
Electronic Supplementary Materials for

Targeted Synthesis of *meso*-Aryl Substituted Aromatic *trans*-Doubly N-confused Dithia/Diselena [18] porphyrins (1.1.1.1) with NIR Absorption: Spectroscopic and Theoretical Characterization

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Materials and Methods:

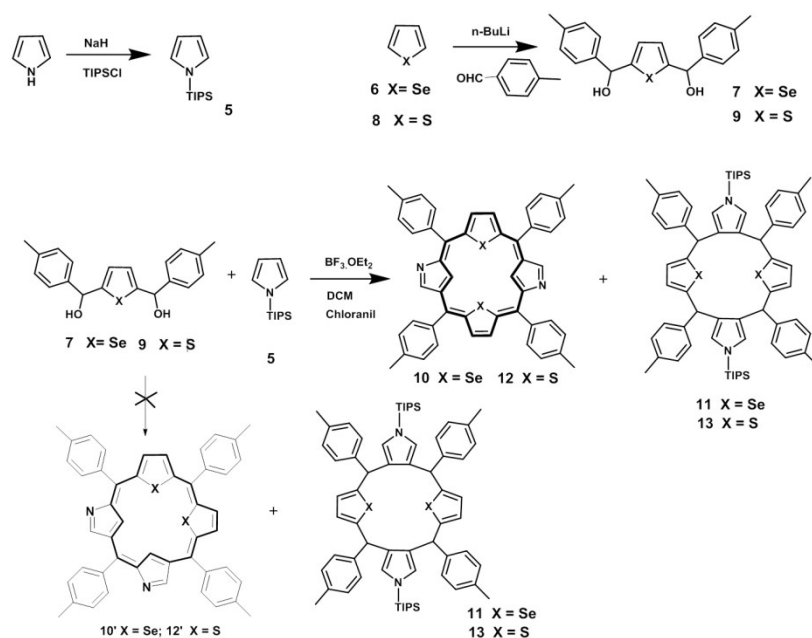
1.1 Electronic absorption spectra were measured using a Perkin Elmer Lambda 950 UV-vis-NIR spectrophotometer. ^1H , and ^{13}C NMR spectra were recorded on a spectrometer (operating as 500.17 MHz for ^1H and 125.91 MHz for ^{13}C) using the residual solvents as the internal references for ^1H [(CHCl_3) ($\delta = 7.26$ ppm), CH_2Cl_2 ($\delta = 5.32$ ppm)]. MALDI-TOF MS data were recorded using BrukerDaltonics 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} and gravity column chromatography were performed using Silica Gel 230-400 mesh.

1.2 Theoretical Calculation

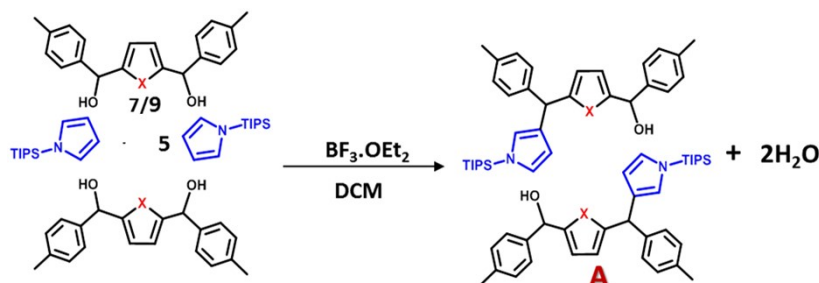
All geometries were optimized using Density Functional theory (DFT) with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP)^{S1} and 6-31G(d,p) and 6-311+G(d) basis sets^{S2} for all the atoms named as **B1b** and **B1c** level of theory. Computed harmonic vibrational frequencies for all the conformers at same level of theory to ascertain that the optimized structures are local minima using Gaussian 16 (A.03).^{S3} While the thermodynamic stability of conformers of **10**, **11**, **12** and **13** were also optimized using B3LYP/6-31G and WB97XD^{S4}/6-31G level of theory considered as **B1** and **B1a**. Further the single point energies at B3LYP/6-311+G (d,p) as **B2** and B3LYP/def2-TZVP^{S5} level of theory (**B2a**) were performed to note the changes in the relative energies of the isomers of **10** and **12**. While for **11** and **13** single point energies were performed at **B2** level of theory. The stimulated steady state absorption spectra were obtained from time dependent density functional (TD-DFT)^{S6} method in presence of dichloromethane solvent with implicit polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM)^{S7} at B3LYP/6-311+G(d) level of theory. The nature of aromaticity of **10/12** were assessed from the nuclear chemical independent shift^{S8} (NICS (0) value and Anisotropy of the current-induced density (ACID)^{S9} that employs gauge independent atomic orbital (GIAO) method^{S10} and the continuous set of gauge transformations (CSGT)^{S11} methods respectively using B1b and B1c level of theory. Using trimethylsilane as a reference, theoretical ^1H NMR chemical shift values are interpreted. AICD plot was plotted using POVray 3.7 for Windows.

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- S5. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.
- S6. (a) C. Adamo and D. Jacquemin, *Chem. Soc. Rev.*, 2013, **42**, 845; (b) G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi and V. Barone, *J. Chem. Phys.*, 2006, **124**, 094107 1.
- S7. (a) S. Miertuš and J. Tomasi, *Chem. Phys.*, 1982, **65**, 239; (b) M. Cossi and V. Barone, *J. Chem. Phys.*, 2000, **112**, 2427.
- S8. P. V. R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao and N. J. R. V. E. Hommea, *J. Am. Chem. Soc.*, 1996, **118**, 6317.
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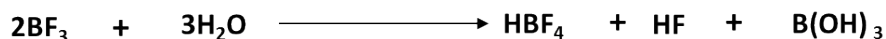
1.3 Synthesis:



Scheme S1. Synthesis of Core modified *trans*-doubly N-confused Porphyrins

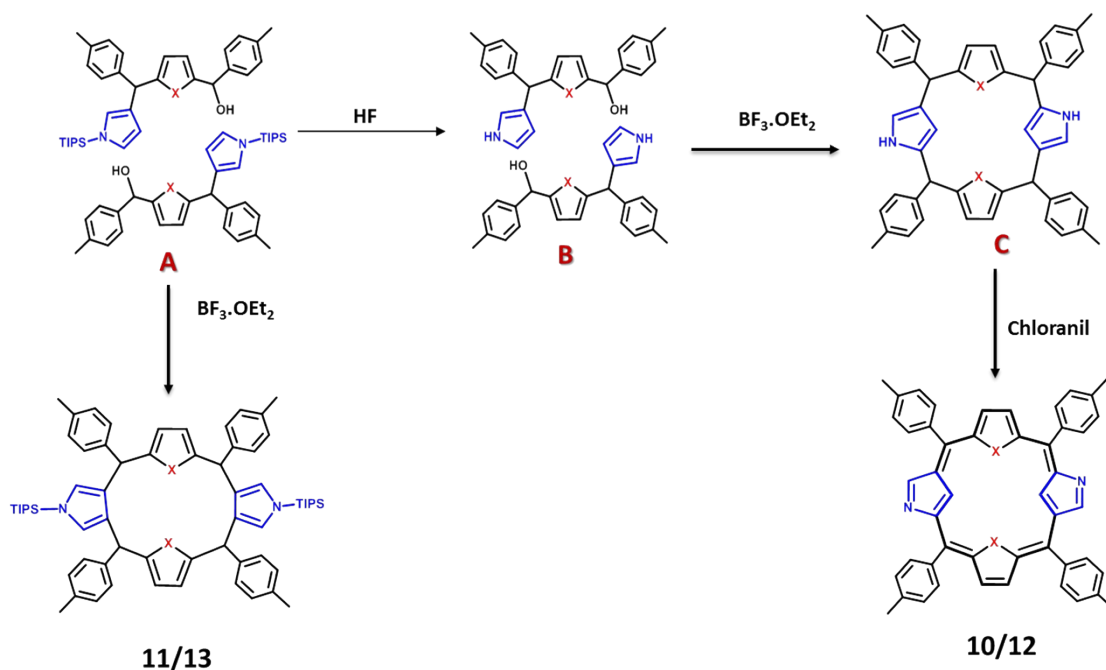


Step 1: TIPS-Pyrrole (owing to steric hindrance of TIPS group, Ref: *Tetrahedron Lett.*, 1981, **22**, 3455) acting as progenitor for mono β -condensation intermediate **A** (Ref: *Chem. Eur. J.*, 2012, **18**, 4380.) catalyzed by Lewis acid (Ref: *Tetrahedron*, 2004, **60**, 11435)



Step 2: Equilibria in the system Boron Trifluoride-Water leading to generation of HF (Ref: *J. Am. Chem. Soc.*, 1951, **73**, 409)

Step 3: HF induced desilylation (Ref: *Chem. Asian J.*, 2016, **11**, 986) of monocondensed intermediate **A** leading to the intermediate **B** followed by Lewis acid catalyzed cyclization (Ref: *Tetrahedron*, 2004, **60**, 11435) leading to the formation of macrocycle **C**. Macrocycle **C** then undergoes chloranil oxidation (Ref: *Chem. Rev.*, 1978, **78**, 317-361; *Angew. Chem. Int. Ed Engl.*, 2015, **54**, 14638.) leading to the formation of **10/12** as major product. Whereas, acid catalyzed cyclization of intermediate **A** leads to macrocycles **11/13** as byproducts in negligible yield due to steric hindrance of TIPS groups.



Scheme S2. Plausible reaction mechanism for formation of **10/12** and **11/13**

1-(triisopropylsilyl)-1H-Pyrrole (5). To a suspension of sodium hydride (60% dispersion in oil, 1.520 g, 31.68 mmol) in tetrahydrofuran (50 mL) was slowly added pyrrole (1.934 g, 28.8 mmol) at 0°C. The mixture was stirred at the same temperature for 1.5 hour. To the mixture was slowly added triisopropylsilyl chloride (5.552 g, 28.8 mmol) at 0°C. The resulting mixture was stirred at same temperature for another 1.5 hours. To the reaction mixture was added ice-water. It was extracted with diethyl ether. The extract was washed with water, dried over anhydrous sodium sulfate and concentrated under reduced pressure to give of 1-(triisopropylsilyl) pyrrole as yellow oil. R_f 0.8 (Hexane). Yield: 6.3 g (99%). HR-ESI-TOF MS (m/z): 224.21[M+H]⁺ (223.11 calc. for [C₁₃H₂₅NSi]⁺).

¹H NMR (500 MHz, CDCl₃, 300K, δ [ppm]): 6.80 (t, 2H); 6.32 (t, 2H); 1.10 (d, Methyl); 1.47 (septet, methine CH). ¹³C NMR (125 MHz, CDCl₃, 300K, δ [ppm]): 11.73; 17.81; 110.034; 124.01.

2, 5 -Bis(p-tolylhydroxymethyl) selenophene (7). To a solution of selenophene (1 g, 7.6 mmol) in 45 mL of n-hexane containing N,N',N,N'- tetramethylenediamine (2.87 mL, 19.08 mmol) under argon atmosphere, n-butyl lithium (12.7 mL, 19.08 mmol) was added slowly and was stirred at room temperature for two hours and later refluxed for two hours. The reaction was then allowed to attain room temperature. *p*-Tolylaldehyde (2.24 mL, 19.08 mmol) was dissolved in 25 mL of tetrahydrofuran (THF) and was added drop wise to the reaction mixture in ice-cold condition. After the addition, the reaction mixture was allowed to attain the room temperature and was stirred for an additional two hours. The reaction was quenched with saturated ammonium chloride solution and was stirred for half an hour. This was then extracted with ether (100 mL). The organic layer was combined and was washed with brine and dried over anhydrous sodium sulphate.

The crude product obtained on evaporation of the solvent was recrystallized from toluene. The solid obtained was identified as **7**. R_f 0.4 (Hexane/EtOAc = 4:1). Yield: 1.6 g (57%). HR-ESI-TOF MS (m/z): 395.16 [M+Na]⁺ (372.06. calc. for [C₂₀H₂₀O₂Se]⁺).

¹H NMR (400 MHz, CDCl₃, 300 K, δ [ppm]): 2.34 (s, 6H); 5.89 (s, 2H); 6.84 (s, 2H); 7.15 (d, 4H, J = 10.4 Hz); 7.30 (d, 4H, J = 10.8 Hz); ¹³C {¹H} NMR (100 MHz, CDCl₃, 300 K, δ [ppm]): 21.29; 74.32; 126.20; 126.31; 129.36; 137.87; 140.62; 155.95.

2, 5-Bis(p-tolylhydroxymethyl) thiophene (9): Thiophene (1.9 mL, 23.7 mmol), N, N, N', N' tetramethylenediamine (9 mL, 59.42 mmol) in dry n-hexane (40 mL), n-butyl lithium (38 mL, 59.42 mmol) and p-Tolylaldehyde (7.0 mL, 59.42 mmol) in 20mL THF under similar reaction conditions as mentioned above gave diol **9**. R_f 0.3 (Hexane/EtOAc = 9:1). Yield: 4.5g (59%). HR-ESI-TOF MS (m/z): 347.23 [M+Na]⁺ (324.12 calc. for [(C₂₀H₂₀O₂S)⁺]).

¹H NMR (400 MHz, CDCl₃, 300 K, δ [ppm]): 2.34 (s, 6H); 5.89 (s, 2H); 6.84 (s, 2H); 7.15 (d, 4H, J = 8 Hz); 7.29 (d, 4H, J = 10 Hz). ¹³C NMR (100 MHz, CDCl₃, 300 K, δ [ppm]): 21.11; 72.35; 124.18; 126.18; 129.14; 137.66; 139.99; 148.21.

General Synthetic Procedure for macrocycles **10** and **11**.

Under nitrogen atmosphere and in dark condition a solution of 186 mg of compound **7** (0.5 mmol), 111.5 mg of 1-(triisopropylsilyl) pyrrole **5** (0.5 mmol) and boron trifluoride diethyl etherate (7 μL) in 250 mL dry dichloromethane was stirred for 1 hour. Then, chloranil (307 mg, 1.25 mmol) was added and opened to air and the reaction mixture was refluxed for another 1 hour. The solvent was removed under reduced pressure and the crude product was filtered by basic alumina column using dichloromethane as eluent followed by repeated silica gel column chromatography using the mixture of 20% dichloromethane - hexane solution the compound **11** was obtained while with 5% Ethylacetate - dichloromethane solution the compound **10** was obtained. After recrystallization, the compound **10** was obtained as dark greenish crystal and **11** as yellow sticky compound respectively.

Compound **10**: R_f 0.2 (CH₂Cl₂/EtOAc = 9:1). Yield. ~ 121 mg (30%). M.P. > 350°C. MALDI-TOF MS (m/z): 801.571 (800.1202 calc. for [C₄₈H₃₆N₂Se₂]⁺). UV-Vis (CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 484.62 (1.89 x 10⁴); 562.38 (1.32 x 10³); 616.38 (1.2 x 10³); 804.61 (1.12 x 10²); 1020 (tailing); [(UV-VIS [CH₂Cl₂, 1% TFA/CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 502.91 (1.04 x 10⁴); 788.45 (4.35 x 10³); 991.92 (2.45 x 10³).

¹H NMR (500 MHz, CDCl₃, 298 K, δ [ppm], TMS): 2.68-2.70 (s, tolyl Me); 7.60-8.34 (d, 16H, tolyl-CH); 9.16-9.18 (brs, 2H, selenophene β-H); 9.48 (d, 1H, selenophene β-H, ³J = 5 Hz); 9.53 (d, 1H, selenophene β-H, ³J = 5 Hz); ¹H NMR (500 MHz, CDCl₃, 243 K δ [ppm], TMS): -0.29 (br, 2H, inner pyrrole β-H); 14.56 (br, 2H, outer pyrrole α-H).

Compound **11**: R_f 0.5 (CH₂Cl₂/Hexane = 1:4). Yield. ~3 mg (<1%). HRMS (m/z): 1118.898 (1118.4347 calc. for [C₆₆H₈₂N₂Se₂Si₂]⁺); UV-Vis (CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 439.17 (1.45 x 10³). ¹H NMR (500 MHz, CDCl₃, 298 K, δ [ppm], TMS): 6.98-7.13 (m, 16H, tolyl-CH); 6.51 (br, 2H, selenophene β-H); 6.41 (s, 2H, α-H of TIPS- Pyrrole); 6.36 (s, 2H, α-H of TIPS- Pyrrole); 6.28 (br, 2H, selenophene β-H); 5.24 (s, 2H, *meso*-CH); 5.18 (s, 2H, *meso*-CH); 2.32 (s, 6H, tolyl Me); 2.30 (s, 6H, tolyl Me); 1.27-1.28 (m, 6H, TIPS-CH); 0.92-1.12 (m, 36H, TIPS-CH₃). ¹³C{¹H} NMR (125 MHz, CDCl₃, δ [ppm]): 11.80, 13.21, 13.64, 13.71, 13.81, 13.91, 17.94, 18.03, 18.34, 18.54, 18.62, 18.70, 21.22, 21.35, 29.86, 45.54, 45.78, 45.82, 122.78, 123.27, 123.53, 123.68, 126.58, 126.72, 127.55, 128.30, 128.47, 128.53, 128.77, 128.86, 129.02, 129.24, 129.31, 129.61, 133.35, 133.46, 141.67, 141.77, 142.44, 142.61, 154.62, 154.90, 155.61, 155.71.

General Synthetic Procedure for **12** and **13**.

Under nitrogen atmosphere and in dark condition a solution of 162.2 mg of compound **9** (0.5 mmol), 111.5 mg of 1-(triisopropylsilyl) pyrrole **5** (0.5 mmol) and boron trifluoride diethyl etherate (7 μL) in 250 mL dry dichloromethane was stirred for 1 hour. Then, chloranil (307 mg, 1.25 mmol) was added and opened to air and the mixture was refluxed for another 1 hour. The solvent was removed under reduced pressure and crude product was filtered by basic alumina column using dichloromethane as eluent followed by repeated silica gel column chromatography using the mixture of 30% dichloromethane - hexane solution, the compound **13** was obtained while with 15% Ethylacetate-dichloromethane solution, the compound **12** was obtained. After recrystallization, the compound **12** was obtained as greenish crystal and **13** as yellow sticky compound.

Compound **12**: R_f 0.1 (CH₂Cl₂/EtOAc = 9:1). Yield. ~71mg (~20%). M.P. > 350°C. MALDI-TOF MS (m/z): 705.646 (704.2320 Calc. for [C₄₈H₃₆N₂S₂]⁺). UV-vis (CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 461.31 (1.89 x 10⁴); 542.47 (broad); 586.81 (broad); 798.61 (1.2 x 10³); 1050 (tailing); [(UV-VIS [CH₂Cl₂, 1% TFA/CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 477.33 (0.89 x 10⁴); 625.73 (2.96 x 10³); 724.63 (2.75 x 10³); 914.07 (1.7 x 10³).

¹H NMR (500 MHz, CDCl₃, 298K, δ [ppm], TMS): 2.70-2.72 (s, 12H, tolyl Me); 7.60-8.35 (d, 16H, tolyl-CH); 9.23-9.24 (brs, 2H, thiophene β-H); 9.53 (d, 1H, thiophene β-H, ³J = 5 Hz); 9.56 (d, 1H, thiophene β-H, ³J = 5 Hz); ¹H NMR (500 MHz, CDCl₃, 243 K, δ [ppm], TMS): -1.09 (br, 2H, inner pyrrole β-H); 14.56 (br, 2H, outer pyrrole α-H).

Compound **13**: R_f 0.3 (CH₂Cl₂/Hexane = 1:4). Yield. ~2.5 mg (<1%). HRMS (m/z): 1022.513 (1022.55 Calc. For [C₆₆H₈₂N₂S₂Si₂]⁺). UV-Vis (CH₂Cl₂, λ [nm], (ε [M⁻¹cm⁻¹]), 298K): 431.3 (1.5 x 10³). ¹H NMR (400 MHz, CDCl₃, 298 K, δ [ppm], TMS): 6.89-7.31 (m, 16H, tolyl-CH); 6.41 (br, 2H, thiophene β-H); 6.26 (s, 2H, α-H of TIPS-Pyrrole); 6.16 (s, 2H, α-H of TIPS- Pyrrole); 6.0 (br, 2H, thiophene β-H); 5.53

(s, 2H, *meso*-CH); 5.49 (s, 2H, *meso*-CH); 2.31 (s, 6H, tolyl Me); 2.32 (s, 6H, tolyl Me); 1.19-1.33 (m, 6H, TIPS-CH); 0.94-1.07 (m, 36H, TIPS-CH₃).

¹³C{¹H} NMR (100 MHz, CDCl₃, δ[ppm]): 11.68, 11.73, 11.87, 13.88, 17.88, 18.02, 18.61, 22.59, 22.85, 43.95, 44.74, 122.97, 123.37, 123.92, 124.09, 124.43, 124.57, 124.73, 124.90, 125.54, 126.01, 126.39, 127.97, 128.05, 128.18, 128.43, 128.53, 128.67, 129.00, 145.18, 145.65, 147.74, 148.38.

