Supporting Information

Aromatic Fused Heterocyclic [22] Macrocycles with NIR Absorption

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Instrumentation and Materials

1.1 Electronic absorption spectra were measured with a PerkinElmer Lambda 950 UV-visible-NIR spectrophotometer, and variable temperature UV-vis NIR spectroscopic study was carried out in Unisoku Scientific cryostat. ^{1}H NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer and chemical shifts were reported as the delta scale in ppm relative to $CHCl_3$ (δ = 7.26 ppm) as internal reference for ^{1}H. MALDI-TOF MS data were recorded using Bruker Daltonics flex Analyser and ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. Cyclic voltammograms were recorded using a platinum working electrode, a platinum wire counter electrode and an Ag/AgCl reference electrode in Bioanalytical Systems EC epsilon. The measurements were carried out in CH_2Cl_2 solution using 0.1 M Bu_4NPF_6 as the supporting electrolyte at a scan rate of 0.1 V/s. Peak potentials were determined from differential pulse voltammetry experiments. The Fc/Fc^+ redox couple was used as an internal standard. All solvents and chemicals were of reagent grade quality, obtained commercially and used without further purification except as noted. For spectral measurements, anhydrous dichloromethane was obtained by refluxing and distillation over CaH_2. Dry THF was obtained by refluxing and distillation over pressed Sodium metal. Thin layer chromatography (TLC) was carried out on alumina sheets coated with silica gel 60 F_{254} (Merck 5554) and gravity column chromatography were performed using Merck Silica Gel 230-400 mesh. Aluminum Oxide (Basic) grade II was purchased from Sigma Aldrich.

1.2 **<u>X-ray Structure Determination</u>**

A suitable shinning blue crystal of size 0.01 x 0.07 x 0.15 mm^3 was mounted on a Rigaku Saturn 724 CCD diffractometer with a fine- focus sealed tube Mo-Kα (λ = 0.71075Å) X-ray source. Total 800 frames were collected at 150K with the exposure time of 16s per frame. Unit cell determination using both high angle and low angle diffraction reveal that compound crystallizes in triclinin P – 1 space group. Data integration and indexing of **6** was done by using crystal clear. All calculations were carried out using the programs in WinGX module[1] and solved by direct methods (SIR-92).[2] The final refinement of the structure was carried out using least-squares method on F^2 using SHELX-97.[3] The final refinement of the solved structure converged at the R value of 0.0843 ($I>2\sigma(I)$). All non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were located from difference Fourier maps.

1.3 **<u>Theoretical Calculation</u>**

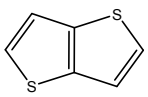
Quantum mechanical calculations were carried out on Gaussian 09W [4] program suite to estimate the

NICS (0) values at the center of the molecular plane of all the two macrocycles. Density functional theory (DFT) with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP) and 6-31G (d) basis set for all the atoms employed in the calculations (SI). The molecular structure obtained from single crystal analysis was used to obtain the geometry optimized structures of **6**. For macrocycle **5** and **7,** since there is no crystal structure available, the molecules were drawn in Gauss View using the default parameters for bond lengths, angles and dihedrals. This initial structure was then subjected to complete geometry optimization based on the DFT-formalism. We have used the B3LYP/6-31G* level of theory to get the minimum energy structure.

References:

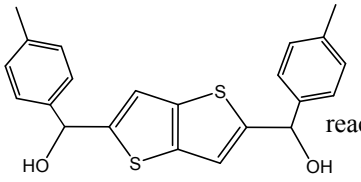
1. L. J. Farrugia, WinGX, Version 1.64.05 *J. Appl. Crystallogr*., 1999, **32**, 837.
2. A. Altomare, G. Cascarano, C. Giacovazzo and A. Gualardi, *J. Appl. Crystallogra*., 1993, **26**, 343.
3. S3. G. M. Sheldrick, SHELXL-97, Program for Structure Refinement, University of Göttingen: Germany, 1997.
4. Gaussian 09, Revision B. 01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, W. H. G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Jr. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Steroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millan, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Incl., Wallingford CT, 2010

General Synthetic Procedure



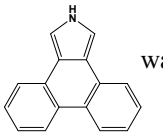
Thieno[3,2-b]thiophene (1): This was synthesized as reported in literature. Yield: 60 %).^{1}H NMR (300 MHz, $CDCl_3$): δ [ppm]: 7.268-7.284 (d, 1H, J=4.8Hz); 7.387-7.404 (d, 1H, J=5Hz). ^{13}C NMR (75 MHz, $CDCl_3$, 300K, δ [ppm]): 119.65, 127.62, 139.73. **HRMS (m/z):**162.90 **[M+Na]** $^{+}$ **(**140.23 calc. for $C_6H_4S_2$).

2,5-Bis(tolylhydroxymethyl)-thieno[3,2-b]thiophene (2): To a 250mL round-bottomed flask equipped with a magnetic bar, Thieno[3,2-b]thiophene **1** (1gm, 7.13mmol) was placed followed by dry THF (40mL). The reaction mixture was stirred under inert atmosphere. N, N, N‘, N‘-Tetramethyl ethylenediamine (3.2mL, 0.021mol) was added followed by stirring for half an hour at room temperature. Afterward n-BuLi in hexane (1.6M) (13.04mL, 0.021mol) was added through rubber septa drop wise,

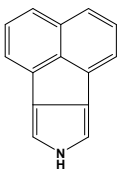


yellow turbidity started forming. The reaction mixture was stirred at room temperature for 2hrs and then heated to 66^{o}C for 1hour. The reaction mixture was brought room temperature after which it was brought to ice cold temperature. At ice cold temperature, Tolylaldehyde (2mL, 0.017mol) in dry THF (40mL) was then added drop wise to the reaction mixture, the reaction mixture was stirred for 2 hours. The reaction mixture was quenched by saturated NH_4Cl (aq) solution, product was extracted by diethyl ether, dried over Na_2SO_4. The crude product was precipitate out by hexane and purified by silicagel column chromatography using hexane-ethyl acetate (1:0.4) solution. The solvent was evaporated and light yellow solid was obtained.

Yield 2.09gm (77.5%).**^{1}H NMR (500MHz,$CDCl_3$, 300K,** δ [ppm]**)**: 2.353(s, 3H); 6.026(s, 1H); 6.979(s, 1H); 7.170-7.186(d, 1H, ^{3}J=8Hz); 7.330-7.346(d, 1H, ^{3}J=8Hz). **^{13}C NMR (125 MHz, $CDCl_3$, 300K,** δ [ppm]**)**: 21.10, 81.714, 117.92, 126.82, 129.19, 137.78, 137.88, 138.205, 148.05. **HRMS (m/z)** 380.593**[M^{+}]** (380.52 calc. for $C_{22}H_{20}O_2S_2$).



Phenanthrene-fused Pyrrole (3): Following the literature reported method, compound **3** was obtained in 85% yield. **^{1}H NMR (300MHz, $CDCl_3$, 300K,** δ [ppm]**):** 7.433-7.481 (m, 4H); 7.579-7.588 (d, 2H, J=2.7Hz); 8.047-8.066 (d, 2H, J= 5.7 Hz); 8.445-8.472 (d, 2H, J=8.1 Hz); 8.948 (brs, 1H). **^{13}C NMR (75MHz, $CDCl_3$, 300K,** δ [ppm]**)**: 110.27, 119.80, 123.24, 123.54, 125.04, 126.88, 128.81, 129.46. **HRMS (m/z)**: 217.83**[M^{+}]** (217.27 calc. for $C_{16}H_{11}N$).



Acenaphthylene-fused Pyrrole (4): Following literature reported method, compound **4** was obtained in 91% yield. **^{1}H NMR (500 MHz, $CDCl_3$, 300K,** δ [ppm]**):** 7.011-7.015 (d, 1H,

^{3}J=2Hz); 7.473-7.502 (t, 1H, ^{3}J=7.5Hz); 7.568-7.582 (d, 1H, ^{3}J=7Hz); 7.614-7.630 (d, 1H, ^{3}J=8Hz); 8.139 (brs, 1H). **^{13}C NMR (125 MHz, $CDCl_3$, 300K, δ [ppm])**: 110.74, 118.64, 124.71, 127.71, 128.85, 131.03, 133.87, 137.89. **HRMS (m/z)**:208.07 [**M+H_2O**]$^{+}$ (191.25 calc. for $C_{14}H_9N$).

General synthetic procedure of Compound 5, 6 and 7: Under nitrogen atmosphere and in dark condition a solution of 380mg of compound **2** (1mmol) and 69μL pyrrole /217mg compound **3**/191mg **4** (1mmol) in 250 mL dry dichloromethane was stirred for 30 minutes. Afterward, catalytic amount of BF_3-Et_2O (0.10mL) was added to the reaction mixture and stirred at RT for 90 minutes. Then 2.5 equivalents DDQ (567mg, 2.5 mmol) was added and opened to air and the mixture was stirred for another 1 hour. The solvent was removed under reduced pressure and compound was filtered by basic alumina followed by repeated silica gel column chromatography with the mixture of 5% methanol-dichloromethane solution. After recrystallization, the title compound was yielded as dark green crystal.

Compound 5: Yield.48mg (~5%). **^{1}H NMR (500 MHz, $CDCl_3$, -40^{o}C, δ [ppm], TMS): -**2.1 (brs, 1H, NH);-0.074 (s, 1H, Inner β-H of Thienothiophene); 2.761 (s, 3H, methyl); 7.851-7.895 (2H, tolyl CH); 8.975 (s, 1H); 9.264 (s, pyrrole β-H) ;9.278 (brs, 2H, tolyl CH). **MALDI-TOF MS (m/z):** 816.10 (Calc. for $C_{52}H_{36}N_2S_4$ exact mass: 816.18). **UV-VIS (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K):** 503(68.73); 530 (50.67); 725 (22.33); 868 (9.22); 957 (5.33). [**(UV-VIS [CH_2Cl_2, 1% TFA/CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K)]:** 509 (93.98); 540 (67.76); 867 (57.6).

Compound 6: Yield.95mg (~8%). **^{1}H NMR (500 MHz, $CDCl_3$, -40^{o}C, δ [ppm], TMS):** -1.543 (brs, 1H); 0.721 (s, 1H), 2.632 (s, 6 H); 7.439-7.445 (br, 2H); 7.488-7.503 (d, 2H, J=7.5Hz); 7.521-7.536 (d, 2H, J=7.5Hz); 8.013-8.029 (d, 2H, J= 8Hz); 8.071-8.087 (d, 2H, J= 8Hz); 8.623-8.637 (d, 2H, J= 7Hz); 8.735 (s, 1H); 8.889-8.905 (d, 2H, J= 8Hz); 9.573-9.587 (d,2H, J= 7Hz); 9.616-9.631 (d, 2H, J= 7.5Hz). **MALDI-TOF MS (m/z):** 1117.278 (Calc. for $C_{76}H_{48}N_2S_4$ exact mass: 1117.27). **UV-VIS (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K):** 557(60.13); 654(7.62); 716(8.53); 969(3.50).**UV-VIS [CH_2Cl_2, 1% TFA/CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K]:** 584 (67.36); 806(16.14); 963(8.98).

Compound 7.: Yield.105mg (~10%) **^{1}H NMR (500MHz, $CDCl_3$, 0^{o}C, δ [ppm], TMS):** -2.028 (brs, 1H); 0.117 (s, 1H); 2.817(s, 3H); 2.831 (s, 3H); 6.593-6.610 (d, 2H, J=8.5Hz); 6.855-6.869 (d, 1H, J=7Hz); 6.982-6.996 (d, 1H, J=7Hz); 7.070-7.091(d, 2H, J=8.5Hz); 7.579-7.618(m, 2H); 8.068-8.083(d, 2H, J=7.5Hz); 8.106-8.121(d, 1H, J=7.5Hz); 8.166-8.199 (t, 1H, J=8.5Hz); 9.055 (s, 1H); 9.303-9.318(d, 1H, J=7.5Hz); 9.337-9.352 (d, 1H, J=7.5Hz). **MALDI-TOF MS (m/z)**: 1065.32 (Calc. for $C_{72}H_{44}N_2S_4$ exact mass: 1065.24).**UV-VIS (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K):** 559(68.80); 661(7.44); 725(8.88); 839(3.12); 939(3.20). **UV-VIS [CH_2Cl_2, 1% TFA/CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^3]), 298K]:** 586(97.12); 850(20.08); 927(12.85).

