Electronic Supplementary Materials for

Fluoride ion Coordination-Induced Turn-On Fluorescence of Tailored N-Methyl N-Confused Tripyrromonomethene Analogues

Manik Jana,[a] Raja Narayansamy,[b] Dandamudi Usharani, *[b,c] Kamini Tripathi, [a] 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] *Central Food Technological Research Institute, Mysore, Karnataka 570020, 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 NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer and chemical shifts were reported as the delta scale in ppm relative to $CHCl_3$ (δ = 7.26 ppm) as internal reference for ^{1}H. MALDI-TOF MS data were recorded using Bruker Daltonics flex Analyser and ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. 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. Transmission electron microscopic (TEM) images was recorded using an ultra-high-resolution field emission gun transmission electron microscope (JEOL, JEM 2100 F) with a 200 kV electron source.

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 suitable shinning orange crystal of size 0.1 x 0.1 x 0.1mm^3 of free base **5** was mounted on a Bruker APEX-III CCD diffractometer with a fine- focus sealed tube Mo-Kα radiation (λ = 0.71073Å) X-ray source. Total 1800 frames were collected at 120 K for free **5** with the exposure time of 20s per frame. Unit cell determination using both high angle and low angle diffraction reveal that compound crystallizes in monoclinic P 21/n space group for **5**. The structures were solved by SHELX-2018/3 using SHELXTL suite of programme. The final refinement of the structure was carried out using least-squares method on F^2 using SHELXL-2018/3. The final refinement of the solved structure converged at the R value of 0.0952 for **5**. All non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were located from difference Fourier maps.

A suitable shinning orange crystal of size 0.1 x 0.1 x 0.1mm^3 of free base **6** was mounted on a Bruker APEX-III CCD diffractometer with a fine- focus sealed tube Mo-Kα radiation (λ = 0.71073Å) X-ray source. Total 1800 frames were collected at 115 K for **6** with the exposure time of 20s per frame. Unit cell determination using both high angle and low angle diffraction reveal that compound crystallizes in monoclinic P 21/n space group for **6**. The structures were solved by SHELX-2018/3 using SHELXTL suite of programme. The final refinement of the structure was carried out using least-squares method on F^2 using SHELXL-2018/3. The final refinement of the solved structure converged at the R value of 0.0607 for **6**. All non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were located from difference Fourier maps.

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

For UV-vis titrations, stock solution of **5** and **6** 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.

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

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 $1/(A-A_0)$ against $1/[G]_n$.

Similarly, for emission titrations also, stock solution of **5**, **6** and guest were prepared in $CHCl_3$. The spectra of these solutions were recorded by means of emission spectroscopy method. Binding constant (K_a) was calculated according to the Benesi-Hildebrand equation stated below.

$$1/(I-I_0) = 1/\{K_a(I_{max}–I_0)\ [G]_n\} + 1/[I_{max}-I_0]$$

Here, I_0 is the emission of the receptor in the absence of guest, I is the emission recorded in the presence of added guest, I_{max} is emission 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 $1/(I-I_0)$ against $1/[G]_n$.

1.4 Job's plot:

The stoichiometry between **5**, **6** and analyte was evaluated by Job's plot method. A solution of **5**, **6** and guest (**G**) of same concentration were mixed in different proportions keeping a final volume of 2 mL. The related compositions for **5** or **6**: **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**]/ [**5** or **6**] + [**G**]. The mole fraction of analytes (X_M) was plotted against absorbance to obtain Job's plot.[S1] The mole fraction at which absorbance / emission intensity appeared to be minimum was taken as the stoichiometry of their interaction.

1.5 Limit of detection (LOD)[S2]:

The limit of detection of **5** and **6** towards F^- and OAc^- ions were evaluated using the data obtained from absorption and emission titrations. A graph of the absorbance and emission of **5** and **6** were plotted repetitively vs. the concentration of F^- and OAc^- ions, respectively to get the slope. The detection limit was calculated using the equation,

$$LOD = \frac{3\sigma}{s}$$

Where, σ = Standard deviation of the blank measurement and s = slope of the graph.

1.6 Fluorescence quantum yield (ΦF)

Fluorescence quantum yield (ΦF) for both samples has been calculated relative to Quinine sulphate dye (0.1 M H_2SO_4, λ_{ex} = 350 nm, Φ = 0.58) as a reference using the following formula:

$$\Phi_S = \Phi_R \times (I_S/I_R) \times (A_R/A_S) \times (\eta_S^2 / \eta_R^2)$$

Where, Φ = quantum yield, I = area under the curve of emission spectrum, A = absorbance at λ_{ex}, η = refractive index of solvent. The subscript **R** and **S** denote the values for the reference substance and samples, respectively. Stock solutions for **5**, **6** were made in $CHCl_3$.

1.7 Transmission Electron Microscopy (TEM): A solution of compounds **5** (1.67 x 10-5 M), **6** (1.73 x 10-5 M) and their aggregates were dropped on carbon-coated copper grids (Ted Pella, Inc.) for 5 min. After removal of excess solution, the sample grid was dried under vacuum. The dried samples were observed with an ultra-high-resolution field emission gun transmission electron microscope (JEOL, JEM 2100 F) with a 200 kV electron source. Images were analyzed with gatan microscopy imaging software.

1.8 Theoretical Calculation

Based on the X-ray crystal structure **5** and **6,** the host-guest complexes of **5**, **6** were generated. A gas phase DFT calculations with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP) [S3] and 6-31G(d,p) basis set [S4] were employed to optimise crystal structures **5**, **6**, $\mathbf{F^-}$, tetra butyl ammonium fluoride (**TBAF**) tetra butyl ammonium acetate (**TBAOAc)** and generated anion complexes [**5-F**]$^-$, [**6-F**]$^-$, [**5-OAc**]$^-$, [**6-OAc**]$^-$ protonated [**6-H**]$^+$ and counter ion complexes [**5-TBAF**], [**6-TBAF**], [**5-TBAOAc**], [**6-TBAOAc**] in gas phase. We observe that gas phase optimisation of **5** and **6** has strong hydrogen bond due to self interaction error. Thus, the lower energy isomer of host-fluoride anion complexes ([**5-F_a**]$^-$ and [**6-F_a**]$^-$) and host-acetate complexes ([**5-OAc_a**]$^-$ and [**6-OAc_a**]$^-$) were optimised in solvent phase in presence of dichloromethane to estimate the interaction energies in charged complexes. Harmonic vibrational frequencies at the same level of theory indicated that all the structures were local minima. To simulate the steady-state absorption spectra, the time-dependent TD-DFT [S5] calculations were employed on the solvent optimized structures in the presence of chloroform solvent for (**5**, **6**), [**5-F_a**]$^-$, [**6-F_a**]$^-$, [**6-H**]$^+$, [**5-OAc_a**]$^-$ and [**6-OAc_a**]$^-$ using the polarizable continuum model (PCM) using the integral equation formalism variant (IEFPCM) [S6] at same level of theory. Further, the complexes were optimised in presence of counter ion tetrabutyl

ammonium ion (TBA) at the same level of theory. Counter poise method [S7] was employed for basis set superimposition error of gas phase and counter ion optimised complexes of **5**, **6**, [**5-F$_a$**]$^-$, [**6-F$_a$**]$^-$, and [**5-TBAF**], and [**6-TBAF**] for obtaining complexation energies. To understand the aggregation phenomena **5** and **6**, dimeric stacked forms with lateral and face-to face overlap were optimised at same level of theory. The local minima structure of dimers of **5** and **6** are confirmed with positive harmonic vibrational frequencies. The steady state absorption spectrum was obtained from the time dependant TD-DFT calculation of local minima in presence of water solvent for dimeric forms of **5** and **6**. All the above-mentioned calculations were performed with the Gaussian16 A03 program. [S8] Electronic structure, excitation analysis was performed using chemcraft, Gauss sum and Multiwfn programs.[S9]

References:

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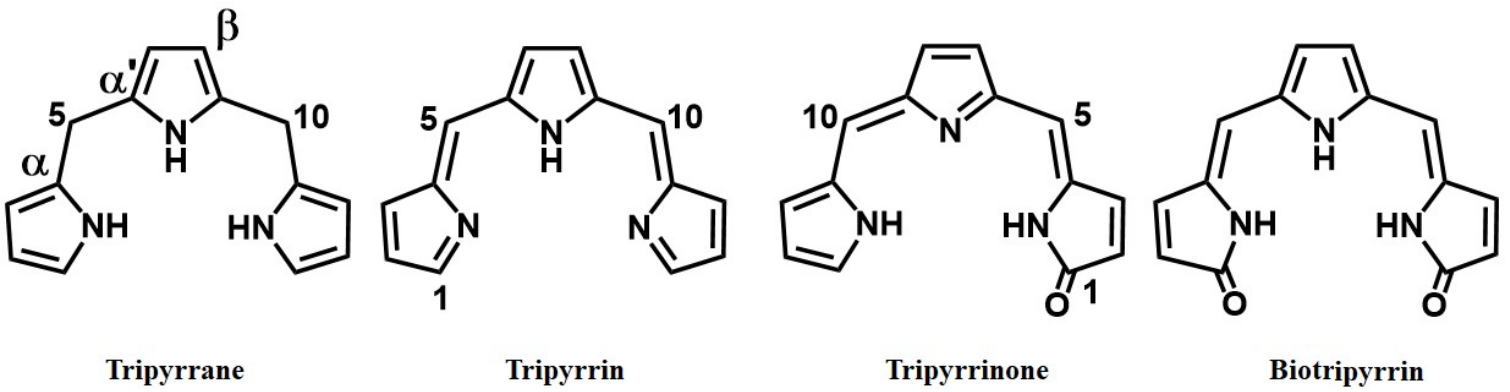


Chart S1. Labelling and nomenclature of Acyclic Tripyrrolic systems

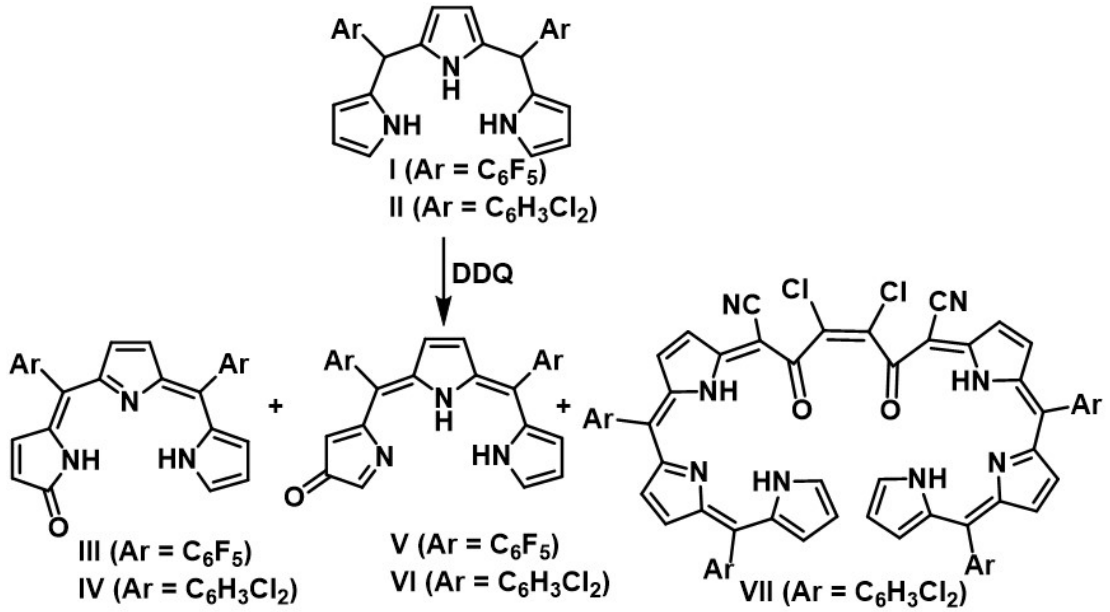
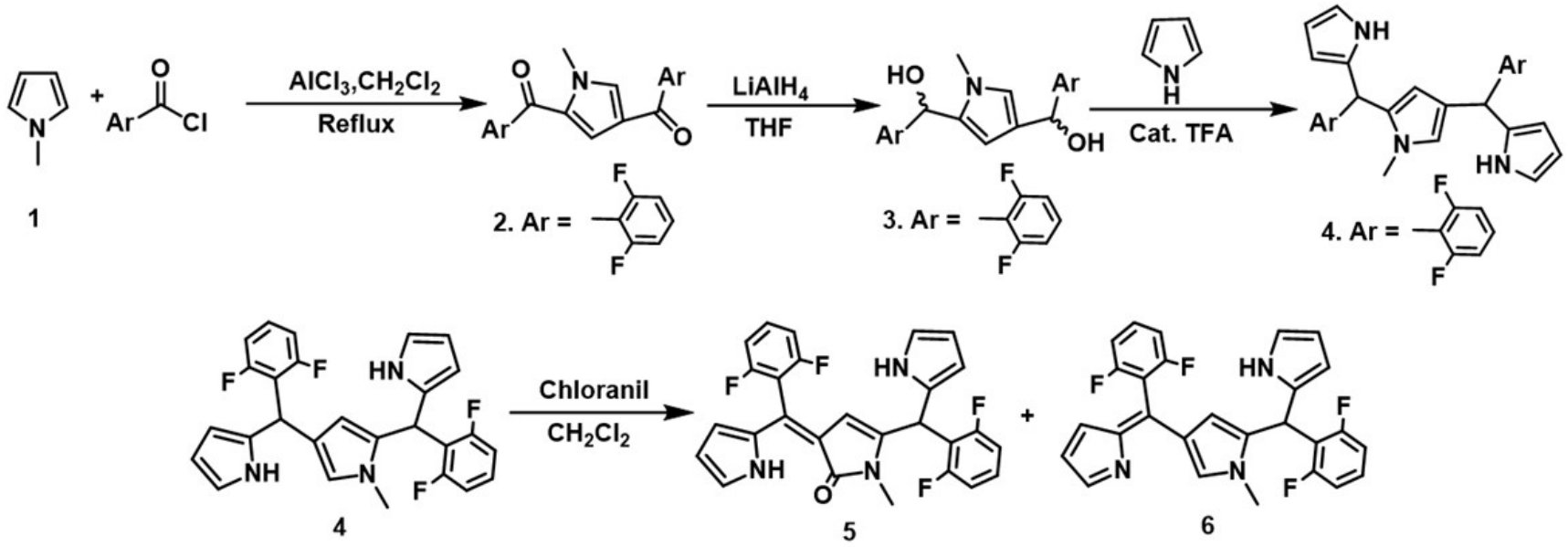


Chart S2. Literature known Oxidation product of Tripyrrolic systems

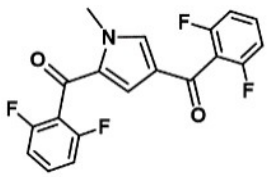
1.9 Synthesis:



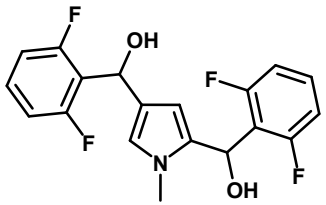
Scheme S1. Synthesis of precursors

Reactant -4	Solvent (CH_2Cl_2) mL	Oxidant (Chloranil) wrt 4	5 (Yield in %)	6 (Yield in %)
1 mmol	740	3 equiv.	21%	14%
1 mmol	250	3 equiv.	40 %	30%
1 mmol	250	1 equiv.	17%	12%
1 mmol	125	1 equiv.	16%	10%

Table S1



Synthesis of **2**: To a stirred solution of 2, 6-difluorobenzoyl chloride (7.07 mL, 56.32 mmol) and anhydrous $AlCl_3$ (7.5 g, 56.32 mmol) in 41 mL dry DCM. N-methyl pyrrole (2 mL, 22.52 mmol) was added drop wise at room temperature. The reaction mixture was refluxed for 22 hours in inert atmosphere. The completion of the reaction mixture was monitored by TLC. It was then quenched with aqueous $NaHCO_3$ in ice cold condition. The organic phase was extracted three times with DCM and after water wash, dried over anhydrous Na_2SO_4. Solvent was removed under reduced pressure. The crude mixture was chromatographed on a silica gel column using hexane-ethyl acetate (4:1) solution. The solvent was evaporated and light-yellow solid was obtained. Yield 3.2 g (39.39%). R_f = 0.4 (20:80 EtOAc/Hexane). ESI-TOF MS (*m/z*) 361.0724 [M^+] (361.0726 calc. for $[C_{19}H_{11}F_4NO_2]^+$).



^{1}H NMR (300 MHz, $CDCl_3$, 300K, δ [ppm]): 4.08 (s, 3H), 6.94-7.00 (m, 4H), 7.07 (s, 1H), 7.31 (s, 1H), 7.35-7.46 (m, 2H,).^{13}C NMR (75 MHz, $CDCl_3$, 300 K, δ [ppm]): 38.49, 111.93, 111.98, 112.02, 112.09, 112.13, 112.19, 117.55, 117.73, 117.91, 123.20, 125.30, 131.73, 131.81, 131,85, 131.89, 131.93, 132.01, 132.93, 136.85, 158.76, 158.81, 158.86, 160.75, 160.80, 160.85, 178.57, 181.65.

Synthesis of **3**: **2** (1.5 g, 4.1 mmol) was reduced with $LiAlH_4$ (1.26 g, 33.2 mmol) in dry THF under N_2 atmosphere for 4 hours at 0° C. The reduced product was extracted with EtOAc and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to yield **3**. Yield 1.45 g (97%). R_f = 0.2 (20:80 EtOAc/ Hexane). ESI-TOF MS (*m/z*) 366.0856 $[M+H]^+$ (366.1039 calc. for $[C_{19}H_{16}F_4NO_2]^+$).

^{1}H NMR (300 MHz, $CDCl_3$, 298 K, δ [ppm]): 2.57 (b, 1H), 2.76 (b, 1H), 3.69 (s, 3H), 5.89 (s, 1H), 6.00 (s, 1H), 6.08 (b, 1H), 6.45 (b, 1H), 6.83-6.96 (m, 4H), 7.17-7.30 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 298 K, δ [ppm]): 34.13, 61.32, 62.92, 107.30, 111.54, 111.70, 111.88, 112.05, 121.75, 123.82, 128.86, 123.82, 128.86, 129.51, 132.34.

Synthesis of **4**: **3** (0.365g, 1 mmol) was immediately reacted with excess pyrrole (43 mL, 623 mmol)) in the presence of catalytic amount of CF_3COOH. After 45 minutes reaction was quenched with DCM and neutralized with 0.1N NaOH solution. The organic phase was extracted with DCM and after water wash for two times, dried over anhydrous Na_2SO_4. The excess solvent was removed in rotary evaporator under reduced pressure. The crude mixture was purified by silica gel column using hexane-ethyl acetate (11:1) solution. Yield 1.45 g (73%).

R_f = 0.4 (15:85 EtOAc/ Hexane). ESI-TOF MS (*m/z*) 464.1745 $[M+H]^+$ (464.1744 calc. for $[C_{27}H_{22}F_4N_3]^+$).

^{1}H NMR (300 MHz, $CDCl_3$, 300K, δ [ppm]): 3.34 (s, 3H, N-Me), 5.71 (s, 1H, α–CH -Py), 5.79 (s, 1H), 5.91-5.96 (m, 4H), 6.10-6.12 (m, 2H), 6.65-6.70 (m, 2H), 6.81-6.90 (m, 4H), 7.09-7.24 (m, 2H), 8.24 (br, 2H, NH). ^{13}C {^{1}H} NMR (75 MHz, $CDCl_3$, 300K, δ [ppm]): 31.9, 32.2, 33.9, 106.1, 107.0, 108.2, 108.3,

108.7, 108.8, 111.7, 111.9, 111.9, 112.0, 112.1, 112.2, 112.3, 116.3, 116.4, 117.2, 117.3, 118.1, 121.2, 121.2, 121.3, 128.1, 128.6, 128.8, 128.9, 129.9, 130.8, 132.6, 159.5, 162.8.

Synthesis of 5, **6:**

Tripyrrane **4** (0.464 g, 1 mmol) was taken in a round bottom flask, to it 250 mL of dry DCM was added and stirred for 15 minutes under nitrogen atmosphere to get a clear solution. After that, *p*-chloranil (0.735 g, 3 mmol) was added and the resulting mixture was refluxed for 90 minutes in open air. After complete removal of solvent from crude mixture by rotary evaporator, the compound was purified by silica gel column chromatography to obtain compound **5** using 80:20 DCM/Hexane as eluent, **6** with 2% EtOAC/DCM as eluent. Extra pure compounds were finally obtained by repeated PTLCs.

[**5**] Yield 190 mg (~40 %). R_f = 0.4 (80:20 CH_2Cl_2/Hexane). HRMS (ESI-TOF) (*m/z*) 477.1464 $[M]^+$ (477.1466 calc. for $[C_{27}H_{19}F_4N_3O]^+$).