2. Supplementary Data:

2.1 Mass Spectra

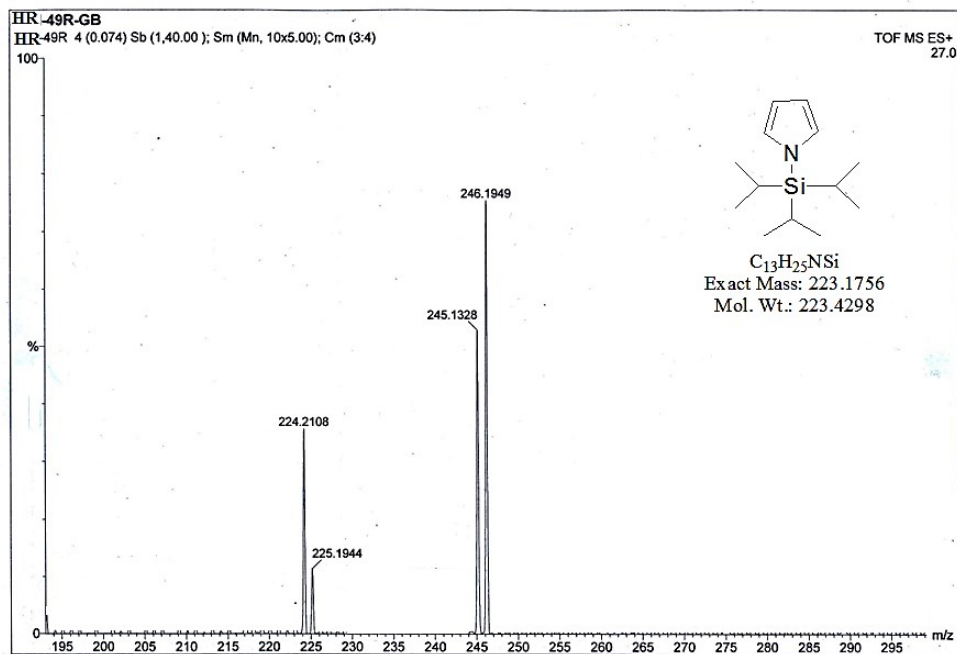


Figure S1. HRMS Spectra of 5

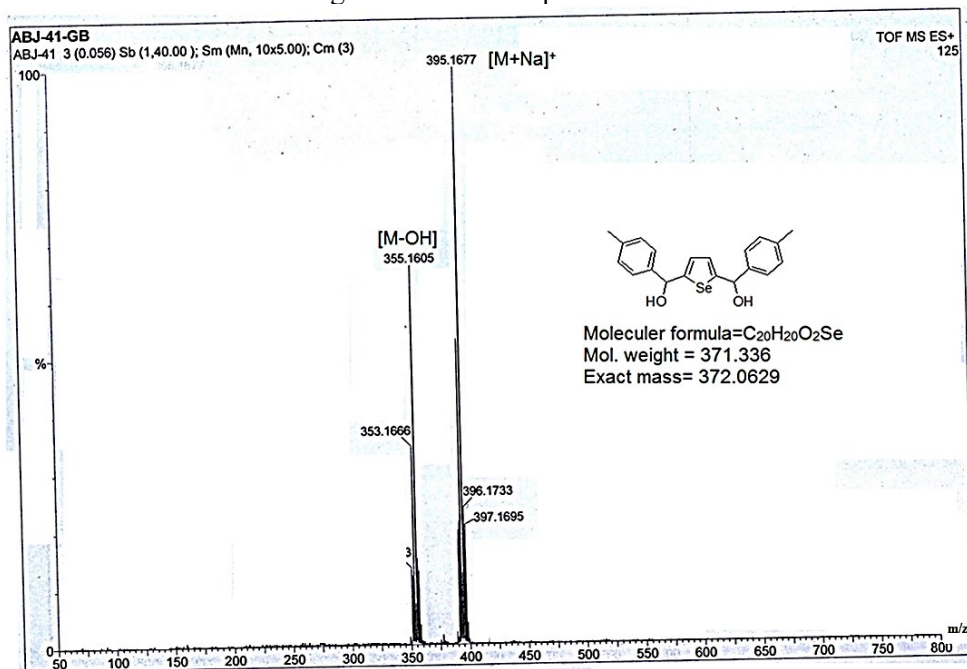


Figure S2. HRMS Spectra of 7

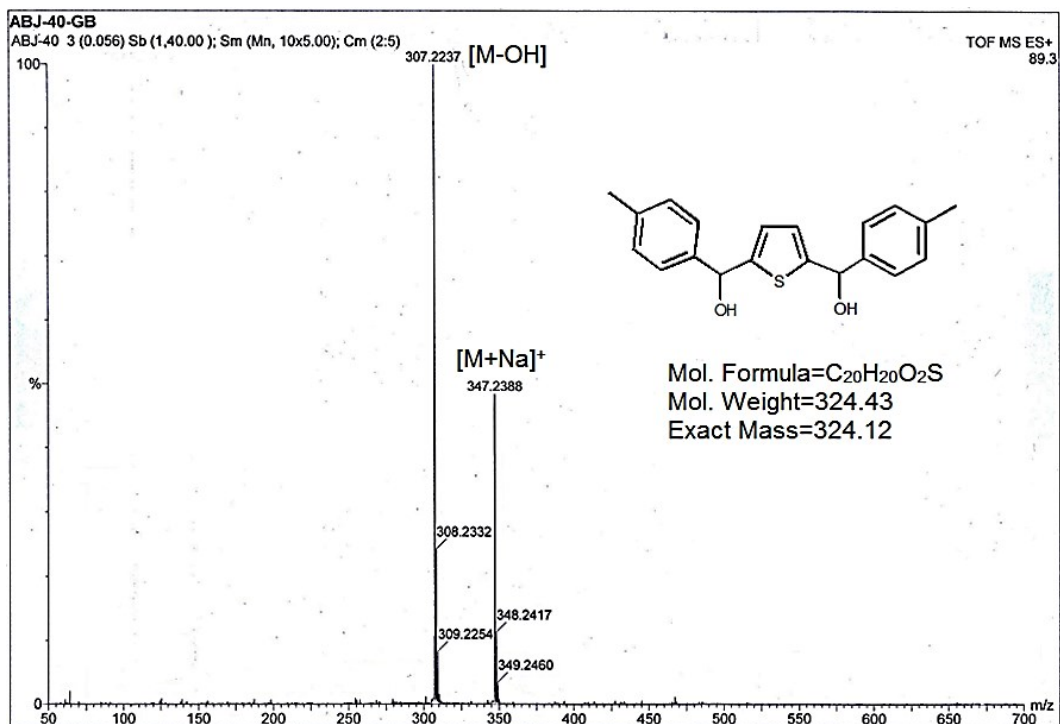


Figure S3. HRMS Spectra of **9**

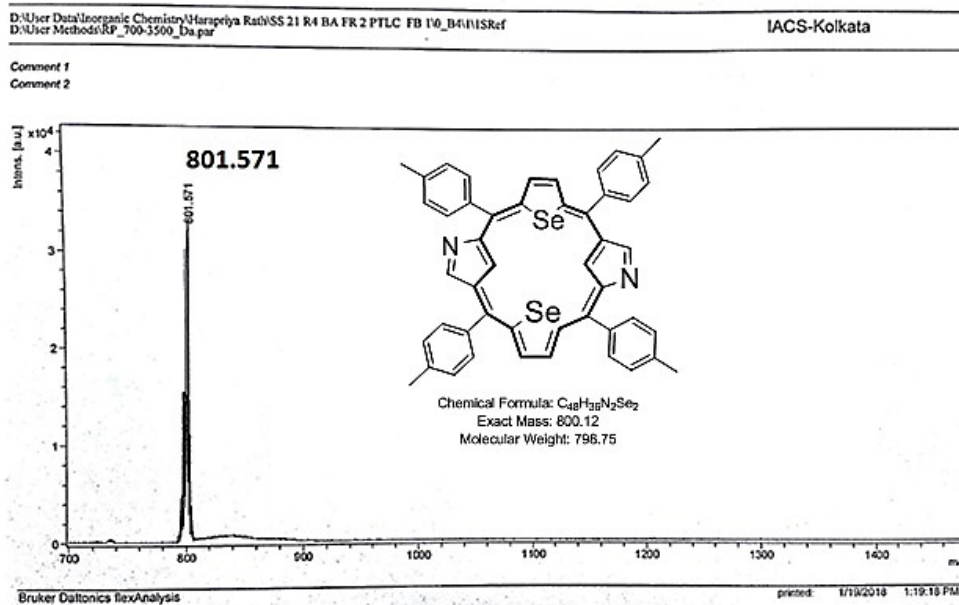


Figure S4. MALDI-TOF MS Spectra of **10**

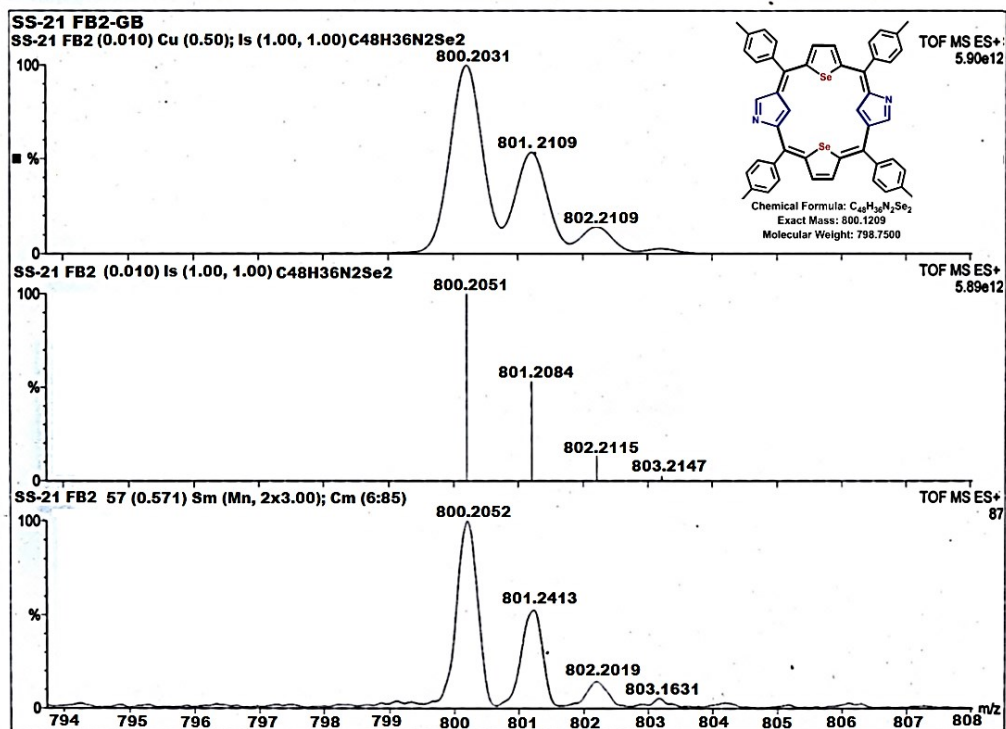


Figure S4a. HRMS Spectra of **10**

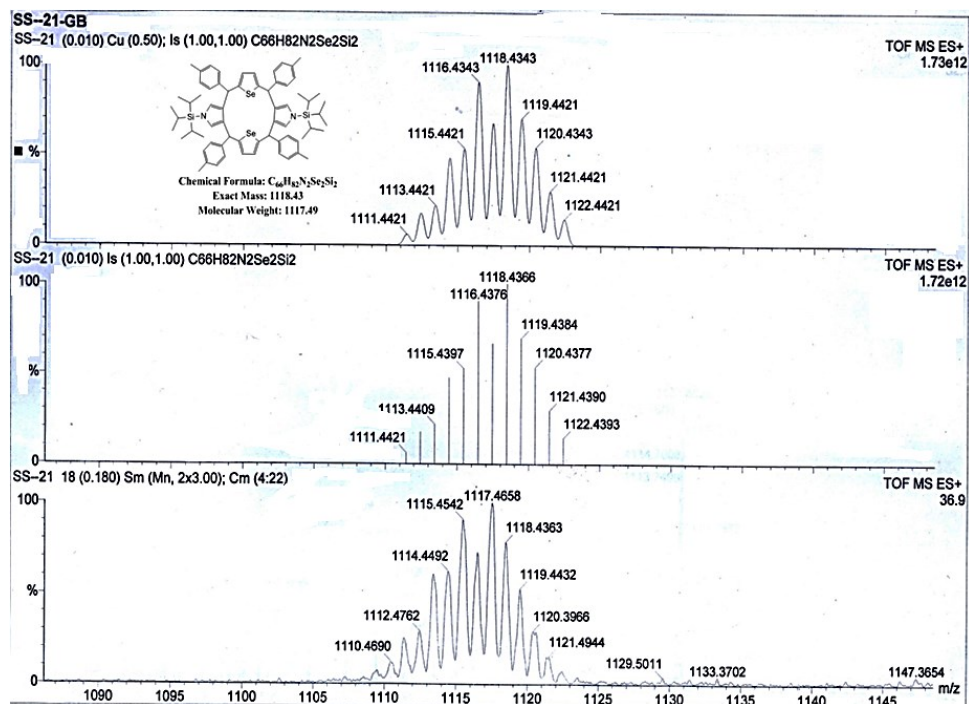


Figure S5. HRMS Spectra of **11**

Comment 1
Comment 2

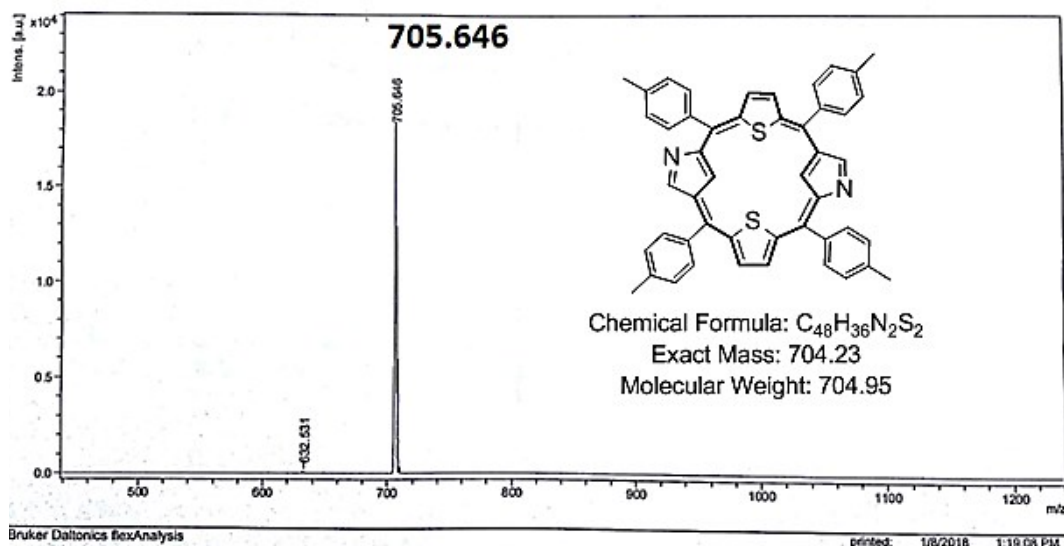


Figure S6. MALDI-TOF MS Spectra of **12**

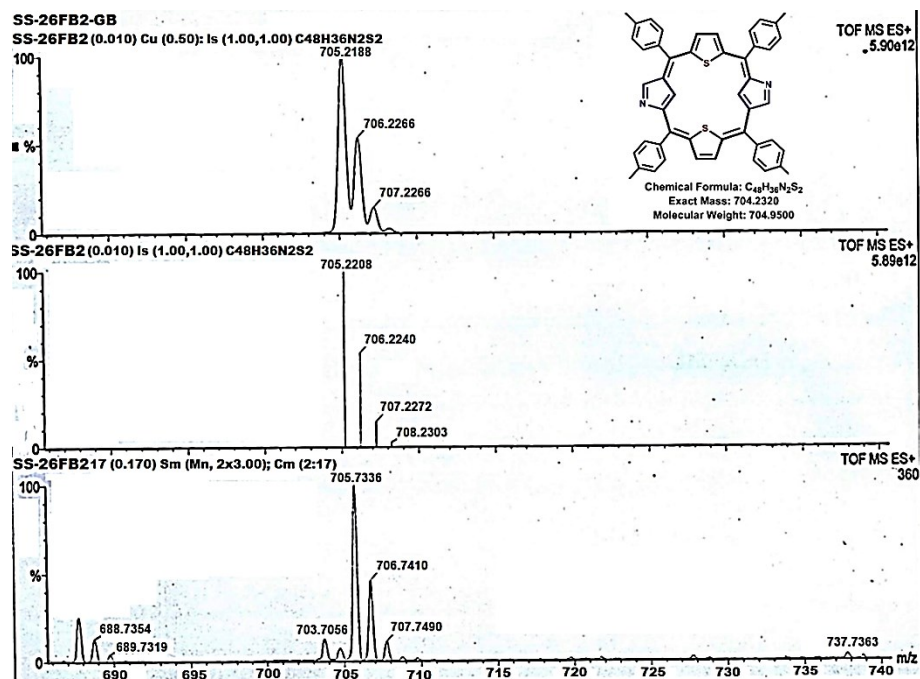


Figure S6a. HRMS Spectra of **12**

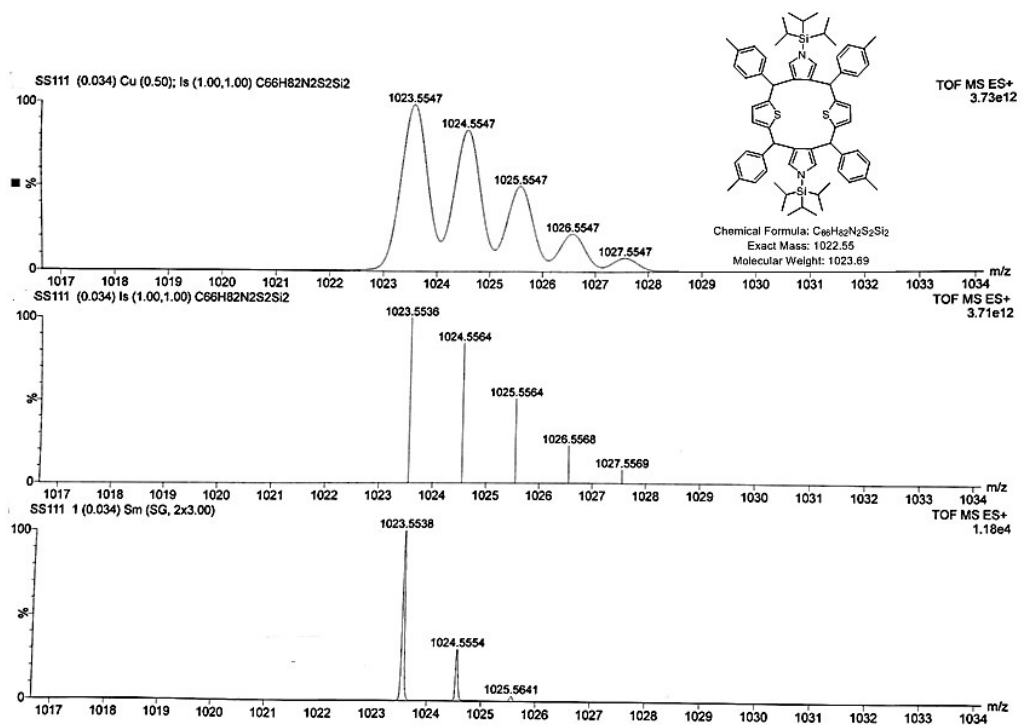


Figure S7. HRMS Spectra of **13**

2.2 Electronic Spectra:

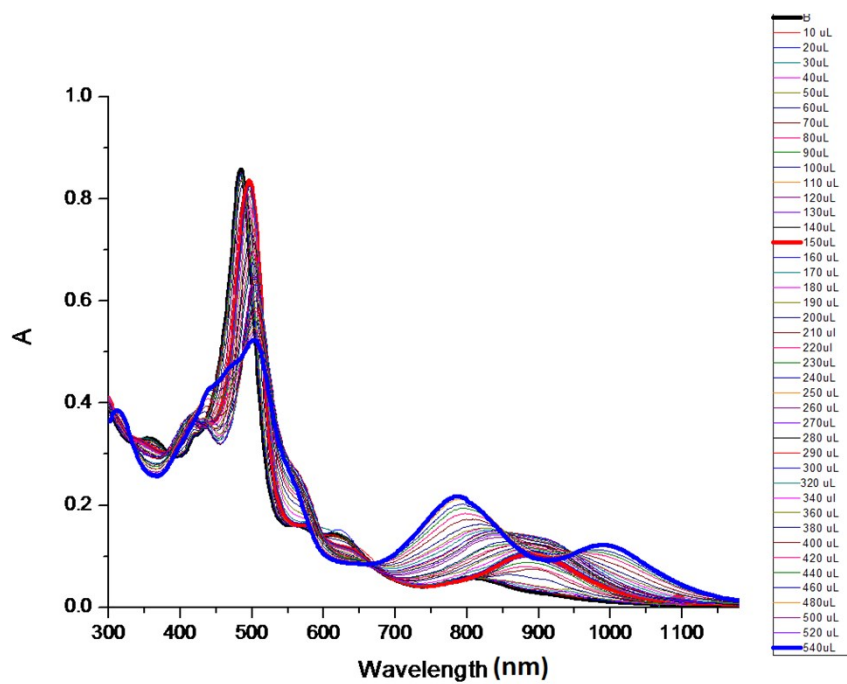


Figure S8. UV-vis-NIR acid titration study of **11** ($\text{CF}_3\text{COOH}/\text{CH}_2\text{Cl}_2$)

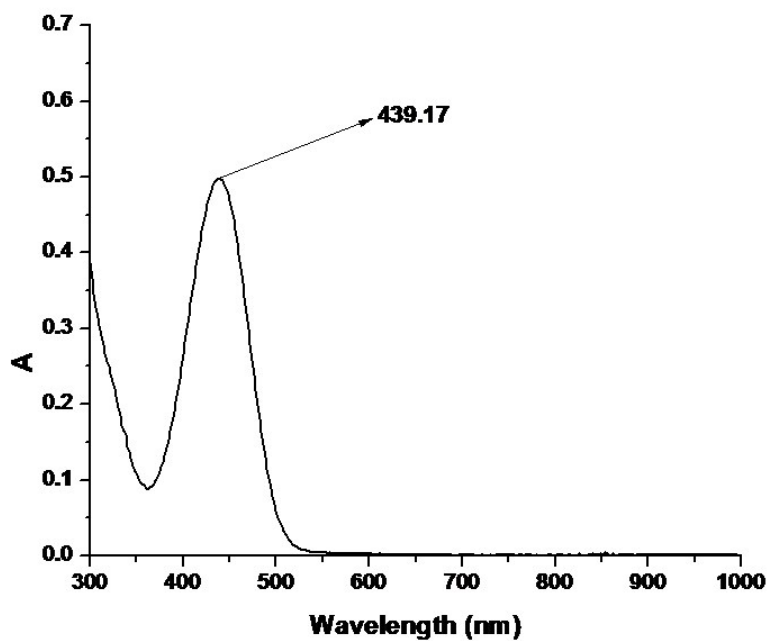


Figure S9. UV-vis spectrum of **11** in CH_2Cl_2

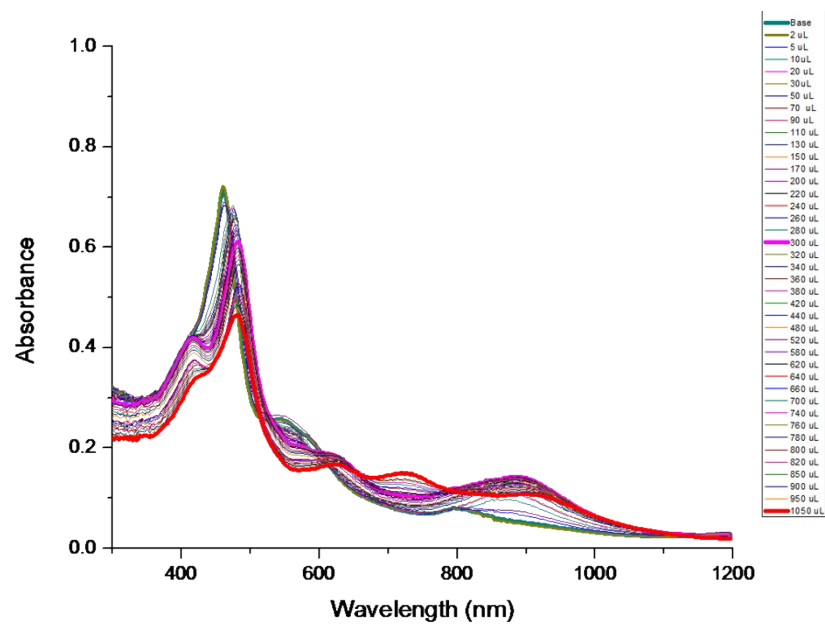


Figure S10. UV-vis-NIR acid titration study of **12** ($\text{CF}_3\text{COOH}/\text{CH}_2\text{Cl}_2$)

