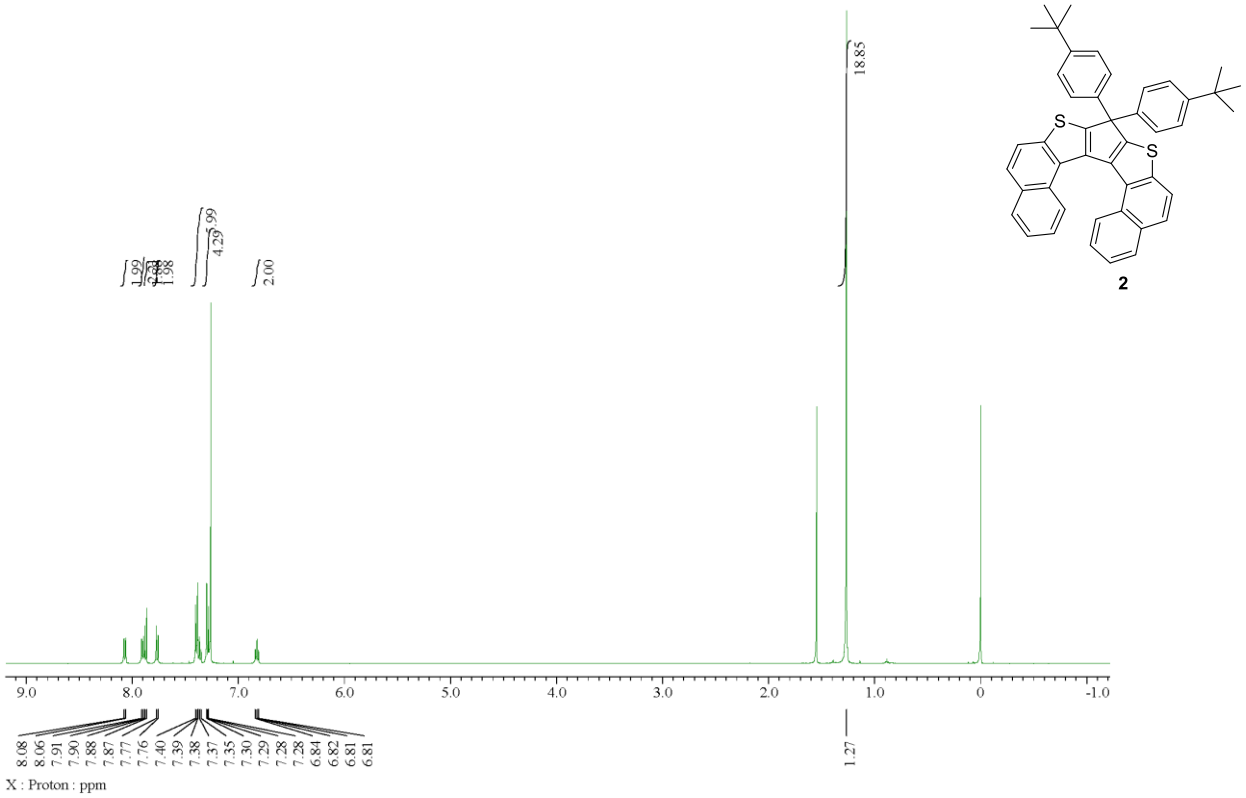


Figure S2. ^{1}H NMR spectrum of **2** (500 MHz, $CDCl_3$).

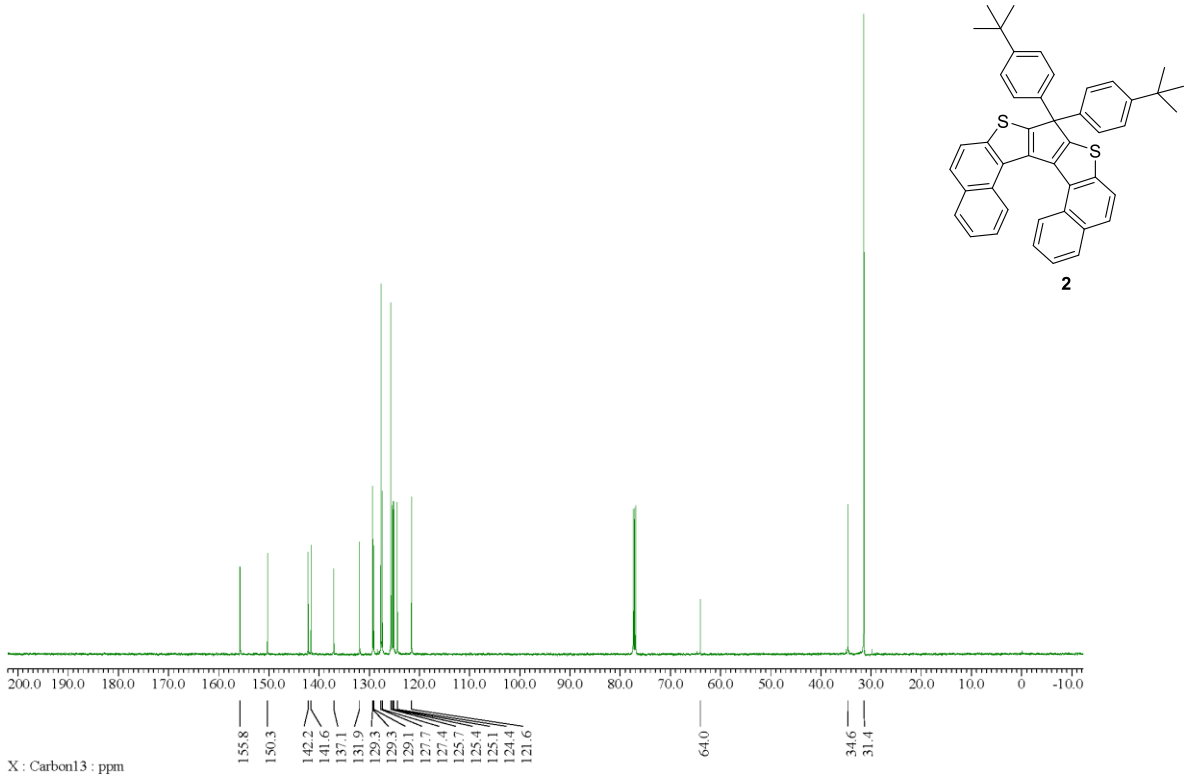


Figure S3. ^{13}C NMR spectrum of **2** (126 MHz, $CDCl_3$).

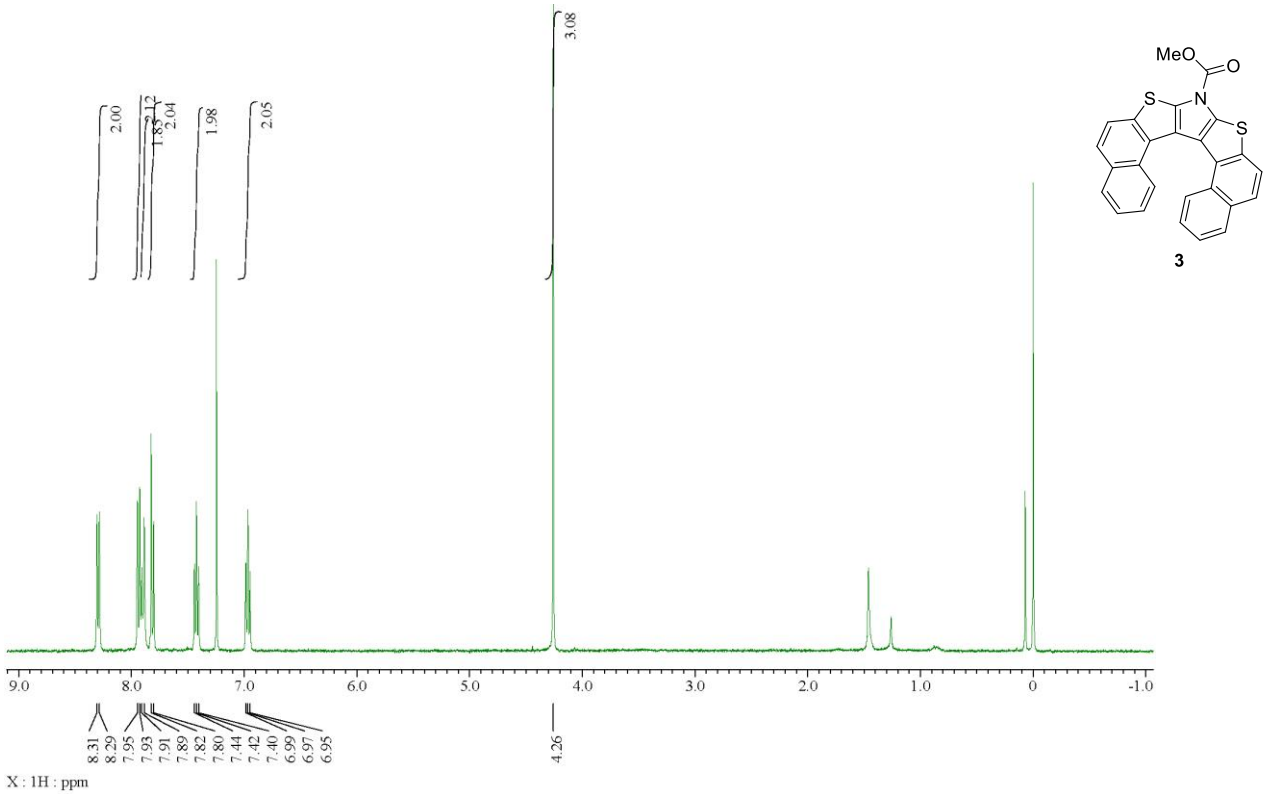


Figure S4. ^{1}H NMR spectrum of **3** (400 MHz, $CDCl_3$).

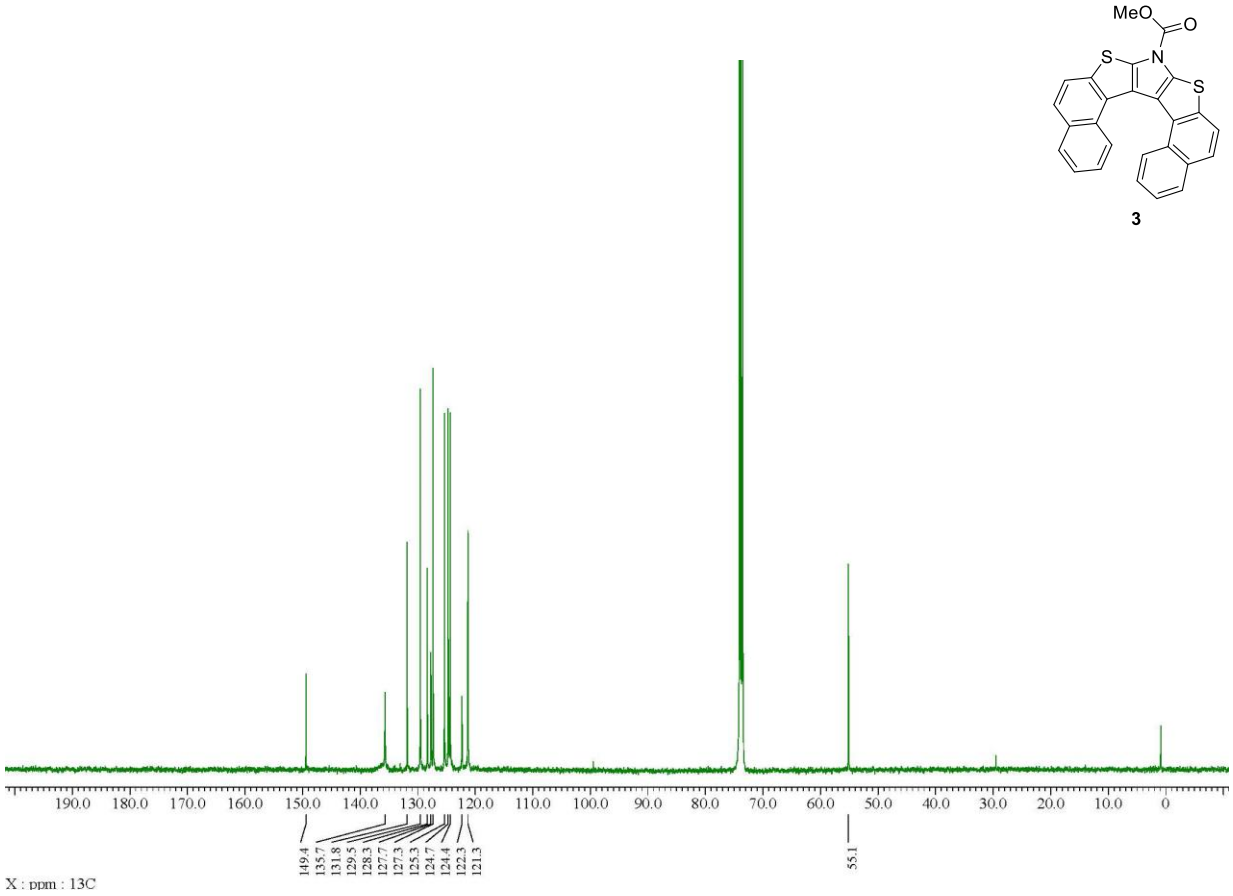


Figure S5. ^{13}C NMR spectrum of **3** (101 MHz, $Cl_2CDCDCl_2$, 60 °C).

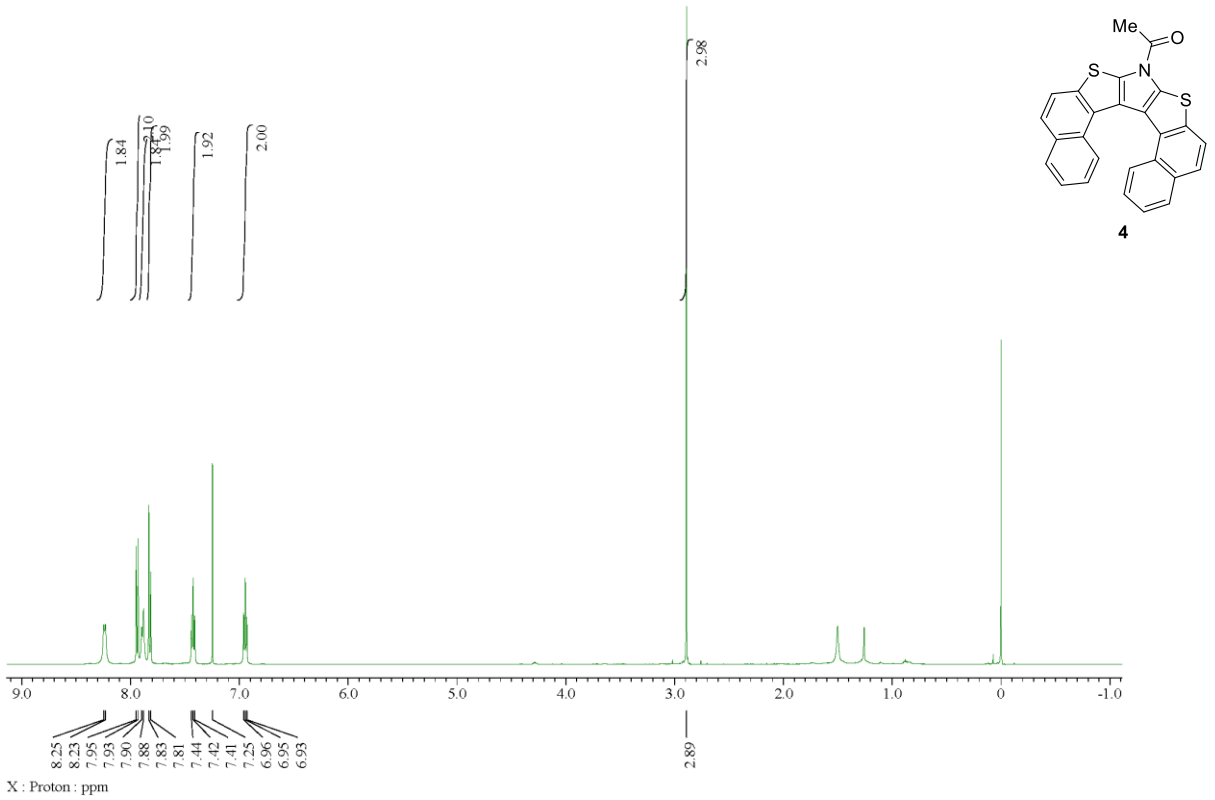


Figure S6. ^{1}H NMR spectrum of **4** (500 MHz, $CDCl_3$, 40 °C).

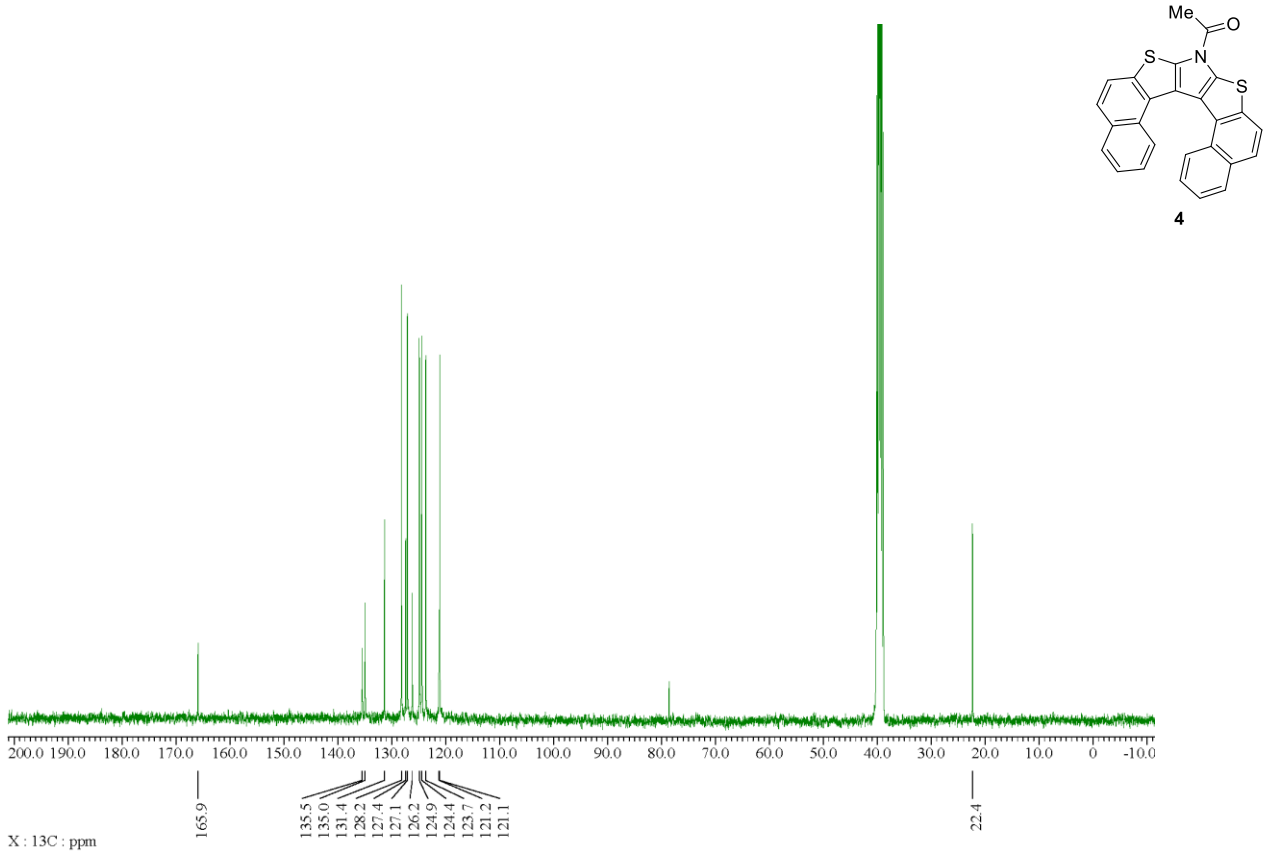


Figure S7. ^{13}C NMR spectrum of **4** (101 MHz, DMSO-d_6, 100 °C).