^{1}H NMR (300 MHz, $CDCl_3$, 300K, δ [ppm]): 2.99 (s, 3H, N-Me), 4.96 (br, 1H), 5.32 (s,1H), 5.58 (br, 1H), 5.97 (br,1H), 6.04 (m, 1H), 6.25 (m,1H), 6.65 (m,1H), 6.85-7.02 (br, 4H, *m*-Ph), 7.14 (br,1H), 7.19-7.29 (m, 1H, *p*-Ph), 7.33-7.43 (m, 1H, *p*-Ph), 8.34 (br 1H), 14.32 (br, 1H). ^{13}C {^{1}H} NMR (75 MHz, $CDCl_3$, 300K, δ [ppm]): 167.76,162.81, 162.10, 159.62, 158.81, 139.92, 131.43, 130.79, 130.66, 130.53, 130.02, 129.88, 129.74, 128.99, 127.14, 124.91, 123.02, 118.64, 118.12, 112.59, 112.55, 112.28, 112.24, 111.89, 111.84, 111.79, 111.55,111.50, 108.64, 108.26,103.61, 103.58, 33.20,33.20, 30.06, 26.97.

UV-vis (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^4]), 298K): 370 (1.52), 444 (1.33).

[**6**] Yield ~138 mg (~30 %). R_f = 0.2 (5:95 EtOAc/CH_2Cl_2). HRMS (ESI-TOF) (*m/z*) 461.1513 $[M]^+$ (461.1515 calcd for $C_{27}H_{19}F_4N_3$).

^{1}H NMR (300 MHz, $CDCl_3$, 300 K, δ [ppm]: 3.40 (s, 3H, N-Me), 5.80 (s, 1H), 5.97 (t, *J* = 3.0 Hz, 1H), 6.07-6.10 (m, 1H), 6.51 (d, *J* = 4.5 Hz, 1H), 6.65 (d, *J* = 4.5 Hz, 1H), 6.71-6.73 (m, 1H), 6.82 (s, 1H), 6.90-7.04 (m, 4H, *m*-Ph), 7.11(d, *J* = 1.9 Hz, 1H), 7.22-7.32 (m,1H, *p*-Ph), 7.38-7.48 (m, 1H, *p*-Ph), 8.03 (s, 1H), 8.77 (s, 1H). ^{13}C {^{1}H} NMR (75 MHz, $CDCl_3$, 300K, δ [ppm]): 162.66, 162.57, 162.14, 161.63, 159.90, 159.38, 159.27, 158.95, 151.40, 134.55, 134.04, 131.65, 131.25, 130.68, 130.55, 130.41,129.59, 129.35, 129.21, 129.08, 128.74,128.49, 125.65, 121.09, 120.88, 117.68,117.38, 117.38, 112.50, 112.32, 112.00, 111.55, 111.50, 111.26, 111.21, 110.27, 108.16, 108.39, 107.52, 107.27, 34.51, 31.86, 29.80.

UV-vis (CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^4]), 298K): 405 (2.38), 555 (0.15).

[**6-H**]$^+$: ^{1}H NMR (300 MHz, $CDCl_3$, 300 K, δ [ppm]: δ 9.68 (s, 1H), 8.58 (s, 1H), 8.42 (s, 1H), 7.56 (ddd, *J* = 14.8, 10.6, 8.3 Hz, 3H), 7.25 (d, *J* = 2.1 Hz, 1H), 7.06 (td, *J* = 8.6, 2.4 Hz, 3H), 6.98 – 6.87 (m, 3H), 6.85 (d, *J* = 16.9 Hz, 1H), 6.70 (d, *J* = 4.5 Hz, 1H), 6.57 (s, 1H), 6.08 (q, *J* = 2.8 Hz, 1H), 5.94 (s, 1H), 5.79 (s, 1H), 3.54 (s, 3H). UV-vis CH_2Cl_2, 1% CF_3COOH/CH_2Cl_2, λ [nm], (ϵ [M^{-1} cm^{-1}x10^4]: 466(4.69).