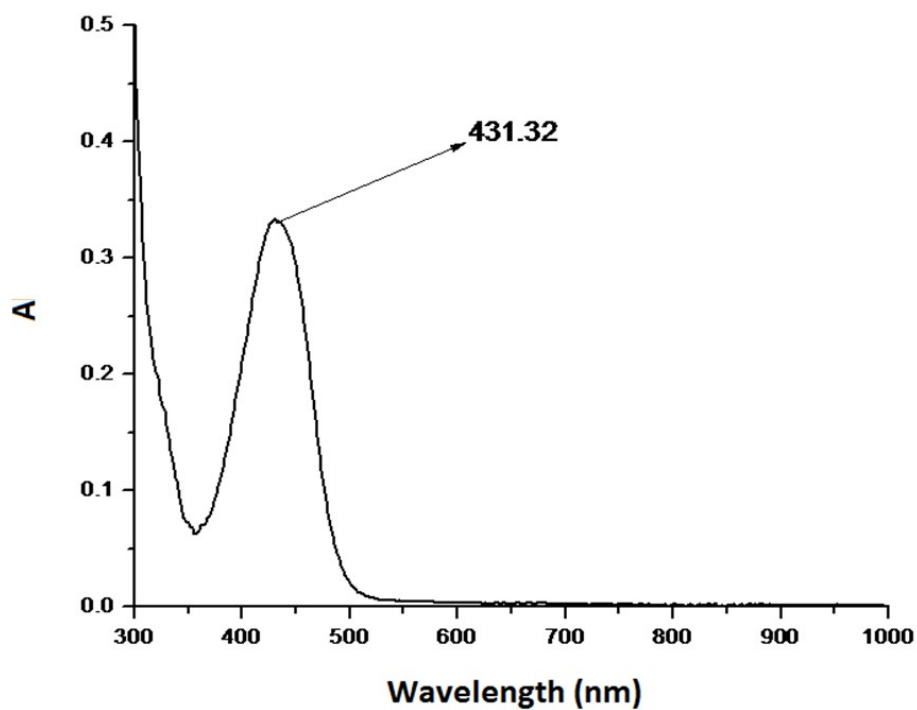


Figure S11. UV-vis spectrum of **13** in CH_2Cl_2

2.3 NMR spectra:

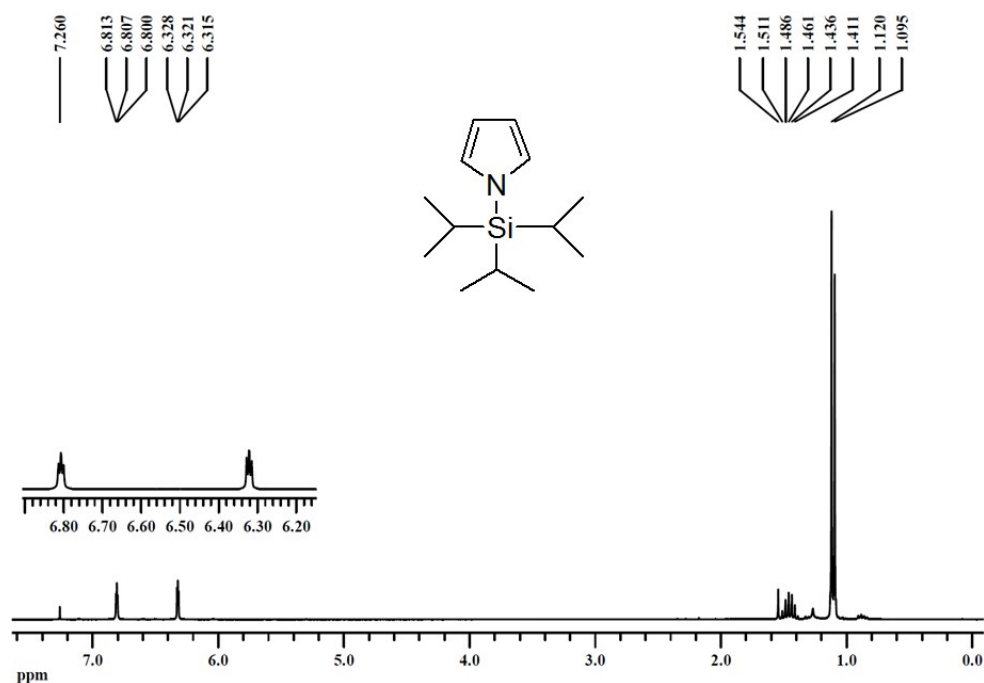


Figure S12. ¹H NMR spectrum of **5** in CDCl₃

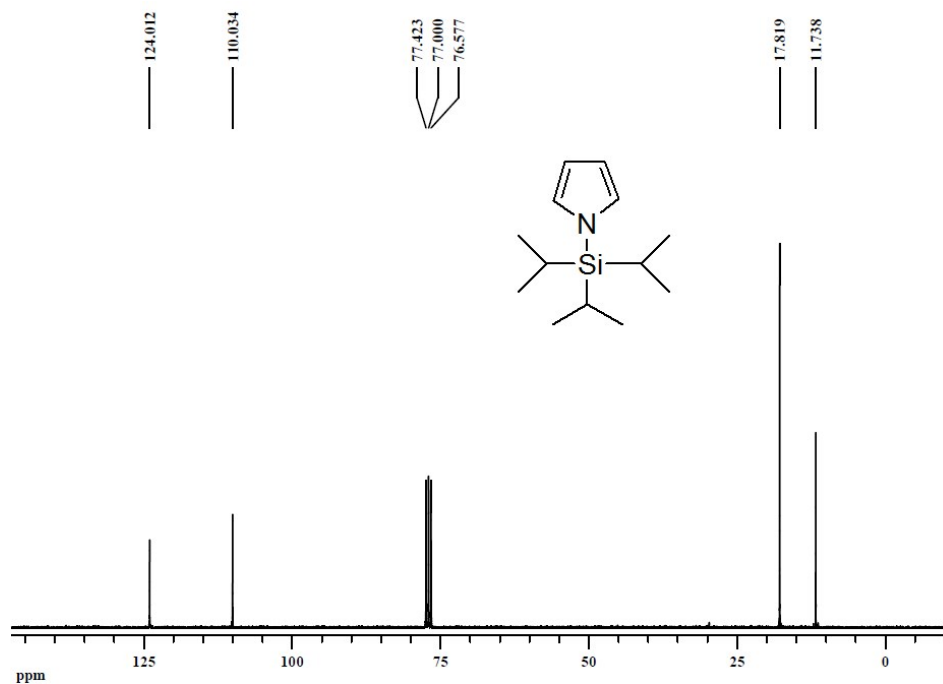


Figure S13. ¹³C NMR spectrum of **5** in CDCl₃

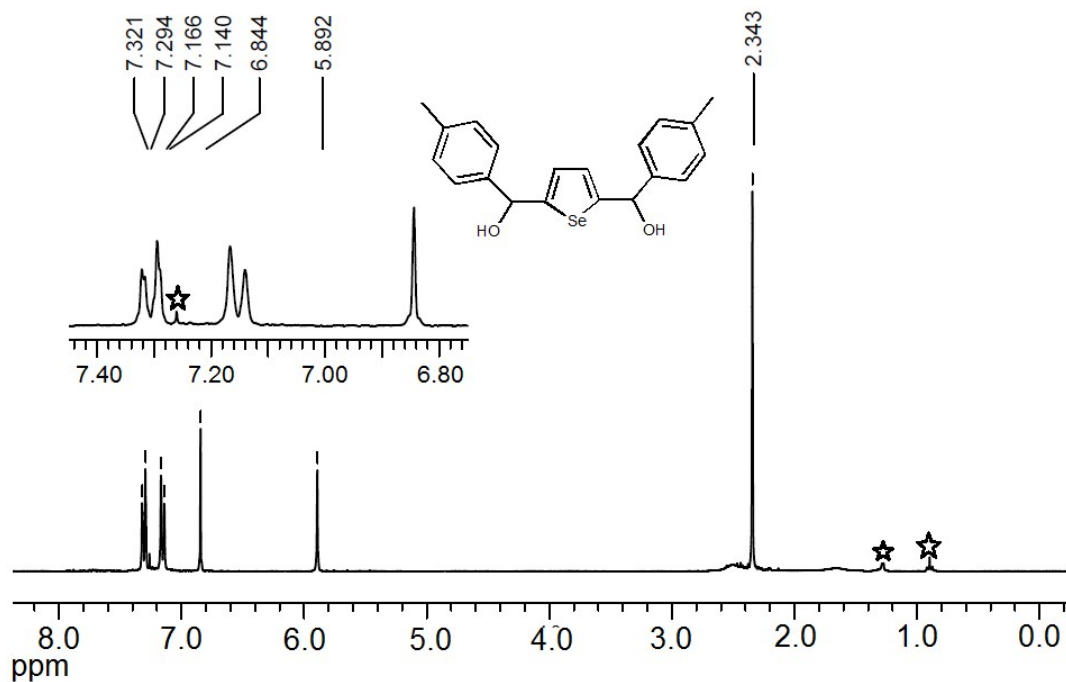


Figure S14. ¹H NMR spectrum of **7** in CDCl₃

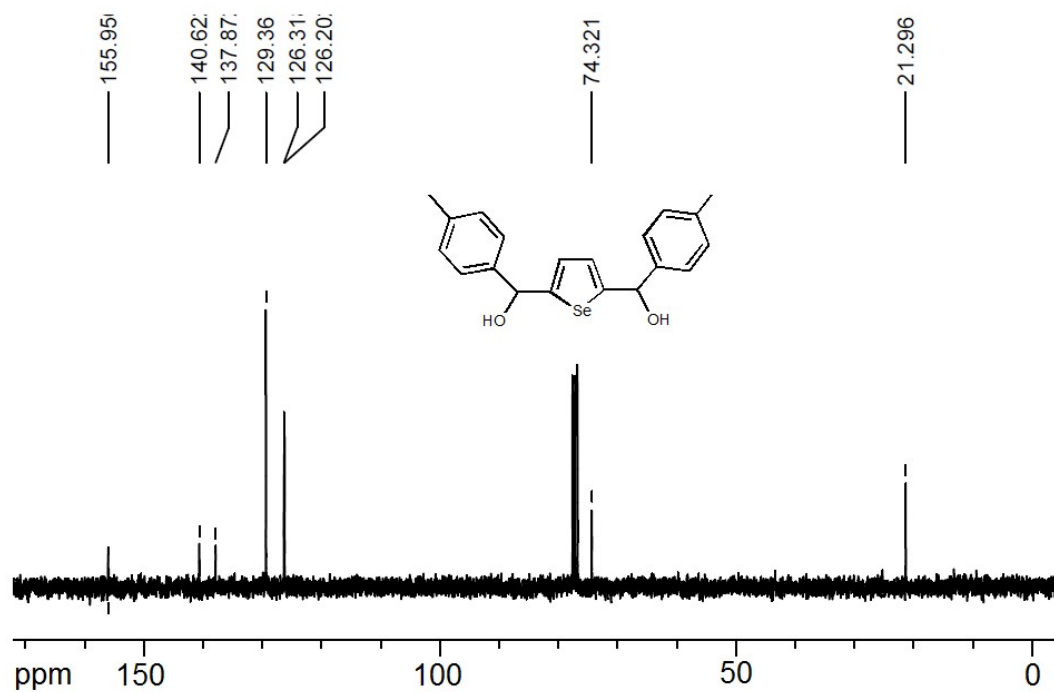


Figure S15. ¹³C NMR spectrum of **7** in CDCl₃

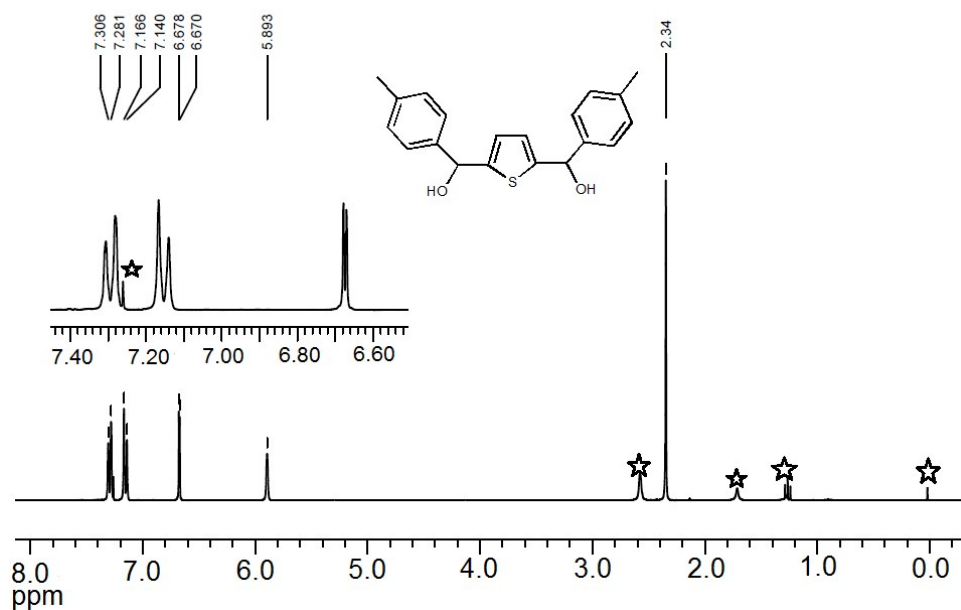


Figure S16. ¹H NMR spectrum of **9** in CDCl₃

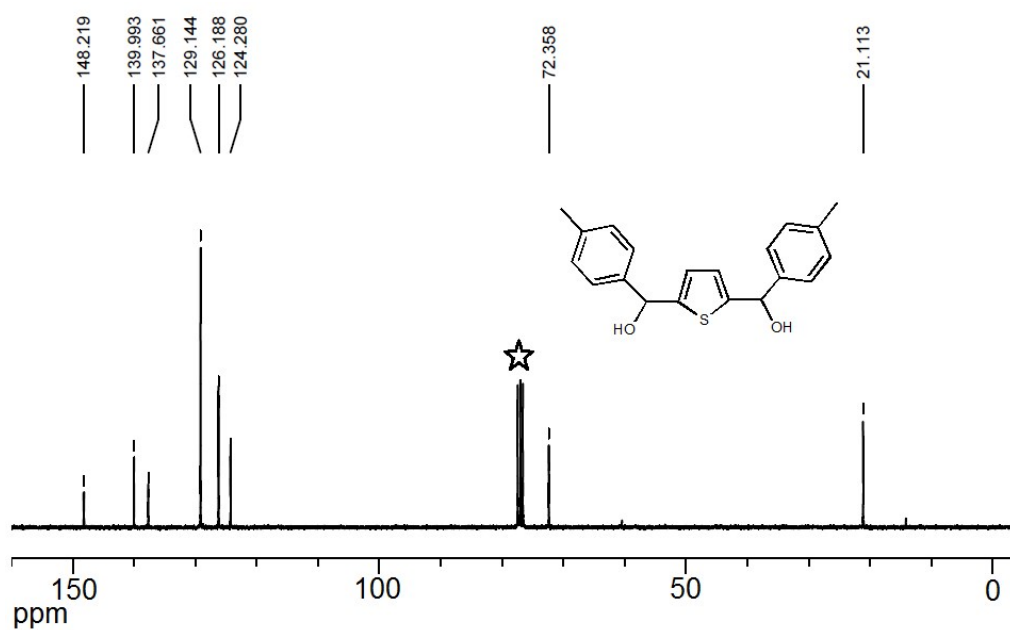


Figure S17. ¹³C NMR spectrum of **9** in CDCl₃

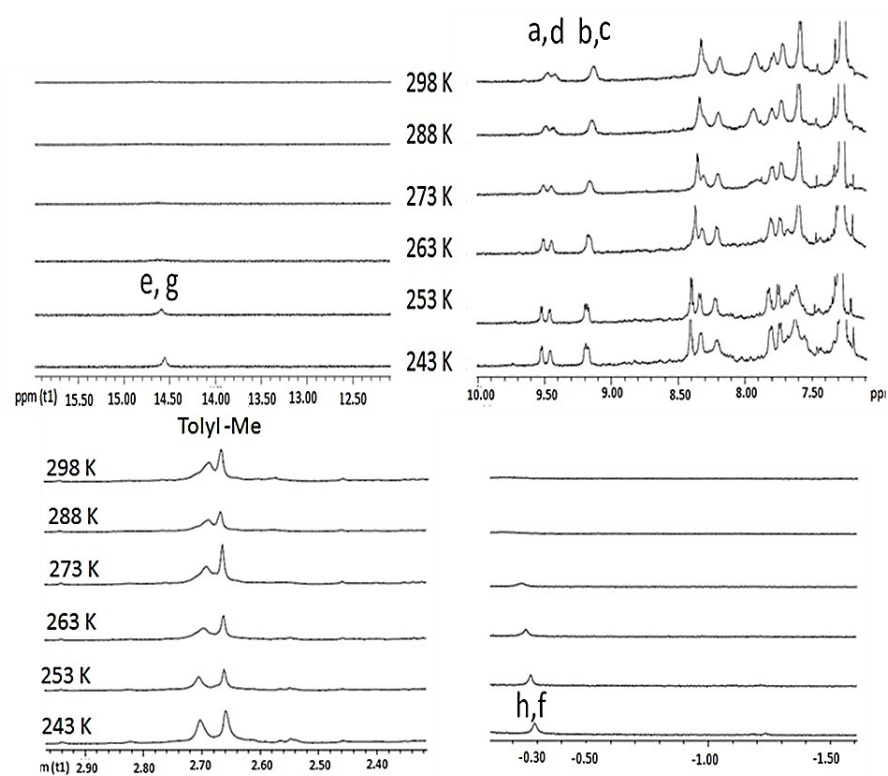


Figure S18. Variable Temperature ^1H NMR spectra of **10** in CDCl_3

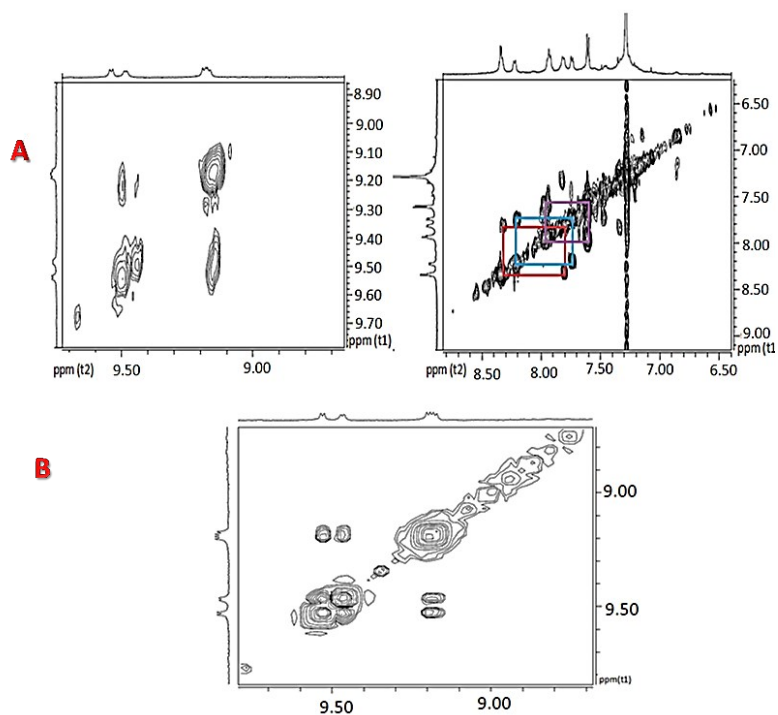


Figure S19. ^1H - ^1H 2D COSY NMR spectra of **10** in CDCl_3 (A: 298 K; B: 253 K)

