Electronic Supplementary Materials for

Rational and Controllable Syntheses of variants of modified N-confused N-fused Porphodimethenes and Porphotrimethene with Adaptive properties

Manik Jana, [a] Sumit Sahoo, [a] Sanjay Kottekad, [b] Dandamudi Usharani [*b, c] and Harapriya Rath[*a]

[a] *School of Chemical Sciences, Indian Association for The Cultivation of Science, 2A/2B Raja S. C. Mullick Road, Jadavpur, Kolkata 700 032, India, E-mail: ichr@iacs.res.in*
[b] *Department of Food Safety and Analytical Quality Control Laboratory, CSIR-Central Food Technological Research Institute, Mysuru 570020 Karnataka, India, E-mail: ushad@cftri.res.in*
[c] *Academy of Scientific and Innovative Research (AcSIR), CSIR-HRDC, Ghaziabad, Uttar Pradesh, India*

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Materials and Methods:

1.1 Electronic absorption spectra were measured with a PerkinElmer Lambda 950 UV-visible-NIR spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVIII 600 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer (operating at 300.132/400.20/600.13 MHz for ^{1}H and 75.47/100.64/150.05 MHz for ^{13}C) using the residual solvents as the internal references for ^{1}H [($CHCl_3$ (δ = 7.26 ppm), CH_2Cl_2 (δ = 5.32 ppm). ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. Fluorescence emission spectra were examined in the Fluoromax-3 instrument (Horiba Jobin Yvon) using a quartz cell of 10 nm path length and slit width of 5 nm for both excitation and emission. 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 X-Ray structure determination.

A specimen of $C_{99}H_{68}Cl_2F_8N_6S_4$, approximate dimensions 0.100 mm x 0.100 mm x 0.100 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 2.42 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 53660 reflections to a maximum θ angle of 26.45° (0.80 Å resolution), of which 18771 were independent (average redundancy 2.859, completeness = 99.1%, R_{int} = 16.23%, R_{sig} =24.49%) and 5816 (30.98%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.72(3) Å, b = 16.498(18) Å, c = 18.03(2) Å, α =94.031(19) °, β = 100.44(4) °, γ = 90.63(4) °, volume = 4586. (11) $Å^3$, are based upon the refinement of the XYZ-centroids of 4152 reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9780 and 0.9780. The final anisotropic full-matrix least-squares refinement on F^2 with 1078 variables converged at R1 = 9.00%, for the observed data and wR2 = 28.39% for all data. The goodness-of-fit was 0.920. The largest peak in the final difference electron density synthesis was 0.414 $e^-/Å^3$ and the largest hole was -0.349 $e^-/Å^3$ with an RMS deviation of 0.068 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.226 g/cm^3 and F (000), 1748 e-.

1.3 Determination of Association Constant by UV-vis Absorption Spectroscopic titration method:

For UV-vis titrations, stock solution of **10-12** were prepared in $CHCl_3$. The solution of the guest was also prepared in $CHCl_3$. The spectra of these solutions were recorded by means of UV-vis absorption methods. Binding constant was calculated according to the Benesi-Hildebrand equation. K_a was calculated following the equation stated below.

$$1/(A\text{-}A_0) = 1/\{K_a(A_{max} - A_0)\,[G]_n\} + 1/[A_{max} - A_0]$$

Here A_0 is the absorbance of receptor in the absence of guest, A is the absorbance recorded in the presence of added guest, A_{max} is absorbance in presence of added $[G]_{max}$ and K_a is the association constant (M^{-1}). The association constant (K_a) could be determined from the slope of the straight line of the plot of $1/(A\text{-}A_0)$ against $1/[G]_n$.

1.4 Job's plot:

The stoichiometry between **10**-**12** and analyte was evaluated by Job's plot method. A solution of **10**-**12** and guest (**G**) of same concentration were mixed in different proportions keeping a final volume of 2 mL. The related compositions for **10/11/12**: **G** (v/v) were 2:0,1.8: 0.2,1.6: 0.4, 1.4:0.6, 1.2:0.8, 1.0:1.0, 0.8:1.2, 0.6:1.4, 0.4:1.6, 0.2:1.8. The solutions thus prepared were used as such to record their absorption spectra. The mole fraction of analyte *i.e.,* (X_M) was calculated using the following equation (X_M) = [**G**]/ [**10** or **11** or **12**] + [**G**]. The mole fraction of analytes (X_M) was plotted against absorbance to obtain Job's plot.[S1] The mole fraction at which absorbance intensity appeared to be minimum was taken as the stoichiometry of their interaction.

1.5 Theoretical Calculation

Based on the X-ray crystal structure of **10**, the geometries for **11** and **12** were modelled. All these macrocycles were fully optimized at the DFT level using B3LYP [S2] with 6-31G (d, p) basis set. [S3] Further fully optimized stationary points were characterized by harmonic analysis to ensure that all the structures are minima on the potential energy surface. Also, the deprotonated [**10**]$^-$, [**12**]$^-$ and with Bu_4N^+ counter ions [**10**$^-$ TBA$^+$], [**12**$^-$ TBA$^+$] and anion bound complexes of **11** with fluoride and acetate ([**11**-F]$^-$, [**11**-OAc]$^-$, [**11**-TBAF] and [**11**-TBOAc]) were optimized with same basis set and ascertained the frequencies to be minima. Also, employed counter poise method [S4] for basis set superimposition error for obtaining binding energies for anion bound complexes. Over the years, polarized continuum model (PCM) [S5] has been reported to be the most successful and cost-effective model to examine the solvent effect. We have used dichloromethane as solvent. Further, the time dependent density functional theory (TD-DFT) [S6] has been used to compute the electronic absorption spectra, singlet vertical excitation energies and oscillator strengths on the ground state optimized geometries of **10**,**11** and **12**. Further, predicted ^{1}H NMR Nuclear Independent Chemical Shifts (NICS) values[7a] with gauge independent atomic orbital (GIAO) method[7b, c] were obtained at the same level of theory with tetramethylsilane as standard reference. All computations were carried out with Gaussian 16 program package. [S8] Electronic structure, excitation analysis was performed using chemcraft, and Multiwfn programs. [S9]

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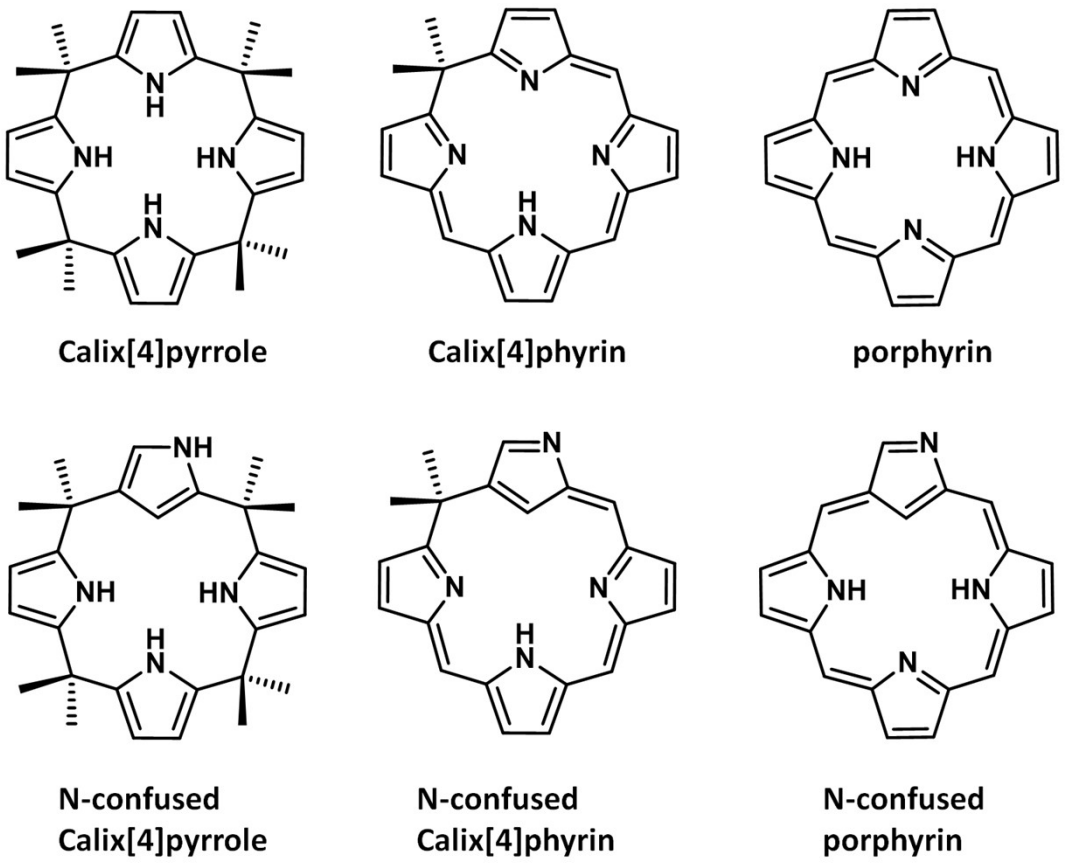


Chart S1. Structural relationship between Calixpyrrole- -calixphyrin -porphyrin

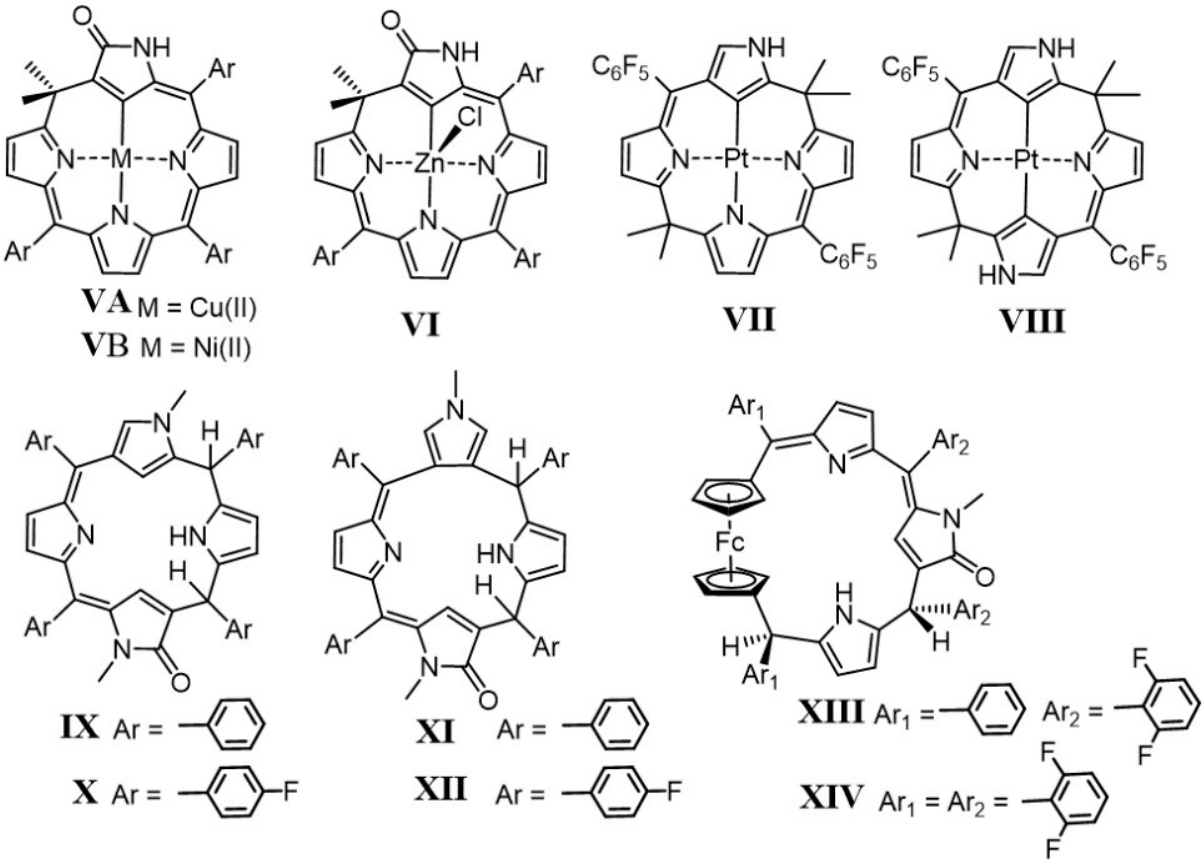
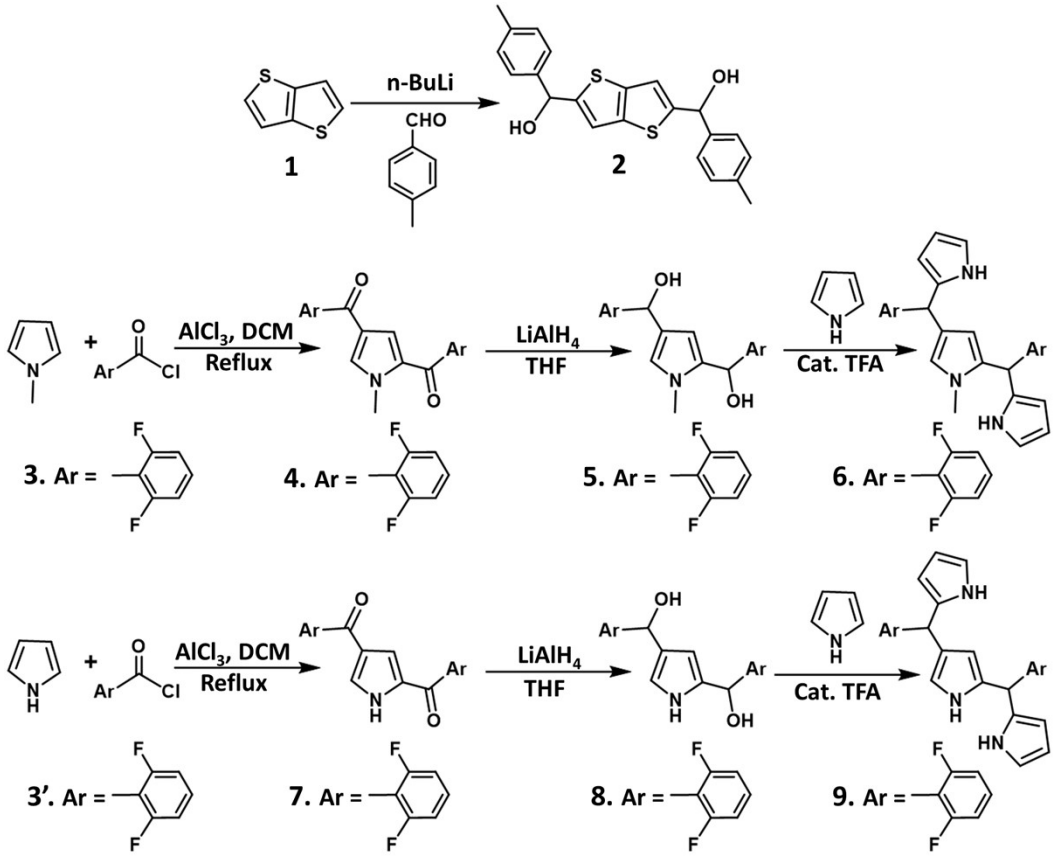
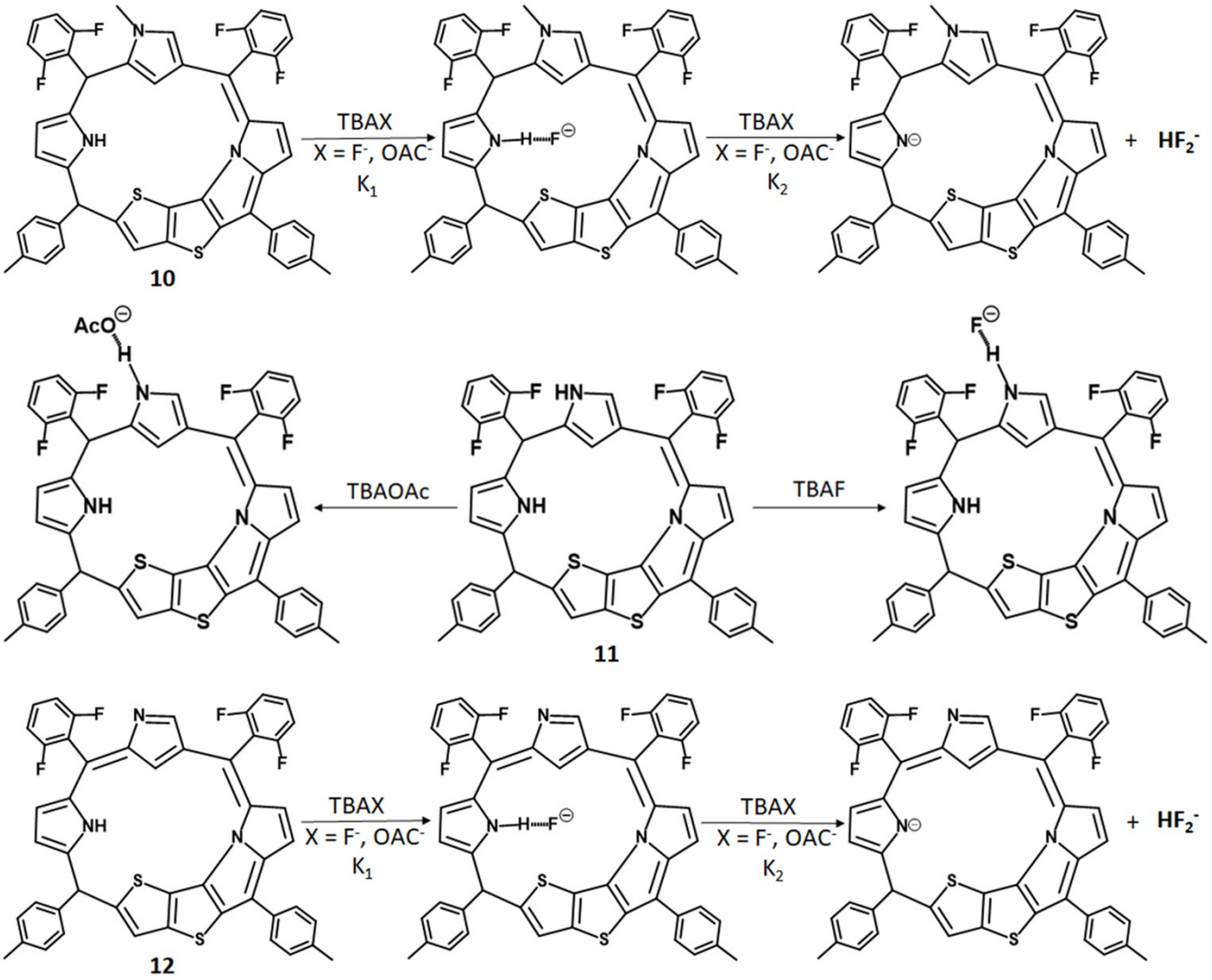


Chart S2. Literature known N-confused calixphyrins

2.0 Synthesis:



Scheme S1. Synthesis of all precursors **2**, [S10] **6**, [S11] and **9** [S12] used for the macrocycles reported in the manuscript



Scheme S2. Calixphyrins **10-12** as anion receptors [anion-receptor association (deprotonation)]

Synthesis of **10**: Tripyrrane **6** (0.463 g, 1 mmol) and diol **2** (0.380 g, 1 mmol) were taken in a round bottom flask, to it 740 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. After that *p*-Toluenesulfonic acid (0.035 g, 0.185 mmol) was added to the reaction mixture and stirred for 90 minutes under dark condition. After that, *p*-chloranil (0.368 g, 1.5 mmol) was added and the resulting mixture was refluxed for 90 minutes in open air. After complete removal of solvent from reaction mixture by rotary evaporator, the compound was filtered through a short pad of basic alumina column. The crude mixture was purified by silica gel (200-400 mesh) column chromatography using 80% dichloromethane/hexane as eluent. The red colored **10** collected from column was evaporated and recrystallized from CH_2Cl_2/Hexane yielding **10** as red crystalline solid.

[**10**] Yield. ~240 mg (~30%). Mp > 350°C. R_f = 0.4 (C_6H_{14}/CH_2Cl_2 = 80:20). HRMS (ESI-TOF) *m/z* calc. for $C_{49}H_{33}F_4N_3S_2$ $[M]^+$, 803.2052; found, 803.2050. Elemental analysis Calc. for $C_{49}H_{33}F_4N_3S_2$: C, 73.21; H, 4.14; N, 5.23. Found: C, 73.68; H, 4.21; N, 5.18. UV-vis (CH_2Cl_2, λ [nm], (ϵ [$M^{-1}cm^{-1} \times 10^4$]), 298K): 330 (2.53), 442 (1.15), 515 (0.84). ^1H NMR ($CDCl_3$, 400 MHz): δ 8.54 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.28 (s, 1H), 7.23 – 7.15 (m, 3H), 7.14 (s, 1H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.94 – 6.86 (m, 5H), 6.80 (t, *J* =

8.6 Hz, 1H), 6.68 (s, 1H), 6.12 (br, 2H), 6.06 (br, 1H), 6.05 (br, 1H), 5.78 (br, 1H), 5.76 (s, 1H, *meso*-CH), 5.7 (s, 1H, *meso*-CH), 3.05 (s, 3H, N-Me), 2.40 (s, 3H, Tol-Me), 2.30 (s, 3H, Tol-Me). ^{13}C {^{1}H} NMR ($CDCl_3$, 101 MHz): δ 162.54, 160.09, 160.0, 151.02, 141.83, 139.33, 136.98, 136.44, 135.94, 135.81, 134.56, 132.54, 131.50, 129.83, 129.65, 129.44, 129.24, 128.90, 128.79, 128.52, 128.22, 127.69, 126.51, 126.40, 126.25, 125.83, 120.93, 119.79, 118.54, 117.52, 115.75, 112.81, 112.38, 112.35, 112.13, 112.10, 111.68, 111.59, 111.46, 111.40, 109.65, 109.59, 109.31, 107.19, 46.85, 34.42, 33.00, 21.38, 21.10.

Synthesis of **11**: Tripyrrane **9** (0.449 g, 1 mmol) and diol **2** (0.380 g, 1 mmol) were taken in a round bottom flask, to it 740 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. After that *p*-Toluenesulfonic acid (0.035 g, 0.185 mmol) was added to the reaction mixture and stirred for 90 minutes under dark condition. After that, *p*-chloranil (0.368 g, 1.5 mmol) was added and the resulting mixture was refluxed for 90 minutes in open air. After complete removal of solvent from reaction mixture by rotary evaporator, the compound was filtered through a short pad of basic alumina column. The crude mixture was purified by silica gel (200-400 mesh) column chromatography using dichloromethane/hexane as eluent. The red colored **11** collected from column were evaporated and recrystallized from CH_2Cl_2/Hexane yielding **11** as red crystalline solid.

[**11**] Yield. ~198 mg (~25%), Mp> 350°C. R_f = 0.3 (EtOAc/CH_2Cl_2 = 1:9). HRMS (ESI-TOF) *m/z* calc. for $C_{48}H_{31}F_4N_3S_2$ $[M]^+$, 789.1896; found, 789.1895. Elemental analysis Calc. for $C_{48}H_{31}F_4N_3S_2$: C, 72.99; H, 3.96; N, 5.32. Found: C, 73.11; H, 4.12; N, 5.29. UV-vis (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1} × 10^4]), 298K): 333 (1.01), 455 (0.48), 541 (0.32). [**11**] ^{1}H NMR ($CDCl_3$,600 MHz): δ 8.63 (s, 1H), 8.46 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 2H), 7.38 – 7.30 (m, 4H), 7.18 (s, 1H), 7.12 (d, *J* = 7.7 Hz, 2H), 7.09 (s, 1H), 7.02 (br, 2H), 6.93 (br, 3H), 6.87 (d, *J* = 5.9 Hz, 1H), 6.84 (s, 1H), 6.06 (d, *J* = 5.4 Hz, 1H), 6.04 (s, 1H), 5.92 (br, 1H), 5.73 (s, 1H, *meso*-CH), 5.66 (s, 1H, *meso*-CH), 5.34 (br, 1H), 2.42 (s, 3H, Tol-Me), 2.35 (s, 3H, Tol-Me). ^{13}C {^{1}H} NMR ($CDCl_3$, 151 MHz): δ 160.34, 153.50, 141.39, 138.71, 137.81, 137.35, 136.66, 136.57, 134.98, 132.71, 130.90, 130.29, 130.23, 129.91, 129.37, 129.32, 129.13, 128.96, 128.67, 128.58, 128.50, 128.41, 128.33, 128.27, 126.58, 126.25, 124.97, 122.42, 118.92, 117.99, 117.93, 116.50, 114.60, 114.21, 112.20, 112.03, 112.02, 111.89, 111.73, 111.57, 108.70, 108.62, 105.93, 104.19, 46.54, 33.30, 21.42, 21.22.

Synthesis of **12**: **11** (0.078 g, 1 mmol) was taken in a round bottom flask, to it 10 mL of dry CH_2Cl_2 and *p*-chloranil (0.245 g, 1 mmol) [or DDQ, 0.272 g, 1mmol] was added and stirred under reflux for 1 hour in air. The reaction mixture was evaporated in a rotary evaporator and was purified by silica gel column chromatography followed by recrystallization from CH_2Cl_2/Hexane to obtain compounds **12** as air stable brownish black solid Yield. ~71 mg (~90%).

[**12**] Yield. ~71 mg (~90%), Mp> 350°C. R_f = 0.4 (C_6H_{14}/CH_2Cl_2= 20:80). HRMS (ESI-TOF) *m/z* calc. for $C_{48}H_{30}F_4N_3S_2$ $[M+H]^+$, 788.1817; found, 788.1818. Elemental analysis Calc. for $C_{48}H_{29}F_4N_3S_2$: C, 73.17; H, 3.71; N, 5.33. Found: C, 73.78; H, 3.87; N, 5.29. UV-vis (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1} × 10^4]), 298K): 333 (0.80), 445 (1.26), 637 (0.16). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.23 (s, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.38 (d, *J* = 6.6 Hz, 4H), 7.25-7.19 (m, 4H), 7.16 (s, 1H), 6.94 (t, *J* = 8.5 Hz, 3H), 6.89 (t, *J* = 8.0 Hz,

2H), 6.75 (d, *J* = 6.0 Hz, 1H), 6.53 (br, 1H), 5.95 (br, 2H), 5.87 (s, 1H), 5.85 (s, 1H), 5.68 (s, 1H, *meso*-CH), 2.41 (s, 3H, Tol-Me), 2.40 (s, 3H, Tol-Me). ^{13}C {^{1}H} NMR ($CDCl_3$, 151 MHz): δ 167.48, 161.81, 161.02, 159.31, 157.15, 152.80, 149.52, 147.21, 144.69, 143.19, 142.33, 140.22, 139.85, 139.39, 138.28, 138.15, 137.97, 137.25, 135.33, 130.93, 130.05, 129.56, 129.46, 129.12, 128.66, 128.14, 128.07, 124.75, 124.60, 124.29, 124.12, 122.30, 121.88, 121.71, 120.47, 119.23, 114.21, 111.82, 111.79, 111.68, 111.65, 111.18, 111.03, 110.18, 95.76, 47.86, 21.44, 21.26.

3. Supplementary Data:

3.1 Mass Spectra

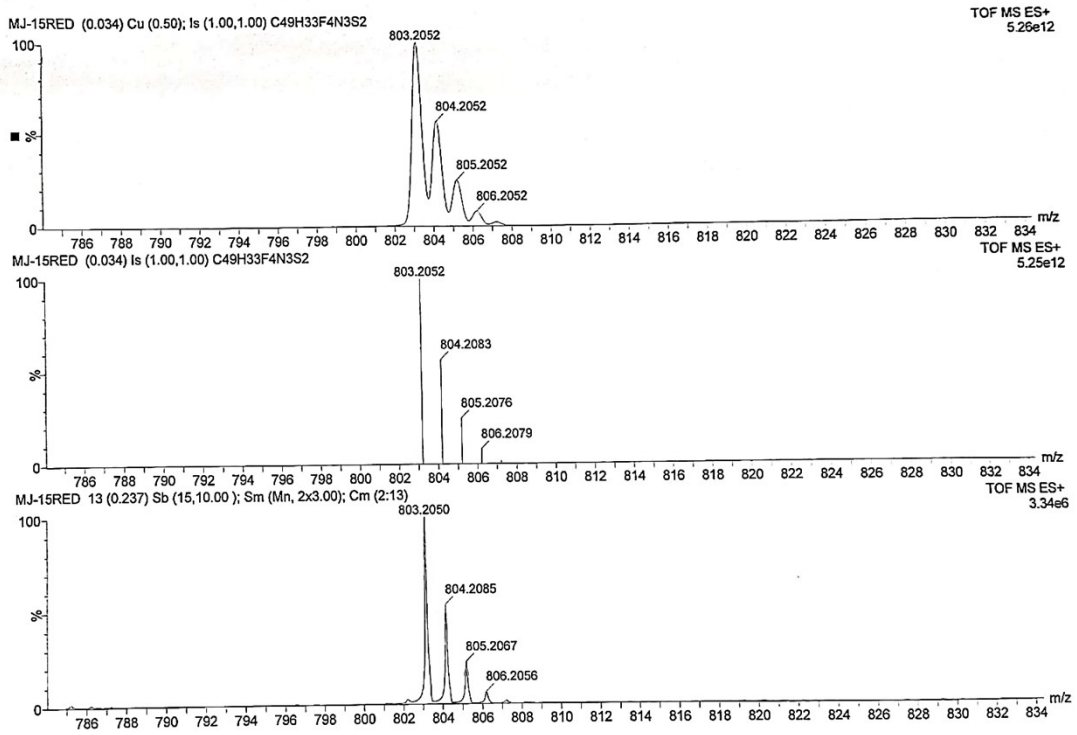


Fig. S1 HRMS Spectra of **10**.

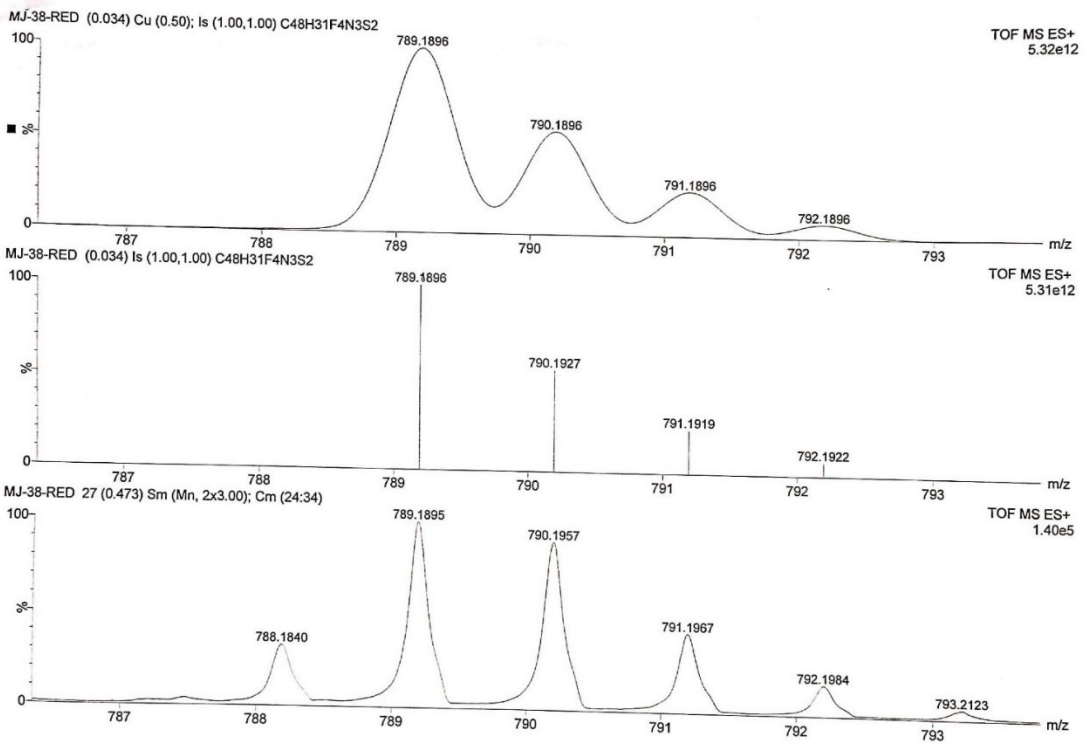


Fig. S2 HRMS Spectra of **11**.

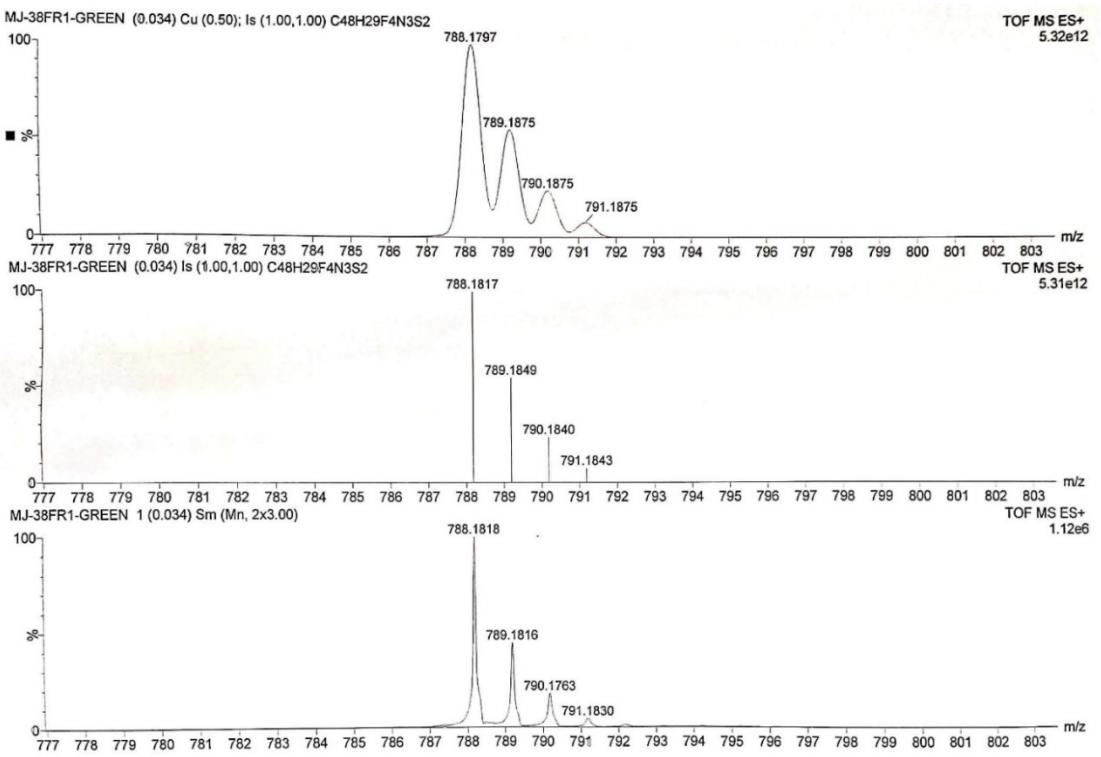


Fig.S3 HRMS Spectra of **12**.

3.2 UV-vis spectra:

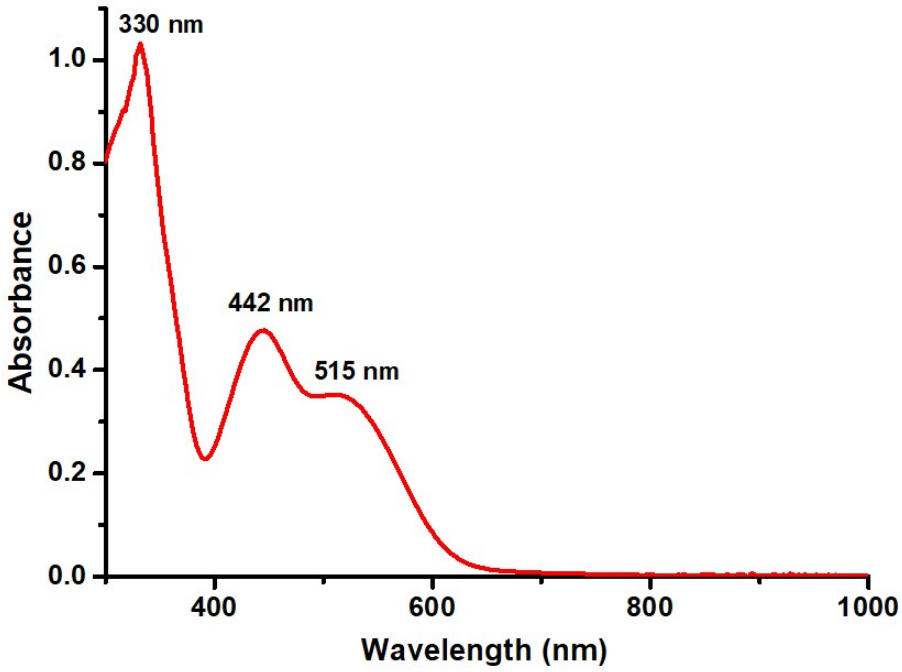


Fig. S4 **UV**-vis Spectra of **10**.

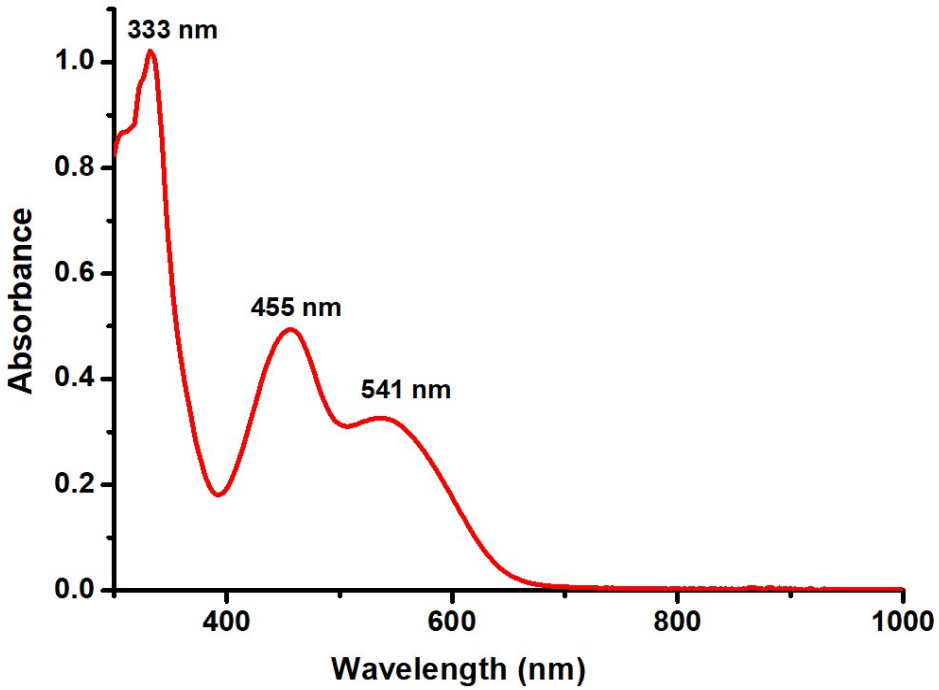


Fig. S5 UV-vis Spectra of **11**.