2. Supplementary Data:

2.1 Mass Spectra

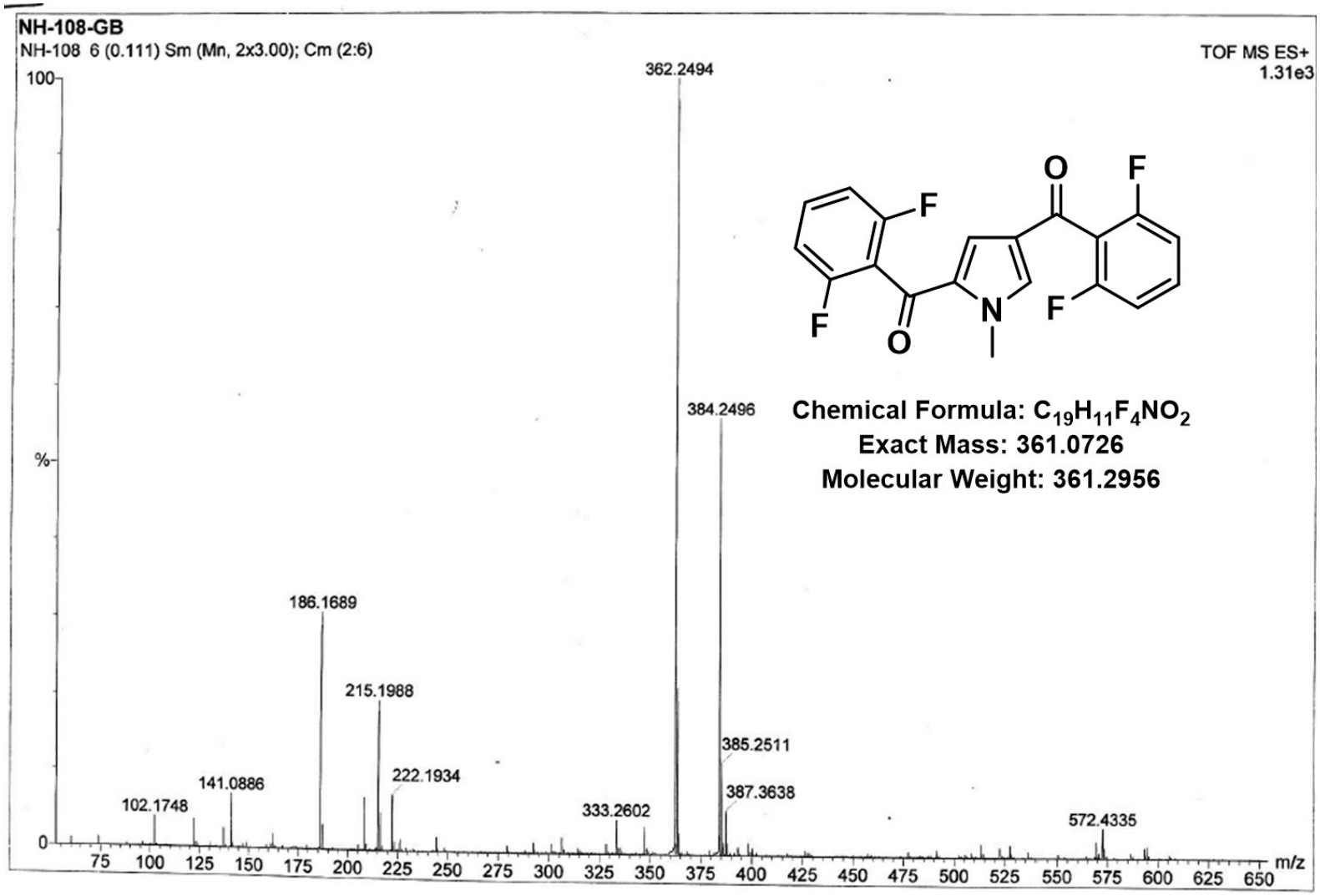


Fig. S1 ESI-MS Spectra of **2**

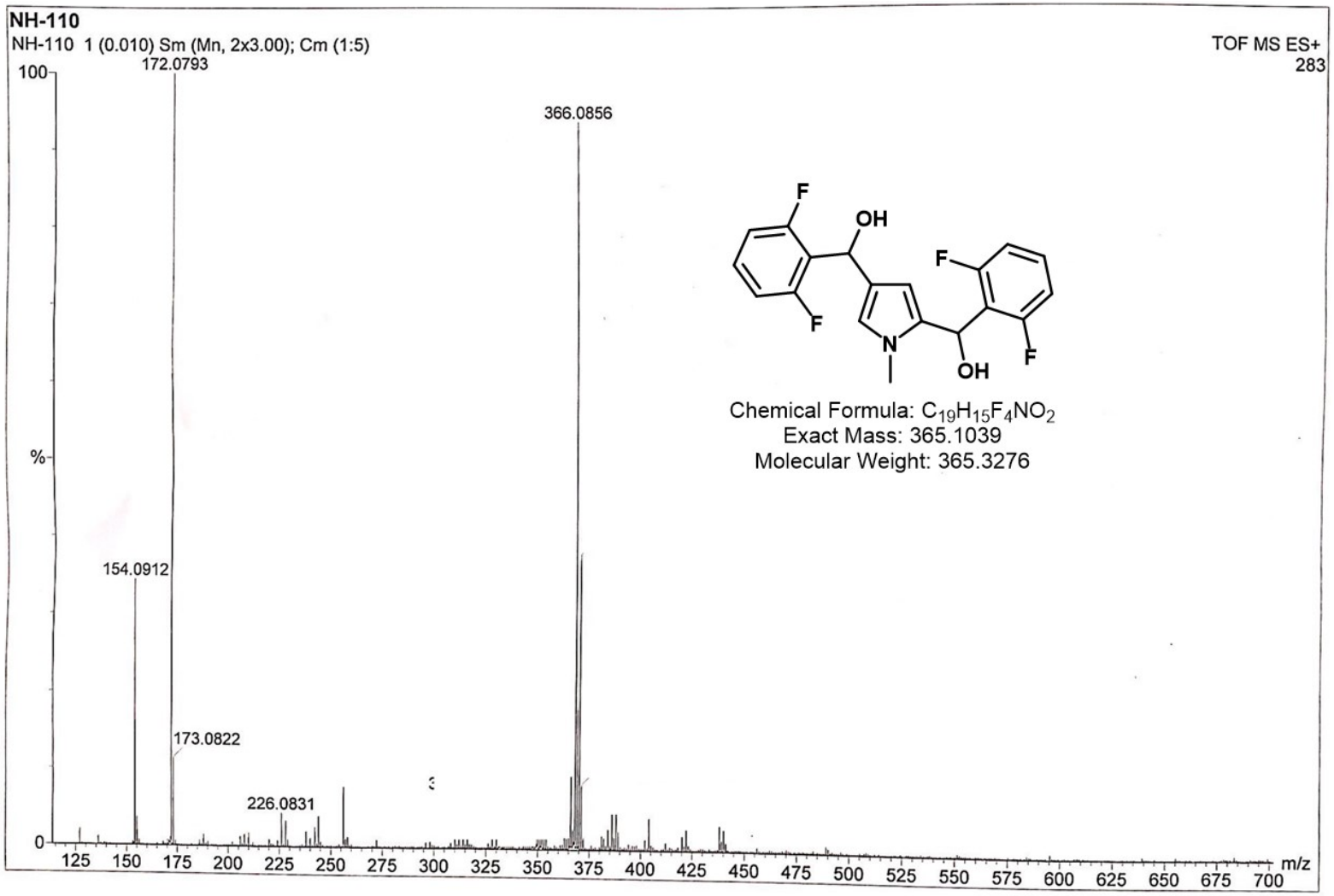


Fig.S2 ESI-MS Spectra of **3**

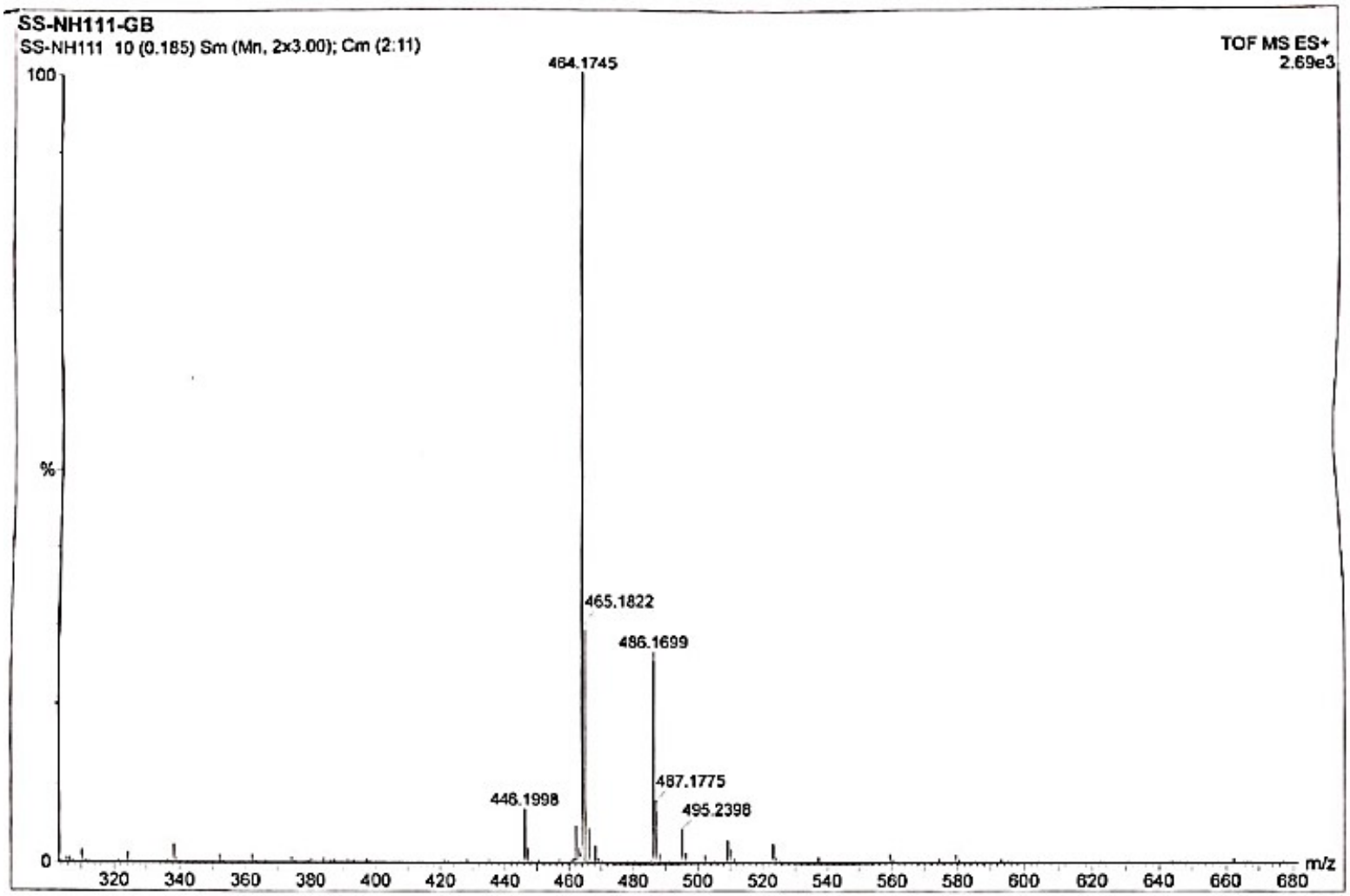


Fig. S3 ESI-MS Spectra of **4**

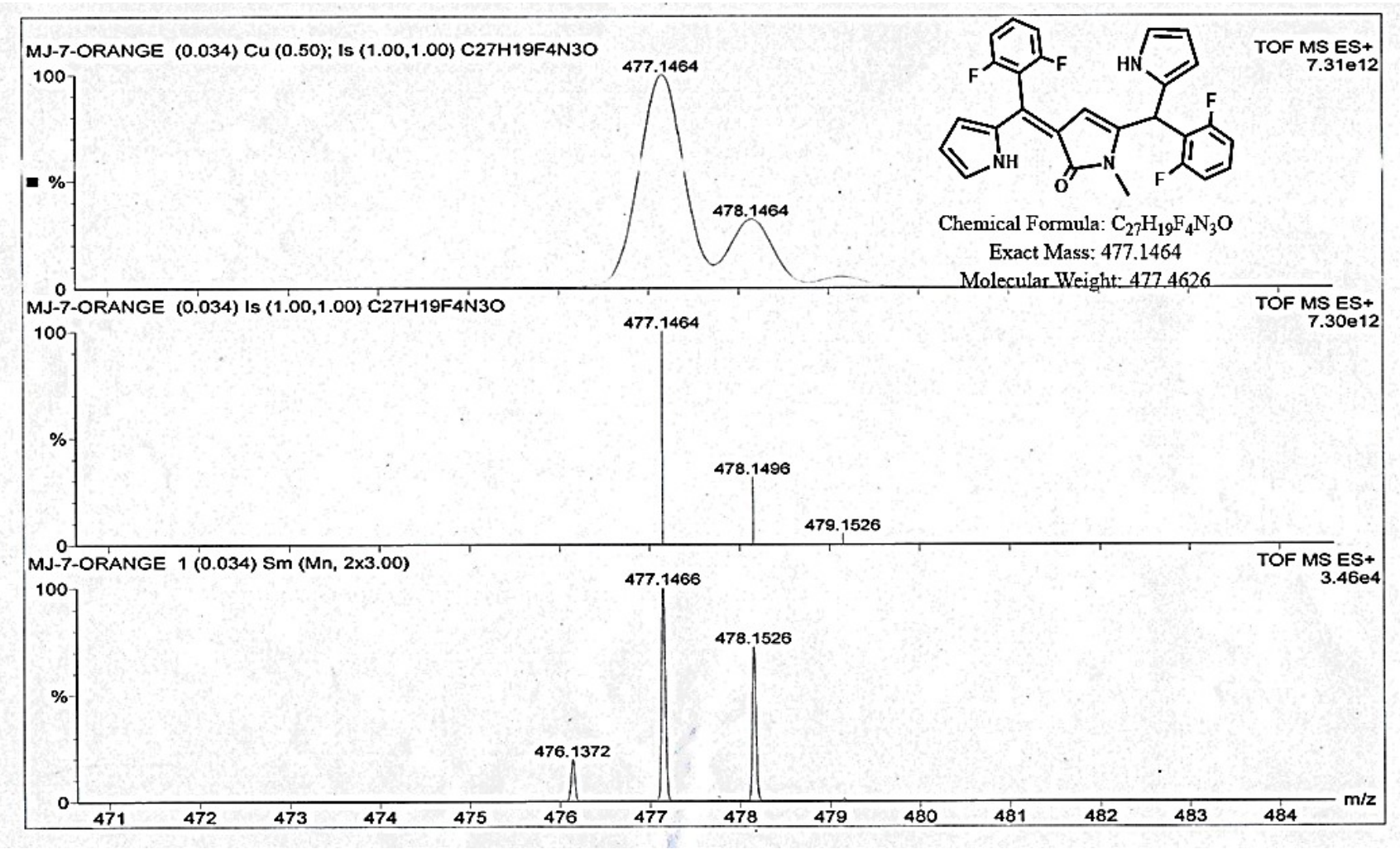


Fig. S4 HRMS Spectra of **5**

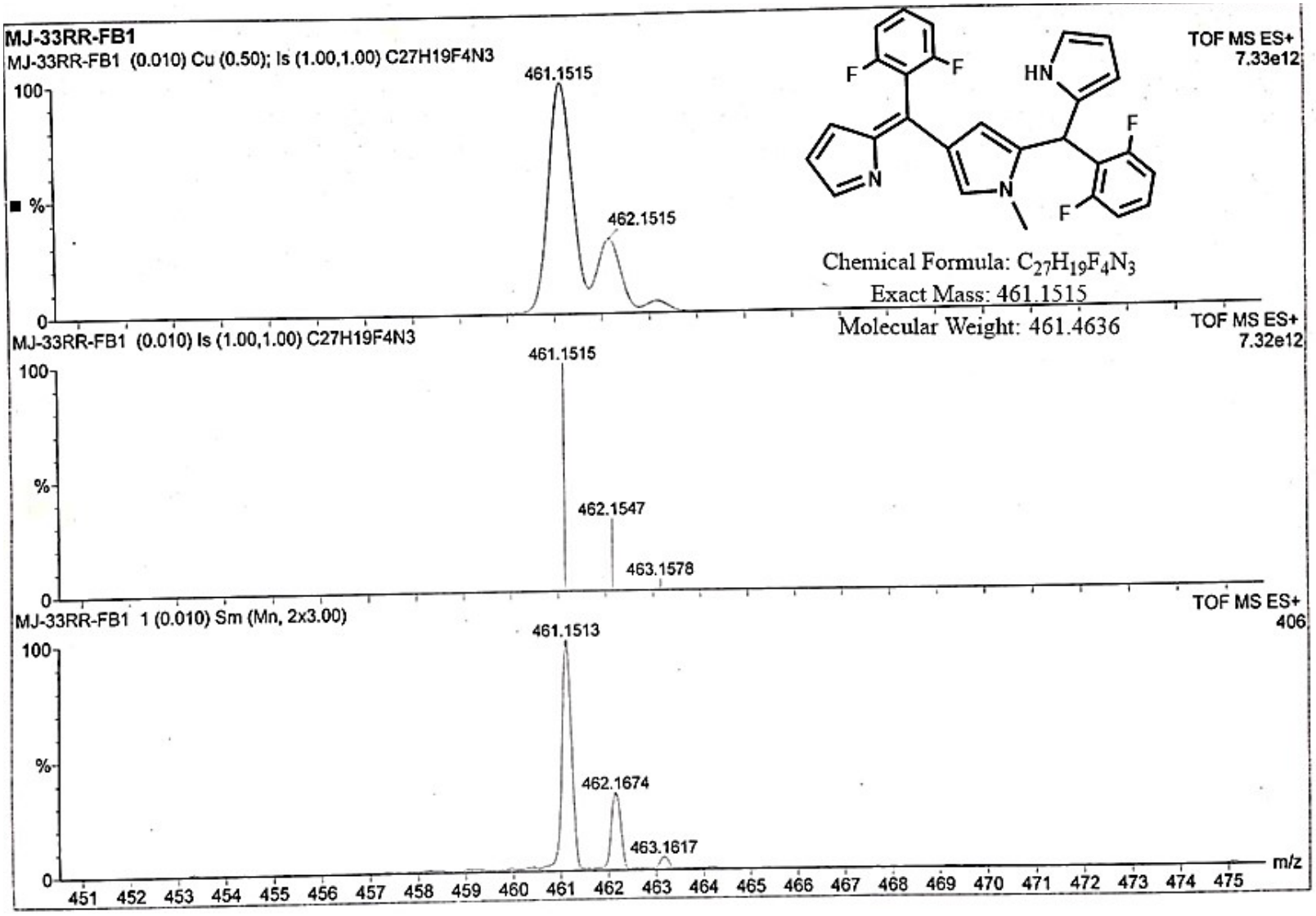


Fig. S5 HRMS Spectra of **6**

2.2 IR spectra:

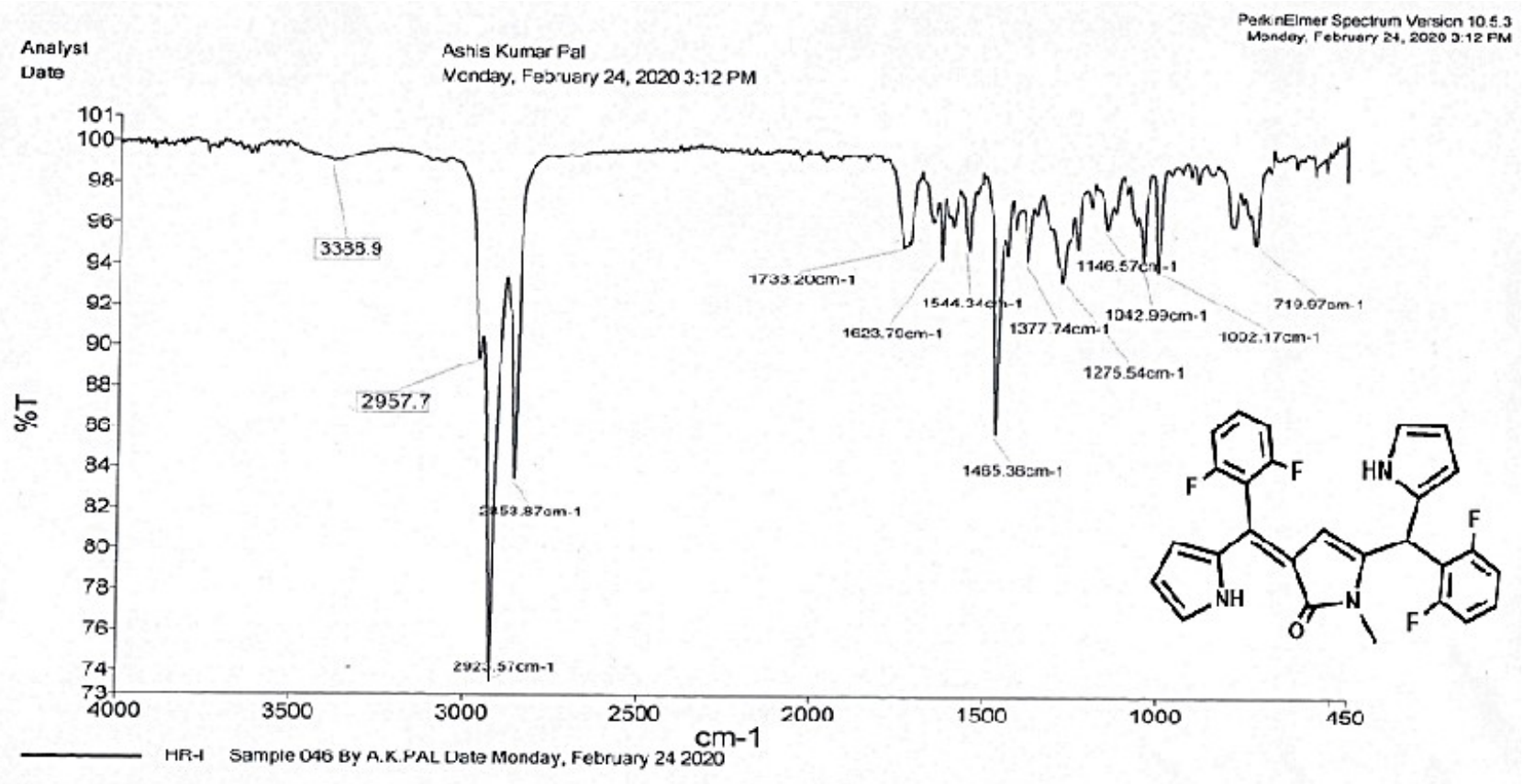


Fig. S6 IR Spectra of **5**

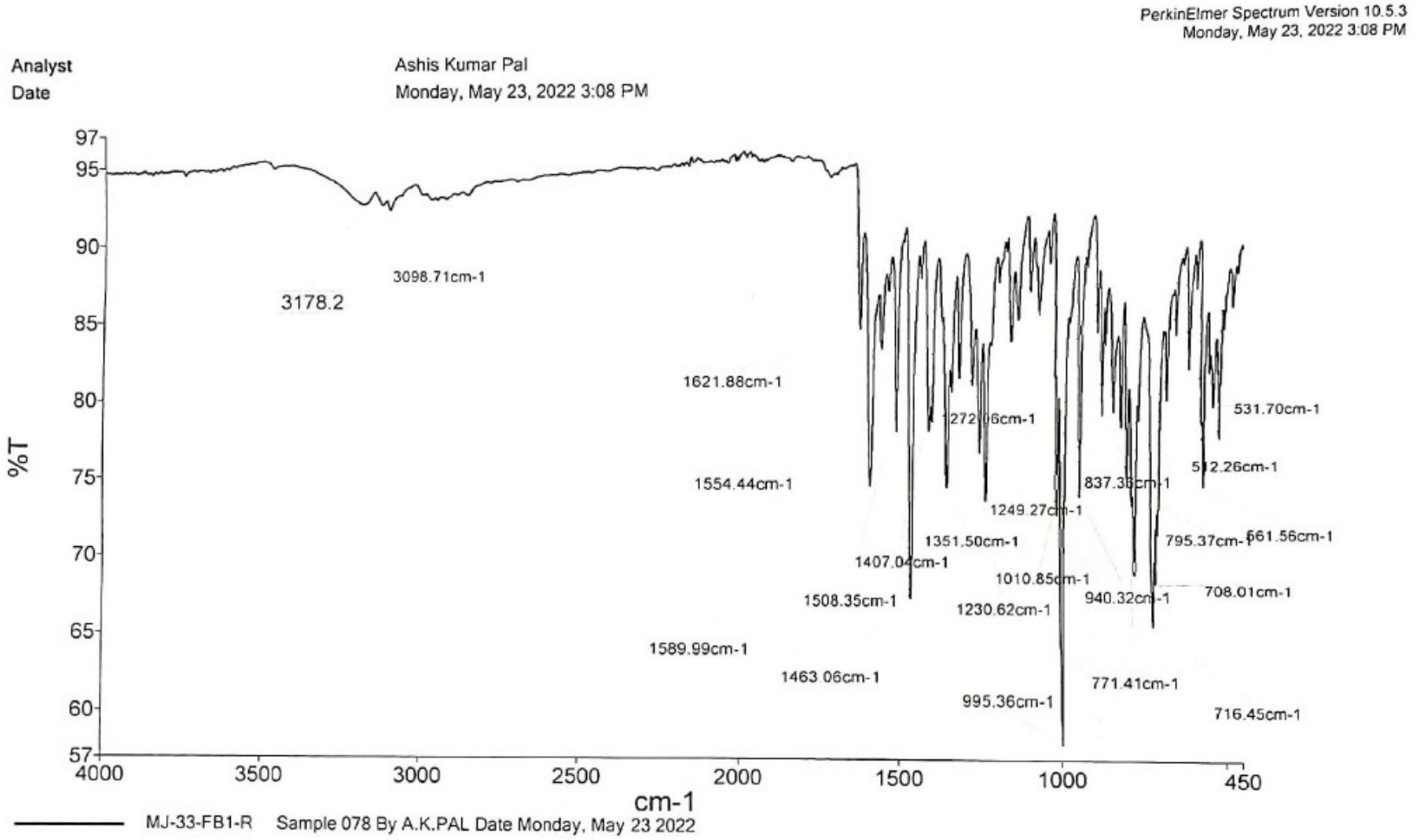


Fig. S7 IR Spectra of **6**

2.3 UV-vis spectra:

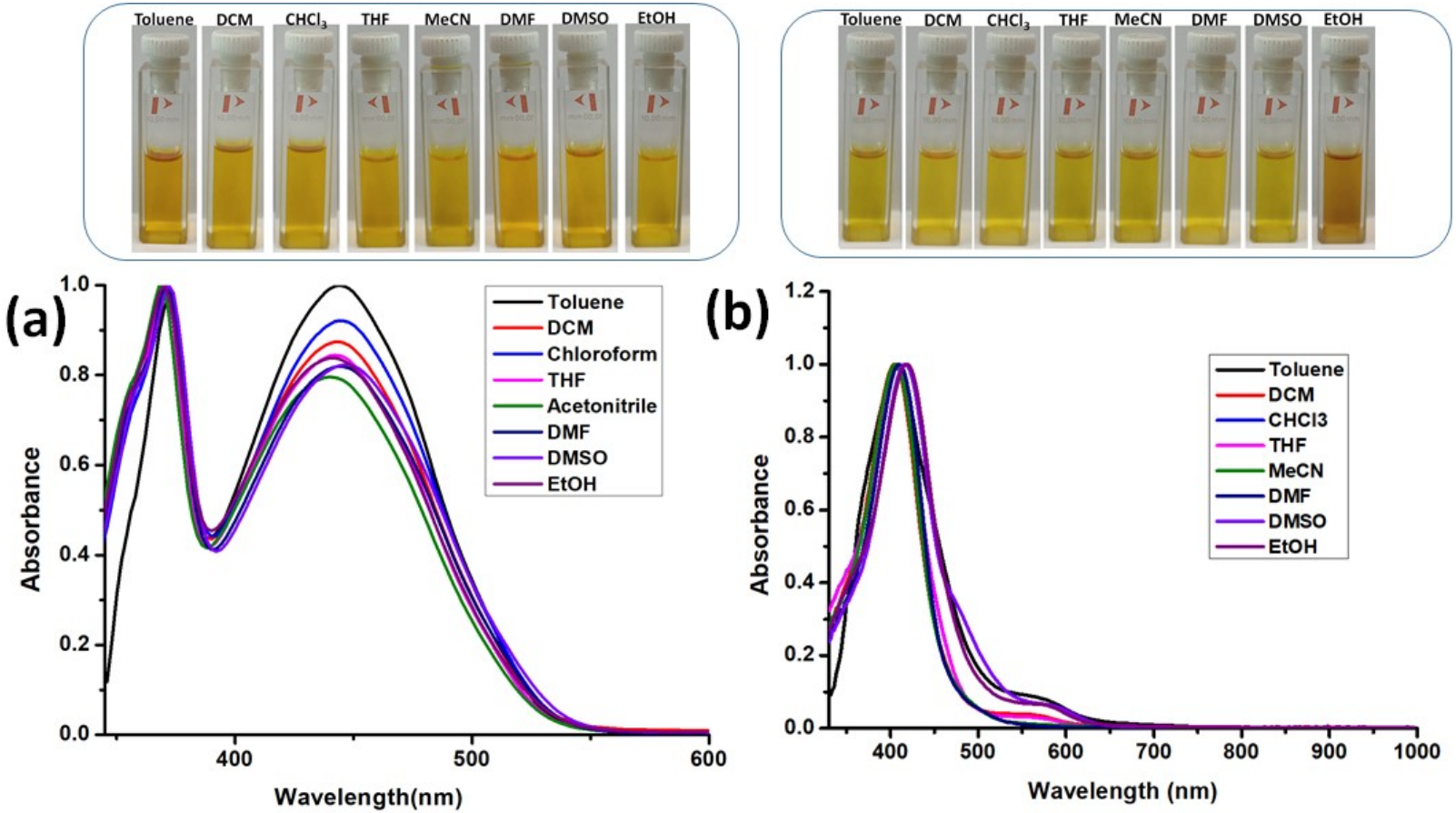


Fig.S8 UV-vis Spectral change induced upon change of solvent systems for receptor **5** (a) **6** (b) at 298 K

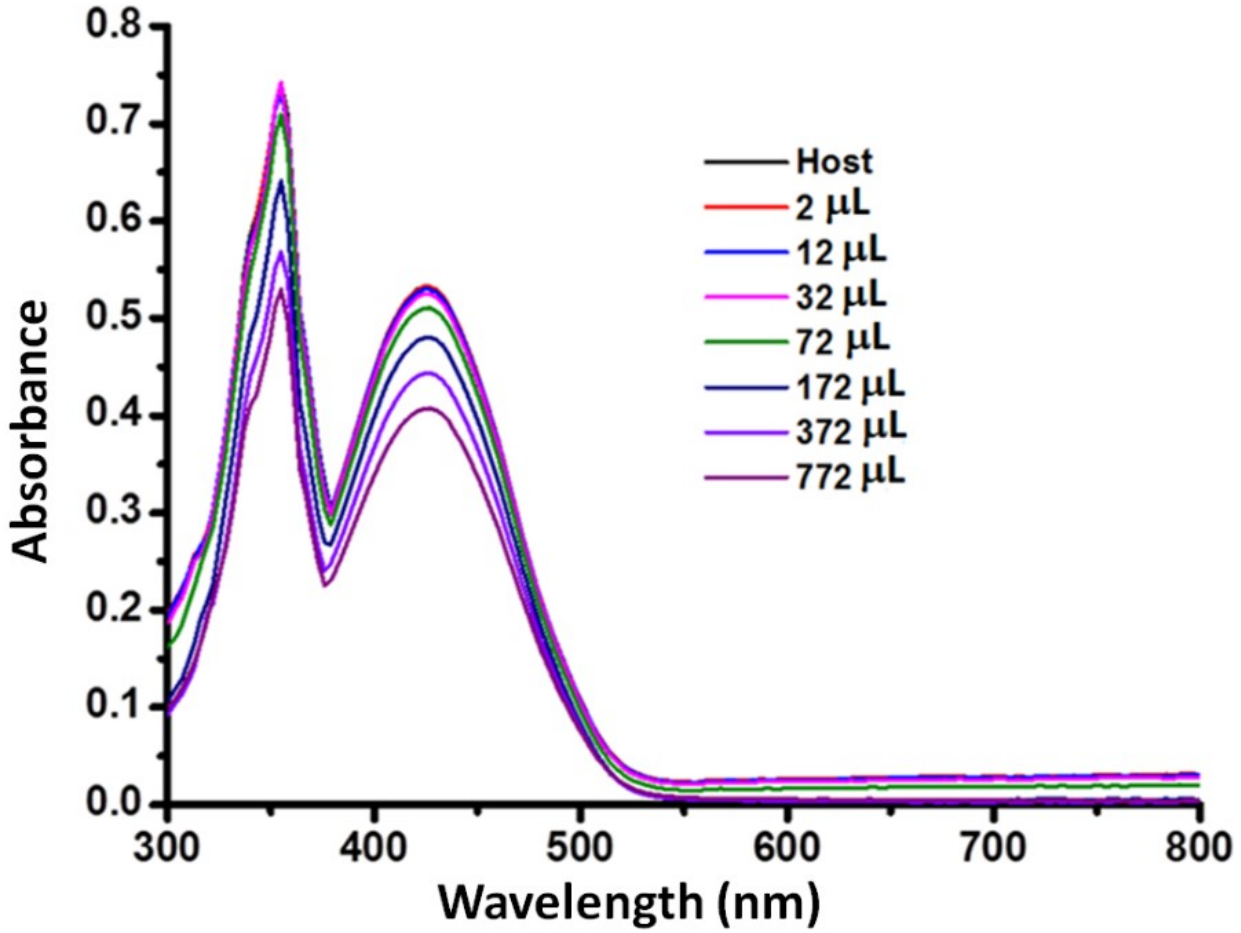


Fig. S9 Change in absorption spectrum of **5** (2.5×10^{-5} M) upon addition of TBABr (5×10^{-2} M) in $CHCl_3$ at 298 K

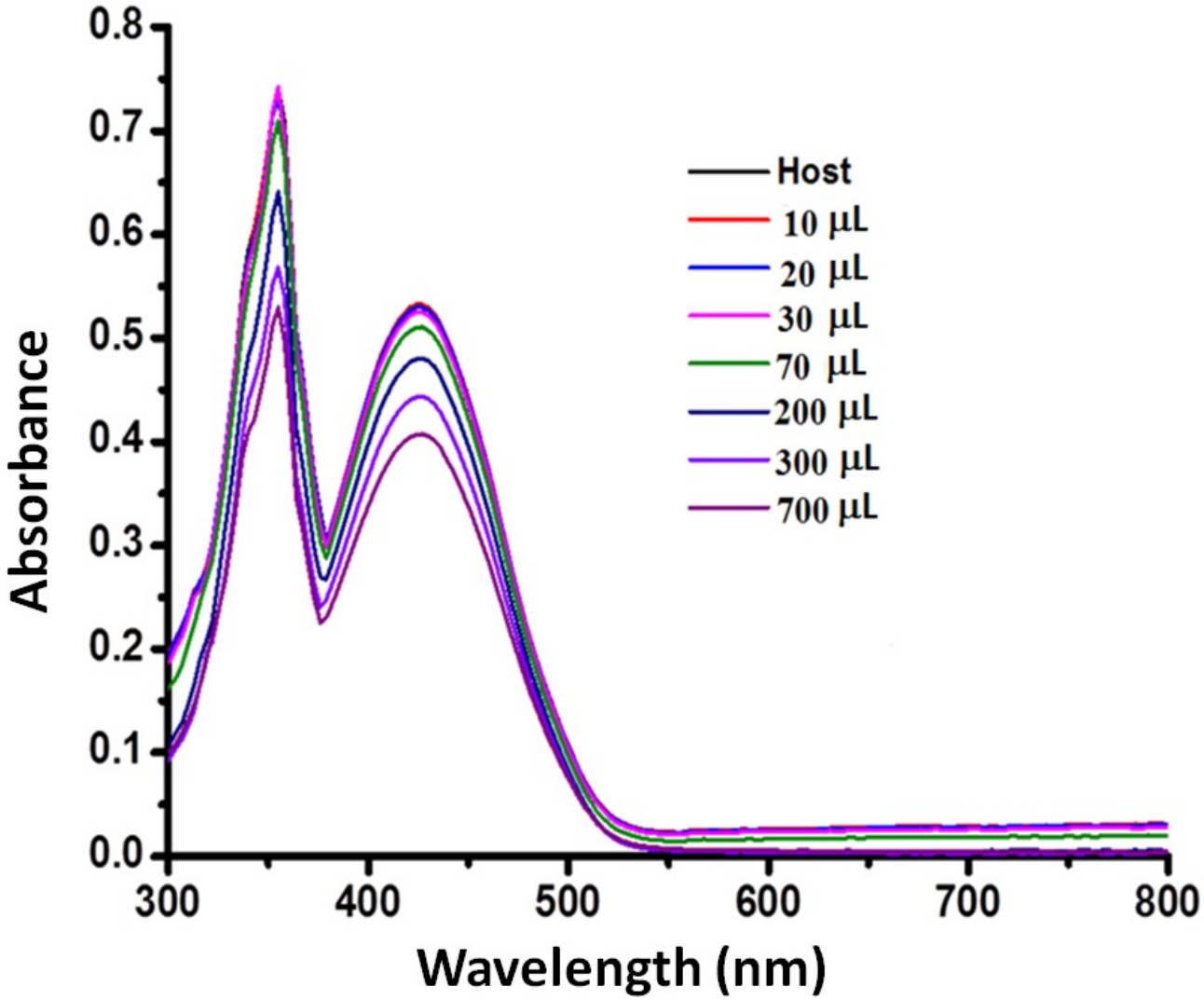


Fig. S10 Change in absorption spectrum of **5** (2.5×10^{-5} M) upon addition of TBACl (5×10^{-2} M) in $CHCl_3$ at 298 K