Supplementary Data

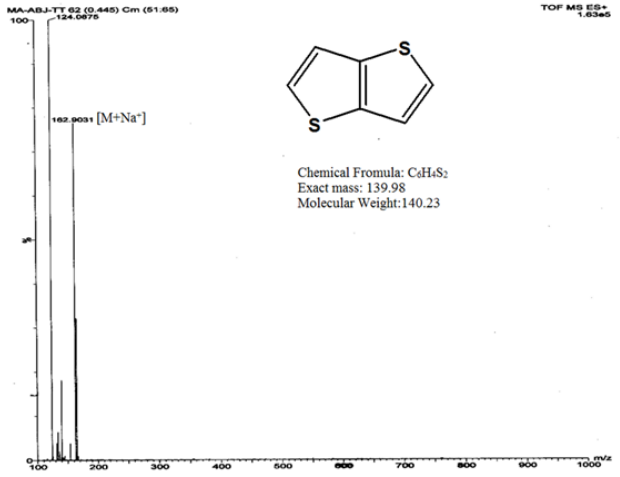


Figure S1. HRMS Spectra of 1

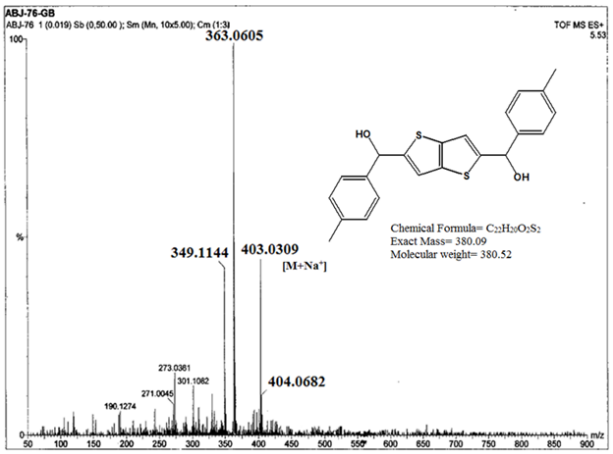


Figure S2. HRMS Spectra of 2

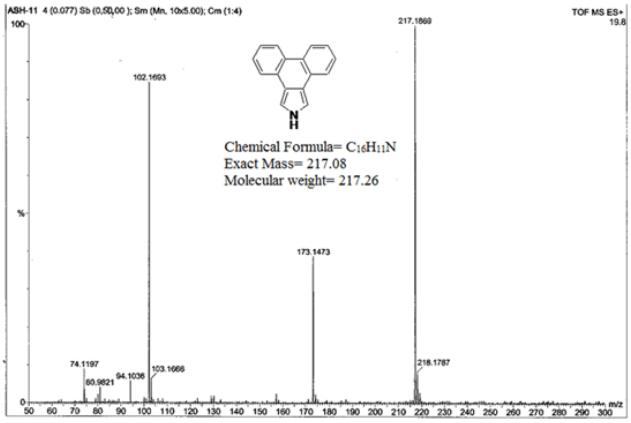


Figure S3. HRMS Spectra of 3

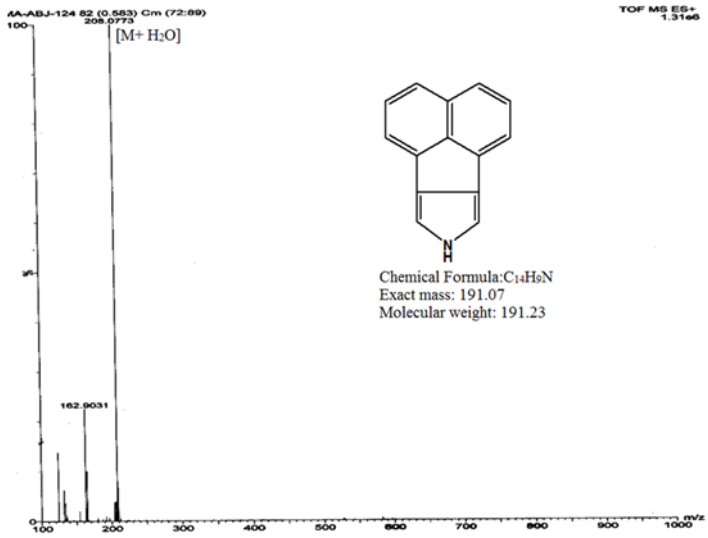


Figure S4. HRMS Spectra of 4

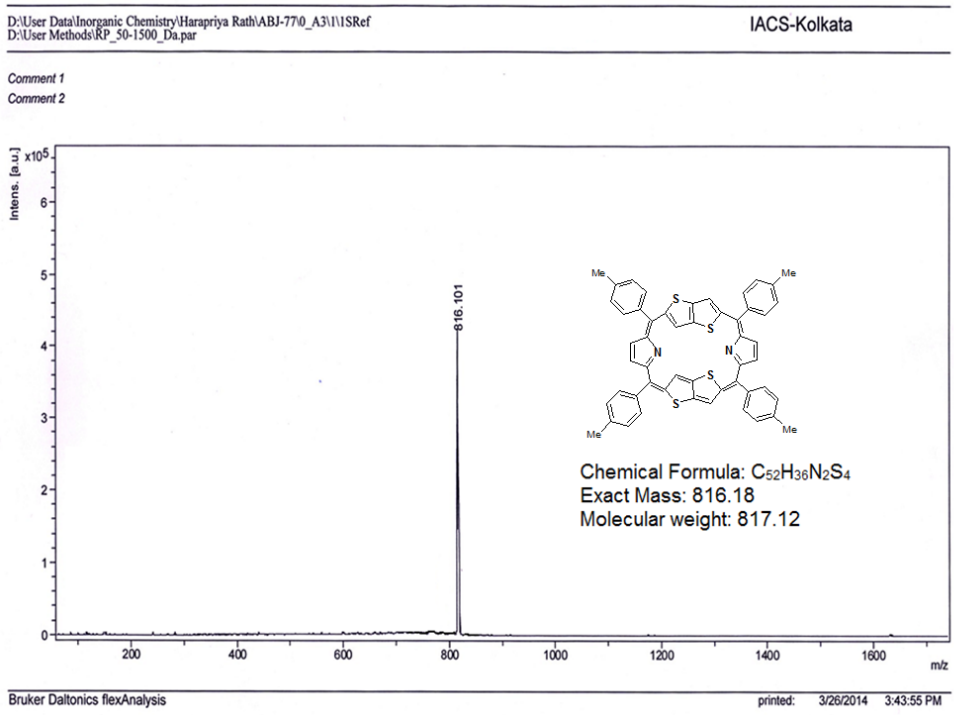


Figure S5. MALDI-TOF MS Spectra of 5

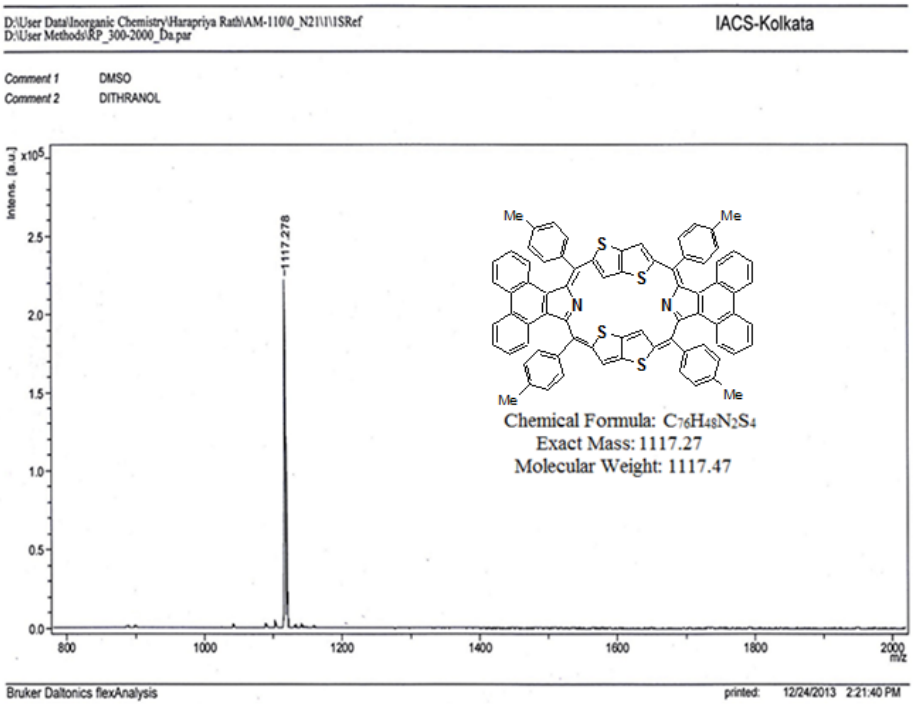


Figure S6. MALDI-TOF MS Spectra of 6

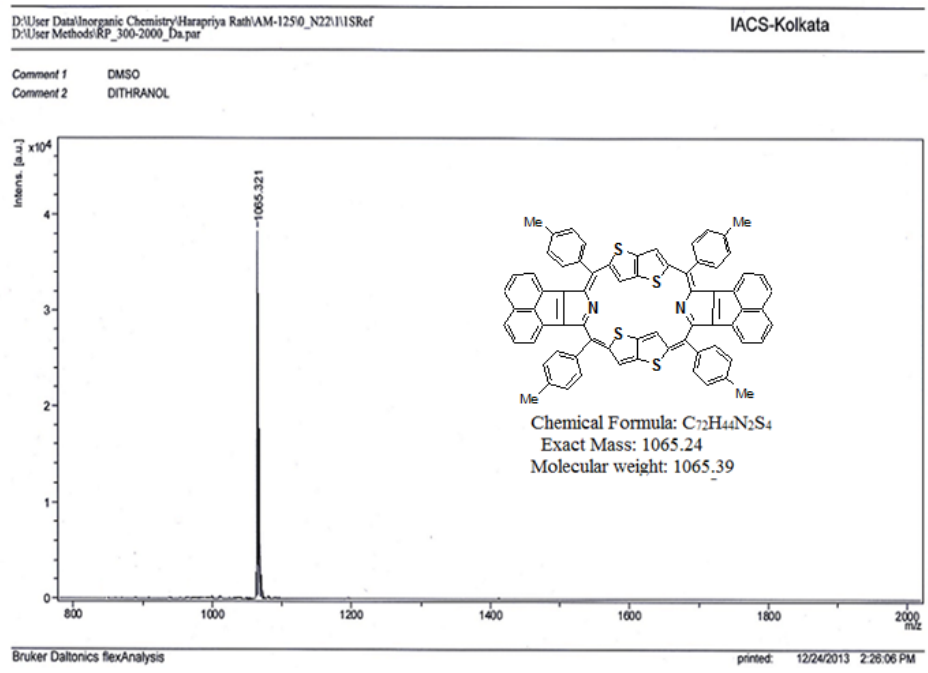


Figure S7. MALDI-TOF MS Spectra of 7

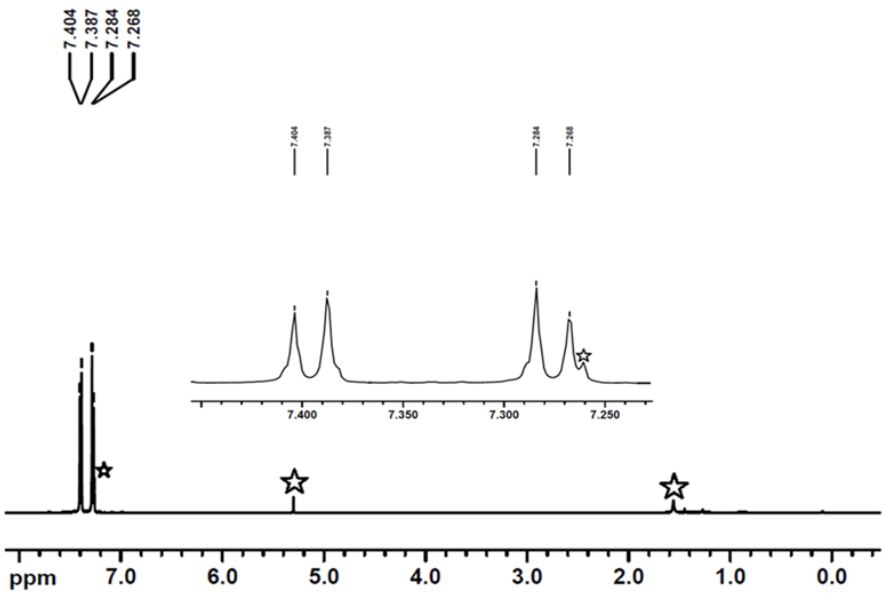


Figure S8. ^{1}H NMR Spectrum of 1

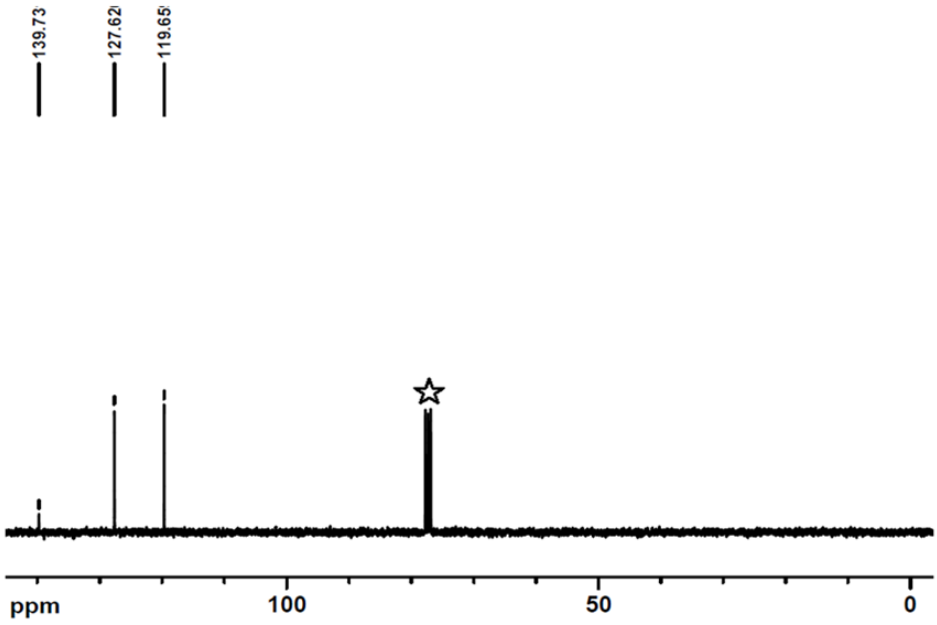


Figure S9. ^{13}C NMR Spectrum of 1

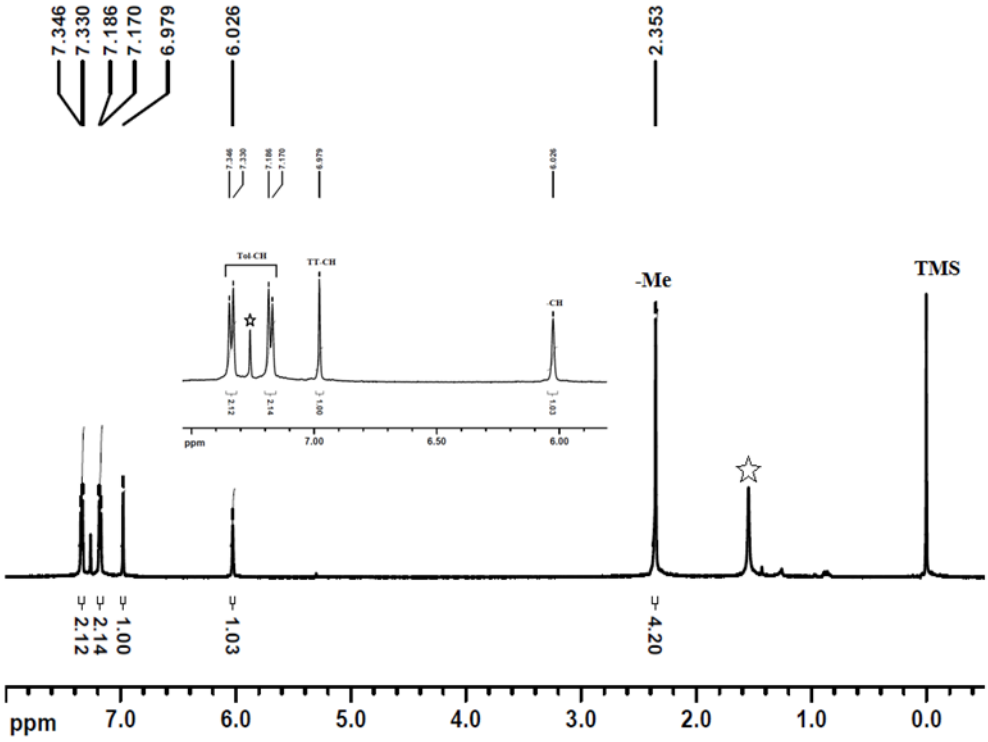


Figure S10. ^{1}H NMR Spectrum of 2