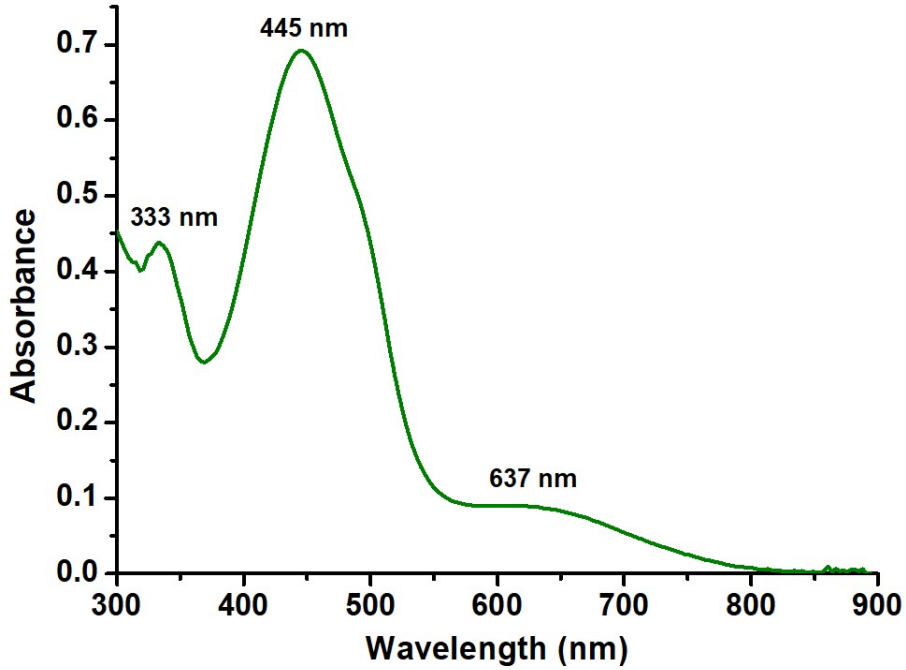


Fig. S6 UV-vis Spectra of **12**.

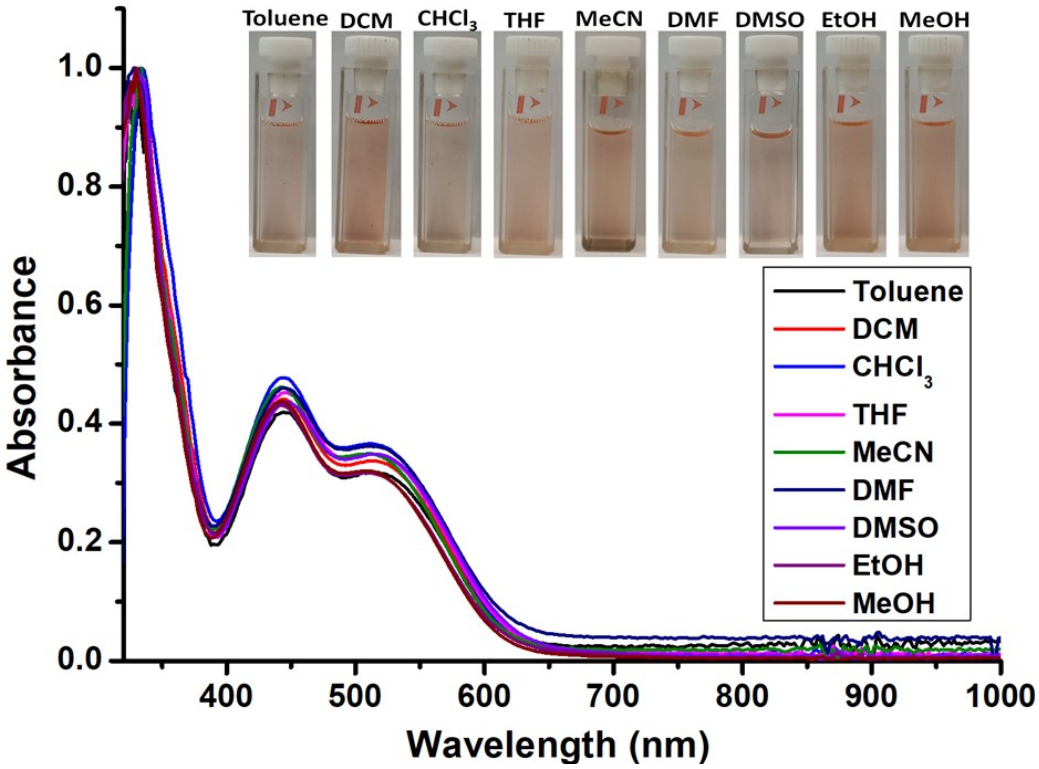


Fig. S7 UV-vis Spectral change induced upon change of solvent systems for receptor **10**.

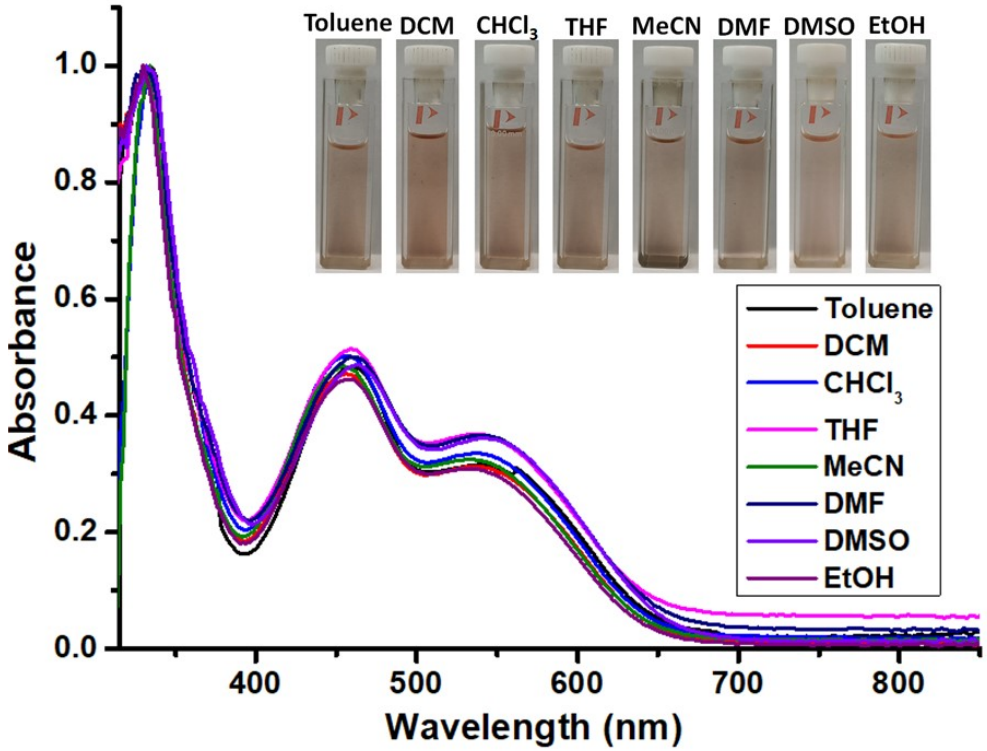


Fig. S8 UV-vis Spectral change induced upon change of solvent systems for receptor **11**.

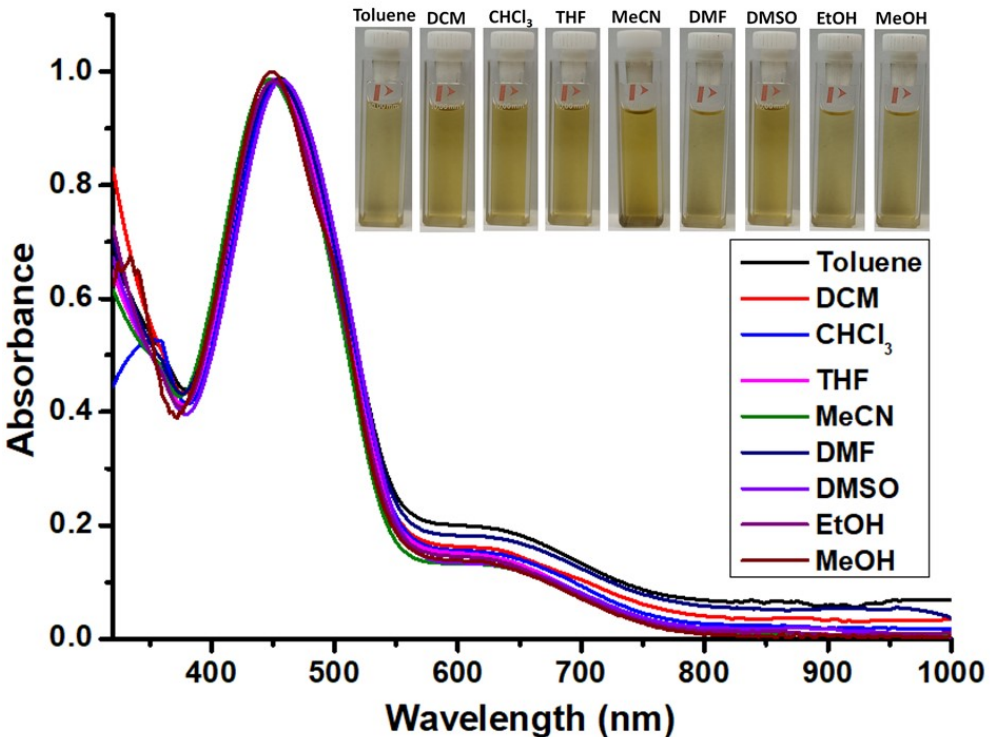


Fig. S9 UV-vis Spectral change induced upon change of solvent systems for receptor **12**.

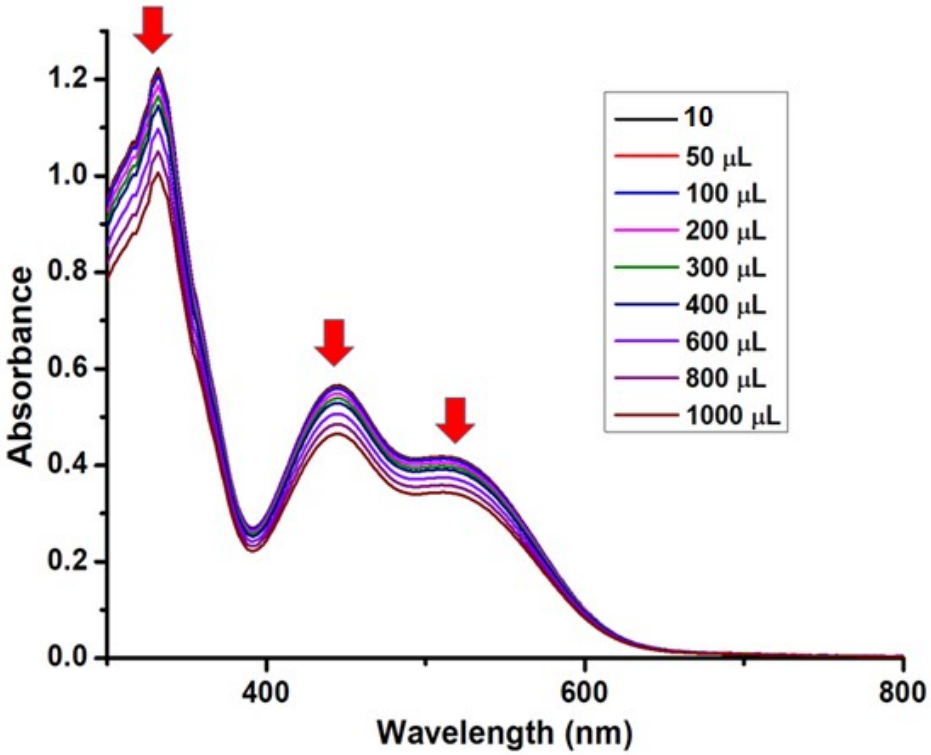


Fig. S10 Change in absorption spectrum of **10** (4.98 x 10^{-5} M) upon addition of TBABr (0.5 M) in $CHCl_3$ at 298 K.

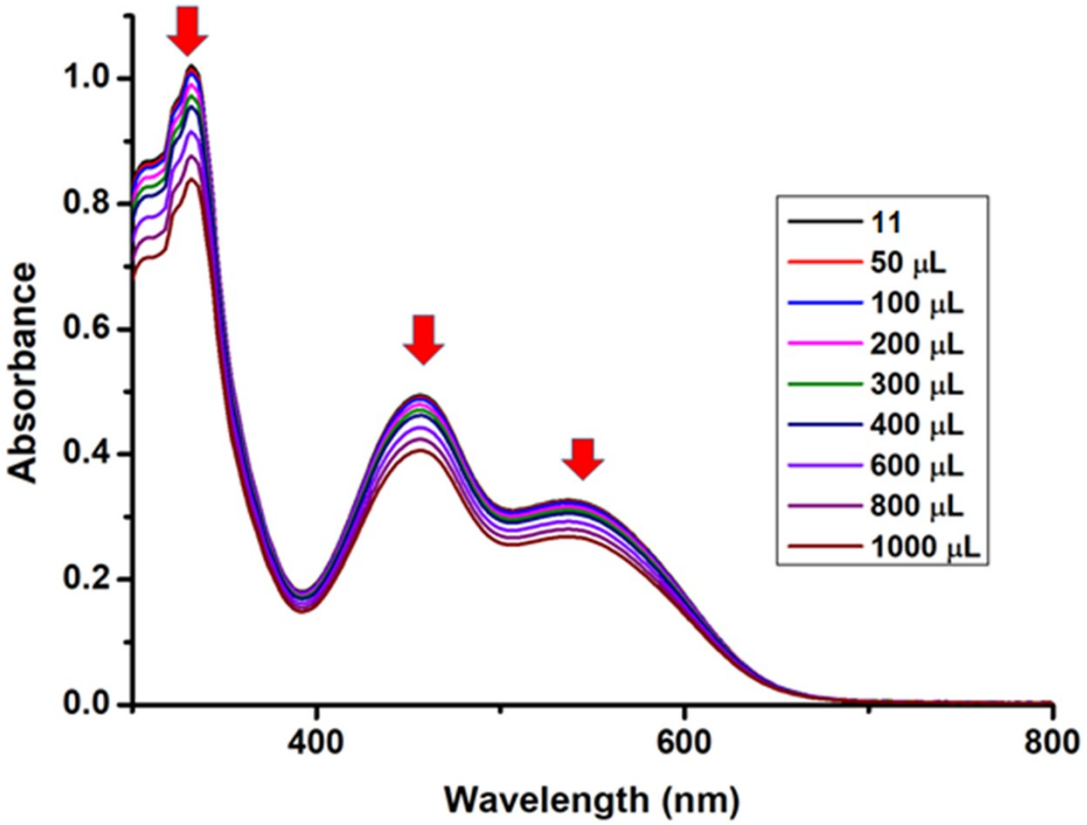


Fig.S11 Change in absorption spectrum of **11** (9.08 x 10^{-5} M) upon addition of TBABr (0.5 M) in $CHCl_3$ at 298 K.

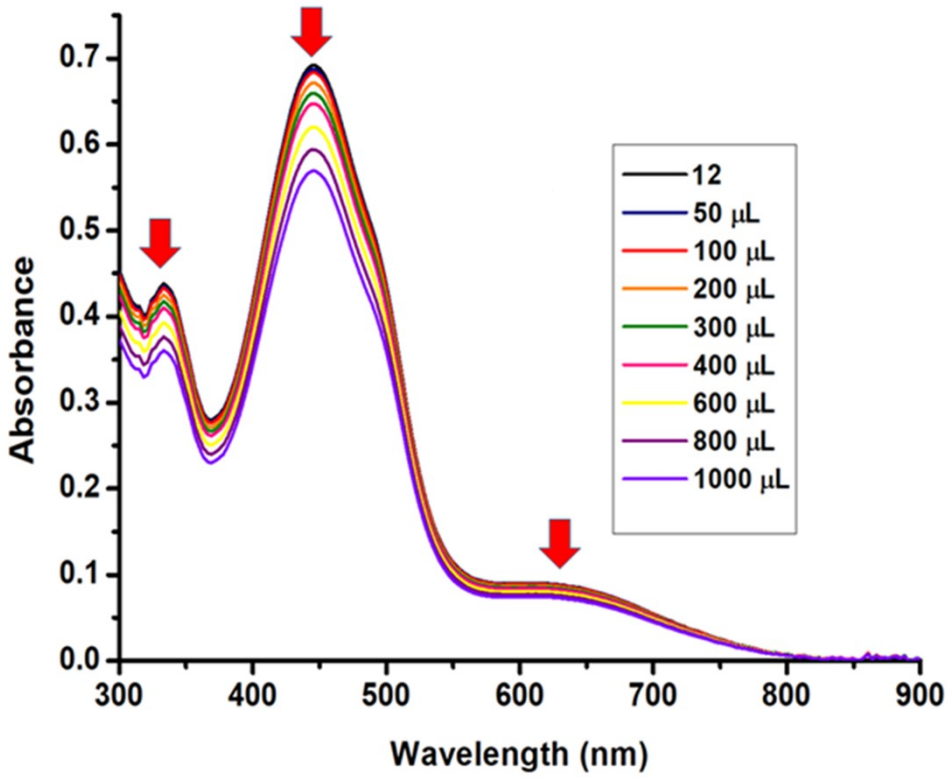


Fig. S12 Change in absorption spectrum of **12** (4.1 x 10^{-5} M) upon addition of TBABr (0.5 M) in $CHCl_3$ at 298 K.

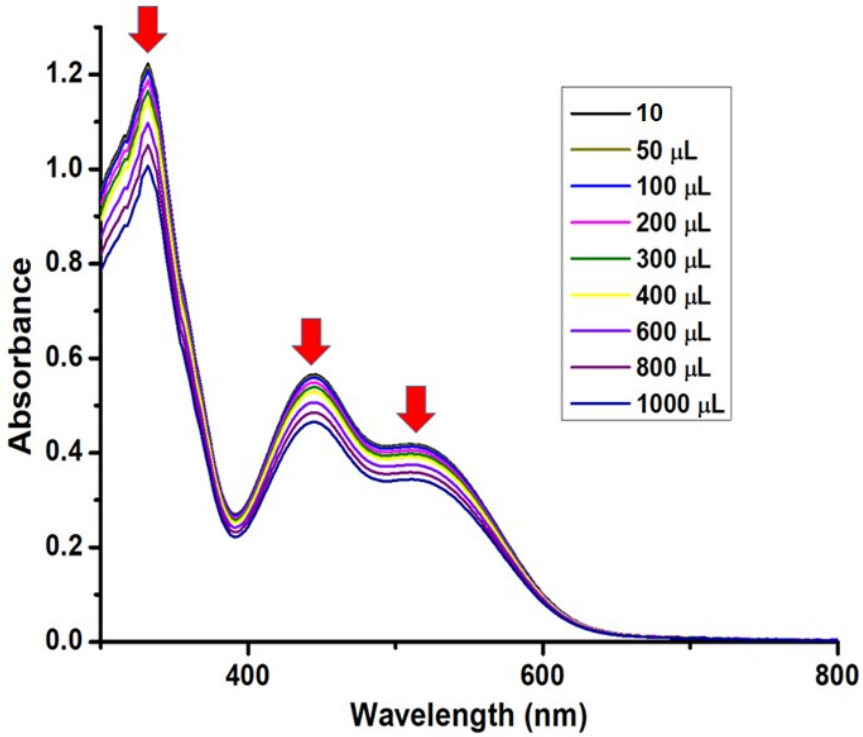


Fig. S13 Change in absorption spectrum of **10** (4.98 x 10^{-5} M) upon addition of TBACl (0.5 M) in $CHCl_3$ at 298 K.

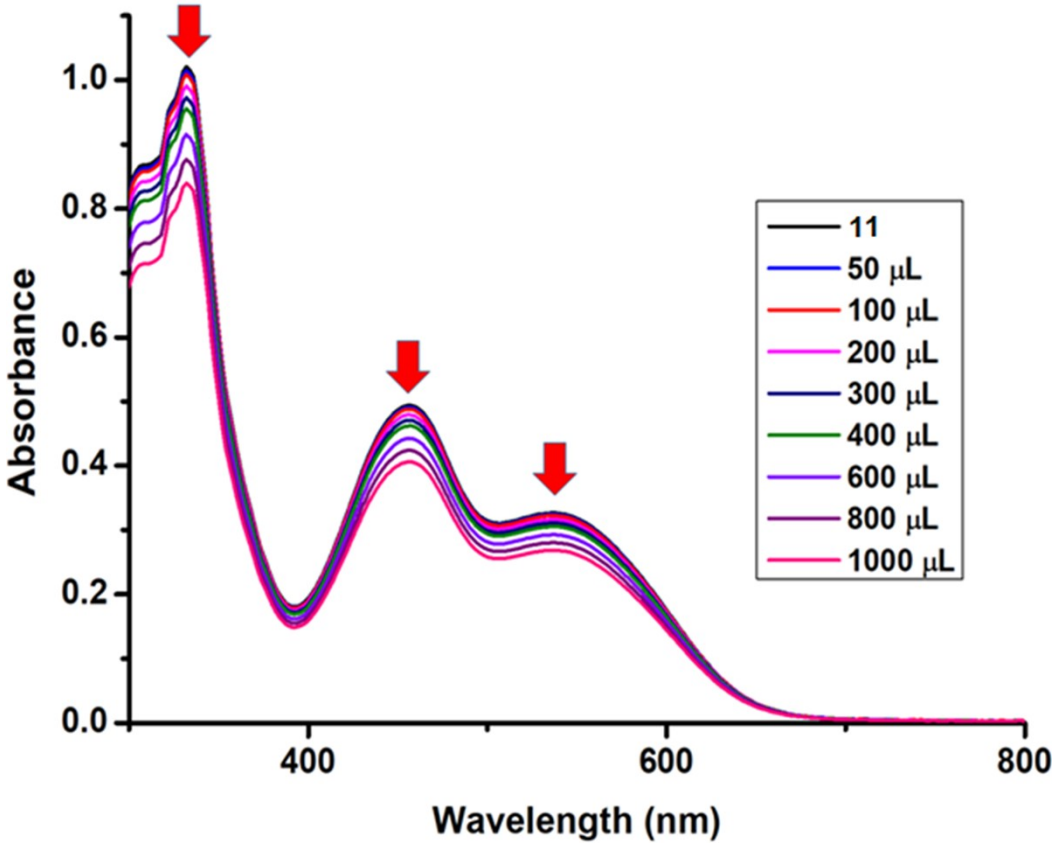


Fig. S14 Change in absorption spectrum of **11** (9.08 x 10^{-5} M) upon addition of TBACl (0.5 M) in $CHCl_3$ at 298 K.

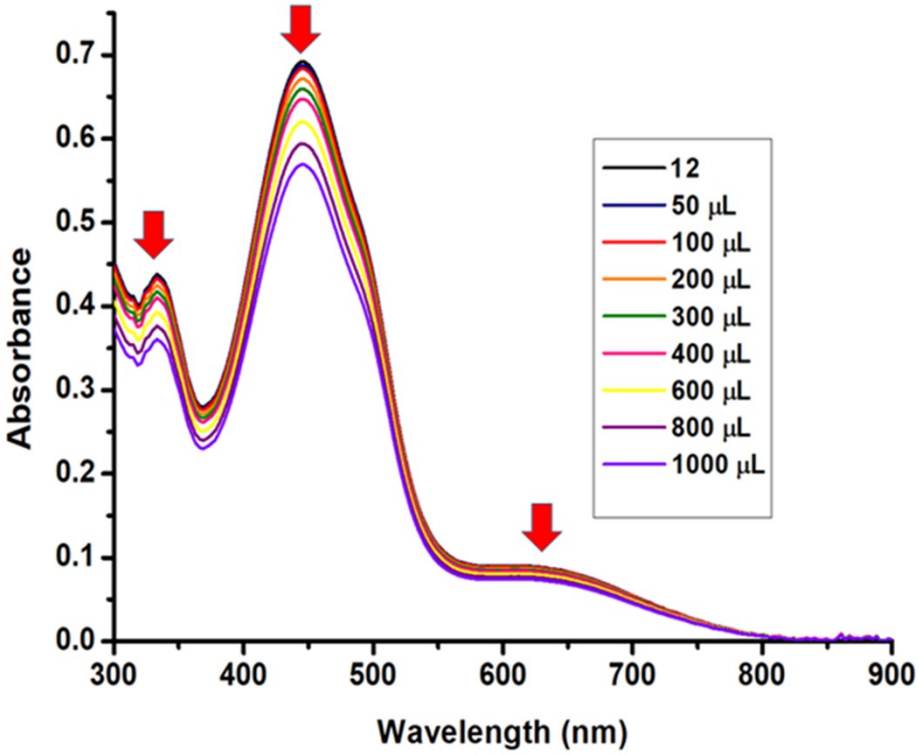


Fig. S15 Change in absorption spectrum of **12** (4.10 x 10^{-5} M) upon addition of TBACl (0.5 M) in $CHCl_3$ at 298 K.

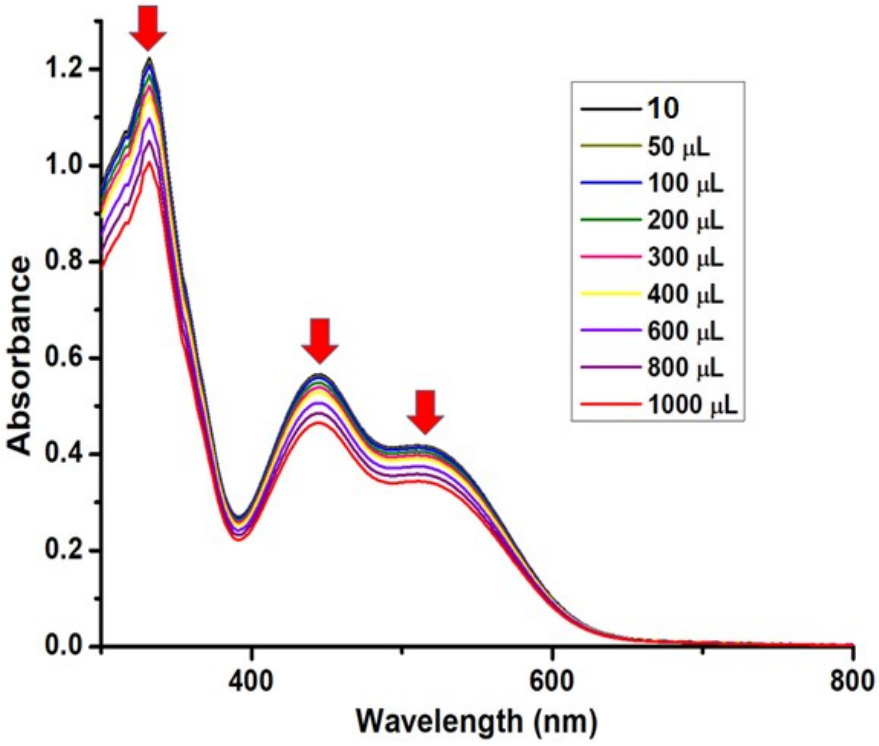


Fig. S16 Change in absorption spectrum of **10** (4.98 x 10^{-5} M) upon addition of TBAI (0.5 M) in $CHCl_3$ at 298 K.

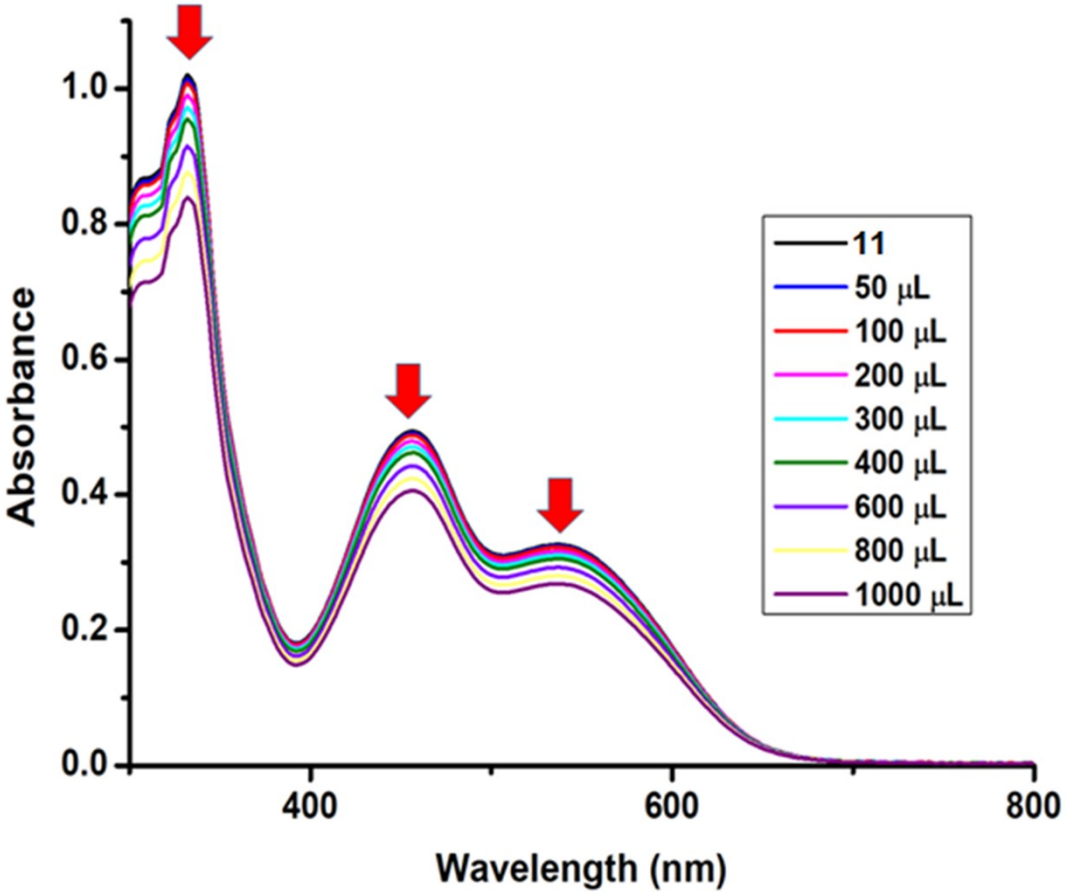


Fig. S17 Change in absorption spectrum of **11** (9.08 x 10^{-5} M) upon addition of TBAI (0.5 M) in $CHCl_3$ at 298 K.

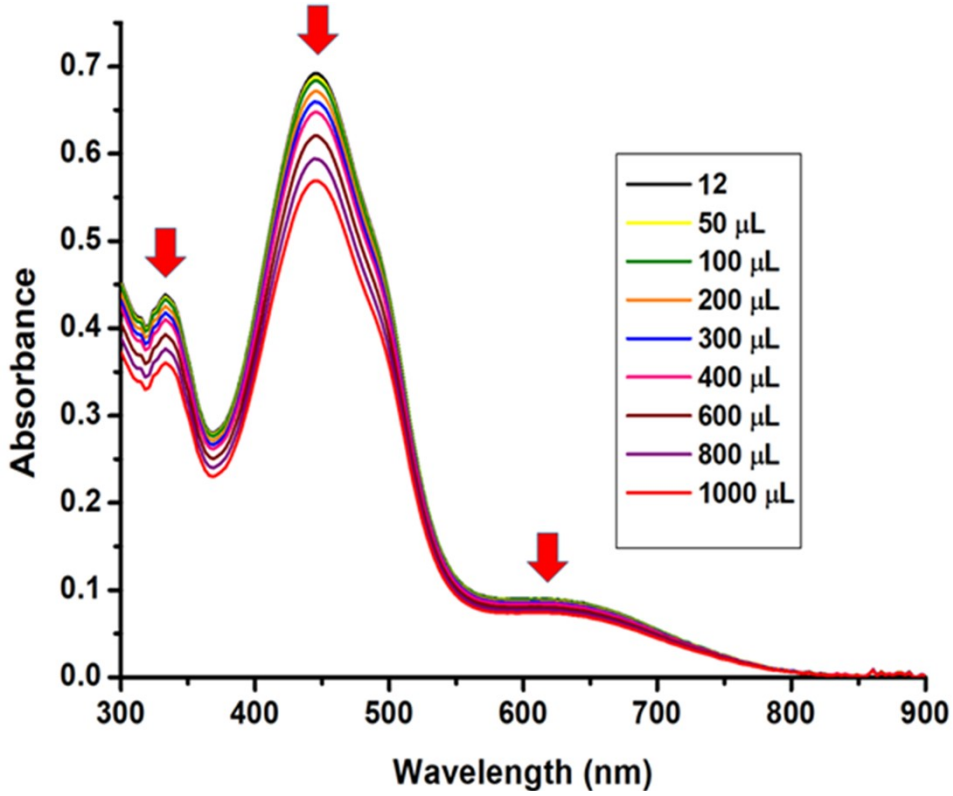


Fig. S18 Change in absorption spectrum of **12** (4.1 x 10^{-5} M) upon addition of TBAI (0.5 M) in $CHCl_3$ at 298 K.

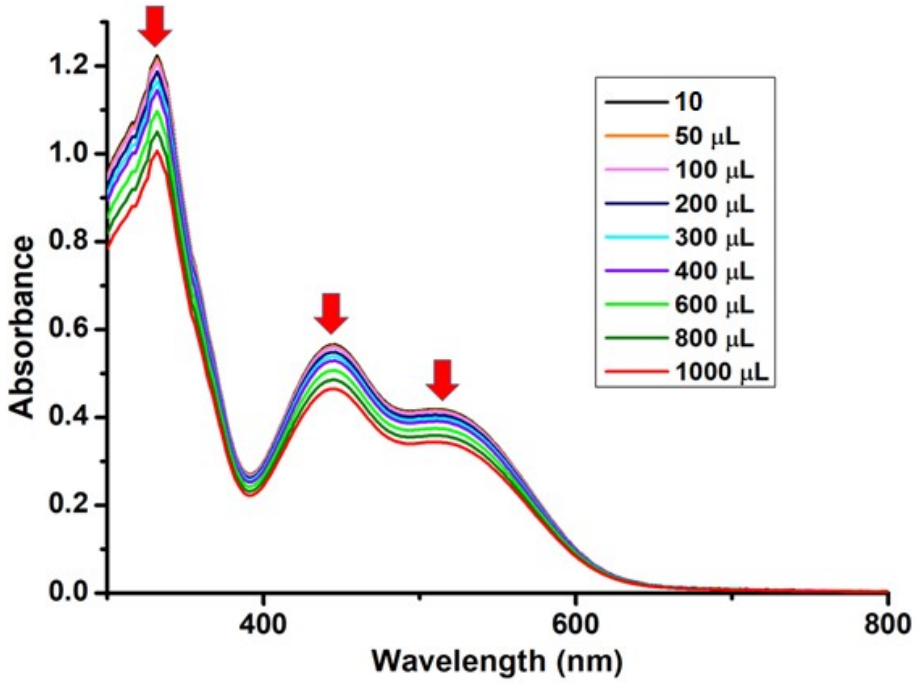


Fig.S19 Change in absorption spectrum of **10** (4.98 x 10^{-5} M) upon addition of $TBAH_2PO_4$ (0.5 M) in $CHCl_3$ at 298 K.

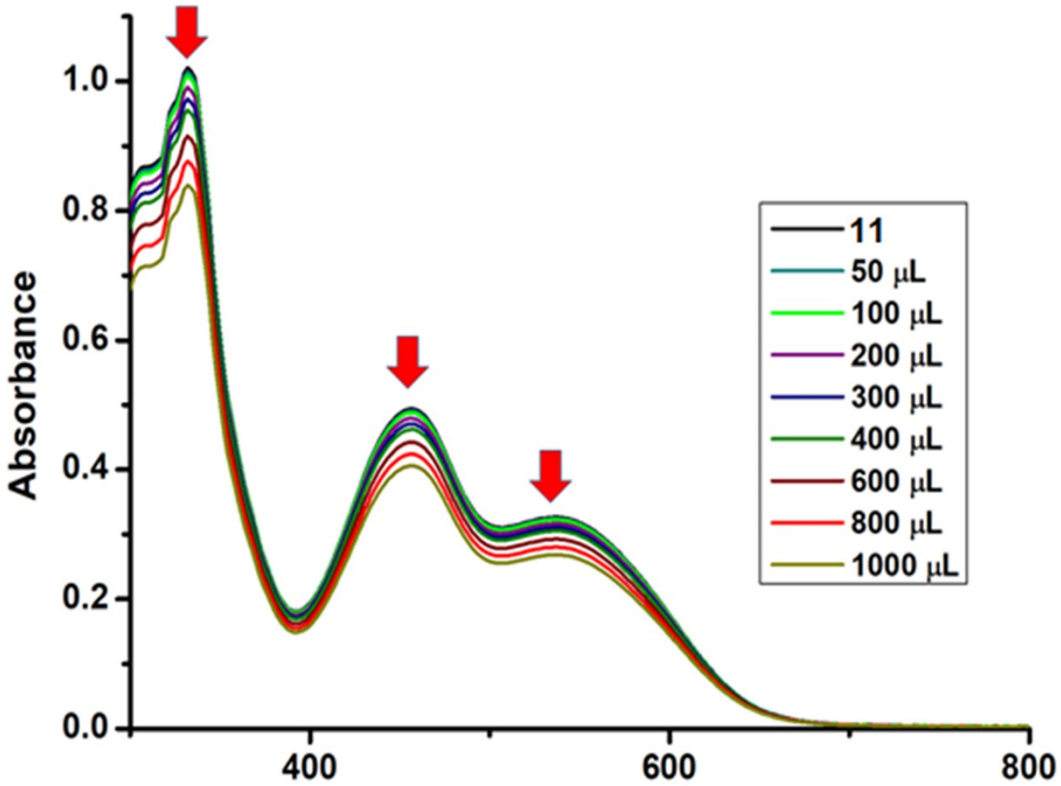


Fig. S20 Change in absorption spectrum of **11** (9.08 x 10^{-5} M) upon addition of $TBAH_2PO_4$ (0.5 M) in $CHCl_3$ at 298 K.