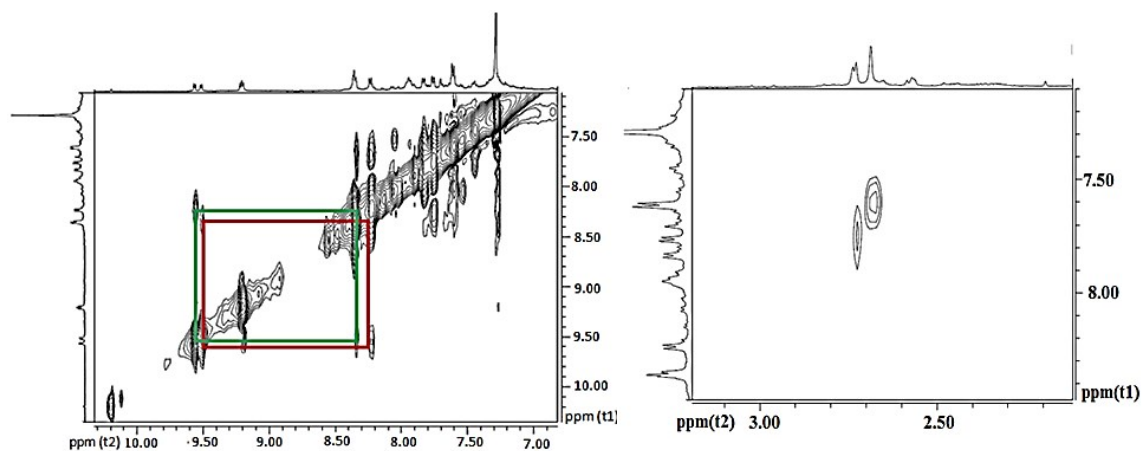


Figure S20. ^1H - ^1H 2D ROESY NMR spectra of **10** in CDCl_3 at 298 K

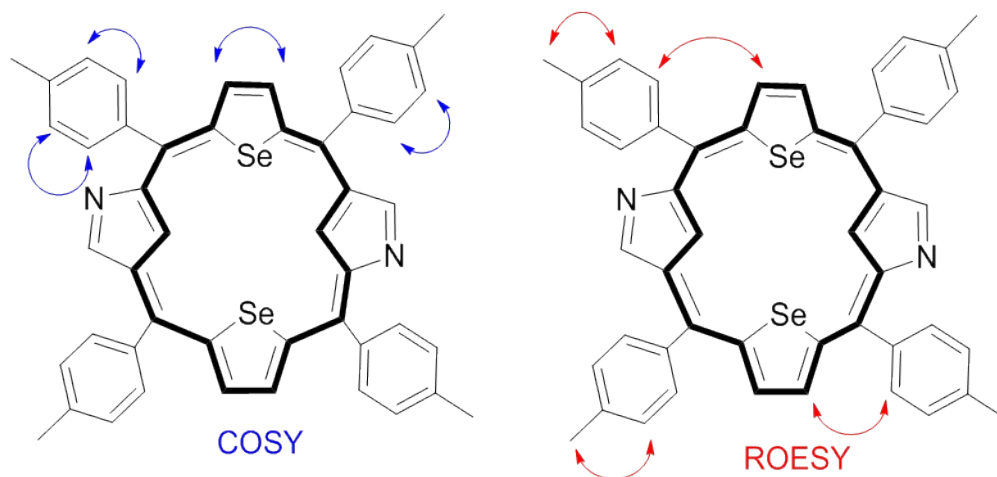


Figure S21. Various Scalar and Dipolar couplings observed in **10** in CDCl_3

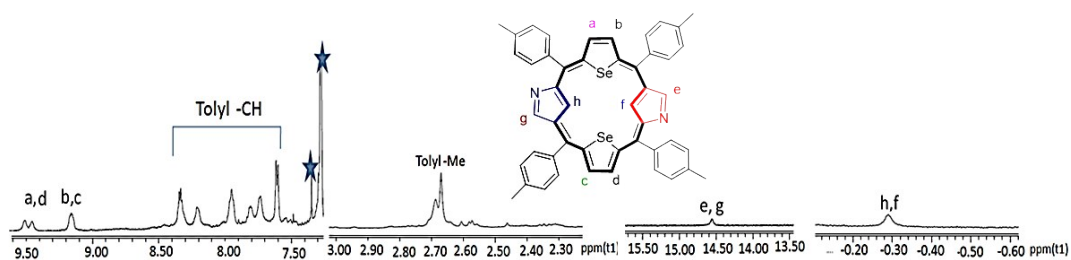


Figure S22. Completely assigned ^1H NMR spectra of **10** in CDCl_3

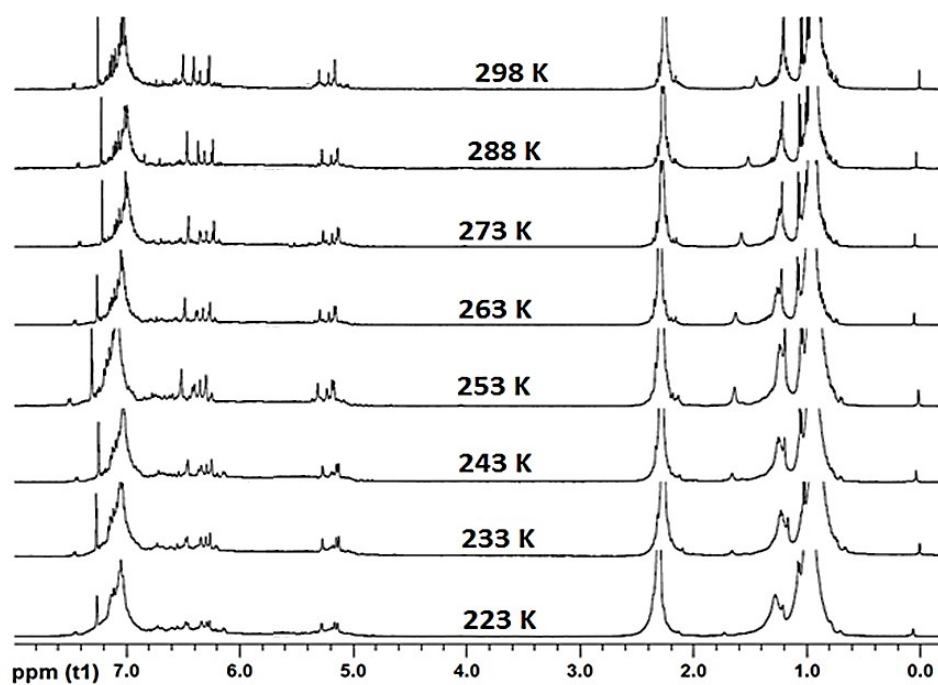


Figure S23. Variable Temperature ^1H NMR spectra of **11** in CDCl_3

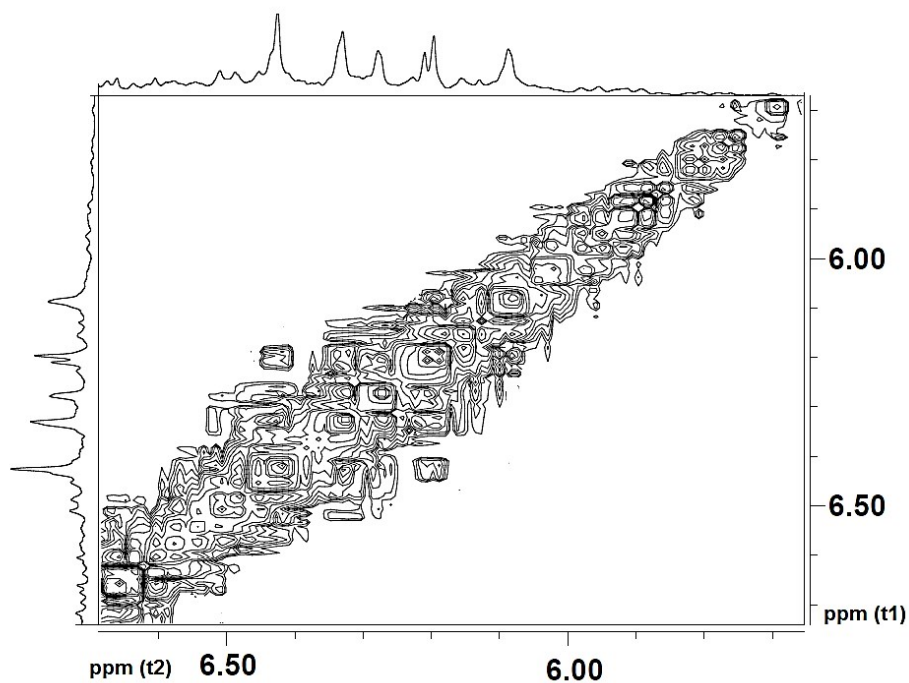


Figure S24. ^1H - ^1H 2D COSY spectra of **11** in CDCl_3 at 298 K

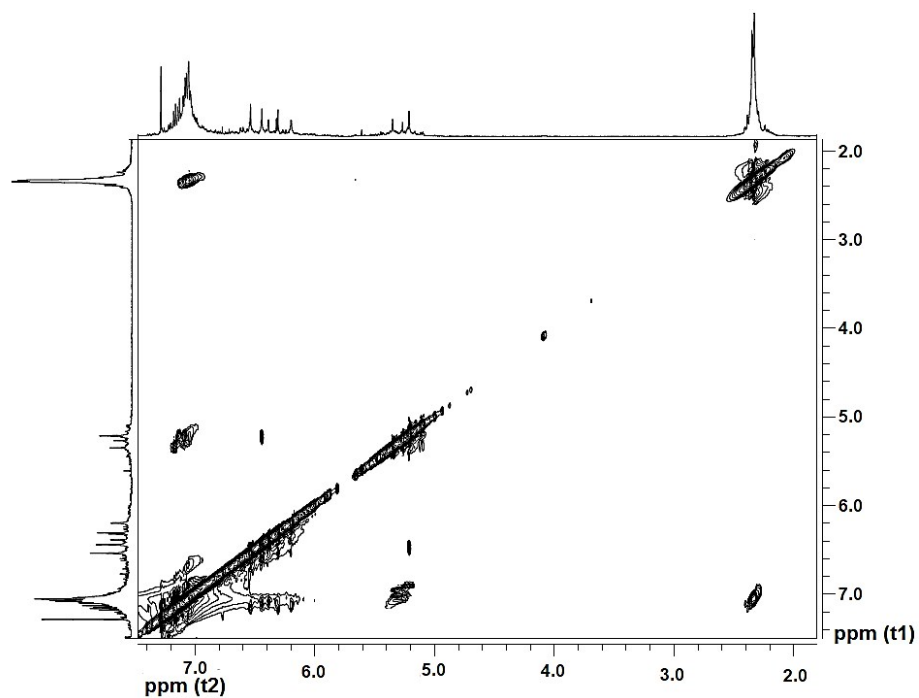


Figure S25. ^1H - ^1H 2D ROESY spectra of **11** in CDCl_3 at 298 K

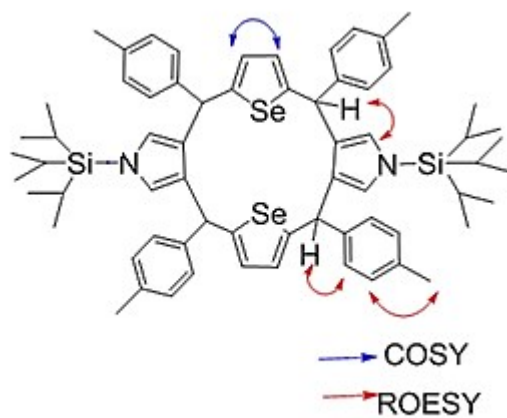


Figure S26. Various scalar and dipolar couplings observed in **11** at 298 K

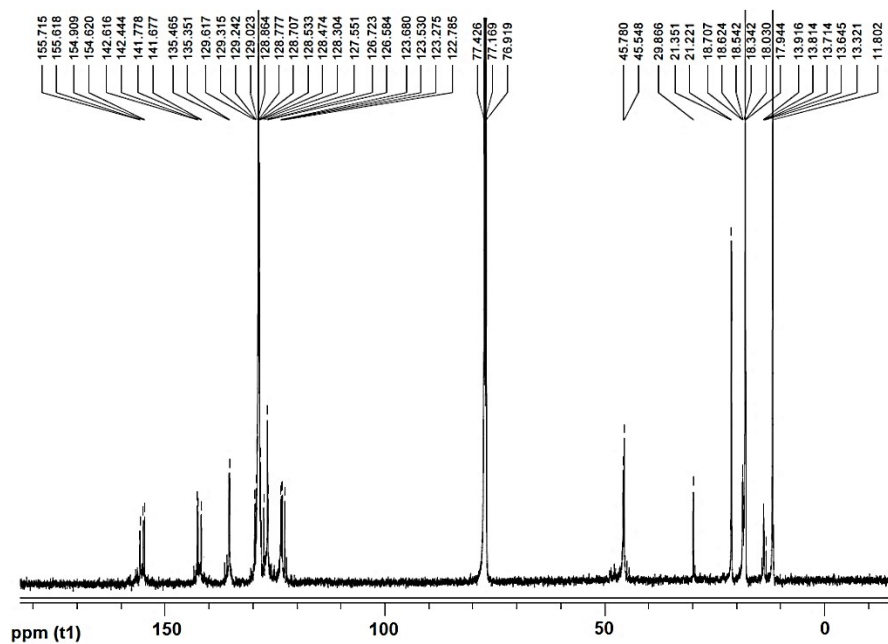


Figure S27. ^{13}C NMR spectra of **11** in CDCl_3 at 298 K

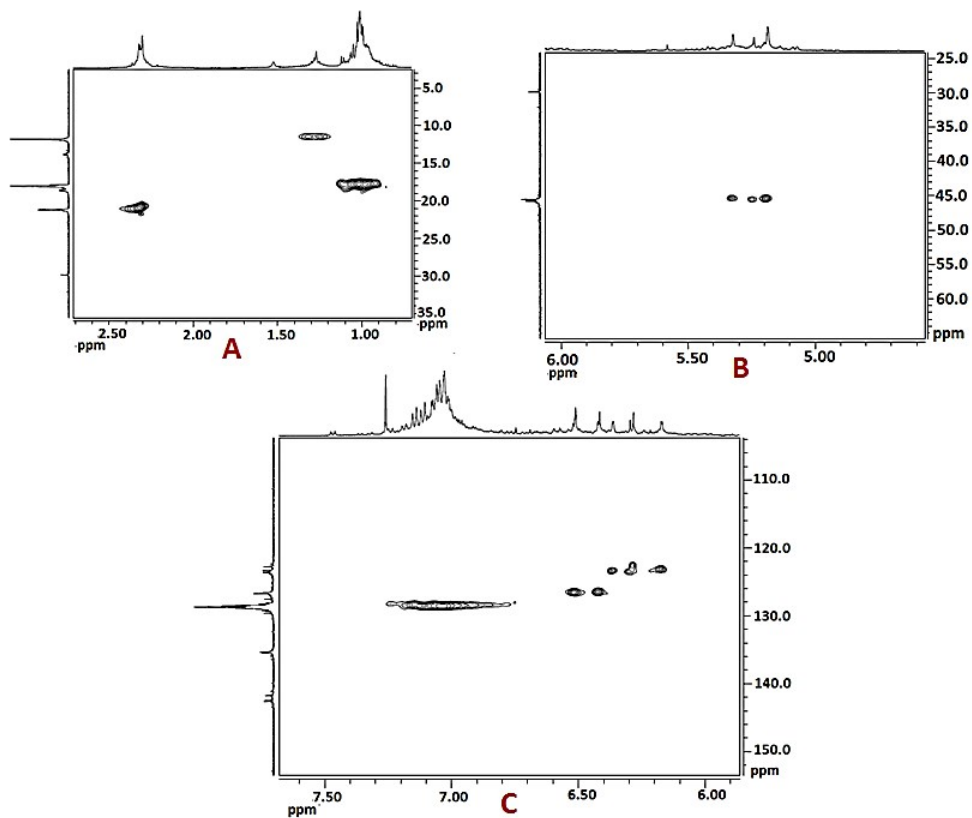


Figure S28. ^1H - ^{13}C 2D HSQC NMR spectra of **11** in CDCl_3 at 298 K

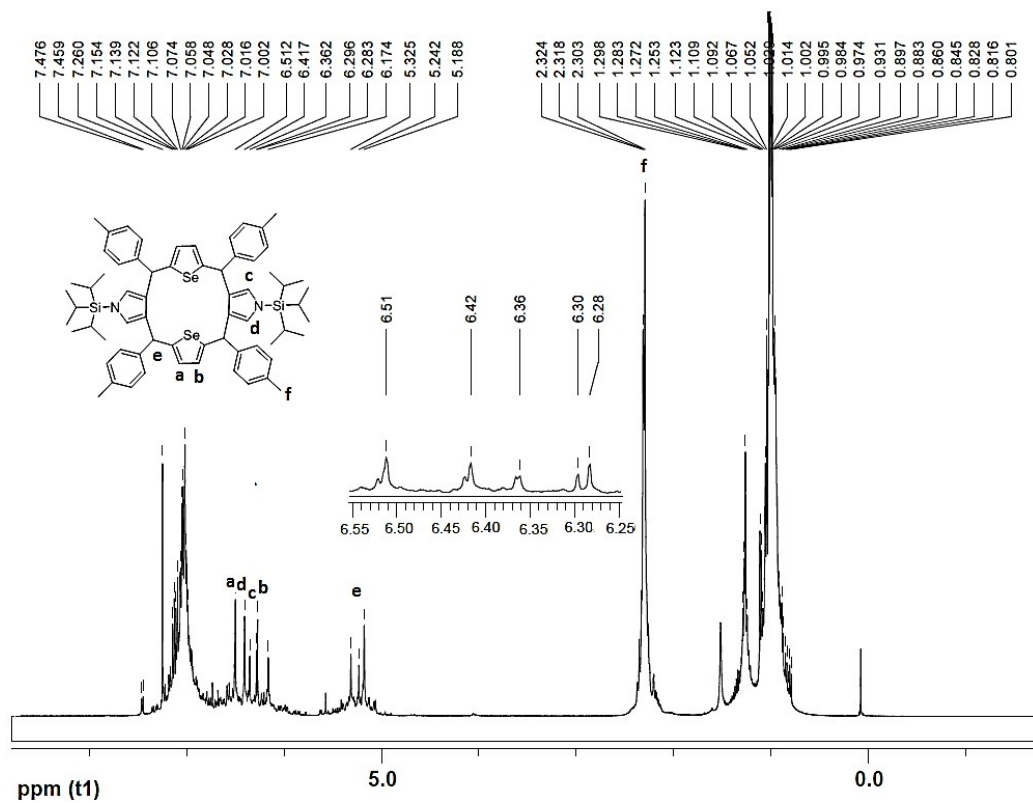


Figure S29. Completely assigned ^1H NMR spectra of **11** in CDCl₃ at 298 K

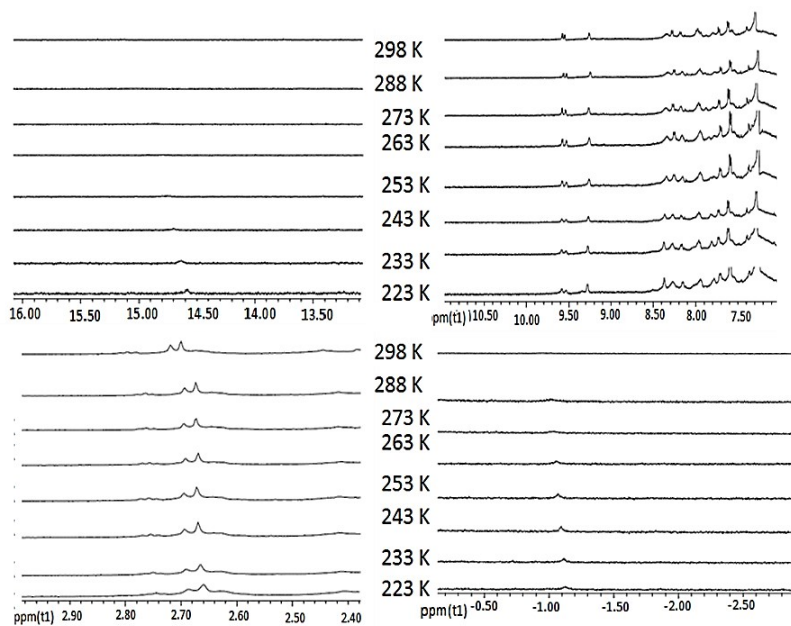


Figure S30. Variable Temperature ^1H NMR spectra of **12** in CDCl₃

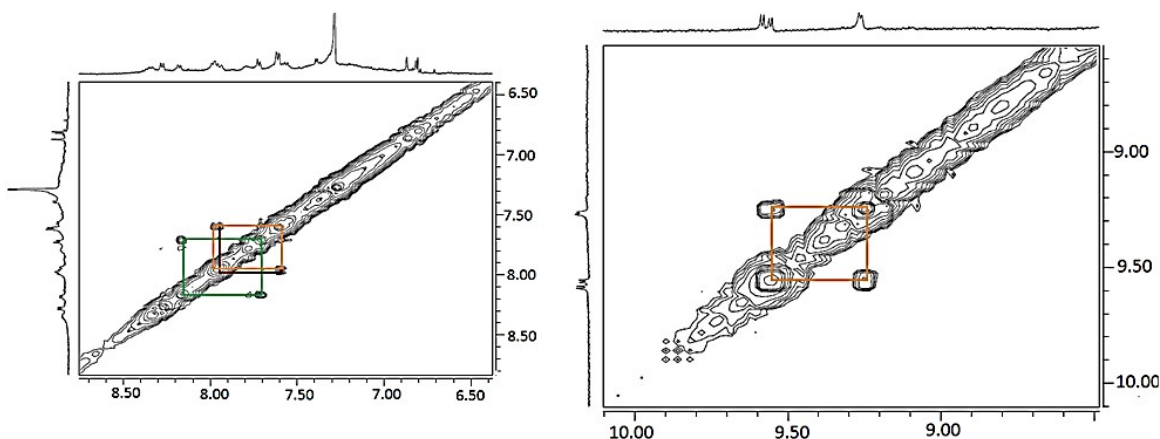


Figure S31. ^1H - ^1H 2D COSY NMR spectra of **12** in CDCl_3 at 298 K

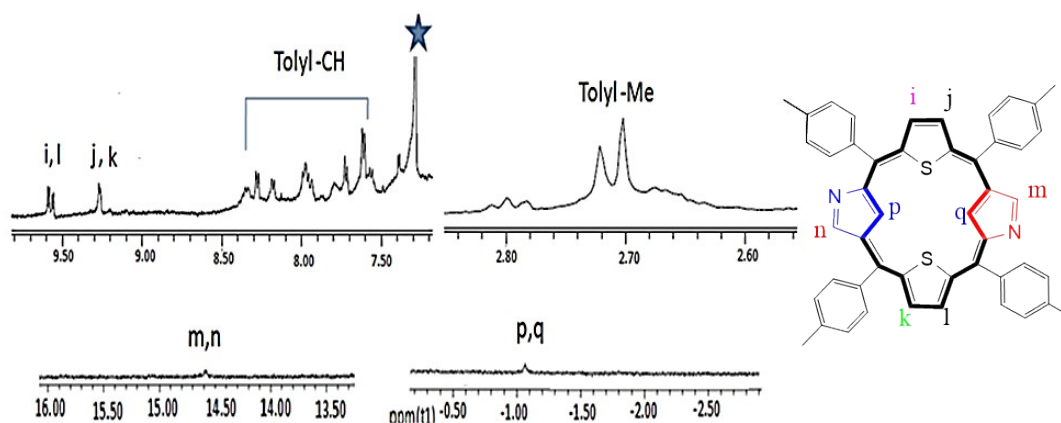


Figure S32. Completely assigned ^1H NMR spectra of **12** in CDCl_3 at 223 K

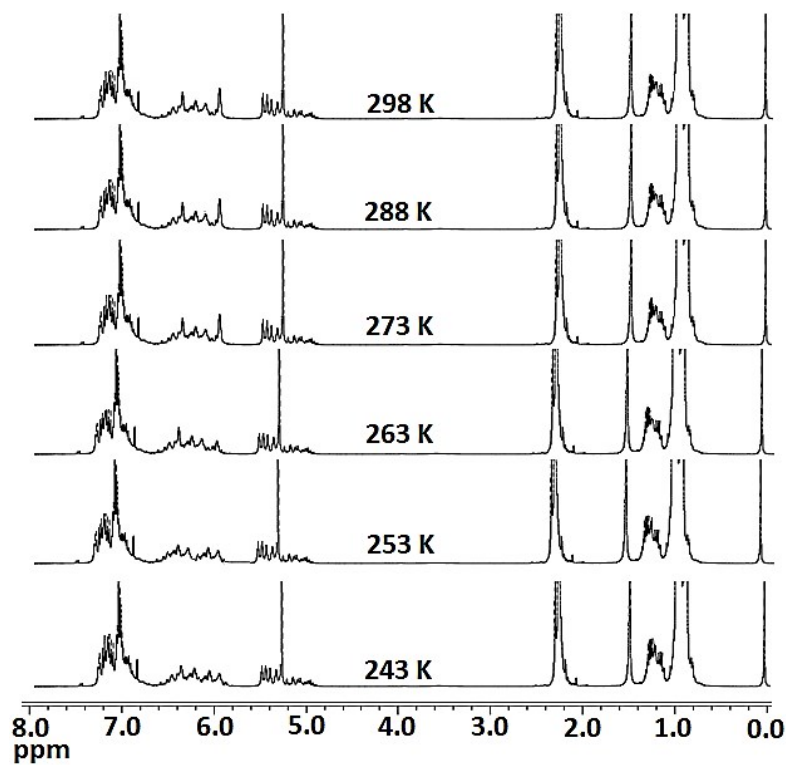


Figure S33. Variable Temperature ^1H NMR spectra of **13** in CD_2Cl_2

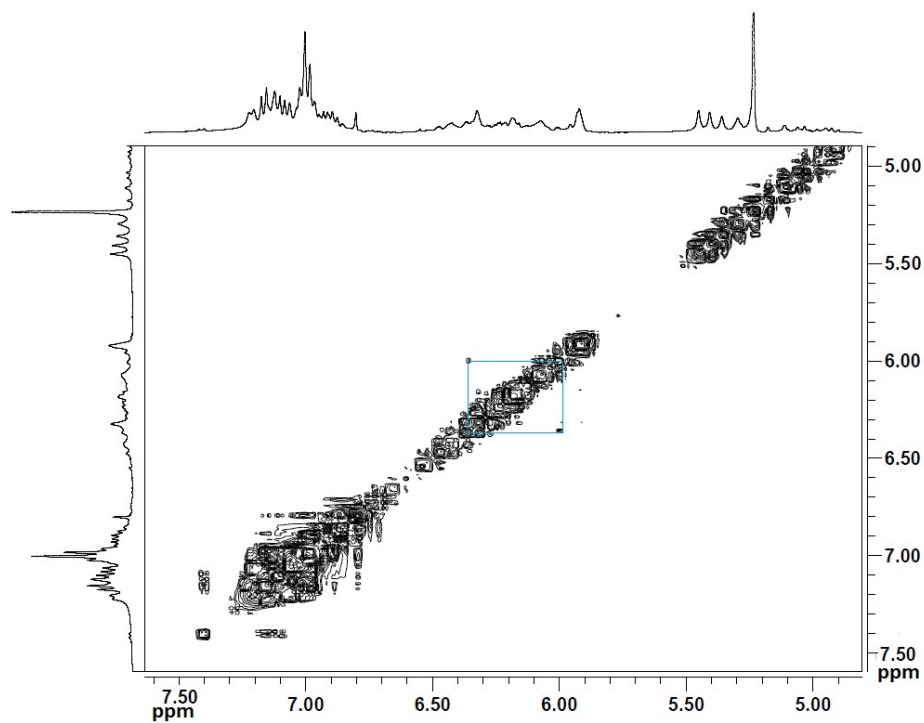


Figure S34. ^1H - ^1H 2D COSY NMR spectra of **13** in CD_2Cl_2 at 298 K

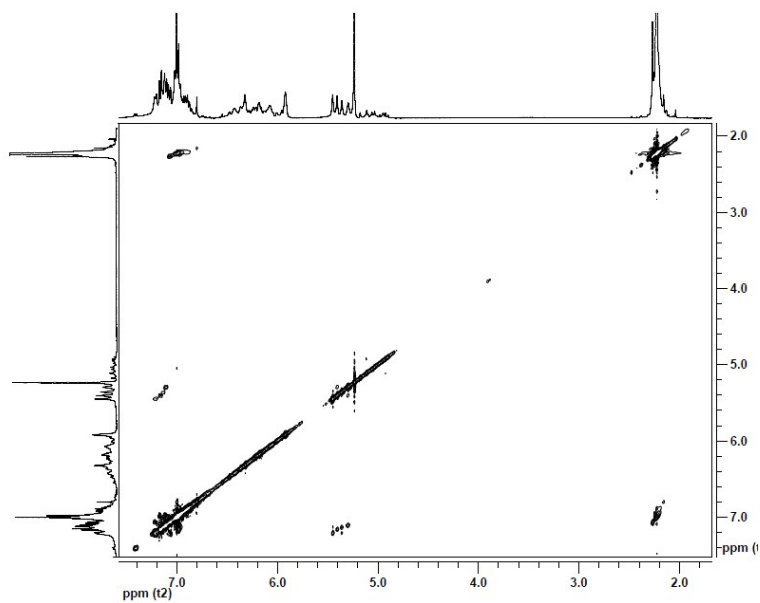


Figure S35. ^1H - ^1H 2D ROESY NMR spectra of **13** in CD_2Cl_2 at 298 K

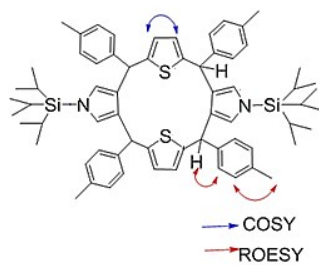


Figure S36. Various scalar and Dipolar couplings observed in **13**

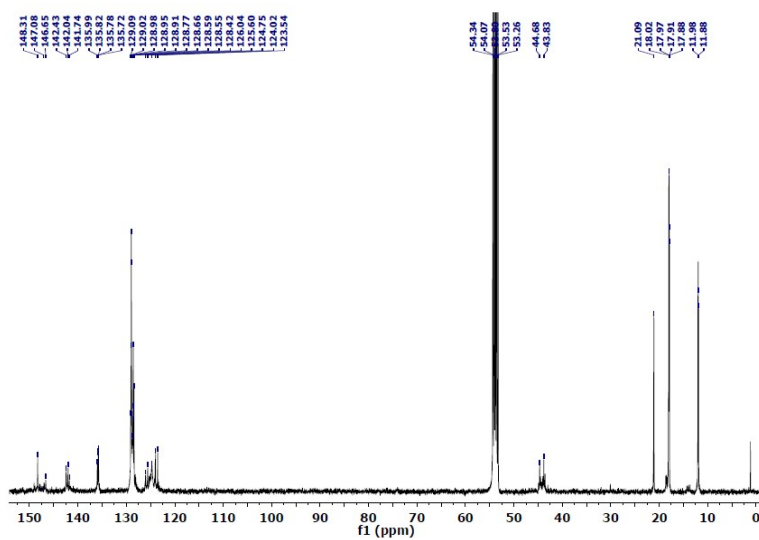


Figure S37. ^{13}C - NMR spectra of **13** in CD_2Cl_2 at 298 K

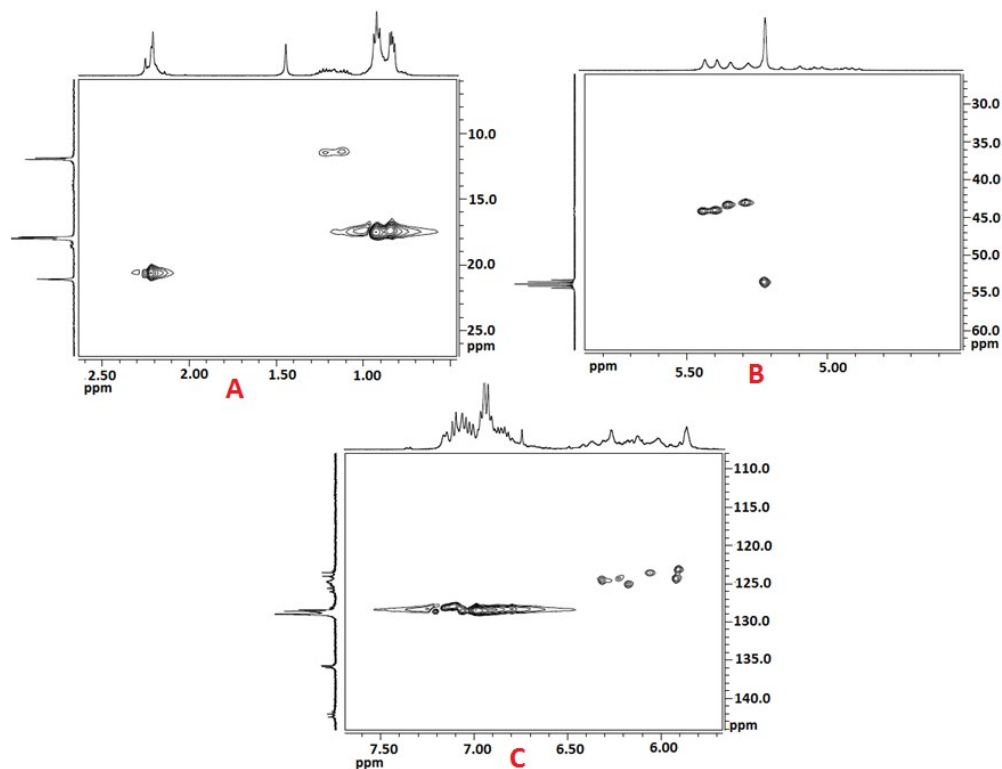


Figure S38. ^1H - ^{13}C 2D HSQC NMR spectra of **13** in CD_2Cl_2 at 298 K

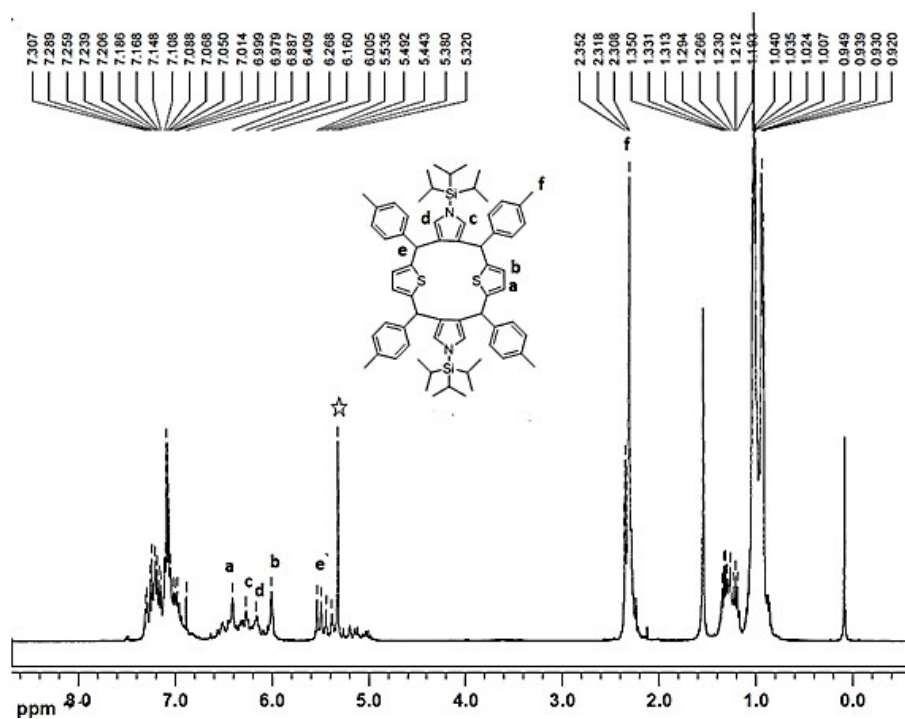


Figure S39. Completely assigned ^1H NMR spectra of **13** in CD_2Cl_2 at 298 K

2.4 Electrochemistry:

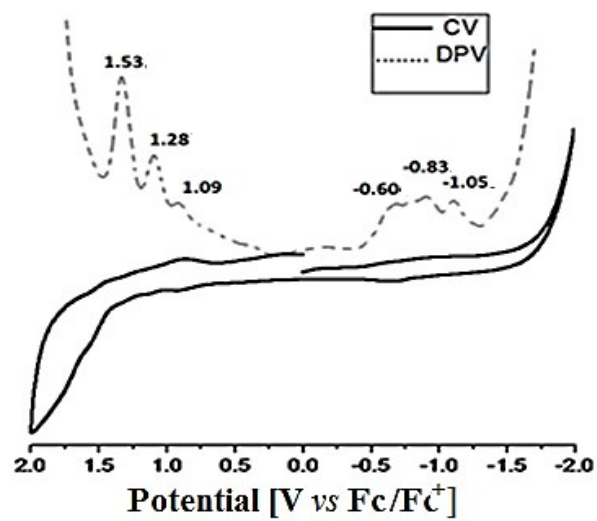


Figure S40. Cyclic Voltammogram of **10**

2.5 Theoretical Studies:

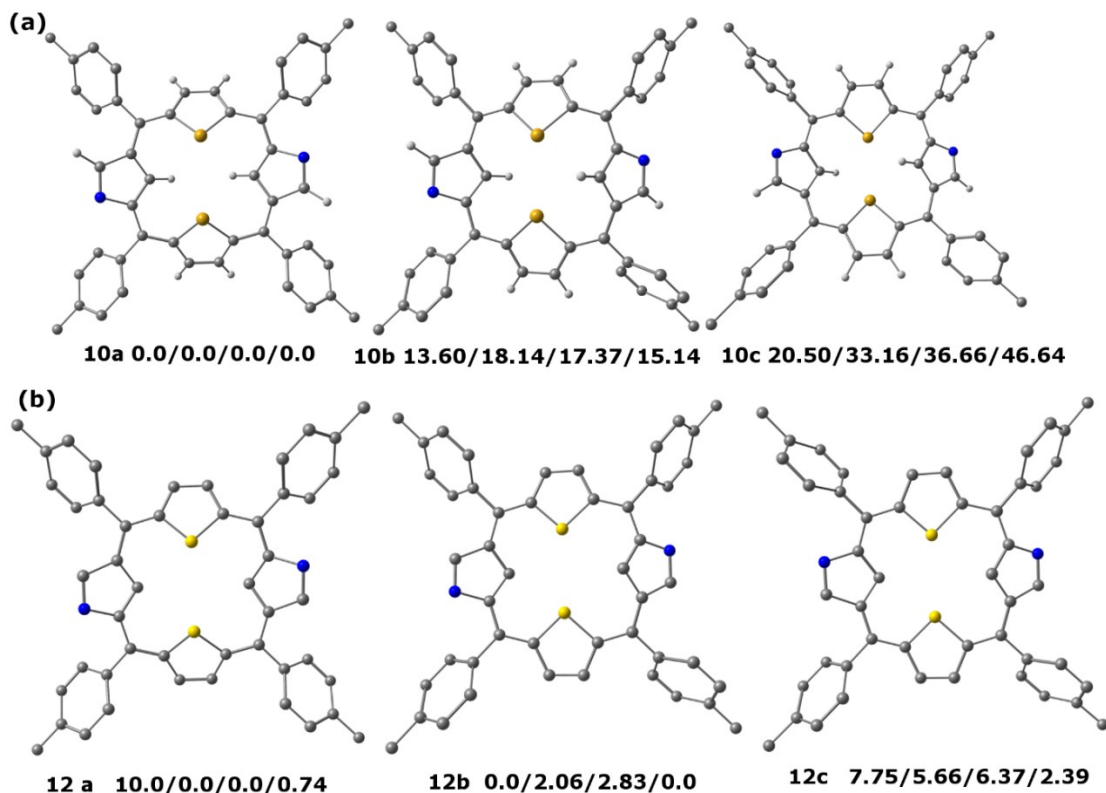


Figure S41. Plausible conformers of **10** (a) and **12** (b). The relative free energies (ΔG , kJ/mol) of conformers are obtained at B1b/B1c/B2/B2a level of theories. For the sake of clarity, the hydrogen atoms are omitted.

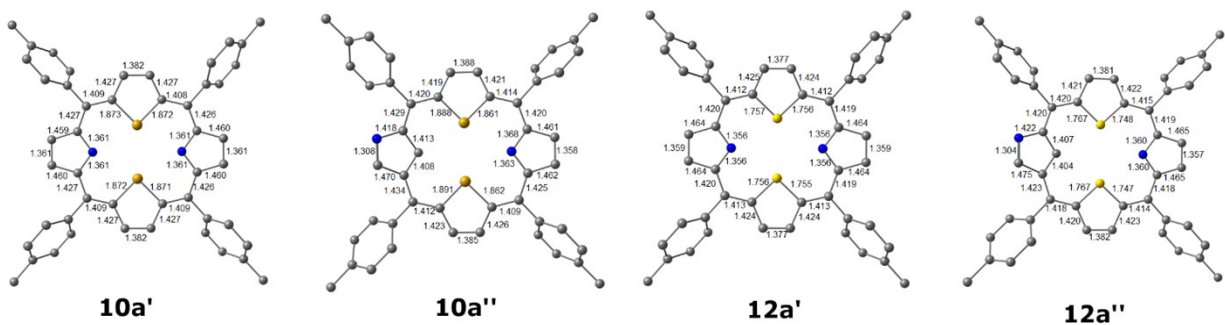


Figure S42. Key bond lengths for free base form of Diselena porphyrin (Se_2TTP , **10a'**), Diselena singly N-confused porphyrin (Se_2CTTP , **10a''**). The relative free energies (ΔG , kJ/mol) of **10a'** and **10a''** are 30.09 and 16.89 kcal/mol lower than Diselena doubly N-confused porphyrin, **10a**. Dithia porphyrin (S_2TTP , **12a'**) and Dithia singly N-confused porphyrin (S_2CTTP , **12a''**) are 30.01 and 14.67 kcal/mol lower than Dithia doubly N-confused porphyrin **12a** at B1b level of theory. For the sake of clarity, the hydrogen atoms are omitted.

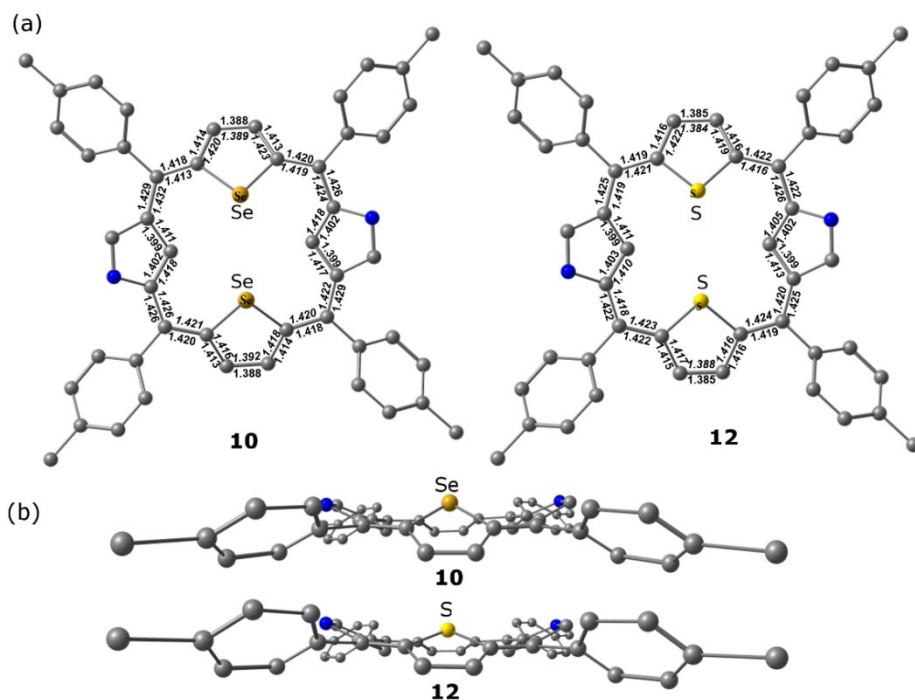


Figure S43. (a) Top view of optimised geometries and key bond length parameters (Å) of free base form of **10** and **12** at **B1c** and **B1b** level of theory. (b) Side view of free base form of **10** and **12**. For the sake of clarity the hydrogen atoms are not shown here.

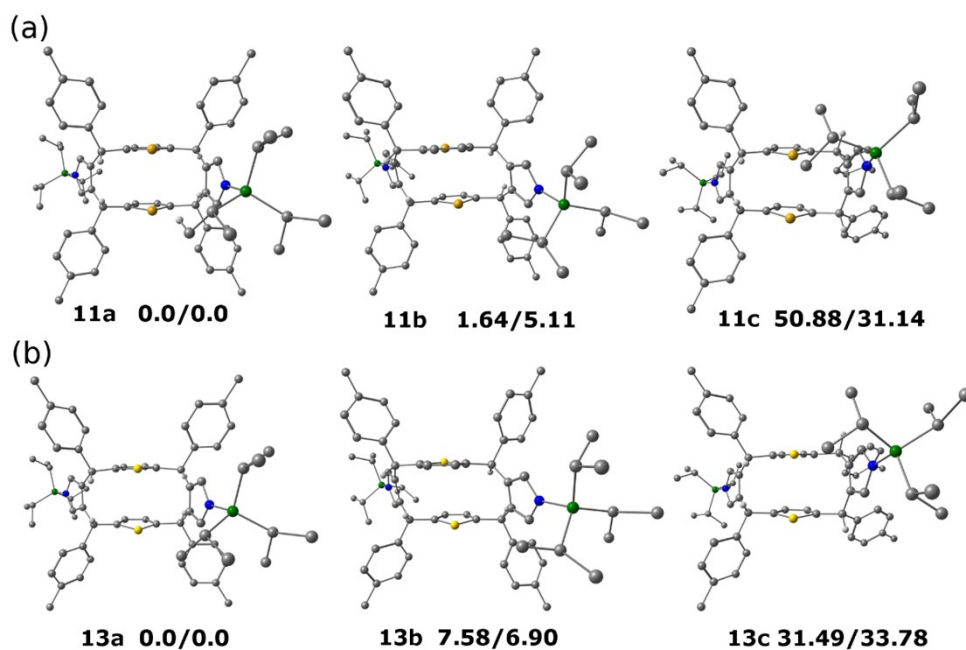


Figure S44. Plausible conformers of **11** and **13**. The relative free energies (ΔG , kJ/mol) of conformers are obtained at B1b/B2 level of theory.

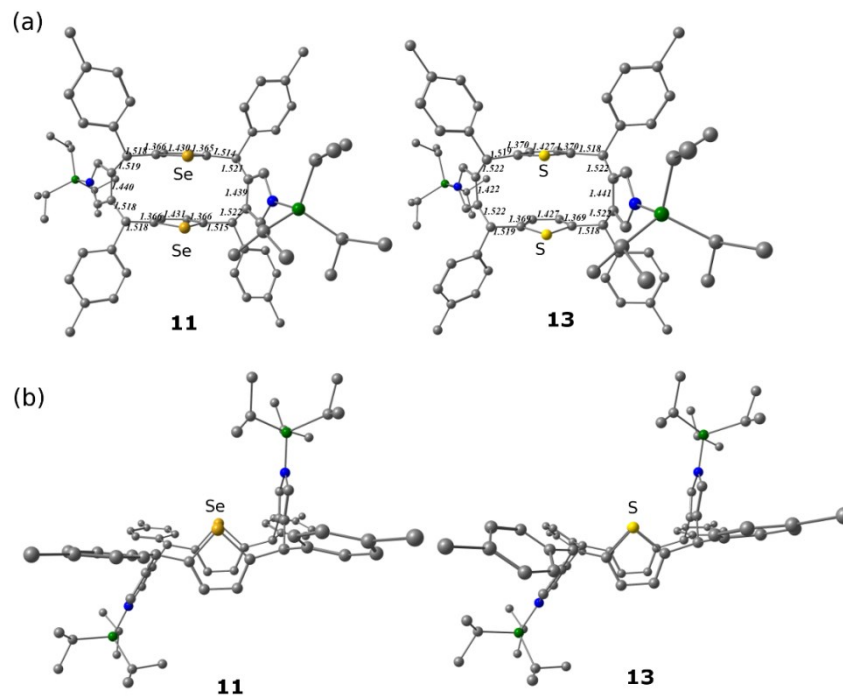