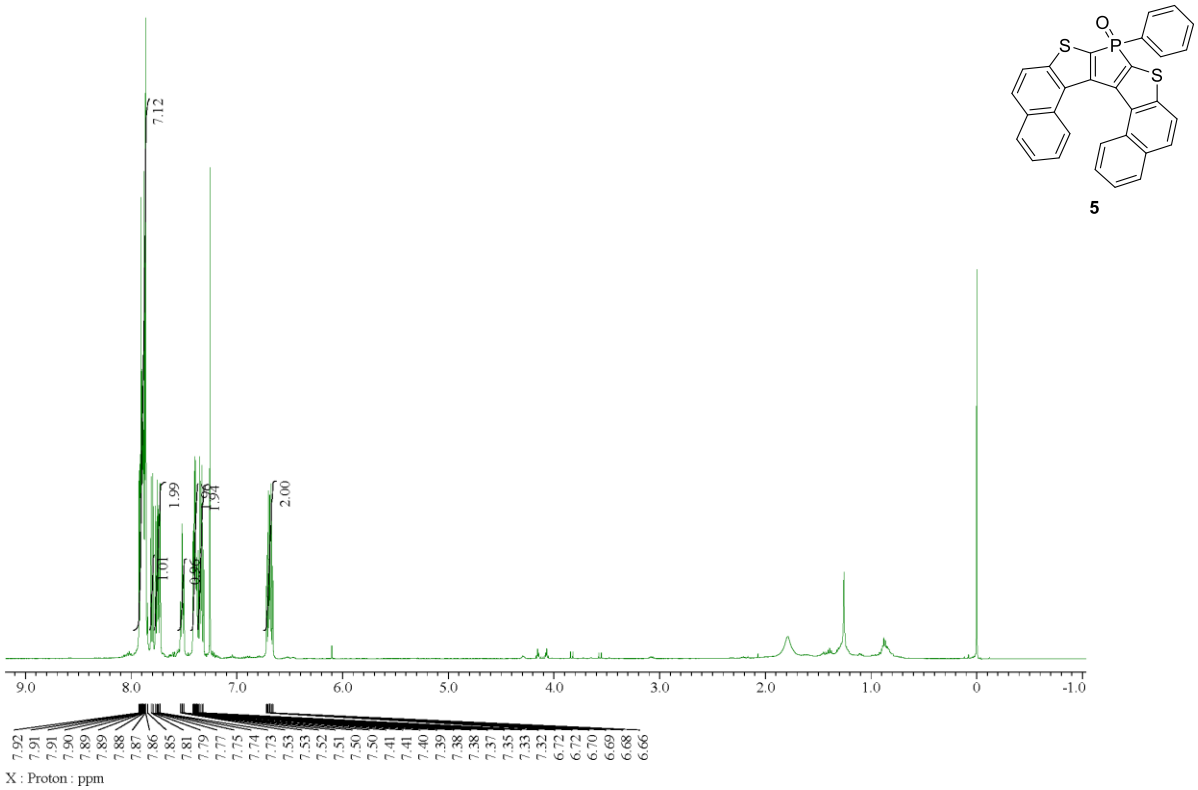


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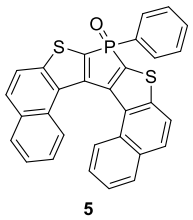
Figure S8. ^{1}H NMR spectrum of **5** (500 MHz, $CDCl_3$).



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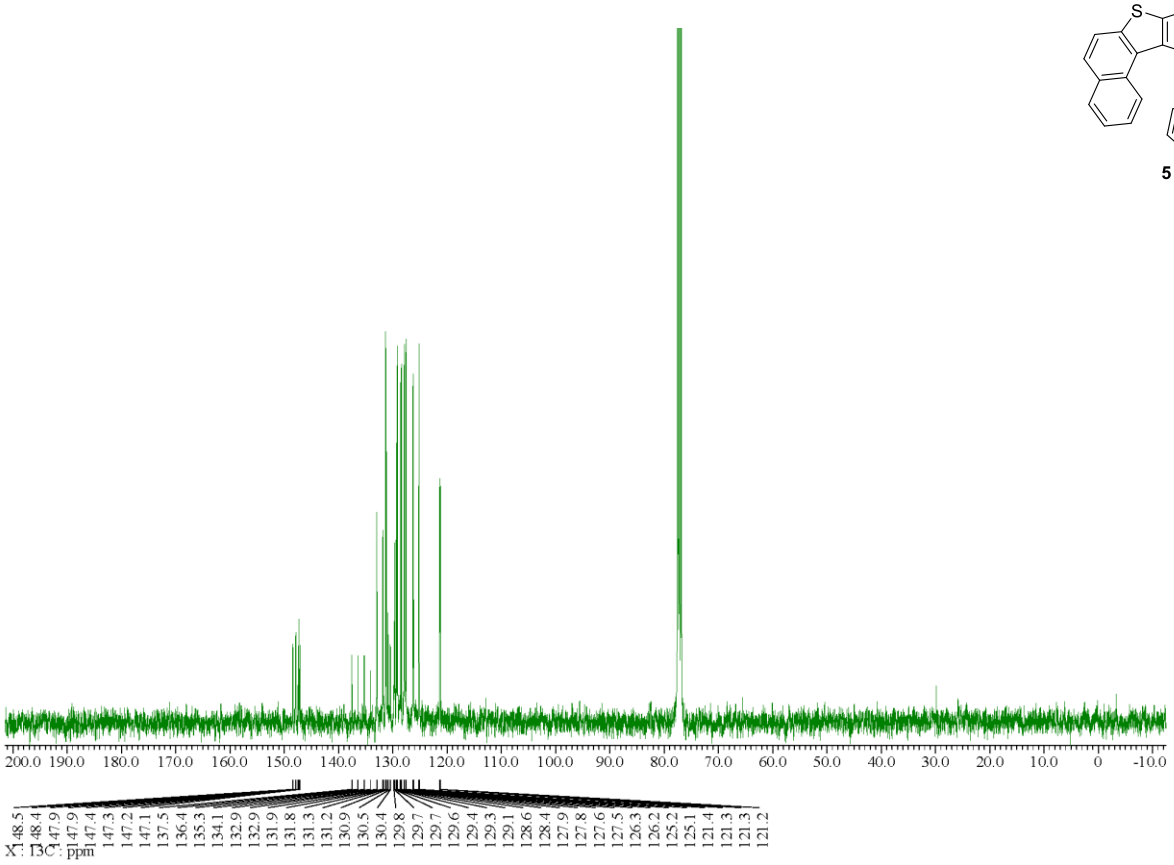

Figure S9. ^{13}C NMR spectrum of **5** (101 MHz, $CDCl_3$).

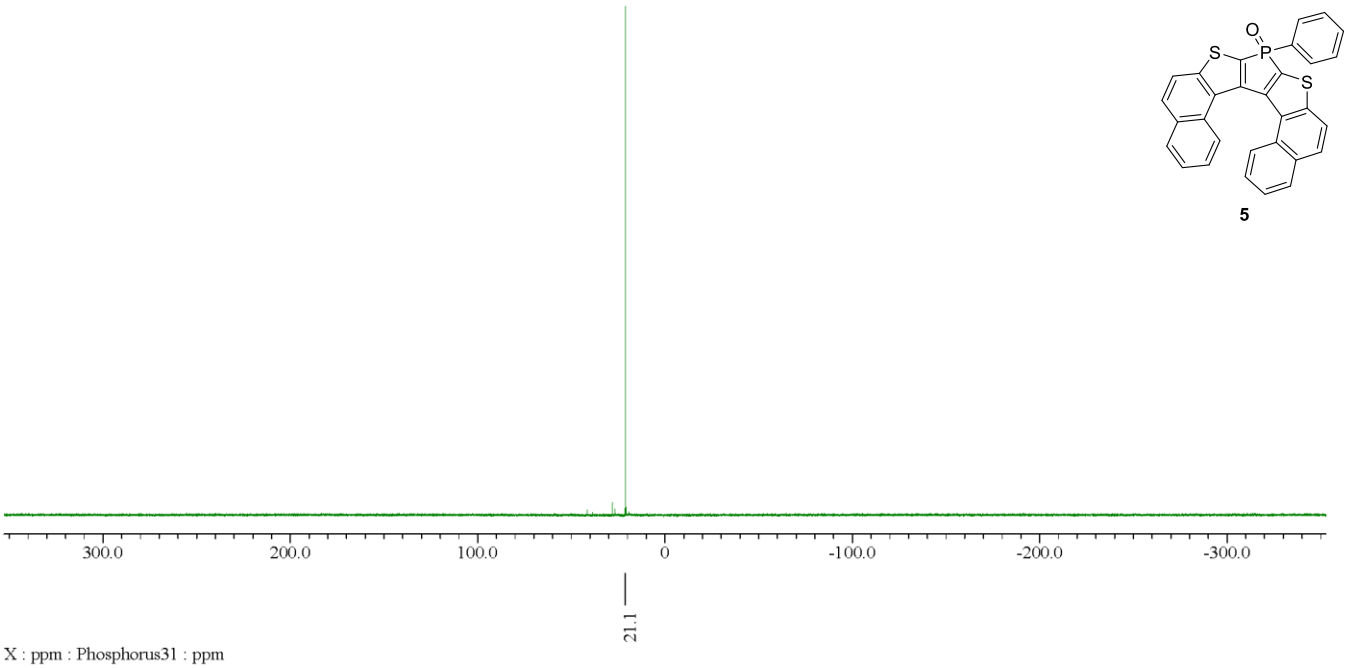

Figure S10. ^{31}P NMR spectrum of **5** (202 MHz, $CDCl_3$).

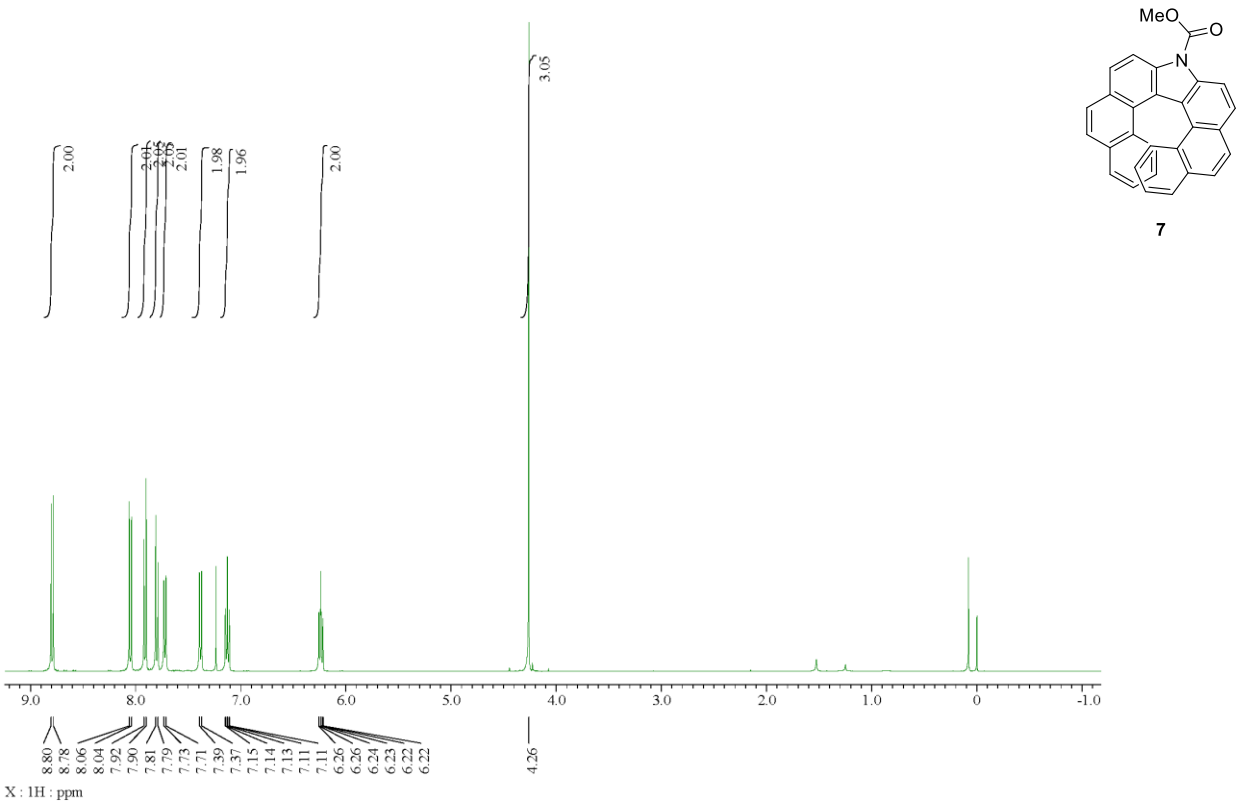

Figure S11. ^{1}H NMR spectrum of **7** (400 MHz, $CDCl_3$).

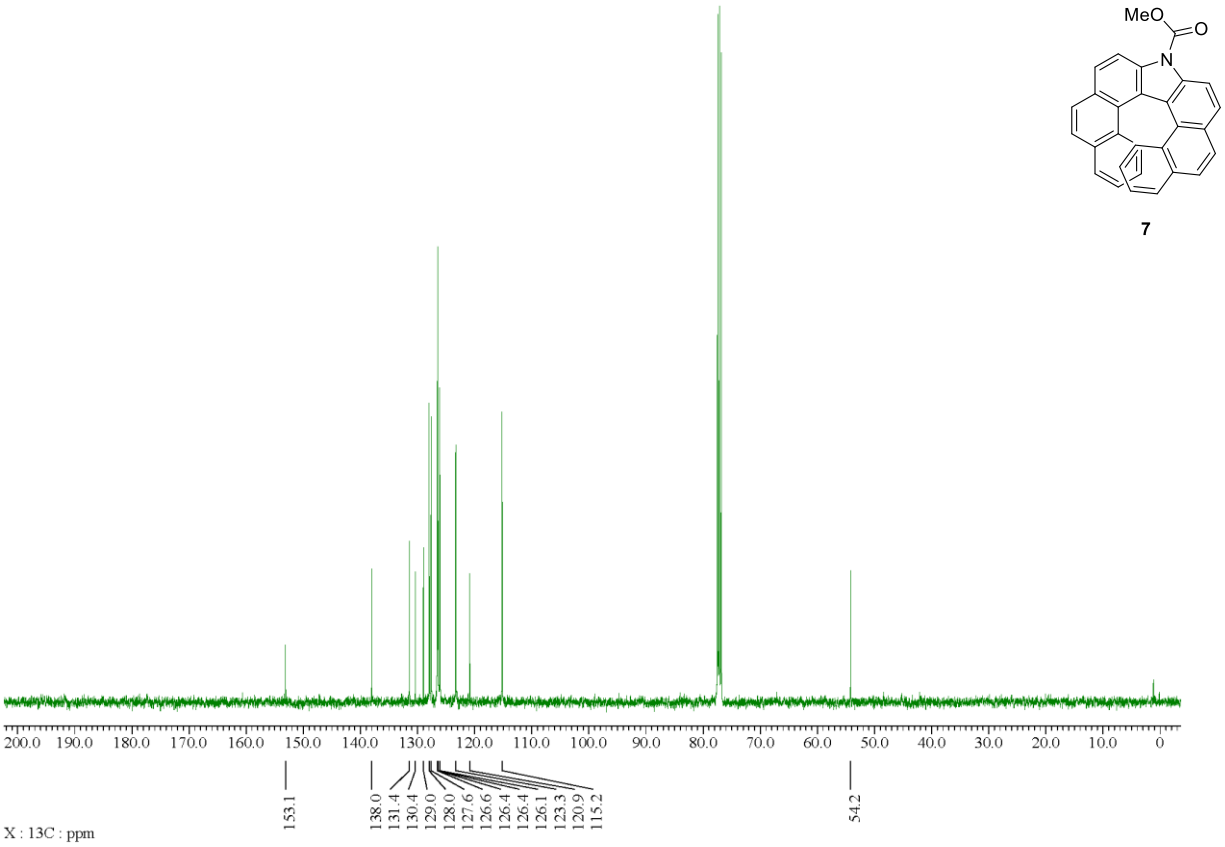

Figure S12. ^{13}C NMR spectrum of **7** (101 MHz, $CDCl_3$).

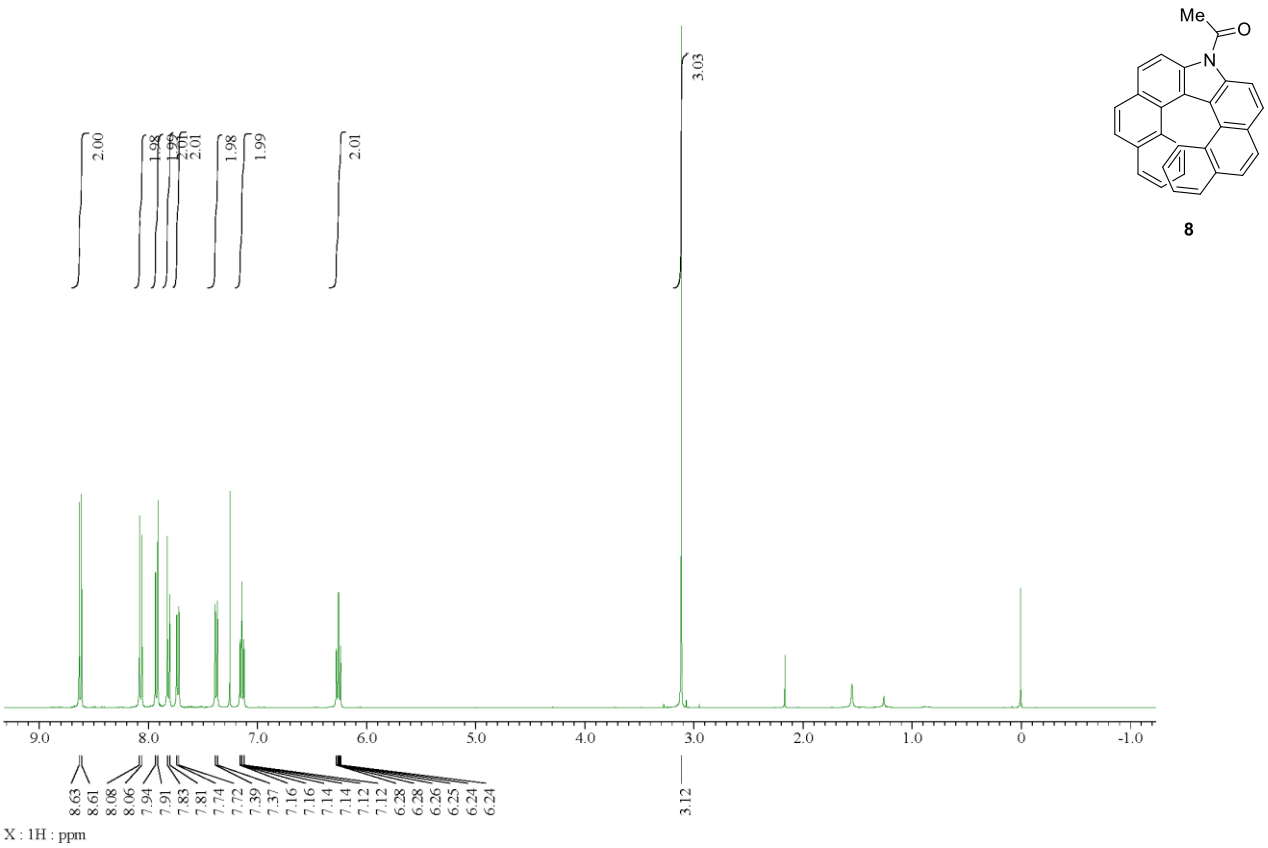

Figure S13. ^{1}H NMR spectrum of **8** (400 MHz, $CDCl_3$).