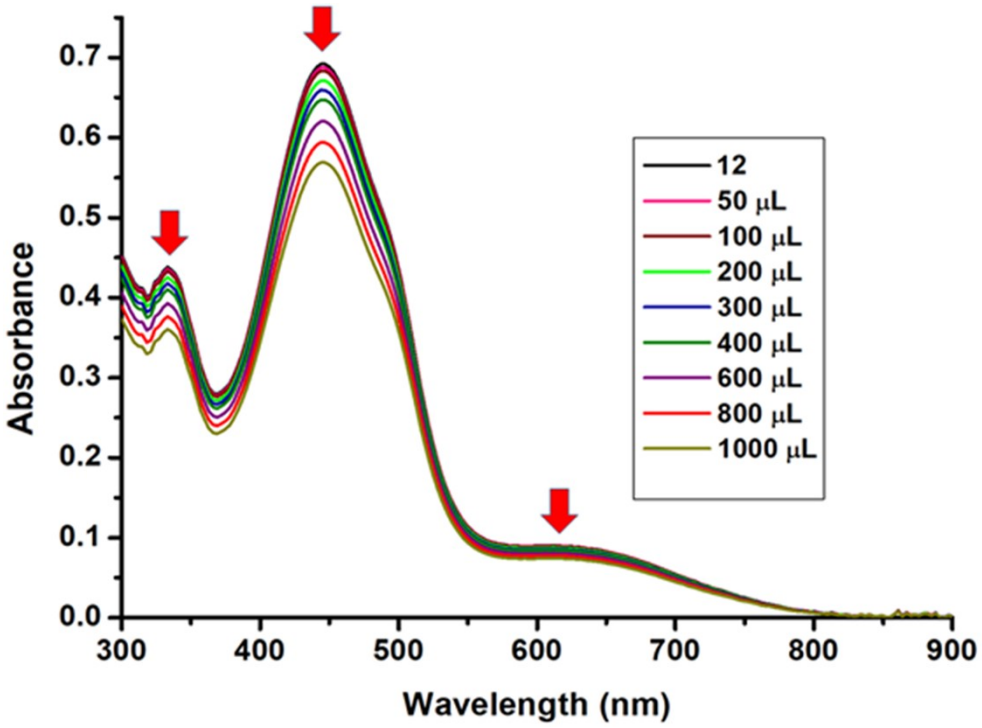


Fig.S21 Change in absorption spectrum of **12** (4.1 x 10^{-5} M) upon addition of $TBAH_2PO_4$ (0.5 M) in $CHCl_3$ at 298 K.

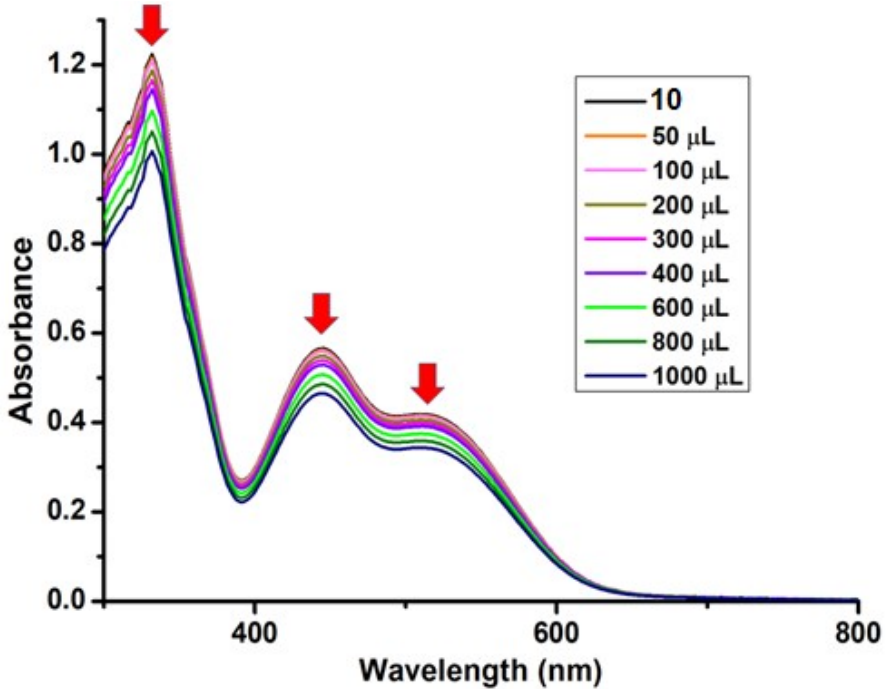


Fig. S22 Change in absorption spectrum of **10** (4.98 x 10^{-5} M) upon addition of $(TBA)_3HP_2O_7$ (0.5 M) in $CHCl_3$ at 298 K.

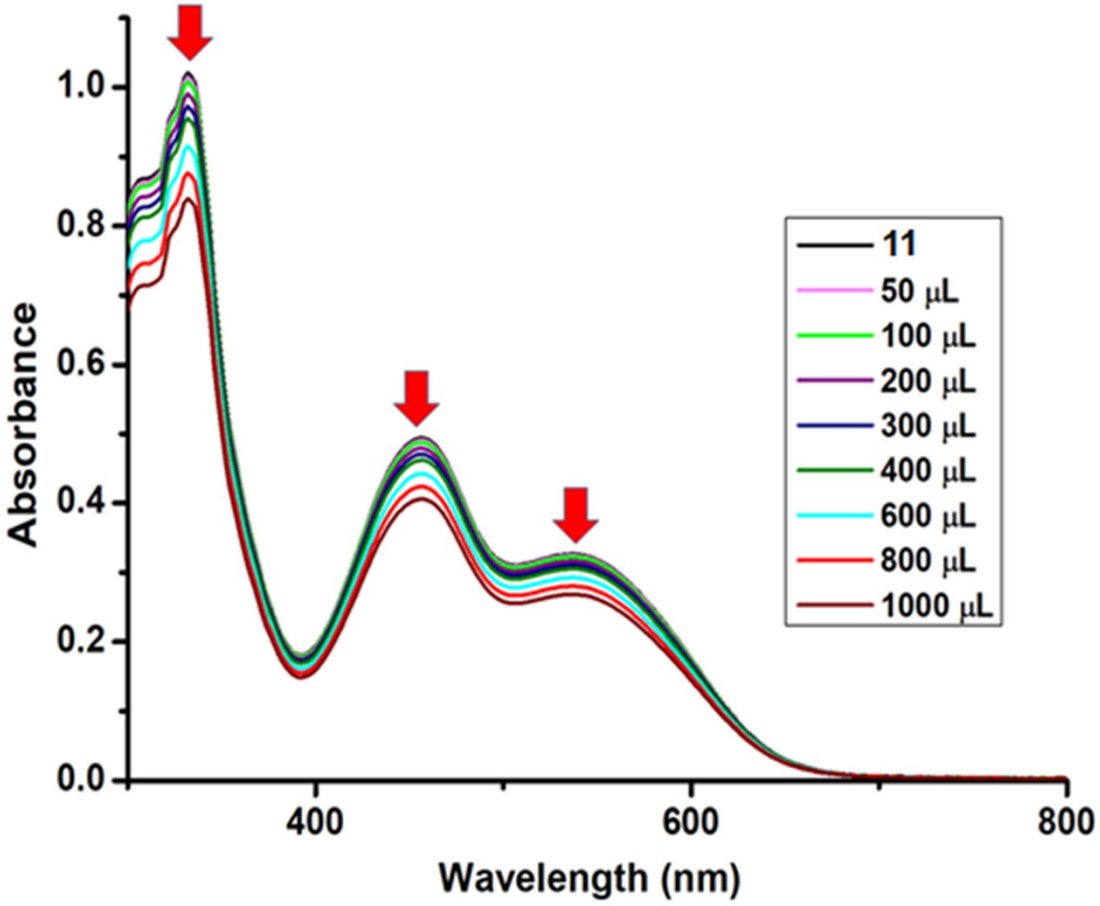


Fig. S23 Change in absorption spectrum of **11** (9.08 x 10^{-5} M) upon addition of $(TBA)_3HP_2O_7$ (0.5 M) in $CHCl_3$ at 298 K.

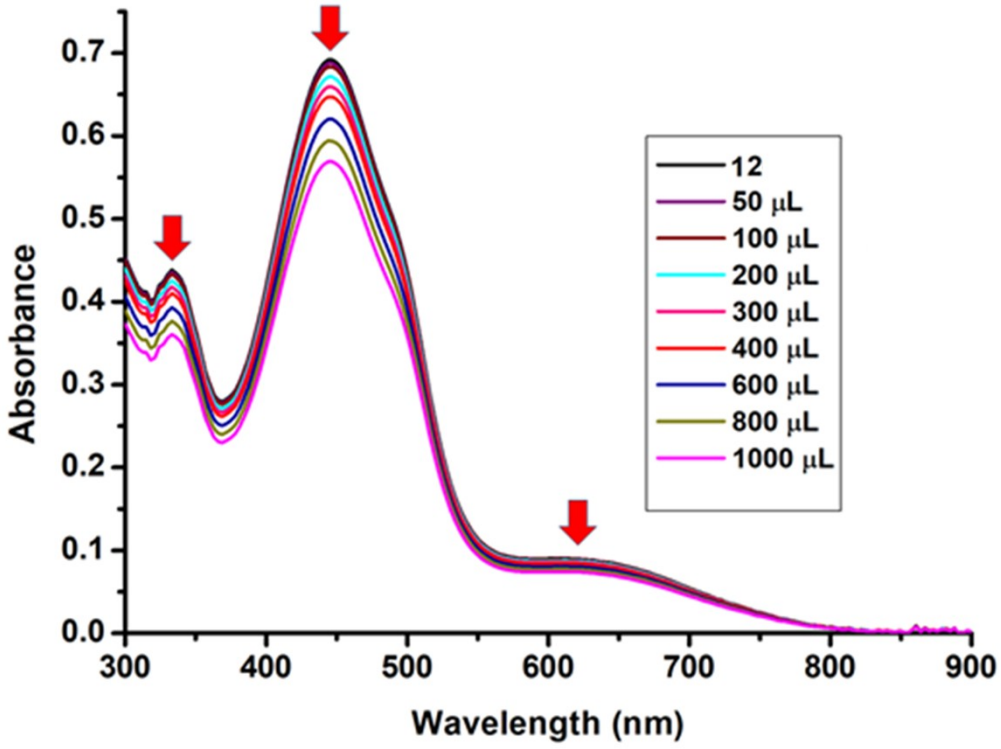


Fig. S24 Change in absorption spectrum of **12** (4.1 x 10^{-5} M) upon addition of $(TBA)_3HP_2O_7$ (0.5 M) in $CHCl_3$ at 298 K.

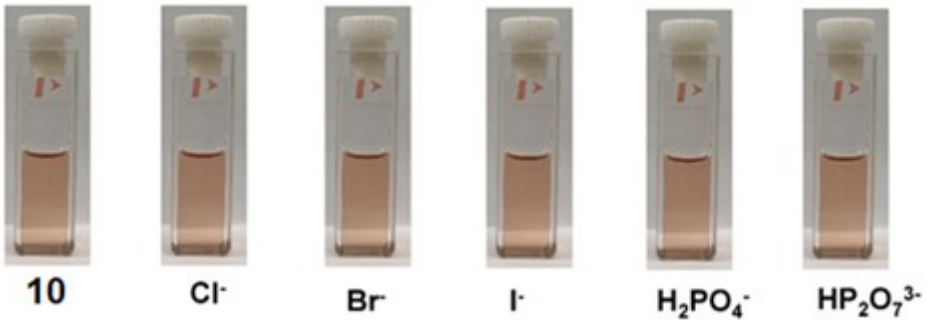


Fig. S25 Color change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **10** in $CHCl_3$ at 298 K.

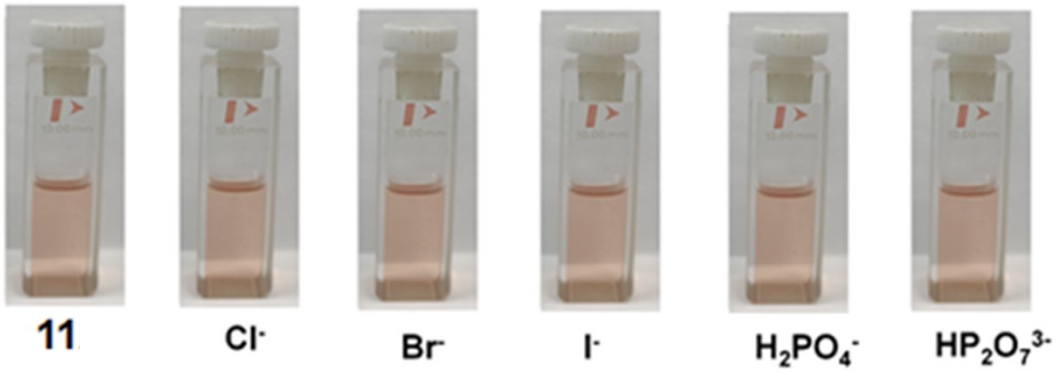


Fig. S26 Color change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **11** in $CHCl_3$ at 298 K.

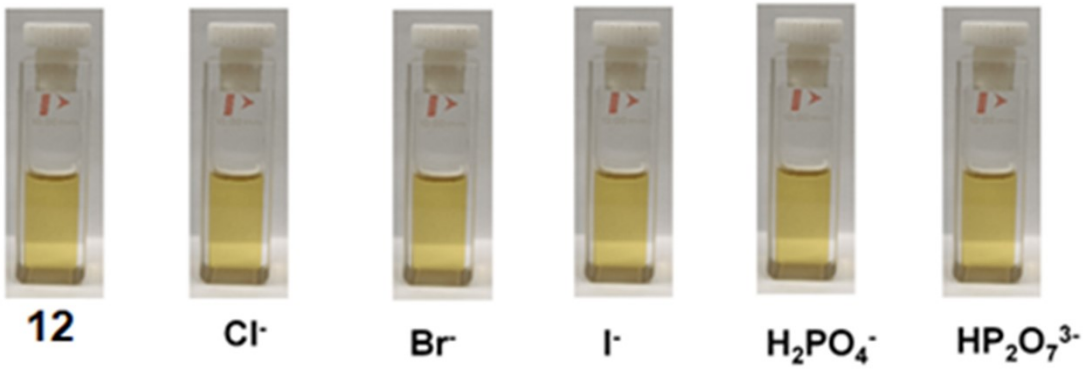


Fig. S27 Color change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **12** in $CHCl_3$ at 298 K.

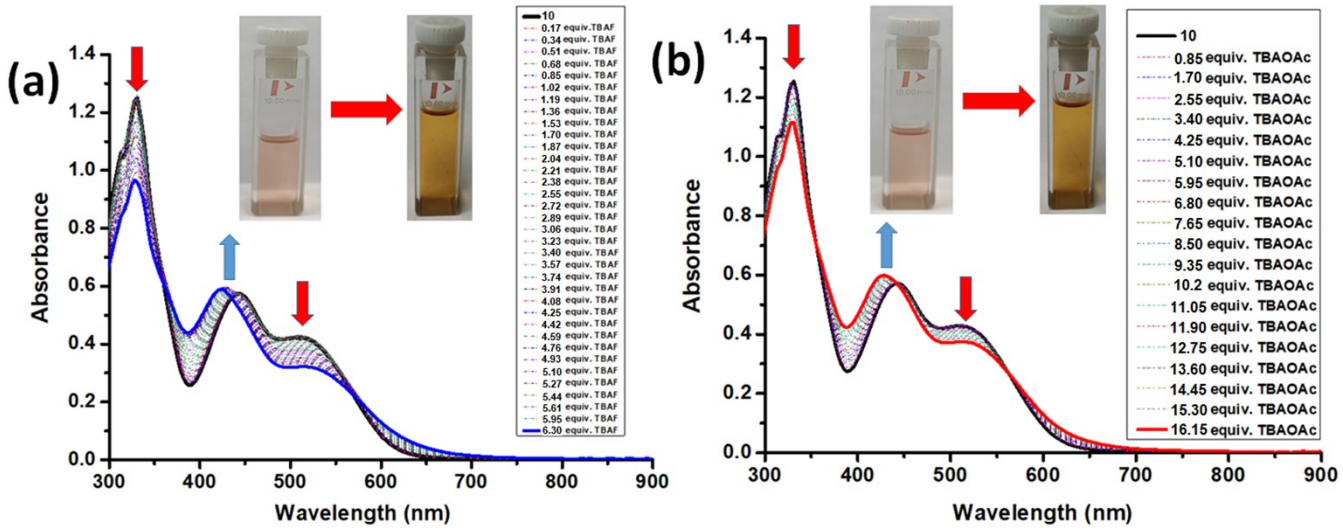


Fig. S28 (a) Change in absorption spectra of **10** (4.98 x 10^{-5} M) upon titration with TBAF (0.05 M) and (b) TBAOAc (0.1 M) in $CHCl_3$ at 298 K.

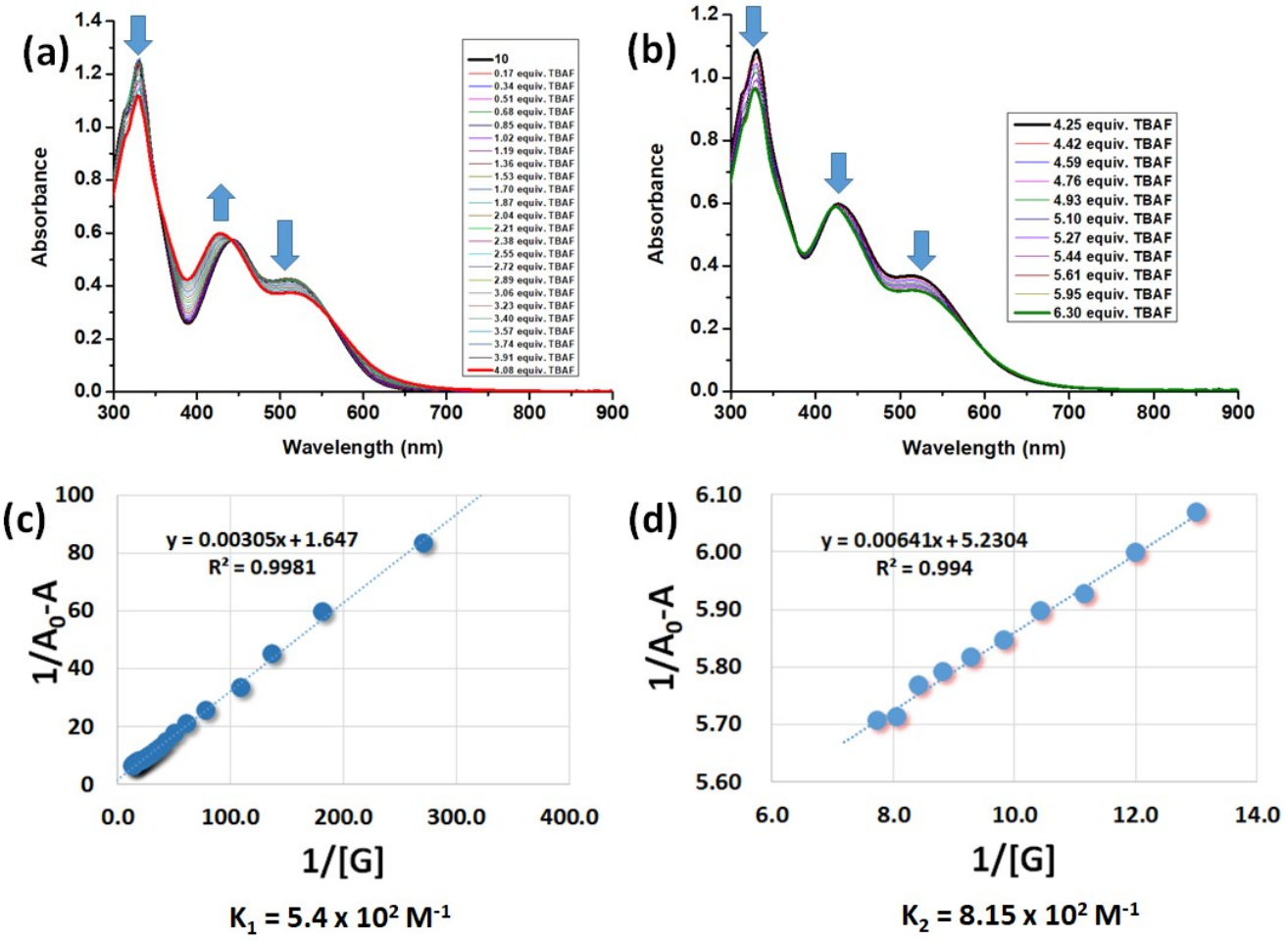


Fig. S28A Change in absorption spectra of **10** (4.98 x 10^{-5} M) upon titration of TBAF (0.05 M) (a) from 0-4.08 equiv of F^- addition and (b) 4.25-6.30 equiv F^- addition in $CHCl_3$ at 298 K. (c) and (d) show B-H plots of [**10**-**F**]$^-$ and [**10**]$^-$ respectively from UV-vis titration experiment to determine binding constant (Some data points in the figure deviated very marginally from the fitting curve. However, the overall fitting of the data points was reasonably good as clearly evident from the R^2 value of >0.98).

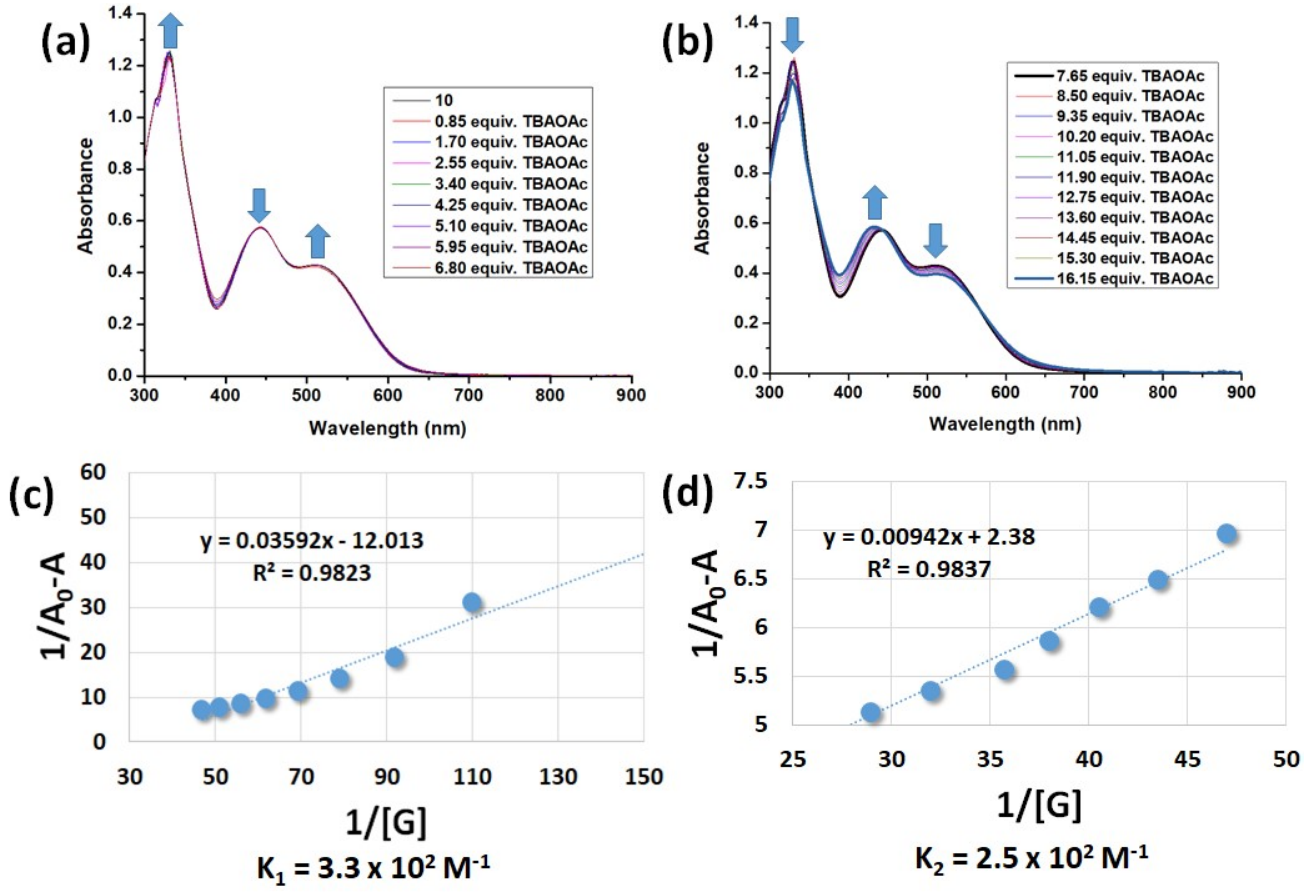


Fig. S28B Change in absorption spectra of **10** (4.98 x 10^{-5} M) upon titration of TBAOAc (0.1 M) (a) from 0-6.8 equiv of AcO^- addition and (b) 7.65-16.15 equiv AcO^- addition in $CHCl_3$ at 298 K. (c) and (d) show B-H plots of [**10**-**OAc**]$^-$ and [**10**]$^-$ respectively from UV-vis titration experiment to determine binding constant (Some data points in the figure deviated very marginally from the fitting curve. However, the overall fitting of the data points was reasonably good as clearly evident from the R^2 value of >0.98).

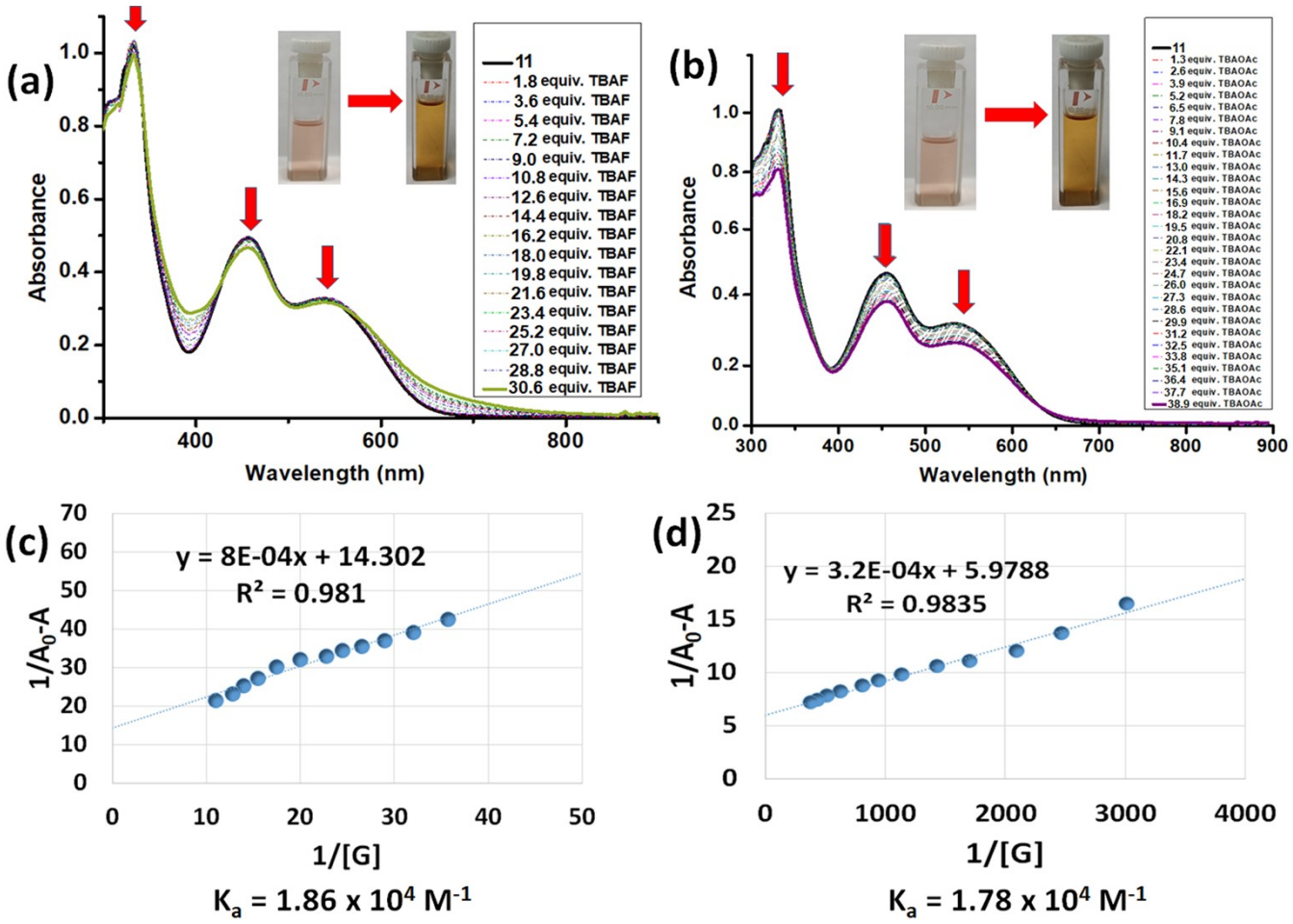


Fig. S29 (a) Change in absorption spectra of **11** (9.08 x 10^{-5} M) upon titration of TBAF (0.05 M) and (b) TBAOAc (0.1 M) in $CHCl_3$ at 298 K. (c) and (d) show B-H plots of [**11**-F]$^-$ and [**11**-OAc]$^-$ respectively from UV-vis titration experiment to determine binding constant for the formation of host-guest complex (Some data points in the figure deviated very marginally from the fitting curve. However, the overall fitting of the data points was reasonably good as clearly evident from the R_2 value of >0.98).

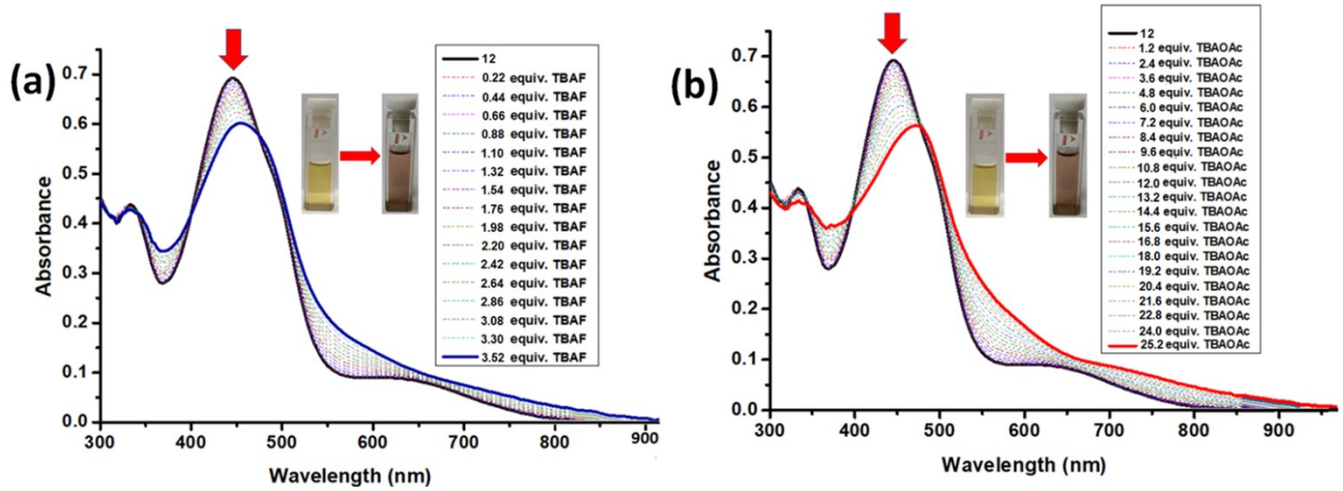


Fig. S30 (a) Change in absorption spectra of **12** (4.10 x 10^{-5} M) upon titration of TBAF (0.05 M) and (b) TBAOAc (0.1 M) in $CHCl_3$ at 298 K.

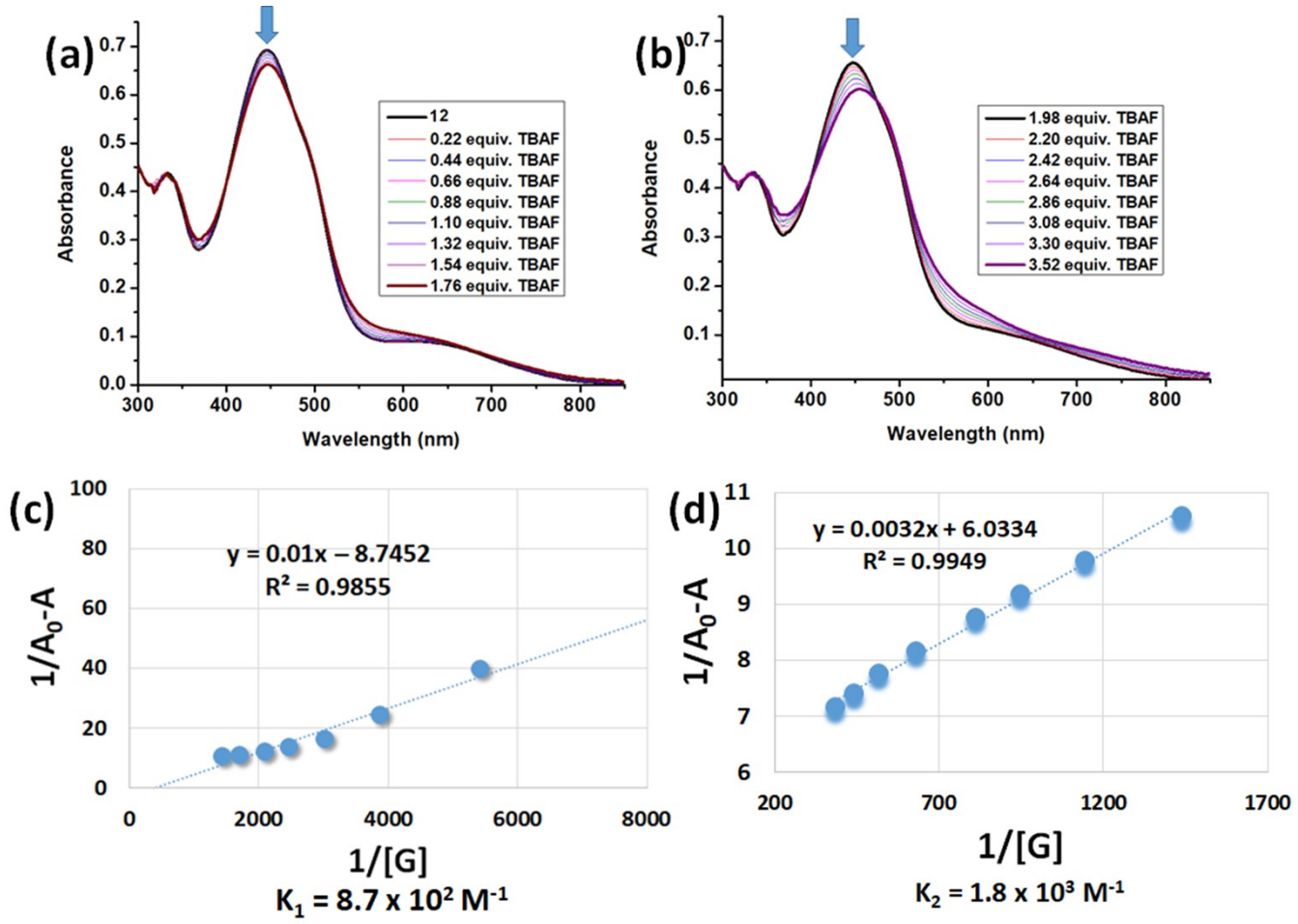


Fig. S30A Change in absorption spectra of **12** (4.10 x 10^{-5} M) upon titration of TBAF (0.05 M) (a) 0-1.76 equiv of F^- and (b) 1.98-3.52 equiv of F^- in $CHCl_3$ at 298 K. (c) and (d) show B-H plots of [**12**-F]$^-$ and [**12**]$^-$ respectively from UV-vis titration experiment to determine binding constant (Some data points in the figure deviated very marginally from the fitting curve. However, the overall fitting of the data points was reasonably good as clearly evident from the R^2 value of >0.98).

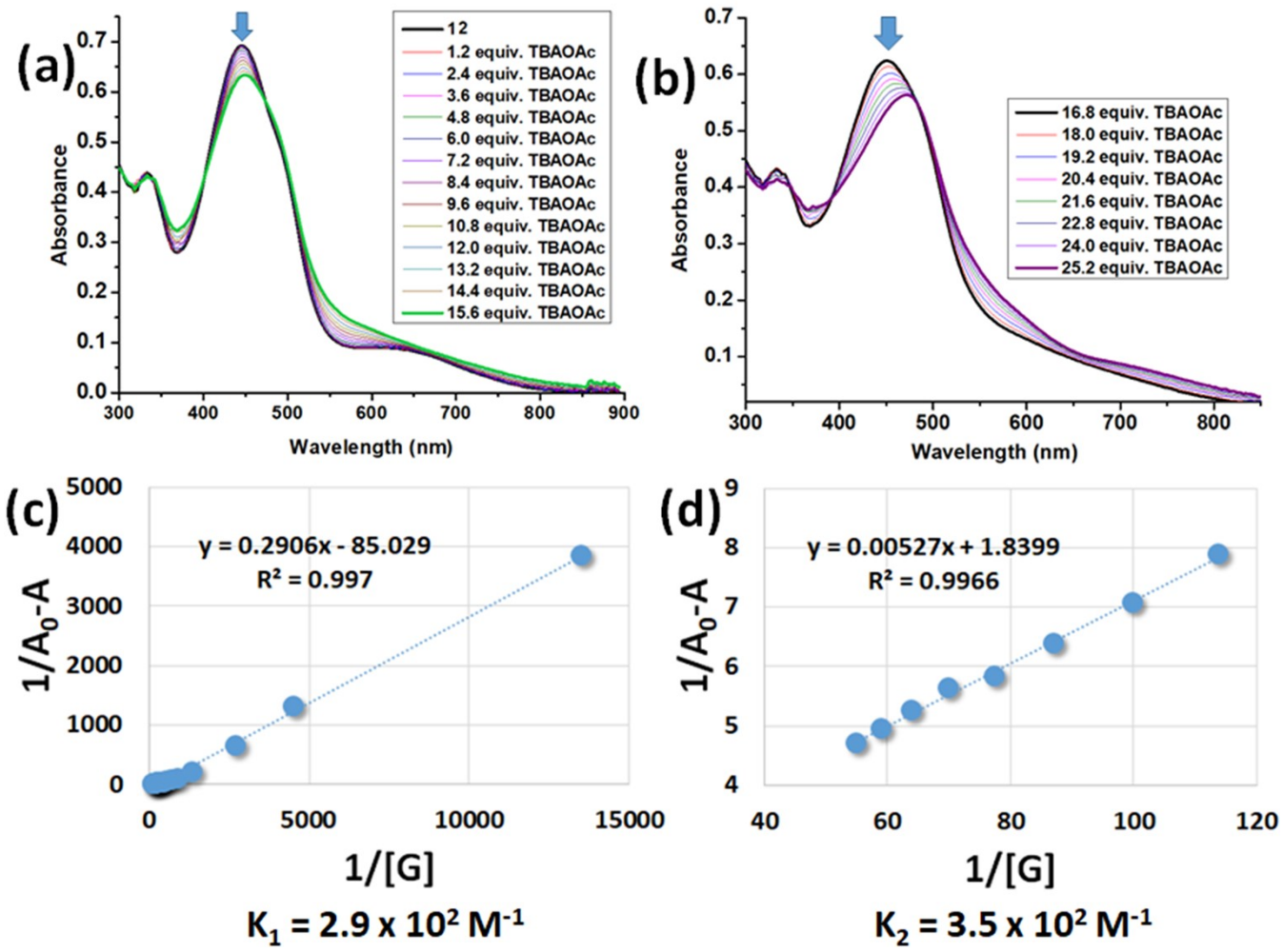


Fig. S30B Change in absorption spectra of **12** (4.10 x 10^{-5} M) upon titration of TBAOAc (0.1 M) (a) 0-15.6 equiv of AcO^- and (b) 16.8 - 25.2 equiv of AcO^- in $CHCl_3$ at 298 K. (c) and (d) show B-H plots of [**12**-OAc]$^-$ and [**12**]$^-$ respectively from UV-vis titration experiment to determine binding constant (Some data points in the figure deviated very marginally from the fitting curve. However, the overall fitting of the data points was reasonably good as clearly evident from the R^2 value of >0.98).