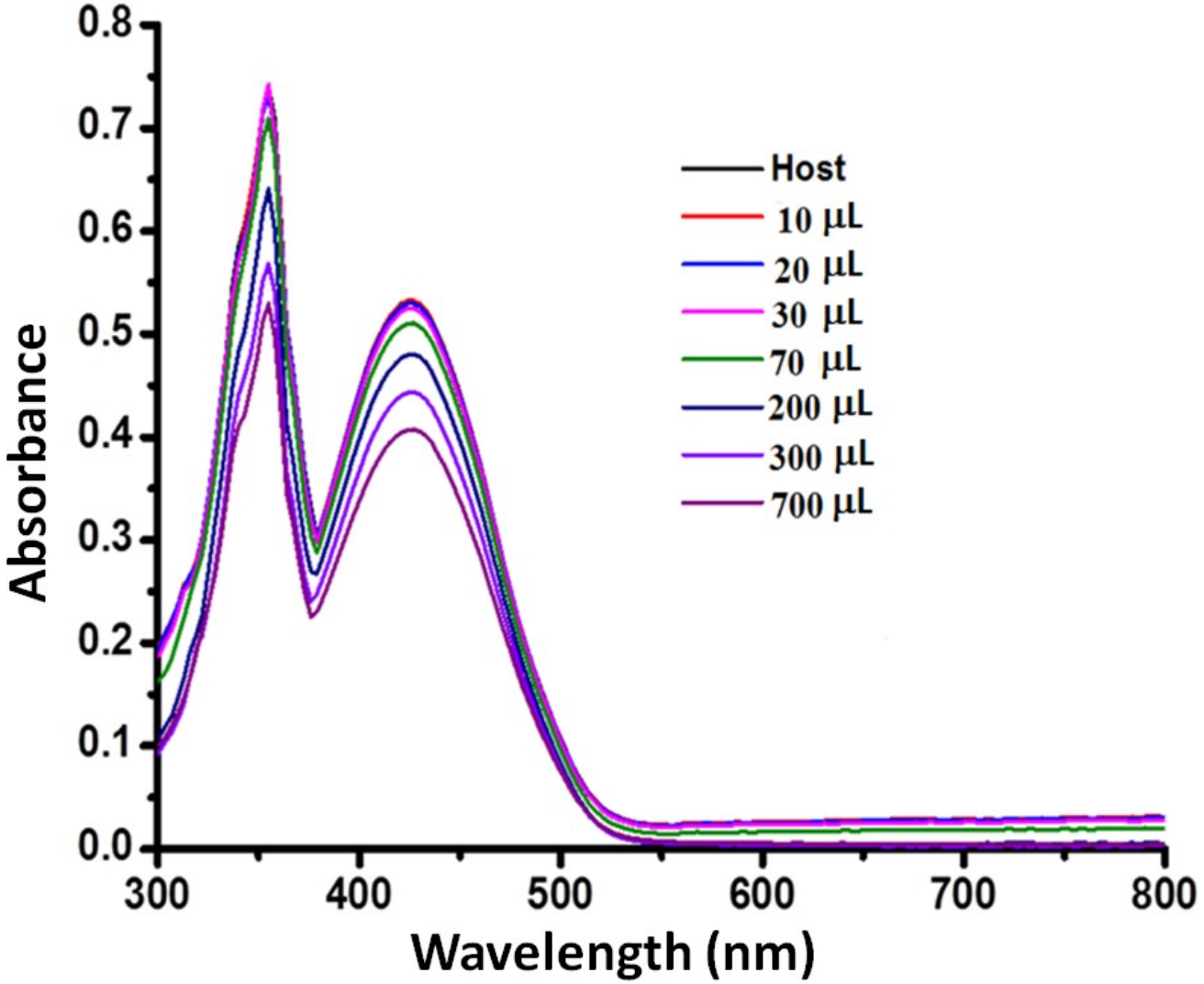


Fig. S11 Change in absorption spectrum of **5** (2.5 x 10^{-5} M) upon addition of TBAI (5 x 10^{-2} M) in $CHCl_3$ at 298 K

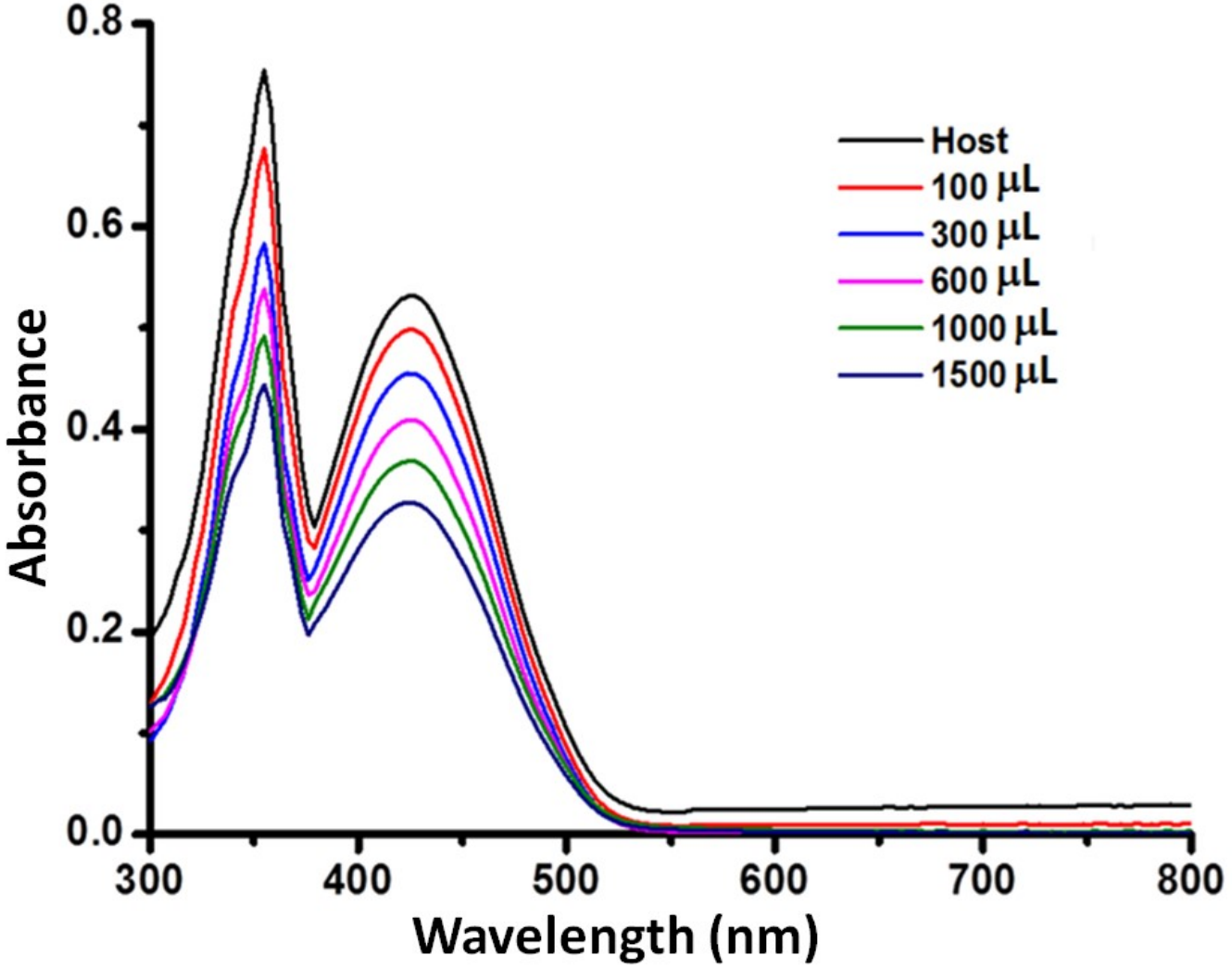


Fig. S12 Change in absorption spectrum of **5** (2.5 x 10^{-5} M) upon addition of $TBAClO_4$ (5 x 10^{-2} M) in $CHCl_3$ at 298 K

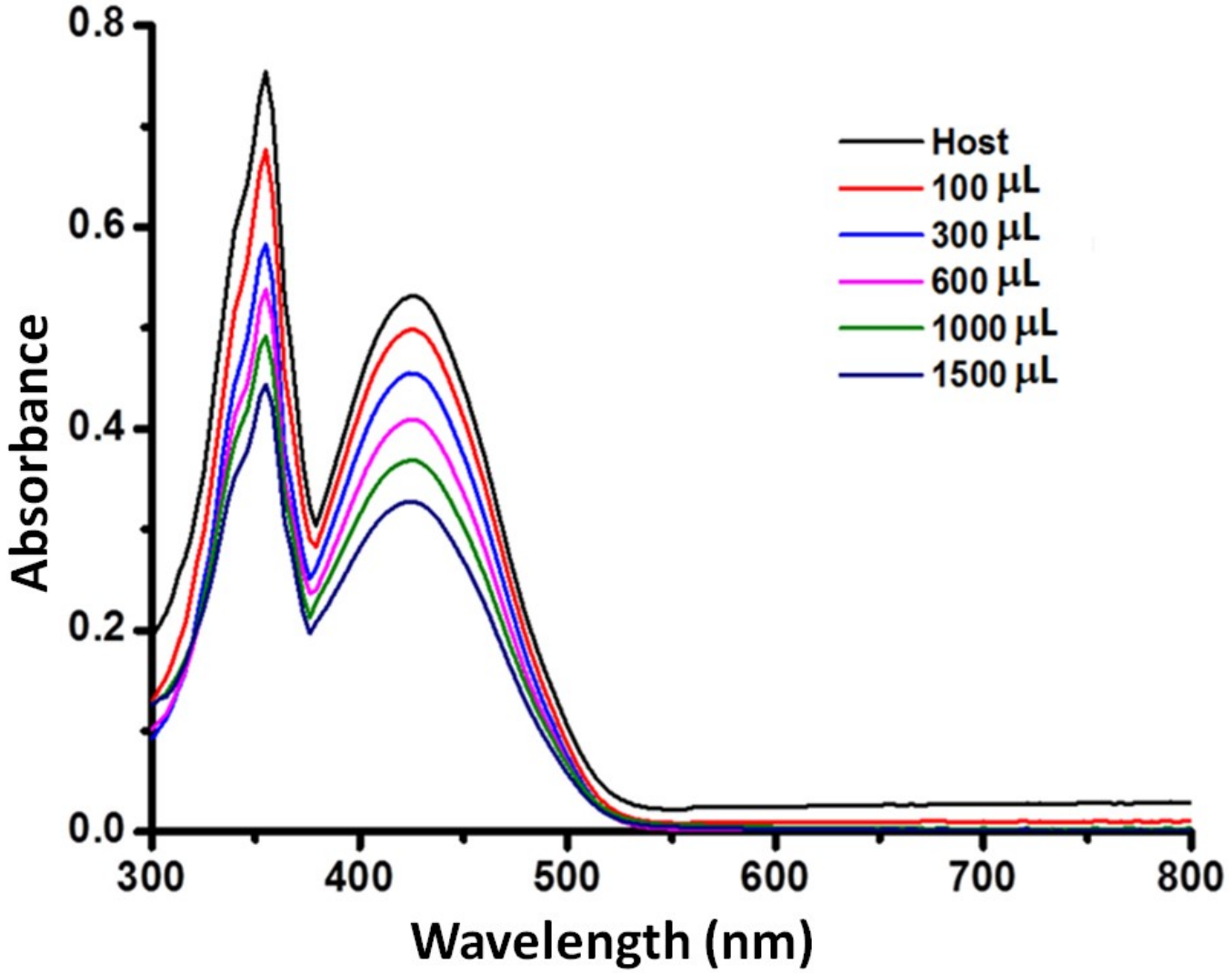


Fig. S13 Change in absorption spectrum of **5** (2.5 x 10^{-5} M) upon addition of $TBAPF_6$ (5 x 10^{-2} M) in $CHCl_3$ at 298 K

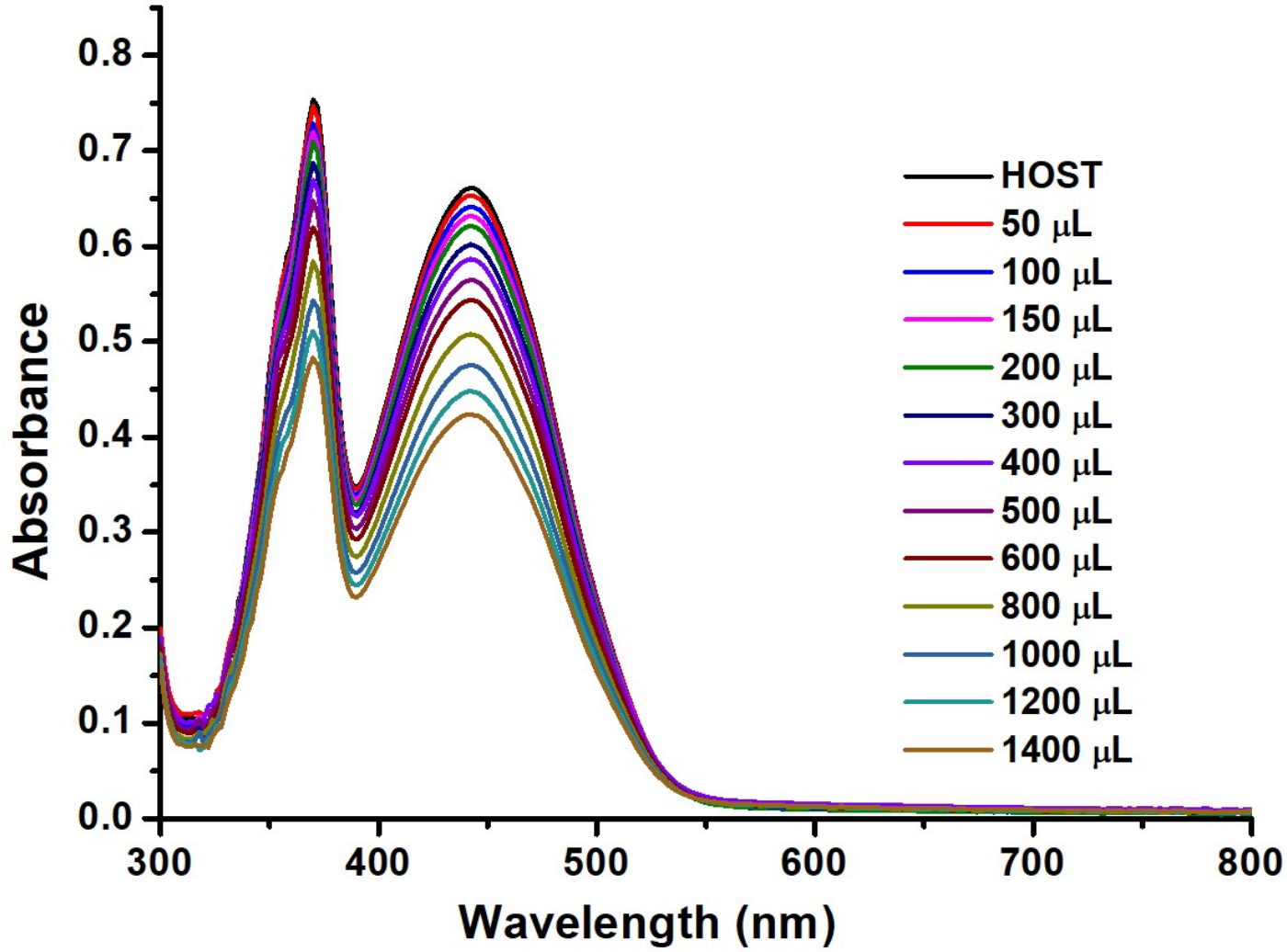


Fig. S13A Change in absorption spectrum of **5** (2.5 x 10^{-5} M) upon addition of $TBAH_2PO_4$ (5 x 10^{-2} M) in $CHCl_3$ at 298 K

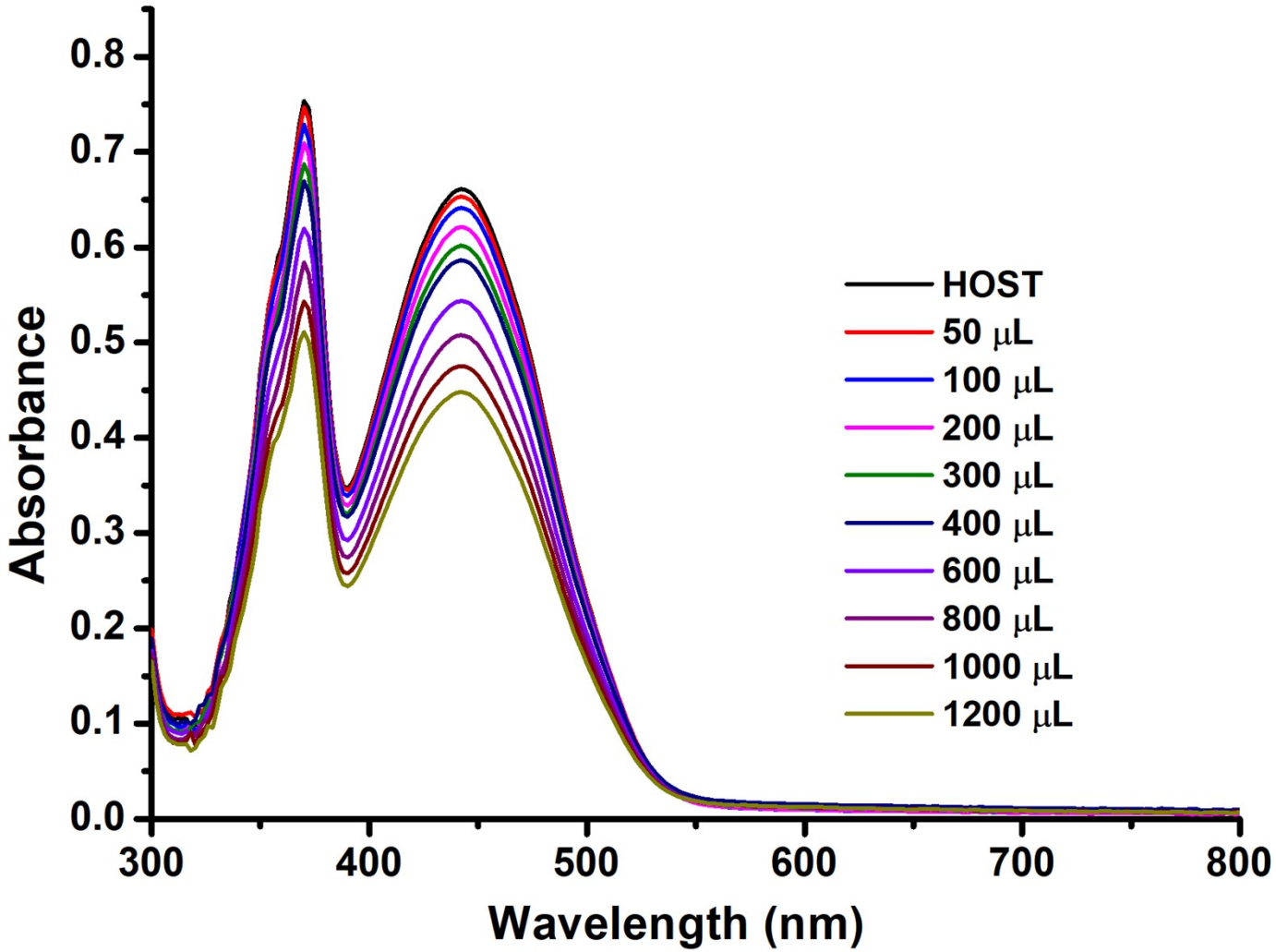


Fig. S13B Change in absorption spectrum of **5** (2.5 x 10^{-5} M) upon addition of $(TBA)_3HP_2O_7$ (5 x 10^{-2} M) in $CHCl_3$ at 298 K

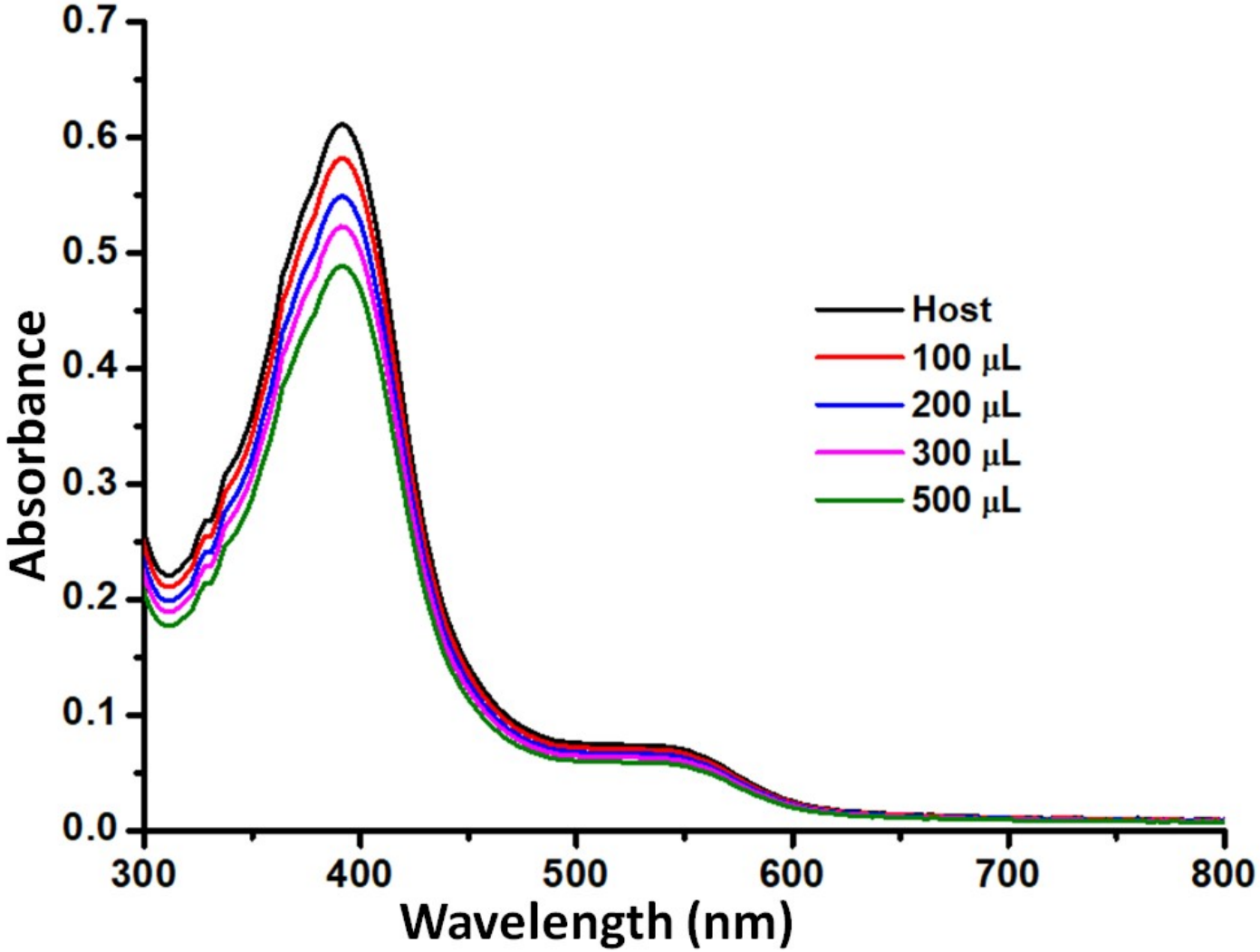


Fig. S14 Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of TBACl (1×10^{-3} M) in $CHCl_3$ at 298 K