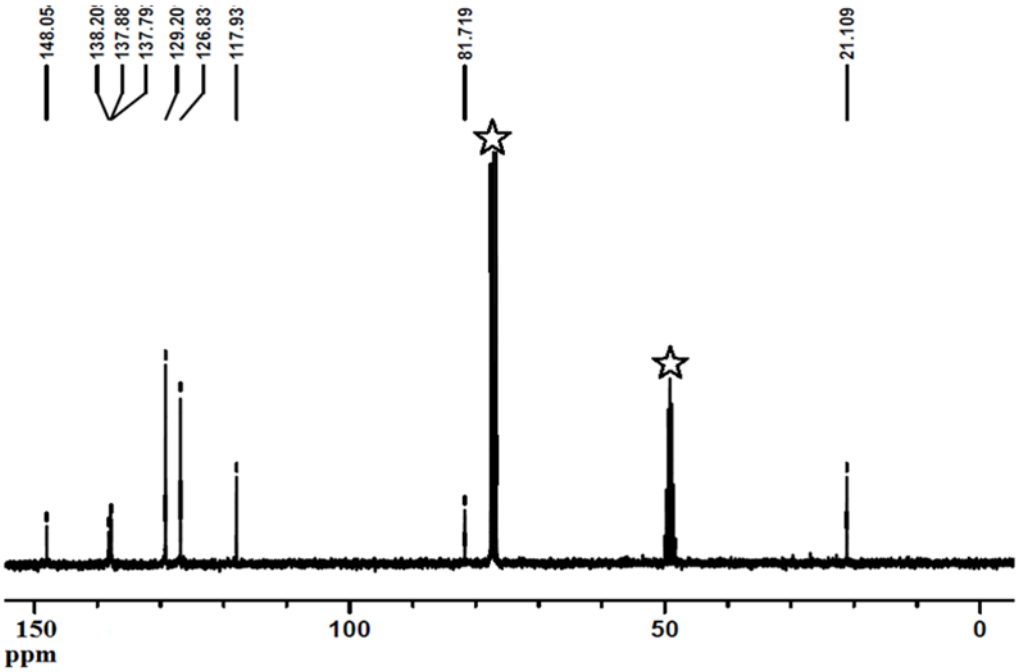


Figure S11. ^{13}C NMR Spectrum of 2

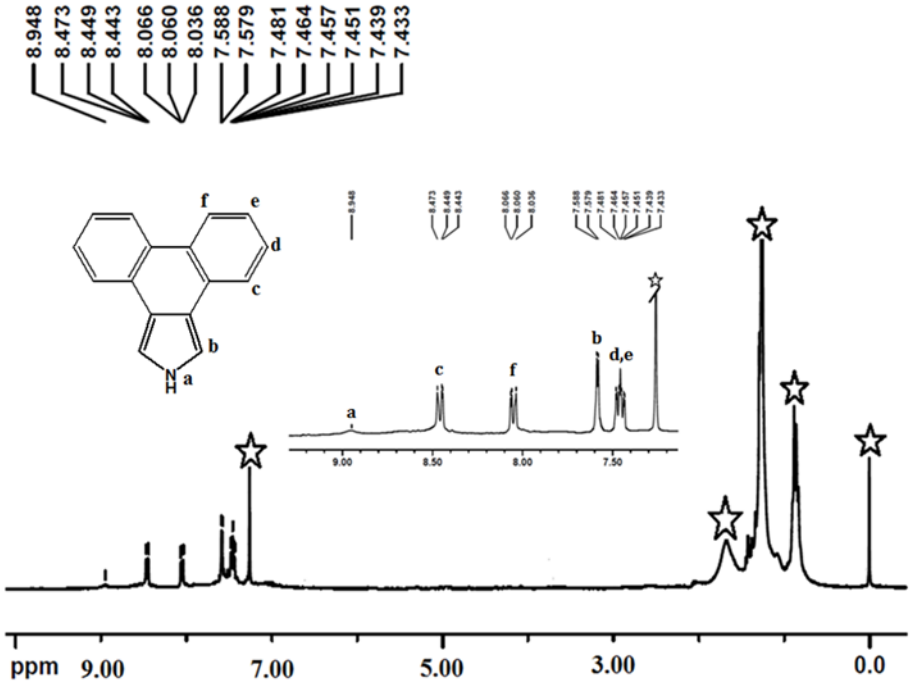


Figure S12. ^{1}H NMR Spectrum of 3

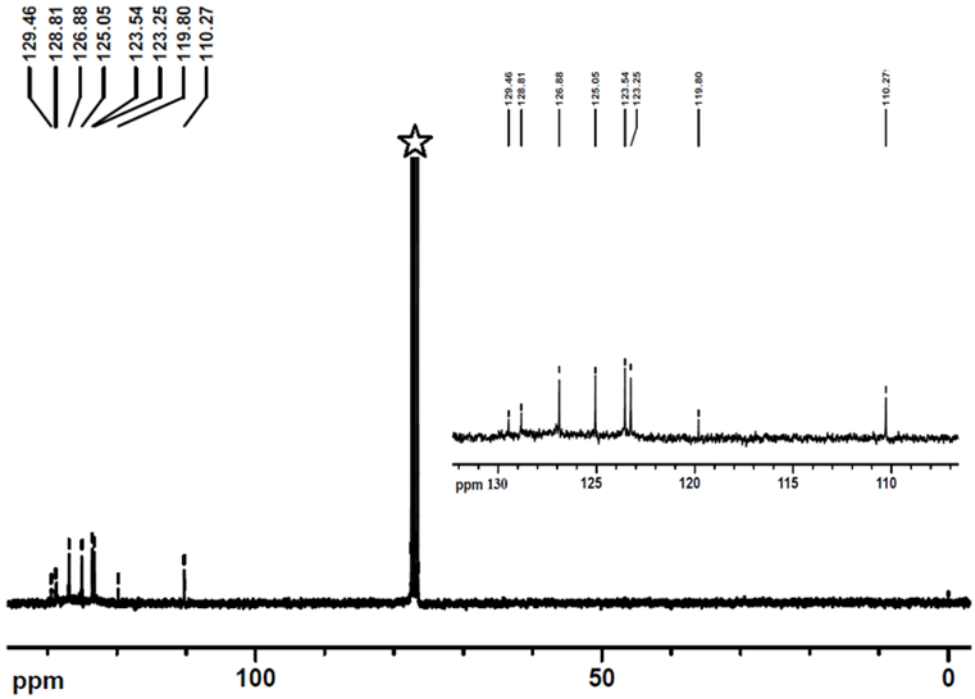


Figure S13. ^{13}C NMR Spectrum of 3

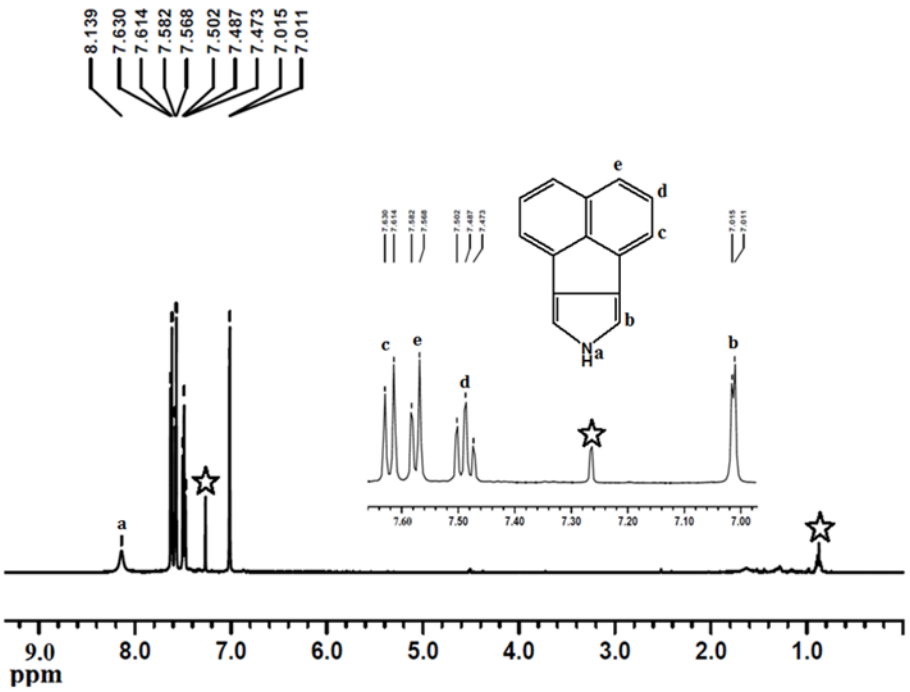


Figure S14. ^{1}H NMR Spectrum of 4

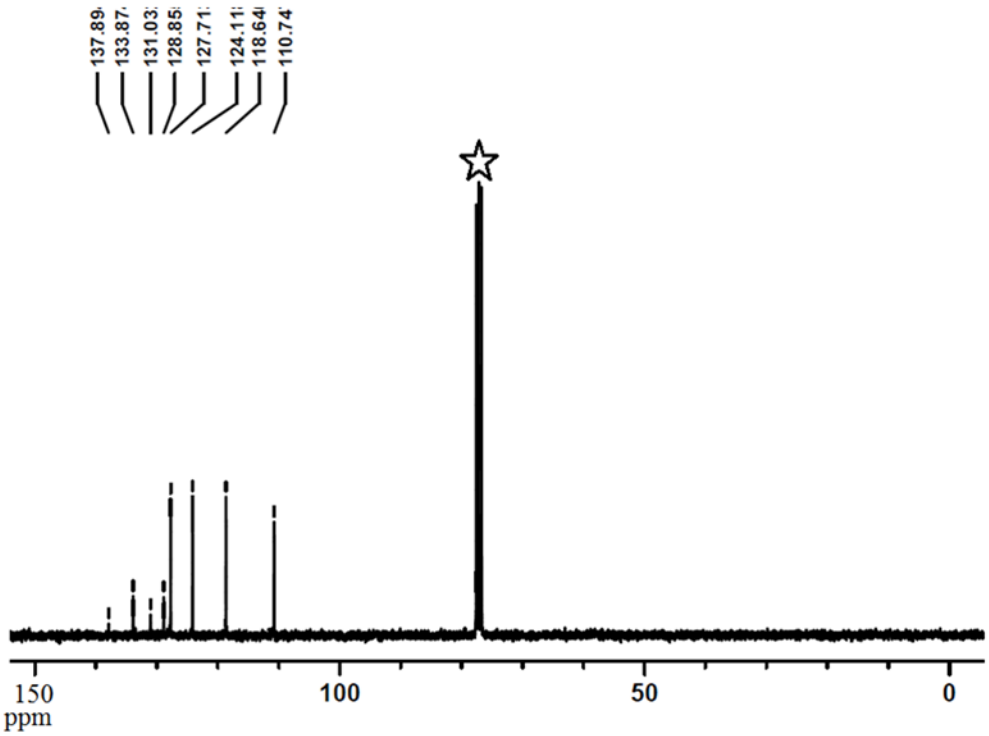


Figure S15. ^{13}C NMR Spectrum of 4

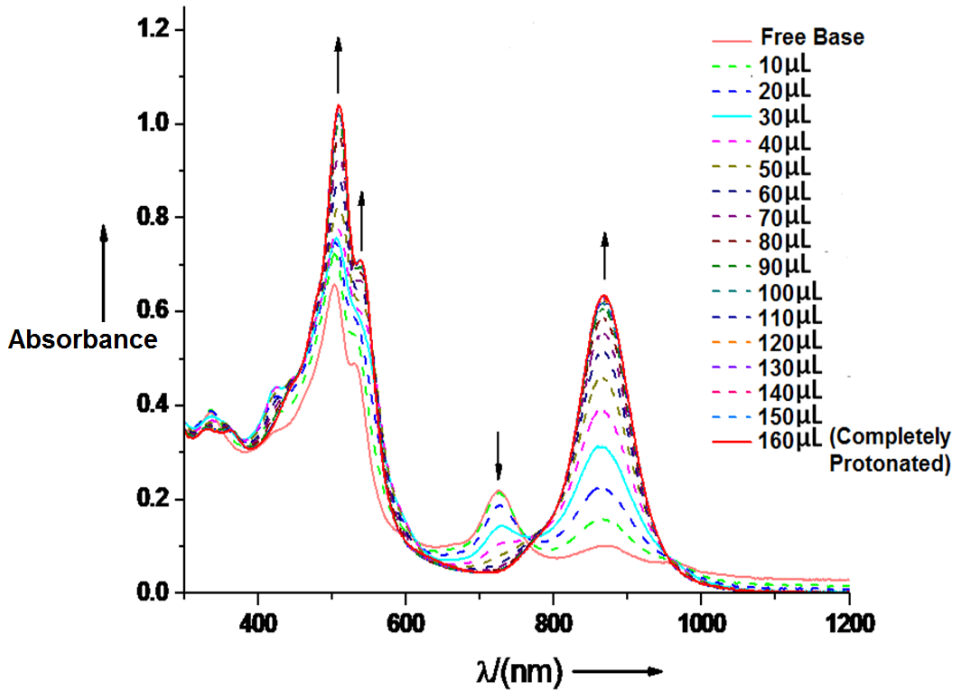


Figure S16. Acid titration UV-vis Spectra of 5 in CH_2Cl_2

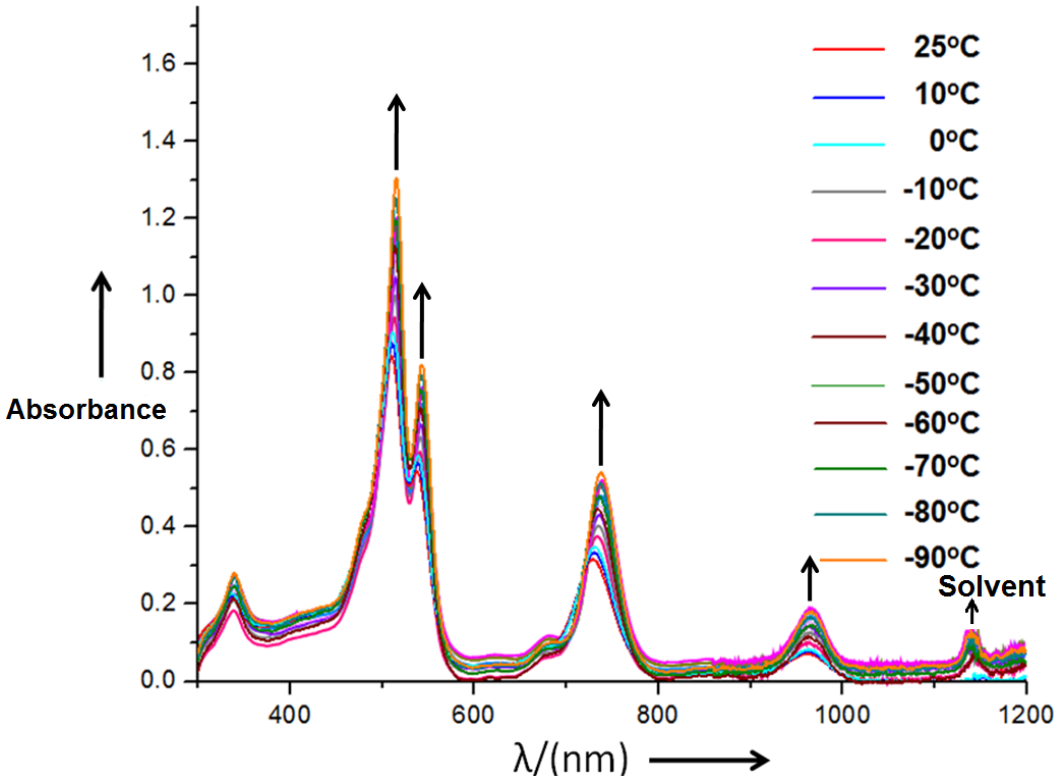


Figure S17. Low Temperature UV-vis Spectra of 5 in Dry Toluene

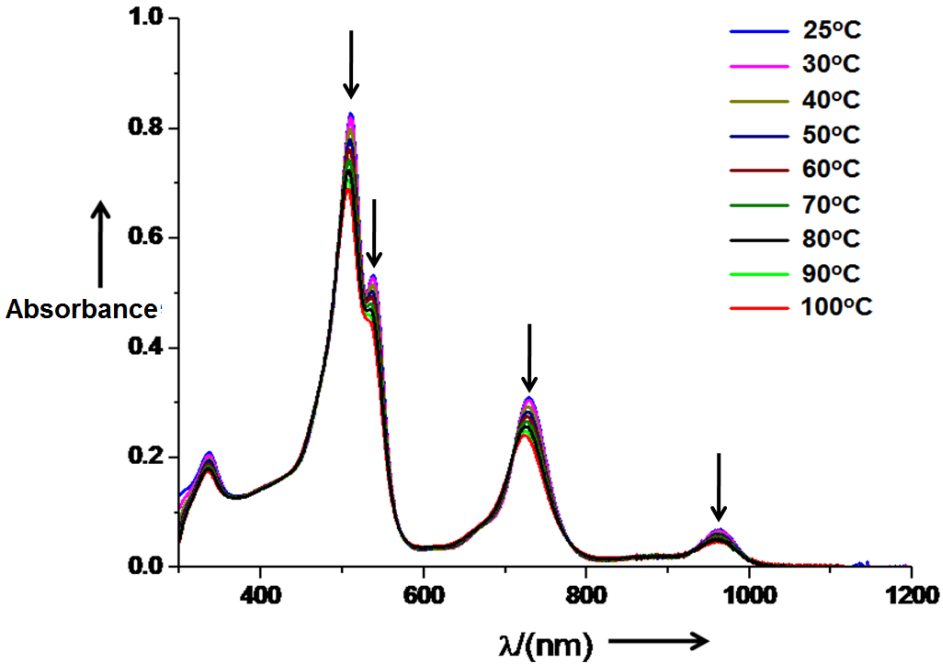


Figure S18. High Temperature UV-vis Spectra of 5 in Dry Toluene

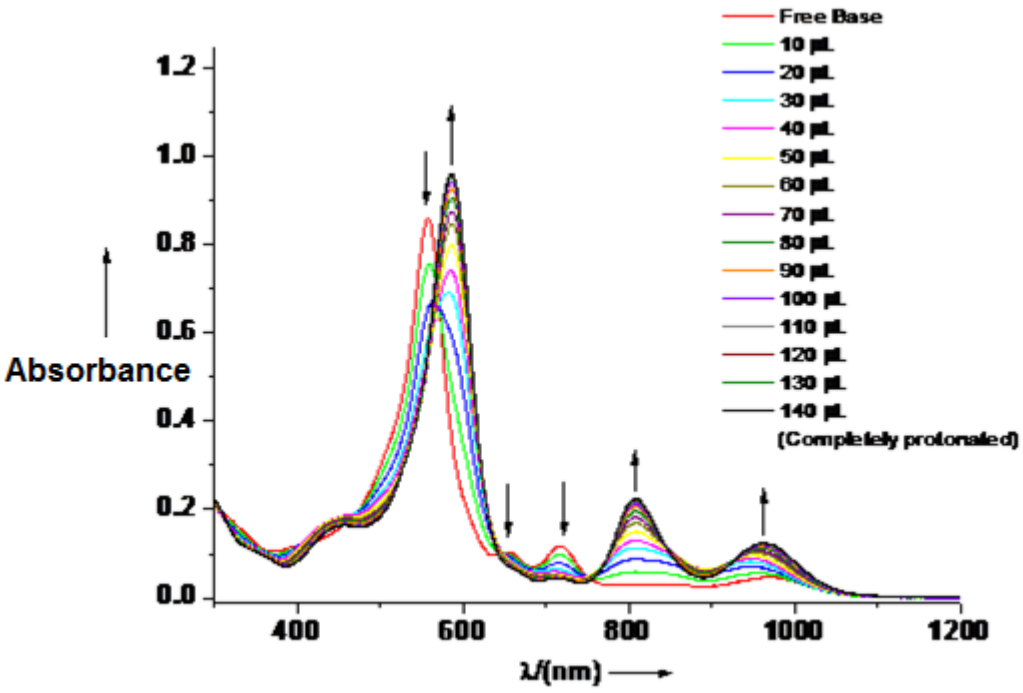


Figure S19. Acid titration UV-vis Spectra of 6 in CH_2Cl_2