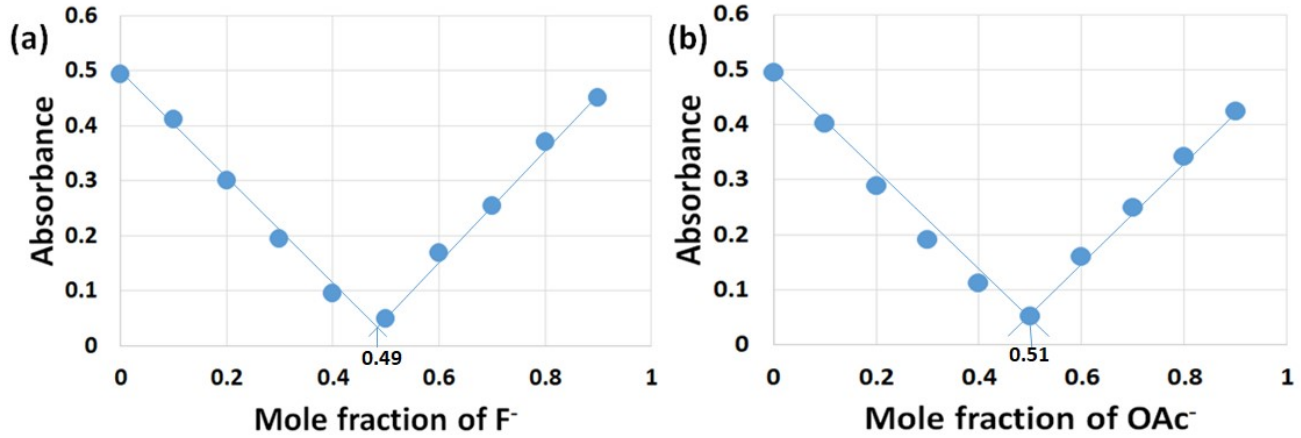


Fig. S31 Job Plot obtained for **11** (9.08 x 10^{-5} M in $CHCl_3$) on variation of its absorbance vs mole fraction of (a) F^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 541 nm; (b) AcO^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 541 nm.

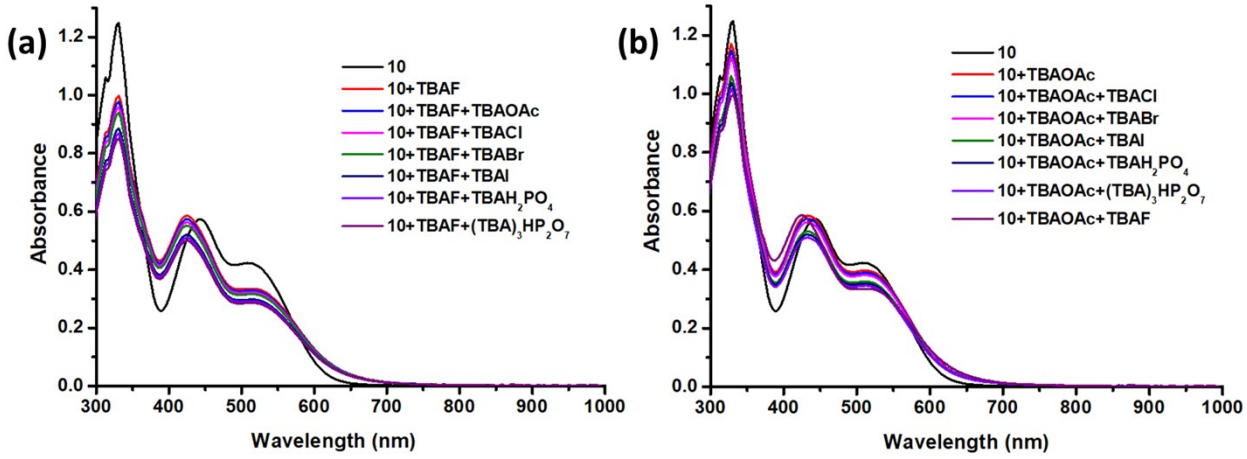


Fig. S32 Competitive Assay experiments of (a) [**10**-TBAF] in the presence of other anions and (b) [**10**-TBAOAc] in the presence of other anions (Absorbance response upon addition of 10 equivalents of F^-, Cl^-, Br^-, I^-, AcO^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

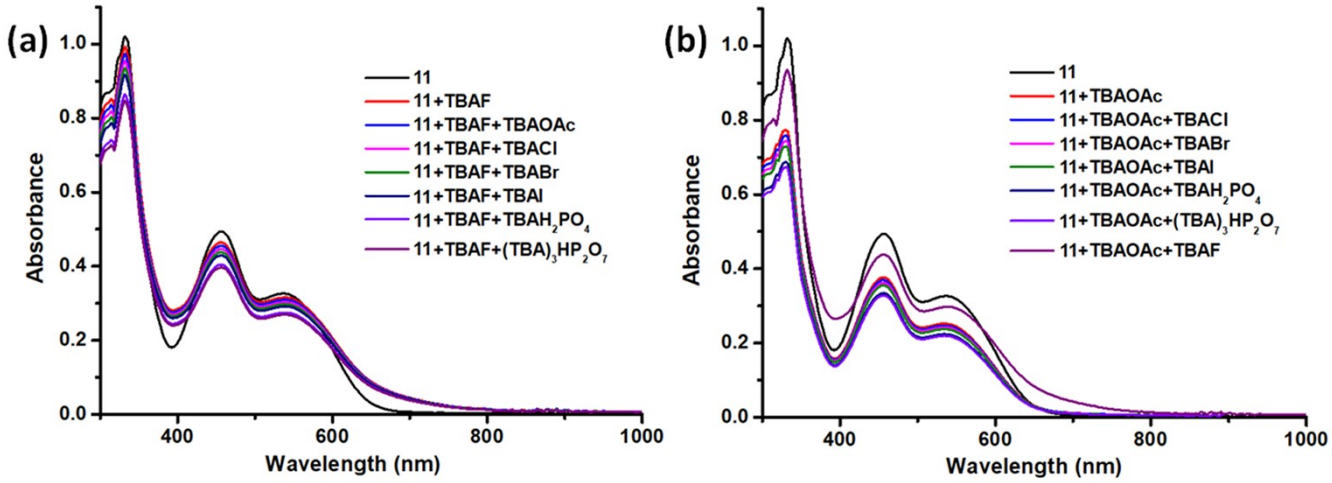


Fig. S33 Competitive Assay experiments of (a) [**11**-TBAF] in the presence of other anions and (b) [**11**-TBAOAc] in the presence of other anions (Absorbance response upon addition of 15 equivalents of F^-, Cl^-, Br^-, I^-, AcO^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

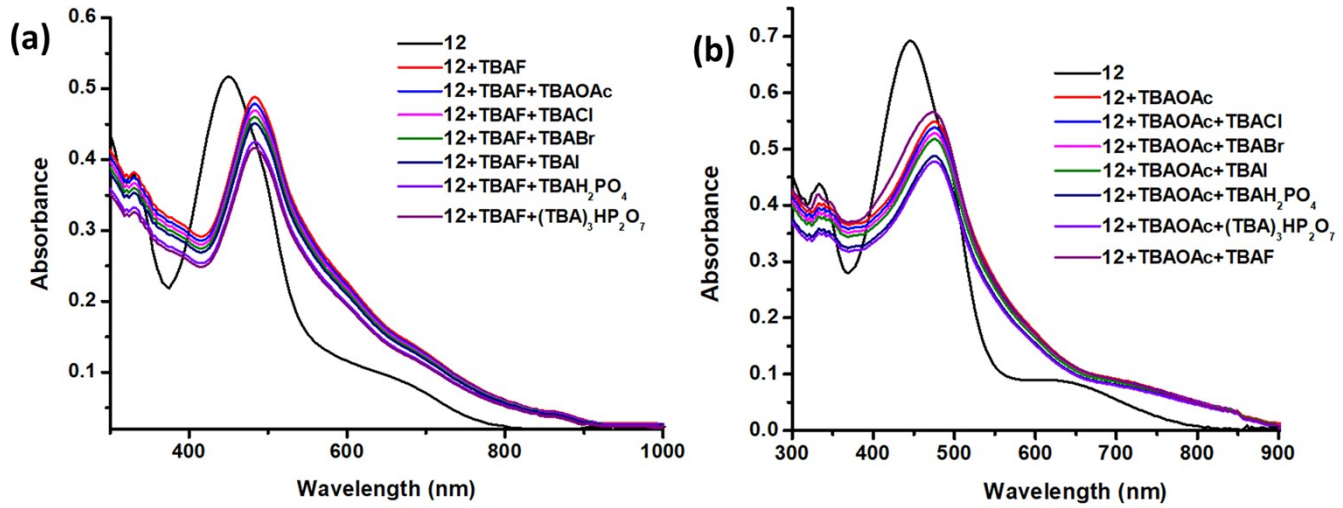


Fig. S34 Competitive Assay experiments of (a) [**12**-TBAF] in the presence of other anions and (b) [**12**-TBAOAc] in the presence of other anions (Absorbance response upon addition of 10 equivalents of F^-, Cl^-, Br^-, I^-, AcO^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

3.3 NMR spectra:

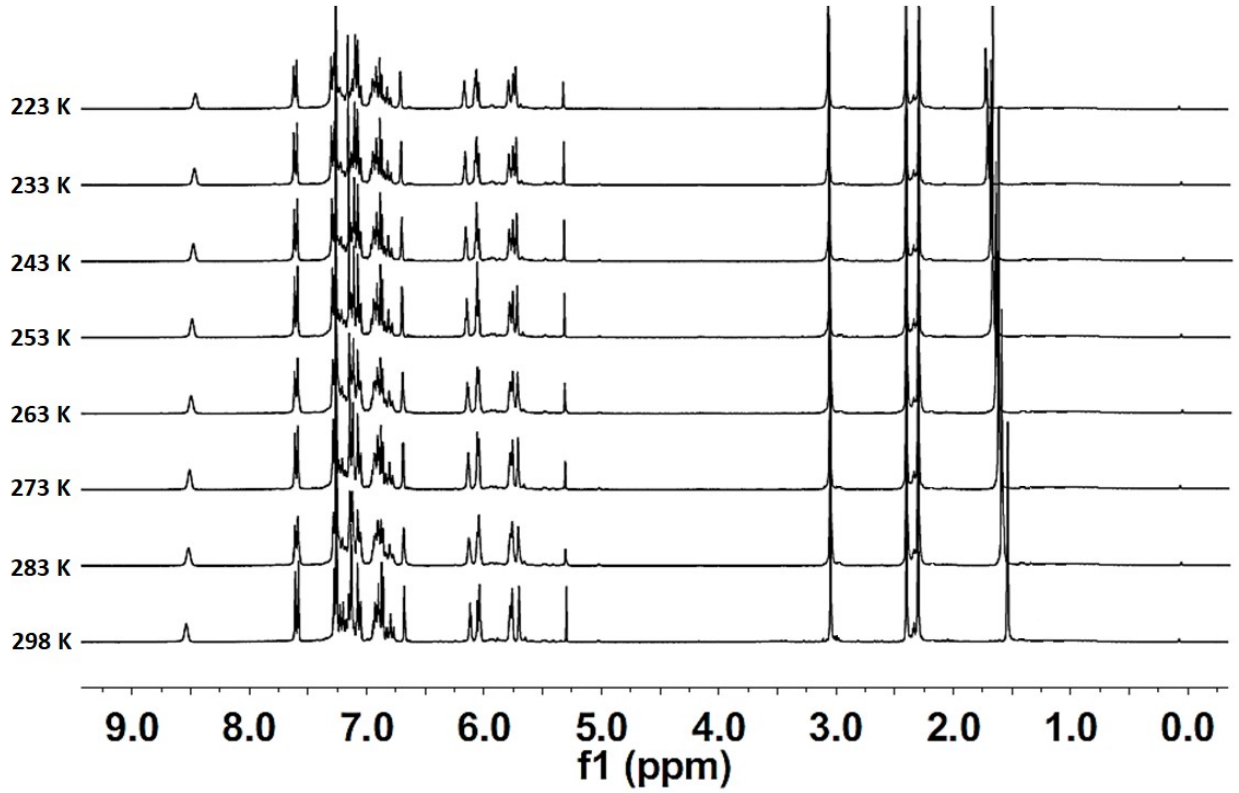
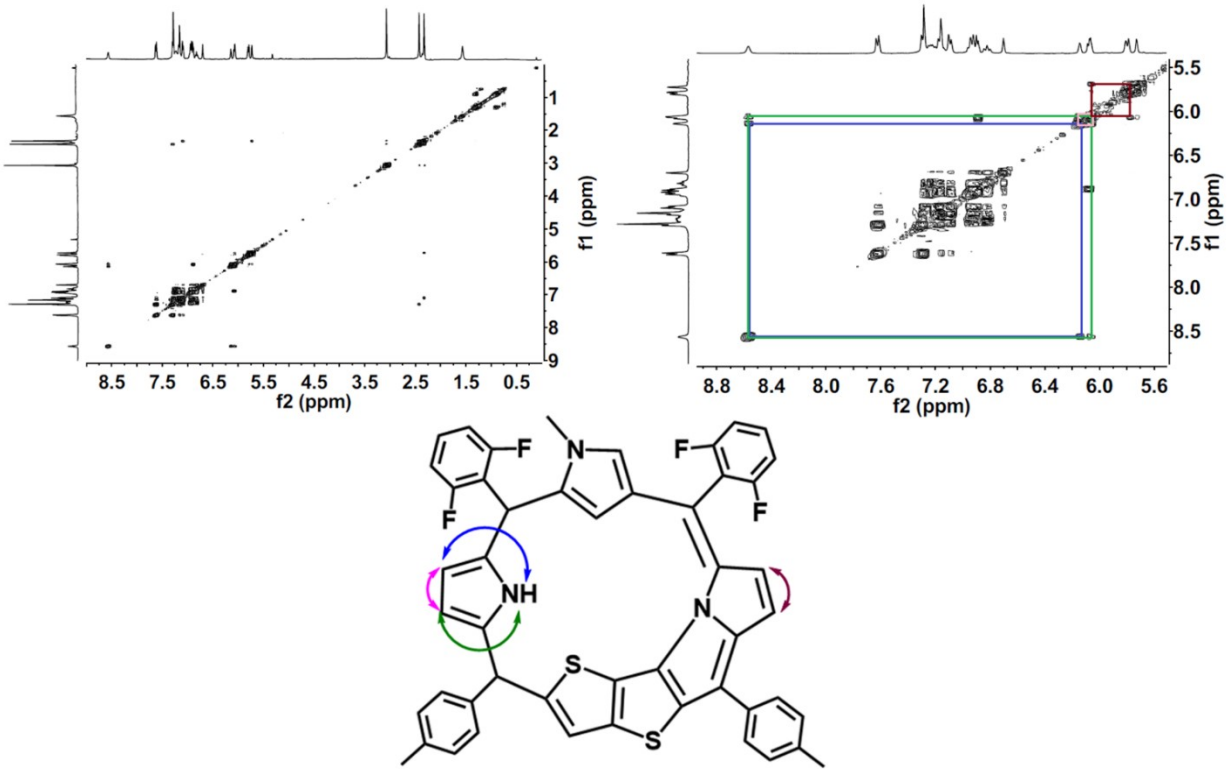


Fig. S35 Low VT ^{1}H NMR spectra of **10** in $CDCl_3$.

Fig.



S36 ^{1}H-^{1}H 2D COSY NMR spectra of **10** in $CDCl_3$ at 298 K.

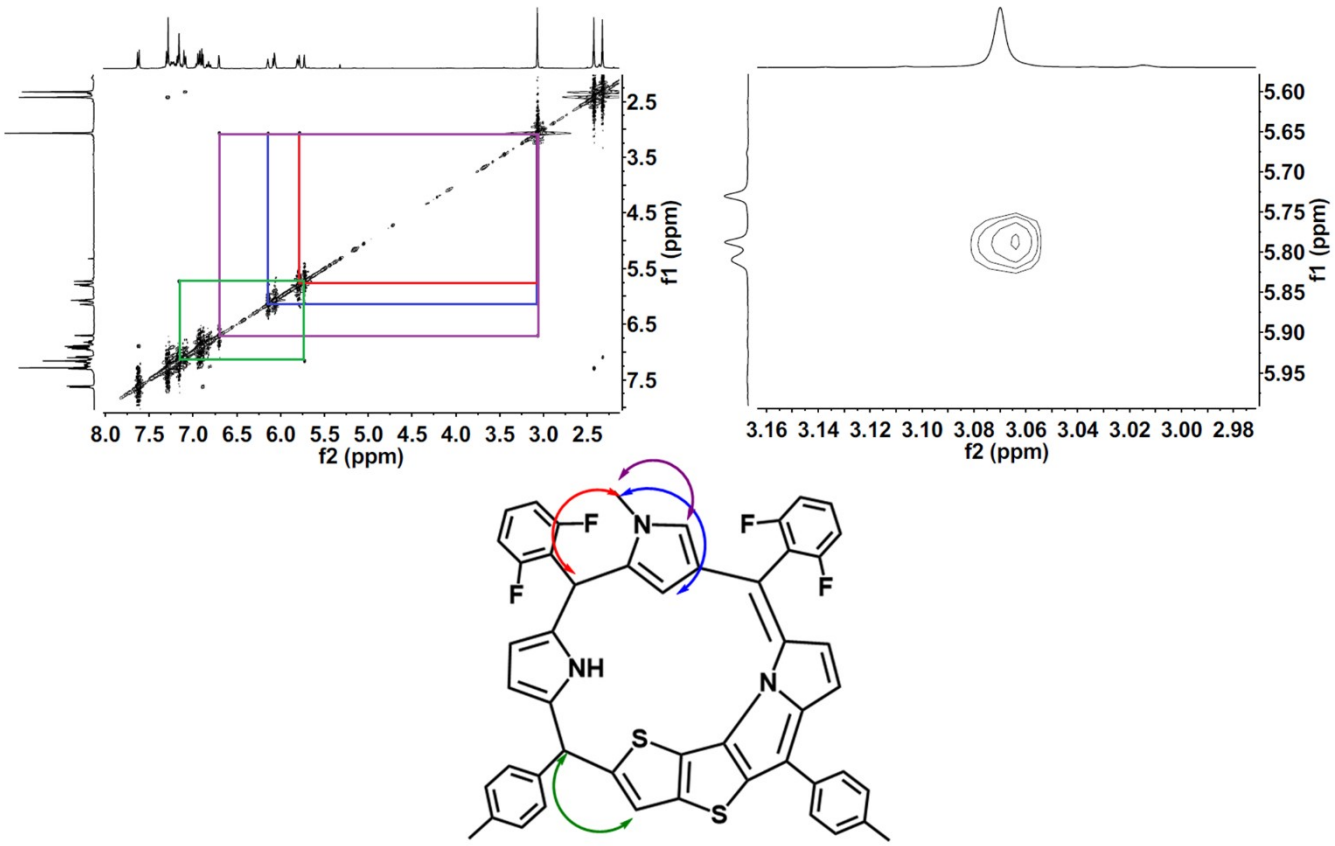


Fig. S37 ^{1}H-^{1}H 2D ROESY NMR spectra of **10** in $CDCl_3$ at 298 K.

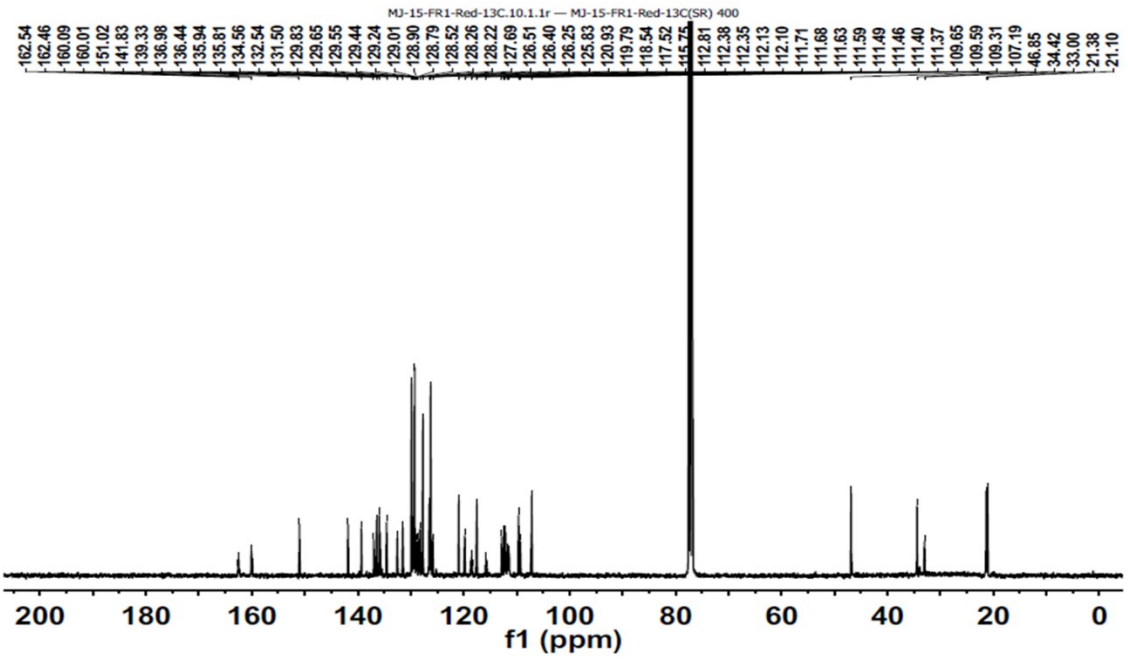
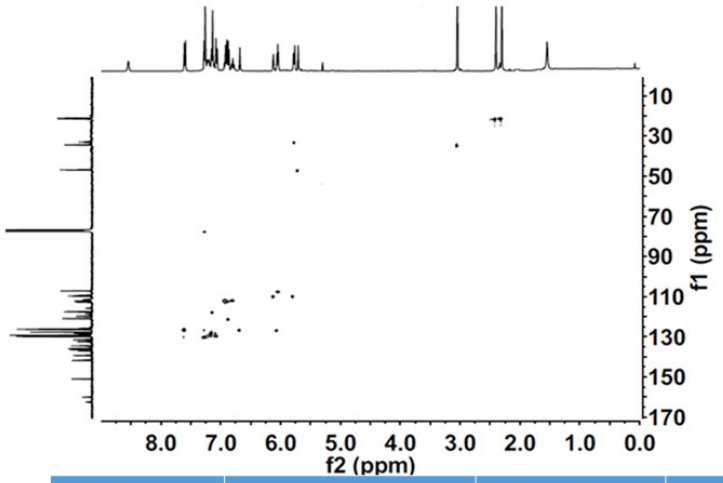
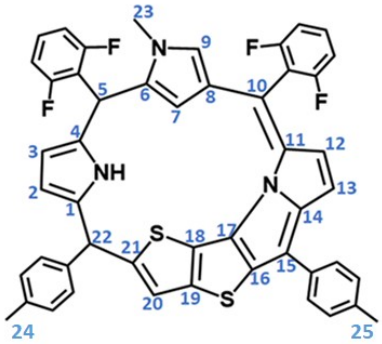


Fig. S38 ^{13}C NMR spectra of **10** in $CDCl_3$ at 298 K.





^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.54(k)	-	6.05 (b)	107.19 (2)
7.14 (i)	117.52 (20)	5.78 (f)	109.31 (13)
6.68 (c)	126.40 (9)	5.76 (g)	33.00 (5)
6.12 (a, d)	109.59 (3), 109.65 (7)	5.70 (h)	46.85 (22)
6.06 (e)	126.25 (12)	3.05 (j)	34.42 (23)
2.40 (m)	21.38 (25)	2.30 (l)	21.10 (24)

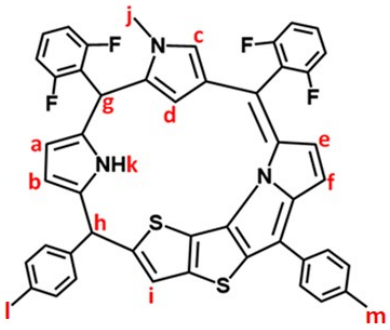
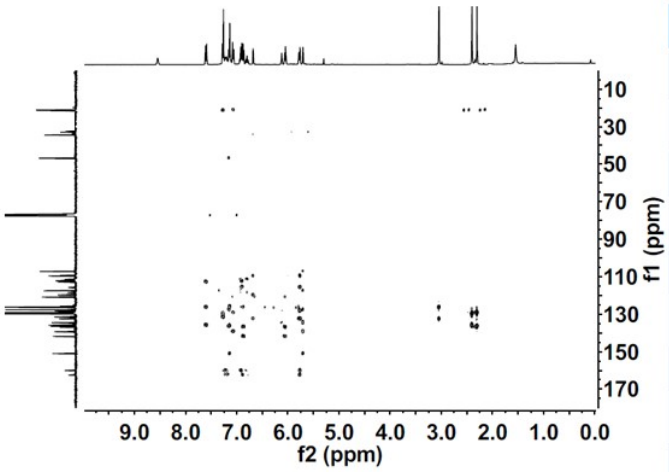
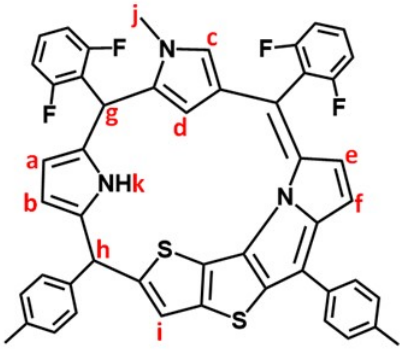


Fig. S39 ^{13}C-^{1}H 2D HSQC NMR spectra of **10** in $CDCl_3$ at 298 K.



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.54 (k)	-	6.12 (a,d)	128.22 (4)
7.14 (i)	126.25 (21)		127.69 (1)
	135.94 (19)		134.56 (6)
	151.02 (18)	6.06 (e)	109.31 (13)
	46.85 (22)		136.44 (11)
6.68 (c)	109.65 (7)		141.83 (14)
	119.79 (10)		120.93 (10)
	132.54 (8)	3.05 (j)	126.25 (9)
	34.42 (23)		132.54 (8)



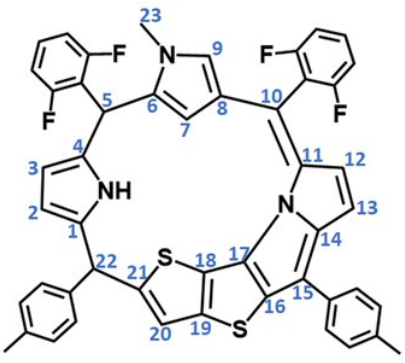


Fig. S40 ^{13}C-^{1}H 2D HMBC NMR spectra of **10** in $CDCl_3$ at 298 K.

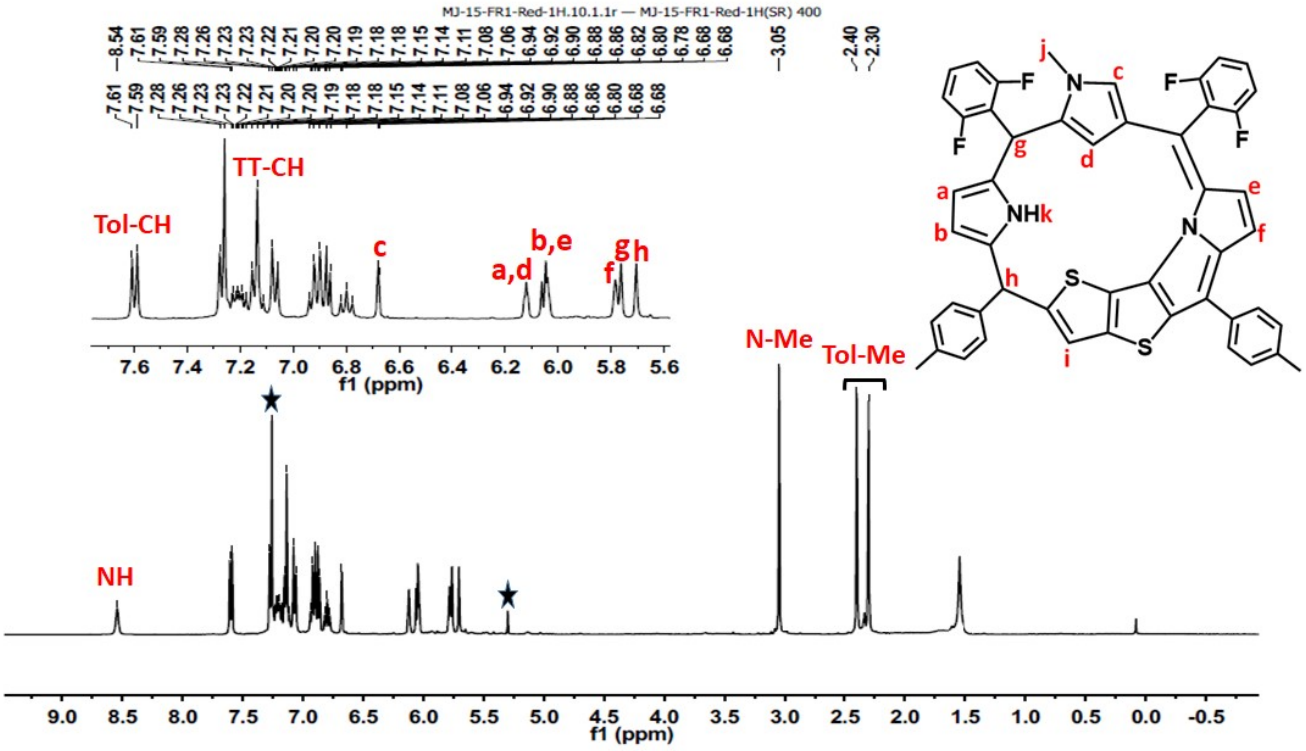


Fig. S41 Completely assigned ^{1}H NMR spectra of **10** in $CDCl_3$ at 298 K.

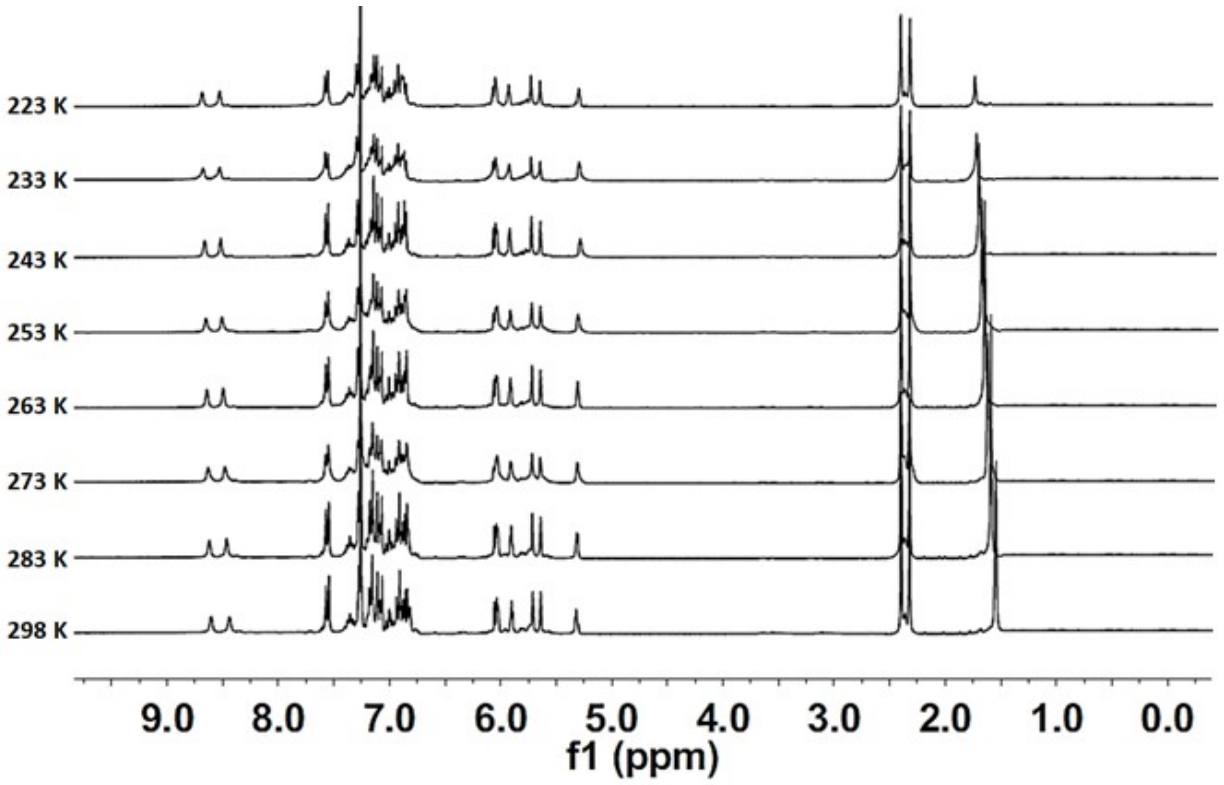


Fig. S42 Low VT ^{1}H NMR spectra of **11** in $CDCl_3$.

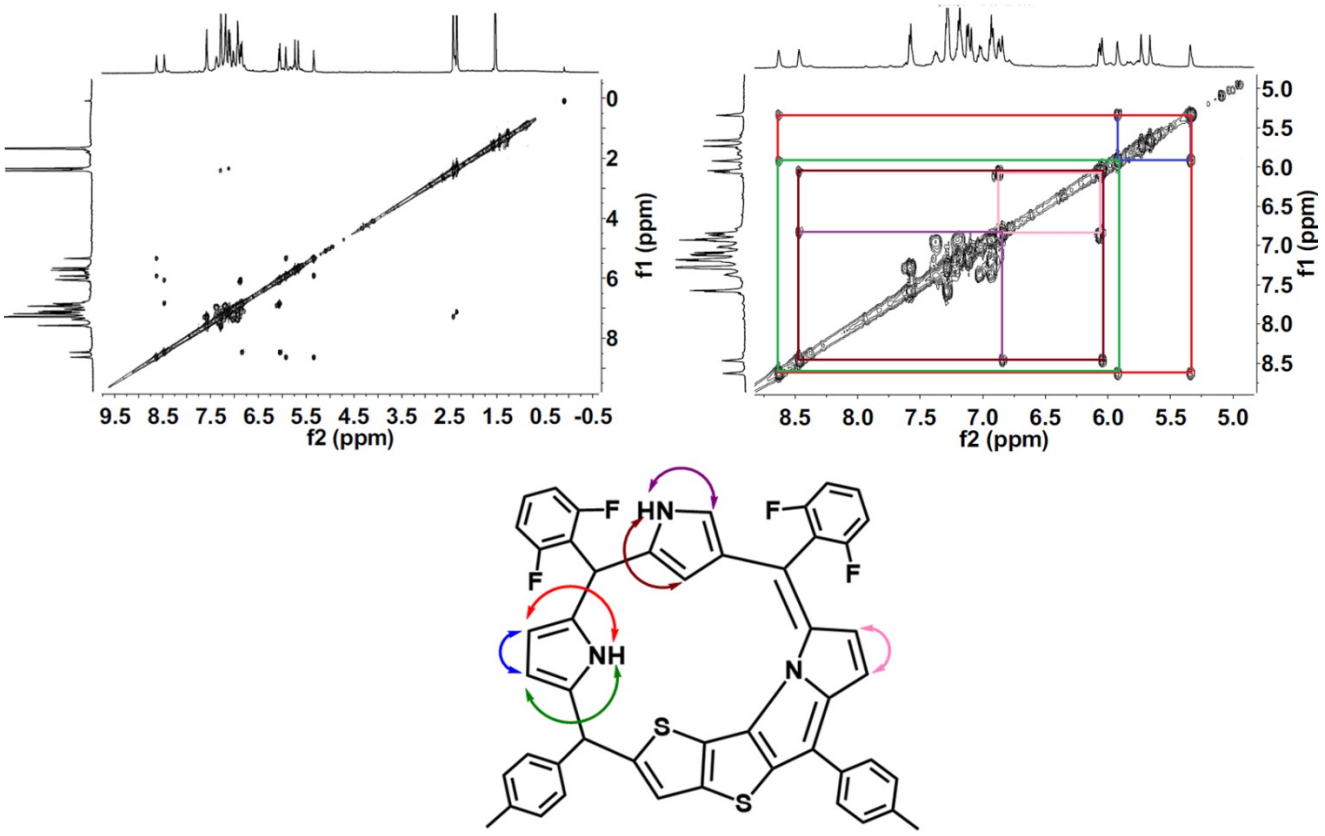


Fig. S43 ^{1}H-^{1}H 2D COSY NMR spectra of **11** in $CDCl_3$ at 298 K.