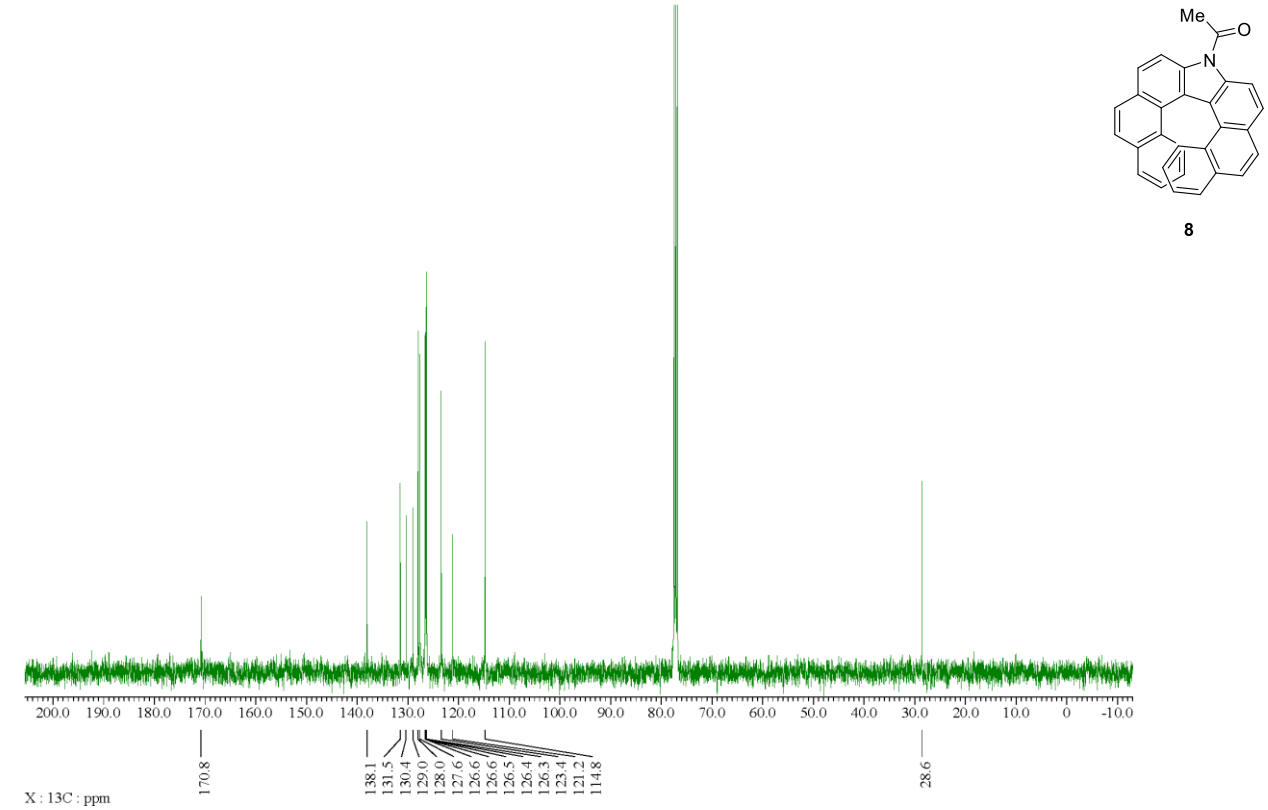

Figure S14. ^{13}C NMR spectrum of **8** (101 MHz, $CDCl_3$).

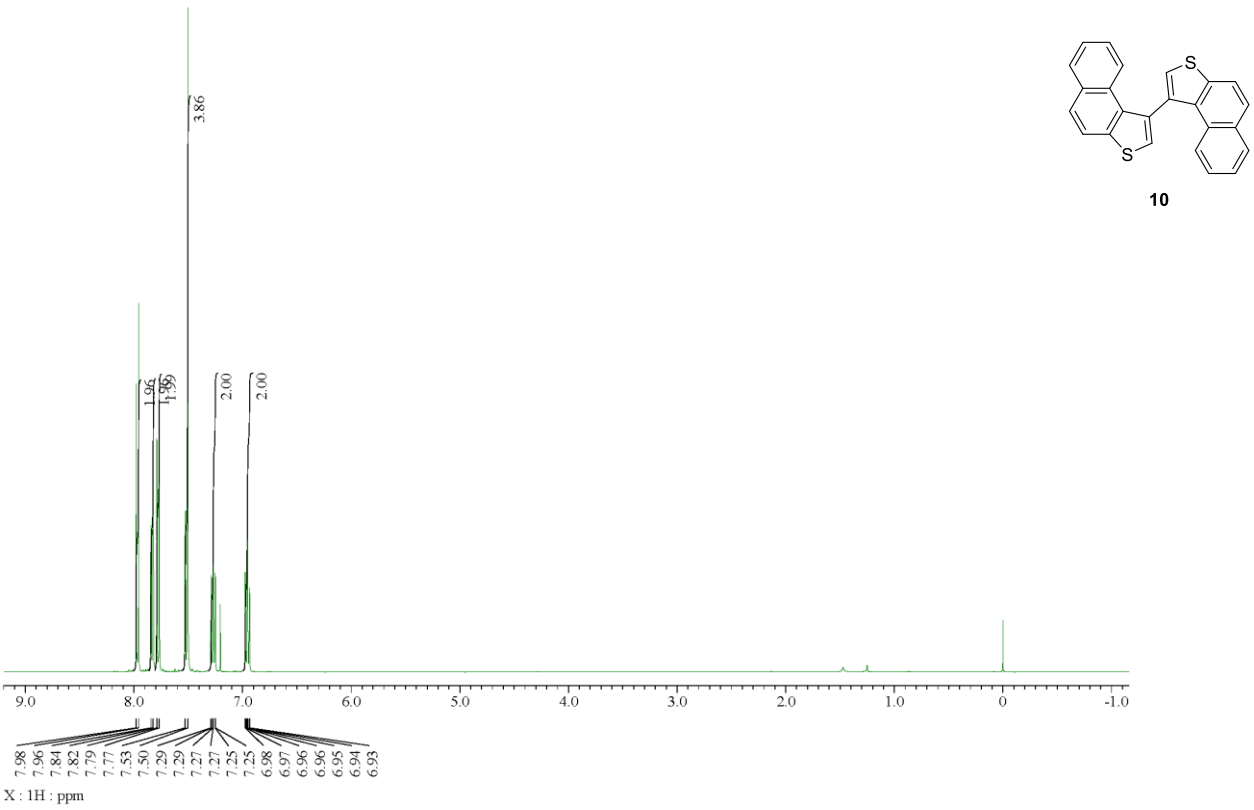

Figure S15. ^{1}H NMR spectrum of **10** (400 MHz, $CDCl_3$).

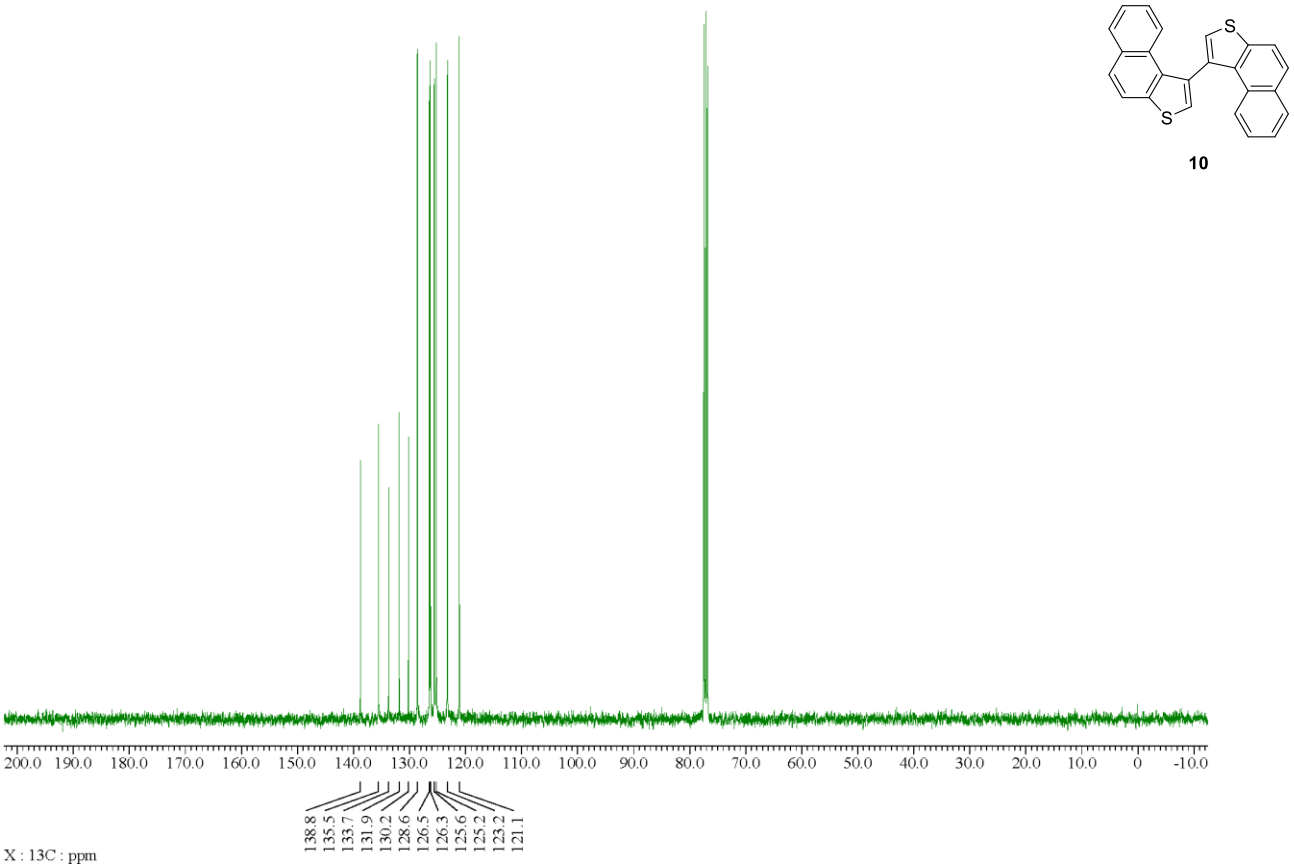

Figure S16. ^{13}C NMR spectrum of **10** (101 MHz, $CDCl_3$).

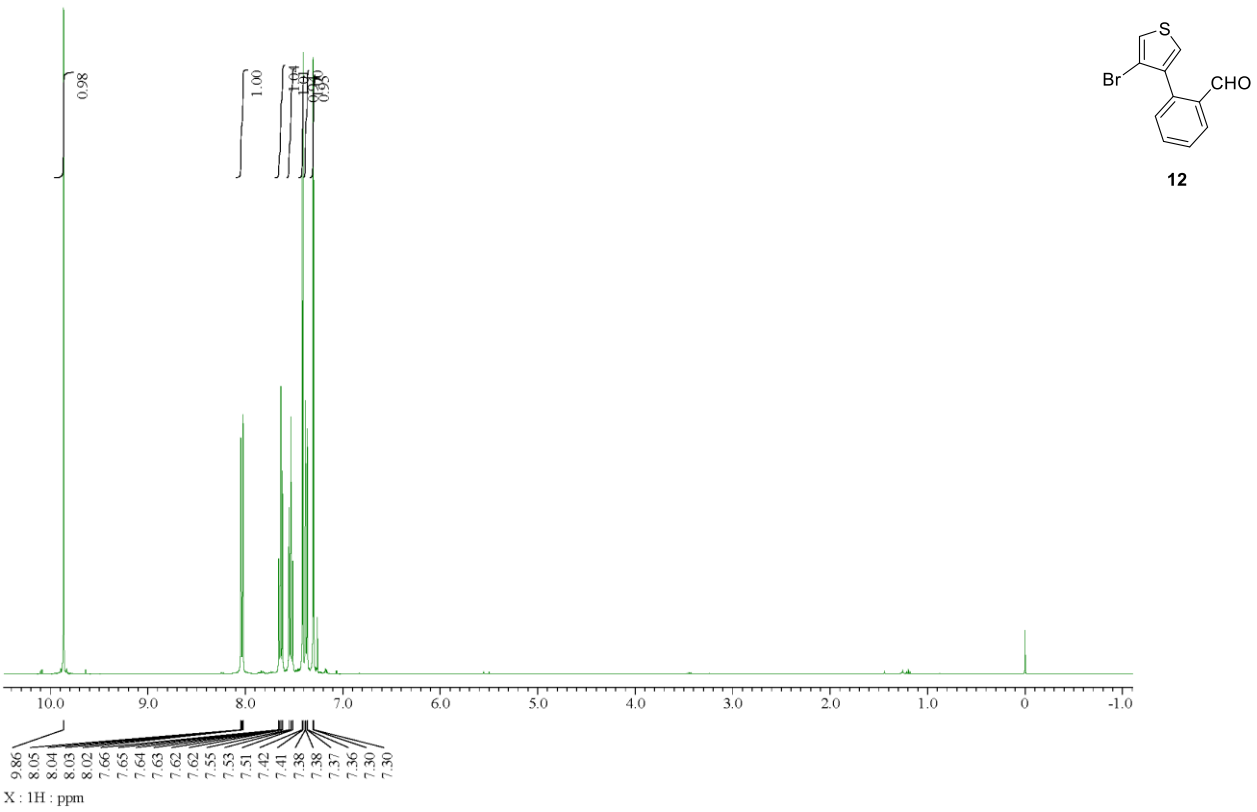

Figure S17. ^{1}H NMR spectrum of **12** (400 MHz, $CDCl_3$).

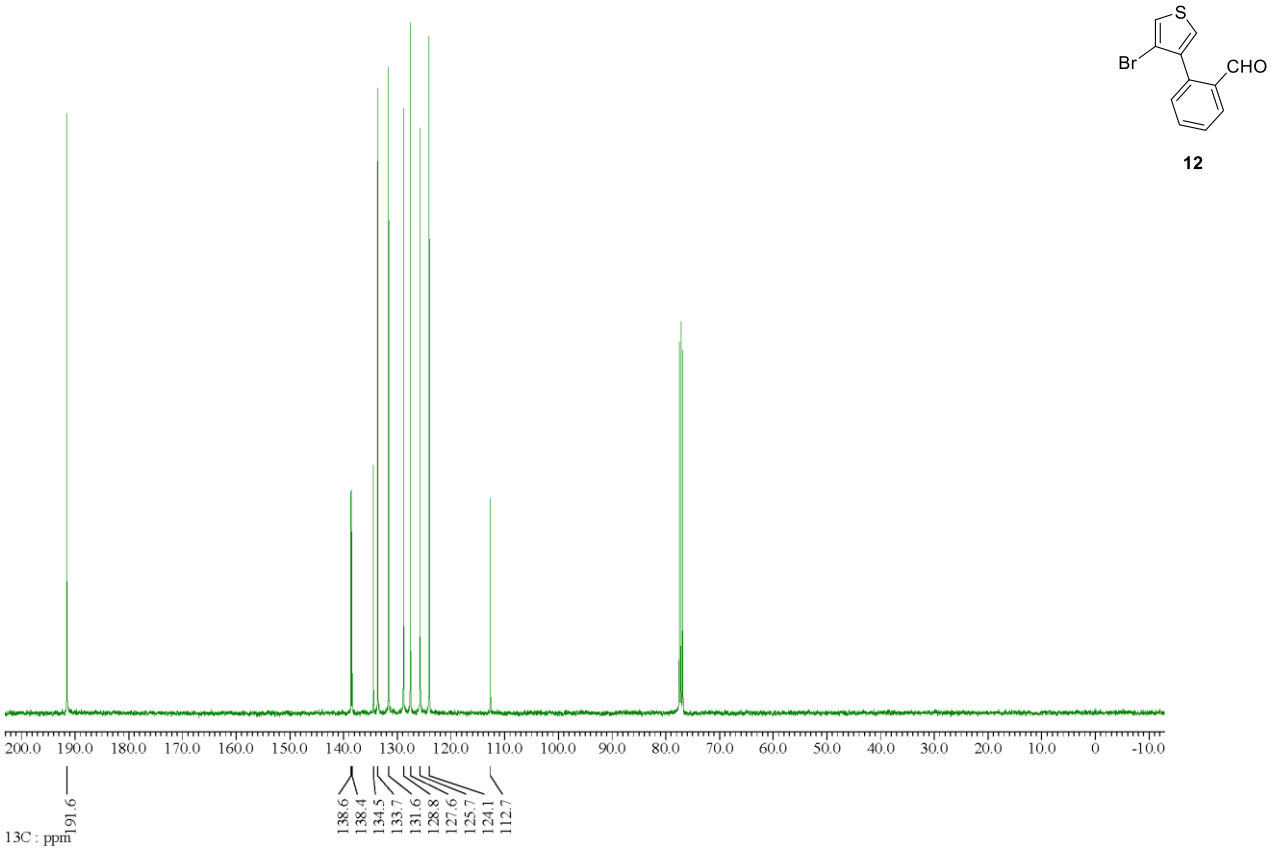

Figure S18. ^{13}C NMR spectrum of **12** (101 MHz, $CDCl_3$).