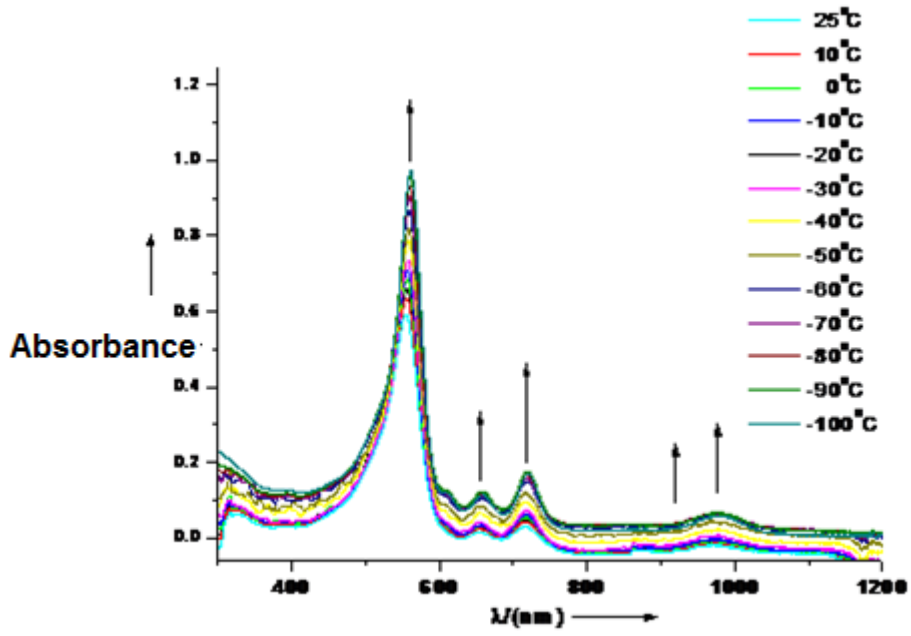


Figure S20. Low Temperature UV-vis Spectra of 6 in Dry THF

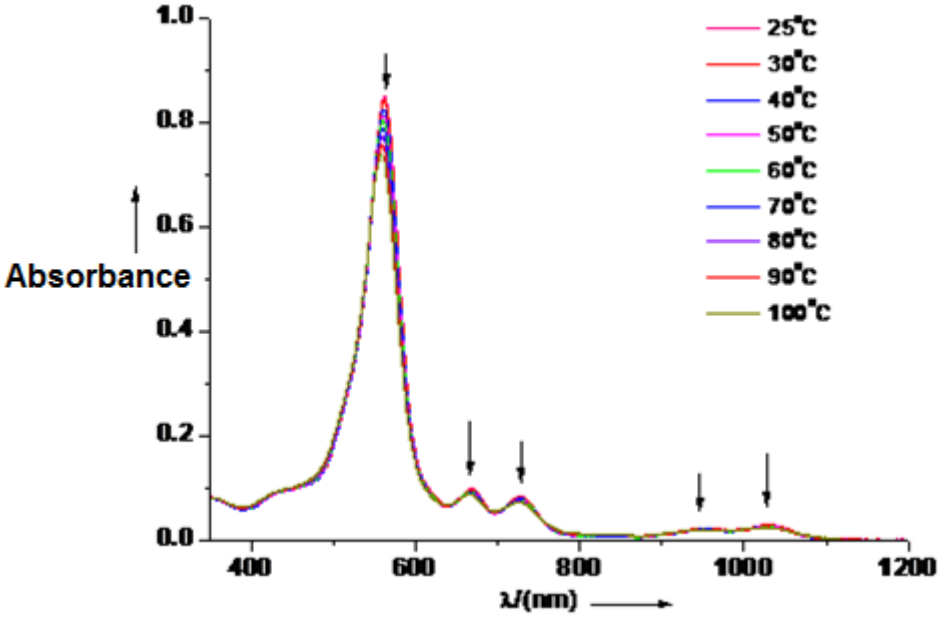


Figure S21. High Temperature UV-vis Spectra of 6 in Dry Toluene

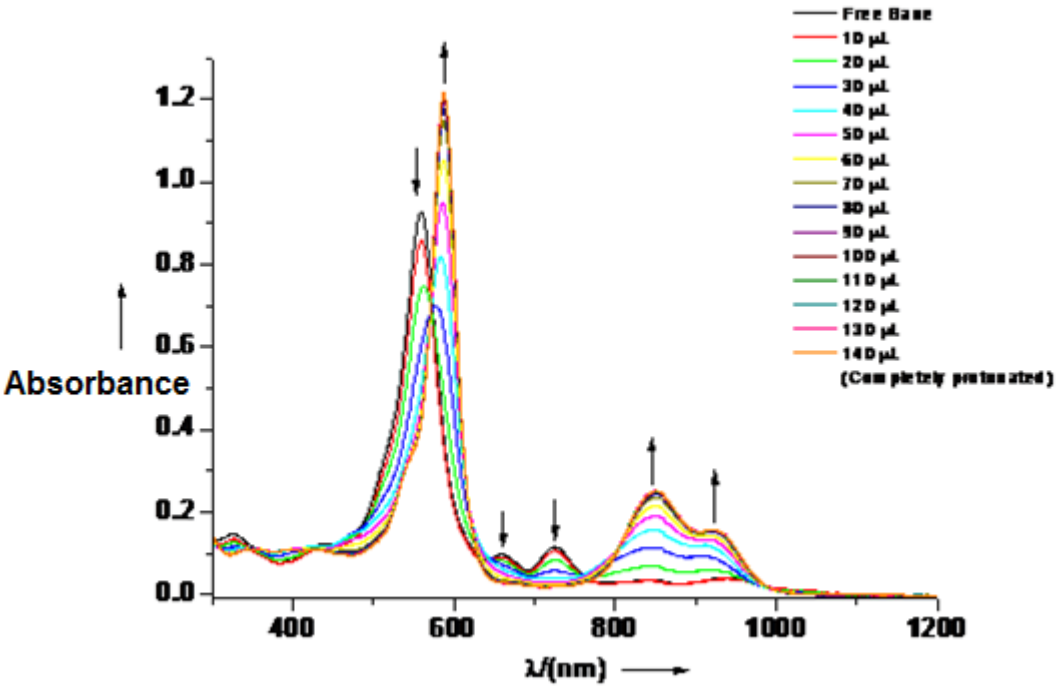


Figure S22. Acid titration UV-vis Spectra of 7 in CH_2Cl_2

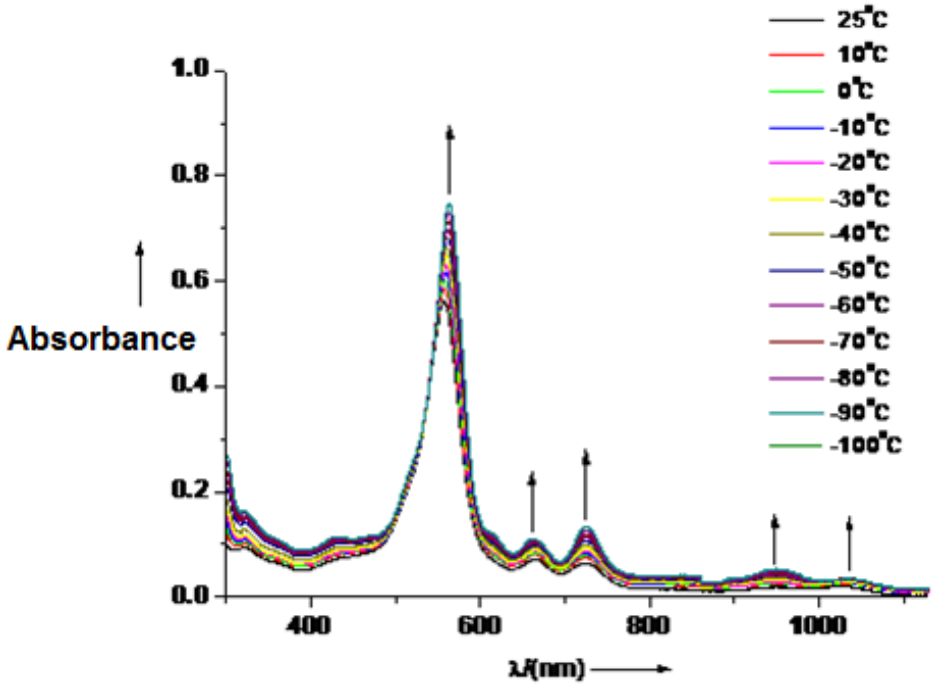


Figure S23. Low Temperature UV-vis Spectra of 7 in Dry THF

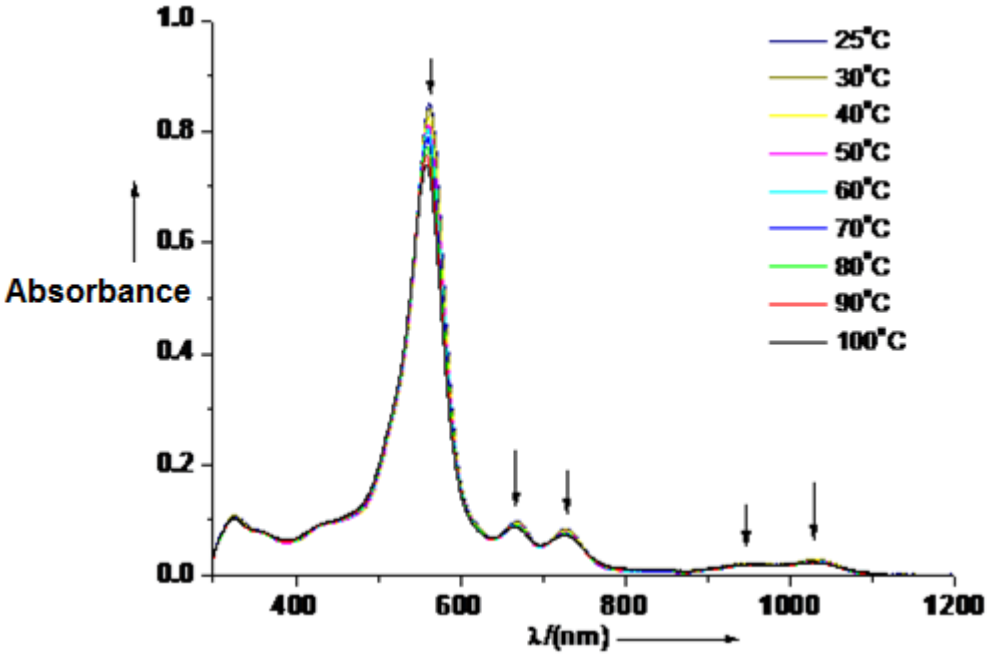


Figure S24. High Temperature UV-vis Spectra of 7 in Dry Toluene

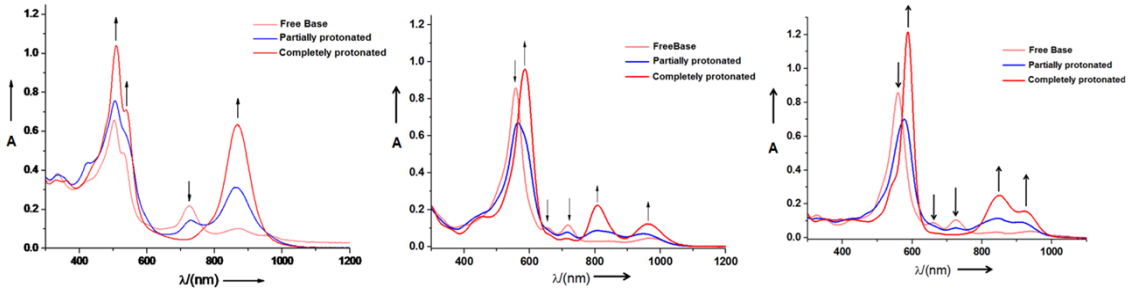


Figure S25. Comparative UV-vis Spectra of free base and protonated forms of 5, 6 and 7 in CH_2Cl_2

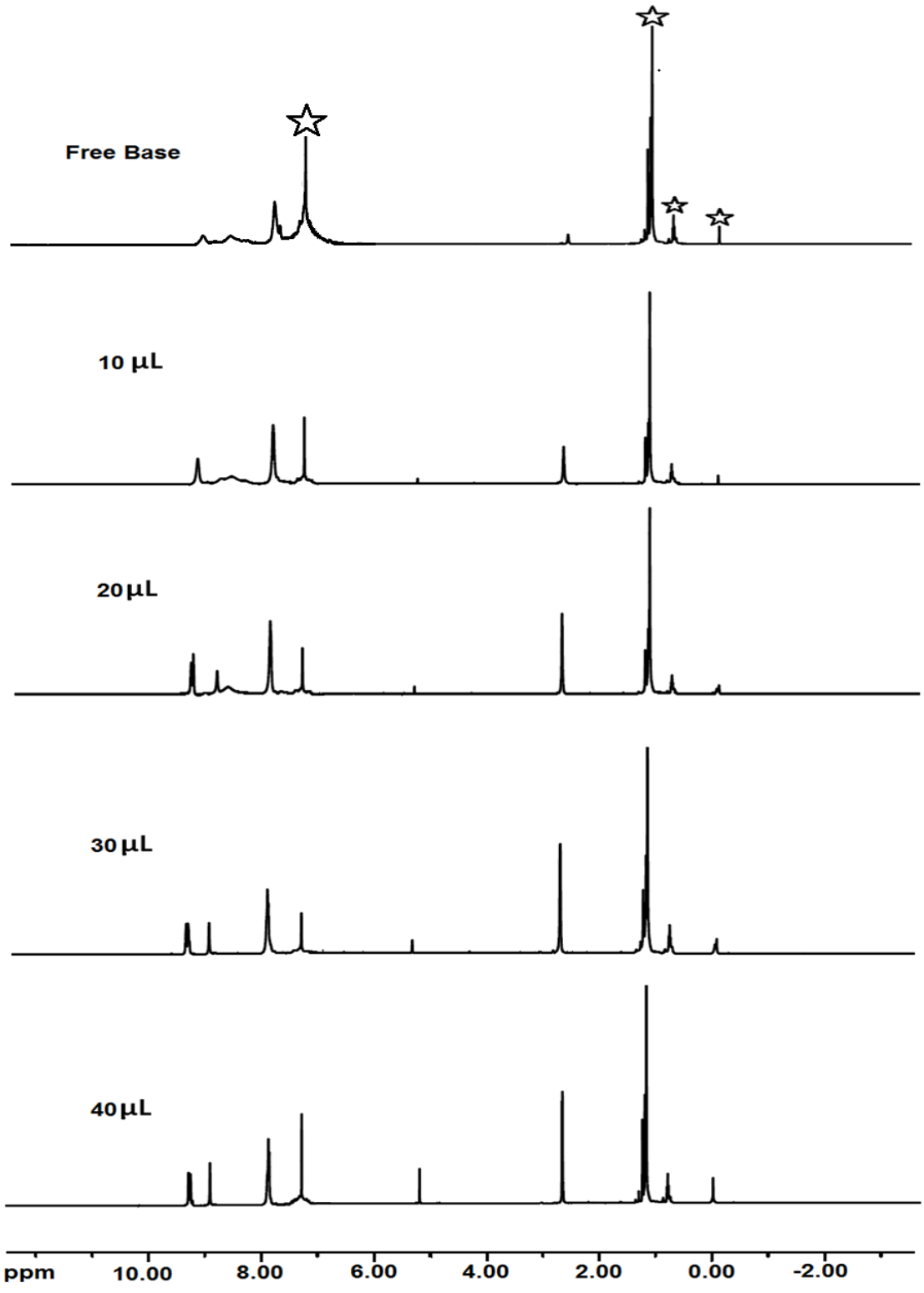


Figure S26. Acid titration ^{1}H NMR Spectra of compound 5 at room temperature (10% TFA-d / $CDCl_3$ mixture)