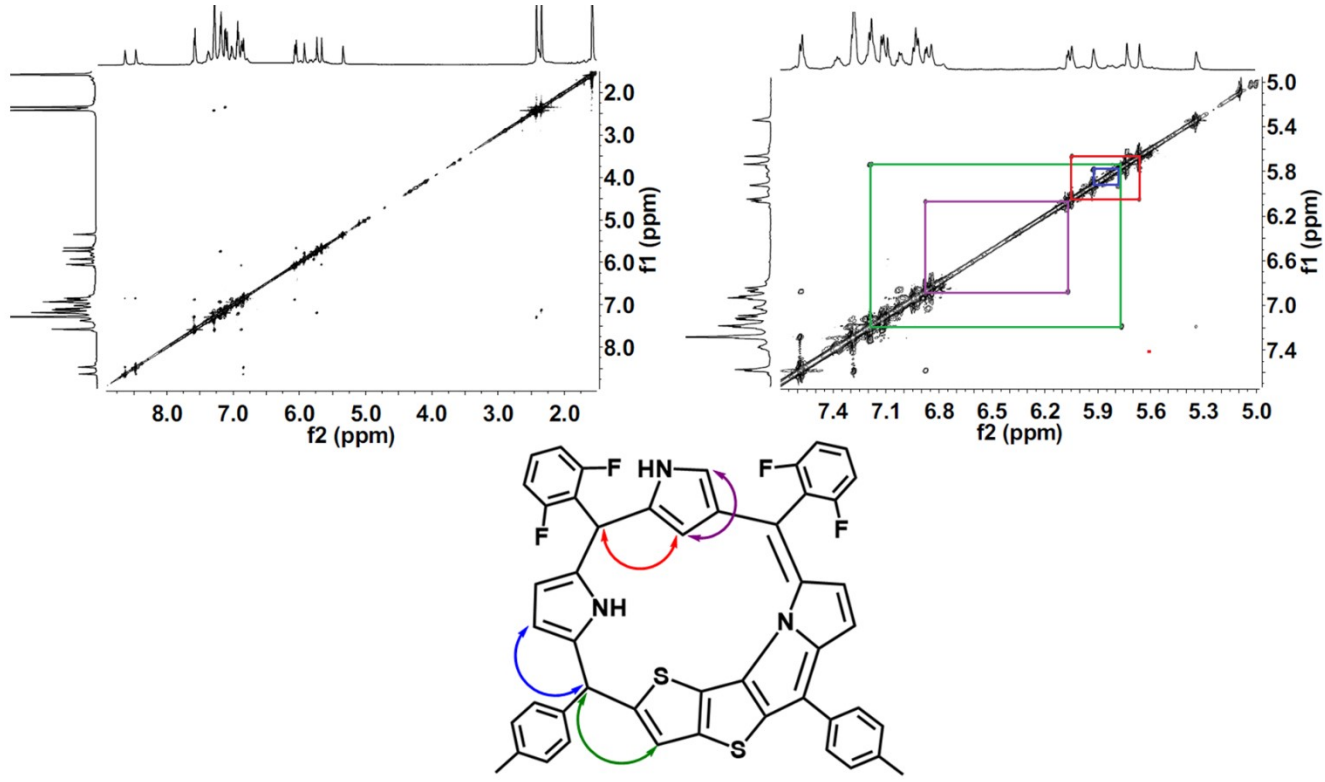


Fig. S44 ^{1}H-^{1}H 2D ROESY NMR spectra of **11** in $CDCl_3$ at 298 K.

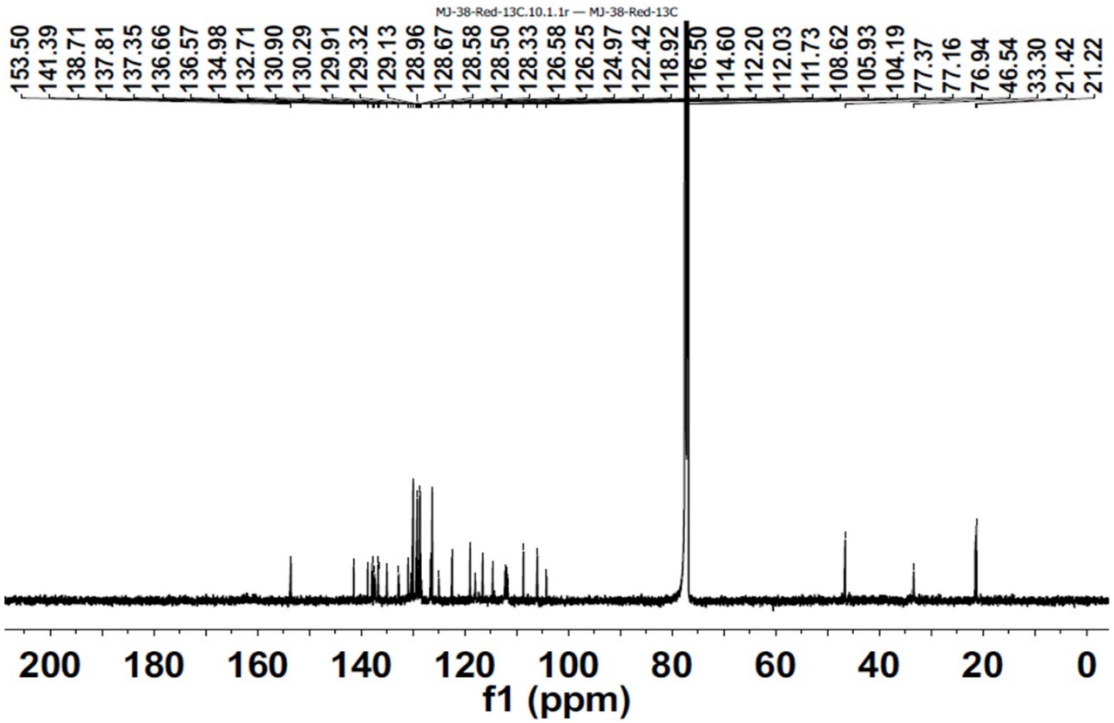
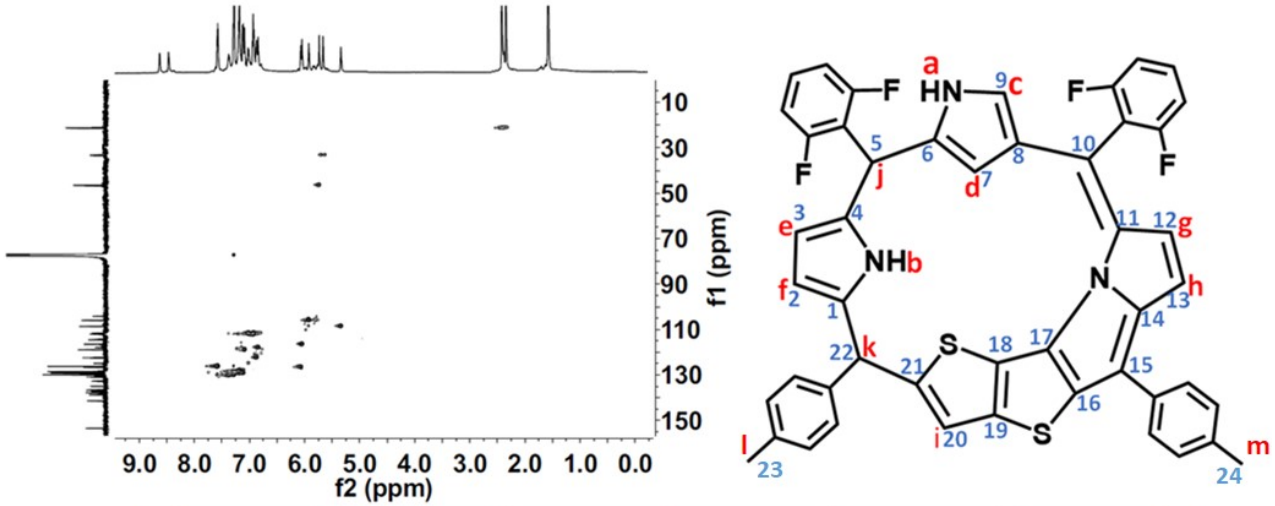
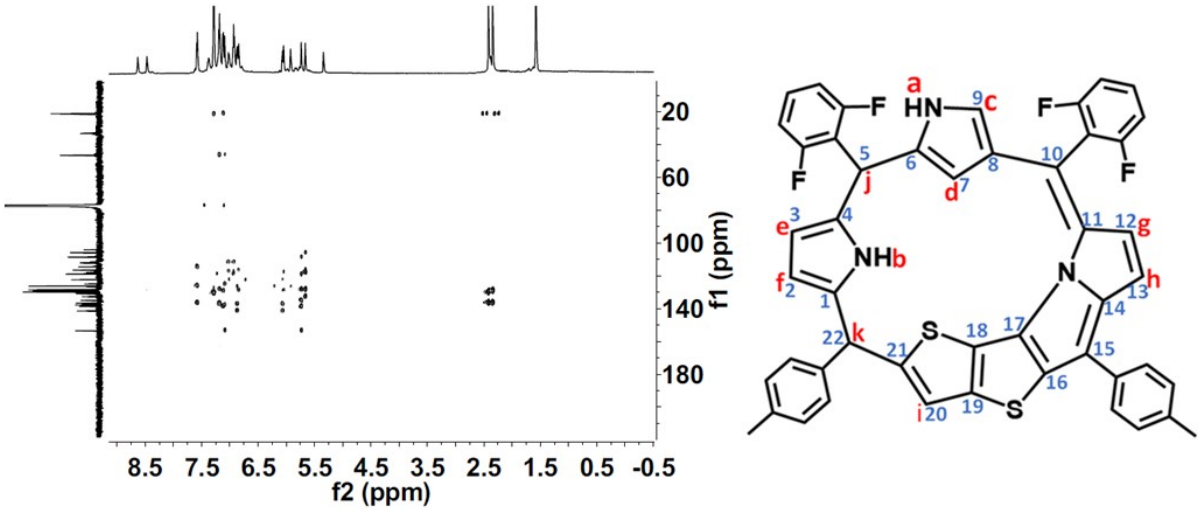


Fig. S45 ^{13}C NMR spectra of **11** in $CDCl_3$ at 298 K.



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.46 (a)	-	5.92 (f)	105.93 (2)	5.73 (k)	46.54 (22)
8.63 (b)	-	6.87 (g)	122.42 (12)	2.42 (m)	21.42 (24)
6.84 (c)	118.92 (9)	6.06 (h)	126.25 (13)	2.35 (l)	21.22 (23)
6.04 (d)	116.50 (7)	7.18 (i)	128.33 (20)		
5.34 (e)	108.62 (3)	5.66 (j)	33.30 (5)		

Fig. S46 ^{1}H-^{13}C 2D HSQC NMR spectra of **11** in $CDCl_3$ at 298 K.



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
6.84 (c)	116.50 (7)	5.66 (j)	108.62 (3)	7.18 (i)	46.54 (22)	5.73 (k)	105.93 (2)
	118.92 (9)		117.93 (4)		126.58(21)		117.99 (1)
	136.66 (8)		116.50 (7)		136.57(19)		128.33(20)
	141.39(10)		137.35 (6)	6.07 (h)	136.66(14)		132.71(19)
6.04(d)	137.35 (6)	6.87(g)	136.66(14)		141.39(10)		
	141.39(10)		141.39(10)				

Fig. S47 ^{1}H-^{13}C 2D HMBC NMR spectra of **11** in $CDCl_3$ at 298 K.

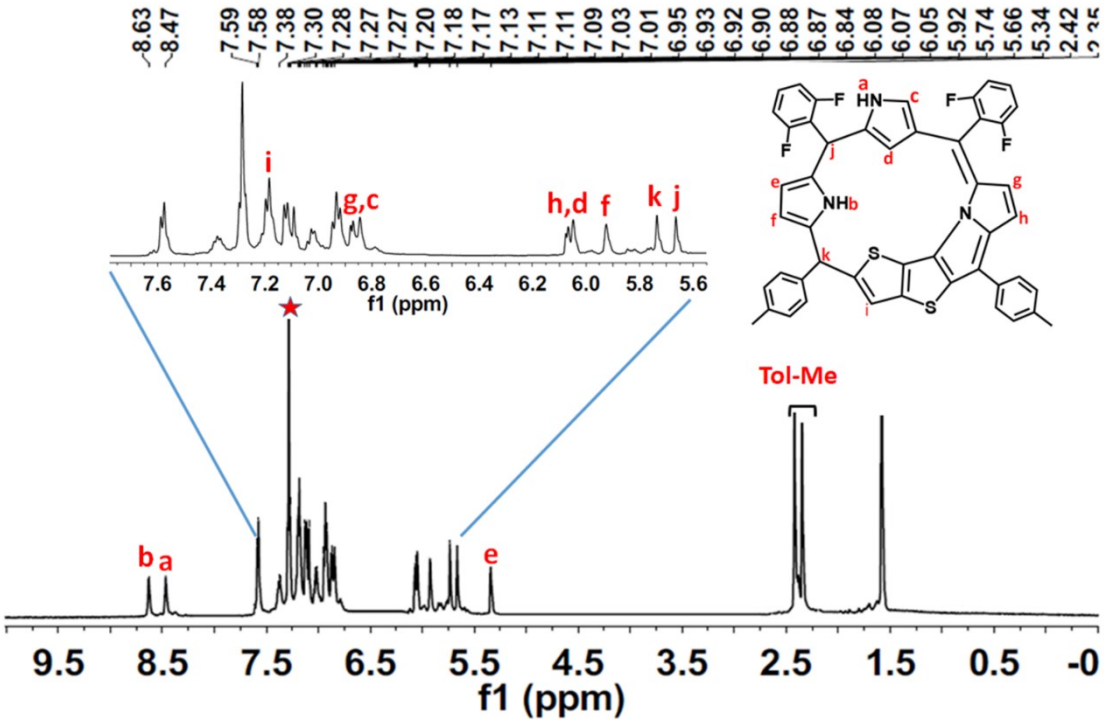


Fig. S48 Completely assigned ^{1}H NMR spectra of **11** in $CDCl_3$ at 298 K.

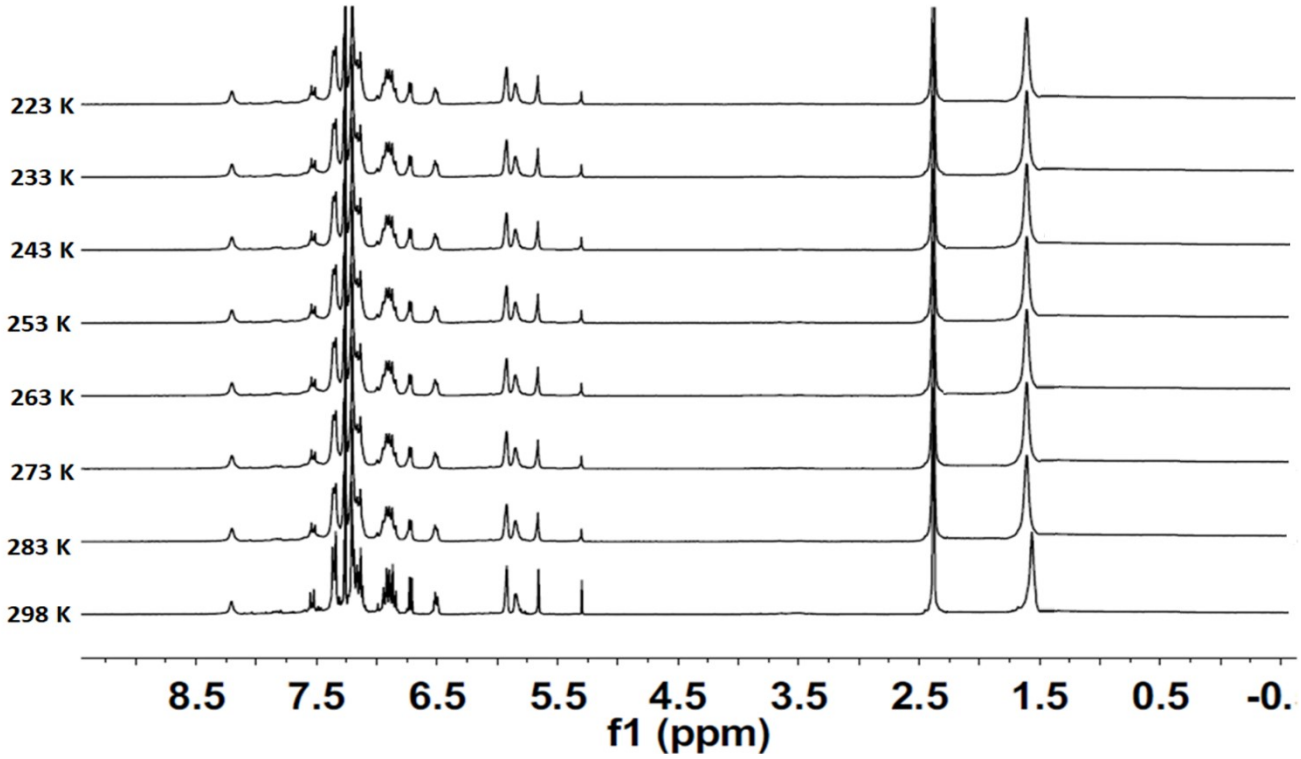


Fig. S49 Low VT ^{1}H NMR spectra of **12** in $CDCl_3$.

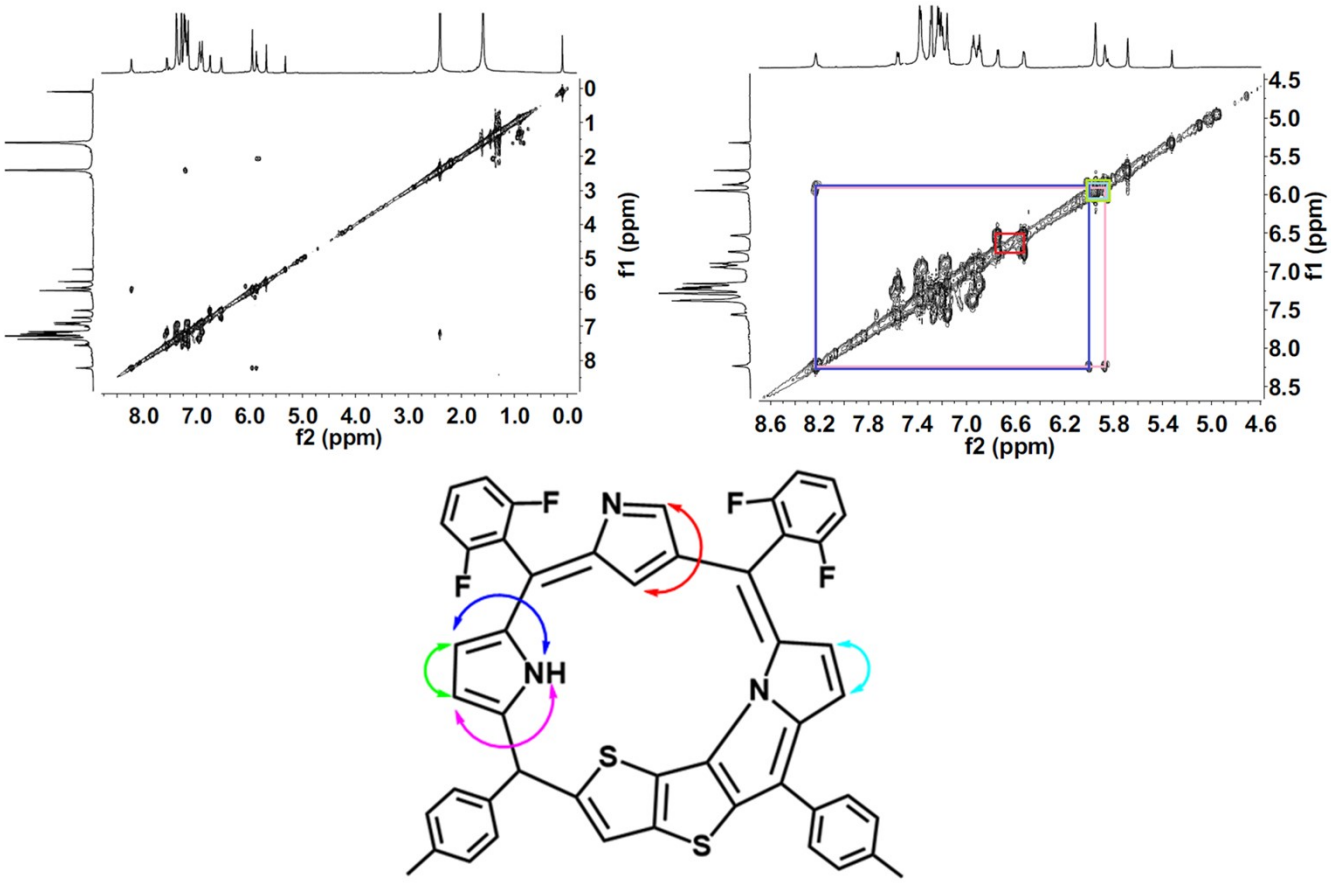


Fig. S50 ^{1}H-^{1}H 2D COSY NMR spectra of **12** in $CDCl_3$ at 298 K.

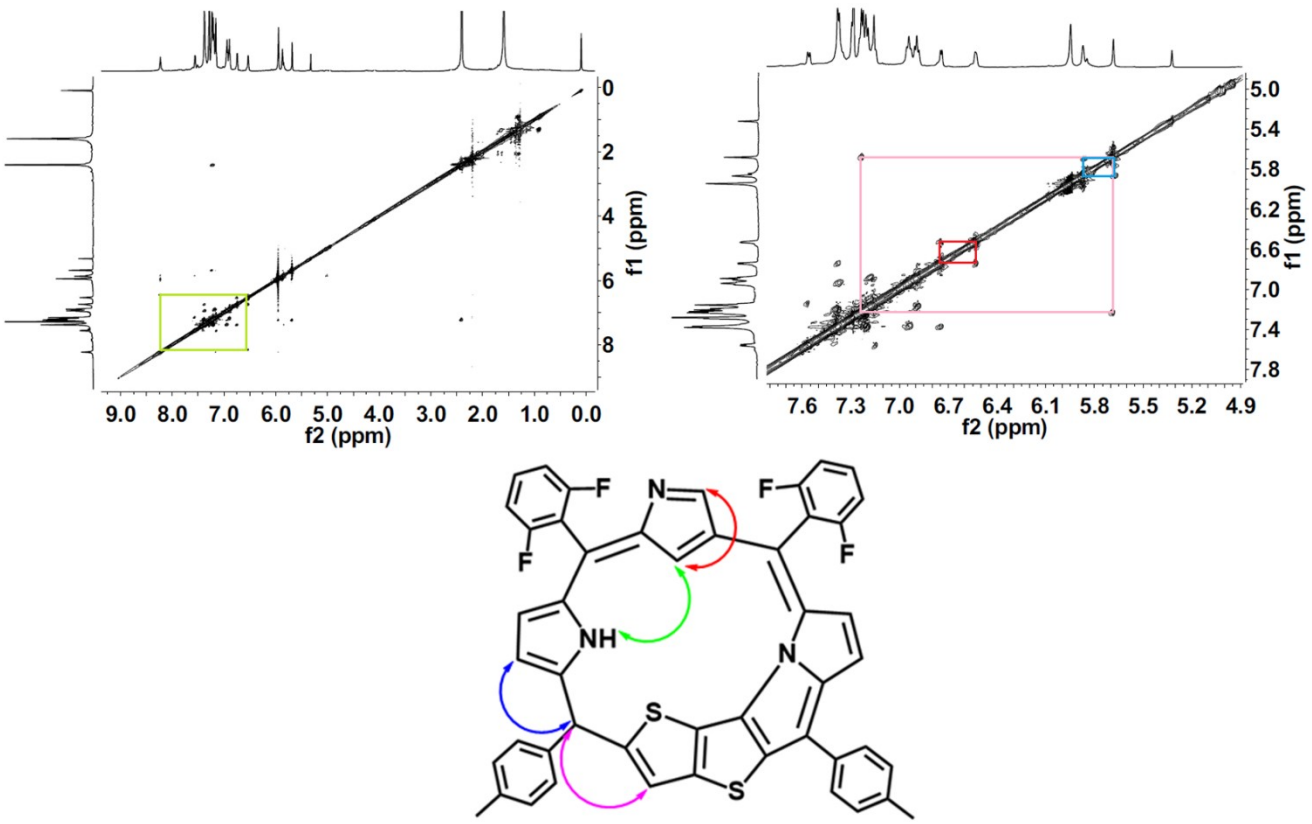


Fig. S51 ^{1}H-^{1}H 2D ROESY NMR spectra of **12** in $CDCl_3$ at 298 K.

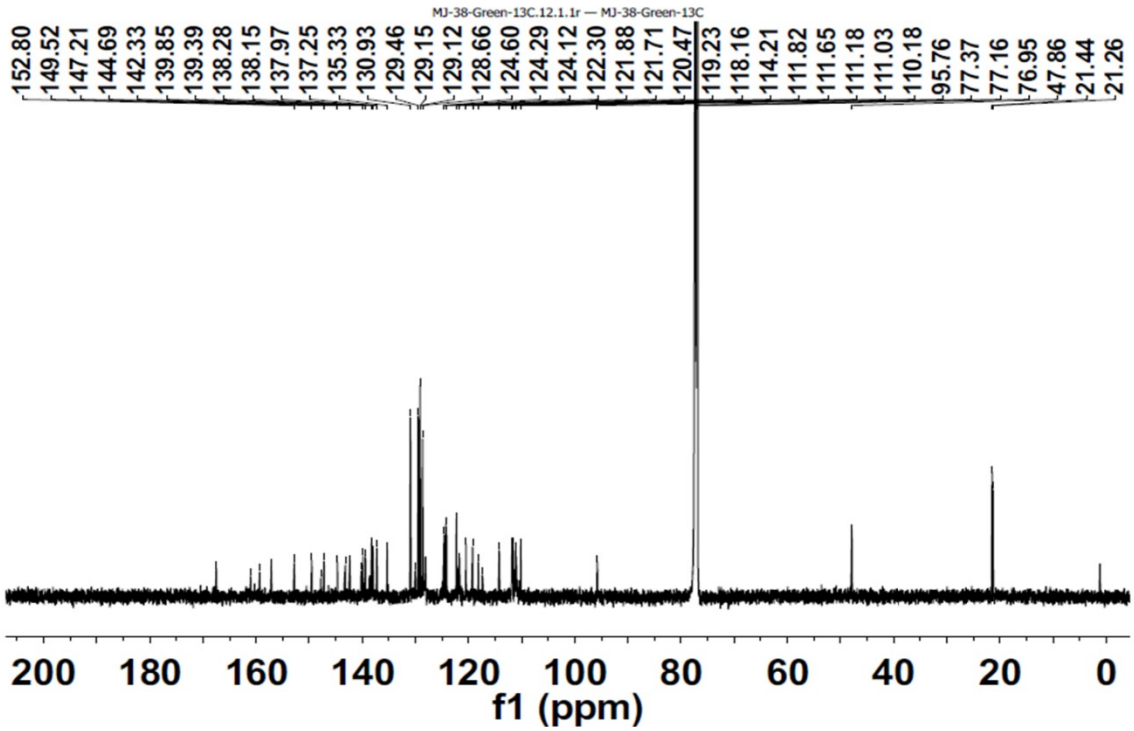
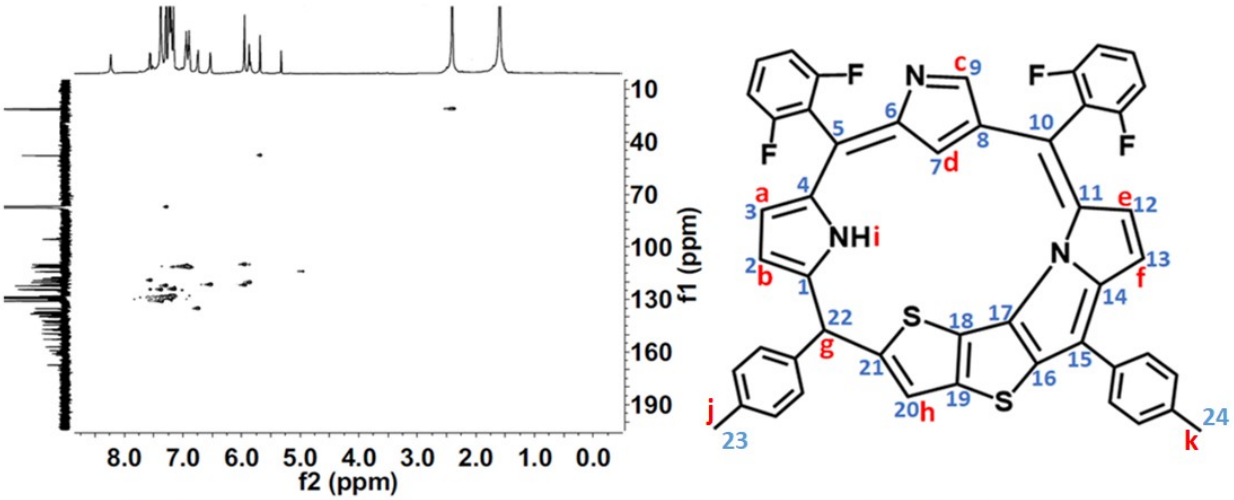
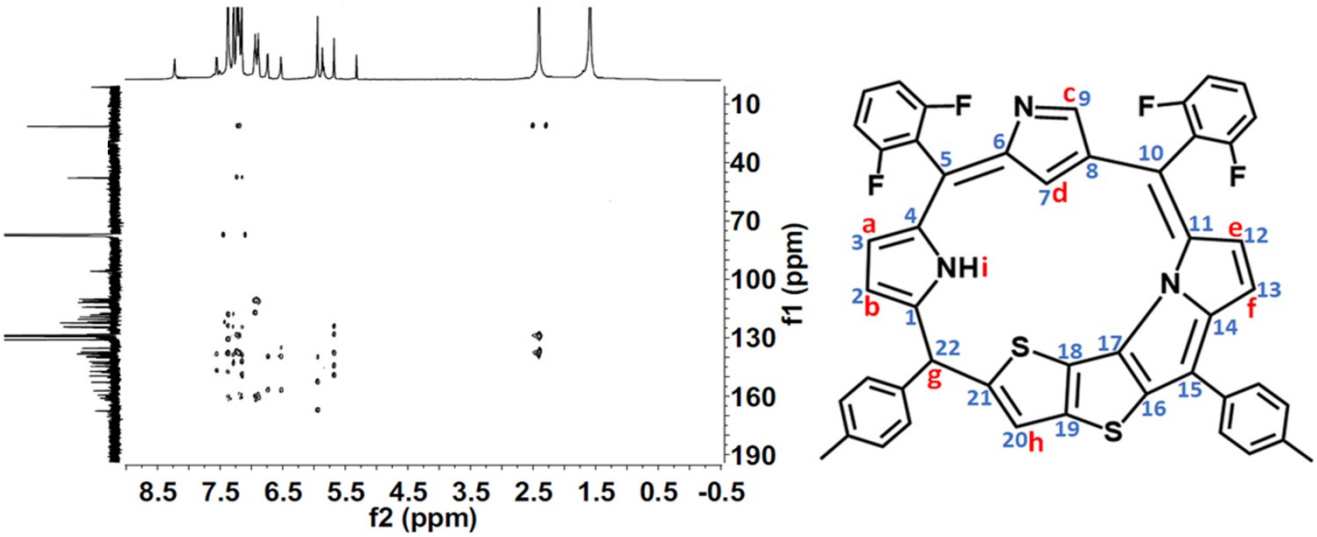


Fig. S52 ^{13}C NMR spectra of **12** in $CDCl_3$ at 298 K.



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.23 (i)	-	5.87 (f)	120.47 (13)
7.16 (h)	124.12 (20)	5.85 (b)	110.03 (2)
6.75 (c)	135.33 (9)	5.68 (g)	47.86 (22)
5.95 (a, e)	110.18 (3), 121.88(12)	6.53 (d)	121.71 (7)
2.40-2.41 (j, k)	21.44 (24), 21.26 (23)		

Fig. S53 ^{1}H-^{13}C 2D HSQC NMR spectra of **12** in $CDCl_3$ at 298 K.



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
7.16 (h)	138.28 (21)	5.95 (a, e)	139.44 (10)
	142.33 (18)		110.03 (2)
	149.52 (19)		128.14 (1)
6.75 (c)	121.71 (7)	5.68 (g)	124.12 (20)
	139.44 (10)		128.14 (1)
6.53 (d)	135.33 (9)		138.28 (21)
	139.44 (10)		149.52 (19)

Fig. S54 ^{1}H-^{13}C 2D HMBC NMR spectra of **12** in $CDCl_3$ at 298 K.

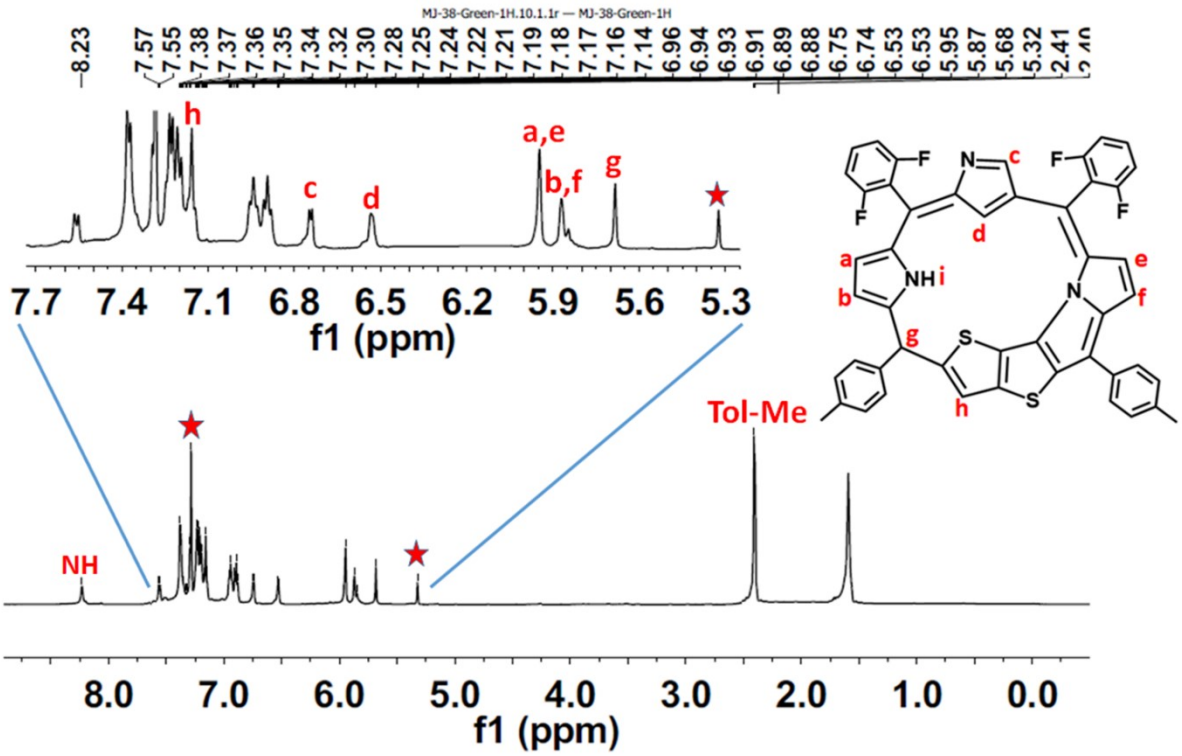


Fig. S55 Completely assigned ^{1}H NMR spectra of **12** in $CDCl_3$ at 263 K.

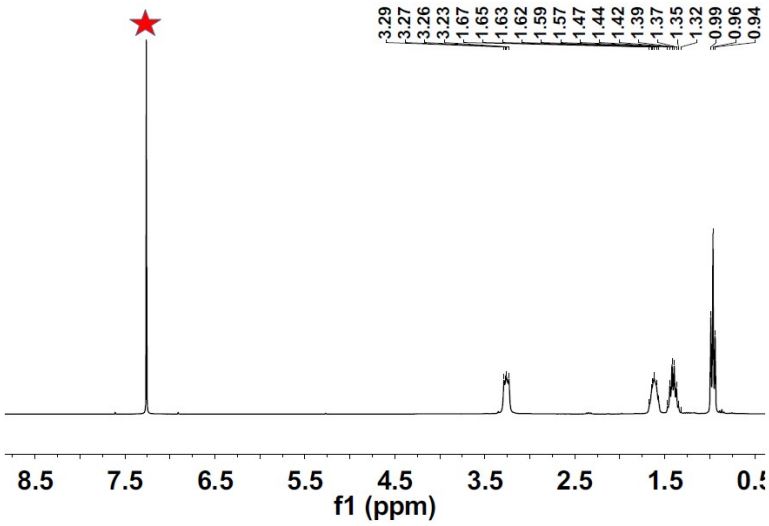


Fig. S56 ^{1}H NMR spectral pattern of TBAF in $CDCl_3$ at 298 K.

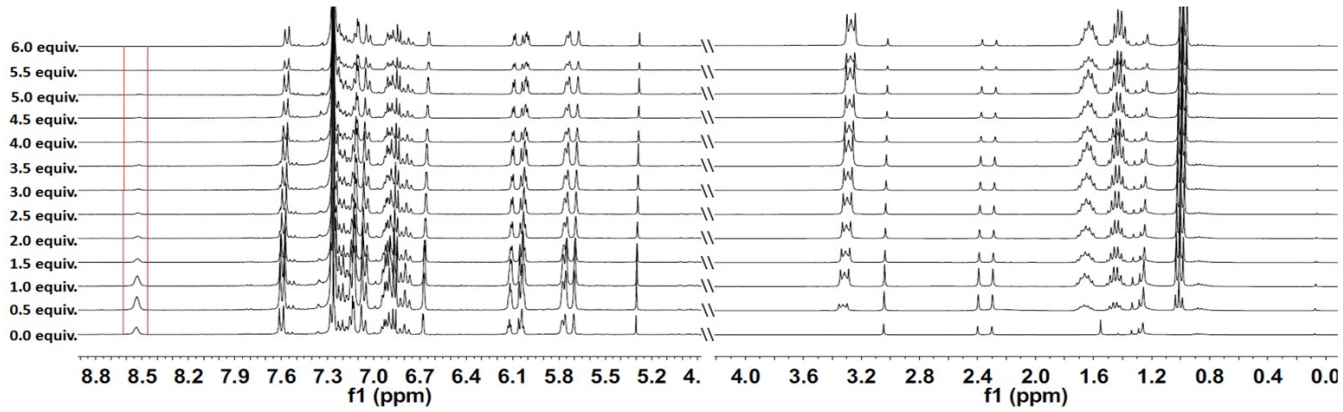


Fig. S57 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.5 M) to **10** (1×10^{-2} M) in $CDCl_3$ at 298 K.

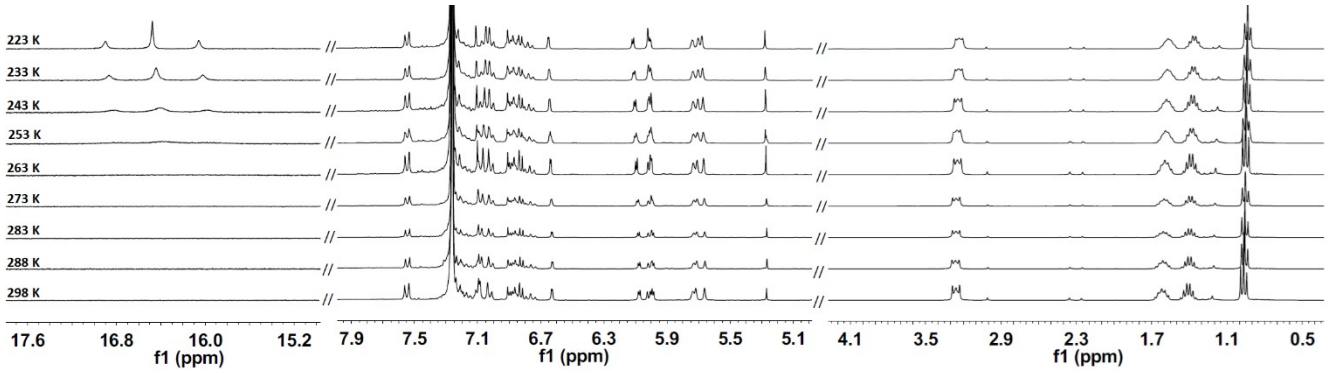


Fig. S58 Low VT ^{1}H NMR spectral pattern observed upon addition of TBAF (1.07 M) to **10** (1×10^{-2} M) in $CDCl_3$.