Figure S45. (a) Top view of optimised geometries and key bond length parameters (Å) of free base form of **11** and **13** at **B1b** level of theory. (b) Side view of free base form of **11** and **13**. For the sake of clarity the hydrogen atoms are not shown here.

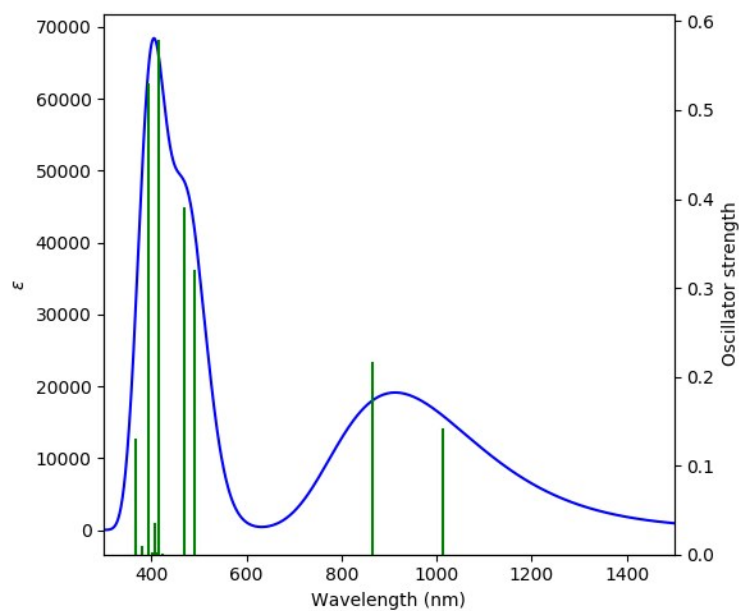


Figure S46. TD-DFT absorption spectrum of free base form of **10** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below. Note that we observe lone pair orbital of Selenium transition to eg orbitals. Mixing of these orbitals in a_{2u} orbitals too.

Table S1. Summary of UV-vis spectral data of free base form of **10**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	9864.161	1013.771	0.1418	Singlet-A	HOMO->LUMO (93%)
2	11545.83	866.1138	0.216	Singlet-A	HOMO->L+1 (93%)
3	19082.27	524.0466	0.0001	Singlet-A	HOMO->L+2 (94%)
4	20405.83	490.0561	0.3195	Singlet-A	H-1->LUMO (45%), H-1->L+1 (39%)
5	21292.23	469.6549	0.3905	Singlet-A	H-1->LUMO (45%), H-1->L+1 (44%)
6	22384.31	446.7416	0.0003	Singlet-A	H-5->LUMO (20%), H-2->LUMO (76%)
7	23565.1	424.3563	0.0008	Singlet-A	H-4->LUMO (48%), HOMO->L+3 (33%)
8	23843.36	419.4039	0.0002	Singlet-A	H-5->LUMO (15%), H-4->L+1 (32%), H-2->L+1 (37%)
9	24018.38	416.3477	0.5795	Singlet-A	H-3->LUMO (85%)
10	24188.57	413.4184	0.0025	Singlet-A	H-4->LUMO (20%), H-4->L+1 (21%), HOMO->L+3 (43%)
11	24546.68	407.3871	0.0355	Singlet-A	H-6->LUMO (77%), H-3->L+1 (10%)
12	24753.16	403.9889	0.0002	Singlet-A	H-5->LUMO (29%), H-2->L+1 (43%)
13	24884.62	401.8546	0.0023	Singlet-A	H-5->LUMO (20%), H-4->LUMO (19%), H-4->L+1 (34%)
14	25466.96	392.6657	0.5299	Singlet-A	H-3->L+1 (81%)
15	26152.53	382.3722	0	Singlet-A	H-7->LUMO (18%), H-5->L+1 (68%)
16	26317.87	379.9699	0.0094	Singlet-A	H-6->L+1 (54%), HOMO->L+4 (40%)
17	26575.97	376.2798	0	Singlet-A	H-8->LUMO (35%), H-7->LUMO (29%), H-5->L+1 (10%)
18	27128.46	368.6166	0.0002	Singlet-A	H-8->LUMO (36%), H-7->LUMO (42%)
19	27158.3	368.2115	0.0358	Singlet-A	H-6->L+1 (29%), HOMO->L+4 (48%)
20	27322.84	365.9942	0.1308	Singlet-A	H-9->LUMO (80%)

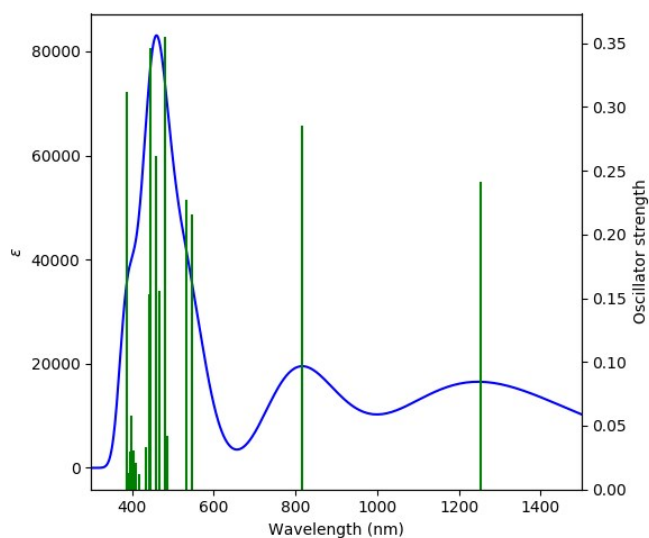
Figure S47. TD-DFT absorption spectrum of partially protonated form of **10** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S2. Summary of UV-vis spectral data of partially protonated form of **10**

No.	Energy (cm-1)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	8142.167	1228.174	0.1706	Singlet-A	HOMO->LUMO (102%)
2	12499.17	800.0529	0.1755	Singlet-A	HOMO->L+1 (89%)
3	16948.13	590.0357	0.1216	Singlet-A	H-1->LUMO (81%)
4	18798.36	531.9612	0.0133	Singlet-A	H-2->LUMO (13%), HOMO->L+2 (76%)
5	19131.47	522.699	0.0388	Singlet-A	H-3->LUMO (15%), H-2->LUMO (58%), HOMO->L+2 (10%)
6	20006.58	499.8355	0.1705	Singlet-A	H-4->LUMO (15%), H-3->LUMO (61%)
7	20826.04	480.1681	0.1354	Singlet-A	H-6->LUMO (16%), H-4->LUMO (63%)
8	21091.4	474.1269	0.0881	Singlet-A	H-5->LUMO (82%)
9	21520.49	464.6735	0.333	Singlet-A	H-6->LUMO (61%), H-4->LUMO (10%)
10	21984.25	454.871	0.296	Singlet-A	H-6->LUMO (10%), H-1->L+1 (58%)
11	22394.79	446.5324	0.1351	Singlet-A	H-7->LUMO (73%), H-1->L+1 (10%)
12	22876.3	437.1336	0.0146	Singlet-A	H-11->LUMO (10%), H-8->LUMO (67%)
13	23269.9	429.7397	0.0262	Singlet-A	H-9->LUMO (79%)
14	24265.19	412.113	0.0133	Singlet-A	H-11->LUMO (57%), H-10->LUMO (12%), H-8->LUMO (14%)
15	24459.57	408.8379	0.0655	Singlet-A	H-2->L+1 (77%)
16	24626.53	406.0662	0.0067	Singlet-A	H-11->LUMO (16%), H-10->LUMO (75%)
17	24949.15	400.8153	0.2342	Singlet-A	H-3->L+1 (60%), HOMO->L+3 (25%)
18	25196.76	396.8764	0.0042	Singlet-A	H-12->LUMO (33%), HOMO->L+3 (43%)
19	25313.71	395.0428	0.0241	Singlet-A	H-13->LUMO (18%), H-12->LUMO (34%), H-5->L+1 (13%), H-3->L+1 (15%)
20	25584.71	390.8584	0.025	Singlet-A	H-12->LUMO (13%), H-6->L+1 (29%), H-4->L+1 (14%)

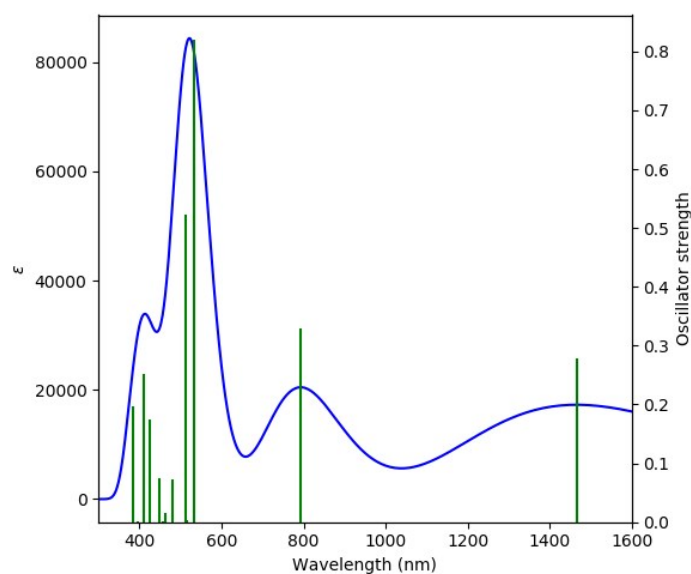
Figure S48. TD-DFT absorption spectrum of fully protonated form of **10** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S3. Summary of UV-vis spectral data of fully protonated form of **10**