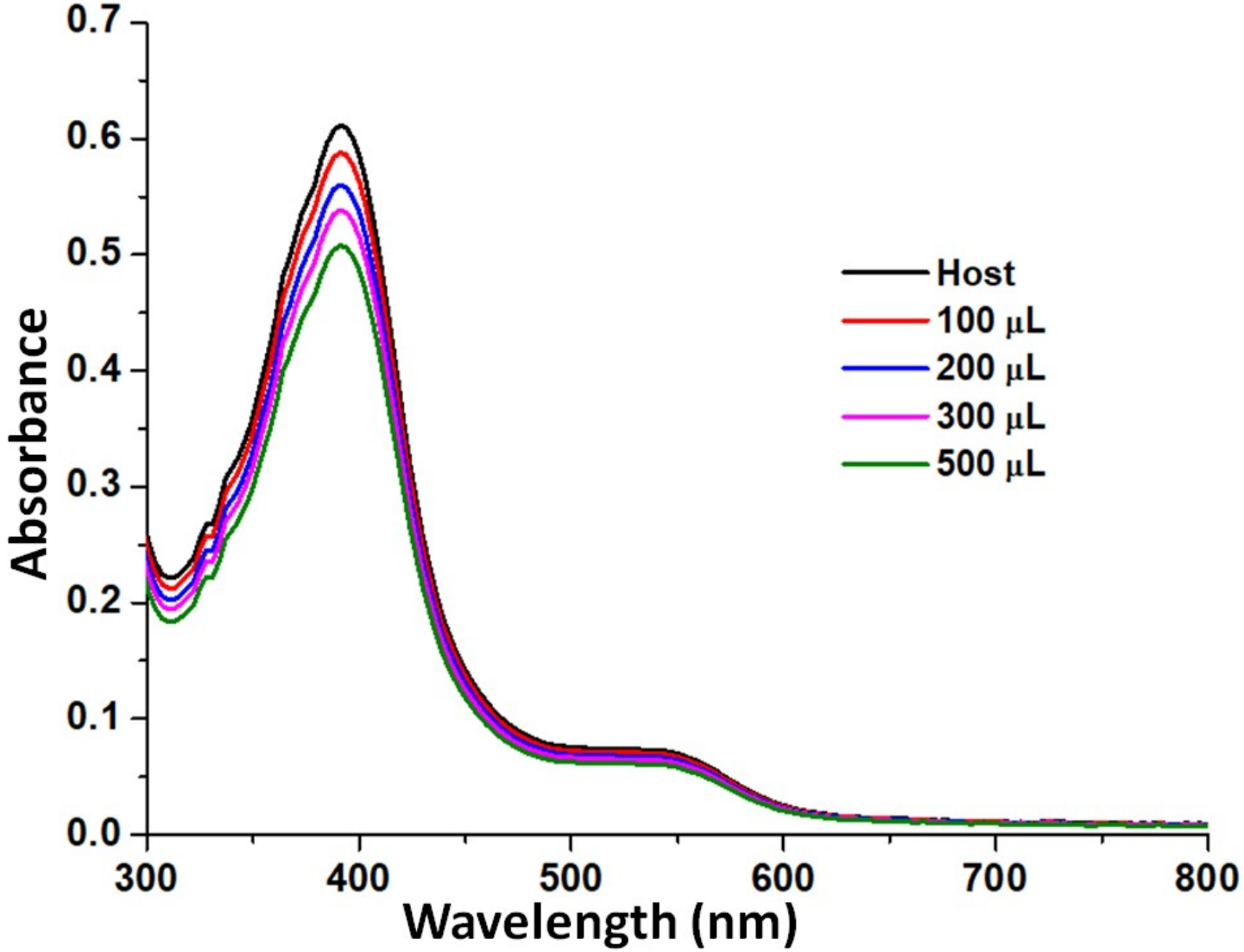


Fig. S15 Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of TBABr (1×10^{-3} M) in $CHCl_3$ at 298 K

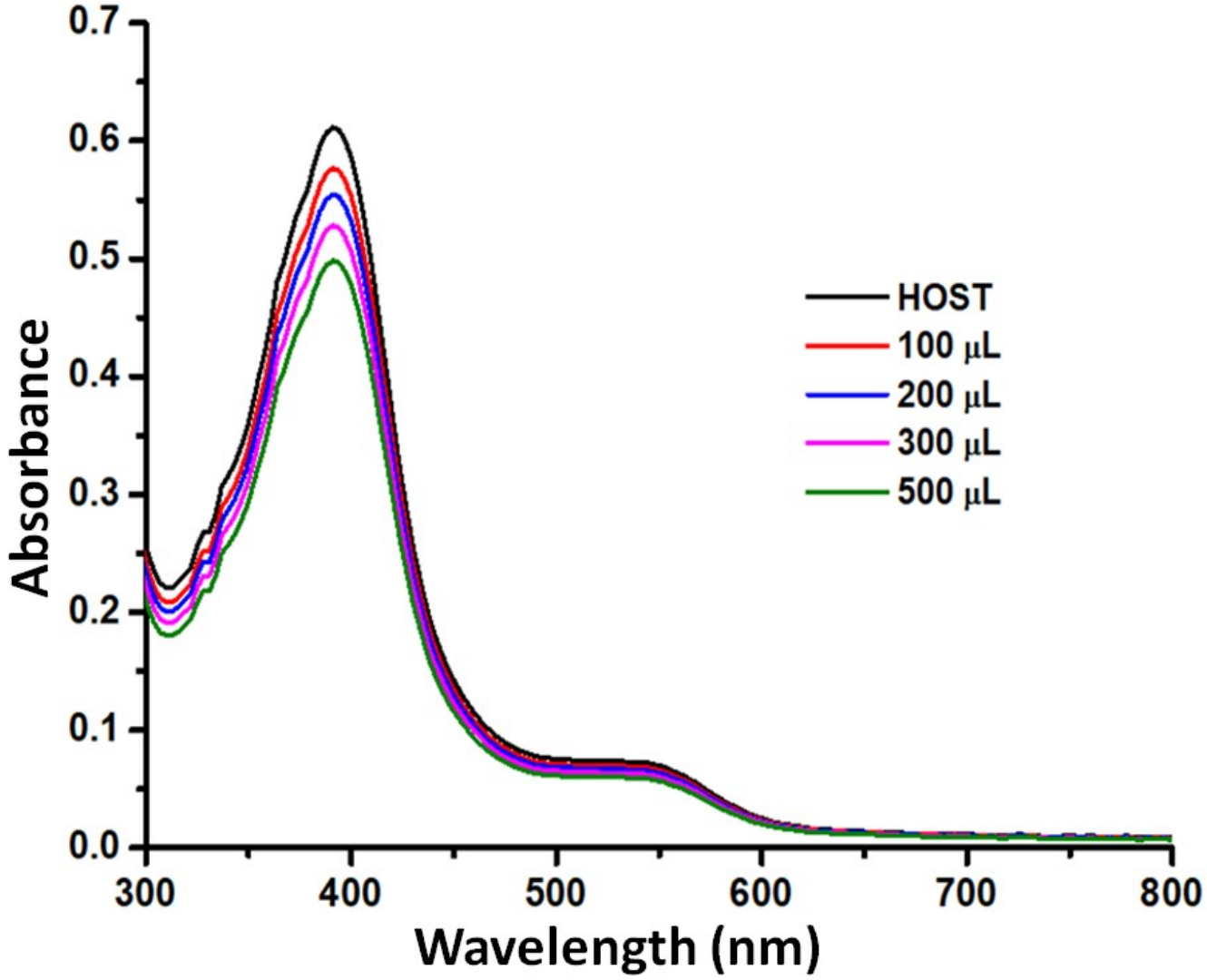


Fig. S16 Change in absorption spectrum of **6** (4.33 x 10^{-5} M) upon addition of TBAI (1 x 10^{-3} M) in $CHCl_3$ at 298 K

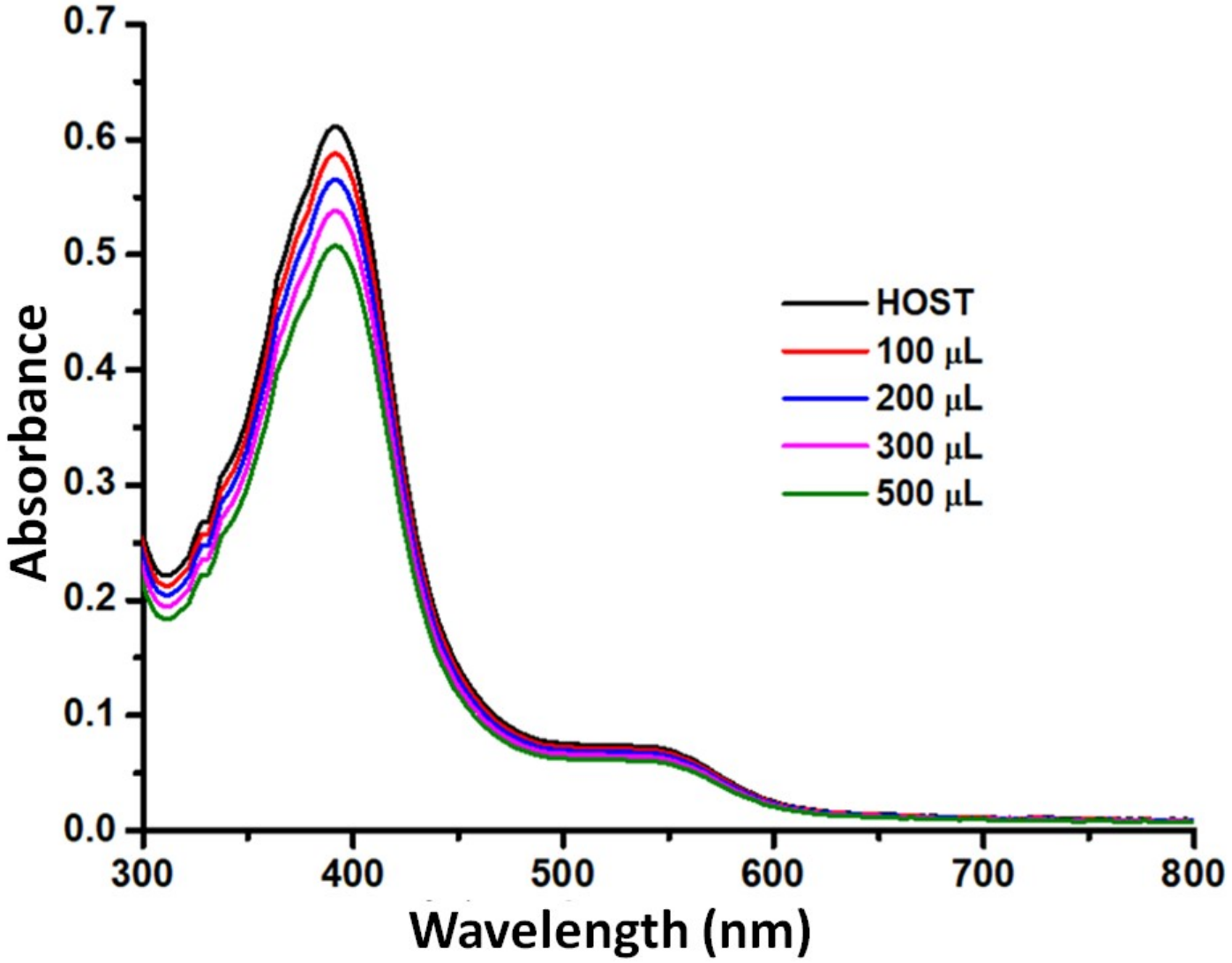


Fig. S17 Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of $TBAClO_4$ (1×10^{-3} M) in $CHCl_3$ at 298 K

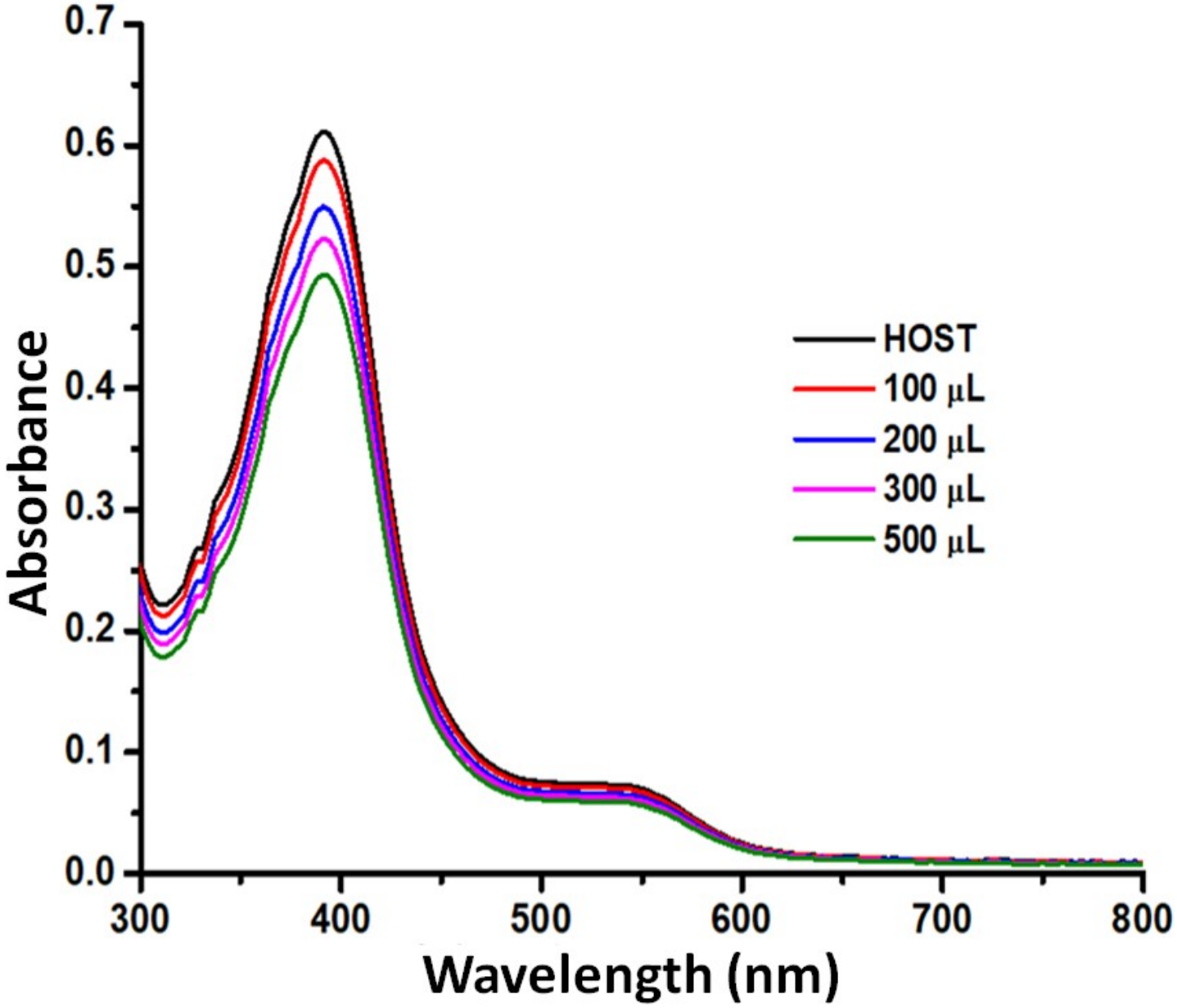


Fig. S18 Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of $TBAPF_6$ (1×10^{-3} M) in $CHCl_3$ at 298 K

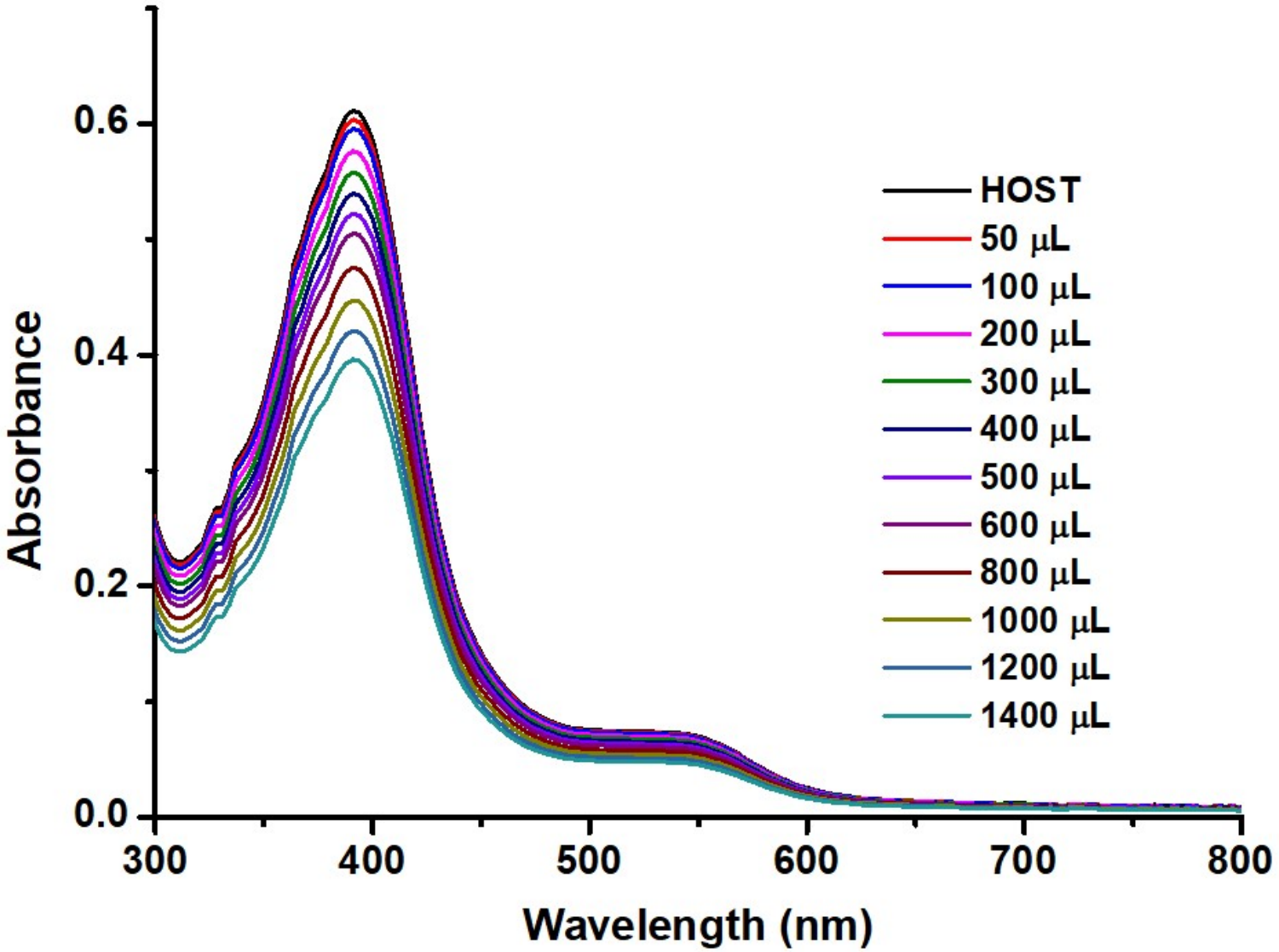


Fig. S18A Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of $TBAH_2PO_4$ (1×10^{-3} M) in $CHCl_3$ at 298 K