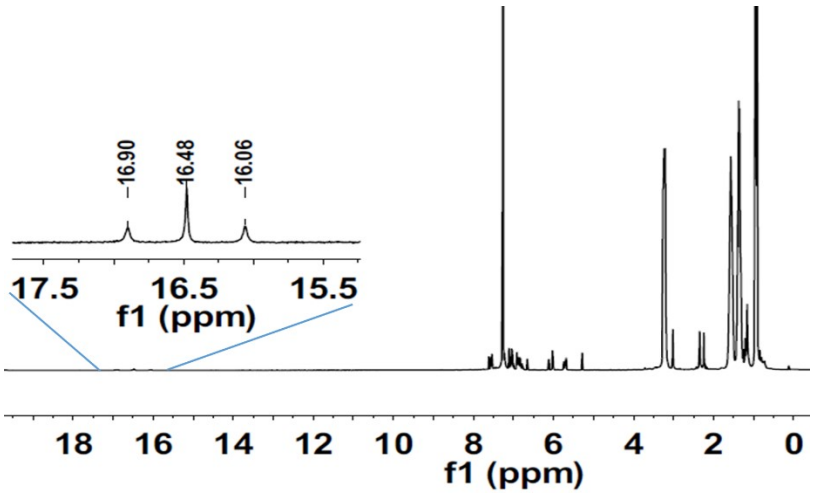


Fig. S59 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.5 M) to **10** (1×10^{-2} M) in $CDCl_3$ at 223 K.

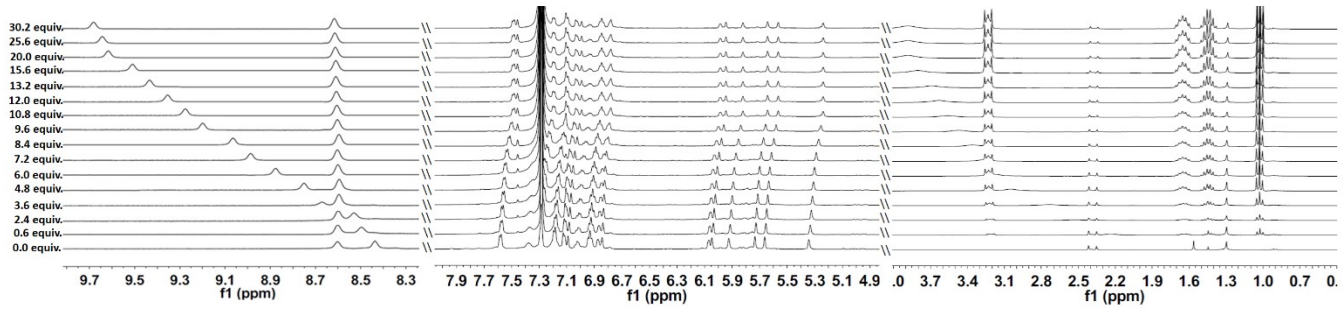


Fig. S60 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.5 M) to **11** (1 × 10^{-2} M) in $CDCl_3$ at 298 K.

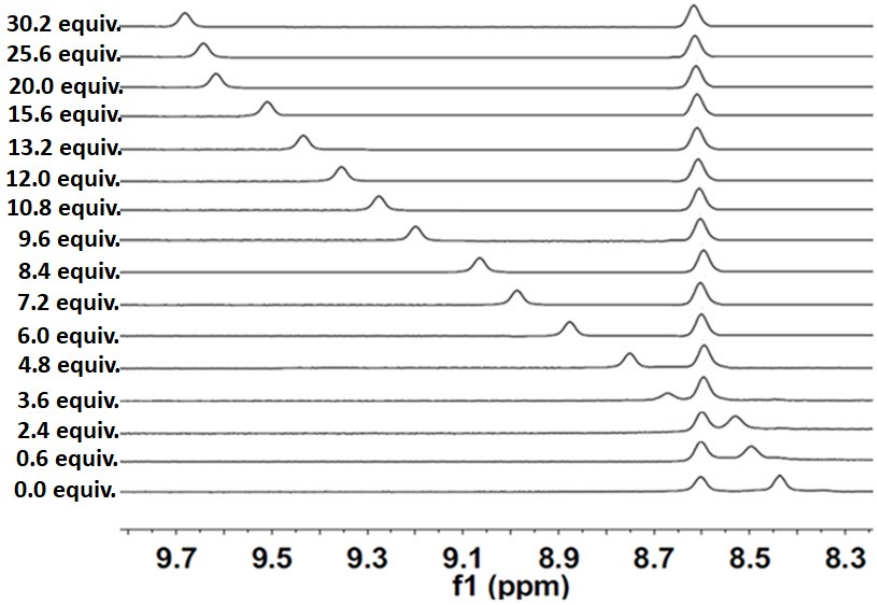


Fig. S60A ^{1}H NMR spectral pattern observed upon addition of TBAF (1.07 M) to **11** (1 × 10^{-2} M) in $CDCl_3$ at 298 K in deshielded region.

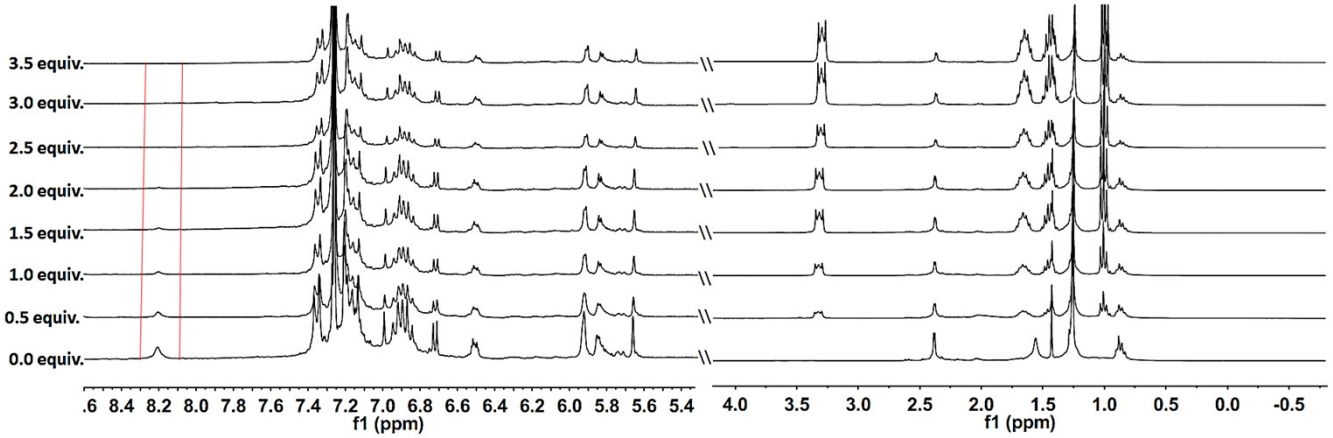


Fig. S61 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.5 M) to **12** (1 × 10^{-2} M) in $CDCl_3$ at 298 K.

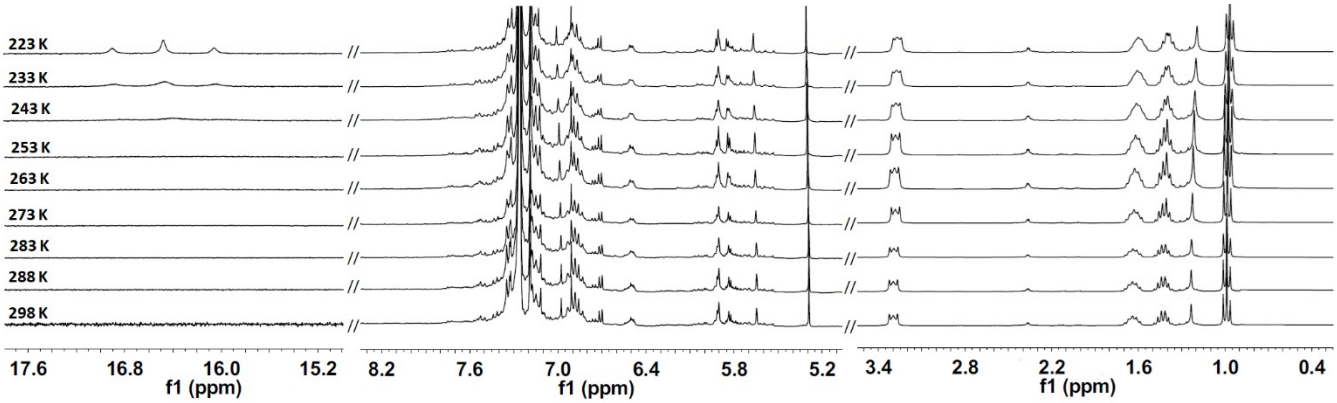


Fig. S62 Low VT ^{1}H NMR spectral pattern observed upon addition of TBAF to **12** in $CDCl_3$.

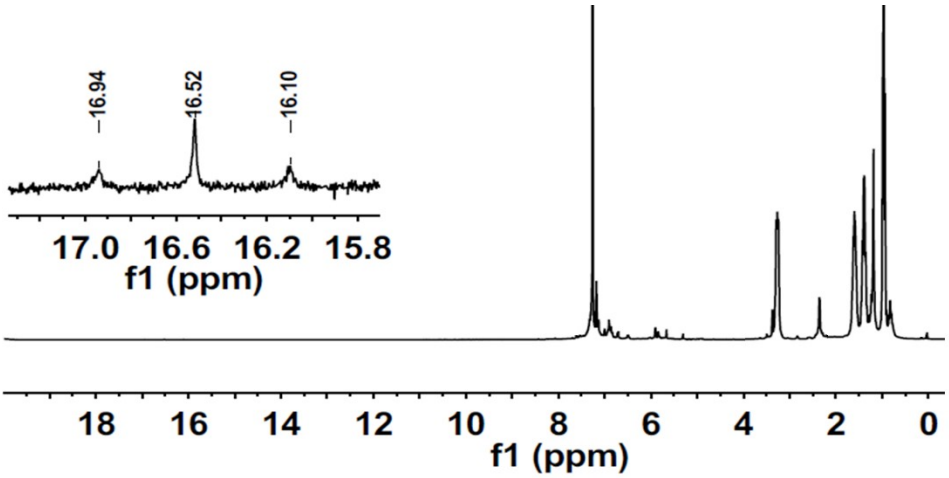


Fig. S63 ^{1}H NMR spectral pattern observed upon addition of TBAF to **12** in $CDCl_3$ at 223 K.

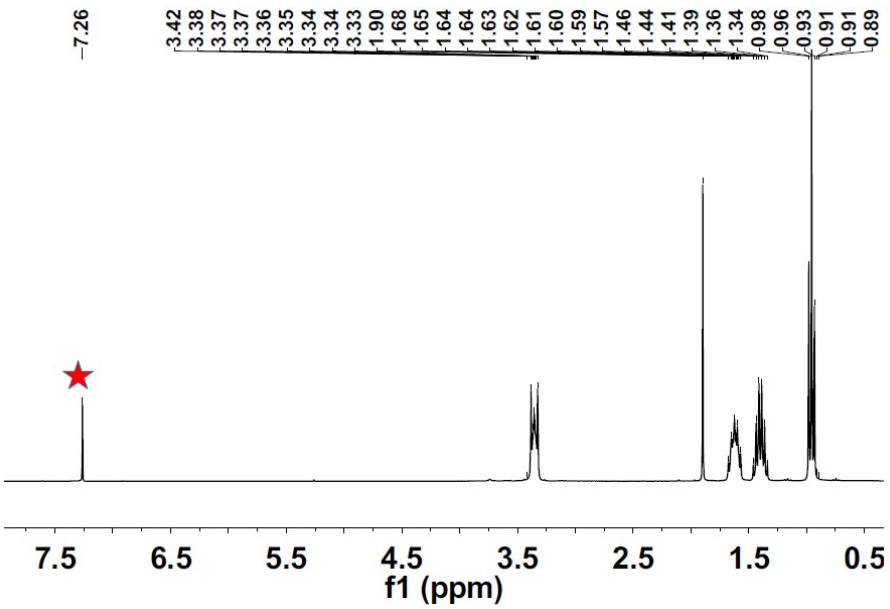


Fig. S64 ^{1}H NMR spectral pattern of TBAOAc in $CDCl_3$ at 298 K.

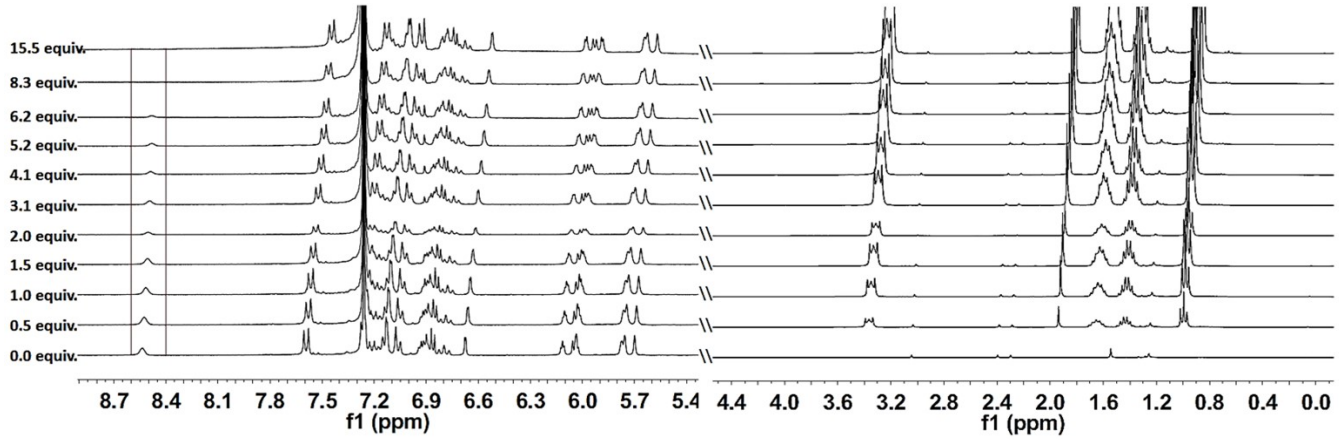


Fig. S65 ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.9 M) to **10** (1 × 10^{-2} M) in $CDCl_3$ at 298 K.

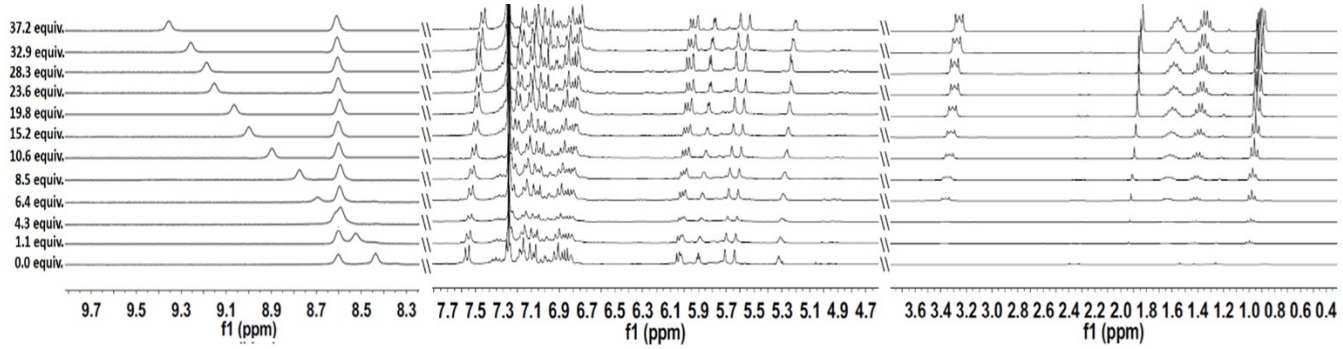


Fig. S66 ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.9 M) to **11** (1 × 10^{-2} M) in $CDCl_3$ at 298 K.

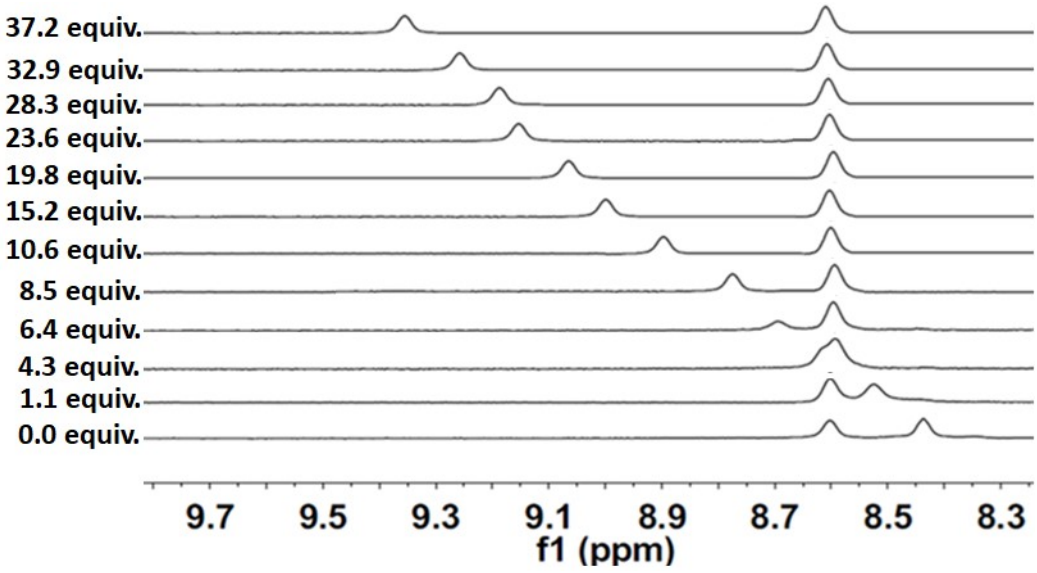


Fig. S66A ^{1}H NMR spectral pattern observed upon addition of TBAOAc to **11** in $CDCl_3$ at 298 K in the deshielded region.

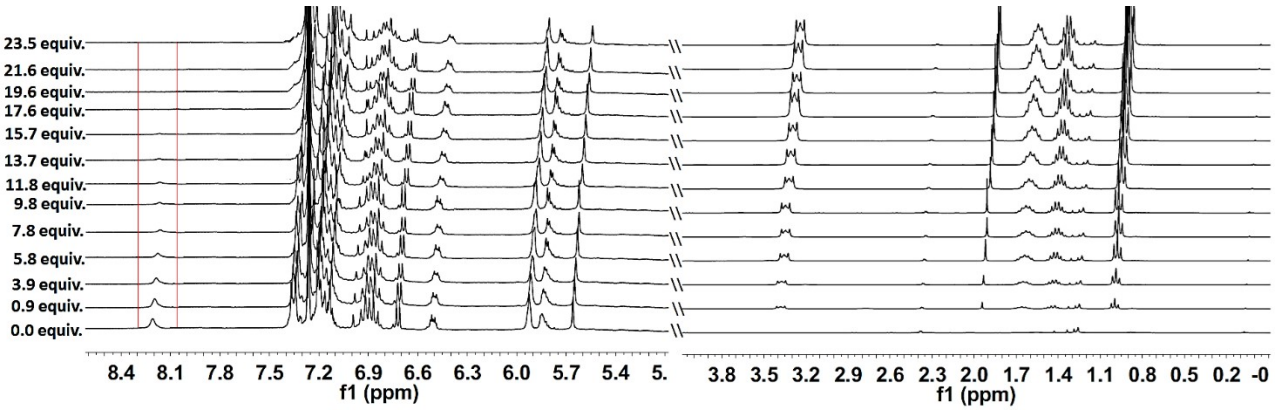


Fig. S67 ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.9 M) to **12** (1 × 10^{-2} M) in $CDCl_3$ at 298 K.

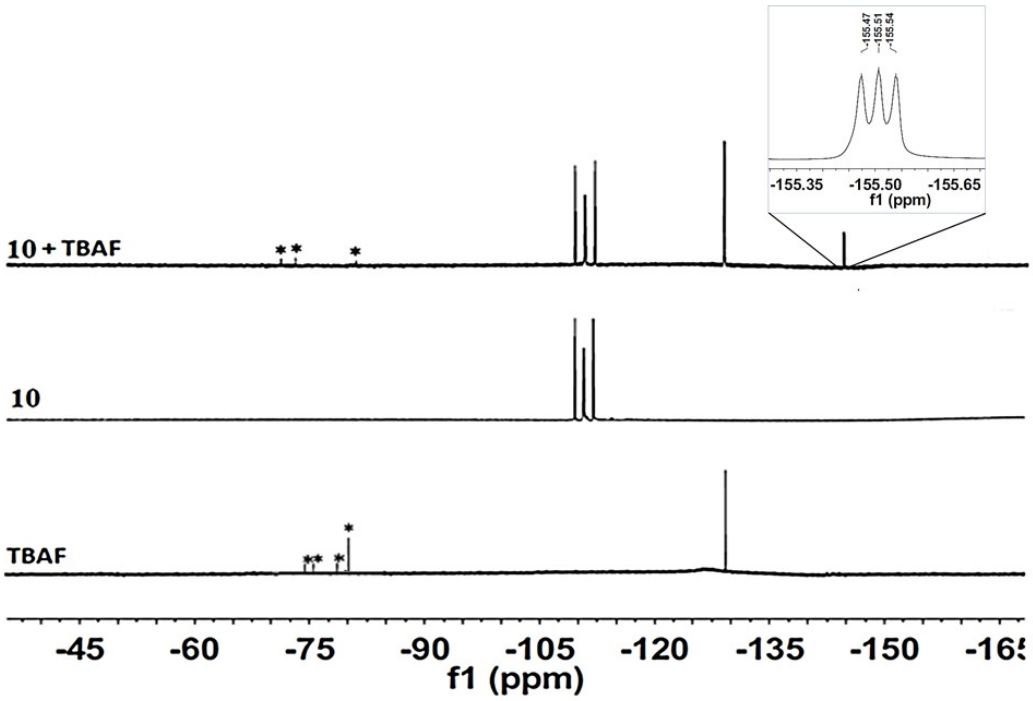


Fig. S68 Comparative ^{19}F NMR spectra for TBAF, **10** in $CDCl_3$ at 298 K and after addition of TBAF (0.5 M) to **10** (1 × 10^{-2} M) in $CDCl_3$ at 223 K (* at -80 to -40 ppm corresponds to unknown impurities in TBAF).

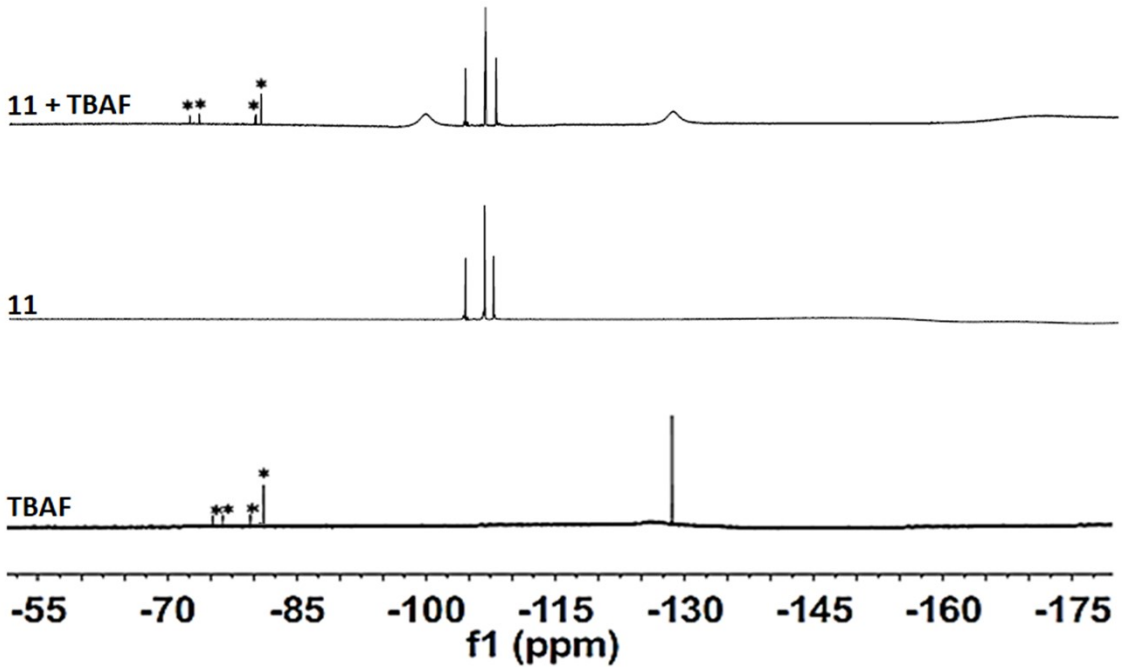


Fig. S69 Comparative ^{19}F NMR spectra for TBAF, **11** in $CDCl_3$ at 298 K and after addition of TBAF (0.5 M) to **11** (1×10^{-2} M) in $CDCl_3$ at 298 K (* at -80 to -40 ppm corresponds to unknown impurities in TBAF).

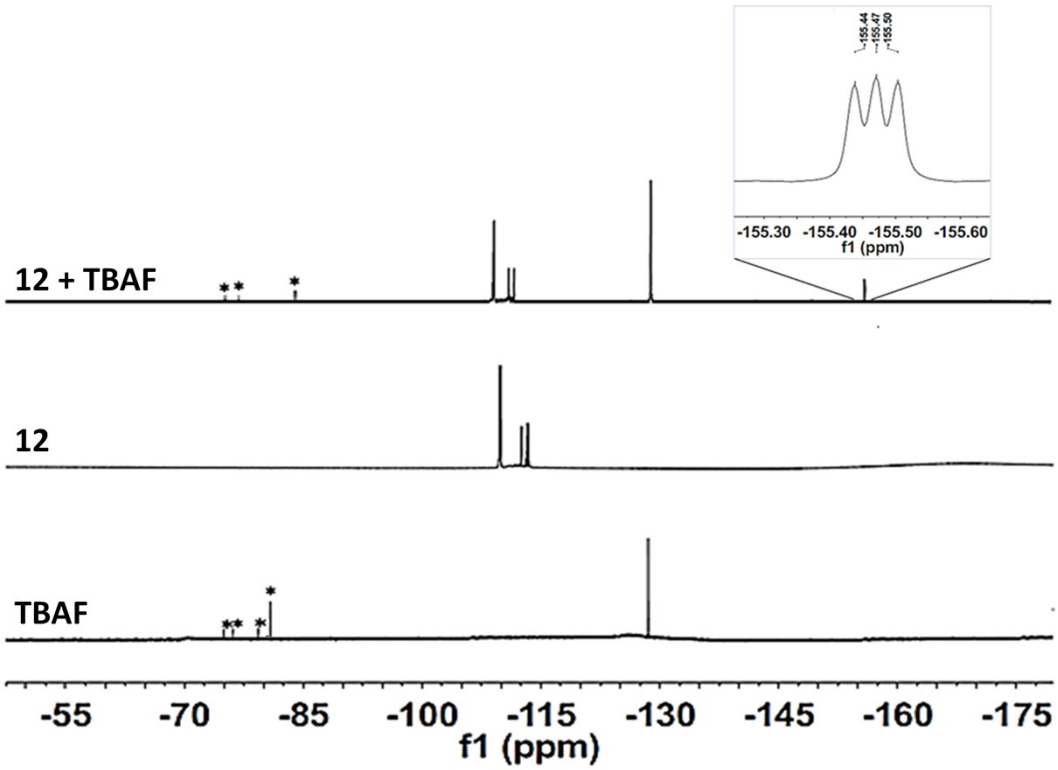


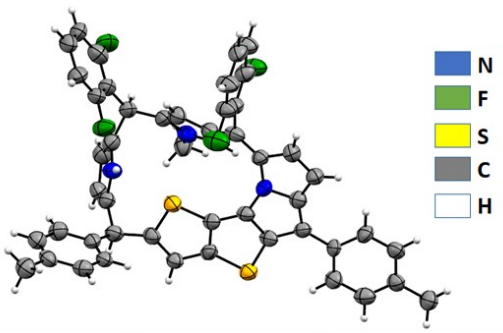
Fig. S70 Comparative ^{19}F NMR spectra for TBAF, **12** in $CDCl_3$ at 298 K and after addition of TBAF (0.5 M) to **12** (1×10^{-2} M) in $CDCl_3$ at 223 K (* at -80 to -40 ppm corresponds to unknown impurities in TBAF).

4. 0 Crystallographic Data

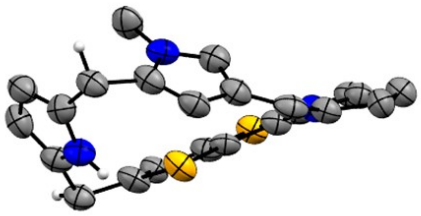
Table S1

Parameters	10
Chemical formula	$C_{49}H_{33}F_4N_3S_2$
Formula weight	803.2052
Temperature (K)	100
Crystal system	Triclinic
Space group	P -1
a (Å); α (°)	15.72(3); 94.031(19)
b (Å); β(°)	16.498(18); 100.44(4)
c (Å); γ (°)	18.03(2); 90.63(4)
V (Å3); Z	4586(11); 2
ρ (calc.) g m-3	1.226
μ(Mo Kα) mm-1	0.227
2θmax (°)	26.454
R(int)	0.0900
Completeness to θ	0.991
Data / param.	18771/5816
GOF	0.919
R1 [F>4σ(F)]	0.0900
wR2 (all data)	0.2839
max. peak/hole (e.Å^{-3})	0.414/-0.349
CCDC	**2252846**

(a)



(b)



(c)

Planes	Dihedral Angle (°)	Planes	Dihedral Angle (°)
Py1-Ar1	45.51	Py3-Ar2	74.44
Py2-Ar1	51.29	Py2-Ar2	66.36
Py1-Ar4	77.40	Py1-Py2	77.73
Th2-Ar4	81.19	Py1-Th2	79.87
Th1-Ar3	20.03	Th1-Py3	20.40
Py3-Ar3	39.69	Py2-Py3	45.23
TP ring-Py1	56.24	TP ring-Py2	57.87

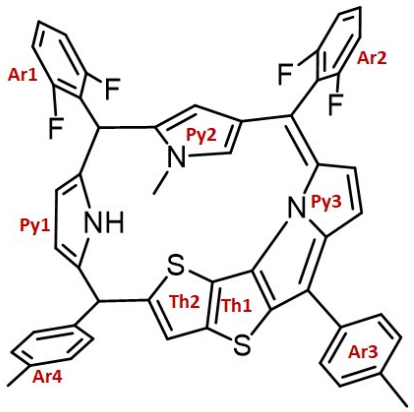


Fig. S71 Crystal structure of **10** (a: top view; b: side view, c: tabulated dihedral angles)

Tp ring: [5.5.5.5] tetracyclic ring

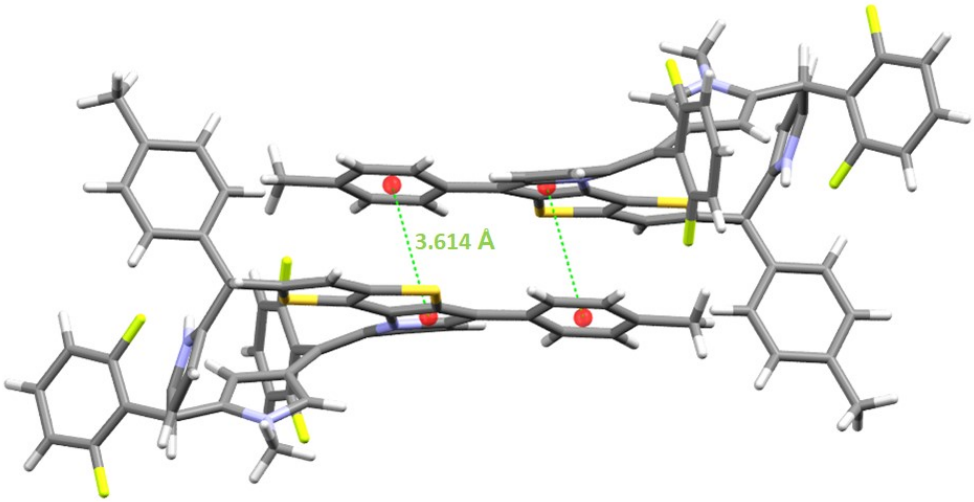


Fig. S72 Crystal structure of **10** showing strong π-π stacking interaction.

5. Theoretical Calculation

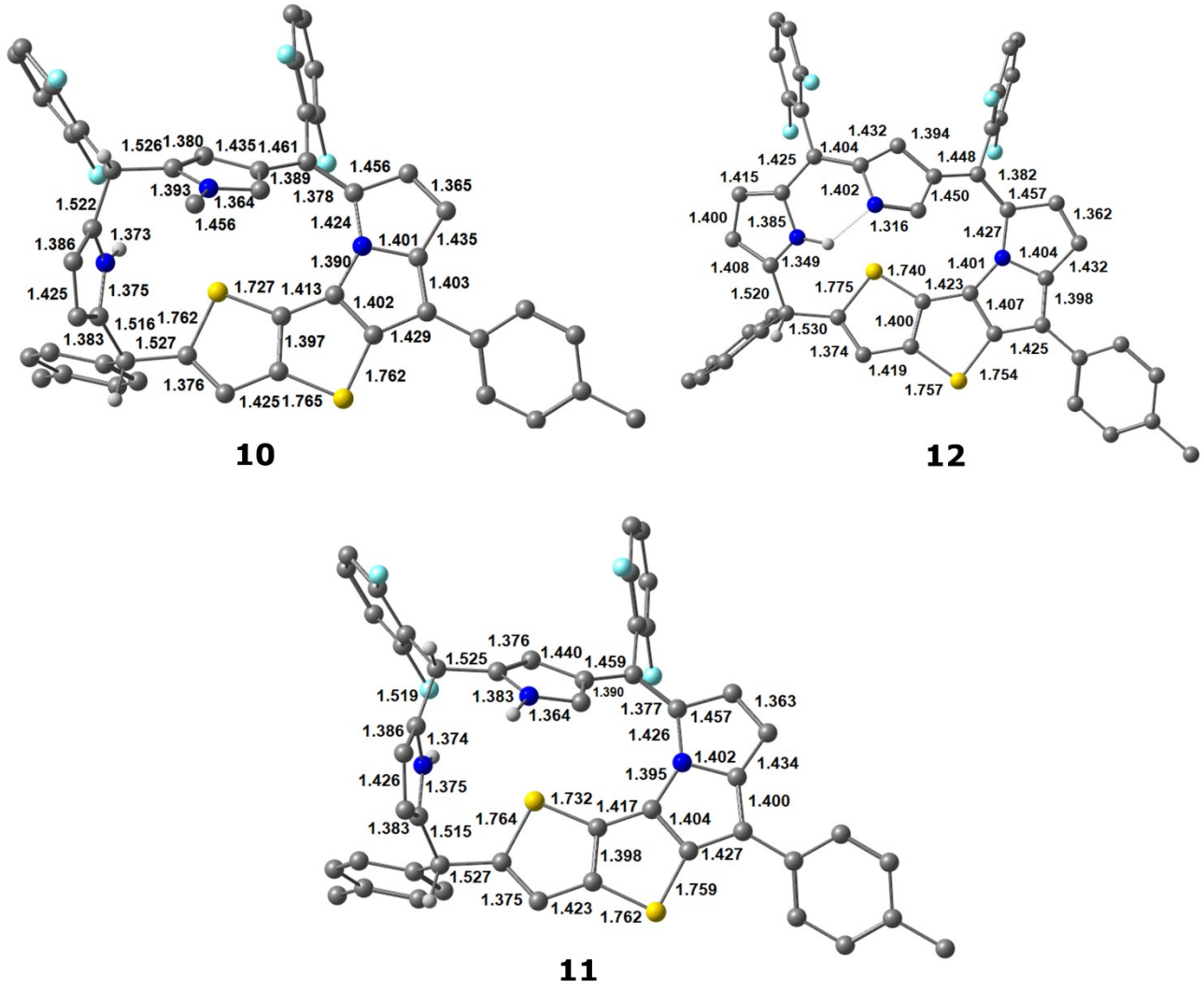


Fig. S73 DFT optimised geometries and key bond length parameters (Å) of **10-12**, at B3LYP/6-31G** level of theory.

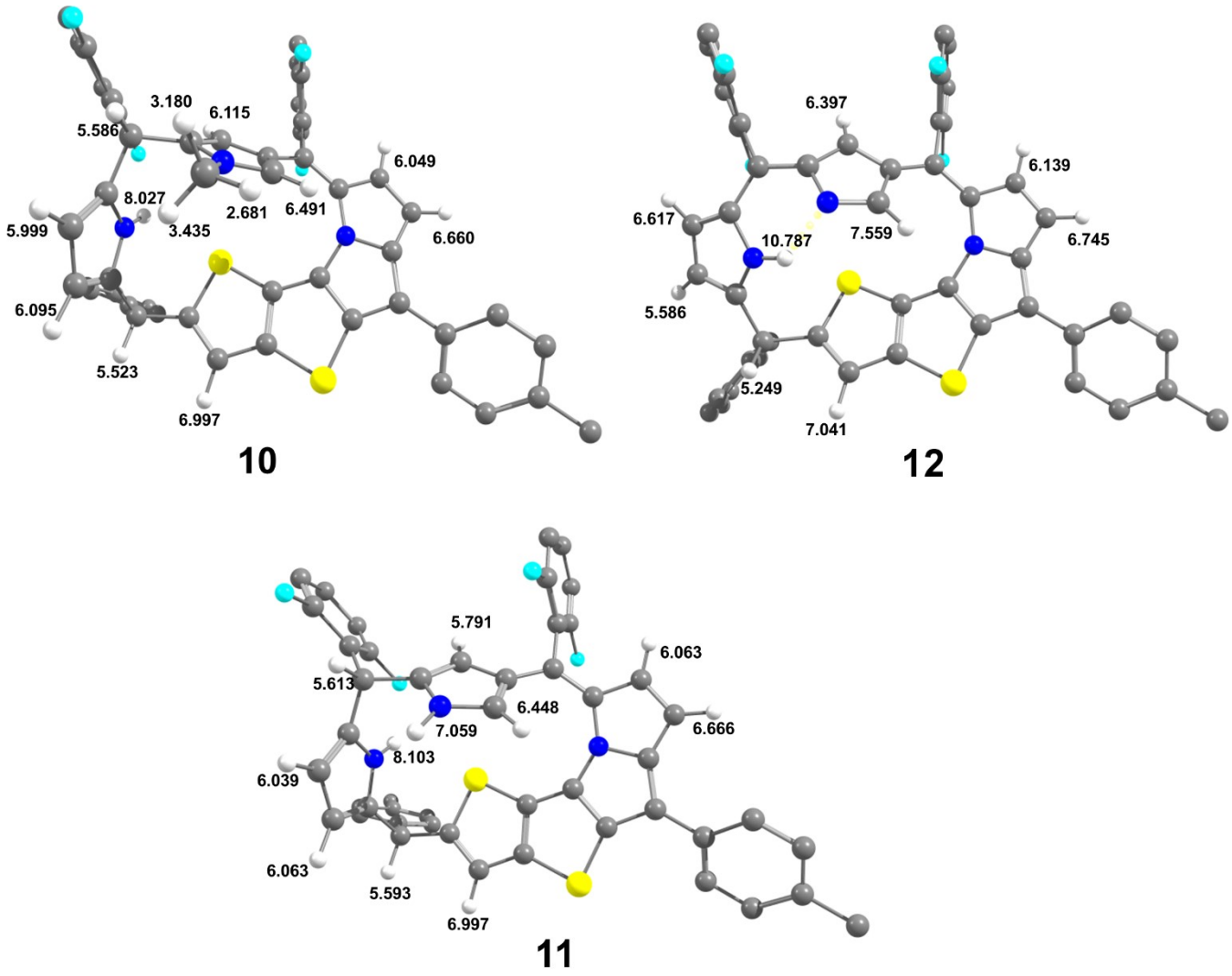


Fig. S74 ^{1}H NMR chemical shifts of DFT optimised geometries of **10-12**, at B3LYP/6-31G** level of theory.