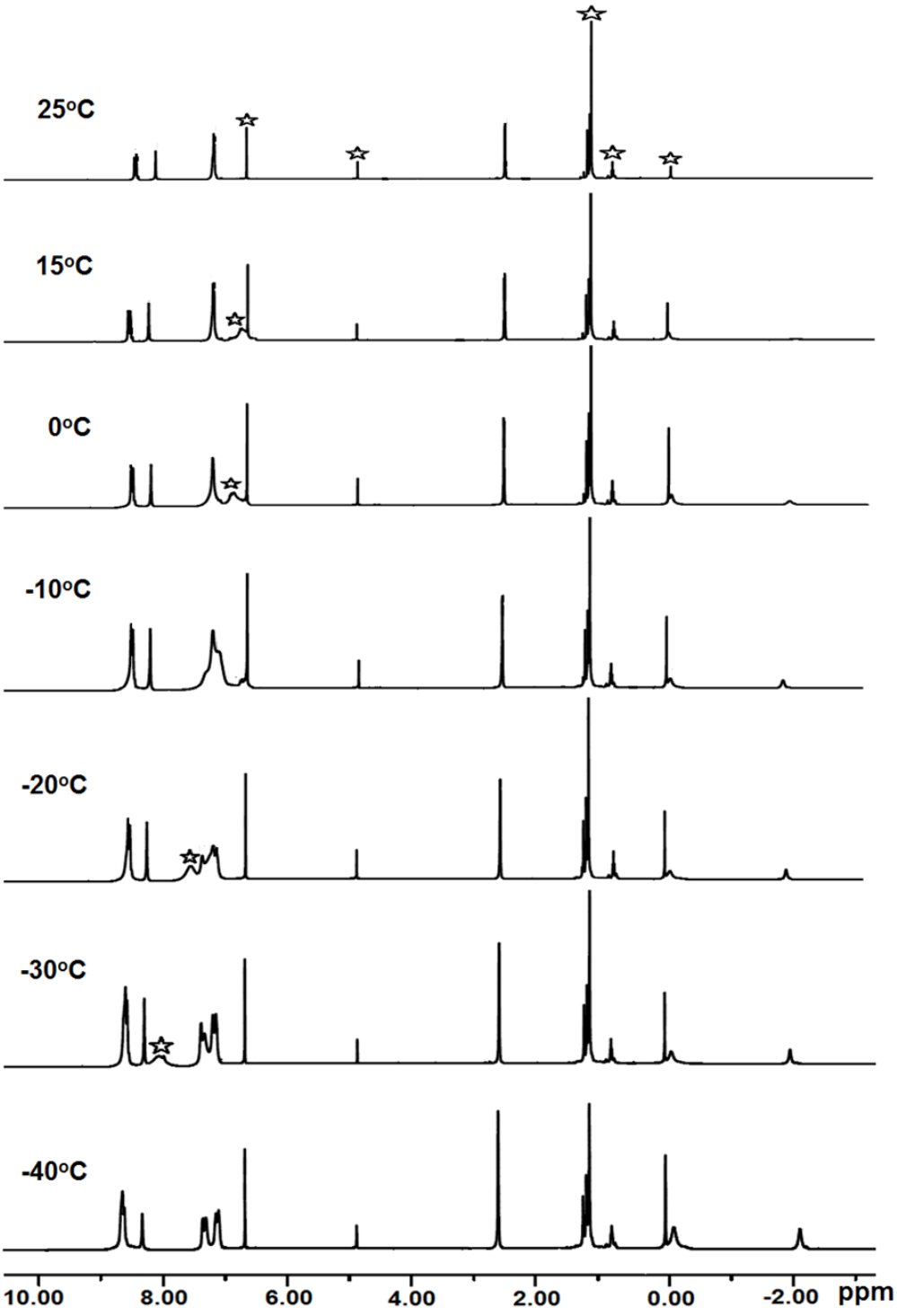


Figure S27. Variable temperature ^{1}H NMR Spectra of protonated 5 (10% TFA-d / $CDCl_3$ mixture)

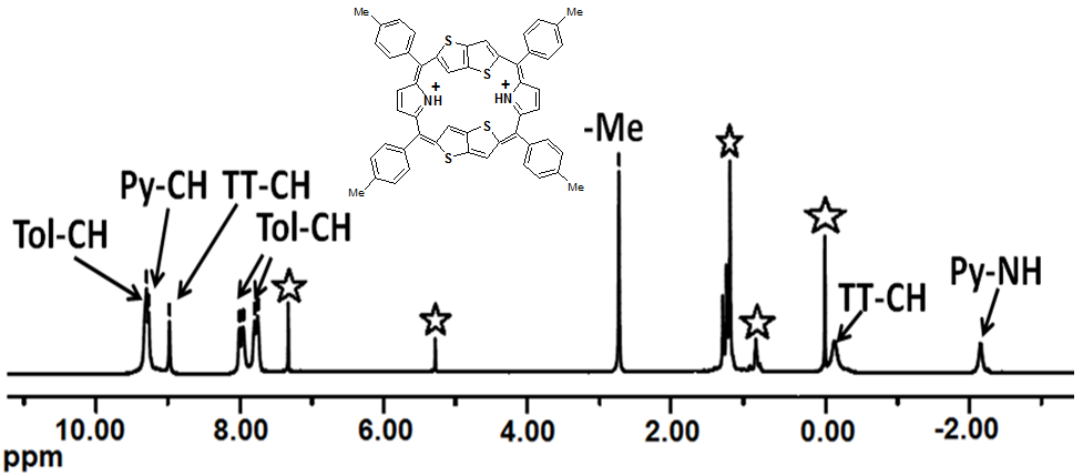


Figure S28. Complete assignment of ^{1}H NMR Spectra of completely protonated 5 at -40^{0}C

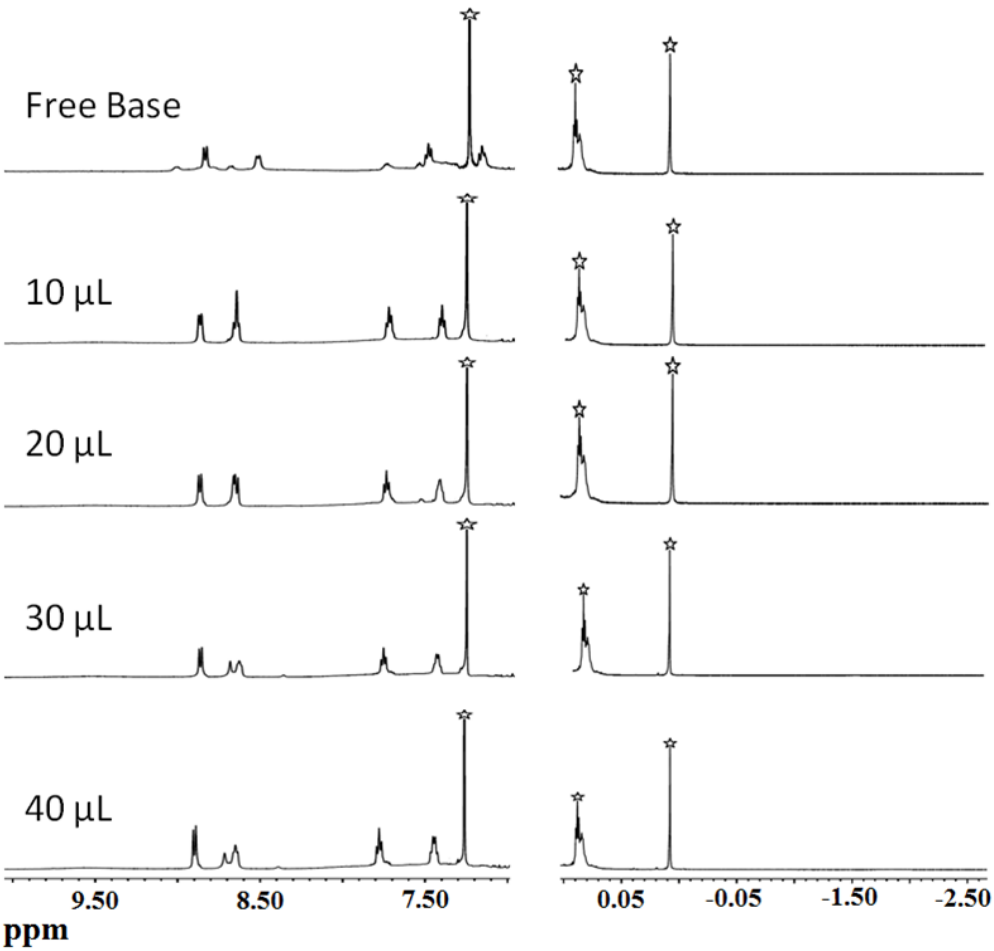


Figure S29. Acid titration ^{1}H NMR Spectra of compound 6 at room temperature (10% TFA-d / $CDCl_3$ mixture)

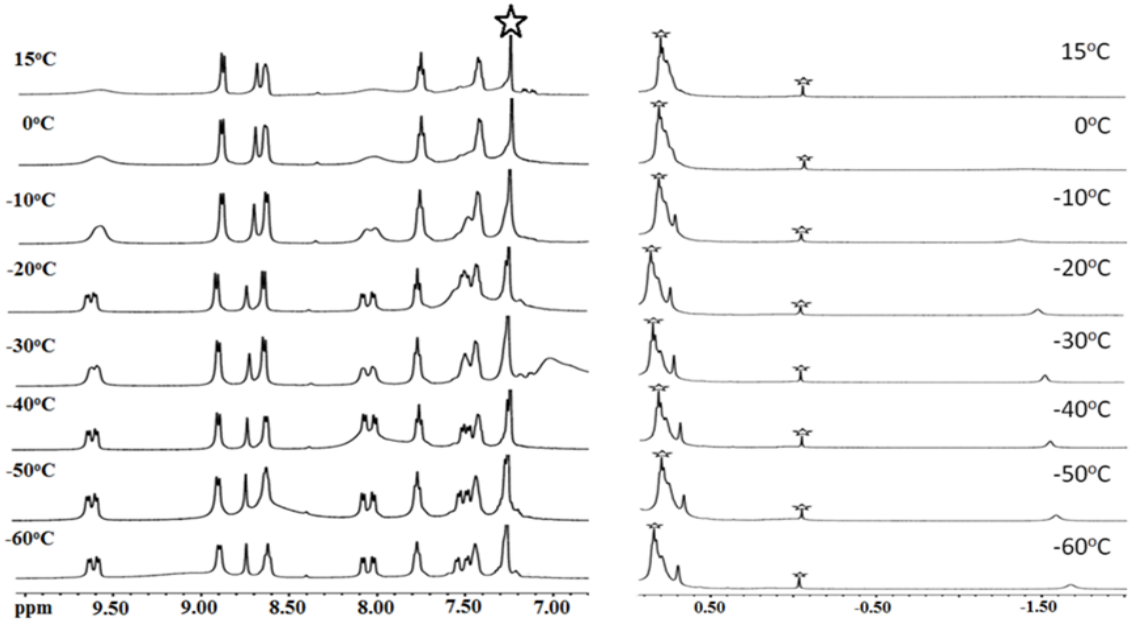


Figure S30. Variable temperature ^{1}H NMR Spectra of protonated 6 (10% TFA-d / $CDCl_3$ mixture)

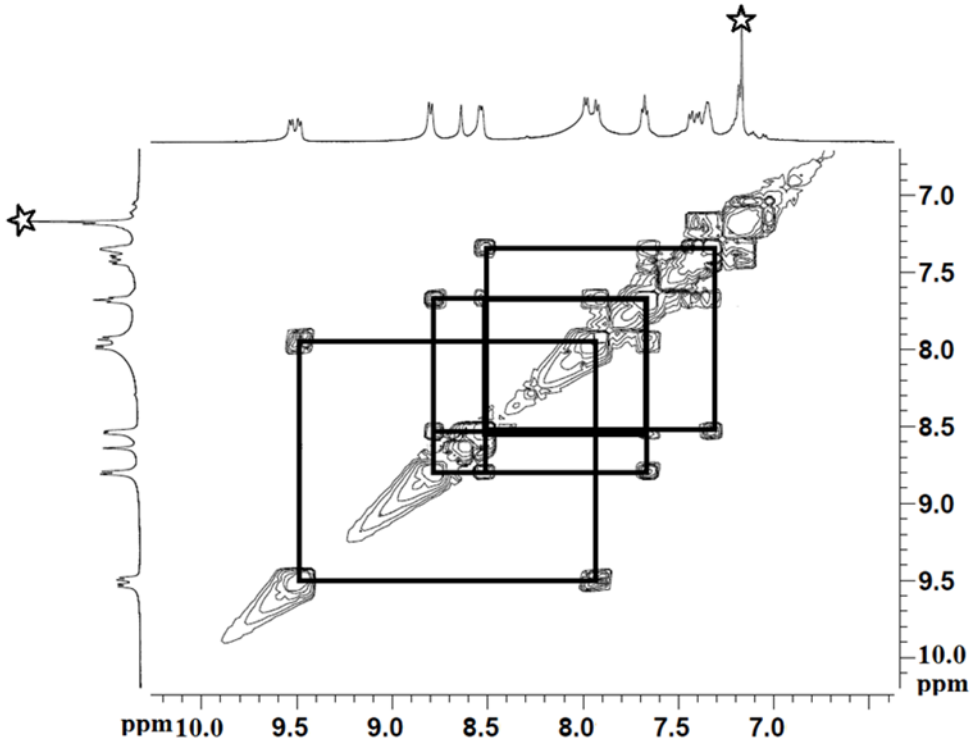


Figure S31. ^{1}H -^{1}H COSY Spectra of completely protonated 6 at -40^{0}C

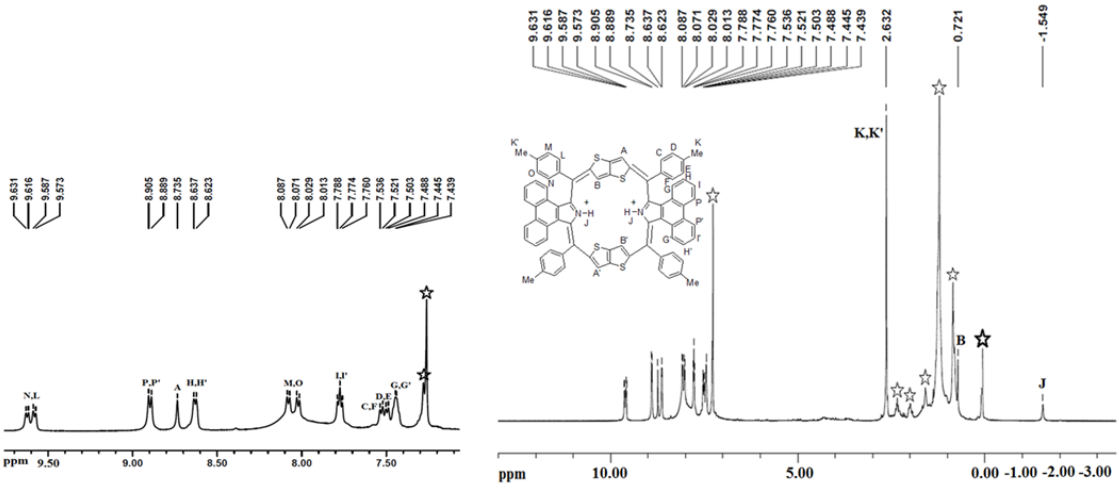


Figure S32. Complete assignment of ^{1}H NMR Spectra of completely protonated 6 at -40^{0}C

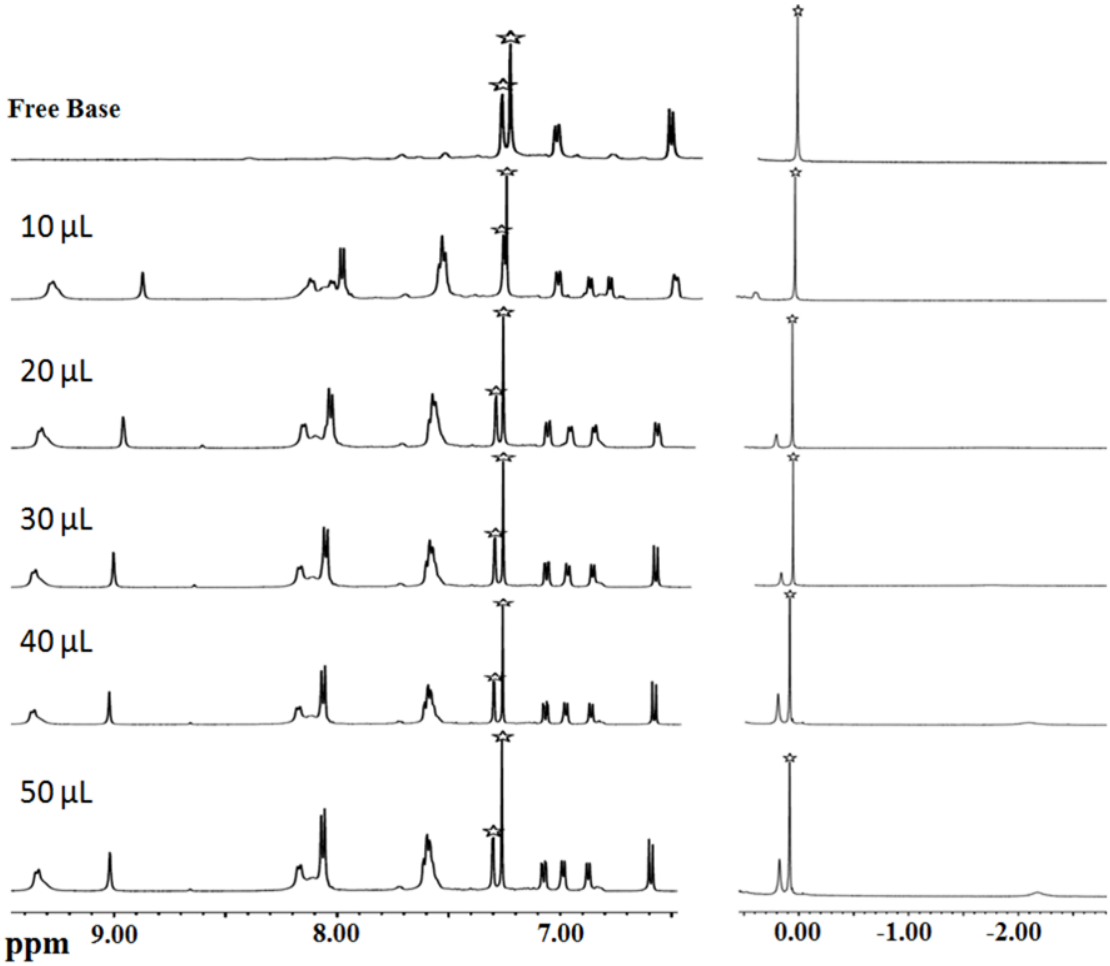


Figure S33. Acid titration ^{1}H NMR Spectra of compound 7 at room temperature (10% TFA-d / $CDCl_3$ mixture)