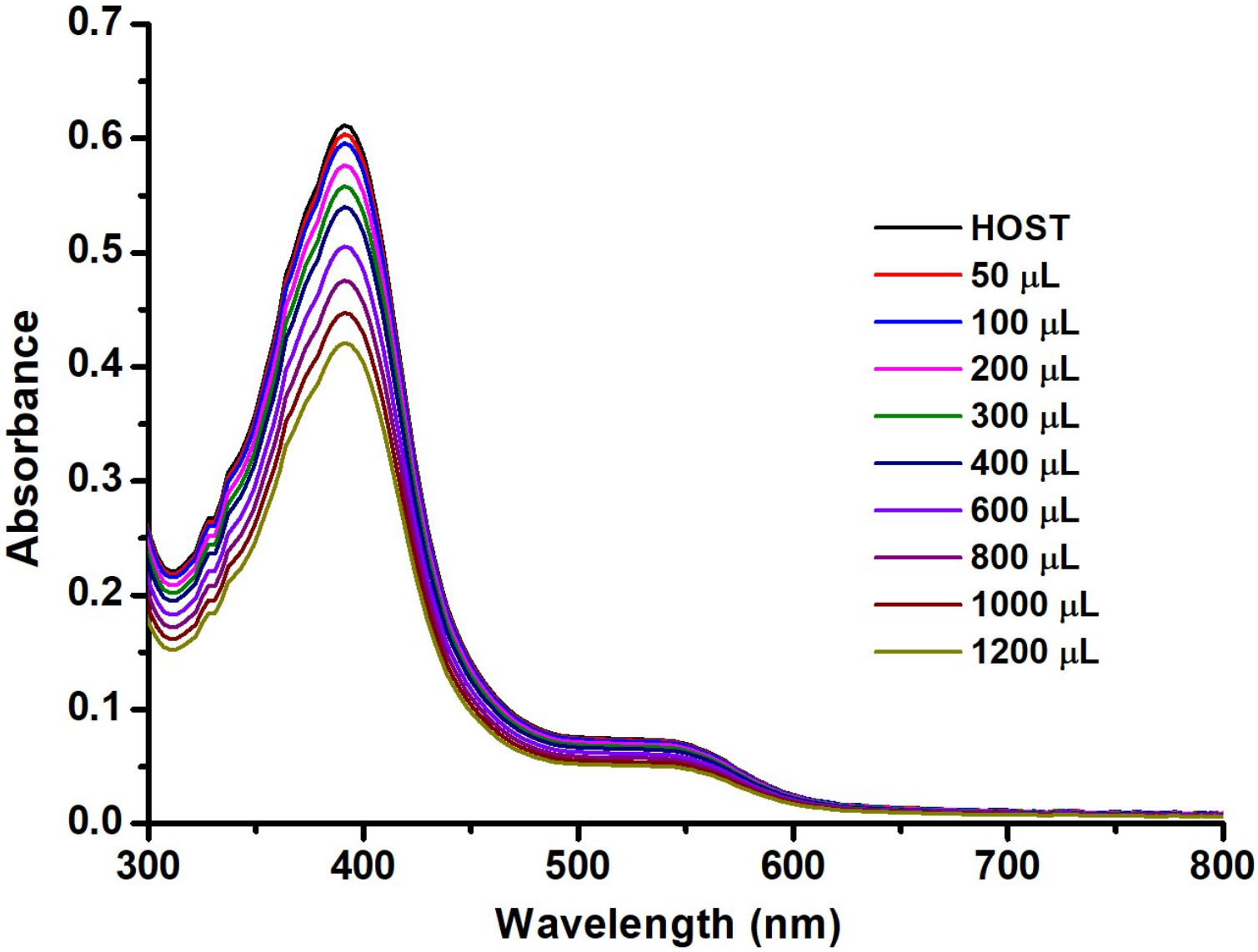


Fig. S18B Change in absorption spectrum of **6** (4.33×10^{-5} M) upon addition of $(TBA)_3HP_2O_7$ (1×10^{-3} M) in $CHCl_3$ at 298 K

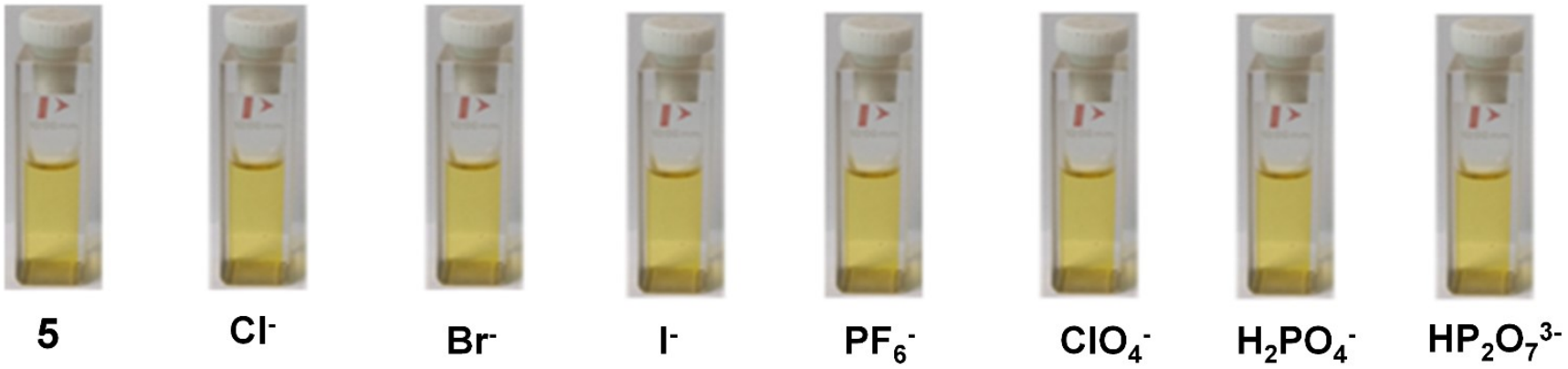


Fig. S19 Color Change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **5** in $CHCl_3$ at 298 K

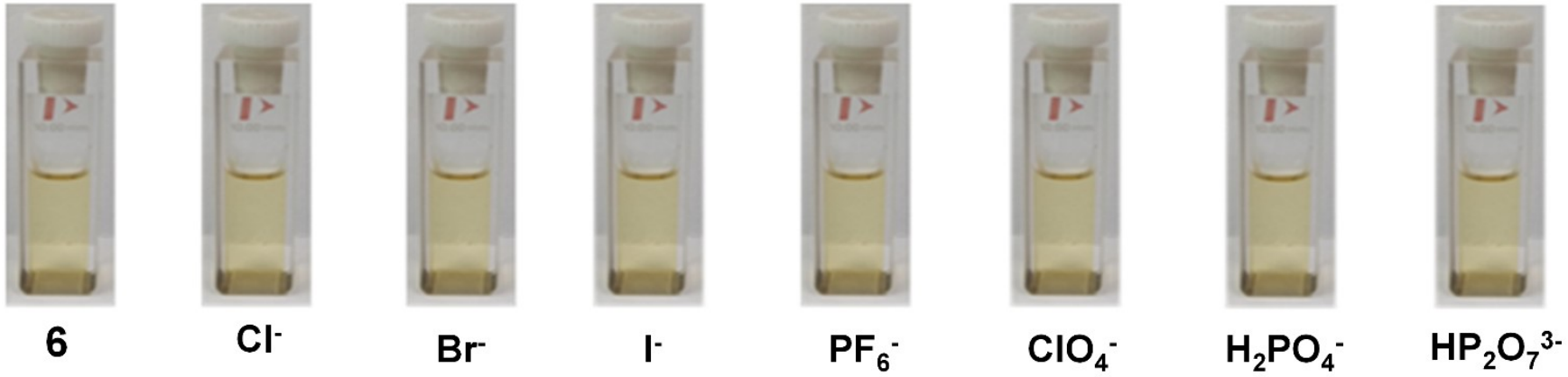


Fig. S20 Color Change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **6** in $CHCl_3$ at 298 K

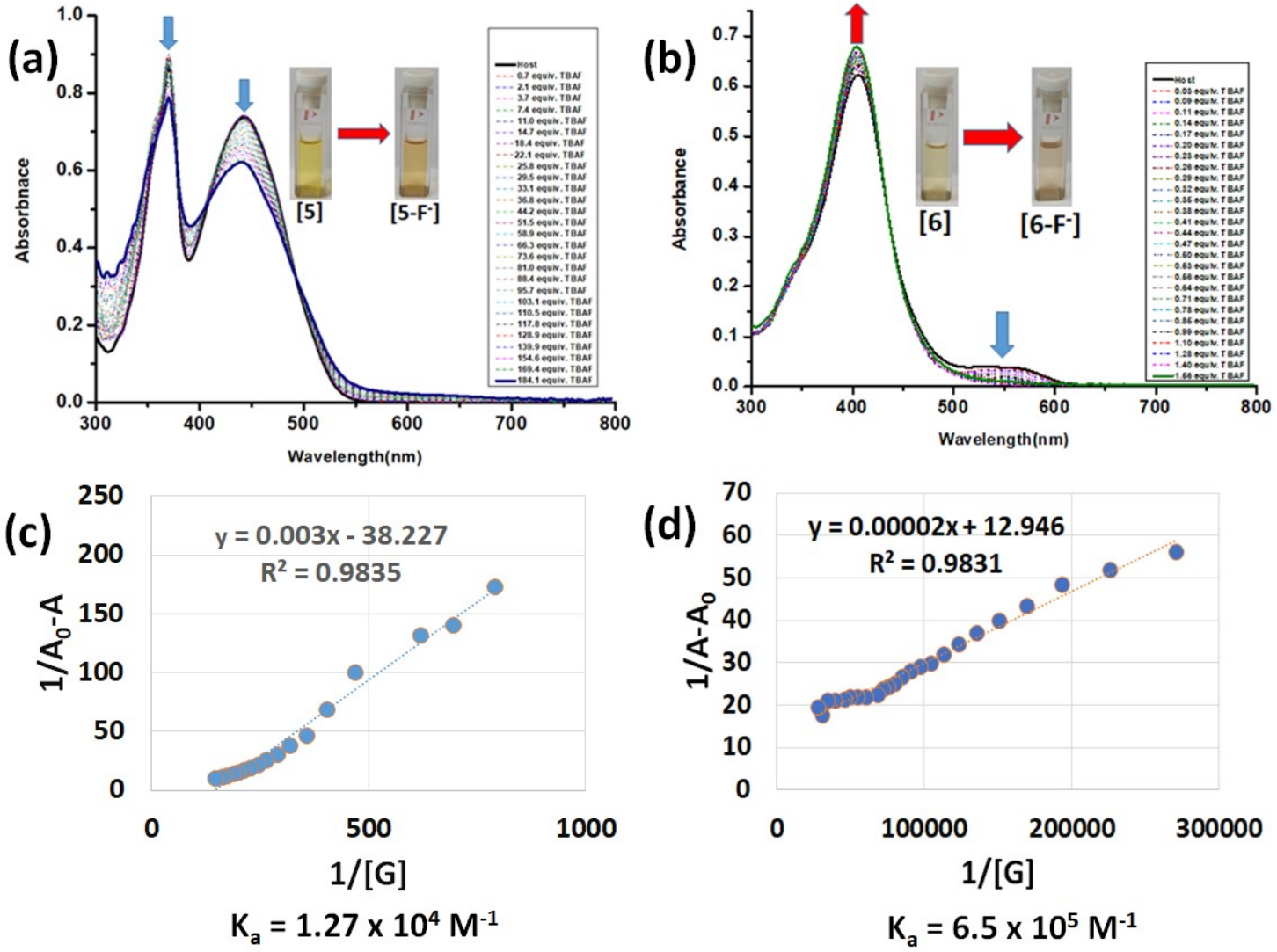


Fig. S21 (a) Change in absorption spectra of **5** (2.5 x 10^{-5} M) upon titration of TBAF (0.05 M) and (b) **6** (4.33 x 10^{-5} M) upon titration of TBAF (0.001 M) in $CHCl_3$ at 298 K. (c) and (d) shows B-H plots of **5** and **6** respectively from UV-vis titration experiment to determine binding 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).

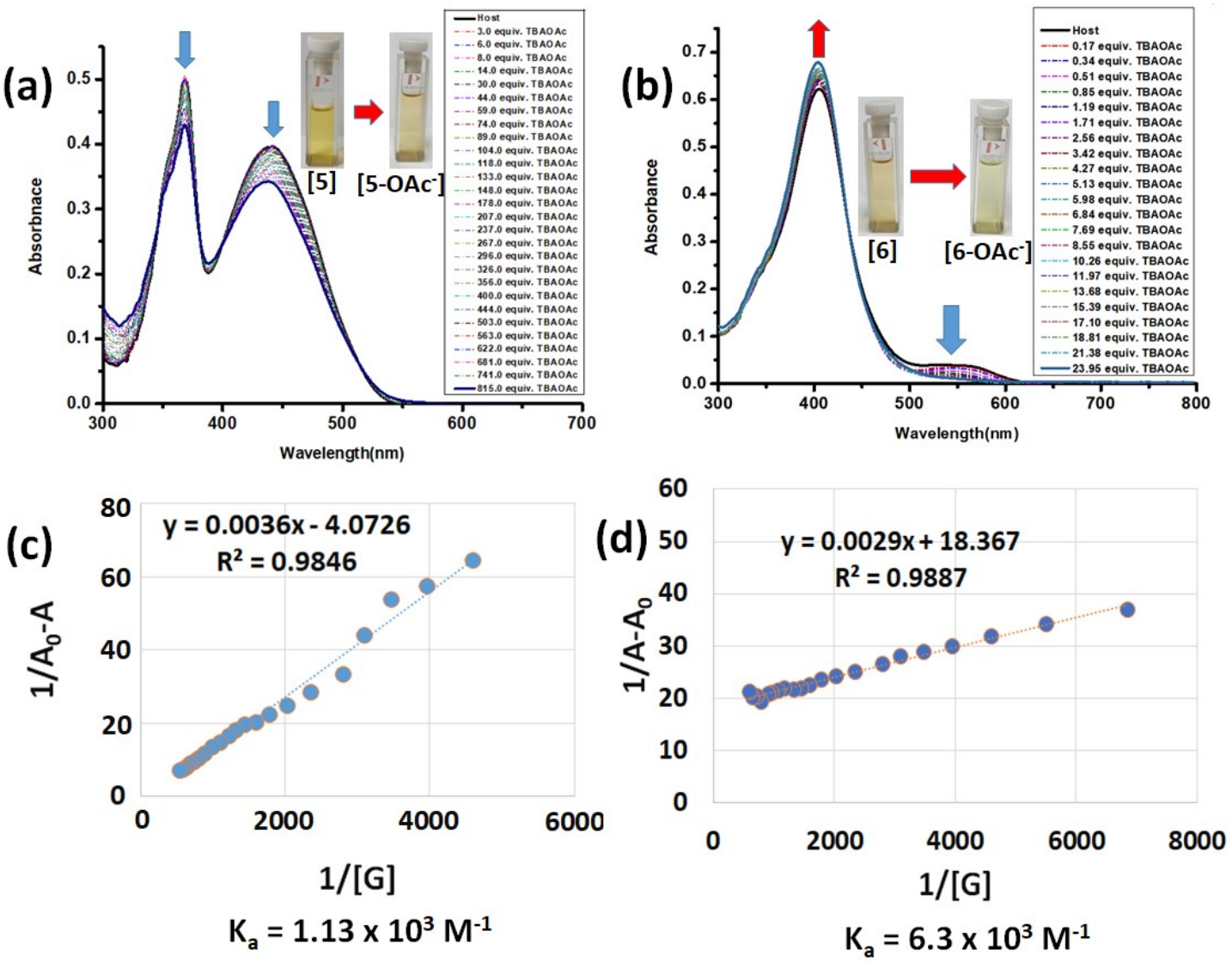


Fig. S22 (a) Change in absorption spectra of **5** (2.5 x 10^{-5} M) upon titration of TBAOAc (0.1 M) and (b) **6** (4.33 x 10^{-5} M) upon titration of TBAOAc (0.01 M) in $CHCl_3$ at 298 K. (c) and (d) shows B-H plots of **5** and **6** respectively from UV-vis titration experiment to determine binding 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).

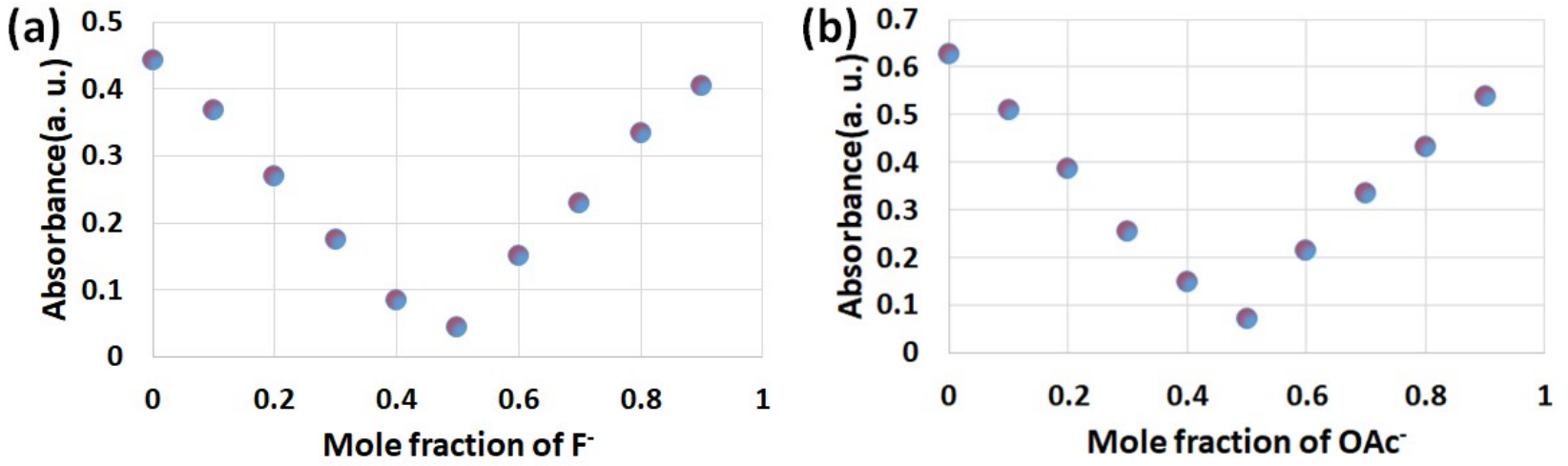


Fig. S23 Job Plot obtained for **5** (2.5 x 10^{-5} M in DCM) on variation of its absorbance vs mole fraction of (a) F^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 442 nm; (b) OAc^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 442 nm.

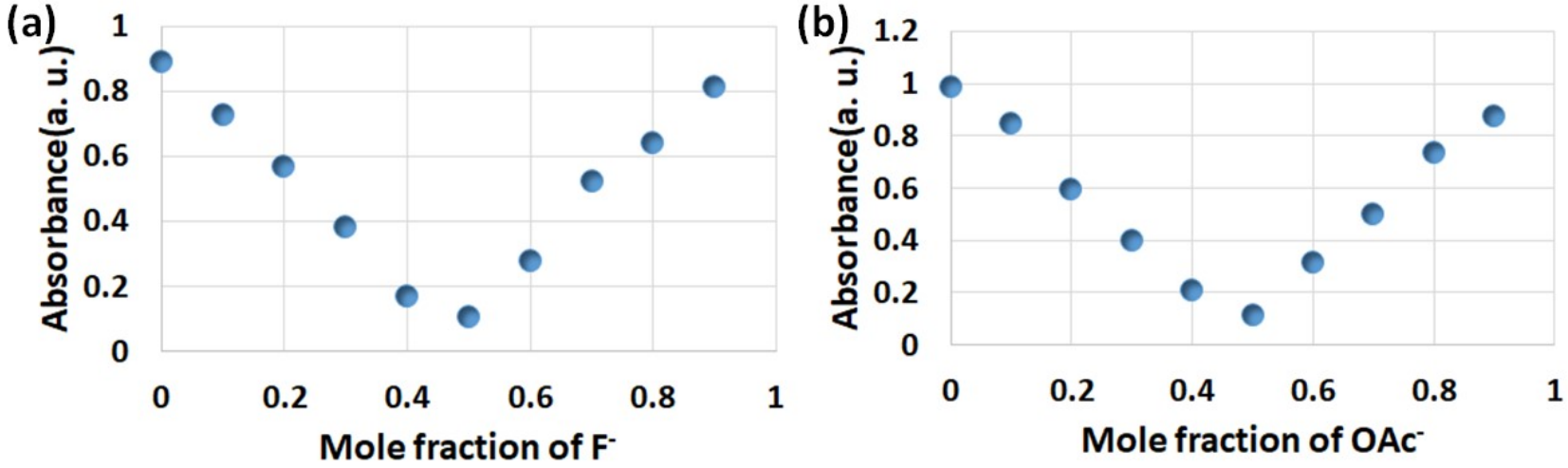


Fig. S24 Job Plot obtained for **6** (4.33 x 10^{-5} M in DCM) on variation of its absorbance vs mole fraction of (a) F^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 405 nm; (b) OAc^- (1.0 x 10^{-5} M in $CHCl_3$) at λ_{max} = 405 nm.