No.	Energy (cm-1)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	7051.705	1418.097	0.2169	Singlet-A	HOMO->LUMO (108%)
2	12795.18	781.5443	0.2015	Singlet-A	HOMO->L+1 (89%)
3	16565.82	603.6525	0	Singlet-A	H-2->LUMO (15%), HOMO->L+2 (83%)
4	18258.78	547.6817	0.0009	Singlet-A	H-2->LUMO (81%), HOMO->L+2 (12%)
5	18450.74	541.9837	0.6542	Singlet-A	H-4->LUMO (13%), H-1->LUMO (78%)
6	18753.2	533.2424	0.2381	Singlet-A	H-4->LUMO (78%)
7	18798.36	531.9612	0.0014	Singlet-A	H-6->LUMO (15%), H-3->LUMO (78%)
8	19381.5	515.9559	0.0551	Singlet-A	H-5->LUMO (92%)
9	19756.55	506.1612	0.0018	Singlet-A	H-8->LUMO (23%), H-6->LUMO (66%)
10	19962.22	500.9462	0	Singlet-A	H-8->LUMO (74%), H-6->LUMO (17%)
11	19998.52	500.0371	0.0282	Singlet-A	H-7->LUMO (87%)
12	20388.89	490.4632	0.0026	Singlet-A	H-9->LUMO (99%)
13	22026.19	454.0049	0.3215	Singlet-A	H-10->LUMO (80%)
14	23379.59	427.7234	0.0139	Singlet-A	H-11->LUMO (85%), H-1->L+1 (11%)
15	24550.71	407.3202	0.0001	Singlet-A	H-12->LUMO (85%), H-2->L+1 (10%)
16	24699.92	404.8596	0	Singlet-A	H-2->L+1 (39%), HOMO->L+3 (41%)
17	24733.8	404.3051	0.1249	Singlet-A	H-11->LUMO (12%), H-4->L+1 (29%), H-1->L+1 (50%)
18	25079.81	398.7271	0.0002	Singlet-A	H-3->L+1 (67%)
19	25230.64	396.3436	0.3679	Singlet-A	H-4->L+1 (64%), H-1->L+1 (30%)
20	25778.29	387.9234	0	Singlet-A	H-9->L+1 (27%), H-8->L+1 (37%), H-6->L+1 (10%), H-3->L+1 (22%)

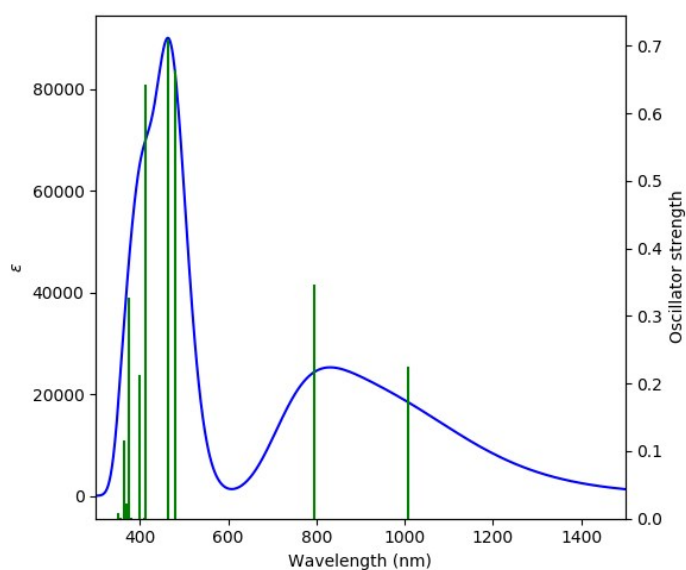
Figure S49. TD-DFT absorption spectrum of free base form of **12** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S4. Summary of UV-vis spectral data of free base form of **12**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	10292.44	971.5868	0.1453	Singlet-A	HOMO->LUMO (93%)
2	12729.85	785.5553	0.2352	Singlet-A	HOMO->L+1 (91%)
3	20381.63	490.6379	0.0001	Singlet-A	HOMO->L+2 (91%)
4	21070.43	474.5988	0.391	Singlet-A	H-3->LUMO (10%), H-1->LUMO (47%), H-1->L+1 (35%)
5	22027.81	453.9716	0.5381	Singlet-A	H-1->LUMO (41%), H-1->L+1 (47%)
6	22479.48	444.8502	0.0001	Singlet-A	H-4->LUMO (20%), H-2->LUMO (74%)
7	24088.55	415.1349	0.0004	Singlet-A	H-4->LUMO (64%), H-2->LUMO (16%)
8	24397.46	409.8787	0.4707	Singlet-A	H-3->LUMO (80%)
9	25073.36	398.8297	0.2966	Singlet-A	H-5->LUMO (74%)
10	25098.36	398.4324	0.0002	Singlet-A	H-2->L+1 (81%)
11	25808.13	387.4748	0.0001	Singlet-A	H-4->L+1 (14%), HOMO->L+3 (74%)
12	26354.97	379.435	0.2411	Singlet-A	H-3->L+1 (87%)
13	26536.45	376.8402	0.0008	Singlet-A	H-9->LUMO (12%), H-7->LUMO (45%), H-4->L+1 (10%)
14	26755.02	373.7616	0	Singlet-A	H-7->LUMO (15%), H-4->L+1 (54%), HOMO->L+3 (12%)
15	27197.82	367.6765	0	Singlet-A	H-6->LUMO (77%), H-4->L+1 (12%)
16	27323.64	365.9834	0.0462	Singlet-A	H-5->L+1 (68%), HOMO->L+4 (21%)
17	27405.11	364.8955	0.1766	Singlet-A	H-8->LUMO (74%)
18	28071.32	356.2355	0.0887	Singlet-A	H-8->L+1 (13%), H-5->L+1 (19%), HOMO->L+4 (59%)
19	28176.98	354.8997	0.0001	Singlet-A	H-9->LUMO (66%), H-7->LUMO (19%)
20	28643.17	349.1234	0.0014	Singlet-A	HOMO->L+5 (90%)

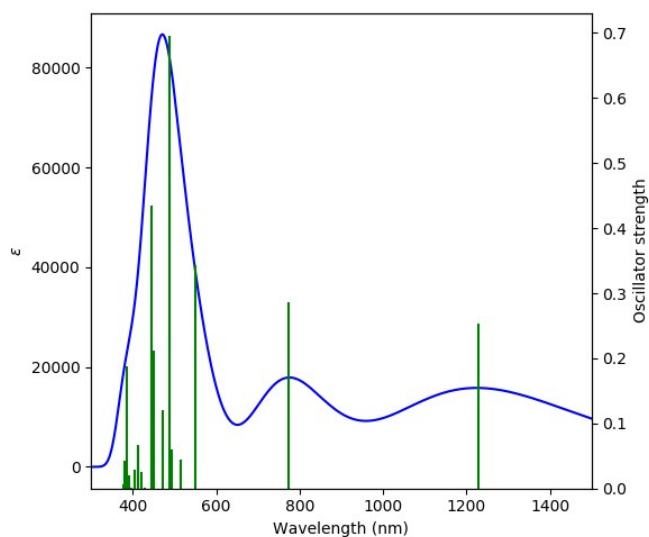
Figure S50. TD-DFT absorption spectrum of partially protonated form of **12** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S5. Summary of UV-vis spectral data of partially protonated form of **12**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	8286.54	1206.776	0.1768	Singlet-A	HOMO->LUMO (101%)
2	13045.21	766.5648	0.1652	Singlet-A	H-1->LUMO (13%), HOMO->L+1 (83%)
3	16565.01	603.6819	0.0982	Singlet-A	H-2->LUMO (14%), H-1->LUMO (73%)
4	18658.02	535.9624	0.03	Singlet-A	H-3->LUMO (75%)
5	19353.27	516.7085	0.0776	Singlet-A	H-4->LUMO (27%), H-3->LUMO (11%), H-2->LUMO (41%), HOMO->L+2 (10%)
6	19436.35	514.4999	0.0354	Singlet-A	H-4->LUMO (11%), H-1->L+1 (12%), HOMO->L+2 (68%)
7	20425.18	489.5917	0.1246	Singlet-A	H-5->LUMO (69%)
8	21013.97	475.8739	0.6506	Singlet-A	H-5->LUMO (14%), H-4->LUMO (45%), H-2->LUMO (21%)
9	21765.68	459.4389	0.1058	Singlet-A	H-6->LUMO (84%)
10	21950.38	455.573	0.2662	Singlet-A	H-8->LUMO (24%), H-1->L+1 (49%)
11	22497.22	444.4993	0.1381	Singlet-A	H-8->LUMO (62%), H-1->L+1 (20%)
12	22710.96	440.316	0.0324	Singlet-A	H-7->LUMO (85%)
13	24150.66	414.0674	0.0447	Singlet-A	H-11->LUMO (23%), H-9->LUMO (59%)
14	24339.39	410.8566	0.0085	Singlet-A	H-12->LUMO (10%), H-11->LUMO (25%), H-10->LUMO (46%), H-9->LUMO (13%)
15	24471.67	408.6358	0.0268	Singlet-A	H-12->LUMO (13%), H-11->LUMO (35%), H-10->LUMO (20%), H-9->LUMO (12%), H-2->L+1 (12%)
16	24569.26	407.0126	0.013	Singlet-A	H-2->L+1 (71%)
17	24850.75	402.4024	0.1197	Singlet-A	H-12->LUMO (13%), H-3->L+1 (68%)
18	25076.58	398.7784	0.047	Singlet-A	H-12->LUMO (46%), H-10->LUMO (11%), H-3->L+1 (24%)
19	25622.62	390.2801	0.0278	Singlet-A	H-13->LUMO (26%), H-4->L+1 (67%)
20	26175.11	382.0423	0.0044	Singlet-A	H-13->LUMO (23%), H-5->L+1 (39%), HOMO->L+3 (21%)

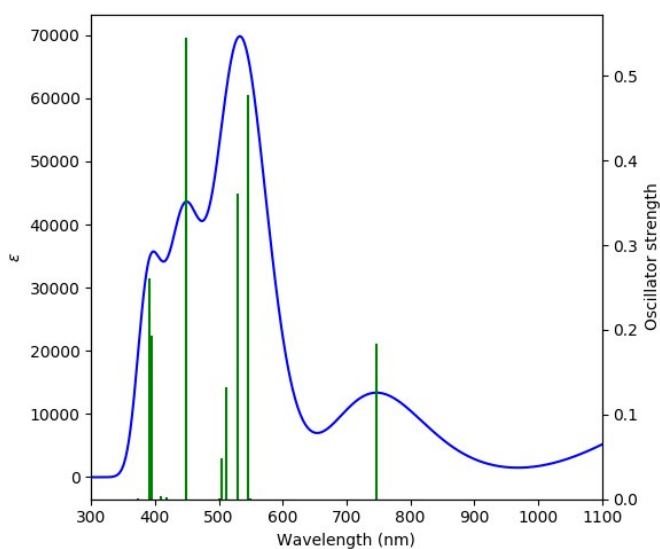
Figure S51. TD-DFT absorption spectrum of fully protonated form of **12** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S6. Summary of UV-vis spectral data of fully protonated form of **12**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator. Strength	Symmetry	Major contributions
1	7167.043	1395.276	0.2216	Singlet-A	HOMO->LUMO (107%)
2	13379.12	747.433	0.1844	Singlet-A	H-1->LUMO (11%), HOMO->L+1 (85%)
3	17019.91	587.5471	0	Singlet-A	H-2->LUMO (28%), HOMO->L+2 (70%)
4	18232.16	548.4813	0.0005	Singlet-A	H-2->LUMO (68%), HOMO->L+2 (24%)
5	18296.69	546.547	0.4776	Singlet-A	H-4->LUMO (33%), H-1->LUMO (62%)
6	18784.65	532.3495	0	Singlet-A	H-5->LUMO (21%), H-3->LUMO (71%)
7	18899.18	529.1234	0.3608	Singlet-A	H-9->LUMO (10%), H-6->LUMO (10%), H-4->LUMO (47%), H-1->LUMO (21%)
8	19515.39	512.4161	0.1319	Singlet-A	H-6->LUMO (86%)
9	19565.4	511.1064	0.0005	Singlet-A	H-5->LUMO (74%), H-3->LUMO (20%)
10	19796.07	505.1507	0.0488	Singlet-A	H-7->LUMO (84%)
11	19945.28	501.3716	0.0005	Singlet-A	H-8->LUMO (95%)
12	22323.01	447.9683	0.5457	Singlet-A	H-9->LUMO (75%)
13	23935.31	417.7928	0.0022	Singlet-A	H-10->LUMO (90%)
14	24382.95	410.1227	0.0003	Singlet-A	H-12->LUMO (87%)
15	24445.05	409.0807	0.0037	Singlet-A	H-11->LUMO (53%), H-4->L+1 (10%), H-1->L+1 (32%)
16	25263.7	395.8248	0	Singlet-A	H-3->L+1 (12%), H-2->L+1 (74%), HOMO->L+3 (10%)
17	25344.36	394.5651	0.1937	Singlet-A	H-11->LUMO (16%), H-4->L+1 (24%), H-1->L+1 (57%)
18	25536.32	391.5991	0.2614	Singlet-A	H-11->LUMO (29%), H-4->L+1 (61%)
19	25566.97	391.1297	0.0001	Singlet-A	H-3->L+1 (84%)
20	26843.74	372.5263	0.0013	Singlet-A	H-5->L+1 (92%)

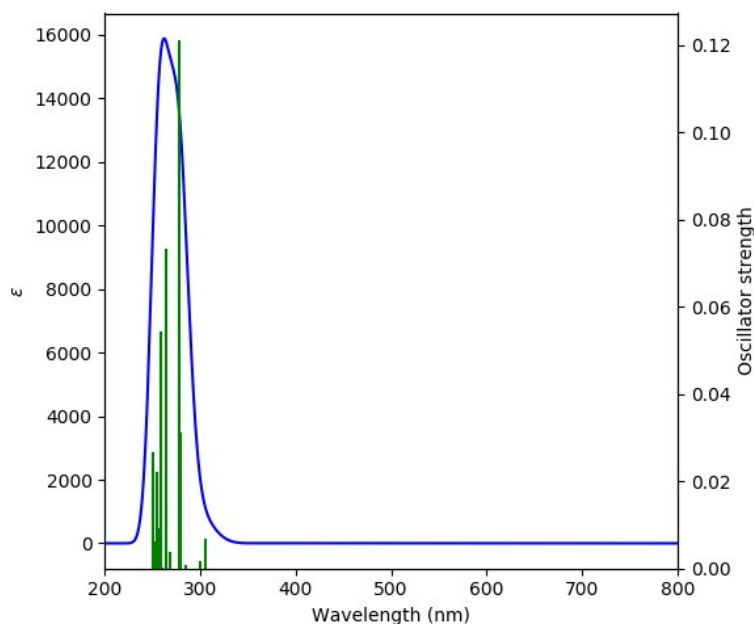
Figure S52. TD-DFT absorption spectrum of free base form of **11** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below.

Table S7. Summary of UV-vis spectral data of free base form of **11**

No.	Energy (cm ⁻¹)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	32685.62	305.945	0.0068	Singlet-A	H-1->LUMO (19%), HOMO->LUMO (79%)
2	33288.92	300.4002	0.0016	Singlet-A	H-1->LUMO (79%), HOMO->LUMO (19%)
3	35055.28	285.2638	0.0009	Singlet-A	H-2->LUMO (97%)
4	35842.47	278.9986	0.0313	Singlet-A	H-4->LUMO (31%), H-3->LUMO (65%)
5	35923.93	278.3659	0.1212	Singlet-A	H-4->LUMO (65%), H-3->LUMO (30%) HOMO->L+2 (27%), HOMO->L+3 (18%), HOMO->L+10 (13%)
6	37349.92	267.7382	0.0038	Singlet-A	H-1->L+2 (28%), H-1->L+3 (13%), H-1->L+5 (13%), H-1->L+10 (15%), HOMO->L+2 (15%)
7	37599.15	265.9635	0	Singlet-A	HOMO->L+1 (87%)
8	37947.58	263.5214	0.0734	Singlet-A	HOMO->L+1 (87%)
9	38422.64	260.2632	0.0002	Singlet-A	HOMO->L+2 (22%), HOMO->L+3 (60%) H-5->LUMO (15%), H-1->L+1 (17%), HOMO->L+4 (50%)
10	38639.6	258.8018	0.0144	Singlet-A	H-1->L+1 (44%), HOMO->L+4 (26%)
11	38725.1	258.2305	0.0543	Singlet-A	H-1->L+3 (10%), HOMO->L+5 (42%)
12	38798.49	257.742	0.0092	Singlet-A	H-5->LUMO (65%), H-1->L+1 (24%) H-1->L+2 (11%), H-1->L+3 (13%), HOMO->L+7 (46%)
13	38812.21	257.6509	0.0057	Singlet-A	H-1->L+2 (24%), H-1->L+3 (18%), HOMO->L+6 (11%), HOMO->L+7 (22%)
14	39188.87	255.1745	0.0222	Singlet-A	H-1->L+4 (14%), HOMO->L+6 (42%), HOMO->L+7 (17%)
15	39242.91	254.8231	0.0025	Singlet-A	H-1->L+4 (52%), HOMO->L+6 (21%)
16	39256.62	254.7341	0.003	Singlet-A	H-1->L+3 (20%), H-1->L+5 (47%)
17	39440.51	253.5464	0.0028	Singlet-A	H-1->L+4 (11%), HOMO->L+8 (50%)
18	39601.82	252.5136	0.0063	Singlet-A	H-1->L+6 (77%)
19	39641.34	252.2619	0.0005	Singlet-A	
20	39891.38	250.6808	0.0268	Singlet-A	

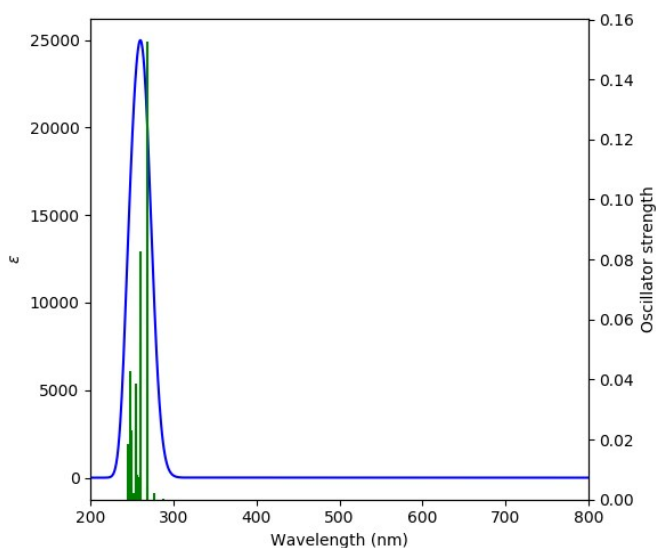
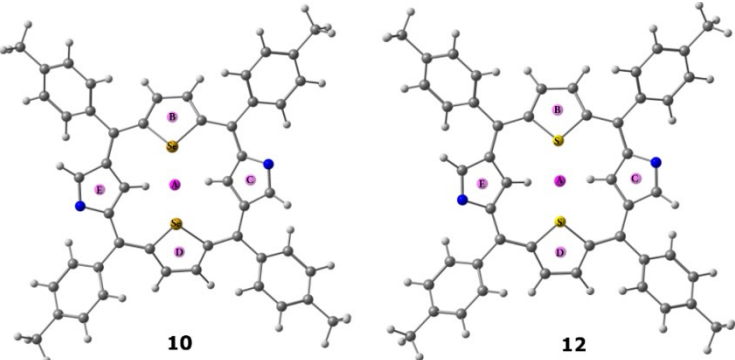
Figure S53. TD-DFT absorption spectrum of free base form of **13** at B3LYP/6-311+G* (B1c) level of theory and the corresponding electronic transitions are shown in the table below

Table S8. Summary of UV-vis spectral data of free base form of **13**

No.	Energy (cm ⁻¹)	Wavelength h (nm)	Osc. Strength	Symmetry	Major contribs
1	34726.2	287.967	0.0002	Singlet-A	HOMO->LUMO (97%)
2	36068.31	277.2517	0.0021	Singlet-A	H-1->LUMO (98%)
3	37282.17	268.2247	0.1527	Singlet-A	H-2->LUMO (85%)
4	37340.24	267.8076	0.004	Singlet-A	H-3->LUMO (90%)
5	38423.45	260.2578	0.0828	Singlet-A	HOMO->L+1 (52%), HOMO->L+2 (21%) HOMO->L+1 (29%), HOMO->L+2 (23%), HOMO->L+3 (30%)
6	38503.3	259.718	0.0524	Singlet-A	H-1->L+2 (14%), HOMO->L+2 (33%), HOMO->L+3 (41%)
7	38680.74	258.5266	0.0076	Singlet-A	H-1->L+1 (12%), HOMO->L+4 (68%)
8	38871.08	257.2606	0.0007	Singlet-A	H-1->L+4 (10%), HOMO->L+5 (54%)
9	39144.51	255.4637	0.0083	Singlet-A	HOMO->L+7 (19%), HOMO->L+8 (50%)
10	39230.81	254.9017	0.0223	Singlet-A	HOMO->L+7 (47%), HOMO->L+8 (20%)
11	39246.94	254.7969	0.0035	Singlet-A	H-1->L+6 (12%), HOMO->L+6 (61%)
12	39267.1	254.6661	0.0387	Singlet-A	H-4->LUMO (82%) H-5->LUMO (21%), H-1->L+1 (31%), HOMO->L+9 (15%)
13	39747.81	251.5862	0.002	Singlet-A	H-3->L+3 (14%), H-1->L+2 (18%), H-1->L+3 (37%)
14	40071.24	249.5556	0.0022	Singlet-A	H-1->L+1 (11%), H-1->L+4 (22%), HOMO->L+9 (23%)
15	40226.1	248.5948	0.0231	Singlet-A	H-5->LUMO (38%), H-3->L+2 (10%)
16	40411.6	247.4537	0.043	Singlet-A	H-5->LUMO (15%), H-3->L+2 (22%), H-1->L+2 (22%)
17	40465.64	247.1232	0.0102	Singlet-A	H-3->L+1 (42%), H-1->L+5 (11%), H-1->L+7 (11%)
18	40487.42	246.9903	0.0113	Singlet-A	H-1->L+5 (25%), H-1->L+8 (11%)
19	40571.3	246.4796	0.0177	Singlet-A	
20	40762.45	245.3238	0.0184	Singlet-A	



	10	B1c	B1b	12	B1c	B1b
A(-5)		-2.415	-2.321	A(-5)	-2.529	-2.401
A(-4)		-3.538	-3.417	A(-4)	-3.705	-3.532
A(-3)		-5.176	-5.027	A(-3)	-5.387	-5.158
A(-2)		-7.166	-7.024	A(-2)	-7.344	-7.098
A(-1)		-8.578	-8.568	A(-1)	-8.551	-8.367
A(0)		-8.503	-8.671	A(0)	-8.289	-8.190
A(1)		-7.252	-7.458	A(1)	-8.387	-8.406
A(2)		-5.876	-5.816	A(2)	-6.920	-6.751
A(3)		-4.374	-4.111	A(3)	-4.863	-4.654
A(4)		-3.015	-2.823	A(4)	-3.275	-3.122
A(5)		-2.065	-1.928	A(5)	-2.065	-2.103
B		-14.90	-16.01	B	-14.94	-16.06
C		3.527	3.239	C	3.940	3.701
D		-14.90	16.01	D	14.96	-16.04
E		3.527	-3.239	E	3.939	3.702

Figure S54. NICS value of free base form of **10** and **12** at B1c [B3LYP/6-311+G(d)] and B1b [B3LYP/6-31G(d,p)] level of theory. A represents the center of macrocycle ring including all the core atoms. While the value in the parenthesis represent the position of dummy atom above and below the plane in angstroms. B and D represents center of thioselenium/thiosulfur rings. C and E represent the Nconfused pyrrole rings.