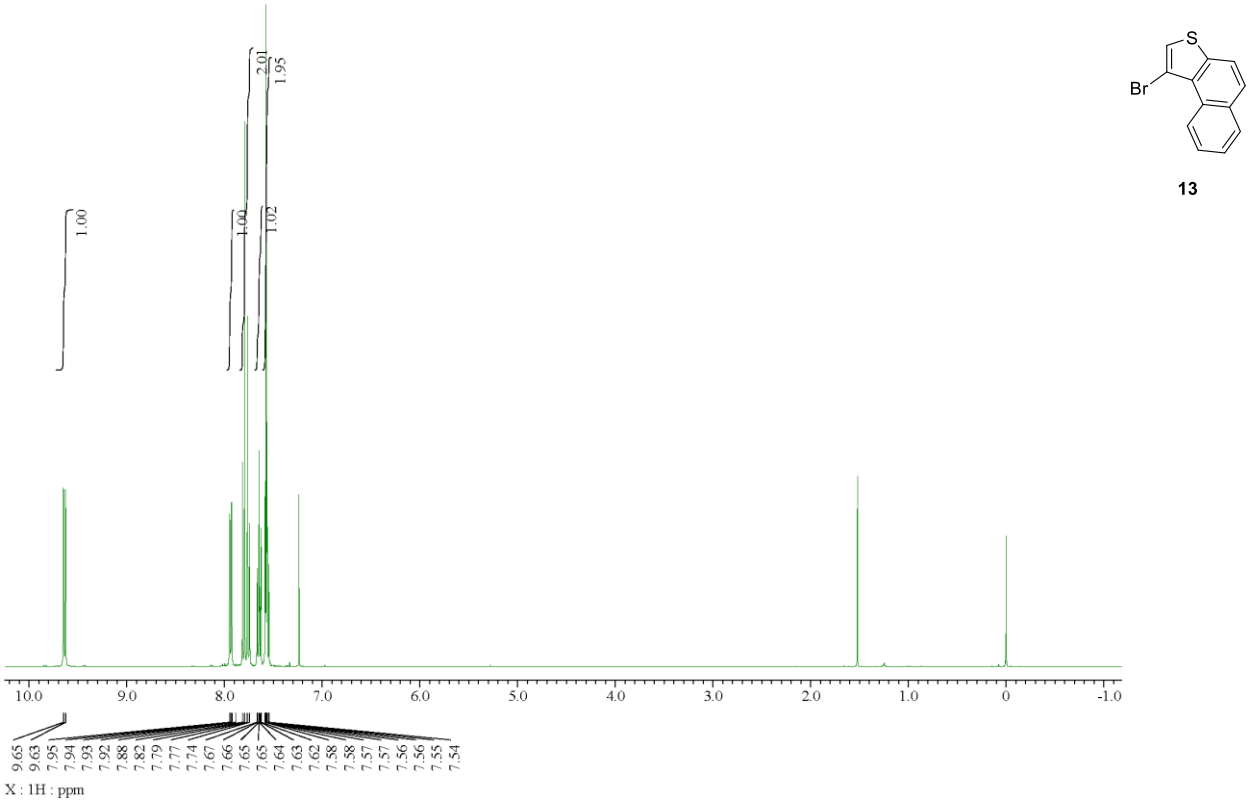

Figure S19. ^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$).

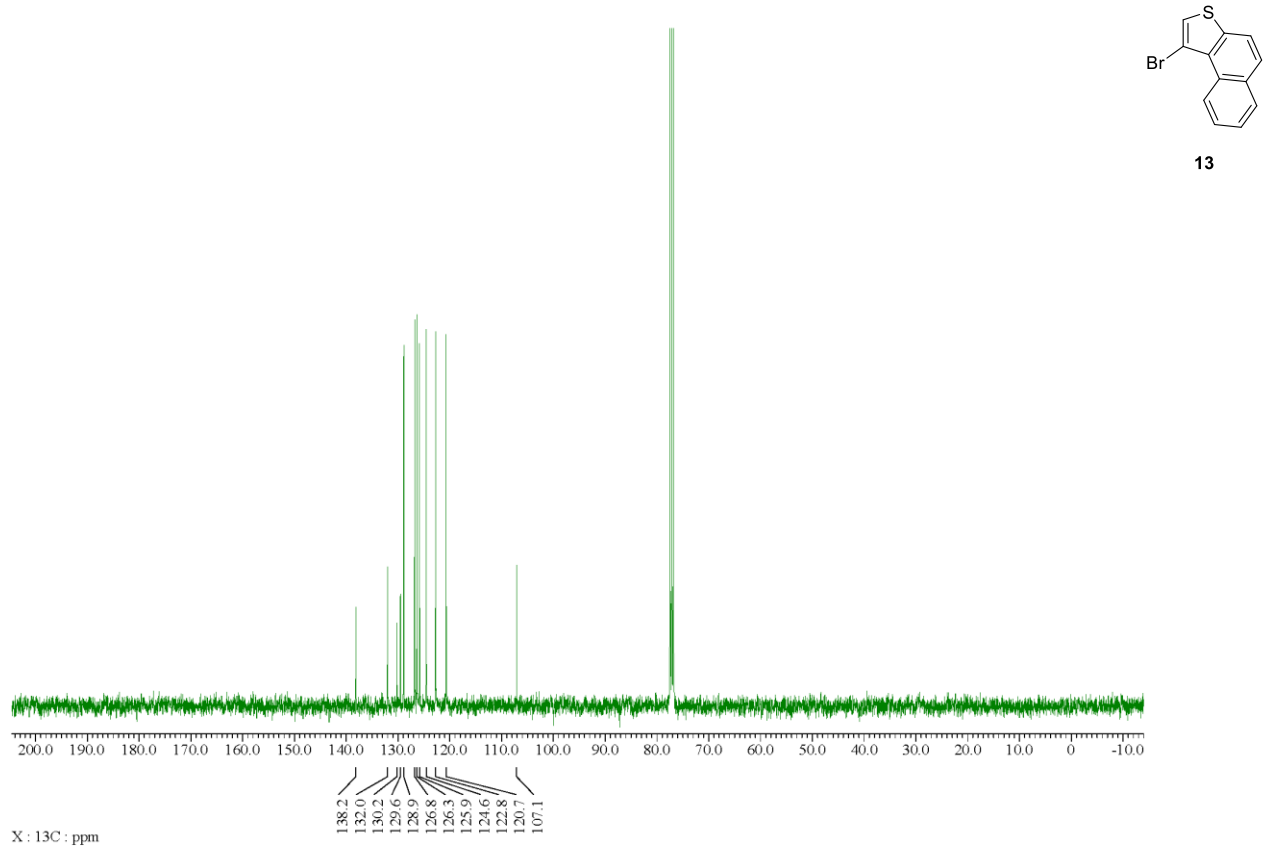

Figure S20. ^{13}C NMR spectrum of **13** (101 MHz, $CDCl_3$)

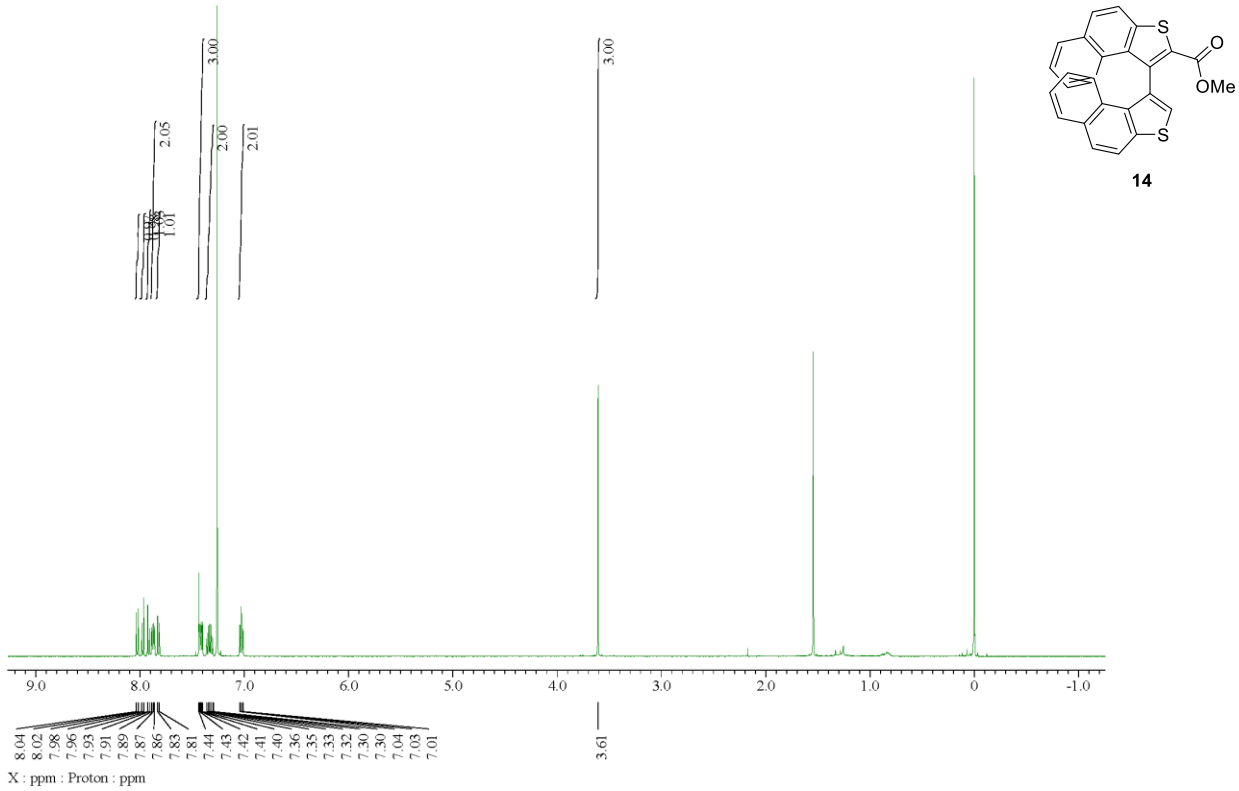

Figure S21. ^{1}H NMR spectrum of **14** (500 MHz, $CDCl_3$).

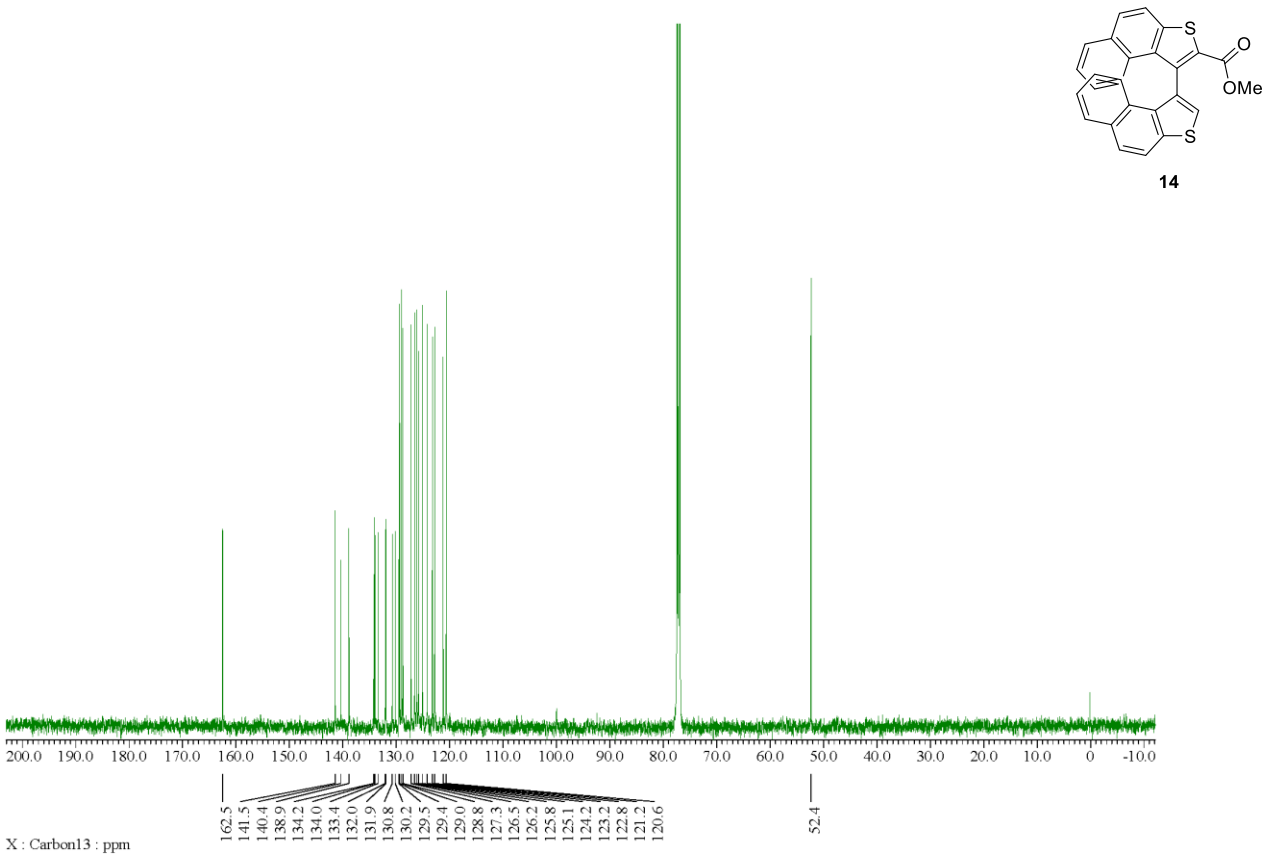

Figure S22. ^{13}C NMR spectrum of **14** (126 MHz, $CDCl_3$)

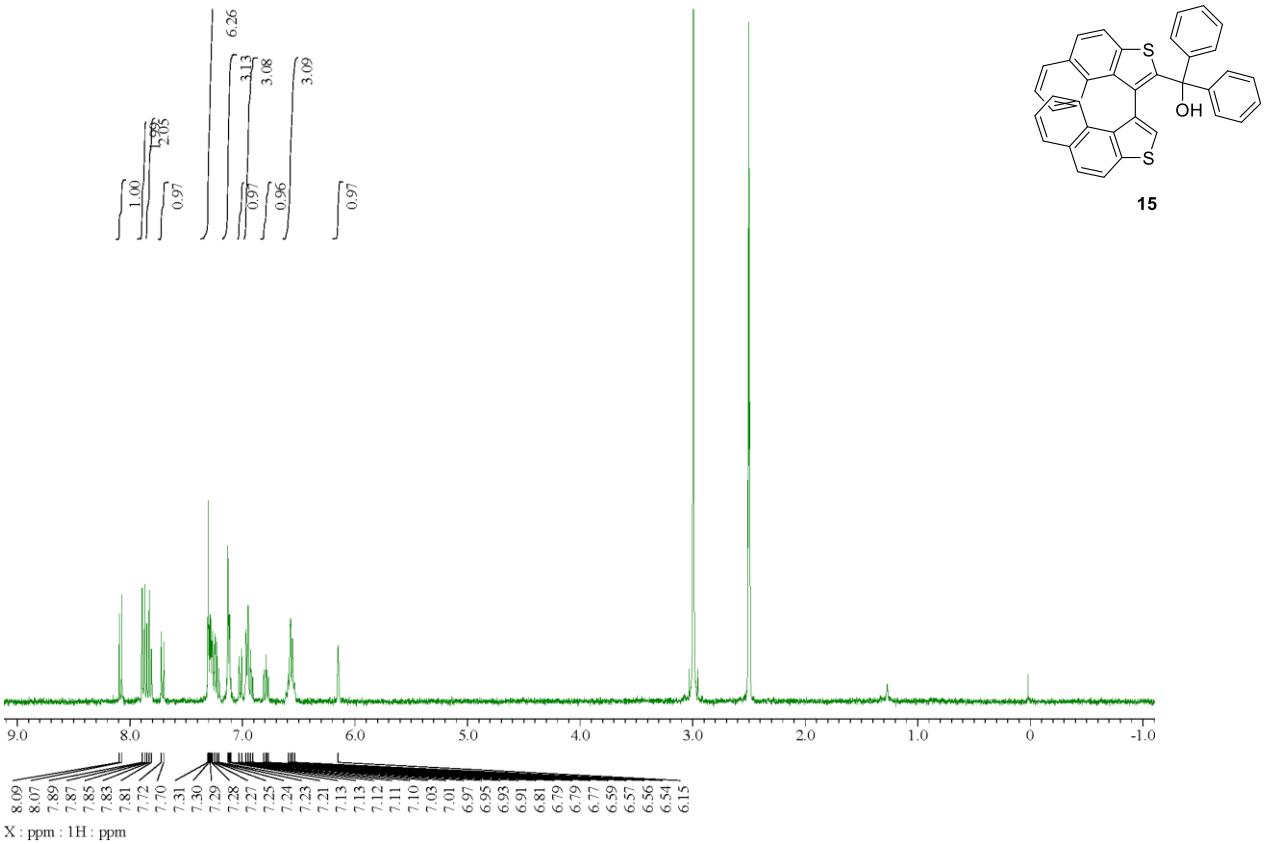

Figure S23. ^{1}H NMR spectrum of **15** (400 MHz, DMSO-d_6, 100 °C).

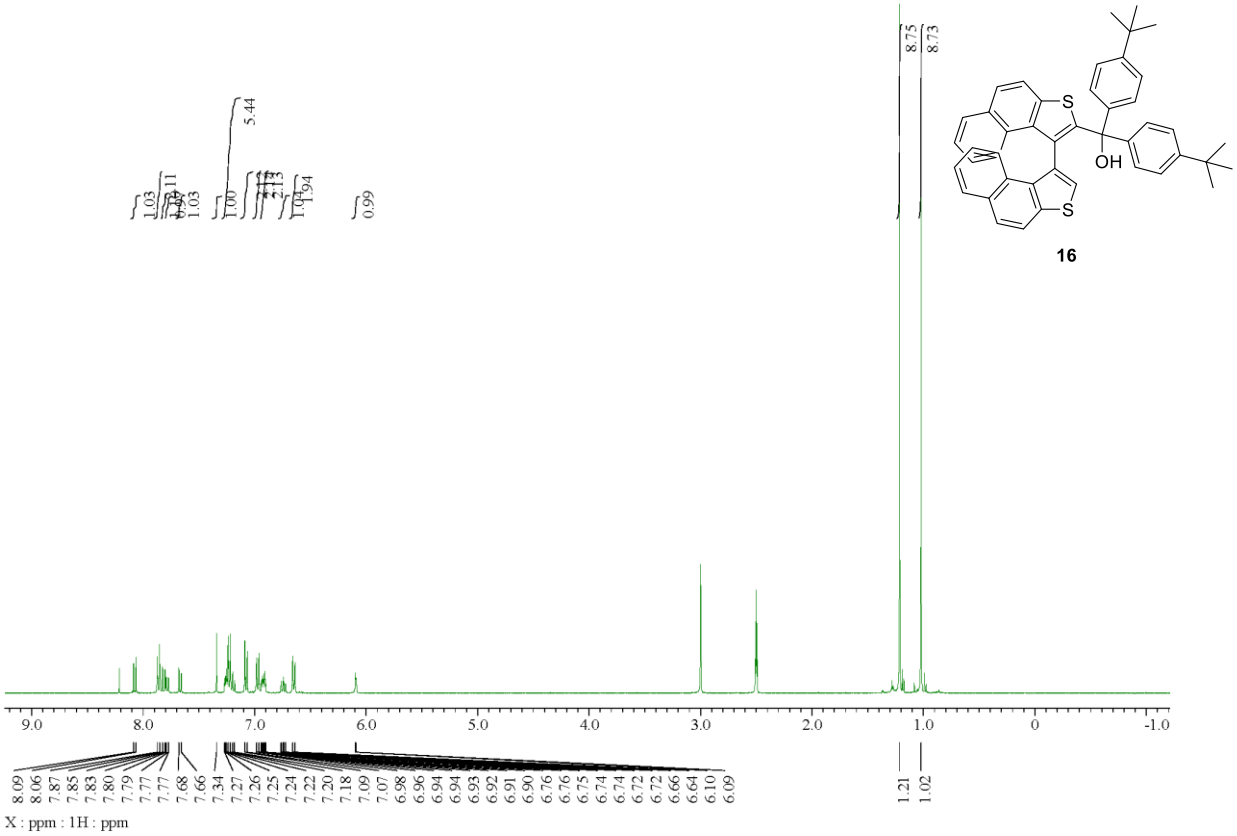

Figure S24. ^{1}H NMR spectrum of **16** (400 MHz, DMSO-d_6, 100 °C).