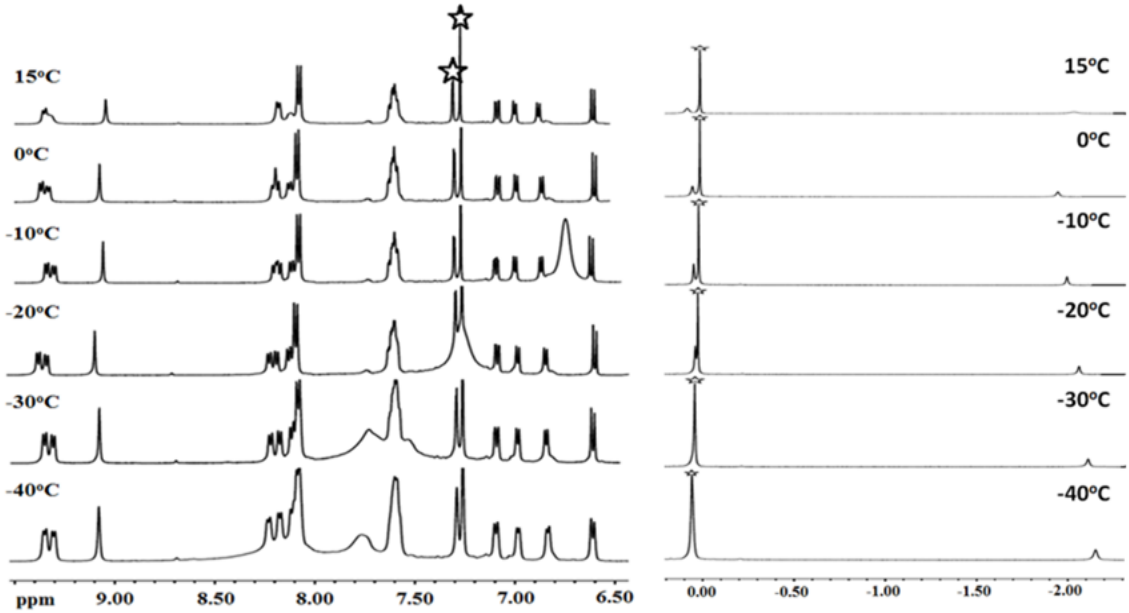


Figure S34. Low VT ^{1}H NMR Spectra of Protonated 7 (10% TFA-d / $CDCl_3$ mixture)

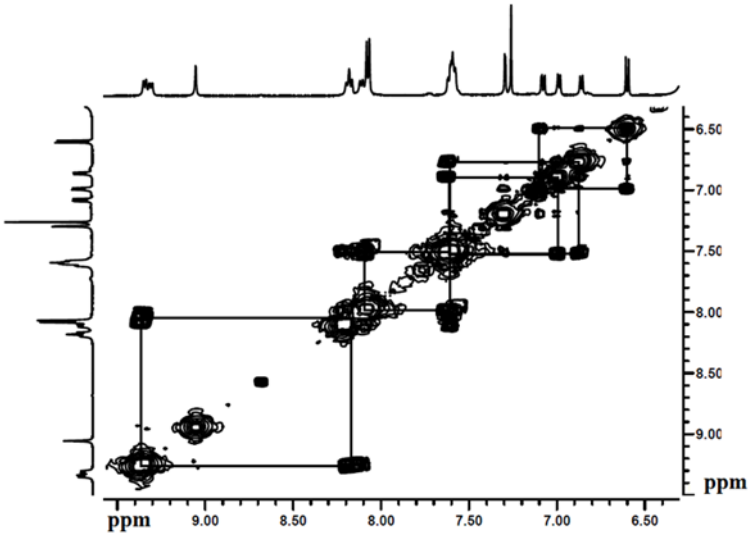


Figure S35. ^{1}H-^{1}H COSY spectra of protonated 7 at $0^{0}C$

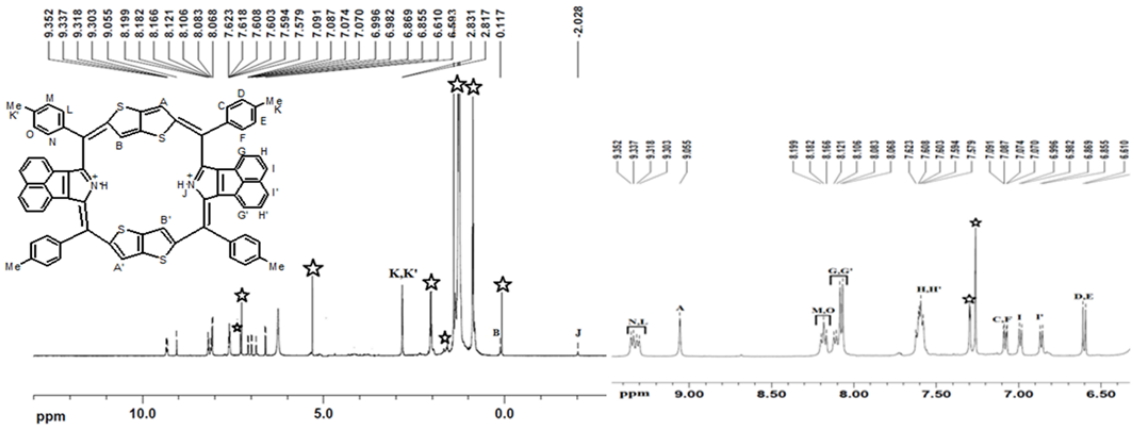


Figure S36.Complete ^{1}H NMR assignment of protonated 7 at 0^{0}C

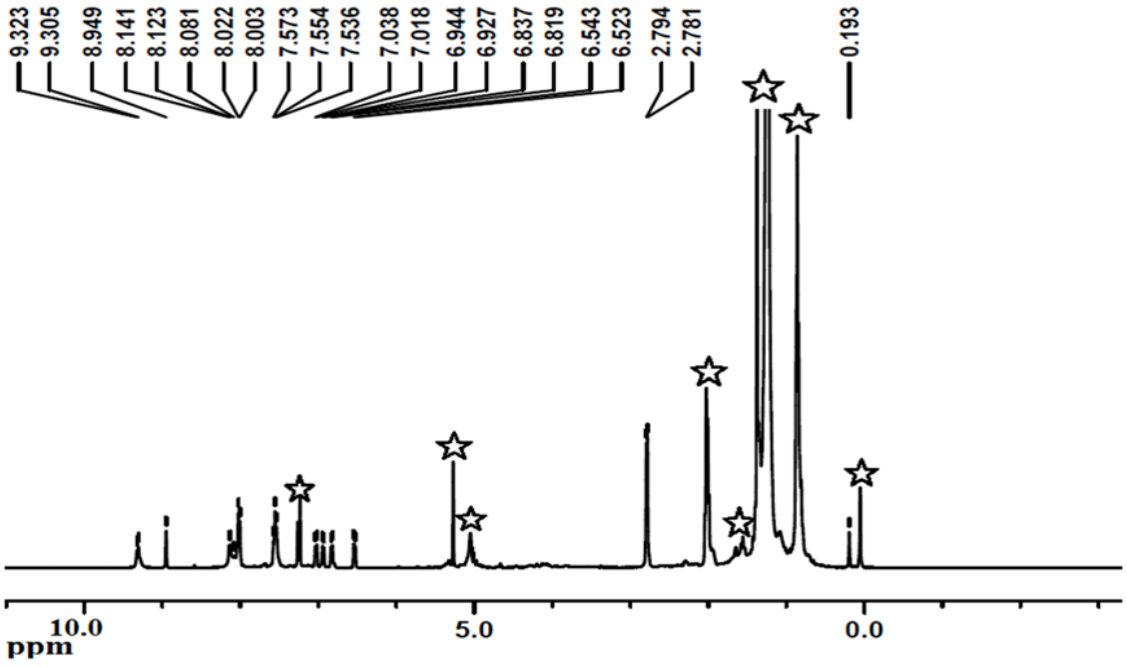


Figure S37. D_2O Exchange spectrum of protonated 7 at RT

☆: Residual solvent peak or solvent impurity

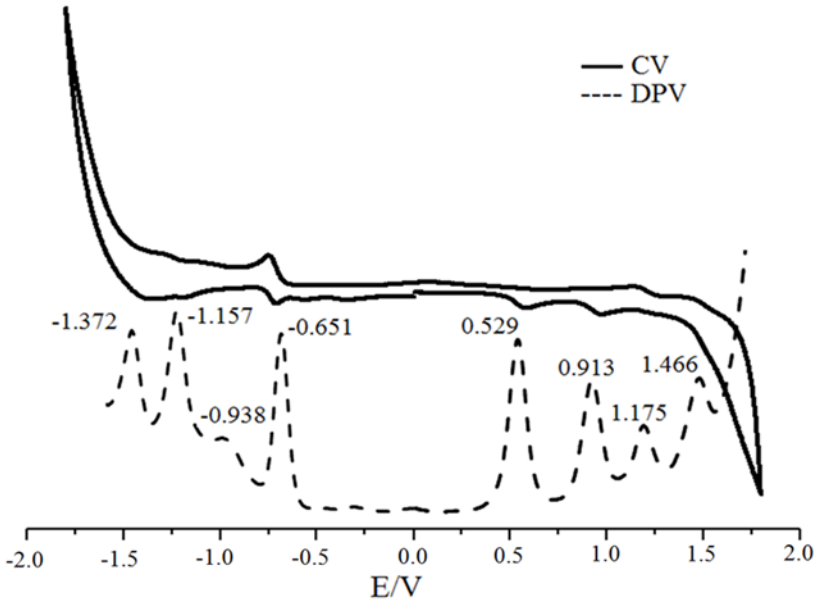


Figure S38. Cyclic Voltammogram of 6 in CH_2Cl_2

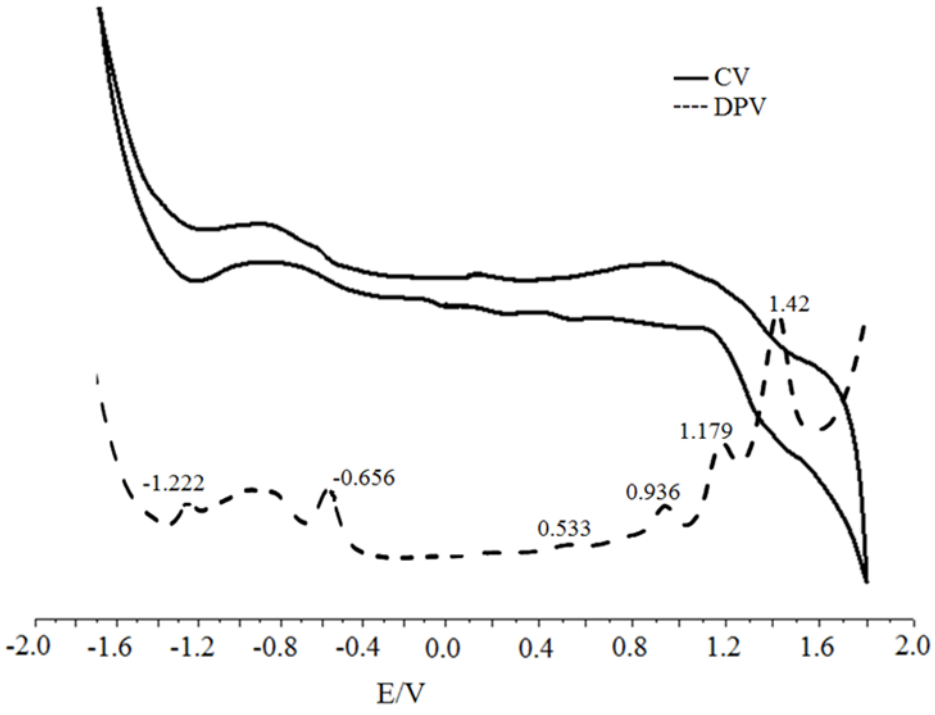


Figure S39. Cyclic Voltammogram of 7 in CH_2Cl_2

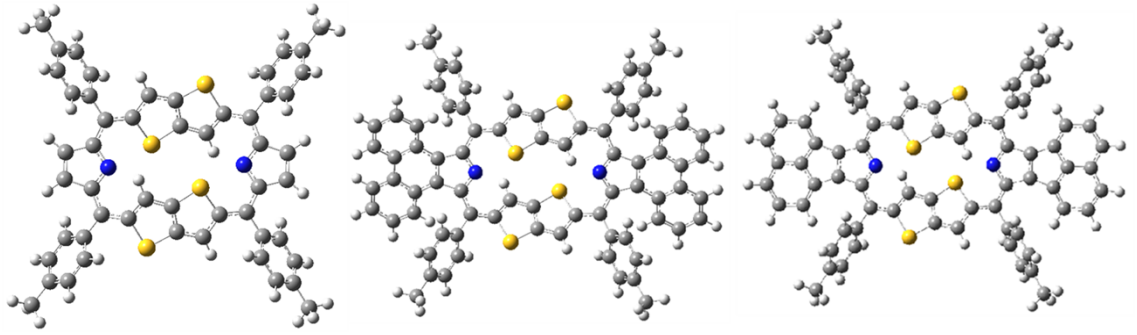


Figure S40. Energy minimized structure of 5, 6 and 7 by DFT method at B3LYP/6-31G* level using Gaussian 09 program (top view)

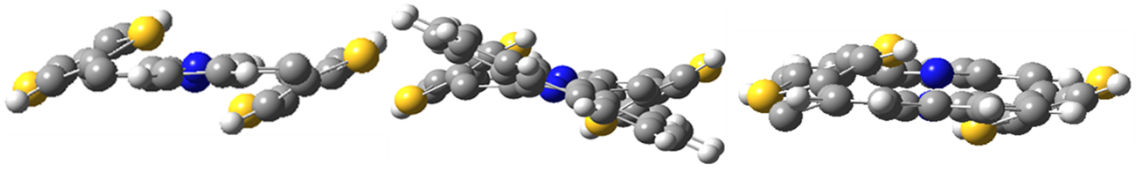


Figure S41. Energy minimized structure of 5, 6 and 7 by DFT method (side view)