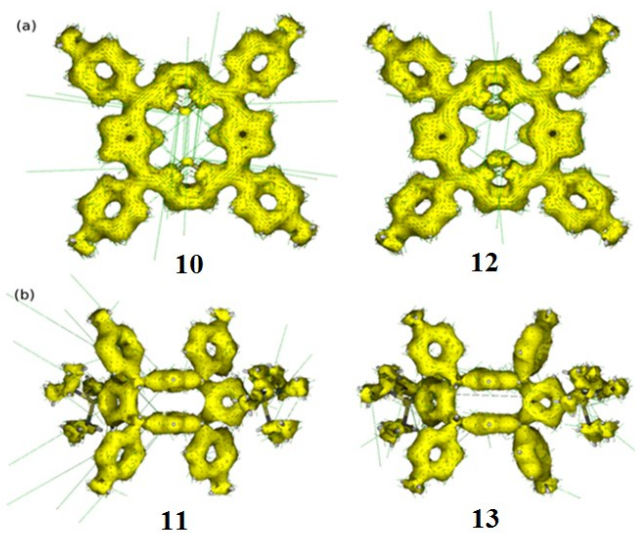


Figure S55. AICD plots of free base form of (a) **10**, **12** (b) **11**, **13** at B1b level of theory

	B1 (B3LYP/6-31G)			B1a (WB97XD/6-31G)		
	E	E+ZPE	G	E	E+ZPE	G
10a	-6758.09684	-6757.39743	-6757.48265	-6757.48833	-6756.77843	-6756.86387
10b	-6758.08597	-6757.38497	-6757.47003	-6757.47568	-6756.76520	-6756.84966
10c	-6758.08073	-6757.37917	-6757.46515	-6757.46916	-6756.75794	-6756.84293
	B1b (B3LYP/6-31G(d,p))			B1c (B3LYP/6-311+G(d))		
	E	E+ZPE	G	E	E+ZPE	G
10a	-6759.0606	-6758.36787	-6758.45312	-6763.72248	-6763.02307	-6763.10829
10b	-6759.0573	-6758.36365	-6758.44792	-6763.71733	-6763.01632	-6763.10138
10c	-6759.053	-6758.35948	-6758.44533	-6763.71124	-6763.00968	-6763.09566
	B2 (B3LYP/6-311G(d,p))			B2a(B3LYP/def2TZVP)		
	E	E+ZPE	G	E	E+ZPE	G
10a	-6763.779697	-6763.08029	-6763.15524	-6764.07448	-6763.37508	-6763.46030
10b	-6763.774834	-6763.07383	-6763.15889	-6764.07047	-6763.36946	-6763.45453
10c	-6763.767119	-6763.06557	-6763.14089	-6764.05811	-6763.35655	-6763.44253
	B1c (B3LYP/6-311+G(d))			B2 (B3LYP/6-311G(d,p))		
	E	E+ZPE	G	E	E+ZPE	G
11a	-8051.90238	-8050.58841	-8050.71230	-8056.76765	-8055.45368	-8055.57757
11b	-8051.90265	-8050.58840	-8050.71167	-8056.7666	-8055.45235	-8055.57562
11c	-8051.88386	-8050.57028	-8050.69292	-8056.75665	-8055.44307	-8055.56571
	B1 (B3LYP/6-31G)			B1a (WB97XD/6-31G)		
	E	E+ZPE	G	E	E+ZPE	G
12a	-2756.06442	-2755.36222	-2755.44548	-2755.37717	-2754.66531	-2754.74891
12b	-2756.06309	-2755.36058	-2755.44406	-2755.37361	-2754.66147	-2754.74484
12c	-2756.05893	-2755.35664	-2755.44259	-2755.36947	-2754.65774	-2754.73883
	B1b (B3LYP/6-31G(d,p))			B1c (B3LYP/6-311+G(d))		
	E	E+ZPE	G	E	E+ZPE	G
12a	-2756.66826	-2755.97288	-2756.05189	-2757.07502	-2756.37282	-2756.456075
12b	-2756.66800	-2755.97256	-2756.05570	-2757.07432	-2756.37181	-2756.455289
12c	-2756.66400	-2755.96890	-2756.04894	-2757.07026	-2756.36798	-2756.45392
	B2 (B3LYP/6-311G(d,p))			B2a(B3LYP/def2TZVP)		
	E	E+ZPE	G	E	E+ZPE	G
12a	-2757.13244	-2756.4302	-2756.51349	-2757.36368	-2756.66148	-2756.74473
12b	-2757.13149	-2756.429	-2756.51245	-2757.36404	-2756.66153	-2756.74501
12c	-2757.12741	-2756.4251	-2756.51107	-2757.36016	-2756.65787	-2756.74382
	B1c (B3LYP/6-311+G(d))			B2 (B3LYP/6-311G(d,p))		
	E	E+ZPE	G	E	E+ZPE	G
13a	-4049.49104	-4048.17641	-4048.30497	-4050.12861	-4048.81397	-4048.30497
13b	-4049.48998	-4048.17522	-4048.30208	-4050.12780	-4048.81304	-4048.30208
13c	-4049.48235	-4048.16740	-4048.29298	-4050.11905	-4048.80410	-4048.29298

Table S9. Total energies and with zero point energy and free energy correction (a.u) for plausible conformers of compounds **10**, **11**, **12** and **13** at **B1**, **B1a**, **B1b**, **B1c**, **B2** and **B2a** level of theory.

Compound	B1		B1a		B1b		B1c		B2		B2a	
	($\Delta E+ZPE$)	ΔG	$\Delta E+ZPE$	ΔG	$\Delta E+ZPE$	ΔG	$\Delta E+ZPE$	ΔG	$\Delta E+ZPE$	ΔG	$\Delta E+ZPE$	ΔG
10a	0.00	0.00	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00
10b	32.72	33.13	34.74	37.3	11.1	13.6	17.73	18.14	16.97	17.37	14.74	15.14
10c	47.93	45.94	53.8	54.98	22.0	20.5	35.15	33.16	38.65	36.66	48.63	46.64
12a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12b	4.32	3.72	10.09	10.70	0.82	-10.00	2.66	2.06	3.33	2.73	-0.14	-0.74
12c	14.66	7.59	19.89	26.47	10.44	7.75	12.73	5.66	13.44	6.37	9.46	2.39

Table S10. Relative energies of **10** and **12** including zero point energy ($\Delta E+ZPE$) and Gibbs free energy (ΔG) in kJ/mol at **B1**, **B1a**, **B1b**, **B1c** **B2** and **B2a** level of theories.

Compound	B1b		B2	
	($\Delta E+ZPE$)	ΔG	$\Delta E+ZPE$	ΔG
11a	0.00	0.00	0.00	0.00
11b	0.03	1.64	3.49	5.11
11c	47.60	50.88	27.85	31.14
13a	0.00	0.00	0.00	0.00
13b	3.11	7.58	2.44	6.90
13c	23.61	31.49	25.91	33.78

Table S11. Relative energies of **11** and **13** including zero point energy ($\Delta E+ZPE$) and Gibbs free energy (ΔG) in kJ/mol at **B1b** and **B2** level of theory

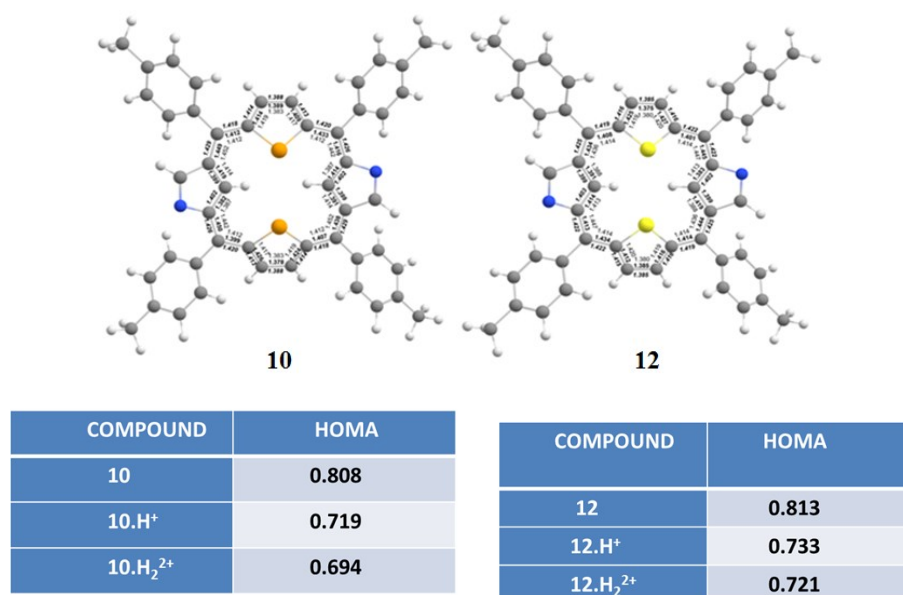


Figure S56. Optimised geometries and key bond length parameters ($\text{\AA}$) of **10** and **12** in freebase form, protonated and doubly protonated forms at B3LYP/6-311+G* level of theory.

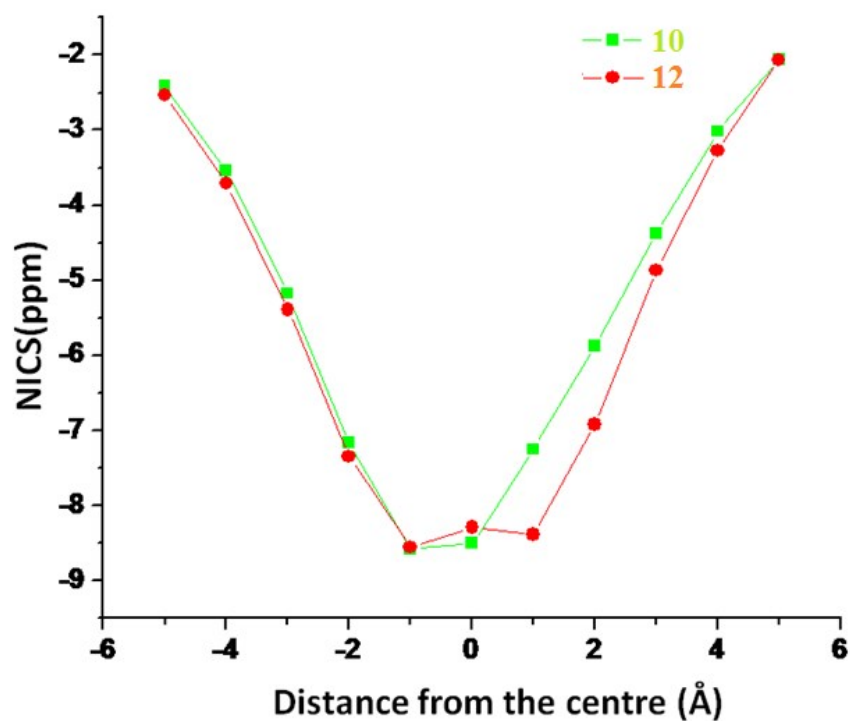


Figure S57. Plot of chemical shift vs distance of probe for **10** and **12**

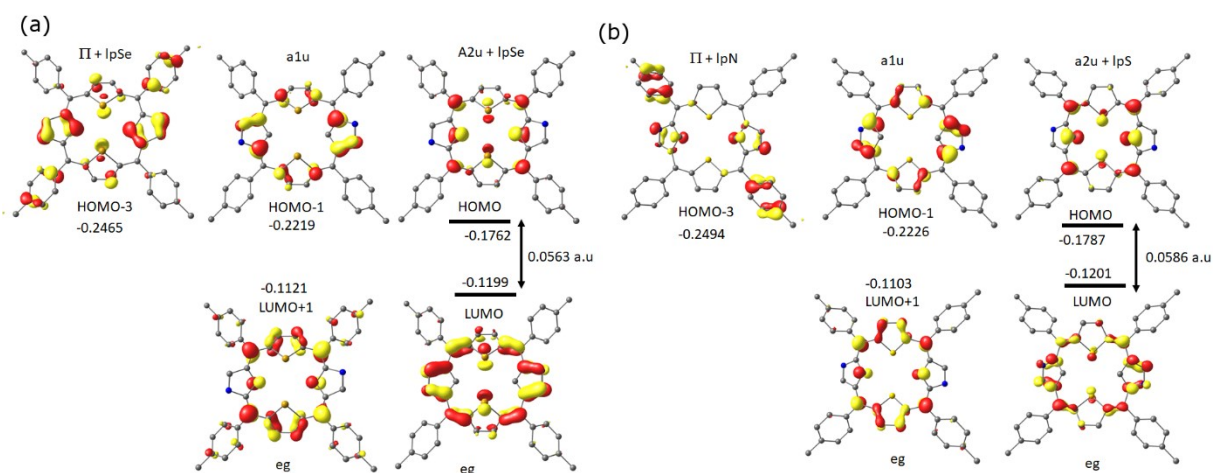


Figure S58. Frontier molecular orbitals for DFT optimised structures of (a) **10** and (b) **12**, at B3LYP/6-311+G (d) level of theory in presence of solvent. The HOMO and LUMO orbitals and the energy gap is also mentioned in a.u.

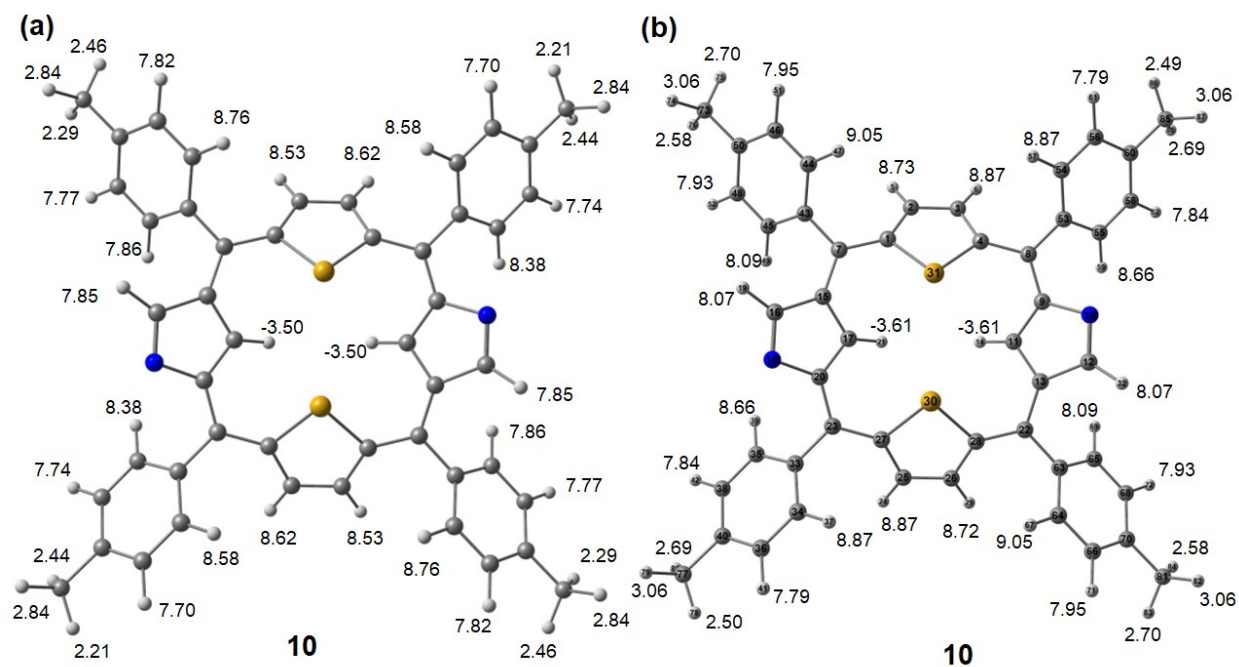


Figure S59. Calculated ^1H -NMR chemical shift values of **10** at B1b and B1c level of theory

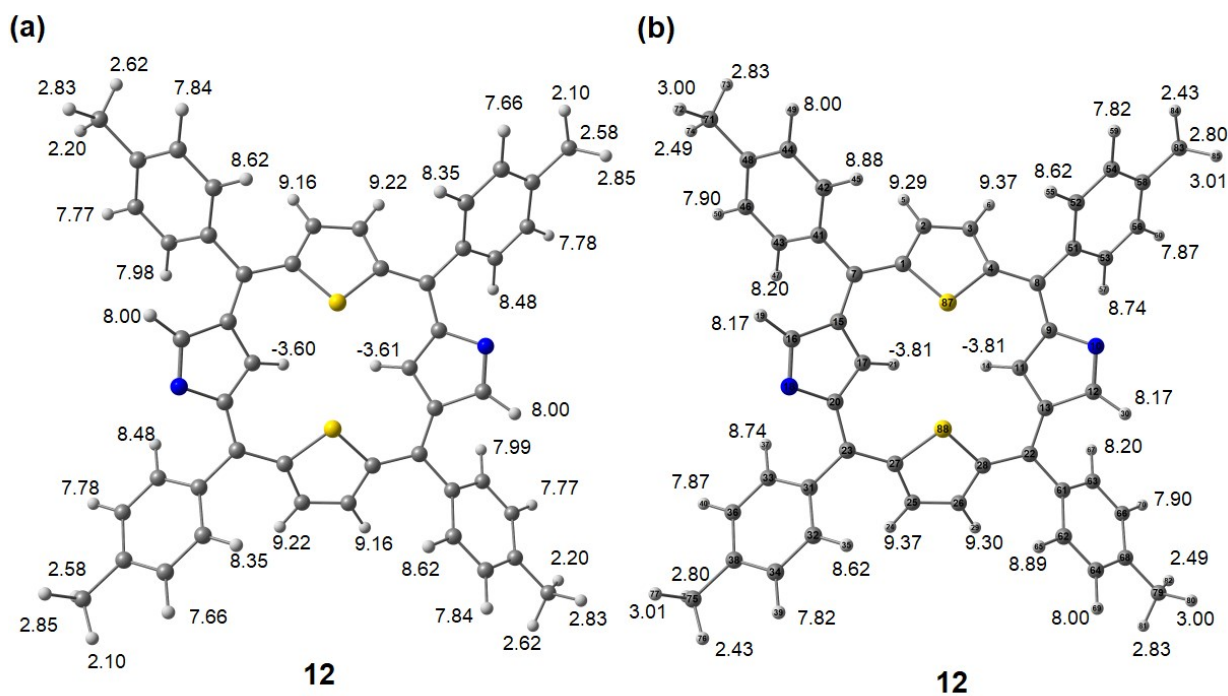


Figure S60. Calculated ^1H -NMR chemical shift values of **12** at B1b and B1c level of theory

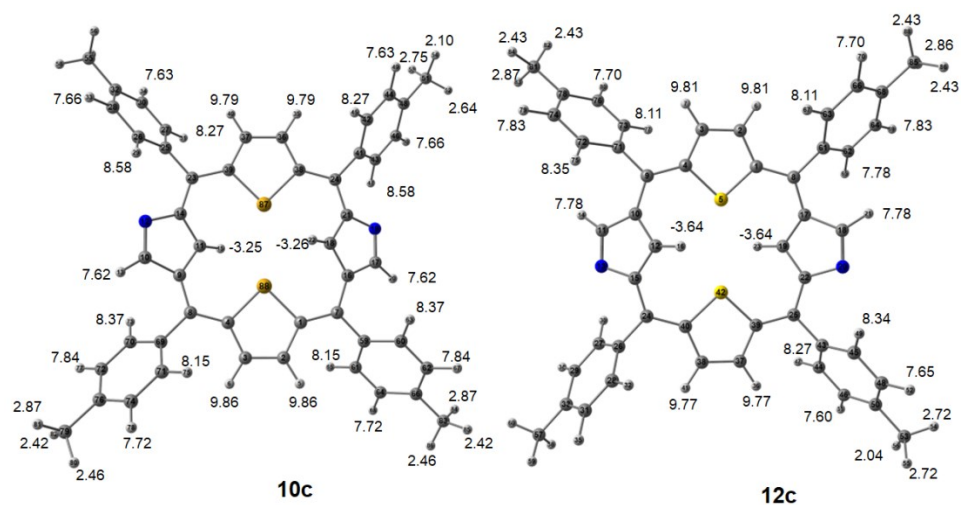


Figure S61. Calculated ^1H -NMR chemical shifts of **10c** and **12c** at B3LYP/6-31G(d,p), B1b level of theory.

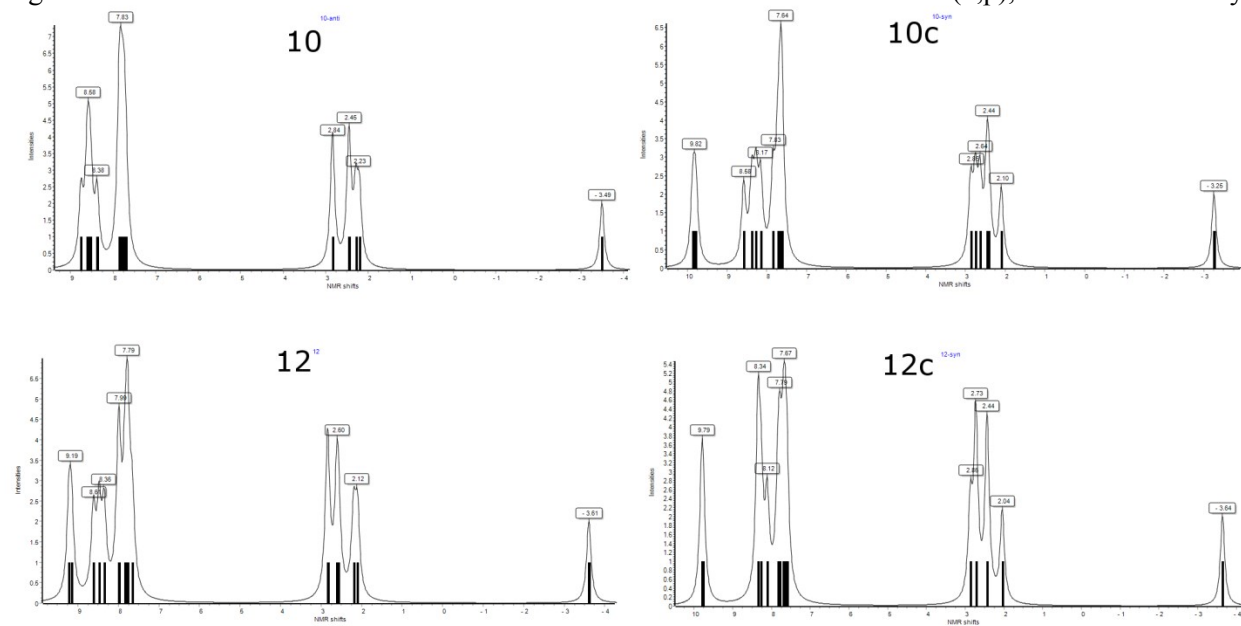


Figure S62. Calculated ^1H -NMR spectral pattern of **10**, **10c**, **12** and **12c** at B3LYP/6-31G(d,p), B1b level of theory.