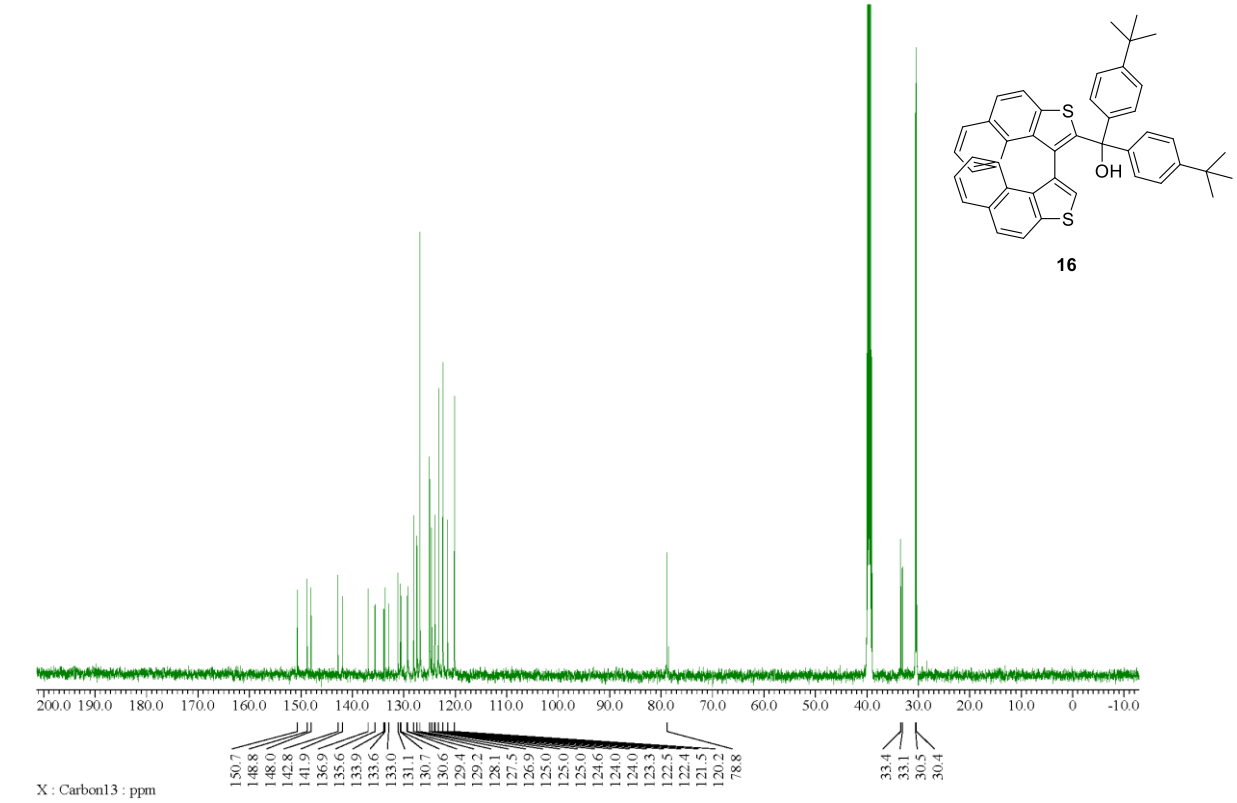

Figure S25. ^{13}C NMR spectrum of **16** (126 MHz, DMSO-d_6, 100 °C)

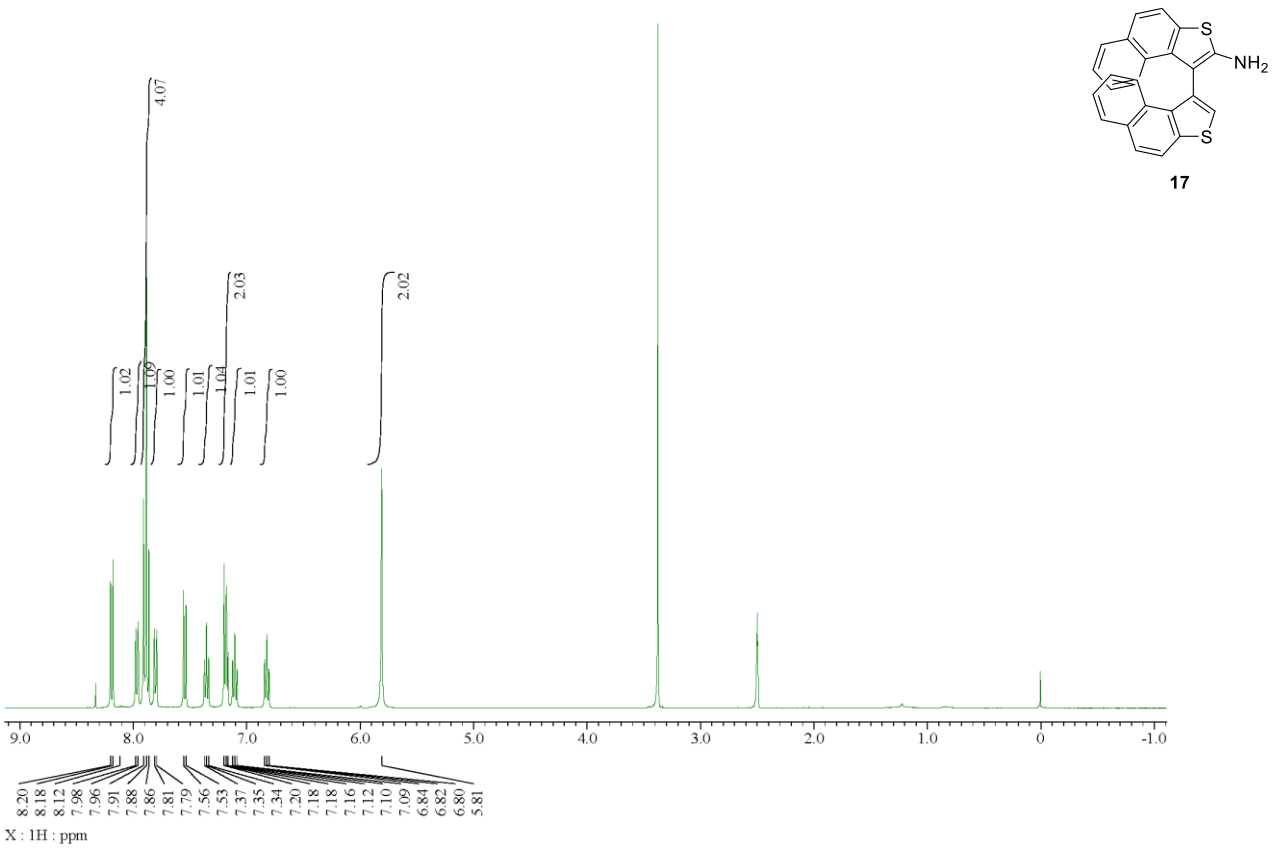

Figure S26. ^{1}H NMR spectrum of **17** (400 MHz, DMSO-d_6).

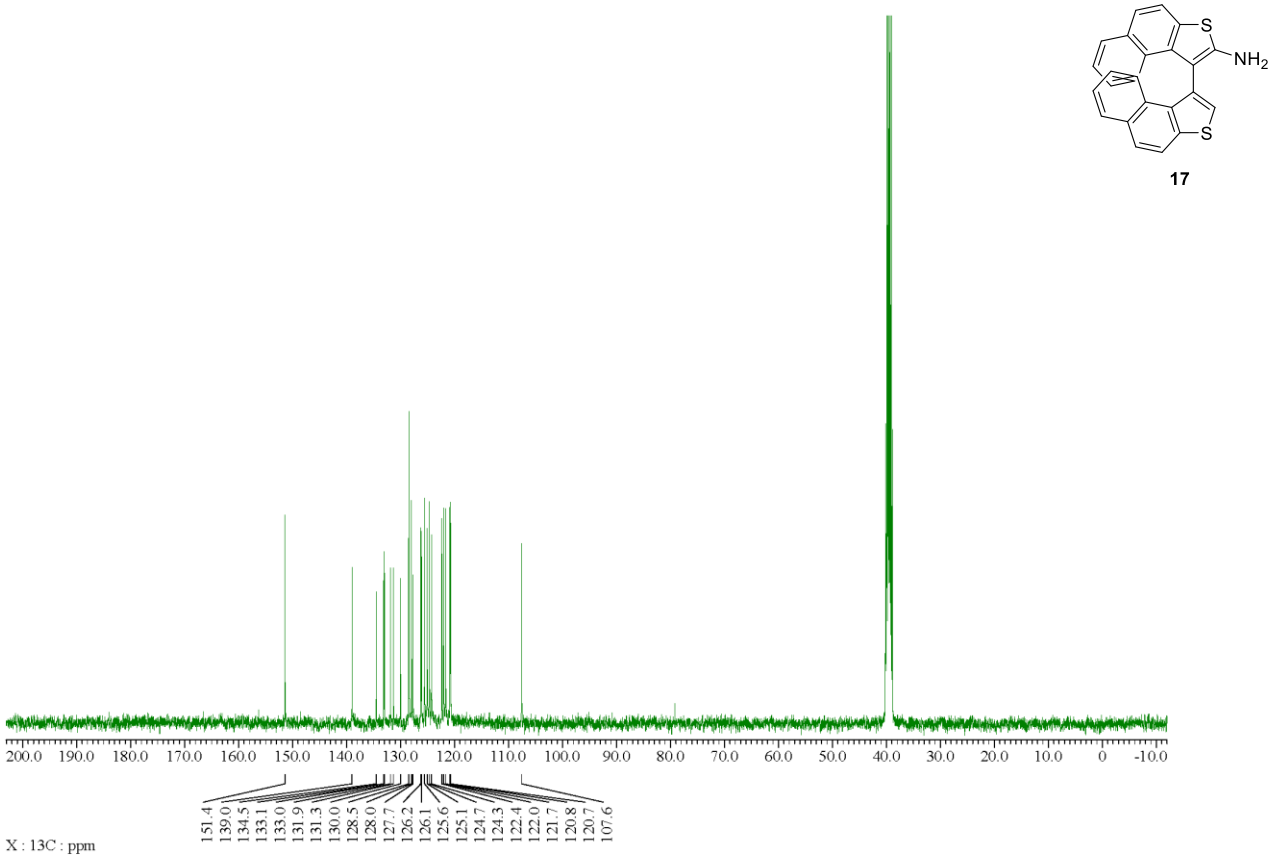

Figure S27. ^{13}C NMR spectrum of **17** (101 MHz, DMSO-d_6)

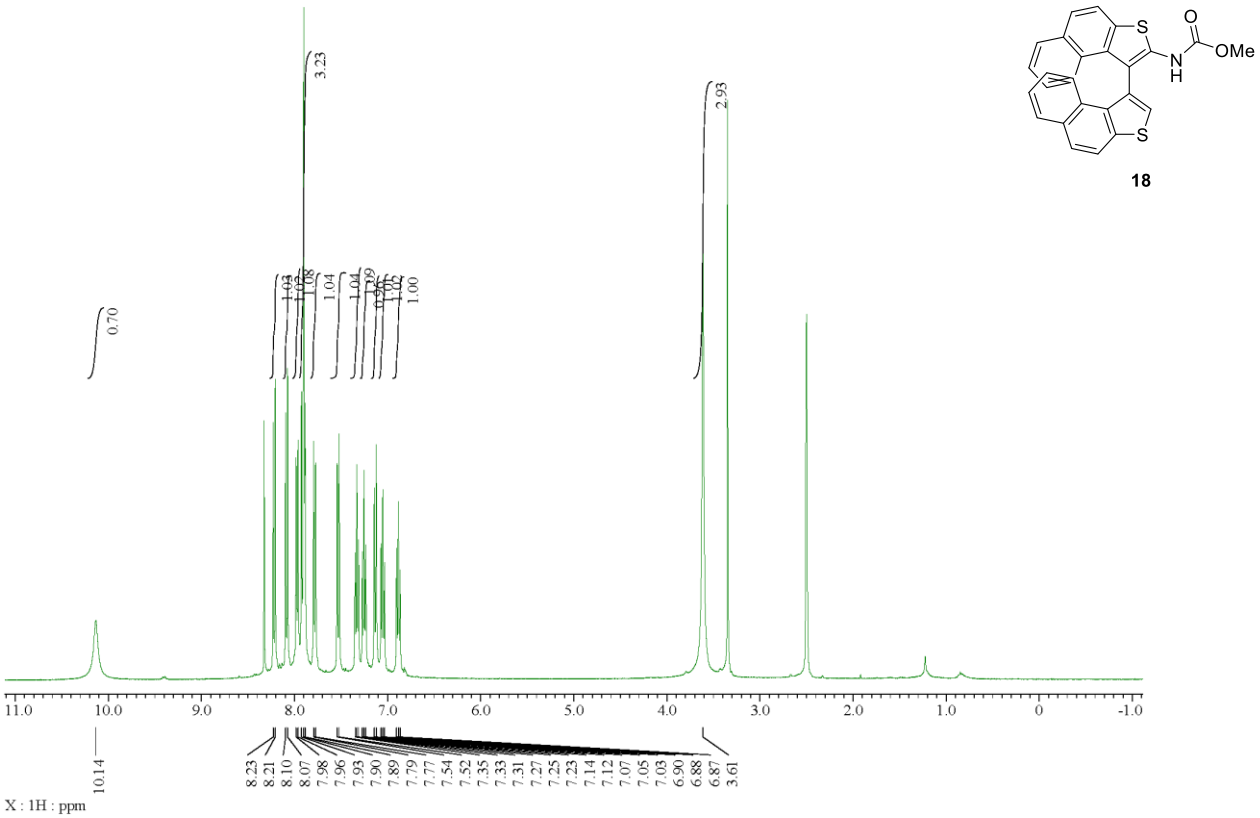

Figure S28. ^{1}H NMR spectrum of **18** (400 MHz, DMSO-d_6).

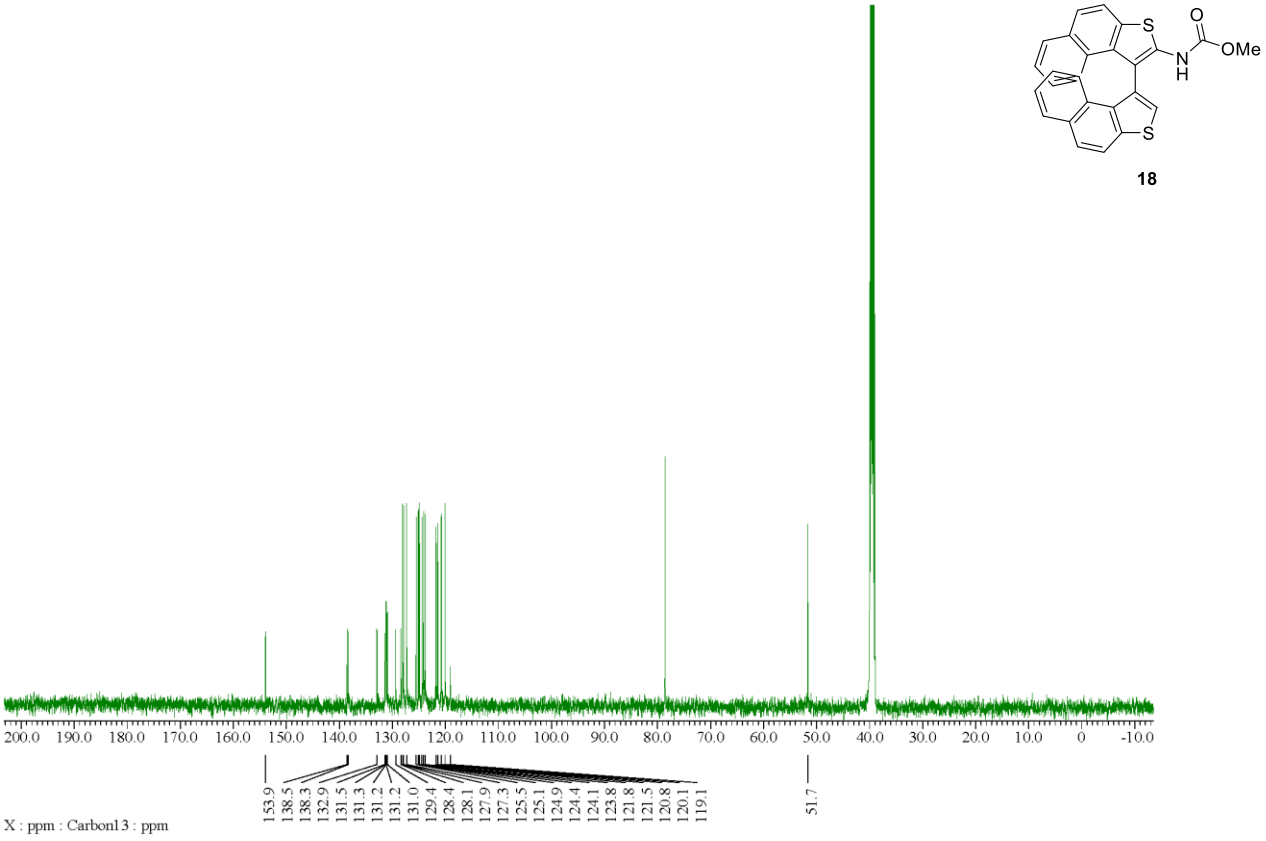

Figure S29. ^{13}C NMR spectrum of **18** (126 MHz, DMSO-d_6, 100 °C)

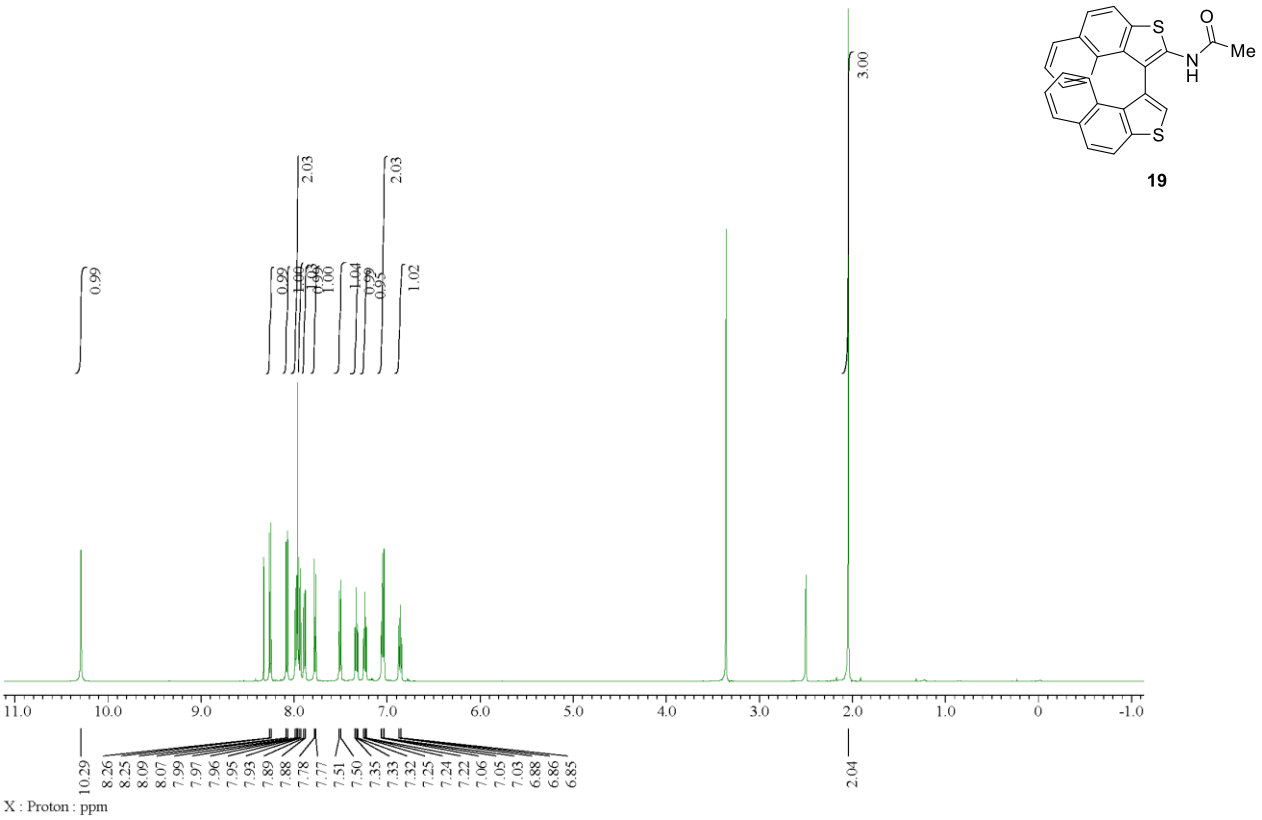

Figure S30. ^{1}H NMR spectrum of **19** (500 MHz, DMSO-d_6).