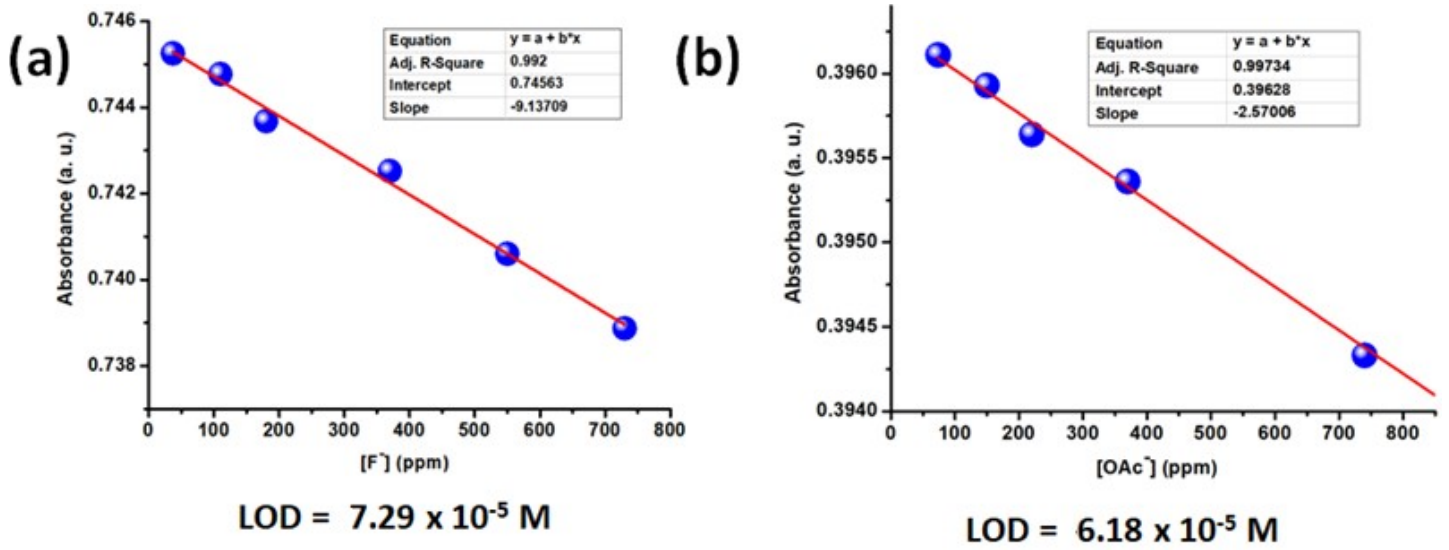


Fig. S25 Calibration curve for the determination of the limit of detection of **5** for (a) F^- and (b) OAc^- ions from absorption titration studies

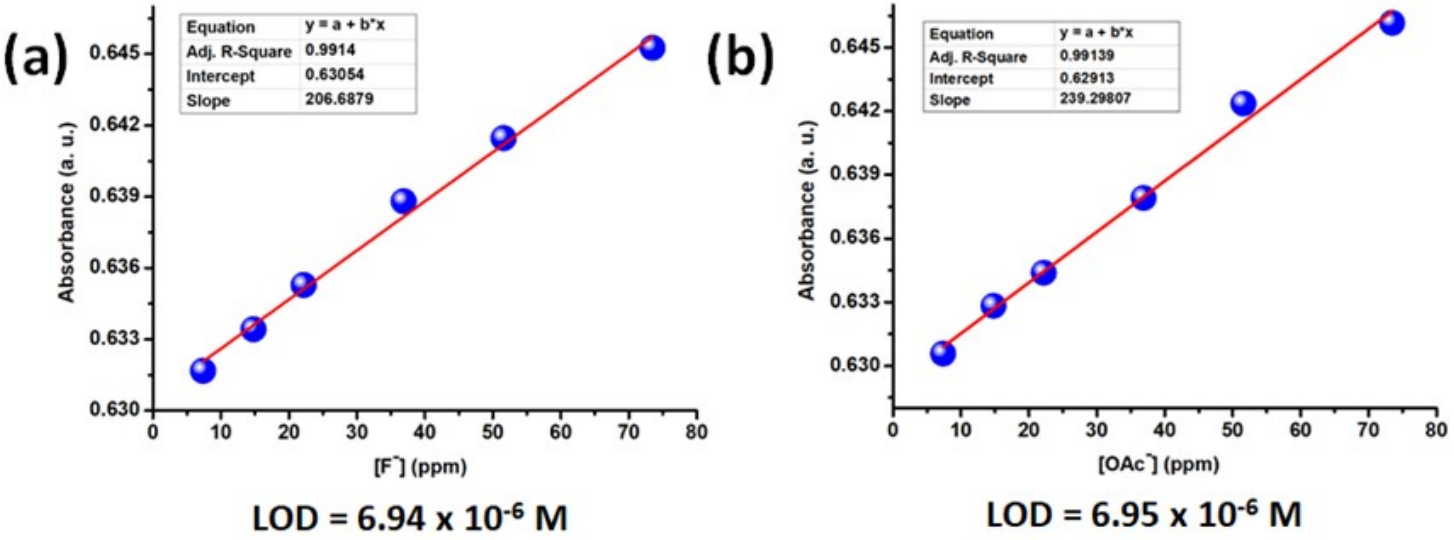


Fig. S26 Calibration curve for the determination of the limit of detection of **6** for (a) F^- and (b) OAc^- ions from absorption titration studies

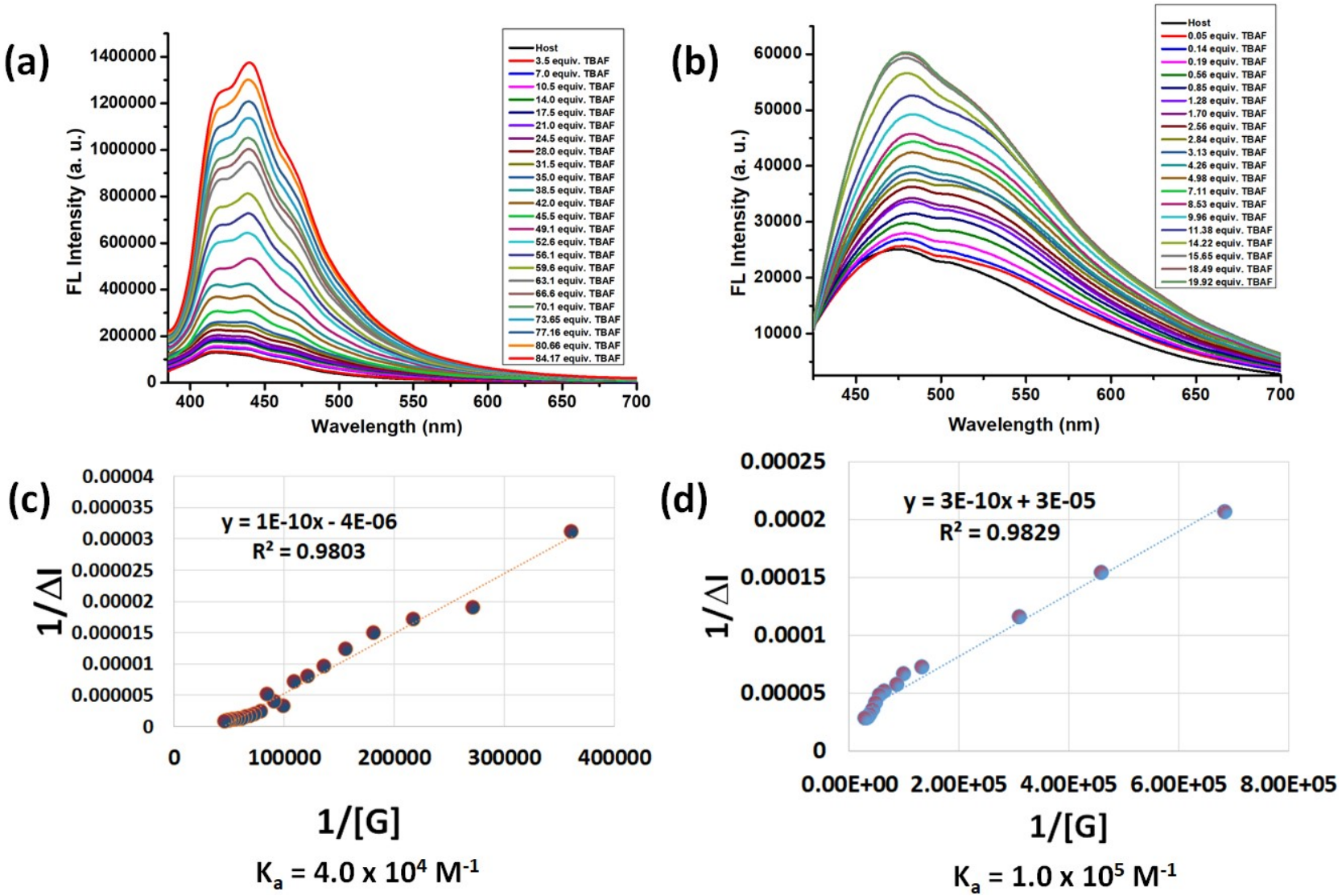


Fig. S27 (a) Change in emission spectra of **5** (2.5 x 10^{-5} M) upon titration of TBAF (0.05 M) and (b) **6** (4.33 x 10^{-5} M) upon titration of TBAF (0.001 M) in $CHCl_3$ at 298 K; (c) and (d) show B-H plots of **5** and **6** respectively from emission titration experiment to determine binding 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).

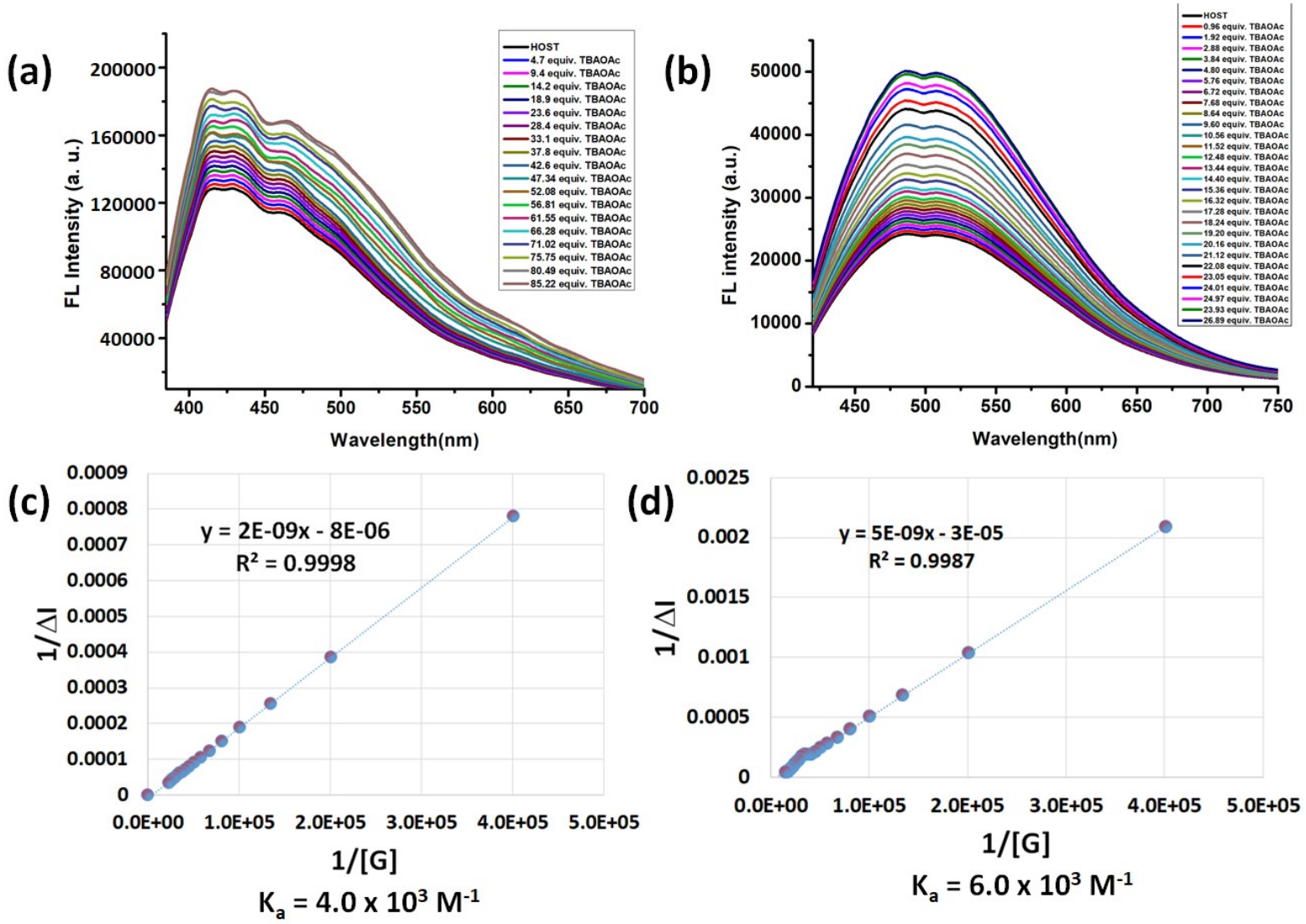


Fig. S28 (a) Change in emission spectra of **5** (2.5 x 10^{-5} M) upon titration of TBAOAc (0.05 M) and (b) **6** (4.33 x 10^{-5} M) upon titration of TBAOAc (0.001 M) in $CHCl_3$ at 298 K; (c) and (d) show B-H plots of **5** and **6** respectively from emission titration experiment to determine binding 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).

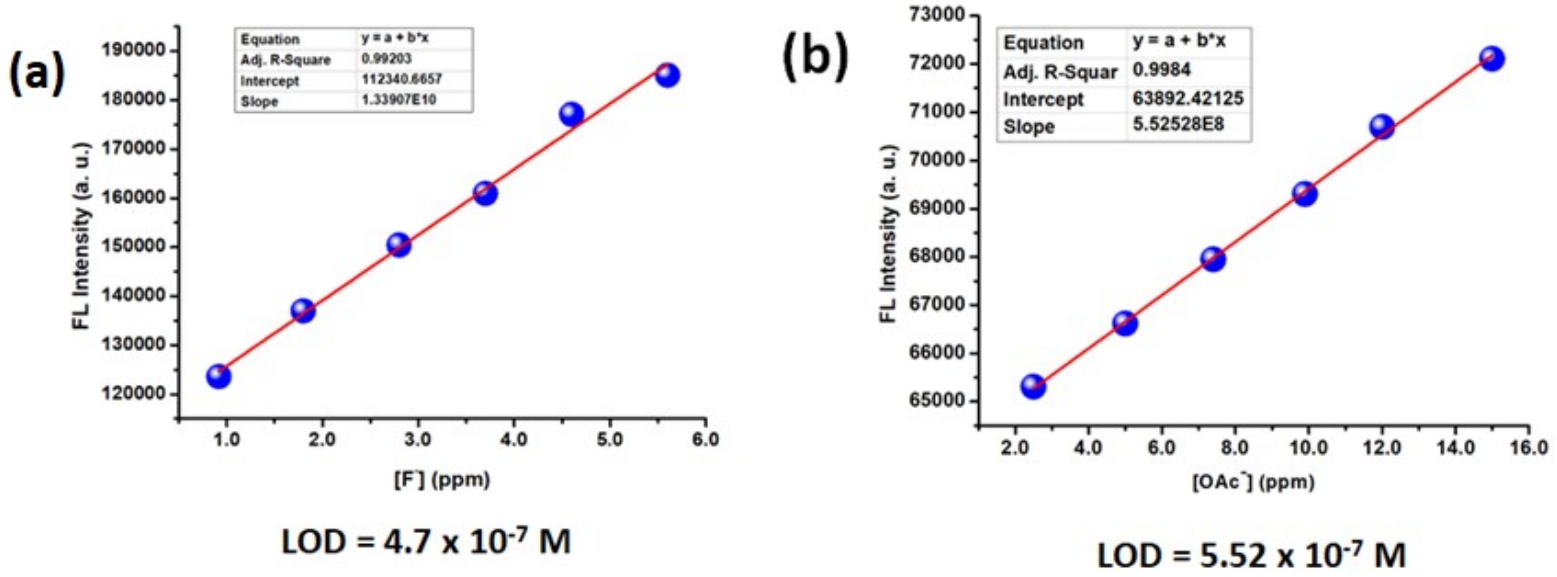


Fig.S29 Calibration curve for the determination of the limit of detection of **5** for (a) F^- and (b) OAc^- ions from emission titration studies

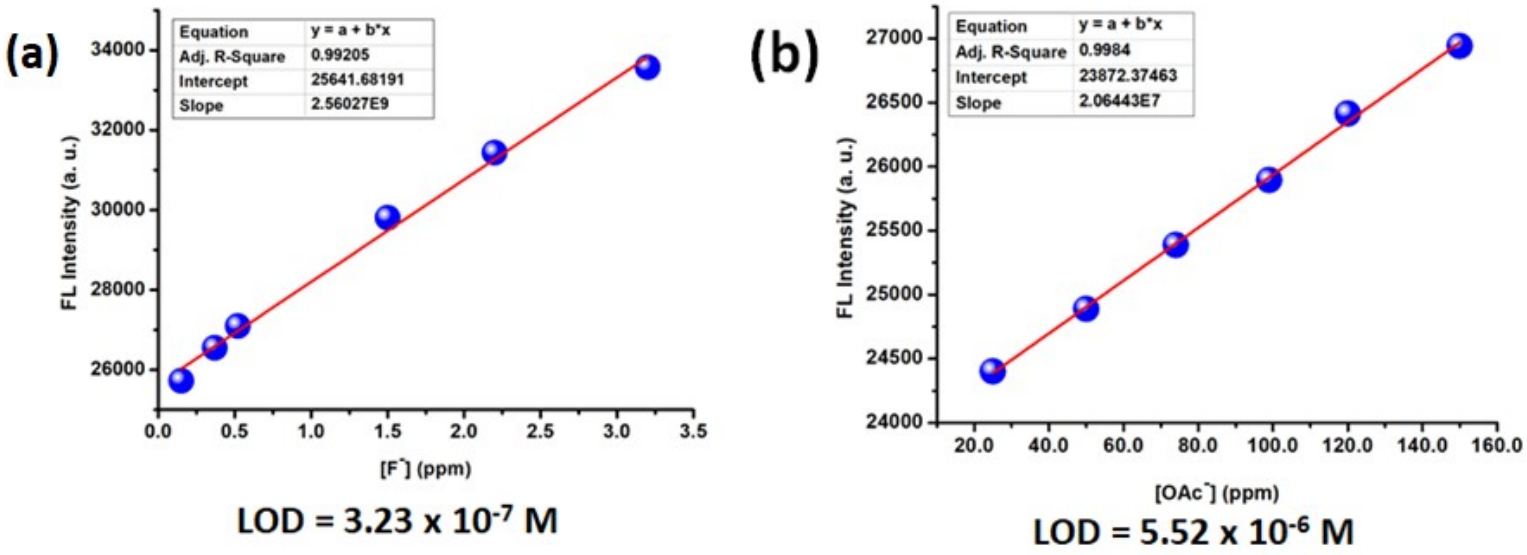


Fig. S30 Calibration curve for the determination of the limit of detection of **6** for (a) F^- and (b) OAc^- ions from emission titration studies

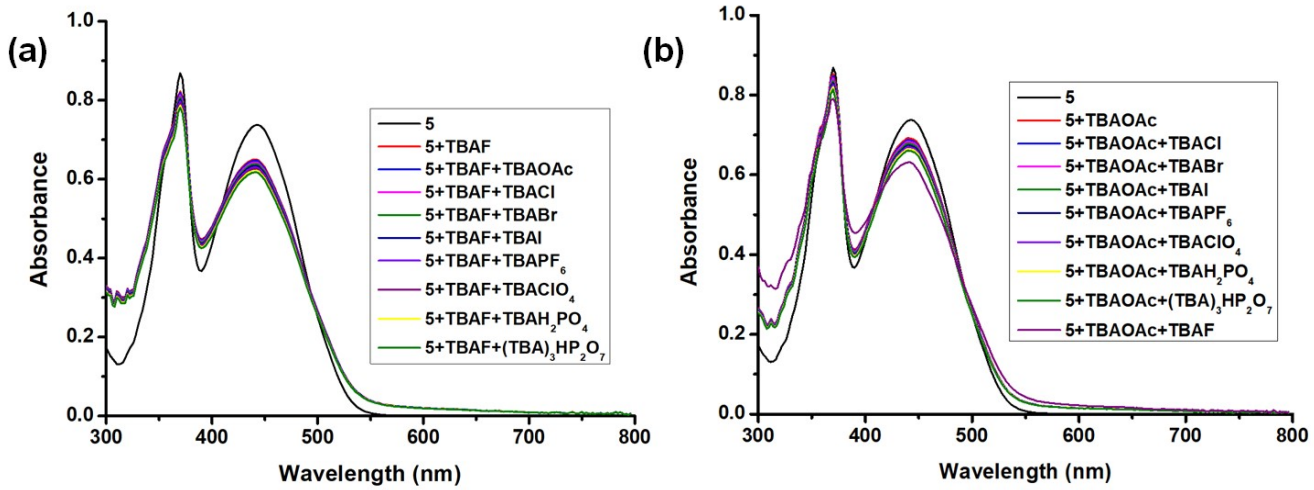


Fig. S31 Competitive Assay experiments of (a) [**5-F**]$^-$ in the presence of other anions and (b) [**5-OAc**]$^-$ in the presence of other anions (Absorbance response upon addition of 100 equivalents of F^-, Cl^-, Br^-, I^-, ClO_4^-, OAc^-, PF_6^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