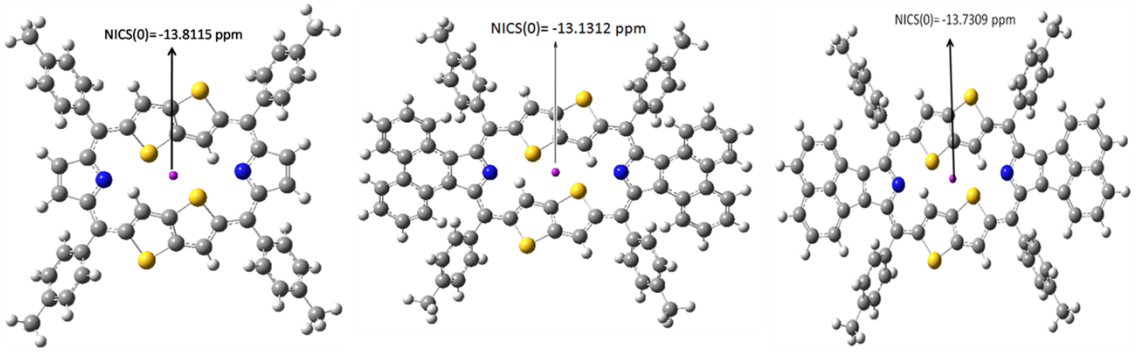


Figure S42. Calculated NICS (0) value for 5, 6 and 7

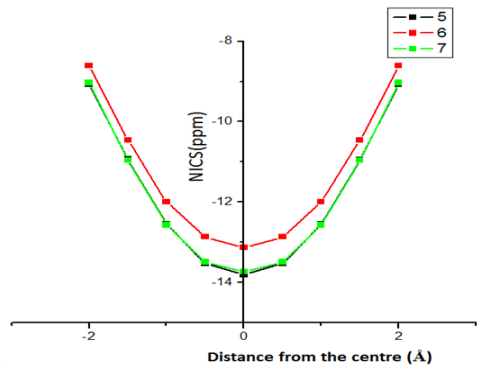


Figure S43. Plot of Chemical shift *vs* distance of NICS probe for 5, 6 and 7

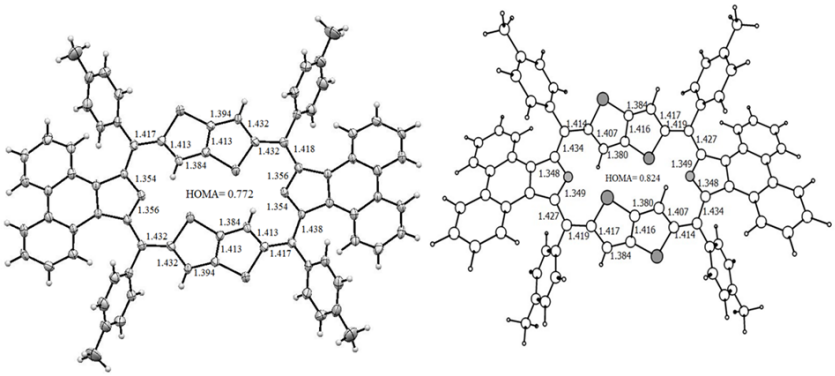


Figure S44. HOMA values from X-ray crystal structure (left) and energy minimized structure (right) of 6

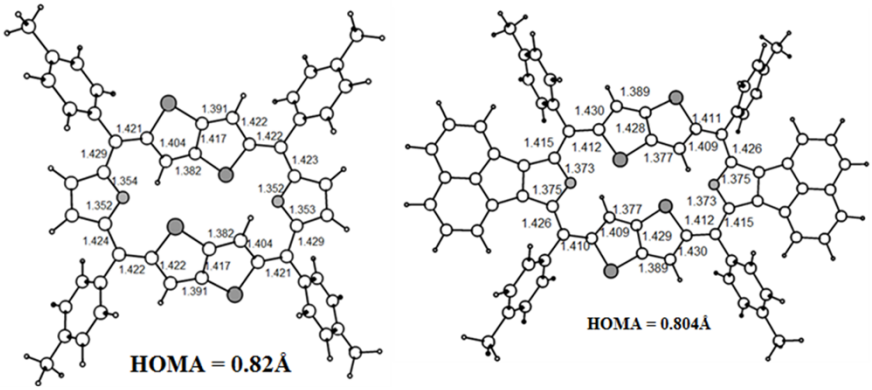


Figure S45. HOMA value from DFT-optimized structure of 5 and 7

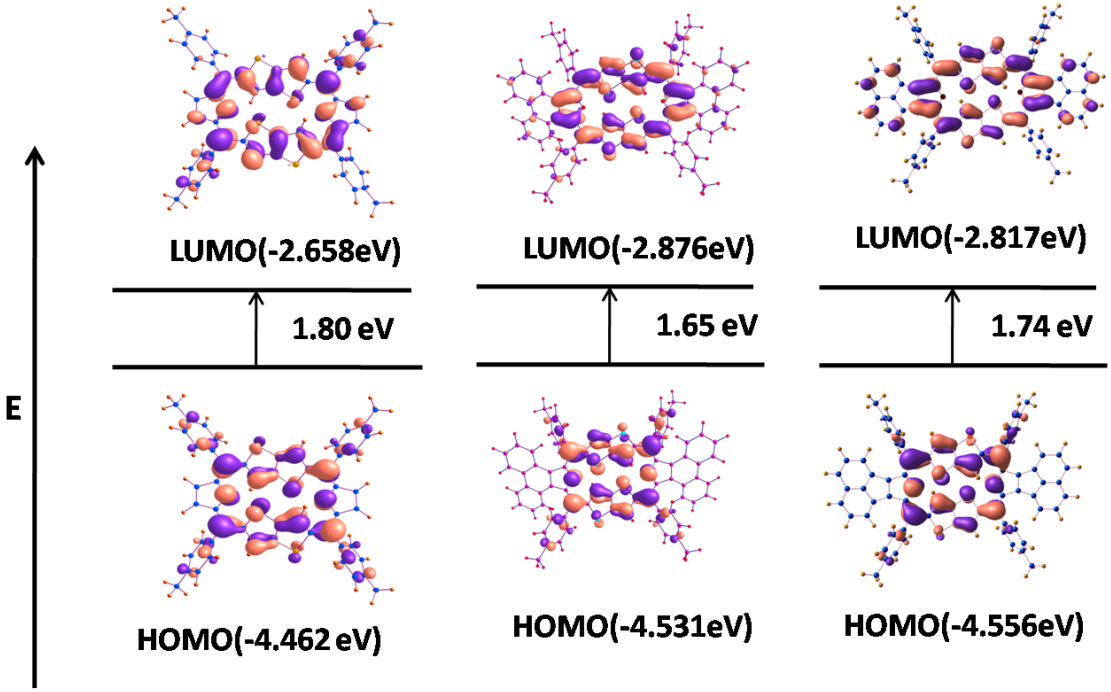


Figure S46. FMO energy diagram from DFT-optimized structure of 5, 6 and 7

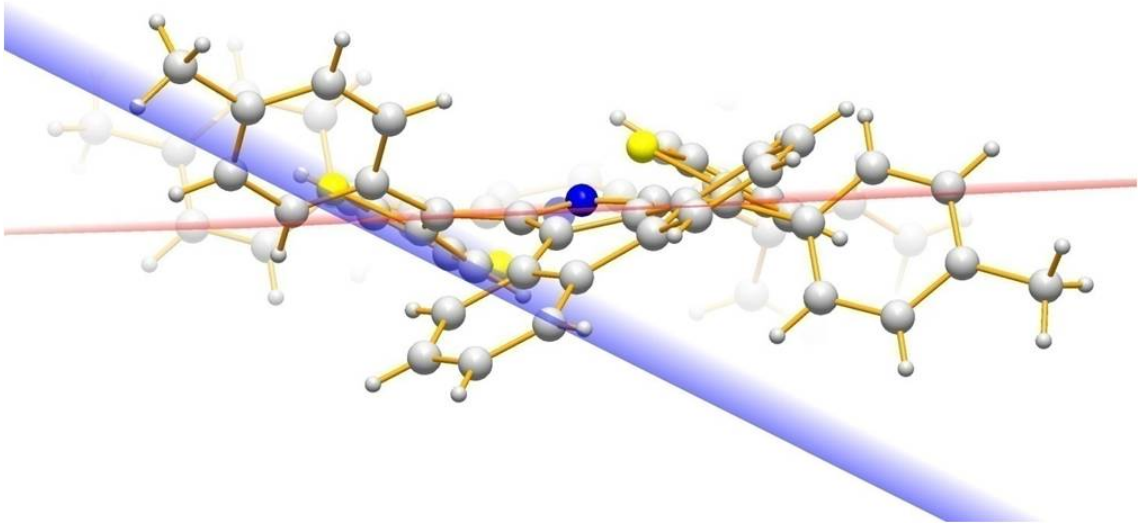


Figure S47. Dihedral Angle between fused thiophene ring plane and Macrocycle plane (defined through *meso* carbons) for 6

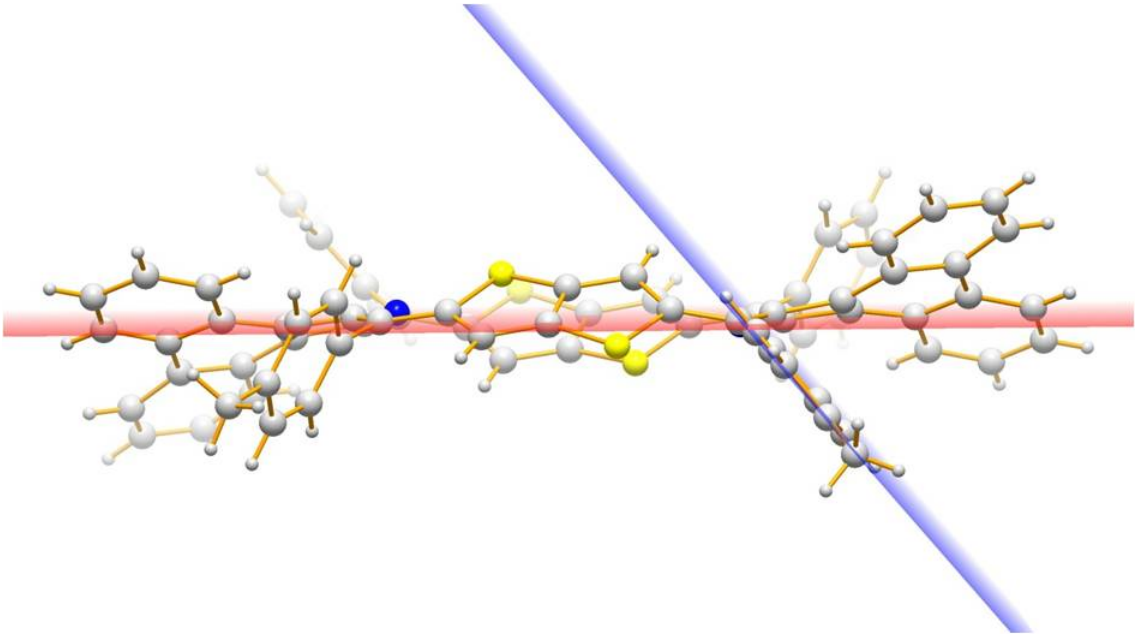


Figure S48. Dihedral Angle between tolyl ring plane (C32, C33, C34, C35, C36, C37) and Macrocycle plane (defined through *meso* carbons) for 6

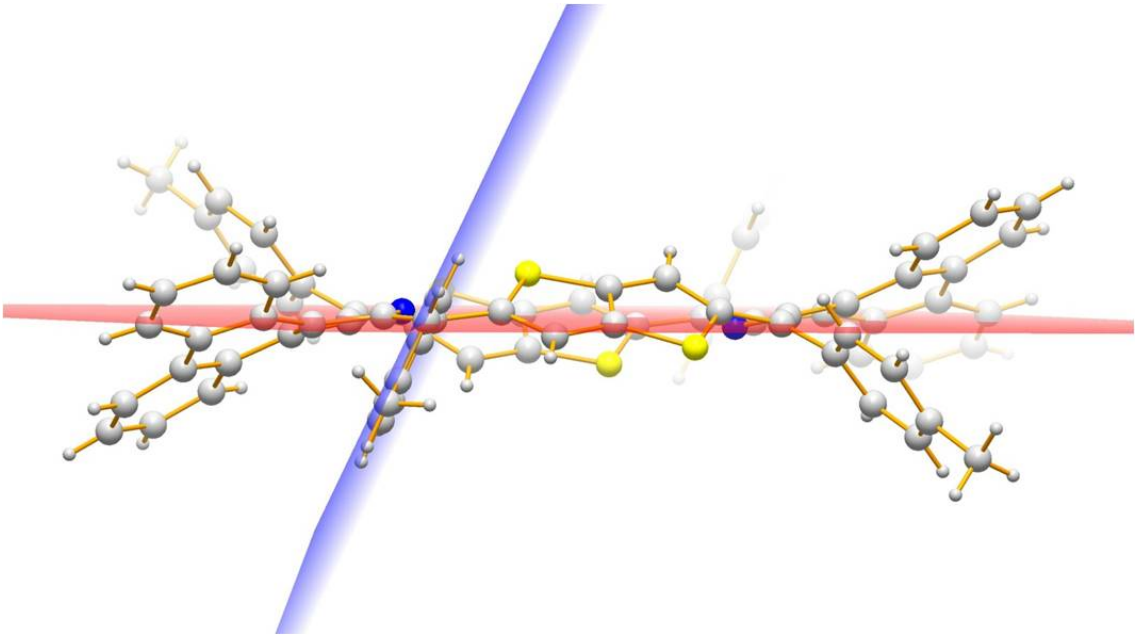


Figure S49. Dihedral Angle between tolyl ring plane (C24, C25, C26, C27, C28, C29) and Macrocycle plane (defined through *meso* carbons) for 6

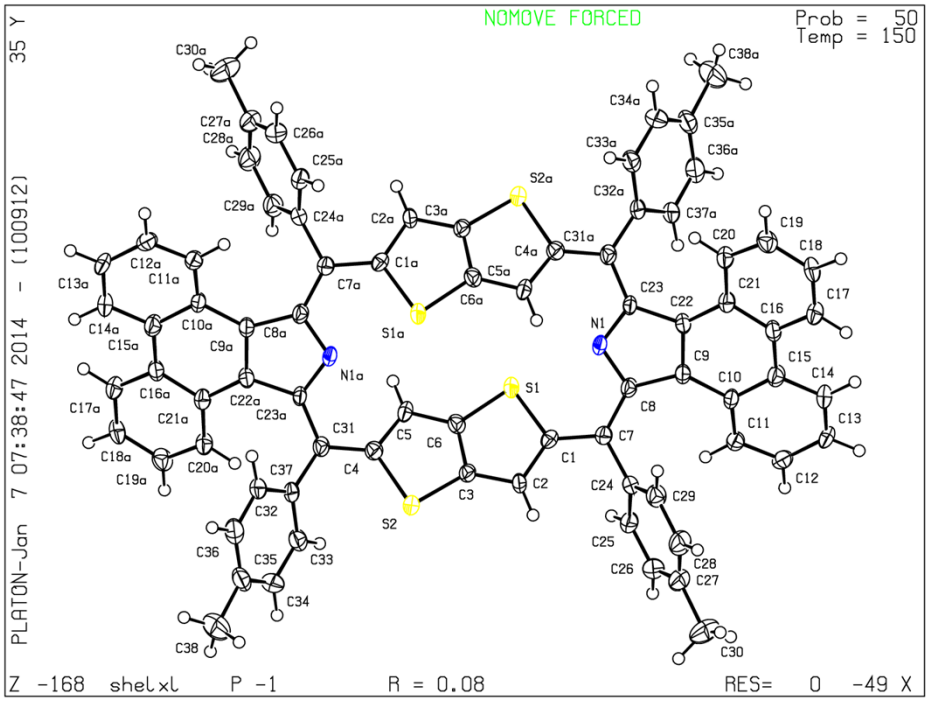


Figure S50. Molecular Structure of 6 with atom labelling

Crystal data and structure refinement for 6

Empirical formula	C76 H48 N2 S4	
Formula weight	1117.40	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.230(5) Å	α= 78.34(2)°.
	B = 14.220(9) Å	β= 76.48(2)°.
	C = 14.339(9) Å	γ = 83.47(3)°.
Volume	1594.0(17) $Å^3$	
Z	1	
Density (calculated)	1.164 Mg/m^3	
Absorption coefficient	0.193 mm^{-1}	
F(000)	582	
Crystal size	0.15 x 0.07 x 0.01 mm^3	
Theta range for data collection	2.66 to 25.00°.	
Index ranges	-9<=h<=6, -16<=k<=16, -17<=l<=15	
Reflections collected	11841	
Independent reflections	5558 [R (int) = 0.0527]	
Completeness to theta = 25.00°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. And min. Transmission	0.9981 and 0.9717	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5558 / 0 / 371	
Goodness-of-fit on F^2	1.128	
Final R indices [I>2sigma (I)]	R1 = 0.0843, wR2 = 0.1643	
R indices (all data)	R1 = 0.1083, wR2 = 0.1759	
Largest diff. Peak and hole	0.346 and -0.305 $e.Å^{-3}$	
CCDC number	990113	

Computational Details: Cartesian Coordinates of DFT- optimized Structure of 5

No.	Atom	X	Y	Z
1	C	-0.703985	3.773054	-0.257178
2	C	0.575104	3.274639	-0.482147
3	C	-1.722284	2.817245	-0.524578
4	C	0.580037	1.959655	-1.009782
5	C	2.859210	2.164979	-0.587639
6	C	1.824482	1.366289	-1.101339
7	C	4.172430	1.726543	-0.269724
8	C	5.265423	2.700240	-0.067734
9	C	4.413147	0.329652	-0.086575
10	C	5.692173	-0.381594	-0.113540
11	C	3.944383	-1.799442	0.119235
12	C	5.398756	-1.710255	-0.003107
13	C	-3.112943	2.946706	-0.258315
14	C	-3.944289	1.799467	-0.119593
15	C	-4.413257	-0.329614	0.086294
16	C	-5.398687	1.710383	0.002564
17	C	-5.692202	0.381754	0.113072
18	C	-1.824510	-1.366227	1.101273
19	C	-0.579968	-1.959573	1.009580
20	C	-2.859133	-2.164786	0.587389
21	C	-0.575061	-3.274351	0.481564
22	C	1.722316	-2.817097	0.524234
23	C	0.704091	-3.772746	0.256466
24	C	3.113115	-2.946568	0.257982
25	C	-4.172526	-1.726369	0.269592
26	C	-3.678287	4.301758	-0.049389
27	C	-4.775356	6.898984	0.335221
28	C	-5.333439	8.284705	0.556718
29	C	-5.043030	5.858578	1.235308
30	C	-4.506939	4.586729	1.051543