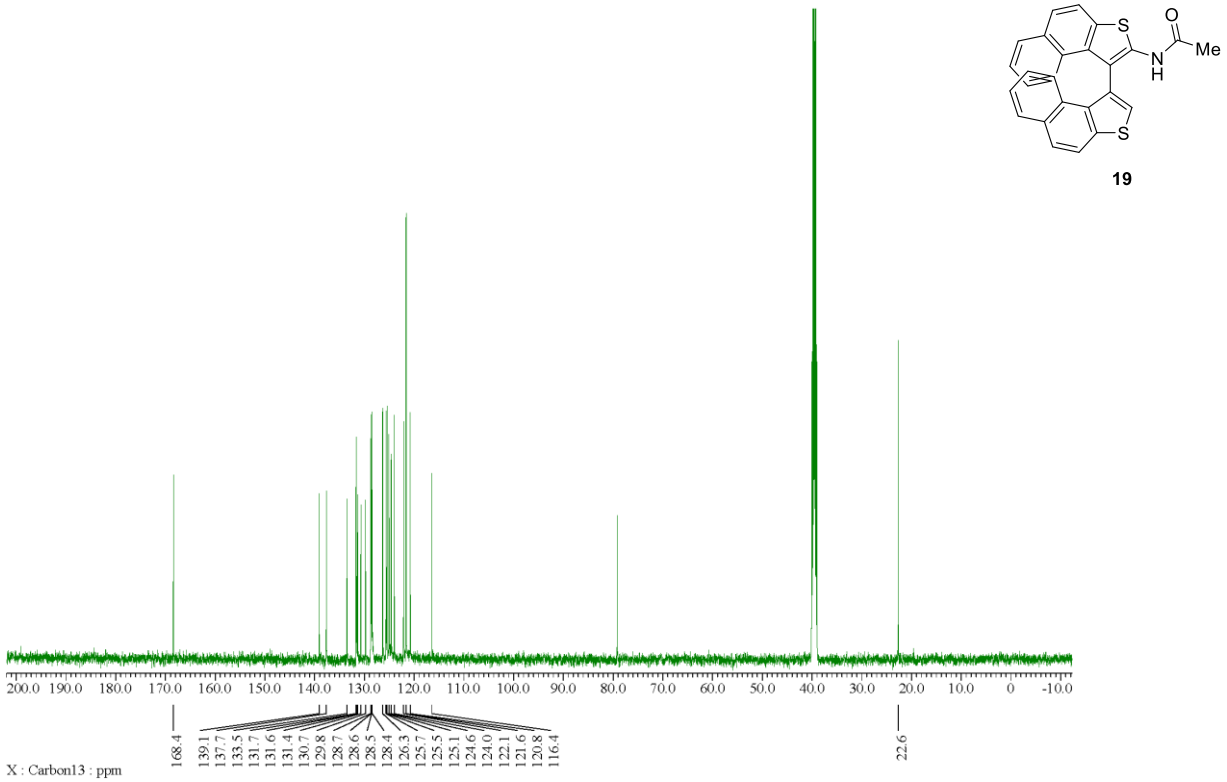

Figure S31. ^{13}C NMR spectrum of **19** (126 MHz, DMSO-d_6)

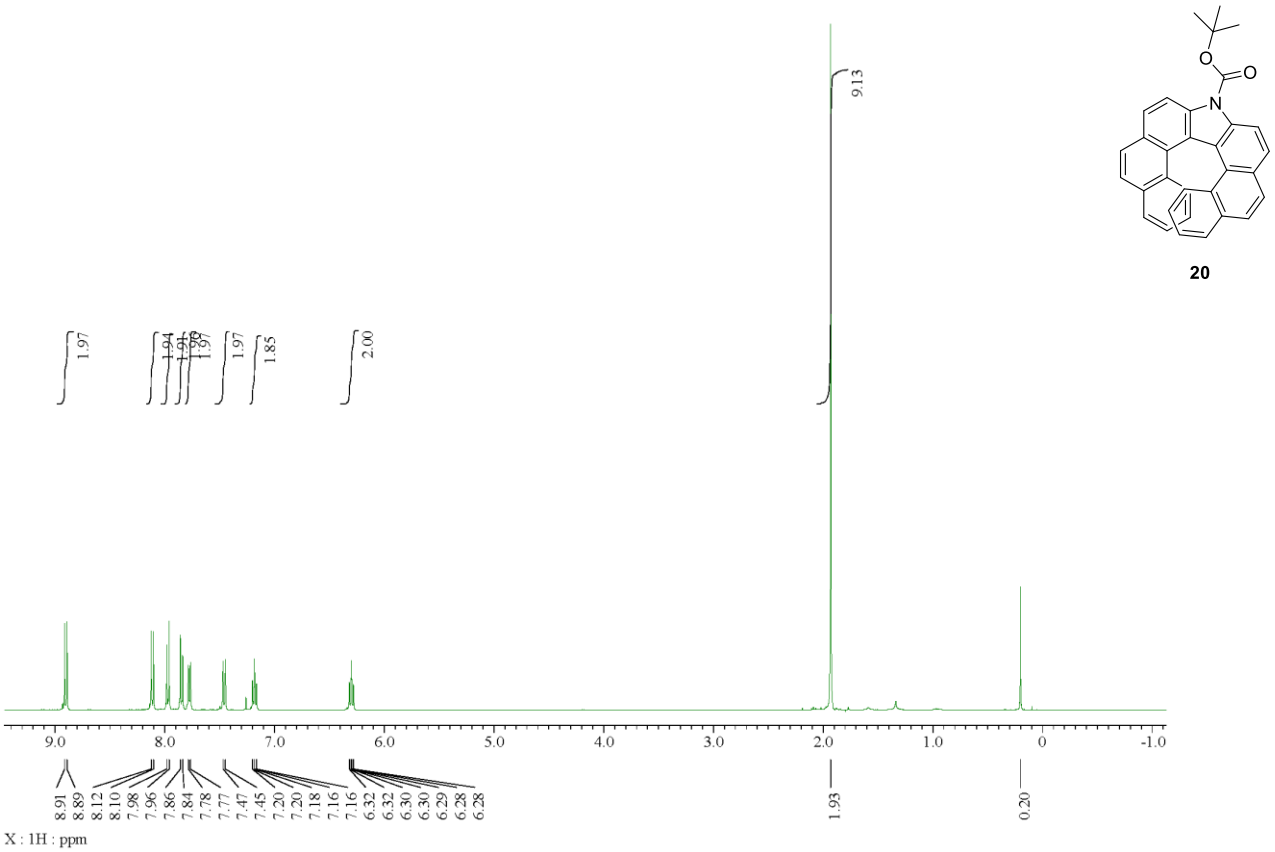

Figure S32. ^{1}H NMR spectrum of **20** (400 MHz, $CDCl_3$)

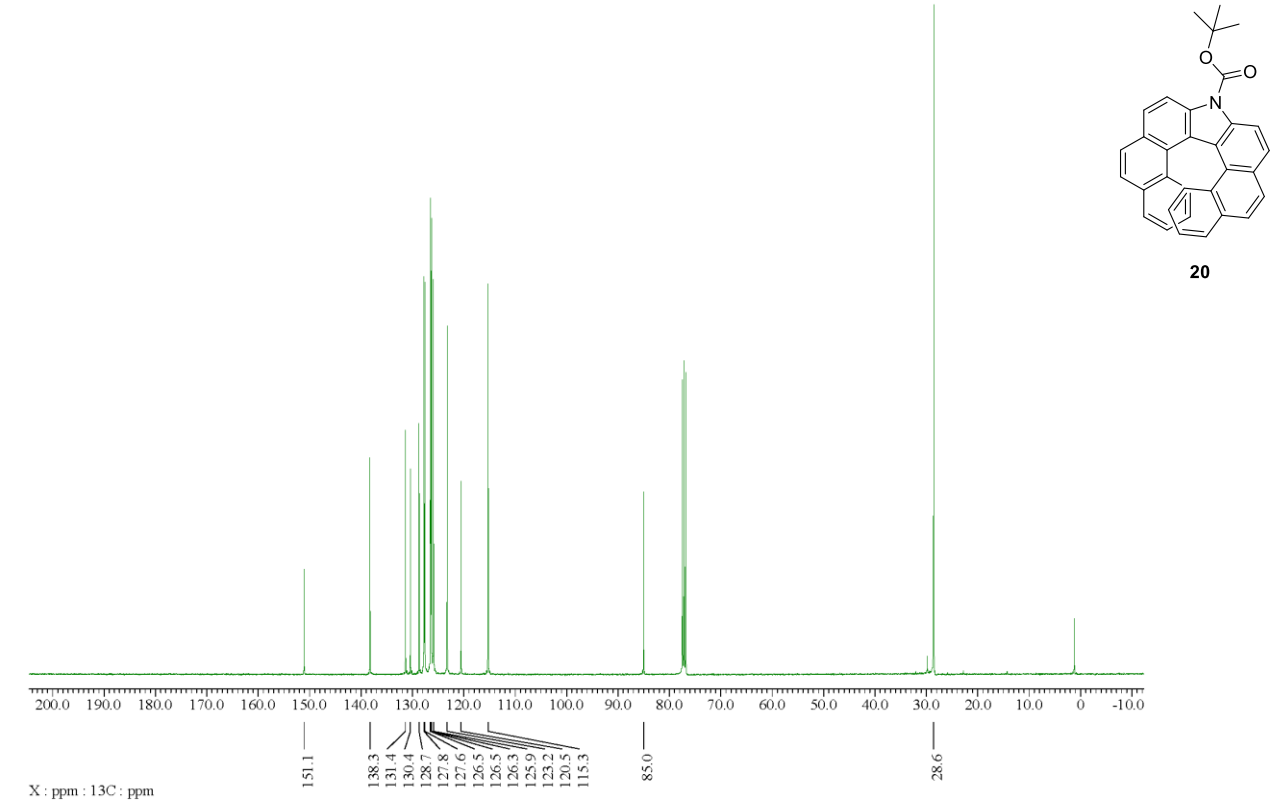

Figure S33. ^{13}C NMR spectrum of **20** (101 MHz, $CDCl_3$)

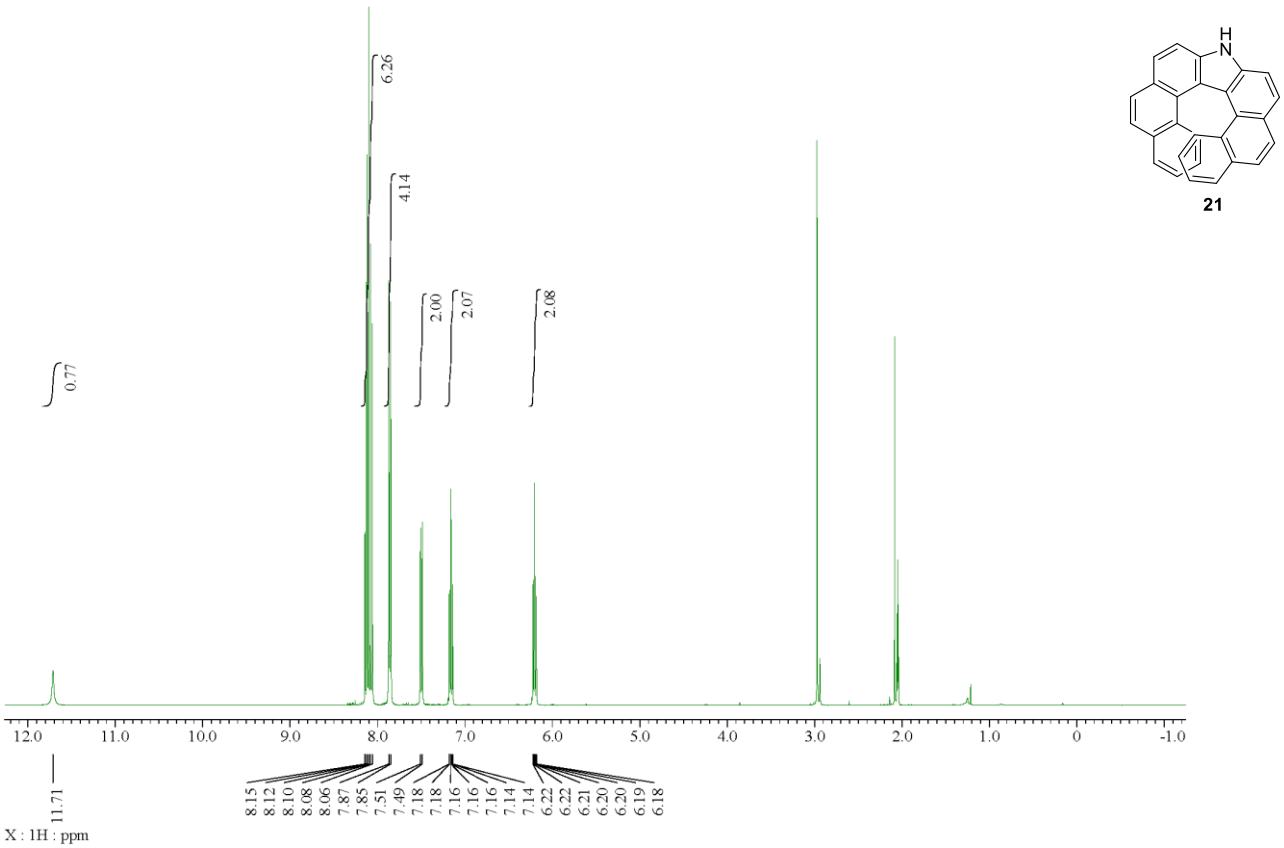

Figure S34. ^{1}H NMR spectrum of **21** (400 MHz, acetone-d_6)

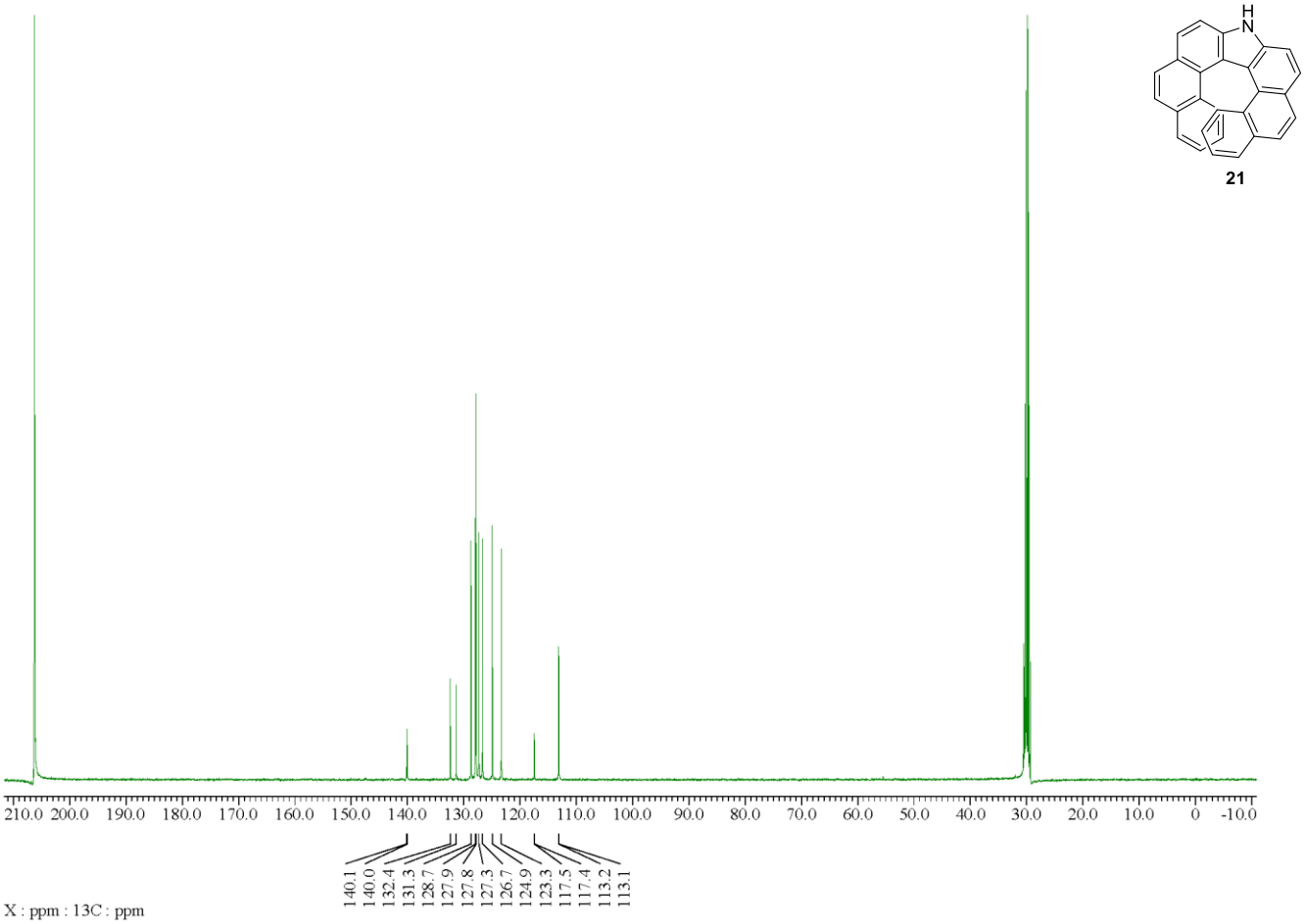

Figure S35. ^{13}C NMR spectrum of **21** (101 MHz, acetone-d_6)

X-ray Analysis

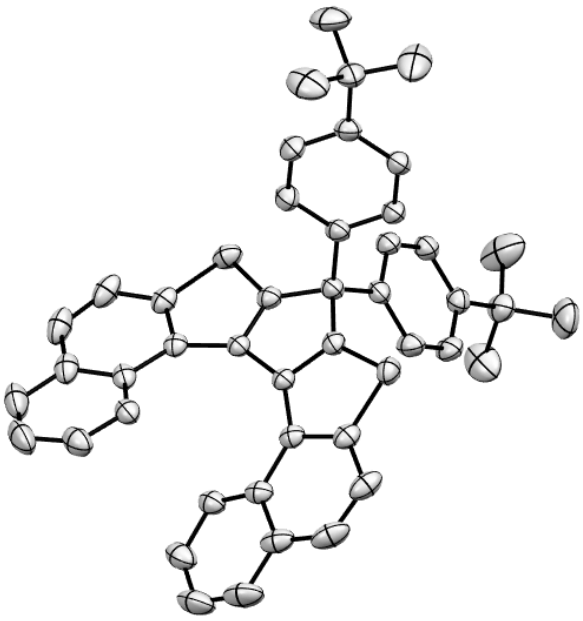

Figure S36. X-ray crystallographic structure of **2** (ORTEP drawing with 50% probability. All hydrogen atoms are omitted for clarity).