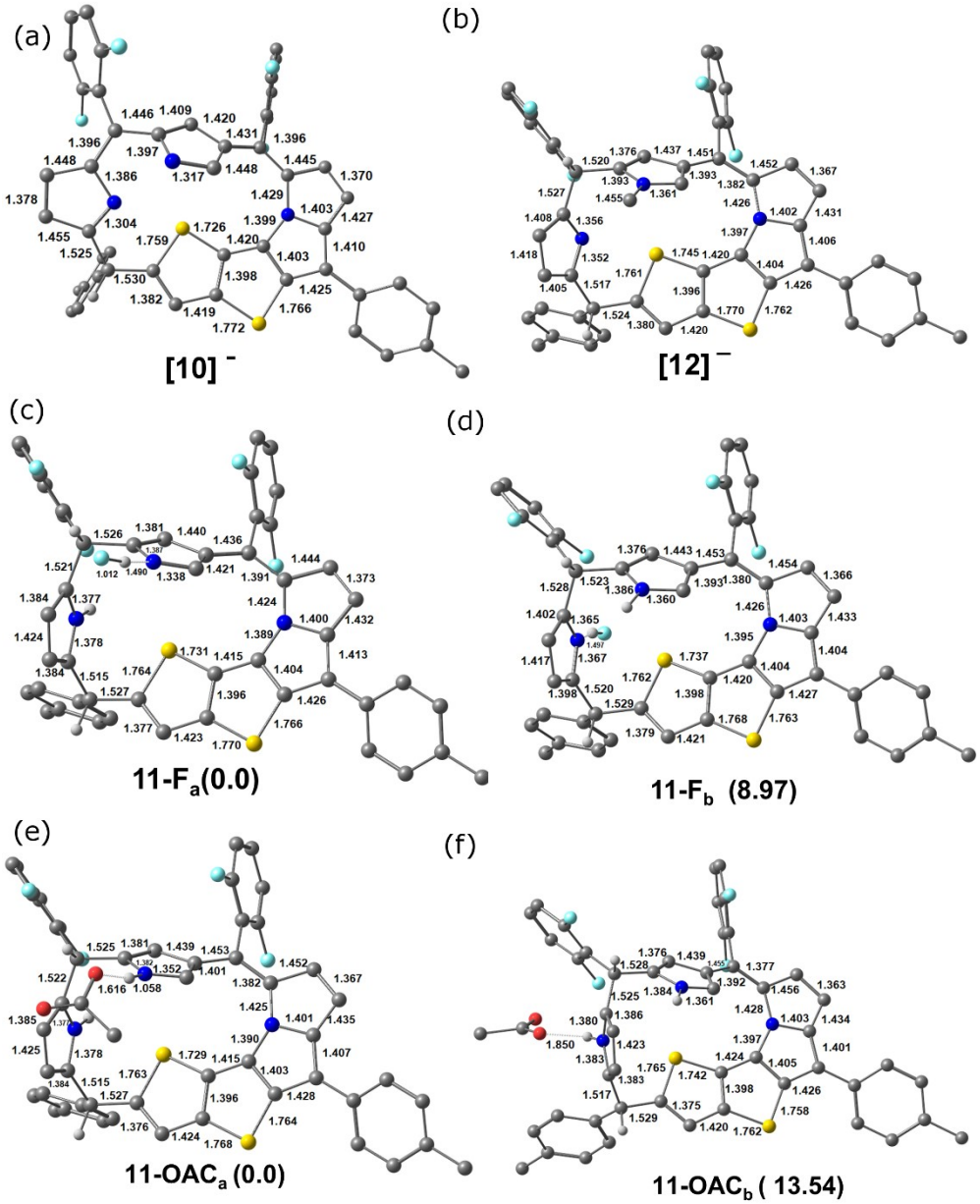


Fig. S75 DFT optimised geometries and key bond length parameters (Å) of (a) [**10**]$^-$, (b) [**12**]$^-$, (c & d) [**11-F**]$^-$**,** (e & f) [**11-AcO**]$^-$ at B3LYP/6-31G** level of theory.

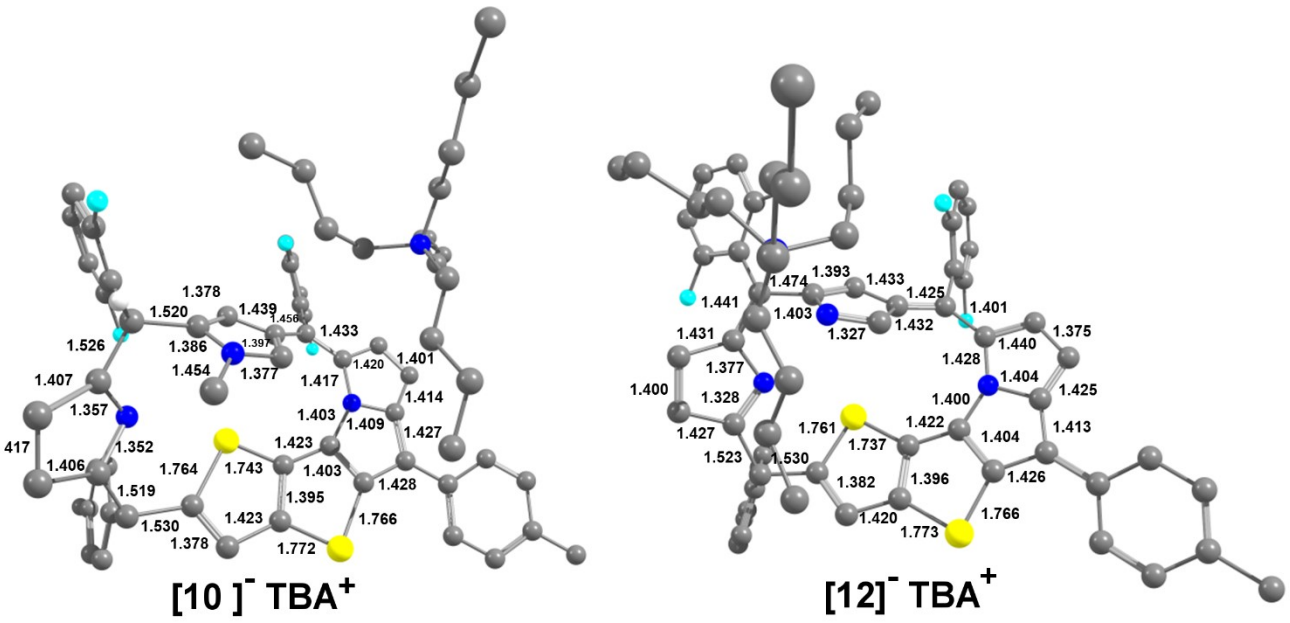


Fig. S76 DFT optimised geometries and key bond length parameters (Å) of (a) [**10**]-**TBA**+ (b) [**12**]-**TBA**+ at B3LYP/6-31G** level of theory.

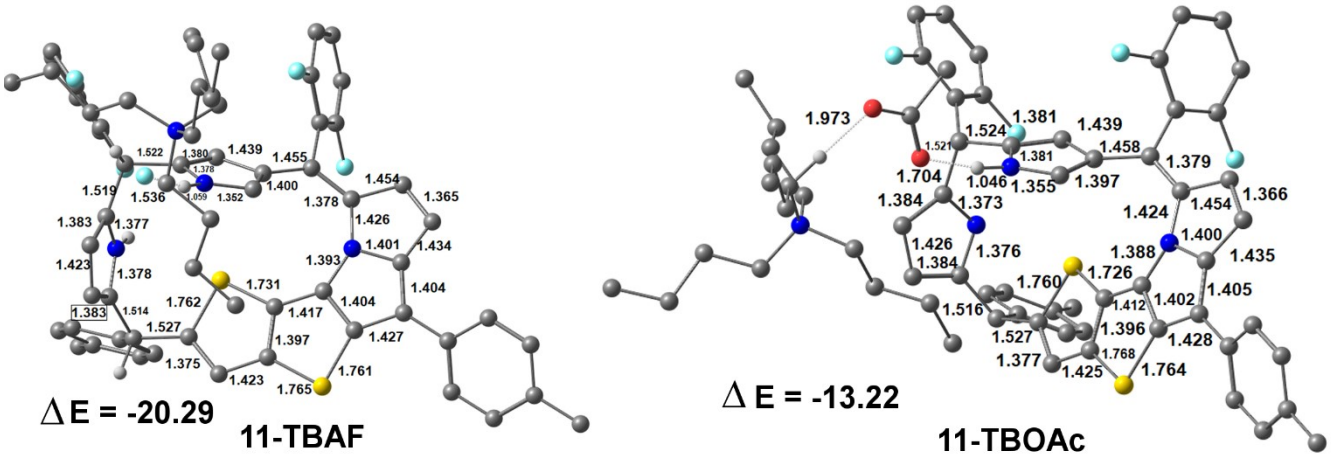


Fig. S77 DFT optimised geometries and key bond length parameters (Å) of (a) **11-TBAF** (b) **11-TBOAc** at B3LYP/6-31G** level of theory.

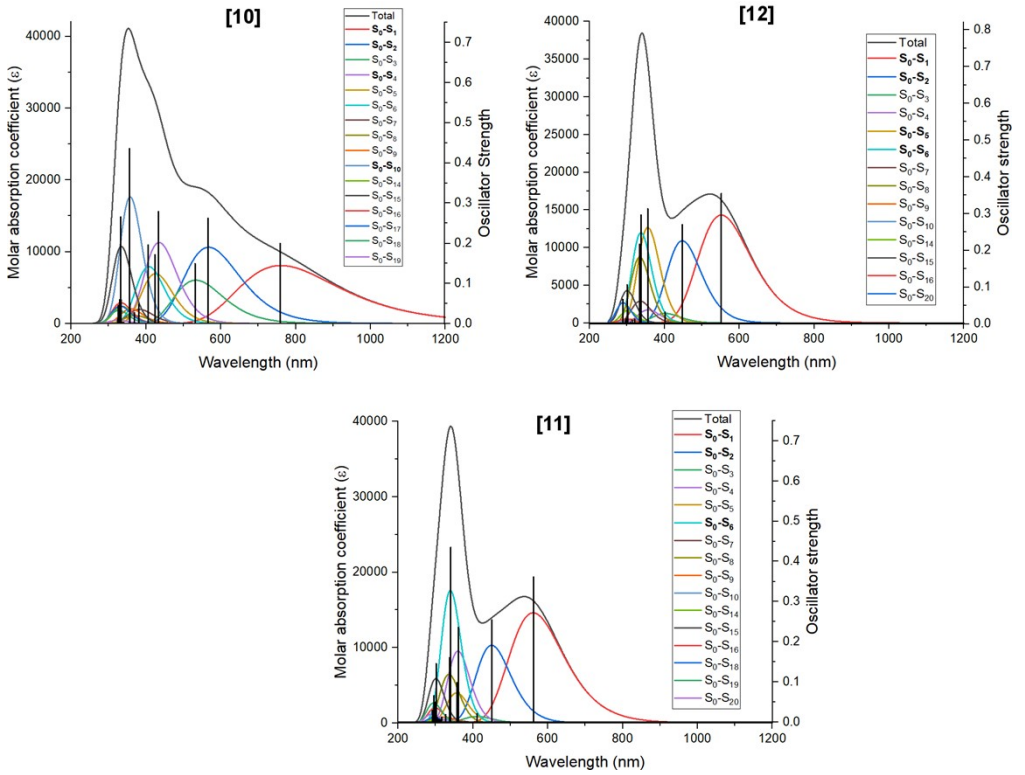


Fig. S78 Steady state absorption spectrum (total) and individual transitions that are predicted from TD-DFT calculation with solvent (dichloromethane using a polarizable continuum model) and at B3LYP/ 6-31G** level of theory for **10**-**12.**

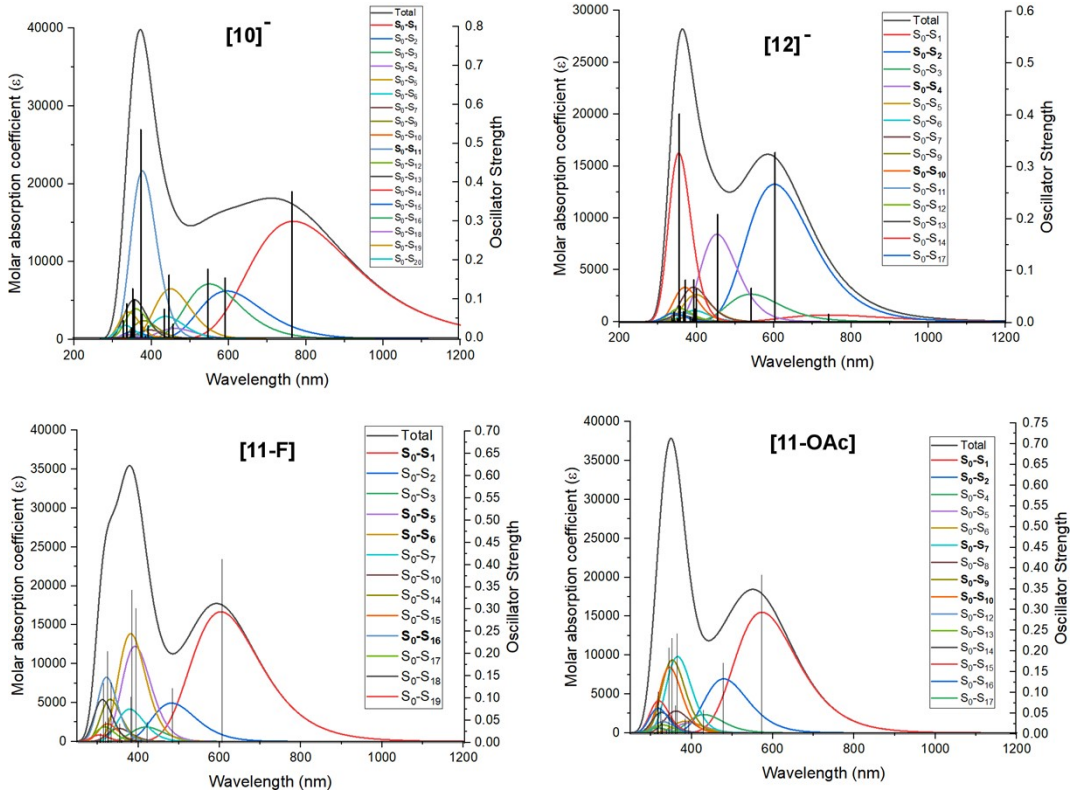


Fig. S79 Steady state absorption spectrum (total) and individual transitions that are predicted from TD-DFT calculation with solvent (dichloromethane using a polarizable continuum model) and at B3LYP/ 6-31G** level of theory for [**10**]$^-$, [**11-F$_a$**]$^-$, [**11-OAC$_a$**]$^-$ and [**12**]$^-$.

Table S2: Summary of UV-vis spectral data of **10** that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.2106**	**560.86**	**0.36130**	**Singlet-A**	**H -> L 97.7%**
2	**2.7553**	**449.98**	**0.25470**	**Singlet-A**	**H-1 -> L 90.7%**
3	3.0242	409.97	0.02130	Singlet-A	H-2 -> L 92.9%
4	**3.4435**	**360.05**	**0.23570**	**Singlet-A**	**H -> L+1 48.5%, H-3 -> L 38.4%, H-4 -> L 5.4%**
5	3.4792	356.36	0.09850	Singlet-A	H-3 -> L 53.4%, H -> L+1 22.7%, H-4 -> L 14.9%
6	**3.6480**	**339.87**	**0.43420**	**Singlet-A**	**H-4 -> L 54.1%, H -> L+1 22.2%, H -> L+3 8.5%, H -> L+2 8.1%**
7	3.6645	338.34	0.01380	Singlet-A	H -> L+3 61.6%, H-4 -> L 17.6%, H -> L+2 9.9%, H-5 -> L 7.7%
8	3.6907	335.94	0.15960	Singlet-A	H -> L+2 73.3%, H -> L+3 13.3%, H-5 -> L 5.2%
9	3.8047	325.87	0.01910	Singlet-A	H-5 -> L 71.2%, H -> L+3 13.0%, H -> L+9 5.8%
10	3.9246	315.92	0.01270	Singlet-A	H -> L+5 58.2%, H -> L+7 22.4%, H -> L+6 8.0%
11	3.9703	312.28	0.00660	Singlet-A	H -> L+6 75.7%, H -> L+5 6.9%, H-8 -> L 6.2%
12	4.0223	308.24	0.00800	Singlet-A	H-6 -> L 74.9%, H -> L+4 17.1%
13	4.0284	307.78	0.00340	Singlet-A	H -> L+4 71.8%, H-6 -> L 17.0%
14	4.0770	304.11	0.01140	Singlet-A	H -> L+7 50.6%, H -> L+5 24.1%, H -> L+8 9.2%
15	4.1182	301.06	0.14530	Singlet-A	H-1 -> L+1 62.3%, H-7 -> L 12.4%, H -> L+9 7.9%
16	4.1461	299.04	0.04970	Singlet-A	H-7 -> L 67.1%, H-1 -> L+1 14.7%, H-13 -> L 5.4%
17	4.1501	298.75	0.00090	Singlet-A	H -> L+8 83.5%, H -> L+7 13.8%
18	4.1596	298.07	0.01840	Singlet-A	H-8 -> L 83.7%, H -> L+6 6.5%
19	4.2022	295.05	0.06550	Singlet-A	H -> L+9 56.8%, H-12 -> L 12.7%, H-1 -> L+1 7.3%
20	4.2567	291.27	0.02990	Singlet-A	H-1 -> L+2 77.4%, H-2 -> L+2 11.1%

Table S3: Summary of UV-vis spectral data of **11** that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.2455**	**552.15**	**0.35390**	**Singlet-A**	**H -> L 97.2%**
2	**2.7682**	**447.89**	**0.26960**	**Singlet-A**	**H-1 -> L 91.2%**
3	3.0816	402.34	0.03150	Singlet-A	H-2 -> L 93.8%
4	3.4763	356.66	0.04350	Singlet-A	H-3 -> L 91.5%
5	**3.4848**	**355.79**	**0.31330**	**Singlet-A**	**H -> L+1 64.4%, H-4 -> L 16.9%, H -> L+2 12.3%**
6	**3.6744**	**337.43**	**0.29610**	**Singlet-A**	**H-4 -> L 43.7%, H -> L+1 29.4%, H -> L+2 16.7%, H -> L+3 6.0%**
7	3.6930	335.73	0.07190	Singlet-A	H -> L+3 33.5%, H -> L+2 31.6%, H-4 -> L 29.1%
8	**3.7105**	334.14	0.21630	**Singlet-A**	**H -> L+3 49.9%, H -> L+2 37.1%**
9	3.8702	320.36	0.01320	Singlet-A	H-5 -> L 69.3%, H -> L+9 8.0%, H -> L+3 7.5%
10	3.9488	313.98	0.01010	Singlet-A	H -> L+5 51.8%, H -> L+7 35.2%
11	4.0041	309.64	0.00510	Singlet-A	H -> L+6 76.6%, H-8 -> L 7.5%
12	4.0512	306.04	0.00070	Singlet-A	H -> L+4 95.7%
13	4.0659	304.94	0.00240	Singlet-A	H-6 -> L 90.9%, H-5 -> L 5.2%
14	4.0970	302.62	0.04100	Singlet-A	H -> L+7 36.5%, H -> L+5 26.3%, H-1 -> L+1 18.2%
15	4.1248	300.58	0.10640	Singlet-A	H-1 -> L+1 58.2%, H -> L+7 13.9%, H -> L+5 10.6%, H -> L+9 5.9%
16	4.1650	297.68	0.01340	Singlet-A	H-8 -> L 83.0%, H -> L+6 7.7%
17	4.1783	296.73	0.00060	Singlet-A	H -> L+8 75.1%, H-7 -> L 7.6%, H -> L+7 5.4%
18	4.1808	296.56	0.00800	Singlet-A	H-7 -> L 37.8%, H -> L+9 15.0%, H -> L+8 14.3%, H-12 -> L 12.3%,
19	4.2306	293.07	0.00130	Singlet-A	H-1 -> L+2 72.6%, H-7 -> L 6.9%, H-2 -> L+2 6.7%
20	4.2778	289.83	0.06650	Singlet-A	H -> L+9 41.1%, H-7 -> L 29.3%, H-1 -> L+2 10.3%

Table S4: Summary of UV-vis spectral data of **12** that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**1.6299**	**760.69**	**0.19980**	**Singlet-A**	**H -> L 97.9%**
2	**2.1838**	**567.75**	**0.26260**	**Singlet-A**	**H-1 -> L 66.9%, H -> L+1 30.7%**
3	2.3249	533.29	0.14940	Singlet-A	H -> L+1 58.5%, H-1 -> L 27.1%, H-2 -> L 12.6%
4	**2.8489**	**435.20**	**0.27900**	**Singlet-A**	**H-1 -> L+1 55.5%, H-2 -> L 37.6%**
5	2.9109	425.93	0.17170	Singlet-A	H-3 -> L 33.5%, H-2 -> L 30.5%, H-1 -> L+1 25.4%
6	3.0391	407.96	0.19600	Singlet-A	H-3 -> L 61.8%, H-2 -> L 17.1%, H-1 -> L+1 11.1%
7	3.2383	382.87	0.04890	Singlet-A	H-4 -> L 90.0%
8	3.3404	371.17	0.02760	Singlet-A	H-2 -> L+1 91.2%
9	3.4460	359.79	0.05060	Singlet-A	H-5 -> L 82.0%, H -> L+2 8.9%
10	**3.4645**	**357.87**	**0.43570**	**Singlet-A**	**H -> L+2 75.2%, H-5 -> L 11.7%**
11	3.6234	342.18	0.00310	Singlet-A	H-9 -> L 97.2%
12	3.6564	339.09	0.00240	Singlet-A	H-6 -> L 93.5%
13	3.6661	338.19	0.00290	Singlet-A	H -> L+3 87.5%
14	3.6916	335.85	0.05910	Singlet-A	H-10 -> L 33.1%, H-11 -> L 18.6%, H-14 -> L 11.0%, H -> L+4 7.8%, H-8 -> L 7.6%,
15	**3.7092**	**334.26**	**0.26540**	**Singlet-A**	**H-3 -> L+1 48.4%, H -> L+4 17.5%, H-4 -> L+1 8.8%, H-10 -> L 6.8%**
16	3.7175	333.51	0.07150	Singlet-A	H-8 -> L 35.7%, H-12 -> L 30.9%, H -> L+4 11.2%, H-3 -> L+1 10.2%
17	3.7359	331.87	0.06030	Singlet-A	H-3 -> L+1 24.1%, H -> L+4 21.9%, H-11 -> L 18.9%, H-8 -> L 14.4%, H-10 -> L 8.0%
18	3.7820	327.83	0.04560	Singlet-A	H-11 -> L 31.0%, H -> L+4 22.9%, H-8 -> L 20.1%, H-10 -> L 13.8%
19	3.8060	325.76	0.01150	Singlet-A	H-12 -> L 40.4%, H-8 -> L 18.5%, H-11 -> L 12.9%, H -> L+4 10.7%, H-10 -> L 7.6%
20	3.8394	322.93	0.00060	Singlet-A	H-7 -> L 89.0%

Table S5: Summary of UV-vis spectral data of [**10**]$^-$ that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	1.6749	740.25	0.01600	Singlet-A	H -> L 99.7%
2	**2.0600**	**601.87**	**0.32760**	**Singlet-A**	**H-1 -> L 98.5%**
3	2.2941	540.45	0.06570	Singlet-A	H-2 -> L 97.2%
4	**2.7367**	**453.04**	**0.20840**	**Singlet-A**	**H-3 -> L 94.4%**
5	3.1105	398.60	0.06460	Singlet-A	H-5 -> L 63.1%, H-4 -> L 33.1%
6	3.1481	393.84	0.02630	Singlet-A	H-4 -> L 45.8%, H-5 -> L 24.1%, H -> L+2 15.0%, H -> L+3 10.6%
7	3.1633	391.95	0.08210	Singlet-A	H -> L+3 42.1%, H -> L+2 28.6%, H-4 -> L 18.7%, H-5 -> L 7.9%
8	3.1952	388.03	0.00640	Singlet-A	H -> L+1 71.0%, H -> L+3 16.1%, H -> L+2 8.5%
9	3.2453	382.04	0.01070	Singlet-A	H -> L+2 38.7%, H -> L+3 26.7%, H -> L+1 25.0%
10	3.3531	369.76	0.08170	Singlet-A	H-6 -> L 74.6%, H-1 -> L+1 13.4%, H-1 -> L+2 6.9%
11	3.3988	364.79	0.02130	Singlet-A	H-1 -> L+1 82.5%, H-6 -> L 13.4%
12	3.4795	356.33	0.03150	Singlet-A	H -> L+6 66.9%, H -> L+5 25.8%
13	3.4890	355.36	0.01620	Singlet-A	H -> L+5 55.2%, H -> L+6 31.5%, H-1 -> L+2 5.2%
14	**3.5016**	**354.08**	**0.40200**	**Singlet-A**	**H-1 -> L+2 77.9%, H -> L+5 7.6%, H-6 -> L 5.7%**
15	3.5521	349.04	0.00700	Singlet-A	H -> L+4 80.3%, H-1 -> L+4 8.4%, H -> L+5 5.3%
16	3.6082	343.62	0.00280	Singlet-A	H -> L+7 85.5%, H -> L+8 8.8%
17	3.6443	340.21	0.02010	Singlet-A	H-1 -> L+4 78.6%, H -> L+8 8.5%, H -> L+4 6.3%
18	3.6562	339.11	0.00380	Singlet-A	H-1 -> L+5 63.5%, H-1 -> L+3 26.8%
19	3.6632	338.46	0.00250	Singlet-A	H -> L+8 64.6%, H -> L+9 16.4%, H-1 -> L+4 6.0%
20	3.6949	335.55	0.00860	Singlet-A	H-1 -> L+3 55.3%, H-1 -> L+5 30.6%, H-2 -> L+3 9.4%

Table S6: Summary of UV-vis spectral data of [**11-F$_a$**]$^-$ that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.0549**	**603.36**	**0.41210**	**Singlet-A**	**H -> L 99.0%**
2	**2.5708**	**482.28**	**0.12190**	**Singlet-A**	**H-1 -> L 94.4%**
3	2.9575	419.22	0.04610	Singlet-A	H-2 -> L 54.9%, H-3 -> L 36.0%
4	3.0619	404.93	0.00690	Singlet-A	H-3 -> L 55.4%, H-2 -> L 39.7%
5	**3.1605**	**392.29**	**0.30250**	**Singlet-A**	**H -> L+1 64.1%, H -> L+3 14.3%, H -> L+2 10.5%, H-3 -> L 5.3%**
6	**3.2474**	**381.80**	**0.34270**	**Singlet-A**	**H -> L+3 82.8%, H -> L+1 12.8%**
7	3.2712	379.02	0.10260	Singlet-A	H -> L+2 83.2%, H -> L+1 14.1%
8	3.4688	357.43	0.00570	Singlet-A	H -> L+7 91.2%, H-4 -> L 6.1%
9	3.4902	355.24	0.00490	Singlet-A	H -> L+8 54.9%, H -> L+4 19.2%, H -> L+6 9.9%, H-4 -> L 8.9%
10	3.5209	352.14	0.04180	Singlet-A	H-4 -> L 70.5%, H -> L+8 8.7%, H -> L+9 6.5%
11	3.5476	349.49	0.00040	Singlet-A	H -> L+4 73.6%, H -> L+8 25.2%
12	3.5697	347.32	0.00240	Singlet-A	H -> L+5 95.8%
13	3.5767	346.64	0.00080	Singlet-A	H -> L+6 88.2%, H -> L+8 8.1%
14	3.7438	331.17	0.13400	Singlet-A	H-1 -> L+1 67.0%, H -> L+9 16.4%, H-1 -> L+2 8.0%
15	3.8190	324.65	0.05590	Singlet-A	H-1 -> L+2 42.5%, H-1 -> L+1 23.0%, H-5 -> L 20.1%, H -> L+9 8.8%
16	3.8471	322.28	0.20460	Singlet-A	H-5 -> L 66.0%, H-1 -> L+2 20.1%, H-1 -> L+3 8.9%
17	3.9093	317.15	0.04640	Singlet-A	H-1 -> L+3 37.6%, H -> L+9 30.1%, H-1 -> L+2 21.8%
18	3.9722	312.13	0.13300	Singlet-A	H-1 -> L+3 47.8%, H -> L+9 29.1%, H-5 -> L 6.6%, H-4 -> L 5.1%
19	4.0723	304.46	0.02060	Singlet-A	H-6 -> L 92.4%
20	4.0838	303.60	0.00510	Singlet-A	H -> L+10 77.5%, H-1 -> L+4 10.6%

Table S7: Summary of UV-vis spectral data of [**11-OAc$_a$**]$^-$ that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.1618**	**573.52**	**0.38340**	**Singlet-A**	**H -> L 98.3%**
2	**2.5850**	**479.63**	**0.17170**	**Singlet-A**	**H-1 -> L 95.6%**
3	2.8277	438.46	0.00050	Singlet-A	H-2 -> L 98.9%
4	2.8770	430.95	0.05820	Singlet-A	H-3 -> L 92.0%
5	3.1394	394.93	0.03200	Singlet-A	H-4 -> L 76.1%, H-5 -> L 17.9%
6	3.2120	386.00	0.03720	Singlet-A	H-5 -> L 70.4%, H-4 -> L 22.2%
7	**3.3878**	**365.97**	**0.24240**	**Singlet-A**	**H -> L+1 70.2%, H-7 -> L 14.1%, H-6 -> L 7.1%**
8	3.4259	361.90	0.06940	Singlet-A	H-6 -> L 84.1%, H -> L+1 8.7%, H-5 -> L 5.7%
9	**3.5118**	**353.05**	**0.23170**	**Singlet-A**	**H -> L+2 48.7%, H -> L+3 41.7%**
10	**3.5818**	**346.15**	**0.20840**	**Singlet-A**	**H-7 -> L 76.6%, H -> L+1 11.2%**
11	3.6439	340.25	0.00940	Singlet-A	H -> L+3 52.2%, H -> L+2 42.8%
12	3.7527	330.39	0.03550	Singlet-A	H -> L+4 77.2%, H -> L+6 10.0%
13	3.7714	328.75	0.02530	Singlet-A	H -> L+5 57.9%, H-8 -> L 27.5%, H-9 -> L 5.7%
14	3.7994	326.33	0.06510	Singlet-A	H-8 -> L 40.0%, H -> L+5 38.1%, H-9 -> L 6.9%, H -> L+9 5.3%
15	3.8783	319.69	0.10200	Singlet-A	H-9 -> L 74.5%, H-8 -> L 11.5%, H-1 -> L+1 9.0%
16	3.8963	318.21	0.07800	Singlet-A	H-1 -> L+1 66.8%, H -> L+6 10.5%, H-9 -> L 5.7%
17	3.9163	316.59	0.01550	Singlet-A	H -> L+6 39.0%, H -> L+8 19.0%, H-1 -> L+1 15.5%, H -> L+4 12.6%, H -> L+7 8.7%
18	3.9465	314.16	0.00060	Singlet-A	H -> L+8 69.2%, H -> L+6 29.5%
19	3.9707	312.25	0.00260	Singlet-A	H -> L+7 88.7%, H -> L+6 5.7%
20	4.0056	309.53	0.00400	Singlet-A	H-1 -> L+2 50.0%, H-1 -> L+3 40.9%

Table S8: Total complexation energy (ΔEcom(corr), kcal/mol), basis set superposition error (BSSE), total energy of complex and fragments (in a.u) and complex energy (raw, kcal/mol) for anion binding of **11**

B1/B3LYP/6-31G**	**Ecorr**	**BSSE**	**Efrag**	**Ecom(raw)**	**Ecom_corr**
[**11**-F$_a$]$^-$	-3307.620716	0.050144587	-3307.420166	-157.31	-125.85
[**11**-OAc$_a$]$^-$	-3436.306027	0.0133508	-3436.255947	-39.8	-31.43
[**11**-TBAF]	-3993.750091	0.028606406	-3993.717755	-38.24	-20.29
[**11**-TBOAc]	-4122.426704	0.012694878	-4122.405635	-21.19	-13.22

Table S9: Summary of UV-vis spectral data of [**12**]$^{-}$ that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP/ 6-31G (d, p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**1.9073**	**650.05**	**0.46460**	**Singlet-A**	**H -> L 96.3%**
2	2.1826	568.06	0.04870	Singlet-A	H-1 -> L 65.9%, H -> L+1 31.9%
3	**2.4532**	**505.40**	**0.36120**	**Singlet-A**	**H -> L+1 63.8%, H-1 -> L 27.9%**
4	2.6453	468.70	0.03290	Singlet-A	H-1 -> L+1 88.3%, H-2 -> L 6.7%
5	2.9007	427.43	0.20970	Singlet-A	H-2 -> L 80.6%
6	3.1093	398.75	0.05460	Singlet-A	H-3 -> L 82.2%
7	3.2385	382.84	0.03980	Singlet-A	H -> L+2 90.6%
8	3.3233	373.08	0.16000	Singlet-A	H -> L+3 85.8%
9	3.3807	366.74	0.09220	Singlet-A	H-4 -> L 55.5%, H-2 -> L+1 20.8%, H -> L+4 5.4%,
10	3.4113	363.45	0.06640	Singlet-A	H -> L+4 60.0%, H-2 -> L+1 27.7%
11	3.4253	361.97	0.04040	Singlet-A	H-2 -> L+1 39.8%, H -> L+4 22.8%, H-4 -> L 20.8%, H-3 -> L 5.2%, H-3 -> L+1 5.0%
12	3.5353	350.70	0.01580	Singlet-A	H -> L+5 95.0%
13	3.5481	349.44	0.00940	Singlet-A	H -> L+6 86.6%
14	3.5780	346.52	0.18330	Singlet-A	H-3 -> L+1 44.2%, H-1 -> L+2 34.7%
15	3.6322	341.35	0.15760	Singlet-A	H-1 -> L+2 31.3%, H-3 -> L+1 21.5%, H-5 -> L 16.7%, H-1 -> L+3 11.2%
16	3.6677	338.04	0.04020	Singlet-A	H-1 -> L+3 63.2%, H-1 -> L+2 12.1%, H-3 -> L+1 6.7%, H-5 -> L 6.0%
17	3.7329	332.14	0.11690	Singlet-A	H-5 -> L 43.4%, H-1 -> L+3 10.0%, H-6 -> L 8.9%, H-3 -> L+1 7.1%, H -> L+7 6.4%
18	3.7517	330.47	0.01390	Singlet-A	H -> L+7 83.1%, H-1 -> L+7 5.2%, H-5 -> L 5.1%
19	3.7580	329.92	0.05030	Singlet-A	H-6 -> L 47.1%, H-7 -> L 13.6%, H-5 -> L 9.4%, H-1 -> L+3 9.3%
20	3.7960	326.62	0.01500	Singlet-A	H-1 -> L+4 76.5%, H-4 -> L+1 6.2%, H -> L+4 5.1%

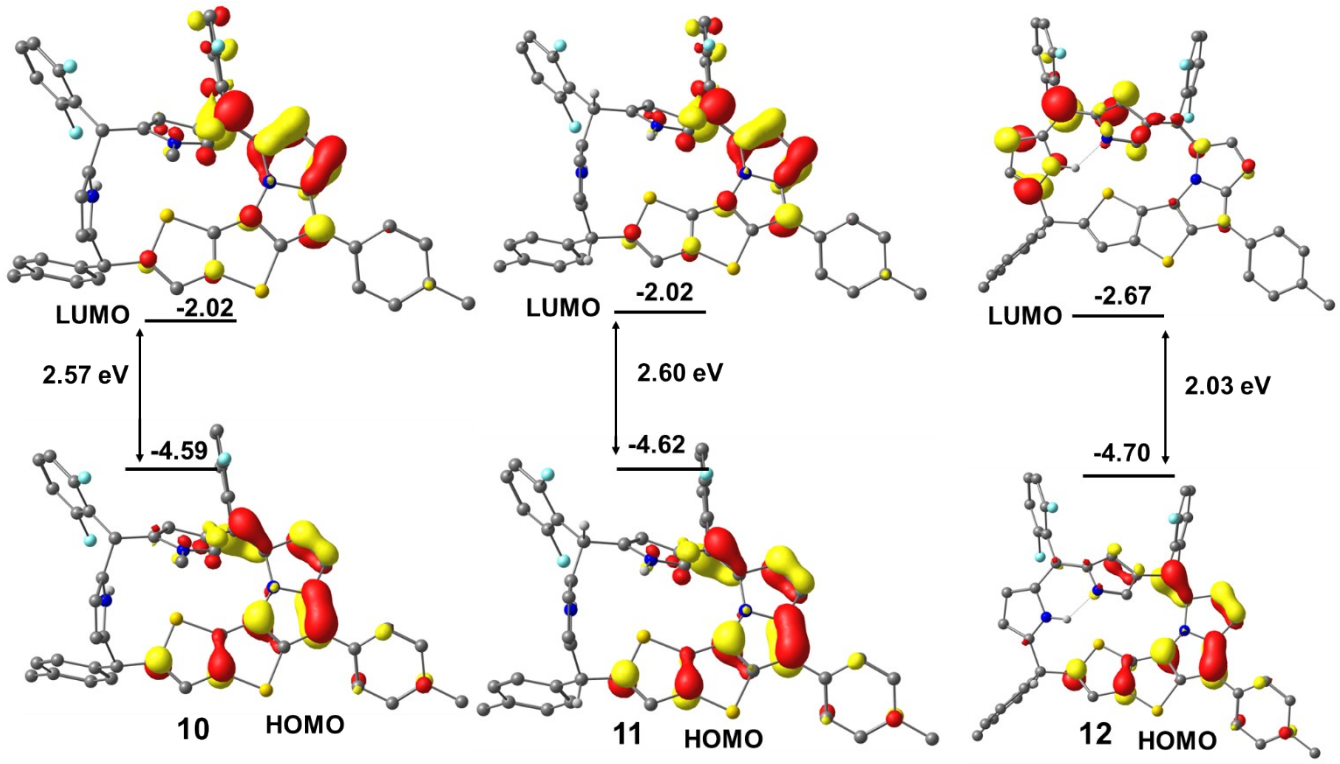


Fig. S80 HOMO-LUMO orbitals for DFT optimized structures of **10** (a), **11** (b), **12** (c) at B3LYP/6-31G** level of theory.