Cartesian Coordinates

10a

Energy = -6759.060562

C, 0.943378, 2.971592, 0.111678
C, 0.162602, 4.002597, 0.688051
C, -1.214539, 3.826813, 0.666762
C, -1.692765, 2.634526, 0.073724
H, 0.629755, 4.841942, 1.191243
H, -1.893265, 4.521102, 1.149397
C, 2.353684, 2.817305, 0.082795
C, -3.021530, 2.132370, -0.001973
C, -3.247519, 0.725758, -0.082316
N, -4.429971, 0.156966, -0.631455
C, -2.363973, -0.289714, 0.314518
C, -4.246143, -1.136238, -0.594375
C, -2.941837, -1.519108, -0.025030
H, -1.441823, -0.150918, 0.849823
C, 2.941863, 1.519068, -0.024962
C, 4.246149, 1.136220, -0.594370
C, 2.363976, 0.289623, 0.314498
N, 4.429933, -0.156983, -0.631566
H, 4.974353, 1.821307, -1.017157
C, 3.247480, -0.725797, -0.082429
H, 1.441836, 0.150811, 0.849816
C, -2.353651, -2.817396, 0.082647
C, 3.021503, -2.132458, -0.002156
H, 1.893293, -4.521482, 1.148629
C, 1.214554, -3.827088, 0.666163
C, -0.162559, -4.002872, 0.687463
C, 1.692789, -2.634640, 0.073378
C, -0.943388, -2.971715, 0.111353
H, -0.629691, -4.842324, 1.190493
Se, 0.221409, -1.681068, -0.639509
Se, -0.221427, 1.681107, -0.639408
H, -4.974350, -1.821311, -1.017182
C, 4.156462, -3.073007, 0.016737
C, 4.071405, -4.330855, -0.610033
C, 5.368482, -2.739231, 0.653417
C, 5.143932, -5.217209, -0.589395
H, 3.163581, -4.599541, -1.140016
C, 6.433439, -3.631111, 0.671016
H, 5.461343, -1.776117, 1.140529
C, 6.345043, -4.886443, 0.050816
H, 5.051623, -6.178137, -1.089376
H, 7.352849, -3.351315, 1.179414
C, 3.221382, 4.006505, 0.186798
C, 2.888345, 5.219690, -0.448237
C, 4.428226, 3.959345, 0.911902
C, 3.722551, 6.328311, -0.357978
H, 1.978503, 5.277015, -1.036785
C, 5.257656, 5.073504, 0.996446
H, 4.695259, 3.046784, 1.434655
C, 4.924616, 6.278323, 0.363036
H, 3.442968, 7.247994, -0.865991
H, 6.176306, 5.010462, 1.574300
C, -4.156426, 3.072991, 0.016795
C, -4.071158, 4.330881, -0.609863

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H, 6.529398, 7.493217, -0.424864
H, 5.278883, 8.413146, 0.412052
H, 6.452216, 7.461315, 1.337451
C, 7.519381, -5.834130, 0.048662
H, 7.204713, -6.863160, -0.146873
H, 8.245686, -5.560283, -0.726913
H, 8.049858, -5.816366, 1.006016
C, -5.841845, -7.474805, 0.430381
H, -6.530171, -7.492700, -0.424084
H, -5.279229, -8.413061, 0.411727
H, -6.451892, -7.461439, 1.338189
C, -7.519142, 5.834361, 0.048327
H, -7.204387, 6.863352, -0.147272
H, -8.245431, 5.560504, -0.727258
H, -8.049666, 5.816710, 1.005658

10b

Energy = -6759.057325

C, -1.134558, -2.960281, -0.197484
C, -0.435613, -4.181111, -0.019919
C, 0.942316, -4.087228, 0.157209
C, 1.498484, -2.786407, 0.090944
H, -0.950537, -5.134859, -0.006209
H, 1.556323, -4.958754, 0.353729
C, -2.528475, -2.689666, -0.233018
C, 2.848550, -2.346230, 0.151417
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N, 4.389129, -0.456981, -0.266366
C, 2.328765, 0.118278, 0.631276
C, 4.285388, 0.844971, -0.233156
C, 2.996155, 1.314661, 0.294332
H, 1.459571, 0.043154, 1.265503
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C, -4.305549, -0.878643, 0.189466
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N, -4.409500, 0.421441, 0.186118
H, -5.074549, -1.503919, 0.630695
C, -3.194028, 0.913044, -0.355388
H, -1.572720, -0.113405, -1.475414

C, 2.493074, 2.653874, 0.241723
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 C, 4.566892, 3.774133, 1.088057
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 H, 2.511706, 4.863215, -1.385366
 C, 5.492337, 4.813926, 1.072794
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 H, 6.453962, 7.474707, -0.800048
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 H, -2.557199, -4.595248, 1.752066
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 H, -6.380493, -5.034473, -1.362244
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 C, 6.071781, -5.201947, -0.205190
 H, 6.998054, -4.050702, 1.364486
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 C, 7.213689, -6.180227, -0.336172
 H, 6.899445, -7.098902, -0.839485

H, 8.036527, -5.750341, -0.920908
 H, 7.622656, -6.451630, 0.642375
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 H, -6.526298, -7.234306, 1.620665
 H, -7.387053, -6.716199, 0.161776
 H, -6.077284, -7.892870, 0.047324
 Se, -0.095748, 1.511702, -0.236061
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 H, 5.065083, 1.481808, -0.638212

10c

Energy = -6759.053026

C, -1.318107, 2.904153, 0.149031
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 C, 0.690271, 4.174855, -0.092545
 C, 1.319686, 2.903474, -0.149162
 H, -1.252921, 5.095537, 0.188881
 H, 1.255625, 5.094891, -0.189031
 C, -2.688704, 2.545888, 0.204608
 C, 2.690105, 2.544510, -0.204702
 C, 3.098583, 1.180799, -0.294654
 C, 4.347647, 0.610915, 0.235317
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 N, 4.363750, -0.694483, 0.233558
 H, 5.166682, 1.183342, 0.657959
 C, 3.108990, -1.102657, -0.284143
 H, 1.521134, 0.028867, -1.347602
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 H, -5.166073, 1.186050, -0.657830
 C, -3.109527, -1.101066, 0.284059
 H, -1.520794, 0.029593, 1.347132
 C, 2.692733, -2.464845, -0.243148
 C, -2.694033, -2.463486, 0.243064
 C, 3.703243, -3.560281, -0.160972
 C, 4.657466, -3.621774, 0.867977
 C, 3.716022, -4.569513, -1.135715
 C, 5.575717, -4.665746, 0.918896
 H, 4.681333, -2.838074, 1.614453
 C, 4.645650, -5.608080, -1.080347
 H, 3.007504, -4.528178, -1.957755
 C, 5.588240, -5.679711, -0.049790
 H, 6.302038, -4.692124, 1.727846
 H, 4.639530, -6.370192, -1.855677
 H, -1.256853, -4.997239, 0.173216
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 C, 0.687290, -4.077707, -0.095244
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 H, 1.254281, -4.997850, -0.173397
 C, -3.705144, -3.558375, 0.160956
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 H, -6.331205, -7.507636, -0.837092
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 H, 7.593081, -6.446907, 0.232209
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 C, 5.844855, 4.556254, -0.803422
 H, 4.913292, 2.840701, -1.704808
 C, 4.674640, 5.541929, 1.045709
 H, 2.842756, 4.586854, 1.628964
 C, 5.779591, 5.548752, 0.182964
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 H, 4.603819, 6.293444, 1.828155
 C, 6.878196, 6.572934, 0.333145
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 H, -7.369919, 6.775426, 0.621939
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11a

Energy = -8051.902382

C, 4.129572, 1.062381, 0.287868
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 C, 3.257801, -0.776344, 1.262635
 C, 4.109058, -1.159475, 0.250169
 N, 4.656174, -0.042177, -0.364424
 C, 2.412715, -1.724455, 2.099594
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 C, 1.018441, 1.701752, 1.608317
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 C, -1.356046, -1.846888, 1.407704
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 Si, -6.929423, -0.034377, 0.950107
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 C, 4.802535, 0.666289, -3.290650
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12a

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 C, 0.882460, -4.030538, 0.581243
 C, 1.411340, -2.809491, 0.098345
 H, -1.053560, -4.931248, 1.000413
 H, 1.517922, -4.818452, 0.964541

C, -2.529690, -2.608897, 0.079398
 C, 2.765270, -2.384711, 0.009168
 C, 3.097334, -1.002615, -0.044641
 N, 4.313155, -0.534036, -0.617636
 C, 2.312587, 0.087089, 0.359685
 C, 4.243046, 0.765043, -0.587818
 C, 2.986299, 1.260832, 0.003666
 H, 1.396026, 0.030826, 0.915283
 C, -2.986206, -1.260945, 0.003390
 C, -4.243027, -0.765087, -0.587867
 C, -2.312592, -0.087398, 0.359673
 N, -4.313306, 0.534004, -0.617319
 H, -5.019170, -1.379452, -1.030703
 C, -3.097494, 1.002519, -0.044336
 H, -1.395995, -0.031178, 0.915215
 C, 2.529796, 2.608580, 0.079948
 C, -2.765408, 2.384415, 0.009750
 H, -1.517975, 4.817157, 0.967611
 C, -0.882514, 4.029612, 0.583551
 C, 0.500845, 4.090371, 0.601651
 C, -1.411288, 2.809124, 0.099511
 C, 1.146641, 2.921565, 0.130088
 H, 1.053651, 4.929935, 1.003467
 H, 5.019183, 1.379448, -1.030602
 C, -3.833626, 3.402375, -0.037569
 C, -3.692656, 4.578614, -0.790825
 C, -5.036748, 3.217796, 0.666277
 C, -4.706977, 5.530062, -0.832597
 H, -2.792678, 4.733558, -1.375764
 C, -6.039820, 4.175947, 0.628093
 H, -5.174262, 2.318166, 1.253465
 C, -5.898109, 5.350257, -0.123101
 H, -4.572804, 6.422812, -1.437048
 H, -6.953987, 4.009193, 1.191521
 C, -3.519700, -3.705856, 0.107255
 C, -3.341822, -4.883666, -0.641066
 C, -4.689863, -3.595074, 0.876806
 C, -4.291140, -5.897112, -0.617785
 H, -2.463771, -4.987664, -1.269110
 C, -5.633531, -4.617300, 0.899433
 H, -4.843677, -2.709198, 1.483245
 C, -5.456340, -5.786077, 0.152558
 H, -4.130215, -6.788529, -1.218116
 H, -6.520804, -4.505636, 1.516217
 C, 3.833756, -3.402433, -0.037756
 C, 3.693609, -4.578443, -0.791510
 C, 5.036340, -3.217790, 0.666976
 C, 4.708175, -5.529655, -0.832848
 H, 2.794102, -4.733379, -1.377177
 C, 6.039666, -4.175698, 0.629210
 H, 5.173239, -2.318304, 1.254541
 C, 5.898757, -5.349808, -0.122442
 H, 4.574640, -6.422239, -1.437685
 H, 6.953401, -4.008899, 1.193327
 C, 3.519569, 3.705733, 0.107444
 C, 3.340930, 4.883690, -0.640482
 C, 4.690232, 3.595049, 0.876251
 C, 4.290051, 5.897317, -0.617609

H, 2.462431, 4.987651, -1.267902
 C, 5.633699, 4.617472, 0.898481
 H, 4.844591, 2.709103, 1.482445
 C, 5.455781, 5.786357, 0.151957
 H, 4.128550, 6.788834, -1.217639
 H, 6.521381, 4.505877, 1.514685
 C, -6.491873, -6.882333, 0.152565
 H, -7.101290, -6.849439, -0.757343
 H, -6.030079, -7.872575, 0.193285
 H, -7.171530, -6.793701, 1.002839
 C, -7.007970, 6.369715, -0.179003
 H, -6.672657, 7.306145, -0.630097
 H, -7.852240, 6.002792, -0.772757
 H, -7.394185, 6.597733, 0.818702
 C, 6.491031, 6.882878, 0.151561
 H, 7.099140, 6.851047, -0.759255
 H, 6.029033, 7.872960, 0.193918
 H, 7.171921, 6.793591, 1.000776
 C, 7.008902, -6.368985, -0.177905
 H, 6.674025, -7.305472, -0.629206
 H, 7.853346, -6.001821, -0.771266
 H, 7.394728, -6.596968, 0.819957
 S, 0.078704, -1.781985, -0.405368
 S, -0.078744, 1.782114, -0.405229

12b

Energy = -2756.668004

C, 1.380777, -2.834541, 0.095590
 C, 0.836657, -4.140505, 0.152308
 C, -0.540919, -4.198738, -0.007230
 C, -1.169574, -2.937832, -0.160796
 S, 0.068113, -1.691767, -0.152068
 H, 1.452905, -5.014409, 0.321720
 H, -1.099085, -5.126412, -0.008137
 C, 2.740486, -2.412057, 0.131797
 C, -2.553258, -2.612081, -0.213929
 C, -3.013508, -1.278116, -0.355000
 C, -4.309191, -0.755983, 0.124127
 C, -2.309522, -0.110360, -0.714925
 N, -4.377019, 0.543563, 0.111408
 H, -5.120781, -1.360420, 0.515404
 C, -3.112319, 0.995365, -0.362906
 H, -1.408422, -0.073828, -1.301115
 C, 3.091625, -1.039940, 0.226863
 N, 4.350307, -0.575457, -0.247195
 C, 2.281973, 0.057066, 0.597723
 C, 4.282475, 0.725558, -0.215726
 C, 2.987422, 1.229517, 0.277099
 H, 1.355162, 0.007754, 1.142106
 C, -2.750788, 2.365669, -0.285863
 C, 2.525615, 2.577491, 0.218773
 C, -3.805817, 3.415705, -0.157766
 C, -4.742335, 3.411470, 0.888689
 C, -3.874985, 4.452366, -1.101156
 C, -5.701526, 4.415058, 0.984433
 H, -4.716965, 2.611755, 1.617999
 C, -4.843867, 5.450702, -1.001039
 H, -3.172203, 4.468259, -1.929100

C, -5.774667, 5.451590, 0.043054
 H, -6.409882, 4.392960, 1.809247
 H, -4.877238, 6.237927, -1.750270
 H, 1.013051, 5.052784, 0.487799
 C, 0.486375, 4.142668, 0.228592
 C, -0.882558, 4.087314, 0.030830
 C, 1.148137, 2.891855, 0.123109
 C, -1.394195, 2.786200, -0.227626
 H, -1.529774, 4.951712, 0.104243
 S, -0.053247, 1.651172, -0.223885
 C, 3.526283, 3.672125, 0.192197
 C, 4.619149, 3.652402, 1.077962
 C, 3.442923, 4.739641, -0.720823
 C, 5.576862, 4.662608, 1.057892
 H, 4.701893, 2.843248, 1.796659
 C, 4.406490, 5.743473, -0.737424
 H, 2.633719, 4.760042, -1.443477
 C, 5.488333, 5.729512, 0.154246
 H, 6.406621, 4.623613, 1.759132
 H, 4.325271, 6.546876, -1.465369
 C, 6.511522, 6.839055, 0.154144
 H, 6.645909, 7.259590, -0.846884
 H, 6.203088, 7.660912, 0.812612
 H, 7.484539, 6.486885, 0.508728
 C, -6.841264, 6.515950, 0.142365
 H, -6.987238, 6.841442, 1.177515
 H, -6.587075, 7.395458, -0.456129
 H, -7.808515, 6.142975, -0.216820
 C, 3.813910, -3.423652, -0.020490
 C, 4.957421, -3.373431, 0.797334
 C, 3.740358, -4.445184, -0.982601
 C, 5.968005, -4.319005, 0.670721
 H, 5.043119, -2.585237, 1.536719
 C, 4.761537, -5.384047, -1.110002
 H, 2.893114, -4.481361, -1.659548
 C, 5.889680, -5.345387, -0.281900
 H, 6.837590, -4.258758, 1.320559
 H, 4.685468, -6.153251, -1.874455
 C, -3.558876, -3.690889, -0.019482
 C, -4.640651, -3.810458, -0.909170
 C, -3.492632, -4.592988, 1.057146
 C, -5.605109, -4.800324, -0.736373
 H, -4.712578, -3.125646, -1.748421
 C, -4.463157, -5.576664, 1.226209
 H, -2.692188, -4.498373, 1.783870
 C, -5.533660, -5.705228, 0.330366
 H, -6.427343, -4.871580, -1.443929
 H, -4.395598, -6.249690, 2.077385
 C, -6.563552, -6.795857, 0.499031
 H, -6.255859, -7.713591, -0.017876
 H, -6.707696, -7.050917, 1.553132
 H, -7.531941, -6.499777, 0.085341
 C, 6.981935, -6.380712, -0.397474
 H, 7.973183, -5.930717, -0.282571
 H, 6.884618, -7.148468, 0.380503
 H, 6.950639, -6.889664, -1.364941
 H, 5.091507, 1.342394, -0.593280

12c

Energy = -2756.664002

C, -1.279398, 2.914011, 0.136495
C, -0.690713, 4.206441, 0.085660
C, 0.683128, 4.207611, -0.085184
C, 1.274009, 2.916189, -0.136208
S, -0.001659, 1.713558, 0.000262
H, -1.278553, 5.111145, 0.177347
H, 1.269429, 5.113318, -0.176821
C, -2.644240, 2.535884, 0.193144
C, 2.639510, 2.540459, -0.193033
C, 3.045788, 1.179048, -0.286946
C, 4.325137, 0.612054, 0.184946
C, 2.294146, 0.039975, -0.623125
N, 4.346060, -0.690286, 0.178769
H, 5.164030, 1.188266, 0.561140
C, 3.061760, -1.096197, -0.278749
H, 1.378484, 0.031129, -1.187357
C, -3.048022, 1.173733, 0.287004
C, -4.326258, 0.604351, -0.185025
C, -2.294263, 0.036073, 0.623215
N, -4.344740, -0.698025, -0.178833
H, -5.166201, 1.178992, -0.561280
C, -3.059700, -1.101537, 0.278735
H, -1.378636, 0.028962, 1.187525
C, 2.650801, -2.450894, -0.225727
C, -2.646239, -2.455477, 0.225708
C, 3.668981, -3.540750, -0.140073
C, 4.593951, -3.608800, 0.914547
C, 3.720957, -4.531853, -1.130868
C, 5.523395, -4.642005, 0.974405
H, 4.585547, -2.839108, 1.676247
C, 4.661008, -5.561063, -1.065880
H, 3.033933, -4.485664, -1.970779
C, 5.575642, -5.638613, -0.011209
H, 6.226455, -4.674089, 1.803453
H, 4.685034, -6.310842, -1.852755
H, -1.272613, -5.014415, 0.160028
C, -0.684257, -4.108833, 0.087815
C, 0.691674, -4.107669, -0.087868
C, -1.271098, -2.820846, 0.170547
C, 1.276310, -2.818683, -0.170615
H, 1.281575, -5.012250, -0.160017
S, 0.001576, -1.620834, -0.000149
C, -3.662446, -3.547168, 0.140067
C, -3.712524, -4.538442, 1.130788
C, -4.587390, -3.616812, -0.914469
C, -4.650711, -5.569351, 1.065809
H, -3.025501, -4.491072, 1.970635
C, -5.514965, -4.651696, -0.974318
H, -4.580460, -2.847041, -1.676104
C, -5.565304, -5.648478, 0.011218
H, -4.673302, -6.319232, 1.852628
H, -6.218051, -4.684985, -1.803297
C, -6.575729, -6.767738, -0.071927
H, -7.595056, -6.378664, -0.172634
H, -6.390384, -7.408761, -0.942113
H, -6.545365, -7.401069, 0.818914

C, 6.588126, -6.756013, 0.071919
H, 6.404259, -7.397103, 0.942367
H, 6.558603, -7.389664, -0.818723
H, 7.606782, -6.365055, 0.172143
C, -3.695751, 3.578974, 0.067647
C, -4.780869, 3.595465, 0.961825
C, -3.664772, 4.556027, -0.943283
C, -5.783209, 4.556211, 0.855129
H, -4.820773, 2.858631, 1.758015
C, -4.672997, 5.510483, -1.046409
H, -2.856998, 4.548181, -1.667988
C, -5.750829, 5.530891, -0.150605
H, -6.602889, 4.551689, 1.569197
H, -4.627659, 6.248082, -1.843856
C, 3.689145, 3.585446, -0.067641
C, 4.774211, 3.603826, -0.961844
C, 3.656407, 4.562529, 0.943201
C, 5.774814, 4.566391, -0.855243
H, 4.815435, 2.866997, -1.757972
C, 4.662906, 5.518817, 1.046231
H, 2.848647, 4.553293, 1.667908
C, 5.740687, 5.541096, 0.150412
H, 6.594489, 4.563292, -1.569324
H, 4.616241, 6.256406, 1.843610
C, 6.844496, 6.562001, 0.284776
H, 6.475915, 7.496531, 0.717936
H, 7.645040, 6.194111, 0.938806
H, 7.297622, 6.791526, -0.684090
C, -6.856479, 6.549787, -0.285078
H, -7.656251, 6.180475, -0.939252
H, -7.310168, 6.778430, 0.683732
H, -6.489540, 7.485014, -0.718132

13a

Energy = -4049.491042

C, 4.214091, -1.064929, -0.079658
C, 3.333324, -0.679006, -1.065603
C, 3.321377, 0.762339, -1.059820
C, 4.194367, 1.156826, -0.070413
N, 4.754710, 0.048077, 0.547587
C, 2.510528, 1.704396, -1.938659
C, 1.071607, 1.843484, -1.475001
C, 2.530482, -1.626084, -1.946508
C, 1.085640, -1.747767, -1.498550
S, 0.625221, 1.830448, 0.215783
C, -1.081625, 1.831169, -0.157304
C, -1.271383, 1.889161, -1.512762
C, -0.053186, 1.902178, -2.254982
C, -0.032711, -1.713013, -2.288070
C, -1.257076, -1.698505, -1.555720
C, -1.079691, -1.731666, -0.198468
S, 0.623285, -1.823360, 0.187801
C, -3.249396, -0.679093, 0.514102
C, -4.496029, -1.062345, 0.072614
N, -5.279613, 0.056099, -0.181409
C, -4.493092, 1.163186, 0.107729
C, -3.248079, 0.762422, 0.536603
C, -2.116345, -1.616348, 0.906075

C, -2.110344, 1.684237, 0.951066
C, 3.237992, 3.039136, -2.157776
C, -2.629724, 3.019667, 1.500592
C, -2.643074, -2.967806, 1.406006
Si, 6.000334, 0.044851, 1.863700
Si, -6.968406, 0.051096, -0.819851
C, 6.364724, 1.900856, 2.181758
C, 5.204668, -0.732411, 3.429717
C, 7.546247, -0.861691, 1.175844
C, 6.966044, 2.211065, 3.568170
C, 7.203577, 2.565523, 1.070201
C, 4.179472, -1.852882, 3.166765
C, 6.233460, -1.202280, 4.480057
C, 8.811034, -0.674017, 2.041627
C, 7.351841, -2.357362, 0.854163
C, -8.115091, -0.888541, 0.397063
C, -7.479920, 1.896443, -0.930766
C, -6.932663, -0.710960, -2.573937
C, -8.665388, 2.161783, -1.882035
C, -7.750771, 2.541314, 0.444246
C, -9.491921, -1.190083, -0.233785
C, -7.538826, -2.158849, 1.051635
C, -6.615019, -2.217988, -2.630032
C, -5.979446, 0.067124, -3.503510
C, -3.121718, 3.075666, 2.812718
C, -3.628219, 4.258740, 3.341878
C, -3.663827, 5.435717, 2.579225
C, -3.175747, 5.376245, 1.270769
C, -2.663115, 4.189960, 0.738764
C, -2.704182, -4.101370, 0.591744
C, -3.226184, -5.303431, 1.076392
C, -3.696399, -5.416046, 2.388179
C, -3.632747, -4.276244, 3.203261
C, -3.116490, -3.076950, 2.721338
C, 2.817544, 4.241324, -1.585959
C, 3.525924, 5.426449, -1.807510
C, 4.668428, 5.452379, -2.610913
C, 5.087526, 4.242566, -3.186093
C, 4.387483, 3.061688, -2.962790
C, 5.418213, 6.736988, -2.874588
C, -4.228777, -6.724536, 2.923296
C, -4.186872, 6.725550, 3.166358
C, 3.253924, -2.966053, -2.150129
C, 4.463305, -2.981775, -2.863876
C, 5.156269, -4.167552, -3.081029
C, 4.670602, -5.390536, -2.591040
C, 3.467950, -5.371959, -1.881865
C, 2.766628, -4.180944, -1.666304
C, 5.423370, -6.676793, -2.837420
H, 4.488402, -2.064122, 0.217108
H, 4.465392, 2.159197, 0.217344
H, 2.436251, 1.236370, -2.930704
H, 2.468140, -1.164724, -2.942928
H, -2.255497, 1.852882, -1.965958
H, -0.011377, 1.900653, -3.339560
H, 0.019837, -1.643370, -3.369872
H, -2.234393, -1.596344, -2.012990
H, -4.888794, -2.059496, -0.046301

H, -4.877346, 2.165739, 0.011814
H, -1.608520, -1.155016, 1.764417
H, -1.597178, 1.194102, 1.790031
H, 5.369594, 2.369730, 2.170546
H, 4.647313, 0.109423, 3.870509
H, 7.729962, -0.347177, 0.220256
H, 7.077147, 3.294777, 3.697631
H, 7.960720, 1.771081, 3.697134
H, 6.334039, 1.850594, 4.385237
H, 7.275775, 3.647314, 1.237545
H, 6.776162, 2.416263, 0.074324
H, 8.226679, 2.174636, 1.051682
H, 3.721697, -2.174113, 4.110833
H, 4.649991, -2.738413, 2.723704
H, 3.376365, -1.532787, 2.499180
H, 5.725121, -1.492429, 5.407989
H, 6.967403, -0.433075, 4.737478
H, 6.784488, -2.081896, 4.129705
H, 9.682075, -1.110305, 1.536846
H, 8.719804, -1.173704, 3.011063
H, 9.041314, 0.377975, 2.232257
H, 8.283280, -2.784287, 0.460998
H, 6.579557, -2.524660, 0.099851
H, 7.087160, -2.936977, 1.745883
H, -8.280112, -0.165350, 1.209317
H, -6.607183, 2.402274, -1.368380
H, -7.956535, -0.579723, -2.956591
H, -8.851023, 3.239596, -1.967029
H, -9.592889, 1.708878, -1.514764
H, -8.488557, 1.780951, -2.892380
H, -7.908301, 3.621835, 0.339640
H, -6.926299, 2.396192, 1.148764
H, -8.655633, 2.128719, 0.904640
H, -10.167818, -1.627836, 0.511134
H, -9.409901, -1.910159, -1.055727
H, -9.982262, -0.295001, -0.629276
H, -8.258834, -2.571732, 1.769545
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