Table S1. Crystallographic data and structure refinement details for compound **2**

Formula	$C_{45}H_{38}S_2$	
Formula weight	642.87	
Temperature	193(2) K	
Wavelength	1.54187 Å	
Crystal system	monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	*a* = 22.8514(4) Å	*α* = 90°
	b = 12.0435(2) Å	*β* = 115.7690(10) °
	c = 13.7823(3) Å	*γ* = 90°
Volume	3415.83(11) Å^3	
Z	4	
Density (calculated)	1.250 g/cm^3	
Absorption coefficient	1.641 mm^{-1}	
F(000)	1360	
Crystal size	0.35 × 0.20 × 0.15 mm^3	
Theta range for data collection	4.253 to 68.240°	
Index ranges	–27<=h<=27, –14<=k<=14, –16<=l<=16	
Reflections collected	29606	
Independent reflections	3113 [R_{int} = 0.0174]	
Completeness to theta	99.4%	
Max. and min. transmission	0.782 and 0.621	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	216/0/3113	
Goodness-of-fit on F^2	1.070	
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0388, wR_2 = 0.1075	
R indices (all data)	R_1 = 0.0415, wR_2 = 0.1098	
Largest diff. peak and hole	0.287 and –0.179 e/Å^3	

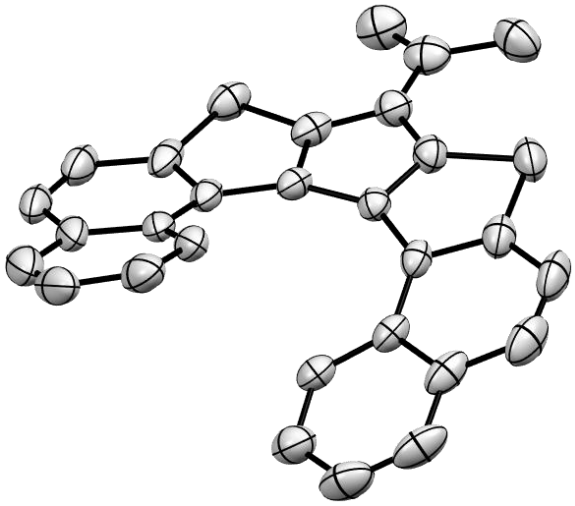

Figure S37. X-ray crystallographic structure of **4** (ORTEP drawing with 50% probability. All hydrogen atoms are omitted for clarity).

Table S2. Crystallographic data and structure refinement details for compound **4**

Formula	$C_{26}H_{15}NOS_2$•0.5($CHCl_3$)	
Formula weight	481.19	
Temperature	193(2) K	
Wavelength	1.54187	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.1314(2) Å	α = 83.5273(7)°
	b = 12.3033(2) Å	β = 85.5012(7) °
	c = 14.3697(3) Å	γ = 81.3505(7)°
Volume	2102.72(7) $Å^3$	
Z	4	
Density (calculated)	1.520 g/cm^3	
Absorption coefficient	4.217 mm^{-1}	
F(000)	988	
Crystal size	0.35 × 0.20 × 0.080 mm^3	
Theta range for data collection	3.101 to 68.229°	
Index ranges	–14<=h<=14, –14<=k<=14, –17<=l<=17	
Reflections collected	39772	
Independent reflections	7590 [R_{int} = 0.0247]	
Completeness to theta	98.5%	
Max. and min. transmission	0.714 and 0.304	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7590/0/577	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2σ (I)]	R_1 = 0.0673, wR_2 = 0.1837	
R indices (all data)	R_1 = 0.0762, wR_2 = 0.1917	
Largest diff. peak and hole	1.753 and –0.719 e/$Å^3$	

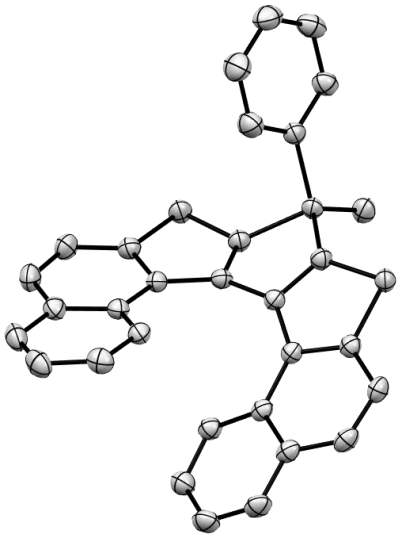

Figure S38. X-ray crystallographic structure of **5** (ORTEP drawing with 50% probability. All hydrogen atoms are omitted for clarity).

Table S3. Crystallographic data and structure refinement details for compound **5**

Formula	$C_{30}H_{17}OPS_2$	
Formula weight	488.52	
Temperature	193(2) K	
Wavelength	1.54187 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.0140(2) Å	α = 90°
	b = 9.11776(17) Å	β = 104.4257(7) °
	c = 21.2612(4) Å	γ = 90°
Volume	2255.54(7) Å^3	
Z	4	
Density (calculated)	1.439 g/cm^3	
Absorption coefficient	2.985 mm^{-1}	
F(000)	1008	
Crystal size	0.50 × 0.40 × 0.15 mm^3	
Theta range for data collection	3.870 to 68.249°	
Index ranges	–14<=h<=14, –10<=k<=10, –25<=l<=25	
Reflections collected	40480	
Independent reflections	4121 [R_{int} = 0.0337]	
Completeness to theta	100%	
Max. and min. transmission	0.639 and 0.220	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4121/0/307	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2σ (I)]	R_1 = 0.0344, wR_2 = 0.0924	
R indices (all data)	R_1 = 0.0352, wR_2 = 0.0931	
Largest diff. peak and hole	0.361 and –0.254 e/Å^3	

Table S4. Summary of Fluorescence Lifetime Measurement of Compounds **1**, **3**–**5**, **7**, and **8**

	τ_1 (ns) [α_1]	τ_2 (ns) [α_2]	τ_{ave} (ns)[a]	Φ (%)	k_r ($\times 10^7$ s^{-1})[b]	k_{nr} ($\times 10^9$ s^{-1})[c]
1	0.49 [1.00]	-	0.49	1.8	3.7	2.0
3	0.16 [0.99]	1.29 [0.01]	0.17	0.29	1.7	5.9
4	0.15 [0.91]	2.26 [0.09]	0.34	0.11	0.32	2.9
5	0.18 [0.94]	0.68 [0.06]	0.21	0.17	0.81	4.8
7	4.16 [0.83]	6.46 [0.17]	4.55	8.4	1.8	0.20
8	3.37 [0.99]	23.8 [0.01]	3.57	12.2	3.4	0.25

[a] $\tau_{ave} = \alpha_1 \cdot \tau_1 + \alpha_2 \cdot \tau_2$. [b] k_r (radiative rate constant) = Φ / τ_{ave}. [c] k_{nr} (non-radiative rate constant) = $(1-\Phi)/\tau_{ave}$.

DFT and TD-DFT Calculation Results

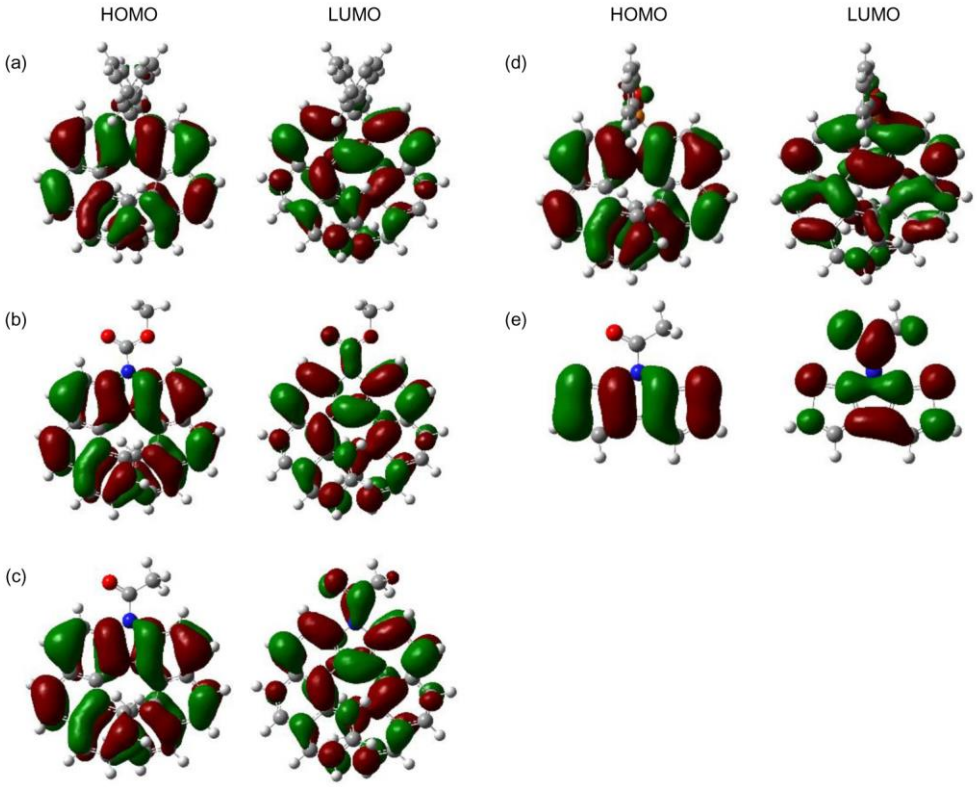

Figure S39. HOMOs and LUMOs of (a) **6**, (b) **7**, (c) **8**, (d) **9**, (e) 1-(7*H*-dithieno[2,3-*b*:3',2'-*d*]-pyrrol-7-yl)ethan-1-one calculated by DFT method at the B3LYP /6-31G(d) level of theory.

Table S5. The selected absorption peaks of compounds **1** and **3-5** calculated by TD–DFT method at the B3LYP /6-31G(d) level of theory.

		transition energy	wavelength	transition configulation	oscillator
1	1	3.3469	370	**HOMO → LUMO (0.700)**	0.0171
	2	3.4457	360	HOMO-1 → LUMO (-0.267)	0.0816
				HOMO → LUMO+1 (0.643)	
	3	3.7989	326	**HOMO-1 → LUMO (0.640)**	0.2725
				HOMO → LUMO+1 (0.260)	
	4	3.8553	322	HOMO-2 → LUMO (0.101)	0.0368
				HOMO-1 → LUMO+1 (0.604)	
				HOMO → LUMO+2 (0.316)	
3	1	3.5620	348	HOMO-1 → LUMO (0.186)	0.0416
				HOMO-1 → LUMO+1 (0.165)	
				HOMO → LUMO (0.632)	
				HOMO → LUMO+1 (0.141)	
	2	3.6419	340	**HOMO-1 → LUMO (0.639)**	0.1207
				HOMO-1 → LUMO+1 (-0.216)	
				HOMO → LUMO (-0.137)	
	3	3.7104	334	HOMO-1 → LUMO (-0.146)	0.0339
				HOMO-1 → LUMO+1 (-0.219)	
				HOMO → LUMO+1 (0.643)	
	4	3.8604	321	HOMO-1 → LUMO (0.128)	0.2121
				HOMO-1 → LUMO+1 (0.602)	
				HOMO → LUMO (-0.221)	
				HOMO → LUMO+1 (0.216)	
4	1	3.4276	362	**HOMO → LUMO (0.691)**	0.0081
				HOMO → LUMO (0.114)	
	2	3.5529	349	HOMO-1 → LUMO (-0.475)	0.0357
				HOMO-1 → LUMO+1 (-0.152)	
				HOMO → LUMO+1 (0.479)	
	3	3.6617	339	HOMO-1 →LUMO (-0.299)	0.0939
				HOMO-1 → LUMO+1 (0.610)	
				HOMO → LUMO+1 (-0.112)	
	4	3.7660	329	HOMO-1 → LUMO (0.409)	0.2647
				HOMO-1 → LUMO+1 (0.284)	
				HOMO → LUMO+1 (0.455)	
5	1	3.0193	411	**HOMO → LUMO (0.701)**	0.0091
	2	3.3503	370	**HOMO-1 → LUMO (0.606)**	0.0096
				HOMO → LUMO+1 (0.353)	
	3	3.6502	3.65	**HOMO-2 → LUMO (0.659)**	0.0698
				HOMO → LUMO+1 (-0.104)	
				HOMO → LUMO+2 (-0.182)	
	4	3.7009	335	HOMO-2 → LUMO (0.116)	0.3325
				HOMO-1 → LUMO (-0.340)	
				HOMO → LUMO+1 (0.583)	

Table S6. The selected absorption peaks of compounds **6-9** calculated by TD–DFT method at the B3LYP /6-31G(d) level of theory.

	excited state	transition energy (eV)	wavelength (nm)	transition configulation (CI expansion coefficient)	oscillator strength *f*
6	1	3.1644	392	**HOMO → LUMO (0.677)** HOMO → LUMO+1 (-0.137)	0.1363
	2	3.4662	358	HOMO-2 → LUMO+2 (0.108) **HOMO-1 → LUMO (0.594)** HOMO → LUMO+2 (0.341)	0.0055
	3	3.4804	356	HOMO-2 → LUMO (0.502) HOMO → LUMO (0.154) **HOMO → LUMO+1 (0.460)**	0.0224
	4	3.7248	333	HOMO-2 → LUMO (-0.486) **HOMO → LUMO+1 (0.496)**	0.0780
7	1	3.2908	377	HOMO-1 → LUMO (0.142) HOMO-1 → LUMO+1 (-0.120) **HOMO → LUMO (0.657)** HOMO → LUMO+2 (-0.134)	0.1442
	2	3.3160	374	**HOMO-1 → LUMO (0.626)** HOMO → LUMO (-0.146) HOMO → LUMO+1 (0.256)	0.0444
	3	3.6304	341	**HOMO-2 → LUMO (0.610)** HOMO → LUMO (0.115) HOMO → LUMO+1 (0.110) HOMO → LUMO+2 (0.295)	0.0343
	4	3.8931	318	HOMO-3 → LUMO (0.101) HOMO-2 → LUMO (-0.311) HOMO-1 → LUMO (-0.109) HOMO-1 → LUMO+1 (0.188) HOMO-1 → LUMO+3 (-0.110) HOMO → LUMO (0.105) **HOMO → LUMO+1 (0.402)** HOMO → LUMO+2 (0.381)	0.0433
8	1	3.2225	385	HOMO-1 → LUMO (0.182) **HOMO → LUMO (0.655)** HOMO → LUMO (-0.108)	0.1344
	2	3.2635	380	**HOMO-1 → LUMO (0.624)** HOMO → LUMO (-0.190) HOMO → LUMO+1 (0.343) HOMO → LUMO+2 (-0.148)	0.0678
	3	3.5390	350	**HOMO-2 → LUMO (0.568)** HOMO → LUMO+1 (0.343) HOMO → LUMO+2 (0.176)	0.0174
	4	3.7770	328	HOMO-2 → LUMO (-0.406) HOMO-1 → LUMO+1 (0.107) HOMO-1 →LUMO+2 (-0.115) **HOMO → LUMO+1 (0.476)** HOMO → LUMO+2 (0.240)	0.0247
9	1	3.0587	405	**HOMO → LUMO (0.691)**	0.0768
	2	3.2576	381	**HOMO-1 → LUMO (0.581)** HOMO → LUMO+1 (-0.378)	0.0113
	3	3.4599	358	HOMO-3 → LUMO+1 (0.105) **HOMO-2 → LUMO (0.618)** HOMO-1 → LUMO (-0.131) HOMO → LUMO (0.232)	0.0228
	4	3.5622	348	**HOMO-2 → LUMO (0.638)** HOMO-1 → LUMO (0.370) HOMO → LUMO+1 (0.567)	0.0012

Table S7. Coordinates (Å) and Absolute Energy of the Optimized Structure for **1**[a]

atom	x	y	z	atom	x	y	z
C	-0.58154	2.63258	3.84664	H	-4.68086	1.47572	10.81437
C	-1.31897	1.87485	4.73819	C	-2.06792	0.78378	8.04504
C	-1.25138	0.47768	4.46954	H	-1.28814	0.57772	7.31848
C	-0.13216	0.24887	3.64116	C	-3.17312	0.13943	10.0902
S	0.54145	1.72277	3.00396	H	-3.29185	-0.5527	10.91955
C	0.32625	-1.04751	3.34637	C	-2.21768	-0.1048	9.11146
H	1.21128	-1.1951	2.73331	H	-1.5841	-0.98597	9.1725
C	-2.04438	-0.669	4.82724	C	-0.90202	4.14715	3.85147
C	-0.38492	-2.14471	3.82751	C	-1.61946	4.65104	2.57277
H	-0.02035	-3.14276	3.5919	C	-2.97933	5.64252	0.29871
C	-1.5757	-1.97533	4.5302	C	-1.77424	6.03721	2.35308
C	-2.33205	-3.09123	4.92311	C	-2.19798	3.77967	1.63032
H	-1.97684	-4.09871	4.71681	C	-2.86322	4.27111	0.50279
C	-3.31432	-0.53791	5.42903	C	-2.43896	6.52644	1.2262
H	-3.75045	0.44113	5.60132	H	-1.37573	6.75592	3.06827
C	-3.56078	-2.93382	5.56389	H	-2.15518	2.70046	1.75656
H	-4.13788	-3.80681	5.85681	H	-3.29801	3.5774	-0.21262
C	-4.0579	-1.65869	5.80343	H	-2.53832	7.59872	1.07878
H	-5.02561	-1.52908	6.28129	H	-3.49957	6.0212	-0.57686
C	-1.9334	4.06268	5.00289	C	0.38774	4.93057	4.20711
C	-2.09192	2.80517	5.55637	C	2.79558	6.29625	4.79096
C	-2.76957	2.83013	6.80896	C	0.73107	5.27292	5.52888
C	-3.44064	4.06696	6.91454	C	1.30862	5.26757	3.19119
S	-2.95577	5.1988	5.68329	C	2.49368	5.94873	3.47885
C	-4.35678	4.33379	7.94757	C	1.91791	5.95472	5.81514
H	-4.88575	5.28225	7.98637	H	0.09057	5.00771	6.36666
C	-2.88855	1.92551	7.92215	H	1.10908	4.99641	2.15509
C	-4.55897	3.37659	8.93954	H	3.18198	6.20114	2.6764
H	-5.27	3.59532	9.73396	H	2.15842	6.21144	6.8439
C	-3.81691	2.19789	8.96059	H	3.71849	6.8233	5.01708
C	-3.9612	1.28799	10.02028				