Table S10: Total energies, zero-point energies and free energy for macrocycles **10**,**11**,**12**, anion bound and deprotonated forms of **10**-**12**.

B1	E	E+ZPE	G	ΔE	ΔE+ZPE	ΔG
10	-3247.070329	-3246.378544	-3246.463106			
11	-3207.761193	-3207.097103	-3207.181404			
12	-3205.82910	-3205.87527	-3205.96000			
gas phase						
[**10**]$^-$	-3246.502322	-3245.826012	-3245.910866			
[**11**-F_a]$^-$	-3307.671551	-3307.009426	-3307.094097	0.00	0.00	0.00
[**11**-F_b]$^-$	-3307.654529	-3306.992622	-3307.07889	10.68	10.54	9.54
[**11**-OAc_a]$^-$	-3436.321352	-3435.608912	-3435.702436	0.00	0.00	0.00
[**11**-OAC_b]$^-$	-3436.300086	-3435.587352	-3435.679639	13.34	13.53	14.31
[12]$^-$	-3205.28853	-3205.33485	-3205.42028			
Solvent						
[**11**-F_a]$^-$	-3307.72619	-3307.064318	-3307.150118	0.00	0.00	0.00
[**11**-F_b]$^-$	-3307.711883	-3307.049555	-3307.134134	8.98	9.26	10.03
[**11**-OAc_a]-	-3436.382922	-3435.66994	-3435.763045	0.00	0.00	0.00
[**11**-OAC_b]$^-$	-3436.361337	-3435.6476	-3435.737134	13.54	14.02	16.26
[**11**-TBAF]	-3993.778698	-3992.606406	-3992.725182			
[**11**-TBOAC]	-4122.439399	-4121.217368	-4121.344117			

6. Cartesian Coordinates

All structures have zero imaginary frequencies, total energies are given in table S10

16	3.673158000	2.687326000	-0.931021000
16	-0.220036000	1.353346000	-0.059230000
9	-0.542690000	-4.757126000	-0.365510000
9	0.895093000	-2.262672000	3.383230000
9	-4.077108000	-0.272673000	0.846984000
9	-5.377748000	-2.494861000	-3.120839000
7	2.747848000	-0.915151000	0.105664000
7	-1.036365000	-1.177788000	-2.429533000
7	-2.975130000	1.538981000	-1.043663000
1	-2.863104000	1.190812000	-0.104495000
6	6.276439000	0.212299000	-0.274764000
6	6.872854000	1.472829000	-0.089634000
1	6.250684000	2.331668000	0.142896000
6	8.254111000	1.631141000	-0.160322000
1	8.683538000	2.617964000	-0.004560000
6	9.101315000	0.545495000	-0.416419000
6	8.508435000	-0.711241000	-0.599916000
1	9.138411000	-1.573361000	-0.806502000
6	7.128467000	-0.876550000	-0.538892000
1	6.698391000	-1.856123000	-0.723312000
6	4.825552000	0.038765000	-0.196078000
6	3.797087000	0.999925000	-0.439342000
6	2.540088000	0.423979000	-0.205748000
6	4.131623000	-1.118500000	0.188175000
6	10.596284000	0.727253000	-0.523927000
1	11.133948000	-0.164895000	-0.188074000
1	10.940302000	1.575107000	0.076008000
1	10.901994000	0.918216000	-1.560660000
6	1.485558000	1.356229000	-0.330158000
6	1.921016000	2.622675000	-0.726721000
6	2.056180000	-2.034899000	0.650020000
6	3.111302000	-2.893786000	1.168692000
1	2.918376000	-3.857867000	1.616028000
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1	5.295538000	-2.820469000	1.057800000
6	0.723925000	-2.370382000	0.540918000
6	-0.210035000	-1.847945000	-0.453363000
6	0.106006000	-1.515378000	-1.764730000
1	1.056439000	-1.545218000	-2.276046000
6	-2.121786000	-1.271055000	-1.561591000
6	-1.633951000	-1.705261000	-0.345714000
1	-2.215415000	-1.858621000	0.550174000
6	0.867821000	3.573005000	-0.863160000
1	1.002237000	4.595627000	-1.197870000
6	-0.360214000	3.042043000	-0.542543000
6	0.209434000	-3.434275000	1.444107000
6	-0.441225000	-4.584160000	0.965591000
6	-0.966315000	-5.569275000	1.791752000
1	-1.445036000	-6.432479000	1.343949000
6	-0.847821000	-5.420834000	3.173729000
1	-1.250494000	-6.181338000	3.834858000
6	-0.211807000	-4.302121000	3.709535000
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6	-3.489821000	-0.748285000	-1.990220000
1	-3.663807000	-1.080122000	-3.017030000
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1	-7.738226000	-2.871976000	0.685957000
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6	-2.126425000	4.661122000	3.073758000
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1	1.067370000	6.740859000	0.626060000
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1	7.473272000	3.292340000	-1.409646000
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6	3.383788000	-1.417850000	-3.325120000
1	3.629244000	-1.063719000	-4.317810000
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6	2.479059000	-4.564998000	2.955216000
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6	3.857554000	-4.803026000	2.981894000
6	4.569504000	-4.640570000	1.785887000
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1	5.406918000	-5.860156000	4.064125000
1	3.880934000	-5.706159000	4.949205000
1	1.200026000	0.440796000	-3.266036000

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16	3.398107000	2.771267000	-0.897174000
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9	0.697152000	-2.935484000	3.160576000
9	-4.679229000	-0.781578000	1.210203000
9	-4.460110000	-3.114645000	-2.883333000
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7	-1.145766000	-0.774462000	-2.190191000
7	-2.730061000	1.317215000	-1.683232000
1	-1.814525000	0.975926000	-1.985717000
6	6.118731000	0.500849000	-0.211262000
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6	2.370301000	0.493388000	-0.040340000
6	4.069452000	-0.957306000	0.298779000
6	10.391367000	1.281317000	-0.547436000
1	10.893445000	1.094799000	0.410564000
1	10.595069000	2.320319000	-0.823033000
1	10.865992000	0.634473000	-1.291747000
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6	1.660164000	2.632905000	-0.678136000
6	2.088158000	-2.101880000	0.587318000
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6	4.382061000	-2.254390000	0.817889000
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6	-0.184530000	-2.076001000	-0.545864000
6	-0.006985000	-1.168580000	-1.662294000
1	0.942049000	-0.830954000	-2.063091000
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6	0.058324000	-5.191553000	3.060798000
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1	-5.861326000	0.777691000	-0.881917000
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1	-3.045763000	7.988642000	3.524222000
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[10]$^{-}$

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7	-2.823543000	1.405529000	-0.988818000
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6	8.209491000	1.739912000	-0.140234000
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6	9.087980000	0.674609000	-0.374208000
6	8.525840000	-0.594998000	-0.566898000
1	9.178201000	-1.441940000	-0.770923000
6	7.149774000	-0.793237000	-0.523340000
1	6.745779000	-1.781085000	-0.720633000
6	4.818329000	0.067893000	-0.216630000
6	3.772101000	1.013882000	-0.426767000
6	2.520316000	0.408199000	-0.232298000
6	4.148257000	-1.123722000	0.109827000
6	10.584224000	0.879994000	-0.397414000
1	11.034041000	0.695061000	0.587397000
1	10.843413000	1.904629000	-0.682704000
1	11.071885000	0.200938000	-1.105015000
6	1.437012000	1.318395000	-0.349904000
6	1.865129000	2.597928000	-0.709204000
6	2.095420000	-2.103491000	0.525466000
6	3.165792000	-2.963446000	0.998104000
1	2.992877000	-3.954230000	1.392878000
6	4.378337000	-2.401512000	0.710607000
1	5.350801000	-2.831201000	0.906171000
6	0.766749000	-2.469975000	0.423562000
6	-0.214791000	-1.941756000	-0.505331000
6	0.032781000	-1.500783000	-1.803117000
1	0.960437000	-1.446928000	-2.352957000
6	-2.191505000	-1.342360000	-1.476047000
6	-1.638139000	-1.858440000	-0.326808000
1	-2.170578000	-2.061216000	0.589029000
6	0.801577000	3.523232000	-0.882423000
1	0.925918000	4.557966000	-1.183396000
6	-0.433144000	2.953653000	-0.648563000
6	0.306967000	-3.580108000	1.304192000
6	-0.301000000	-4.741912000	0.800053000
6	-0.783129000	-5.769113000	1.602271000
1	-1.233917000	-6.635541000	1.131803000
6	-0.664974000	-5.653911000	2.987181000
1	-1.038323000	-6.445080000	3.629945000
6	-0.068162000	-4.526214000	3.547855000
1	0.032890000	-4.399494000	4.619752000
6	0.400404000	-3.524114000	2.704446000
6	-1.278629000	-0.638644000	-3.736033000
1	-0.279506000	-0.439962000	-4.127689000
1	-1.860890000	0.286581000	-3.726590000
1	-1.774072000	-1.366223000	-4.390213000
6	-3.581639000	-0.828052000	-1.812262000
1	-3.819947000	-1.171871000	-2.824083000
6	-4.683081000	-1.426202000	-0.937609000
6	-4.858560000	-1.160922000	0.427202000
6	-5.916502000	-1.663388000	1.180205000
1	-5.972360000	-1.406757000	2.232223000
6	-6.867339000	-2.474610000	0.563441000
1	-7.699486000	-2.870874000	1.137447000
6	-6.745002000	-2.778347000	-0.790791000
1	-7.458915000	-3.407391000	-1.310810000
6	-5.665898000	-2.252767000	-1.493223000
6	-1.799541000	3.618101000	-0.770142000
1	-1.649515000	4.487331000	-1.428158000
6	-2.766349000	2.672568000	-1.457352000
6	-3.565531000	0.697398000	-1.875667000
6	-4.030098000	1.524803000	-2.916455000
1	-4.651253000	1.232891000	-3.757837000
6	-3.505817000	2.813696000	-2.643426000
1	-3.633555000	3.713075000	-3.237436000
6	-2.319655000	4.181416000	0.570567000
6	-1.456972000	4.650941000	1.567736000
1	-0.383681000	4.563107000	1.428061000
6	-1.953036000	5.221530000	2.741039000
1	-1.255874000	5.572910000	3.499840000
6	-3.328890000	5.345073000	2.961765000
6	-4.190554000	4.879260000	1.960433000
1	-5.267025000	4.960360000	2.102252000
6	-3.697369000	4.304944000	0.790354000
1	-4.377334000	3.934529000	0.029348000
6	-3.867647000	5.926800000	4.248704000
1	-4.079040000	5.143754000	4.989131000
1	-4.803530000	6.471612000	4.082779000
1	-3.152658000	6.618520000	4.706636000

[11-F$_a$]$^{-}$

16	-3.699764000	-2.706820000	-0.868910000
16	0.183360000	-1.308786000	-0.022788000
9	0.474341000	4.832875000	-0.096551000
9	-0.949171000	1.978416000	3.394566000
9	4.101528000	0.313940000	0.886901000
9	5.408977000	2.466133000	-3.123228000
7	-2.810238000	0.928555000	0.079120000
7	1.061604000	1.231552000	-2.390435000
7	2.998550000	-1.504503000	-1.015026000
1	2.957504000	-1.182569000	-0.061196000
6	-6.324419000	-0.222806000	-0.328361000
6	-6.921168000	-1.496200000	-0.237494000
1	-6.297081000	-2.367293000	-0.063964000
6	-8.301494000	-1.658659000	-0.331984000
1	-8.722872000	-2.658960000	-0.253338000
6	-9.157846000	-0.567402000	-0.516436000
6	-8.569074000	0.702838000	-0.610778000
1	-9.202228000	1.574419000	-0.767963000
6	-7.192764000	0.873704000	-0.526102000
1	-6.770888000	1.866280000	-0.645600000
6	-4.882161000	-0.043994000	-0.231322000
6	-3.846627000	-1.006181000	-0.418289000
6	-2.593161000	-0.418326000	-0.188124000
6	-4.192780000	1.138130000	0.129056000
6	-10.654688000	-0.743128000	-0.618511000
1	-11.184185000	-0.183870000	0.163223000
1	-10.938410000	-1.795472000	-0.520376000
1	-11.041312000	-0.385640000	-1.581317000
6	-1.525978000	-1.341530000	-0.284775000
6	-1.945854000	-2.621685000	-0.652885000
6	-2.125277000	2.050319000	0.621433000
6	-3.171655000	2.933392000	1.065795000
1	-2.979341000	3.912280000	1.482984000
6	-4.401616000	2.414520000	0.736884000
1	-5.363482000	2.873025000	0.916173000
6	-0.761442000	2.342132000	0.568909000
6	0.187857000	1.850331000	-0.378686000
6	-0.068170000	1.503106000	-1.739184000
1	-1.024872000	1.529053000	-2.247359000
6	2.097544000	1.342976000	-1.471790000
6	1.619845000	1.756523000	-0.245140000
1	2.182624000	1.903700000	0.665653000
6	-0.884234000	-3.560399000	-0.772723000
1	-1.005018000	-4.588486000	-1.097535000
6	0.339131000	-3.006936000	-0.465327000
6	-0.269571000	3.330934000	1.573224000
6	0.362371000	4.530255000	1.207544000
6	0.855278000	5.449556000	2.127401000
1	1.322366000	6.357518000	1.762991000
6	0.726243000	5.176435000	3.488796000
1	1.107816000	5.881909000	4.220634000
6	0.108160000	4.001511000	3.912964000
1	-0.002379000	3.753849000	4.962657000
6	-0.373830000	3.114138000	2.955719000
6	3.449987000	0.818362000	-1.943275000
1	3.554321000	1.164606000	-2.973871000
6	4.659307000	1.344630000	-1.180383000
6	4.954059000	1.086677000	0.160867000
6	6.071154000	1.573440000	0.829481000
1	6.211390000	1.318203000	1.873685000
6	6.971927000	2.375551000	0.131420000
1	7.851694000	2.767748000	0.631989000
6	6.739337000	2.673485000	-1.209428000
1	7.413679000	3.294169000	-1.788575000
6	5.602435000	2.157431000	-1.822913000
6	1.726482000	-3.629893000	-0.593479000
1	1.581279000	-4.564466000	-1.153093000
6	2.582934000	-2.738268000	-1.467231000
6	3.352154000	-0.693906000	-2.070700000
6	3.233087000	-1.453701000	-3.220373000
1	3.350647000	-1.064355000	-4.220330000
6	2.752198000	-2.737493000	-2.840587000
1	2.483440000	-3.550553000	-3.502477000
6	2.382683000	-4.007718000	0.745457000
6	1.627994000	-4.215018000	1.905120000
1	0.554530000	-4.057414000	1.873501000
6	2.236707000	-4.618998000	3.093839000
1	1.624557000	-4.769493000	3.980568000
6	3.618123000	-4.829138000	3.168100000
6	4.370501000	-4.627330000	2.003840000
1	5.446826000	-4.785537000	2.028299000
6	3.766053000	-4.221796000	0.815516000
1	4.369374000	-4.063132000	-0.073755000
6	4.280789000	-5.227658000	4.466336000
1	4.621866000	-4.348771000	5.028770000
1	5.158446000	-5.858790000	4.291807000
1	3.592212000	-5.778649000	5.114805000
1	1.548582000	1.049603000	-3.857102000
9	2.080854000	0.998001000	-4.693562000

[11-F_b]$^-$

16	-3.547480000	-2.797789000	-0.891623000
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9	-0.032909000	4.952850000	-0.764136000
9	-1.065425000	2.675041000	3.246959000
9	3.836561000	1.116718000	0.988028000
9	5.554948000	2.290284000	-3.258796000
7	-2.870114000	0.861301000	0.127377000
7	0.977357000	1.050433000	-2.294255000
7	3.027581000	-1.269396000	-1.034397000
1	2.990588000	-1.158114000	0.501265000
6	-6.305862000	-0.502665000	-0.294143000
6	-6.819863000	-1.804988000	-0.138305000
1	-6.141964000	-2.620529000	0.093413000
6	-8.184707000	-2.059352000	-0.238873000
1	-8.544973000	-3.077355000	-0.105399000
6	-9.103440000	-1.033894000	-0.496413000
6	-8.596211000	0.263420000	-0.650720000
1	-9.281555000	1.083003000	-0.857939000
6	-7.232743000	0.525013000	-0.560589000
1	-6.870887000	1.535103000	-0.723715000
6	-4.874463000	-0.232567000	-0.186276000
6	-3.782654000	-1.129821000	-0.377215000
6	-2.564158000	-0.476396000	-0.131612000
6	-4.265908000	0.981863000	0.172827000
6	-10.579816000	-1.320230000	-0.637327000
1	-11.186753000	-0.467905000	-0.314366000
1	-10.877493000	-2.189514000	-0.041958000
1	-10.853237000	-1.534193000	-1.679317000
6	-1.439143000	-1.335565000	-0.249213000
6	-1.802077000	-2.614477000	-0.682544000
6	-2.267756000	2.076423000	0.562407000
6	-3.382130000	2.896581000	1.004522000
1	-3.262033000	3.907281000	1.366477000
6	-4.563482000	2.264712000	0.732682000
1	-5.557153000	2.652553000	0.907356000

6	-0.969651000	2.522235000	0.396688000
6	0.024773000	1.987236000	-0.512347000
6	-0.219859000	1.314627000	-1.708690000
1	-1.152234000	1.039593000	-2.176202000
6	2.022893000	1.483377000	-1.492059000
6	1.460025000	2.106088000	-0.405365000
1	1.994025000	2.535053000	0.426746000
6	-0.700156000	-3.492295000	-0.844504000
1	-0.765607000	-4.497055000	-1.247606000
6	0.497566000	-2.905691000	-0.489754000
6	-0.570518000	3.723404000	1.183207000
6	-0.078130000	4.891606000	0.579556000
6	0.343637000	6.007513000	1.292364000
1	0.705688000	6.872684000	0.748648000
6	0.280881000	5.978933000	2.685395000
1	0.608595000	6.840016000	3.259502000
6	-0.201921000	4.848758000	3.342461000
1	-0.256723000	4.789057000	4.423451000
6	-0.613727000	3.756154000	2.586216000
6	3.413357000	1.051992000	-1.939599000
1	3.530769000	1.420753000	-2.963565000
6	4.598799000	1.645417000	-1.187244000
6	4.793097000	1.627673000	0.199188000
6	5.930304000	2.131278000	0.826682000
1	5.993709000	2.070380000	1.907196000
6	6.945492000	2.686816000	0.052489000
1	7.839358000	3.079895000	0.527187000
6	6.810370000	2.737824000	-1.333764000
1	7.573114000	3.163557000	-1.975961000
6	5.654463000	2.221095000	-1.906548000
6	1.893664000	-3.477036000	-0.741667000
1	1.714766000	-4.338722000	-1.402032000
6	2.686960000	-2.478479000	-1.566842000
6	3.386191000	-0.467986000	-2.074658000
6	3.302549000	-1.169381000	-3.288311000
1	3.549369000	-0.785469000	-4.272650000
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1	2.648047000	-3.289626000	-3.636267000
6	2.595223000	-4.048831000	0.498697000
6	1.867941000	-4.628367000	1.542865000
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6	2.514298000	-5.248927000	2.611520000
1	1.921622000	-5.685873000	3.413332000
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6	4.634992000	-4.741273000	1.622110000
1	5.722923000	-4.774783000	1.642496000
6	3.991150000	-4.117121000	0.555997000
1	4.570728000	-3.664315000	-0.242032000
6	4.612635000	-5.949975000	3.852073000
1	4.843909000	-5.209732000	4.629511000
1	5.561306000	-6.410310000	3.554791000
1	3.994662000	-6.724727000	4.318606000
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9	2.844511000	-1.269245000	1.476522000

[11-OAc$_a$]$^-$

16	-3.764782000	2.670193000	0.862429000
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9	0.430059000	-4.781346000	-0.322285000
9	-1.266949000	-1.972488000	-3.726708000
9	3.936026000	-0.230582000	-1.444889000
9	5.517167000	-2.508364000	2.390678000
7	-2.898703000	-0.920296000	-0.263978000
7	1.124717000	-1.357479000	1.949696000
7	2.930931000	1.517007000	0.586017000
1	2.837065000	1.237775000	-0.377164000
6	-6.399193000	0.199831000	0.316891000
6	-7.003011000	1.469877000	0.235143000
1	-6.388650000	2.340552000	0.027819000
6	-8.378838000	1.625726000	0.378238000
1	-8.809713000	2.621972000	0.302626000
6	-9.219934000	0.529349000	0.606864000
6	-8.623086000	-0.736229000	0.687386000
1	-9.246145000	-1.609231000	0.871278000
6	-7.248105000	-0.899926000	0.554515000
1	-6.815188000	-1.889343000	0.662268000
6	-4.957326000	0.029458000	0.163404000
6	-3.917845000	0.987575000	0.357320000
6	-2.673500000	0.414309000	0.056177000
6	-4.283236000	-1.127912000	-0.271064000
6	-10.707872000	0.707440000	0.795539000
1	-11.265554000	-0.162813000	0.433904000
1	-11.076422000	1.588849000	0.260819000
1	-10.968342000	0.839817000	1.854162000
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6	-2.022144000	2.603681000	0.573295000
6	-2.238688000	-2.013350000	-0.896015000
6	-3.314245000	-2.868754000	-1.356106000
1	-3.142874000	-3.821626000	-1.836428000
6	-4.520176000	-2.369292000	-0.945411000
1	-5.491314000	-2.815705000	-1.105496000
6	-0.889415000	-2.321125000	-0.917042000
6	0.119015000	-1.855298000	0.010914000
6	-0.065675000	-1.638854000	1.387017000
1	-0.962115000	-1.745334000	1.980655000
6	2.112295000	-1.350758000	0.982664000
6	1.530081000	-1.686579000	-0.222728000
1	2.020907000	-1.734129000	-1.183056000
6	-0.963763000	3.550015000	0.676015000
1	-1.081143000	4.570152000	1.025000000
6	0.250198000	3.015097000	0.307617000
6	-0.445623000	-3.302682000	-1.946880000
6	0.236431000	-4.486411000	-1.618098000
6	0.698402000	-5.393874000	-2.564273000
1	1.209294000	-6.288579000	-2.227238000
6	0.482513000	-5.126963000	-3.915954000
1	0.838333000	-5.824007000	-4.668287000
6	-0.189743000	-3.969411000	-4.304224000
1	-0.368023000	-3.727336000	-5.345776000
6	-0.636038000	-3.091647000	-3.321868000
6	3.481186000	-0.825469000	1.400712000
1	3.643819000	-1.201895000	2.416422000
6	4.640335000	-1.324024000	0.543710000
6	4.847268000	-1.013926000	-0.802410000
6	5.924972000	-1.459516000	-1.557723000
1	5.997253000	-1.164336000	-2.598298000
6	6.877138000	-2.272888000	-0.945582000
1	7.729472000	-2.633028000	-1.513203000
6	6.731709000	-2.623640000	0.394556000
1	7.448515000	-3.254761000	0.907498000
6	5.629248000	-2.147823000	1.098118000
6	1.636113000	3.654159000	0.353184000
1	1.525874000	4.561225000	0.963298000
6	2.573693000	2.740504000	1.111952000
6	3.394116000	0.681931000	1.582654000
6	3.403117000	1.409340000	2.759523000

1	3.650150000	1.018207000	3.741436000
6	2.886161000	2.701484000	2.459252000
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6	2.170783000	4.097568000	-1.020073000
6	1.320858000	4.345373000	-2.103441000
1	0.254434000	4.176392000	-1.991928000
6	1.825784000	4.805562000	-3.320097000
1	1.141014000	4.986987000	-4.145843000
6	3.194647000	5.033836000	-3.498936000
6	4.042349000	4.791304000	-2.410401000
1	5.111603000	4.962547000	-2.516442000
6	3.541959000	4.329191000	-1.194741000
1	4.217494000	4.139592000	-0.365571000
6	3.744205000	5.494636000	-4.828924000
1	4.034421000	4.643980000	-5.459192000
1	4.634505000	6.118855000	-4.700424000
1	3.003564000	6.073922000	-5.389414000
1	1.370782000	-1.270755000	2.988781000
8	2.213736000	-1.302573000	4.280539000
6	2.214478000	-0.599153000	5.353309000
8	3.131960000	0.135598000	5.757449000
6	0.928050000	-0.701886000	6.202075000
1	1.042183000	-0.183203000	7.157373000
1	0.089196000	-0.254996000	5.654163000
1	0.670990000	-1.752470000	6.377268000

[11-OAc$_b$]$^-$

16	-3.752640000	-2.905257000	-0.836989000
16	0.034211000	-1.126189000	-0.282684000
9	-0.691012000	5.077985000	-0.861115000
9	-1.430568000	2.704007000	3.157755000
9	3.229497000	1.046957000	0.771625000
9	5.034781000	3.004484000	-3.123102000
7	-3.228465000	0.807806000	0.087956000
7	0.513706000	1.358210000	-2.505800000
7	2.846858000	-1.064779000	-1.336687000
1	3.352988000	-0.998334000	-0.430638000
6	-6.591225000	-0.793085000	-0.063228000
6	-7.001164000	-2.115207000	0.193021000
1	-6.257812000	-2.872877000	0.421546000
6	-8.349790000	-2.463366000	0.197099000
1	-8.630773000	-3.492798000	0.406439000
6	-9.350154000	-1.513971000	-0.050819000
6	-8.944027000	-0.195765000	-0.303468000
1	-9.695047000	0.564786000	-0.504132000
6	-7.597971000	0.158433000	-0.317628000
1	-7.318321000	1.180656000	-0.552497000
6	-5.174659000	-0.422944000	-0.067442000
6	-4.041301000	-1.242932000	-0.342577000
6	-2.852674000	-0.505871000	-0.203911000
6	-4.623565000	0.827665000	0.238991000
6	-10.809339000	-1.901717000	-0.076526000
1	-11.448848000	-1.076367000	0.251093000
1	-11.005610000	-2.761826000	0.570603000
1	-11.130849000	-2.177796000	-1.088973000
6	-1.693389000	-1.306959000	-0.407400000
6	-2.015316000	-2.616579000	-0.776330000
6	-2.687920000	2.059475000	0.511645000
6	-3.830765000	2.794077000	1.035564000
1	-3.758305000	3.804770000	1.409525000
6	-4.976802000	2.084700000	0.830650000
1	-5.982828000	2.398847000	1.069769000
6	-1.436359000	2.595716000	0.306261000
6	-0.442584000	2.136198000	-0.652366000
6	-0.687052000	1.565349000	-1.898433000
1	-1.617569000	1.330811000	-2.391966000
6	1.555672000	1.735765000	-1.676064000
6	0.986260000	2.265368000	-0.540879000
1	1.514941000	2.643931000	0.318534000
6	-0.889033000	-3.445856000	-1.023574000
1	-0.945205000	-4.471438000	-1.371116000
6	0.300410000	-2.790748000	-0.806861000
6	-1.080186000	3.808924000	1.094326000
6	-0.680991000	5.009701000	0.486402000
6	-0.299861000	6.141575000	1.194154000
1	-0.012472000	7.034754000	0.651501000
6	-0.307112000	6.093095000	2.588866000
1	-0.010710000	6.966272000	3.160526000
6	-0.694268000	4.929181000	3.251762000
1	-0.702525000	4.859510000	4.333311000
6	-1.069844000	3.823400000	2.498038000
6	2.978243000	1.374953000	-2.101820000
1	3.135806000	1.811358000	-3.093081000
6	4.073789000	1.963802000	-1.225800000
6	4.189992000	1.757361000	0.151636000
6	5.225463000	2.267953000	0.925453000
1	5.263683000	1.996968000	1.973053000
6	6.203203000	3.042165000	0.304493000
1	7.025253000	3.444317000	0.887971000
6	6.135491000	3.299342000	-1.065979000
1	6.877999000	3.900228000	-1.578443000
6	5.083474000	2.752291000	-1.788314000
6	1.706453000	-3.320390000	-1.091297000
1	1.545772000	-4.150465000	-1.793841000
6	2.443560000	-2.265106000	-1.893907000
6	3.009584000	-0.130808000	-2.340173000
6	2.746880000	-0.753985000	-3.550500000
1	2.766107000	-0.274718000	-4.521746000
6	2.385325000	-2.100853000	-3.266254000
1	2.041032000	-2.844355000	-3.973563000
6	2.419812000	-3.932096000	0.122617000
6	1.689749000	-4.546370000	1.148181000
1	0.605199000	-4.500348000	1.135584000
6	2.334118000	-5.223975000	2.182763000
1	1.740497000	-5.691134000	2.965429000
6	3.730906000	-5.312188000	2.230634000
6	4.455586000	-4.691234000	1.206432000
1	5.542214000	-4.730658000	1.221671000
6	3.815814000	-4.008661000	0.171963000
1	4.410987000	-3.500579000	-0.576935000
6	4.432396000	-6.018926000	3.366685000
1	4.700550000	-5.316032000	4.165161000
1	5.359899000	-6.493868000	3.031391000
1	3.796746000	-6.790283000	3.812473000
1	0.648553000	0.803029000	-3.339520000
8	5.090534000	-0.615057000	2.544890000
6	5.576044000	-1.083093000	1.489346000
8	5.017783000	-1.192969000	0.351514000
6	7.044812000	-1.575939000	1.533335000
1	7.120933000	-2.590239000	1.125345000
1	7.668706000	-0.933104000	0.900334000
1	7.444268000	-1.562437000	2.551381000

[11-TBAF]

16	-4.509503000	1.742422000	-2.503029000
16	-2.163573000	-1.375643000	-0.914276000

9	0.749793000	0.536364000	4.156194000
9	-3.713513000	-1.019800000	4.050151000
9	0.037227000	-4.578119000	0.957377000
9	4.490170000	-2.979604000	0.880534000
7	-3.103948000	1.664205000	1.093562000
7	1.016708000	-0.208933000	0.137176000
7	0.010285000	-3.286665000	-1.586012000
1	-0.539428000	-3.719967000	-0.860744000
6	-5.408352000	4.332401000	-0.104536000
6	-6.422442000	4.319588000	-1.080340000
1	-6.576976000	3.428172000	-1.680398000
6	-7.252087000	5.421091000	-1.270910000
1	-8.026168000	5.375865000	-2.033591000
6	-7.116491000	6.580955000	-0.497386000
6	-6.102985000	6.598687000	0.470426000
1	-5.958994000	7.491098000	1.075592000
6	-5.263916000	5.505378000	0.661213000
1	-4.462111000	5.567699000	1.390367000
6	-4.532670000	3.178972000	0.100125000
6	-4.180220000	2.148900000	-0.821765000
6	-3.343486000	1.208467000	-0.200475000
6	-3.882593000	2.812770000	1.288882000
6	-8.041612000	7.759823000	-0.683673000
1	-8.924781000	7.682503000	-0.036220000
1	-8.402454000	7.827356000	-1.714670000
1	-7.543608000	8.703104000	-0.437994000
6	-3.026729000	0.119223000	-1.049925000
6	-3.575799000	0.255380000	-2.327445000
6	-2.596658000	1.206340000	2.345120000
6	-3.188158000	2.101141000	3.326886000
1	-2.966168000	2.044592000	4.382666000
6	-3.907997000	3.075469000	2.698018000
1	-4.425180000	3.900795000	3.166372000
6	-1.619440000	0.268369000	2.598552000
6	-0.623342000	-0.222832000	1.659071000
6	0.052052000	0.548782000	0.706287000
1	-0.072696000	1.594031000	0.462943000
6	0.988416000	-1.479439000	0.670600000
6	0.002653000	-1.517784000	1.635339000
1	-0.297549000	-2.377093000	2.216364000
6	-3.272502000	-0.824526000	-3.203313000
1	-3.580204000	-0.879743000	-4.241770000
6	-2.514060000	-1.794148000	-2.589940000
6	-1.488465000	-0.217769000	4.000675000
6	-0.290128000	-0.108131000	4.725137000
6	-0.122571000	-0.597470000	6.013733000
1	0.832495000	-0.464992000	6.509006000
6	-1.197121000	-1.235519000	6.634354000
1	-1.085633000	-1.624842000	7.641233000
6	-2.413868000	-1.371789000	5.968564000
1	-3.265860000	-1.866358000	6.420721000
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6	1.868692000	-2.508252000	-0.025109000
1	2.797551000	-1.978612000	-0.252132000
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1	0.968901000	-6.516516000	2.325755000
6	3.066020000	-5.944330000	2.388065000
1	3.379787000	-6.797965000	2.979809000
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1	-1.978739000	-2.925811000	-4.287202000
6	-0.414211000	-3.044616000	-2.874588000
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6	-3.923188000	-4.380107000	-2.359134000
1	-4.450752000	-3.443746000	-2.208094000
6	-4.567011000	-5.587864000	-2.087546000
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6	-3.920291000	-6.814634000	-2.273669000
6	-2.602961000	-6.790165000	-2.750332000
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1	-0.932452000	-5.593109000	-3.385356000
6	-4.606992000	-8.119409000	-1.945233000
1	-4.397563000	-8.432056000	-0.914283000
1	-4.268980000	-8.926845000	-2.602370000
1	-5.693543000	-8.035705000	-2.043507000
1	1.797627000	0.057420000	-0.527051000
9	3.189301000	0.041690000	-1.177379000
7	5.404817000	2.900484000	-1.034257000
6	6.562757000	1.886236000	-0.953555000
6	6.253842000	0.414127000	-1.251070000
1	6.983471000	1.999466000	0.047440000
1	7.314387000	2.239761000	-1.664813000
6	7.427699000	-0.464359000	-0.788500000
1	5.310967000	0.077748000	-0.810627000
1	6.122593000	0.285748000	-2.331189000
6	7.226667000	-1.939511000	-1.148946000
1	8.365959000	-0.101445000	-1.233125000
1	7.549060000	-0.368439000	0.299093000
1	8.080074000	-2.541751000	-0.821394000
1	6.326769000	-2.341768000	-0.675570000
1	7.122478000	-2.070622000	-2.231501000
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1	4.037999000	1.434737000	-1.797886000
1	4.982983000	2.354257000	-3.020275000
6	2.258032000	2.613143000	-3.353556000
1	2.600252000	3.418973000	-1.391735000
1	3.413095000	4.320924000	-2.675685000
6	0.945428000	3.363984000	-3.588043000
1	2.799869000	2.513845000	-4.304097000
1	2.060748000	1.595929000	-2.997642000
1	0.324571000	2.844739000	-4.323667000
1	0.361146000	3.441470000	-2.664905000
1	1.122258000	4.380761000	-3.958277000
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1	4.008846000	3.901058000	0.159313000
1	5.516950000	3.514154000	0.977187000
6	4.925174000	1.221579000	2.091121000
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6	4.190211000	0.068097000	2.781222000

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1	5.130841000	4.933922000	-1.529412000
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1	7.929856000	4.158755000	-0.524100000
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1	6.775844000	6.849871000	-1.428669000
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8	-4.484949000	1.439883000	-2.893867000
6	-2.705124000	0.143662000	-3.822801000
1	-3.130650000	0.458720000	-4.776943000
1	-1.625494000	0.316125000	-3.817574000
1	-2.861485000	-0.935072000	-3.708900000
7	-5.599492000	2.398236000	0.349858000
6	-5.483621000	0.856382000	0.242859000
6	-6.555727000	0.107955000	-0.552054000
1	-5.446593000	0.498787000	1.275141000
1	-4.516594000	0.679723000	-0.238576000
6	-6.318557000	-1.408197000	-0.433890000
1	-7.571487000	0.335801000	-0.208431000
1	-6.478487000	0.388628000	-1.605611000
6	-7.352539000	-2.220563000	-1.219169000
1	-5.316154000	-1.650260000	-0.805407000
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1	-8.369800000	-2.033623000	-0.855944000
1	-7.325865000	-1.965579000	-2.283756000
6	-6.249708000	2.951776000	-0.921710000

6	-6.397997000	4.470156000	-1.013570000
1	-7.234655000	2.490031000	-0.984529000
1	-5.629503000	2.556062000	-1.737253000
6	-7.110481000	4.836570000	-2.327734000
1	-6.974431000	4.877766000	-0.172633000
1	-5.421523000	4.964879000	-1.002699000
6	-7.266223000	6.348251000	-2.513383000
1	-6.546548000	4.414501000	-3.167969000
1	-8.099476000	4.359816000	-2.351120000
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1	-7.850410000	6.793491000	-1.699899000
1	-6.291537000	6.847807000	-2.534622000
1	-3.707214000	2.646940000	-0.526995000
6	-6.341877000	2.816597000	1.604075000
6	-7.816979000	2.432895000	1.703399000
1	-6.231448000	3.901410000	1.678536000
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1	-7.931046000	1.344700000	1.669690000
1	-7.855412000	2.559578000	3.865388000
1	-8.309417000	4.050663000	3.056896000
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6	-3.294593000	2.475281000	1.574635000
1	-3.703062000	2.784965000	2.544796000
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1	-1.938155000	4.154431000	1.347903000
1	-1.456813000	2.702028000	0.476917000
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1	-1.343284000	3.047176000	3.537728000
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[12]$^{-}$

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9	-4.289299000	-3.187087000	-2.623506000
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6	8.203032000	1.619156000	-0.226528000
1	8.625007000	2.611056000	-0.076337000
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6	8.469179000	-0.715007000	-0.684568000
1	9.101811000	-1.571018000	-0.912518000
6	7.091455000	-0.890994000	-0.612024000
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6	2.026121000	-2.158264000	0.429452000
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6	4.310265000	-2.497803000	0.554271000
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6	-0.356593000	-2.013894000	-0.486904000
6	-0.232881000	-1.346495000	-1.765950000
1	0.690601000	-1.219134000	-2.322734000
6	-2.350457000	-1.358991000	-1.322885000
6	-1.758105000	-2.088842000	-0.273863000
1	-2.256161000	-2.462466000	0.612113000
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[10]$^-$ TBA$^+$

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[12]$^-$ TBA$^+$
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