31	C	-3.951442	6.616107	-0.762436
32	C	-3.409922	5.347280	-0.951775
33	C	-5.265428	-2.700286	0.068056
34	C	-7.366142	-4.580337	-0.315035
35	C	-7.201921	-3.490713	-1.182026
36	C	-6.176256	-2.568550	-0.998119
37	C	-6.457328	-4.716465	0.742666
38	C	-5.428310	-3.798529	0.933571
39	C	-8.498775	-5.561026	-0.503303
40	C	3.678313	-4.301671	0.049080
41	C	4.775045	-6.899061	-0.335426
42	C	3.409667	-5.347180	0.951417
43	C	3.951035	-6.616068	0.762141
44	C	4.507013	-4.586771	-1.051777
45	C	5.042939	-5.858699	-1.235490
46	C	5.332970	-8.284853	-0.556863
47	C	7.366302	4.579882	0.316476
48	C	5.428773	3.798639	-0.932964
49	C	6.457855	4.716382	-0.741501
50	C	6.175881	2.568121	0.998708
51	C	7.201638	3.490082	1.183155
52	C	8.499016	5.560362	0.505331
53	S	-2.219939	-3.792223	0.135728
54	S	1.020655	-1.303132	1.146399
55	S	-1.020576	1.303060	-1.146304
56	S	2.220036	3.792663	-0.136605
57	N	-3.406604	0.559999	-0.079467
58	N	3.406619	-0.559893	0.079217
59	H	-6.309583	8.250226	1.052373
60	H	-4.668109	8.883987	1.193009
61	H	-5.451727	8.825317	-0.388248
62	H	-5.675093	6.049168	2.100033
63	H	-4.714510	3.805126	1.776020

64	H	-3.736691	7.399595	-1.485924
65	H	-2.790806	5.150601	-1.822146
66	H	-6.097371	2.536049	-0.019201
67	H	-6.668331	-0.065168	0.248150
68	H	-6.054810	-1.749737	-1.700476
69	H	-7.881160	-3.369859	-2.023169
70	H	-6.560698	-5.551141	1.432474
71	H	-4.753815	-3.917236	1.776225
72	H	-8.735116	-5.702088	-1.563546
73	H	-9.415578	-5.208222	-0.011645
74	H	-8.257138	-6.539870	-0.076185
75	H	-2.001726	-0.355203	1.430696
76	H	0.929966	-4.744260	-0.164728
77	H	2.790438	-5.150427	1.821689
78	H	3.736079	-7.399529	1.485598
79	H	5.450938	-8.825536	0.388103
80	H	4.667717	-8.883992	-1.193365
81	H	6.309255	-8.250488	-1.052246
82	H	5.675052	-6.049374	-2.100158
83	H	4.714722	-3.805215	-1.776263
84	H	6.097498	-2.535873	0.018604
85	H	6.668242	0.065474	-0.248598
86	H	6.054092	1.749144	1.700828
87	H	7.880599	3.368911	2.024478
88	H	4.754598	3.917624	-1.775837
89	H	6.561585	5.551191	-1.431094
90	H	8.257665	6.539335	0.078346
91	H	9.415929	5.207539	0.013887
92	H	8.735046	5.701141	1.565681
93	H	-0.929885	4.744678	0.163750
94	H	2.001651	0.355187	-1.430539

Computational Details: Cartesian Coordinates of DFT- optimized Structure of 6

No	Atom	X	Y	Z
1	S	1.249400	-1.075677	-1.252233
2	S	-1.533753	-3.969321	-0.008429
3	N	3.549490	0.004420	-0.068964
4	C	2.179210	-2.419128	-0.539283
5	C	1.317739	-3.484453	-0.177998
6	H	1.683862	-4.373643	0.312266
7	C	-0.016409	-3.205438	-0.419908
8	C	-2.446162	-2.527038	-0.578447
9	C	-1.567248	-1.587125	-1.146715
10	H	-1.921825	-0.647209	-1.533682
11	C	-0.239941	-1.949481	-1.035307
12	C	3.580009	-2.364788	-0.321383
13	C	4.274328	-1.119930	-0.246610
14	C	5.708738	-0.778862	-0.189258
15	C	6.914052	-1.461693	-0.596351
16	C	6.903447	-2.632623	-1.385872
17	H	5.958280	-3.067471	-1.670629
18	C	8.071649	-3.210646	-1.835997
19	H	8.029559	-4.102753	-2.450580
20	C	9.306741	-2.629237	-1.518314
21	H	10.228479	-3.072968	-1.877621
22	C	9.345738	-1.468840	-0.772289
23	H	10.306016	-1.009207	-0.579210
24	C	8.168622	-0.851090	-0.297795
25	C	8.206935	0.392732	0.464345
26	C	9.409701	0.900231	1.001123
27	H	10.331685	0.351725	0.860388
28	C	9.439879	2.064020	1.742293
29	H	10.378718	2.421888	2.149845

30	C	8.249608	2.760578	1.992449
31	H	8.258908	3.656666	2.602595
32	C	7.057922	2.291095	1.481627
33	H	6.143765	2.81416	1.714691
34	C	7.001415	1.120068	0.694075
35	C	5.762483	0.556576	0.212463
36	C	4.369864	1.043371	0.185855
37	C	4.252868	-3.642401	0.026859
38	C	4.105760	-4.789734	-0.766342
39	H	3.513268	-4.736378	-1.672606
40	C	4.733478	-5.982812	-0.422789
41	H	4.614445	-6.850113	-1.064276
42	C	5.518449	-6.082439	0.729503
43	C	5.655039	-4.940086	1.527315
44	H	6.254331	-4.988463	2.431035
45	C	5.039200	-3.743887	1.185226
46	H	5.158117	-2.876233	1.822963
47	C	6.193094	-7.376731	1.111592
48	H	7.264442	-7.230674	1.277504
49	H	6.072779	-8.133662	0.334178
50	H	5.774700	-7.781378	2.038989
51	C	-3.821710	-2.364616	-0.292945
52	C	-4.615461	-3.552678	0.096034
53	C	-4.561415	-4.747364	-0.638434
54	H	-3.960354	-4.793696	-1.539023
55	C	-5.298208	-5.861019	-0.249105
56	H	-5.245678	-6.766979	-0.844253
57	C	-6.108866	-5.831374	0.888678
58	C	-6.155200	-4.642333	1.627268
59	H	-6.768871	-4.592369	2.521240
60	C	-5.427964	-3.525789	1.241950
61	H	-5.473635	-2.622039	1.837293
62	C	-6.916569	-7.033264	1.311141

63	H	-6.693243	-7.317286	2.343900
64	H	-6.712516	-7.895567	0.673612
65	H	-7.989834	-6.823879	1.258801
66	S	-1.249398	1.075646	1.252279
67	S	1.533751	3.969292	0.008481
68	N	-3.549486	-0.004453	0.068972
69	C	-2.179207	2.419097	0.539332
70	C	-1.317743	3.484428	0.178063
71	H	-1.683868	4.373623	-0.312191
72	C	0.016409	3.205409	0.419963
73	C	2.446161	2.527005	0.578481
74	C	1.567254	1.587090	1.146749
75	H	1.921832	0.647171	1.533707
76	C	0.239943	1.949447	1.035349
77	C	-3.580008	2.364755	0.321424
78	C	-4.274322	1.119905	0.246608
79	C	-5.708731	0.778857	0.189178
80	C	-6.914051	1.461719	0.596194
81	C	-6.903457	2.632677	1.385675
82	H	-5.958292	3.067519	1.670451
83	C	-8.071667	3.210733	1.835734
84	H	-8.029589	4.102860	2.450288
85	C	-9.306757	2.629332	1.518019
86	H	-10.228502	3.073091	1.877273
87	C	-9.345742	1.468915	0.772025
88	H	-10.306021	1.009295	0.578917
89	C	-8.168617	0.851132	0.297597
90	C	-8.206917	-0.392703	-0.464525
91	C	-9.409668	-0.900187	-1.001350
92	H	-10.331650	-0.351666	-0.860659
93	C	-9.439831	-2.063979	-1.742517
94	H	-10.378658	-2.421834	-2.150108
95	C	-8.249559	-2.760553	-1.992621

96	H	-8.258846	-3.656642	-2.602767
97	C	-7.057889	-2.291086	-1.481751
98	H	-6.143729	-2.814163	-1.714777
99	C	-7.001397	-1.120059	-0.694198
100	C	-5.762476	-0.556583	-0.212534
101	C	-4.369861	-1.043391	-0.185868
102	C	-4.252877	3.642378	-0.026764
103	C	-4.105752	4.789686	0.766471
104	H	-3.513235	4.736303	1.672717
105	C	-4.733484	5.982771	0.422971
106	H	-4.614437	6.850053	1.064482
107	C	-5.518485	6.082432	-0.729298
108	C	-5.655093	4.940103	-1.527142
109	H	-6.254411	4.988506	-2.430843
110	C	-5.039241	3.743896	-1.185106
111	H	-5.158173	2.876261	-1.822866
112	C	-6.193140	7.376735	-1.111331
113	H	-7.264481	7.230674	-1.277275
114	H	-6.072851	8.133626	-0.333873
115	H	-5.774730	7.781439	-2.038697
116	C	3.821710	2.364586	0.292965
117	C	4.615460	3.552660	-0.095978
118	C	4.561409	4.747326	0.638524
119	H	3.960342	4.793631	1.539110
120	C	5.298205	5.860992	0.249231
121	H	5.245672	6.766900	0.844406
122	C	6.108870	5.831379	-0.888547
123	C	6.155210	4.642359	-1.627171
124	H	6.768888	4.592420	-2.521140
125	C	5.427972	3.525804	-1.241890
126	H	5.473647	2.622070	-1.837257
127	C	6.916567	7.033284	-1.310978
128	H	6.693144	7.317411	-2.343687

129	H	6.712603	7.895534	-0.673348
130	H	7.989831	6.823863	-1.258768
131	Bq	0	0	0

Computational Details: Cartesian Coordinates of DFT- optimized Structure of 7

No	Atom	X	Y	Z
1	C	1.329571	-3.610466	-0.446323
2	C	-0.016363	-3.309795	-0.607764
3	C	2.171356	-2.466969	-0.612878
4	C	-0.237601	-1.952669	-0.995100
5	C	-2.443325	-2.573040	-0.587121
6	C	-1.559386	-1.568191	-1.029313
7	C	0.237559	1.952128	0.995188
8	C	2.443298	2.572335	0.587255
9	C	0.016441	3.309325	0.608236
10	C	-2.171311	2.466622	0.612923
11	C	-1.329521	3.610097	0.446740
12	C	-4.303896	-1.068632	-0.015976
13	C	-4.223792	1.164344	0.232098
14	C	-5.684085	-0.586879	-0.042119
15	C	-5.632778	0.810777	0.104173
16	C	-7.084861	-0.999685	-0.234031
17	C	-7.002220	1.349335	0.080829
18	C	-7.840636	0.210878	-0.136612
19	C	-7.770633	-2.175719	-0.474231
20	C	-9.189602	-2.132002	-0.603195
21	C	-9.233074	0.274693	-0.243760
22	C	-9.911653	-0.957578	-0.488516
23	C	-7.606115	2.584793	0.221458
24	C	-9.026120	2.671011	0.131241

25	C	-9.825751	1.565867	-0.099125
26	C	4.223825	-1.164501	-0.232659
27	C	4.304131	1.068489	0.015325
28	C	5.632907	-0.810948	-0.105575
29	C	5.684425	0.586713	0.040515
30	C	7.002274	-1.349678	-0.083273
31	C	7.085486	0.999410	0.230963
32	C	7.841011	-0.211293	0.133197
33	C	7.605864	-2.585241	-0.224319
34	C	9.025933	-2.671639	-0.135464
35	C	9.233567	-0.275260	0.238807
36	C	9.825927	-1.566537	0.093858
37	C	9.912614	0.957021	0.482188
38	C	9.190877	2.131614	0.596987
39	C	7.771764	2.175466	0.469661
40	C	3.563031	-2.406597	-0.382101
41	C	4.648850	3.564585	-0.034024
42	C	-3.563009	2.406311	0.381850
43	C	-3.795369	-2.382667	-0.233331
44	C	-4.649046	-3.564479	0.035557
45	C	-6.232959	-5.841013	0.595713
46	C	-4.766708	-4.604352	-0.902015
47	C	-5.553456	-5.722703	-0.623863
48	C	-5.335828	-3.678992	1.258377
49	C	-6.110750	-4.801211	1.531876
50	C	-7.072738	-7.065156	0.911342
51	C	-4.294965	3.687446	0.173107
52	C	-4.426769	4.618960	1.214278
53	C	-5.104723	5.820711	1.006712
54	C	-4.847569	3.992744	-1.080822
55	C	-5.513476	5.199985	-1.284637
56	C	-5.653725	6.131789	-0.245406
57	C	5.335456	3.681345	-1.255793

58	C	6.112486	4.803840	-1.526273
59	C	6.235548	5.840570	-0.588191
60	C	5.556417	5.719301	0.632411
61	C	4.768281	4.602072	0.907076
62	C	7.062353	7.074064	-0.901103
63	C	4.295077	-3.687653	-0.173206
64	C	5.654039	-6.131861	0.245530
65	C	5.514239	-5.199713	1.284500
66	C	4.848211	-3.992546	1.080578
67	C	5.104512	-5.821181	-1.006476
68	C	4.426499	-4.619496	-1.214150
69	C	6.359570	-7.455367	0.480717
70	S	1.225370	-1.022702	-1.041348
71	S	-1.550025	-4.114646	-0.308086
72	S	-1.225441	1.022240	1.041186
73	S	1.550184	4.114065	0.308638
74	N	3.477134	-0.013430	-0.174870
75	N	-3.477026	0.013162	0.174650
76	H	1.731386	-4.566747	-0.147980
77	H	-1.912967	-0.573675	-1.231073
78	H	-4.257234	-4.520555	-1.854774
79	H	-5.644164	-6.510992	-1.363325
80	H	-7.166095	-7.713176	0.034801
81	H	-6.614165	-7.648655	1.719356
82	H	-8.079051	-6.776402	1.235992
83	H	-6.627962	-4.875915	2.482681
84	H	-5.247838	-2.882916	1.987405
85	H	-7.255702	-3.121936	-0.560688
86	H	-9.715074	-3.060938	-0.793803
87	H	-10.991892	-0.965738	-0.586112
88	H	-10.902888	1.673095	-0.168627
89	H	-9.488138	3.645218	0.244639
90	H	-7.026466	3.480796	0.391290

91	H	-4.752237	3.278141	-1.889312
92	H	-5.933452	5.421484	-2.260114
93	H	-5.211158	6.524501	1.825437
94	H	-4.008766	4.387976	2.186941
95	H	-5.663622	8.190977	-0.904421
96	H	5.650194	6.504346	1.375132
97	H	4.260092	4.515026	1.860236
98	H	6.631666	4.879437	-2.475739
99	H	5.248167	2.886674	-1.986437
100	H	6.471526	7.792565	-1.484066
101	H	7.949487	6.814296	-1.488137
102	H	7.387849	7.572417	0.017378
103	H	9.716658	3.060659	0.786167
104	H	7.257312	3.121940	0.555826
105	H	10.992974	0.965077	0.578453
106	H	10.903126	-1.673869	0.162235
107	H	9.487717	-3.645924	-0.249150
108	H	7.025932	-3.481176	-0.393526
109	H	7.189622	-7.338173	1.185156
110	H	6.754579	-7.861591	-0.455742
111	H	5.662783	-8.192098	0.901185
112	H	5.934652	-5.420880	2.259863
113	H	4.753217	-3.277688	1.888884
114	H	5.210662	-6.525200	-1.825044
115	H	4.008151	-4.388796	-2.186731
116	H	1.912885	0.572879	1.230604
117	H	-1.731262	4.566478	0.148610
118	C	3.795469	2.382201	0.233417
119	C	1.559370	1.567480	1.029156
120	C	-6.359375	7.455259	-0.480516
121	H	-7.191726	7.337255	-1.182126
122	H	-6.751269	7.863155	0.456518
123	Bq	0	0	0