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S8. Coordinates (Å) and Absolute Energy of the Optimized Structure for **3**[a]

atom	x	y	z	atom	x	y	z
H	-3.78644	-1.39211	-2.114	C	-1.11279	0.85852	2.00007
C	-2.77455	-1.28779	-1.73178	C	-1.40158	3.26739	1.91674
H	-2.44381	-3.40122	-1.65071	C	-2.44074	0.70551	2.40333
C	-2.01017	-2.42191	-1.45915	C	-0.57963	2.13056	1.69934
C	-0.9295	0.10807	-1.04908	C	-0.87131	4.5479	1.77627
C	-0.69739	-2.30714	-0.97434	H	-2.83129	-0.28797	2.60833
C	-2.22858	-0.02426	-1.54347	H	-0.49539	-0.03234	1.93817
C	-0.15649	-1.02226	-0.70616	C	0.48099	4.73738	1.50029
C	0.08544	-3.44496	-0.7921	H	-1.49328	5.42445	1.94788
H	-2.80904	0.86378	-1.77993	H	0.90079	5.73941	1.48028
H	-0.5239	1.11008	-0.94964	C	1.29609	3.61424	1.27539
C	1.42476	-3.34194	-0.42297	C	0.77591	2.30123	1.24542
H	-0.31954	-4.43304	-1.00249	C	1.81709	1.45078	0.79282
H	2.04884	-4.22993	-0.37008	S	3.02751	3.64588	1.06469
C	1.96159	-2.07227	-0.1471	C	3.05571	1.99654	0.83464
C	1.1697	-0.90162	-0.15889	N	4.02502	1.02484	0.65457
C	1.96984	0.14847	0.35985	C	5.4249	1.13316	0.70006
S	3.6422	-1.73368	0.18265	O	6.1536	0.17353	0.49802
C	3.29372	-0.12224	0.40971	O	5.80757	2.40108	0.99118
H	-4.29209	1.70259	2.85217	C	7.22257	2.57503	1.05384
C	-3.25757	1.8208	2.54114	H	7.65102	1.95109	1.84449
H	-3.38514	3.95609	2.461	H	7.42516	3.62292	1.29176
C	-2.73846	3.0943	2.30968	H	7.68056	2.34447	0.08684

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S9. Coordinates (Å) and Absolute Energy of the Optimized Structure for **4**[a]

atom	x	y	z	atom	x	y	z
H	-3.81834	-1.39677	-1.99441	C	-0.88618	0.88722	1.90484
C	-2.78253	-1.27585	-1.68868	C	-1.2354	3.28845	1.83657
H	-2.42009	-3.38388	-1.60745	C	-2.17516	0.70624	2.41016
C	-1.98582	-2.39729	-1.45964	C	-0.40679	2.16942	1.55965
C	-0.911	0.15063	-1.15813	C	-0.74748	4.58007	1.65146
C	-0.64288	-2.26066	-1.07313	H	-2.52601	-0.29456	2.64833
C	-2.24078	-0.00358	-1.55477	H	-0.25503	0.01052	1.79893
C	-0.10049	-0.96619	-0.86022	C	0.57428	4.79905	1.26994
C	0.16574	-3.38647	-0.93404	H	-1.37377	5.44327	1.86867
H	-2.84866	0.8745	-1.75747	H	0.96888	5.80999	1.21408
H	-0.51317	1.15905	-1.09882	C	1.39507	3.69388	0.98508
C	1.52669	-3.26248	-0.66336	C	0.90522	2.36879	1.00089
H	-0.24132	-4.38191	-1.10184	C	1.92799	1.54065	0.47151
H	2.16298	-4.14309	-0.64338	S	3.10331	3.7649	0.63716
C	2.06503	-1.98264	-0.44344	C	3.14975	2.11533	0.41093
C	1.26061	-0.82358	-0.41325	N	4.13291	1.17471	0.15437
C	2.08385	0.24139	0.0346	C	5.51844	1.41933	0.09449
S	3.75567	-1.6169	-0.23819	O	5.953	2.54338	0.31999
C	3.41688	0.00009	-0.01766	C	6.39872	0.26115	-0.25156
H	-4.00837	1.66391	2.99828	H	7.43276	0.61635	-0.31826
C	-3.00406	1.80352	2.60741	H	6.1355	-0.15028	-1.22876
H	-3.18571	3.93514	2.53106	H	6.36557	-0.49768	0.53335
C	-2.5335	3.08719	2.33257				

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S10. Coordinates (Å) and Absolute Energy of the Optimized Structure for **5**[a]

atom	x	y	z	atom	x	y	z
H	-2.34101	1.27536	-5.21753	C	-0.56868	2.71934	0.38371
C	-1.65698	0.92239	-4.4504	C	-0.34211	5.09558	0.87372
H	-2.08902	-1.13995	-4.82512	H	-3.45512	0.9647	-0.20533
C	-1.51328	-0.44482	-4.21752	H	-1.06305	0.61336	0.11706
C	-0.02576	1.37632	-2.73229	C	1.01181	4.92749	1.15209
C	-0.62853	-0.9203	-3.23638	H	-0.77596	6.08705	0.99031
C	-0.90319	1.8311	-3.71868	H	1.60728	5.76781	1.4993
C	0.09974	0.00079	-2.43813	C	1.58725	3.65328	1.00671
C	-0.4444	-2.28994	-3.06477	C	0.85729	2.54802	0.51638
H	-0.99189	2.89699	-3.91264	C	2.96141	1.66943	0.95169
H	0.57187	2.11609	-2.20988	C	1.77604	1.47137	0.27787
C	0.49854	-2.77929	-2.16429	S	3.21168	3.22728	1.45934
H	-0.99369	-3.00184	-3.67816	P	3.87011	0.18433	1.08221
H	0.6903	-3.84711	-2.09985	O	5.21767	0.257	0.42088
C	1.21768	-1.87276	-1.36597	C	3.72525	-0.36535	2.747
C	0.96925	-0.48275	-1.39432	C	3.59634	-1.25881	5.41229
C	2.69429	-0.70341	0.14515	C	4.88566	-0.75502	3.43481
C	1.69838	0.12731	-0.31974	C	2.49736	-0.43347	3.42465
S	2.52991	-2.29077	-0.30327	C	2.43387	-0.87667	4.74739
H	-4.42077	3.2447	-0.06095	C	4.82302	-1.19839	4.75663
C	-3.35245	3.09589	0.07158	H	5.85186	-0.7116	2.93213
H	-2.97382	5.16981	0.43962	H	1.57377	-0.14089	2.9295
C	-2.52462	4.18289	0.34889	H	1.4758	-0.9232	5.25967
C	-1.43837	1.63029	0.15547	H	5.73214	-1.4959	5.27349
C	-1.14287	4.01003	0.52841	H	3.54636	-1.60354	6.44204
C	-2.81192	1.81915	-0.01071				

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S11. Coordinates (Å) and Absolute Energy of the Optimized Structure for **6**[a]

atom	x	y	z	atom	x	y	z
H	5.8245892	1.9519825	-2.0528943	H	3.7604959	-4.3861668	-1.4584906
C	4.8589207	1.9046579	-1.5568345	C	3.3215388	-2.7042744	-0.1519299
H	5.3130341	3.4691337	-0.1583212	C	4.5778204	-2.7419359	0.4954563
C	4.5778204	2.741936	-0.4954563	C	2.3441004	-1.7415323	0.2501267
C	2.6463469	0.9379987	-1.3744789	C	4.8589207	-1.9046578	1.5568345
C	3.3215387	2.7042745	0.1519299	H	5.3130342	-3.4691336	0.1583212
C	3.8705091	1.0147381	-2.0137083	H	5.8245892	-1.9519823	2.0528944
C	2.3441004	1.7415323	-0.2501267	C	3.8705091	-1.0147381	2.0137084
C	2.9955879	3.6758609	1.1541014	H	4.0638236	-0.3843362	2.8772413
H	4.0638236	0.3843362	-2.8772413	C	2.6463469	-0.9379987	1.3744789
H	1.8946753	0.2635289	-1.7625359	C	-2.2672977	0	0
C	1.7323158	3.7605374	1.6456947	C	-3.1225751	0.5783689	-1.1515901
H	3.7604958	4.3861669	1.4584906	C	-4.6053781	1.504238	-3.3700987
H	1.4595996	4.550142	2.3417207	C	-4.2993426	-0.0710391	-1.5583387
C	0.7162216	2.8199644	1.264827	C	-2.7013229	1.6965703	-1.8850226
C	-0.6112553	3.0171714	1.7069593	C	-3.4352565	2.1553818	-2.9803115
C	1.0518166	1.7061284	0.4273602	C	-5.0326928	0.3858014	-2.6536797
C	-1.6238471	2.1731921	1.2970294	H	-4.6556477	-0.9344937	-1.0052714
H	-0.8297639	3.8776953	2.334242	H	-1.791621	2.2154665	-1.6027158
H	-2.656748	2.3721569	1.5642749	H	-3.0870369	3.0272945	-3.5280565
C	-1.2886023	1.0284886	0.5682845	H	-5.9421962	-0.1343865	-2.9433682
C	0.0428853	0.6990777	0.2631088	H	-5.1780584	1.8641155	-4.2206737
H	-2.6567479	-2.372157	-1.5642749	C	-3.1225751	-0.5783689	1.15159
C	-1.6238471	-2.1731921	-1.2970294	C	-4.6053779	-1.504238	3.3700987
H	-0.8297638	-3.8776953	-2.3342419	C	-2.701323	-1.6965706	1.8850223
C	-0.6112552	-3.0171714	-1.7069592	C	-4.2993424	0.0710393	1.558339
C	0.0428854	-0.6990777	-0.2631088	C	-5.0326925	-0.3858012	2.65368
C	0.7162216	-2.8199644	-1.264827	C	-3.4352566	-2.1553821	2.9803112
C	-1.2886023	-1.0284886	-0.5682845	H	-1.7916213	-2.2154669	1.6027152
C	1.0518166	-1.7061284	-0.4273602	H	-4.6556473	0.9344941	1.0052719
C	1.732316	-3.7605374	-1.6456947	H	-5.9421957	0.1343868	2.9433687
H	1.8946752	-0.2635289	1.762536	H	-3.0870371	-3.027295	3.528056
C	2.995588	-3.6758608	-1.1541015	H	-5.1780582	-1.8641155	4.2206738
H	1.4595998	-4.550142	-2.3417207				

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S12. Coordinates (Å) and Absolute Energy of the Optimized Structure for **7**[a]

atom	x	y	z	atom	x	y	z
H	-4.52553	1.76807	-0.96539	C	0.6301	-0.57488	2.54527
C	-3.49788	1.48302	-0.76024	C	-0.87829	-1.0452	4.40892
H	-3.00669	1.23911	-2.82492	C	1.63389	-0.28429	3.47497
C	-2.63265	1.17453	-1.80535	C	-0.61082	-1.17158	3.01747
C	-1.70511	1.07821	0.79567	C	-2.12594	-1.41004	4.91993
C	-1.29839	0.80738	-1.55827	H	-0.35729	-2.2105	0.42683
C	-3.0281	1.45196	0.54223	C	-3.10506	-1.95493	4.09588
C	-0.8102	0.69094	-0.2314	H	-2.35235	-1.28057	5.97652
C	-0.44206	0.58356	-2.63721	H	-4.06599	-2.21858	4.53253
H	-3.68131	1.71759	1.36884	C	-2.8368	-2.22591	2.75378
H	-1.37363	1.11419	1.82904	C	-3.81651	-2.86511	1.97417
C	0.90533	0.30601	-2.43013	C	-1.57554	-1.88432	2.20112
H	-0.80416	0.67554	-3.65902	C	-3.56027	-3.2294	0.65607
H	1.55188	0.20419	-3.29956	H	-4.79003	-3.10189	2.3982
C	1.42036	0.1697	-1.1389	H	-4.32484	-3.72612	0.06614
C	2.78859	-0.03329	-0.98335	C	-2.31026	-2.98147	0.1141
C	0.55601	0.25548	-0.01329	H	-2.08156	-3.28696	-0.90314
C	3.36847	-0.09579	0.27869	C	-1.33528	-2.33651	0.88089
H	3.44279	-0.07984	-1.85253	N	2.82538	-0.05811	2.77538
H	4.44829	-0.1735	0.35506	C	4.0853	0.16598	3.38924
C	2.53227	-0.09331	1.40586	O	4.25018	0.0635	4.59671
C	1.13787	-0.10001	1.27113	O	5.03022	0.52083	2.48199
H	2.1305	0.0096	5.58145	C	6.3109	0.78414	3.05526
C	1.37314	-0.26733	4.8532	H	6.99382	1.05858	2.24654
H	-0.11416	-0.5161	6.3589	H	6.70137	-0.11105	3.54938
C	0.09256	-0.58083	5.29183	H	6.25191	1.62129	3.75787

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S13. Coordinates (Å) and Absolute Energy of the Optimized Structure for **8**[a]

atom	x	y	z	atom	x	y	z
H	-4.47796	1.88334	-0.93083	C	0.64045	-0.63048	2.52166
C	-3.45811	1.56468	-0.73625	C	-0.85464	-1.10238	4.3962
H	-2.99638	1.30658	-2.80605	C	1.65965	-0.36779	3.44304
C	-2.614	1.22929	-1.79044	C	-0.6064	-1.21161	2.99974
C	-1.66515	1.09754	0.80198	C	-2.10302	-1.44989	4.91738
C	-1.2904	0.81746	-1.55721	H	-0.40414	-2.22682	0.39506
C	-2.97753	1.51456	0.56181	C	-3.10373	-1.96031	4.09746
C	-0.79305	0.68592	-0.23534	H	-2.31329	-1.33289	5.97877
C	-0.45363	0.56126	-2.64471	H	-4.06452	-2.21062	4.54218
H	-3.61454	1.79811	1.39514	C	-2.85742	-2.21602	2.74835
H	-1.32416	1.11655	1.83282	C	-3.85995	-2.82268	1.97175
C	0.88444	0.23176	-2.45193	C	-1.59558	-1.89325	2.18561
H	-0.82376	0.66327	-3.66278	C	-3.62699	-3.17433	0.646
H	1.51561	0.09949	-3.32855	H	-4.83332	-3.04445	2.40421
C	1.40869	0.08127	-1.16601	H	-4.40892	-3.64642	0.05861
C	2.76757	-0.1861	-1.02276	C	-2.37779	-2.94728	0.09331
C	0.56091	0.20884	-0.03223	H	-2.16695	-3.24529	-0.92998
C	3.35979	-0.25814	0.23378	C	-1.38029	-2.33425	0.85742
H	3.40601	-0.28197	-1.89986	N	2.83941	-0.10997	2.73412
H	4.43172	-0.40619	0.29427	C	4.08661	0.18567	3.34191
C	2.5401	-0.18164	1.36946	O	4.27854	-0.07695	4.52537
C	1.14485	-0.15546	1.24669	C	5.12572	0.84783	2.49252
H	2.1844	-0.11196	5.54679	H	5.81391	1.38925	3.15105
C	1.41456	-0.36947	4.82436	H	4.69058	1.58945	1.81869
H	-0.05631	-0.62091	6.34495	H	5.70736	0.09882	1.95191
C	0.13536	-0.67156	5.27435				

[a]Calculated by DFT method [B3LYP/6-31G(d)]

Table S14. Coordinates (Å) and Absolute Energy of the Optimized Structure for **9**[a]

atom	x	y	z	atom	x	y	z
H	-5.9973899	-0.4784728	-1.7513836	C	-0.4735581	1.6105585	-0.3210869
C	-4.9915597	-0.7381688	-1.4329057	C	-1.1497333	3.9133809	-0.9628769
H	-5.6265802	-2.3598171	-0.1770492	H	-0.8718288	-0.1114583	1.8032515
C	-4.7859727	-1.7782239	-0.5482354	C	-2.219186	3.8669706	-0.1277005
C	-2.6014677	-0.3603845	-1.5356484	H	-0.9703054	4.7852413	-1.586872
C	-3.4826992	-2.1388645	-0.1364516	H	-2.923161	4.6941617	-0.0796325
C	-3.8831315	-0.0444458	-1.9497963	C	-2.3917423	2.7675195	0.776307
C	-2.3589536	-1.3784795	-0.5841955	C	-3.3912984	2.8197983	1.7743379
C	-3.2770264	-3.31318	0.6598119	C	-1.4990904	1.6532808	0.7198347
H	-4.0286835	0.7396746	-2.6876108	C	-3.4848214	1.839431	2.7421281
H	-1.766537	0.1675172	-1.9761963	H	-4.0708997	3.6687188	1.7832117
C	-2.0224304	-3.7738233	0.9001224	H	-4.2505313	1.8969184	3.5108162
H	-4.1473899	-3.8664948	1.0040324	C	-2.5552916	0.7845936	2.744922
H	-1.8672701	-4.7123324	1.426313	H	-2.5881152	0.0332819	3.5290878
C	-0.8625836	-3.0432792	0.4711904	C	-1.5887511	0.697496	1.7587178
C	0.4171755	-3.6148987	0.6494094	P	2.7058635	-0.6813327	-1.1048411
C	-1.0180684	-1.7551028	-0.1421579	O	3.3479493	-1.3120961	-2.3073385
C	1.5440863	-2.9613088	0.1933232	C	3.9511793	-0.1480206	0.1238206
H	0.4903743	-4.6012718	1.1002145	C	5.9464828	0.6068752	1.9330315
H	2.5198074	-3.437924	0.2206012	C	5.2994753	-0.3735715	-0.1810211
C	1.4107116	-1.6489093	-0.2721951	C	3.6066264	0.4587698	1.3407883
C	0.1741672	-0.9810687	-0.3212055	C	4.6018919	0.8339733	2.2413926
H	2.8165429	2.0873232	-2.4254239	C	6.2940418	0.0040254	0.7235089
C	1.8753469	1.9525773	-1.90011	H	5.552113	-0.8443087	-1.1265115
H	1.0900437	3.8947103	-2.3854323	H	2.5631687	0.6418329	1.5845755
C	0.9328532	2.9602458	-1.8529949	H	4.3304496	1.3045369	3.1826101
C	0.3528706	0.4833823	-0.6381705	H	7.3388774	-0.1728196	0.4824639
C	-0.2222699	2.8202481	-1.0521431	H	6.7209337	0.9010681	2.6366233
C	1.5718658	0.7263823	-1.2998119				

[a]Calculated by DFT method [B3LYP/6-31G(d)]