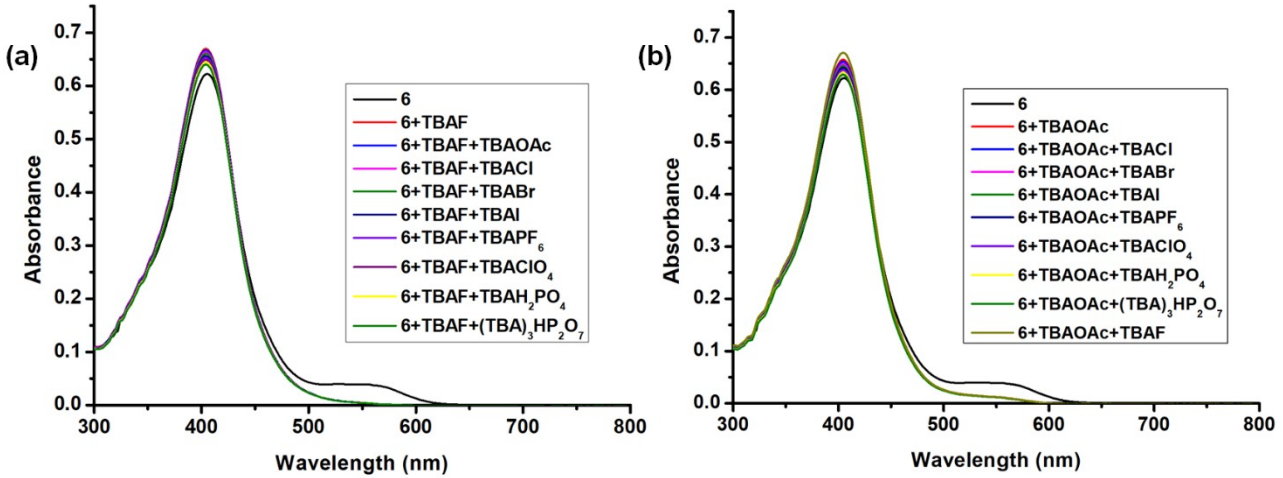


Fig. S32 Competitive Assay experiments of (a) [**6-F**]$^-$ in the presence of other anions and (b) [**6-OAc**]$^-$ in the presence of other anions (Absorbance response upon addition of 10 equivalents of F^-, Cl^-, Br^-, I^-, ClO_4^-, OAc^- PF_6^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

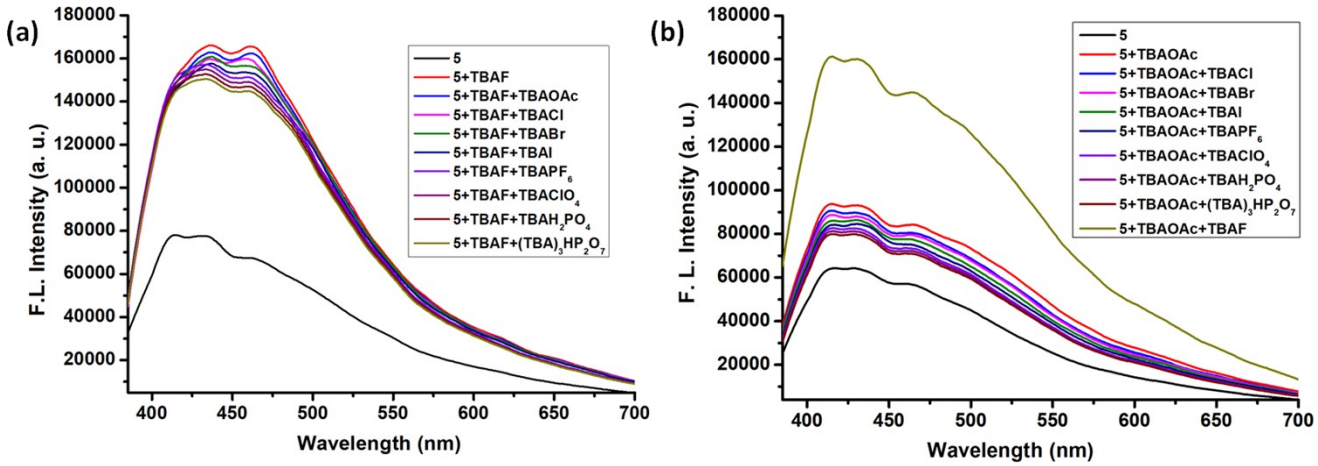


Fig. S33 Competitive Emission Assay experiments of (a) [**5-F**]$^-$ in the presence of other anions and (b) [**5-OAc**]$^-$ in the presence of other anions (Emission response upon addition of 70 equivalents of F^-, Cl^-, Br^-, I^-, ClO_4^-, OAc^-, PF_6^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

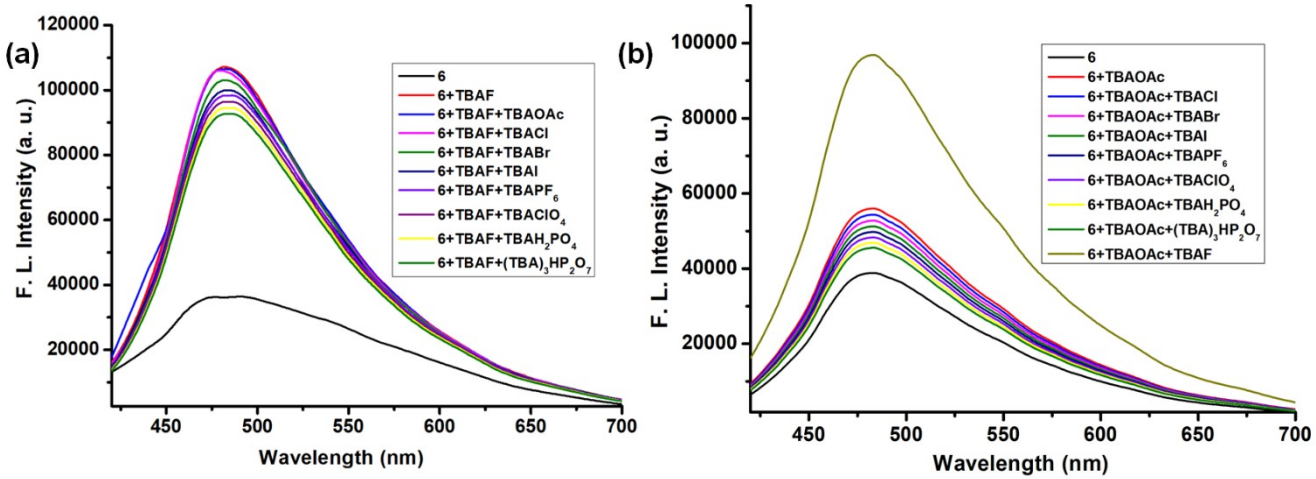


Fig. S34 Competitive Emission Assay experiments of (a) [**6-F**]$^-$ in the presence of other anions and (b) [**6-OAc**]$^-$ in the presence of other anions (Emission response upon addition of 20 equivalents of F^-, Cl^-, Br^-, I^-, ClO_4^-, OAc^- PF_6^-, $H_2PO_4^-$ and $HP_2O_7^{3-}$ in the form of their TBA salts).

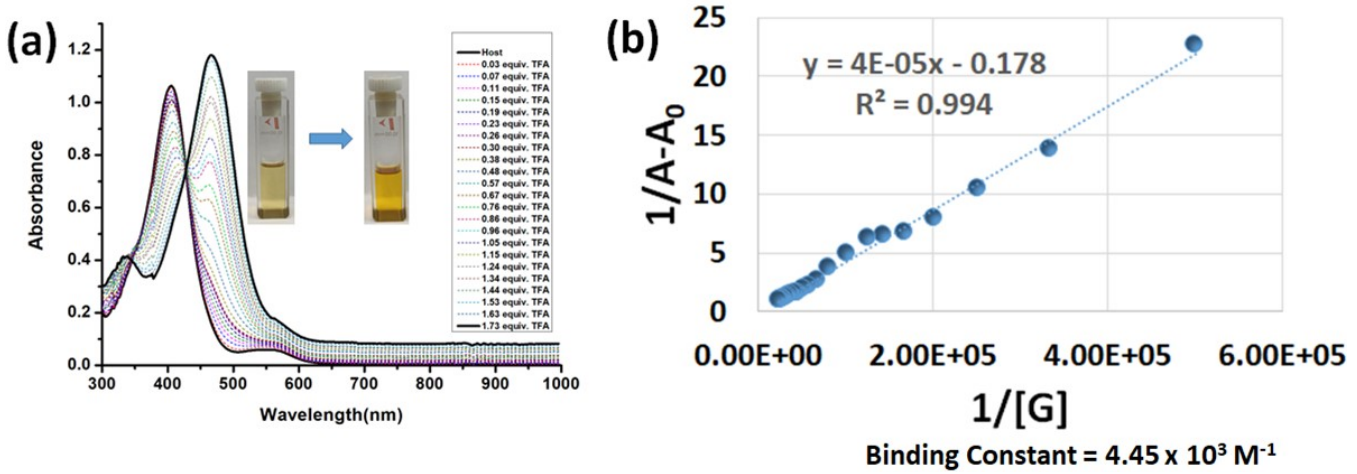


Fig. S35 (a) Change in absorption spectra of **6** (4.33 x 10^{-5} M) upon titration with CF_3COOH (0.001 M) in $CHCl_3$ at 298 K. (b) shows B-H plots of **6** from UV-vis titration experiment to determine binding constant for the formation of host-guest complex (Some data points in the figure deviated 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 >0.99).

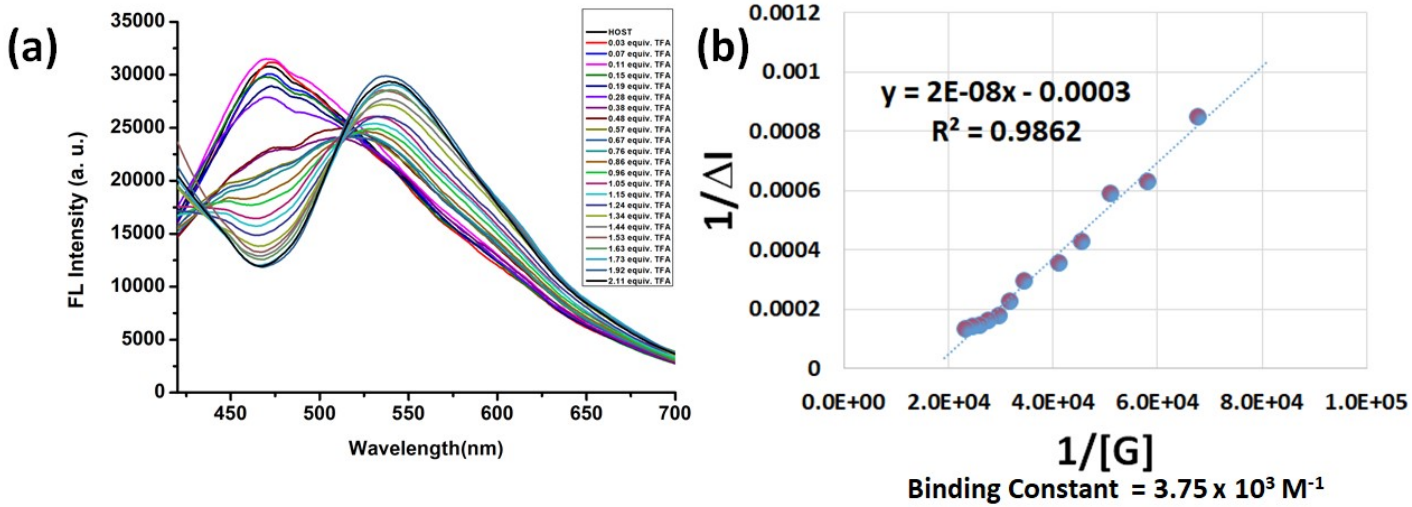


Fig. S36 (a) Change in Emission spectra of **6** (4.33 x 10^{-5} M) upon titration with CF_3COOH (0.001 M) in $CHCl_3$ at 298 K. (b) shows B-H plots of **6** from emission titration experiment to determine binding constant for the formation of host-guest complex (Some data points in the figure deviated 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).

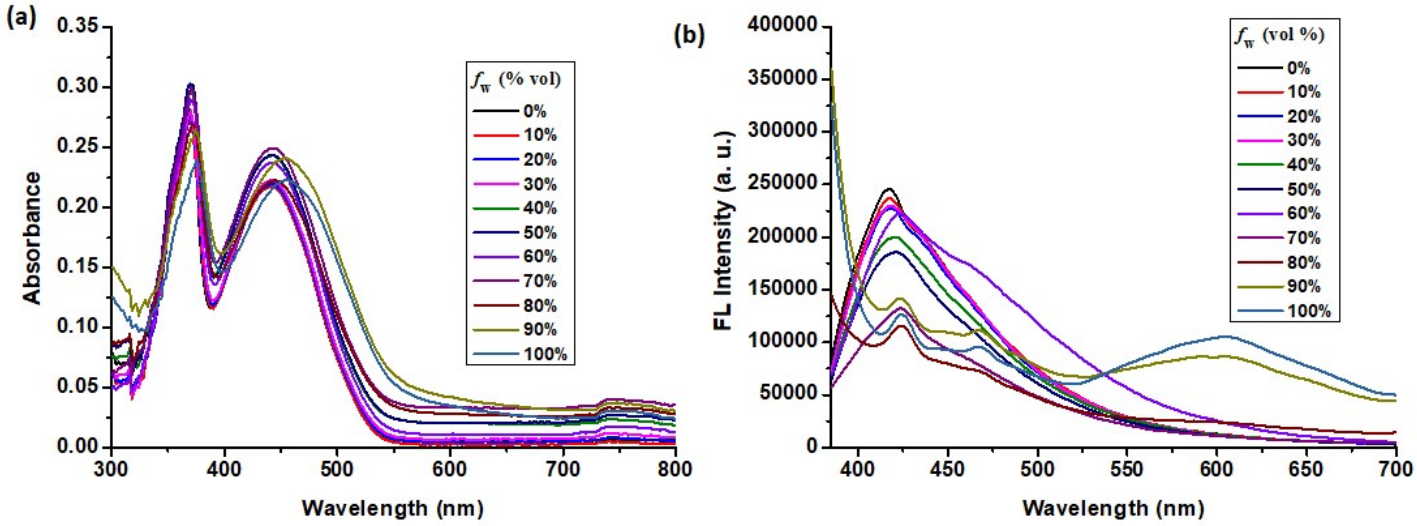


Fig. S37 (a) Change in absorption and (b) Emission spectra of **5** (1.73 × 10^{-5} M) (λ_{ex}=370 nm and λ_{em} = 425 nm) upon gradual increasing of water fraction in CH_3CN at 298 K.

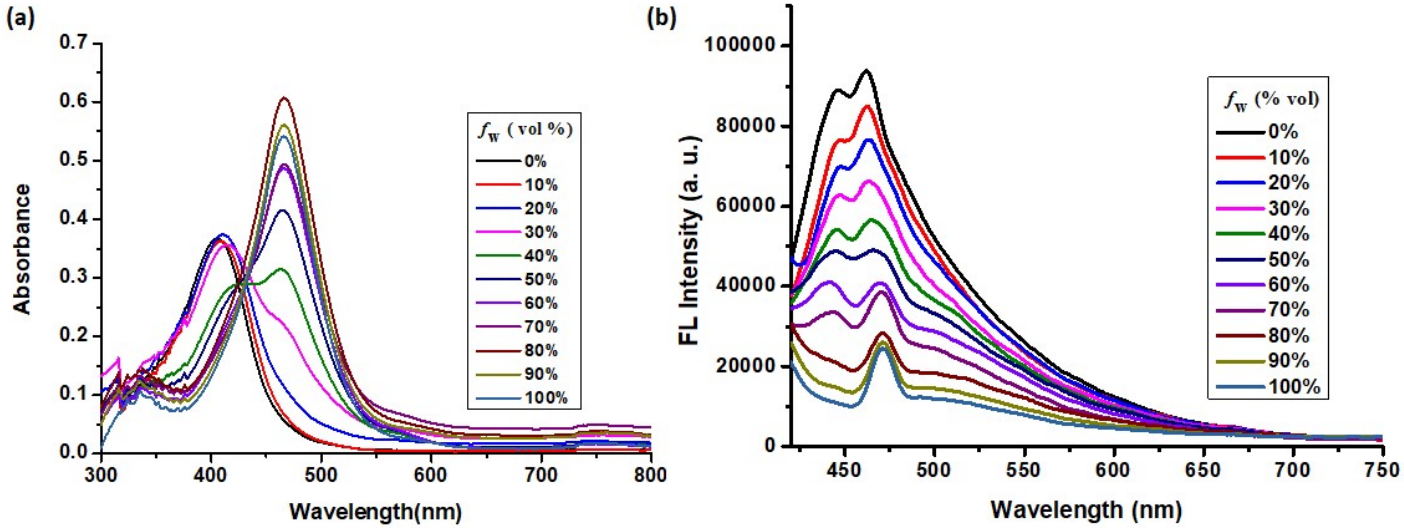


Fig. S38 (a) Change in absorption and (b) Emission spectra of **6** (1.73 × 10^{-5} M) (λ_{ex}=370 nm and λ_{em} = 425 nm) upon gradual increasing of water fraction in CH_3CN at 298 K.

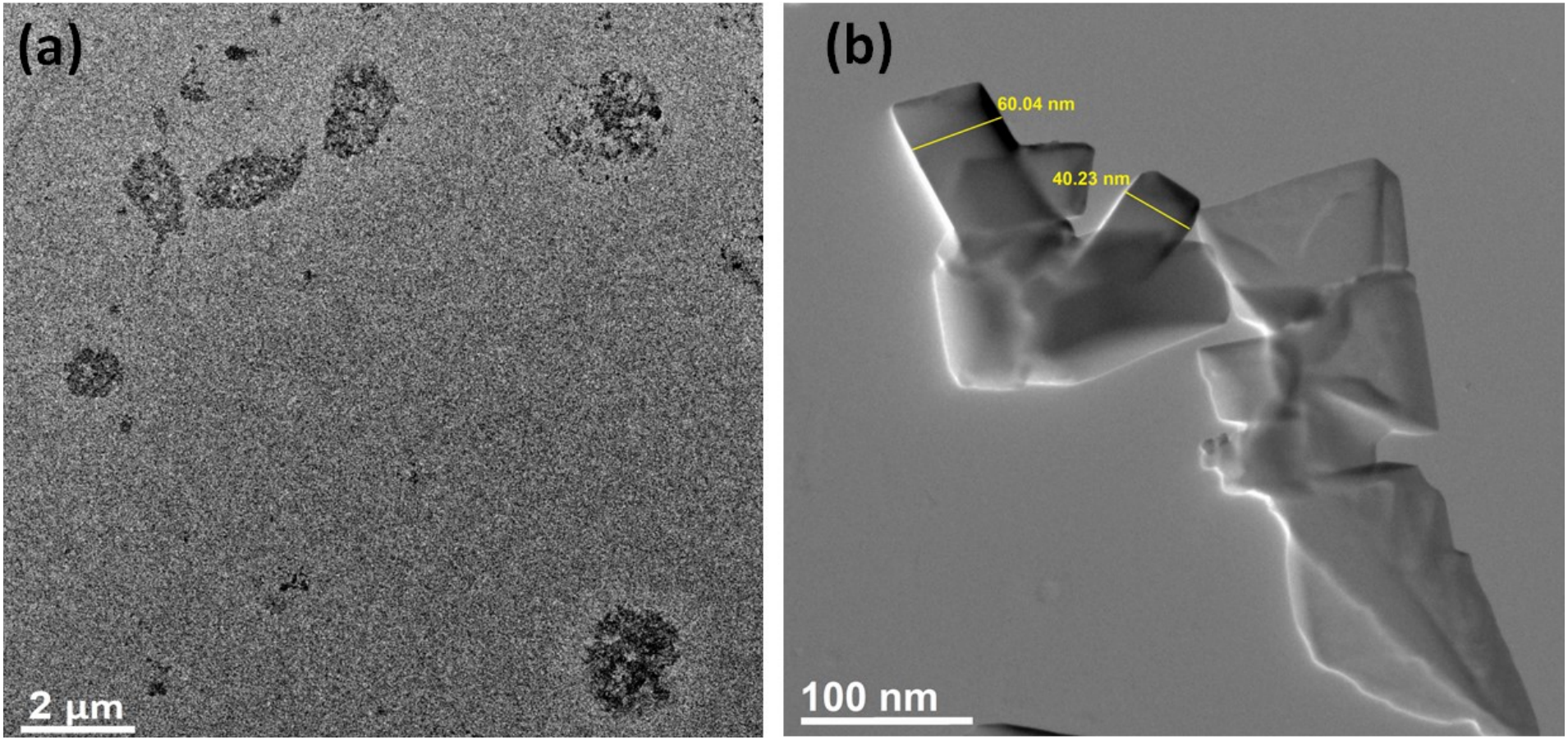


Fig. S39 UHR-FEG-TEM figure of **5** (a) at 0% water and (b) 100% water fraction at 298 K.

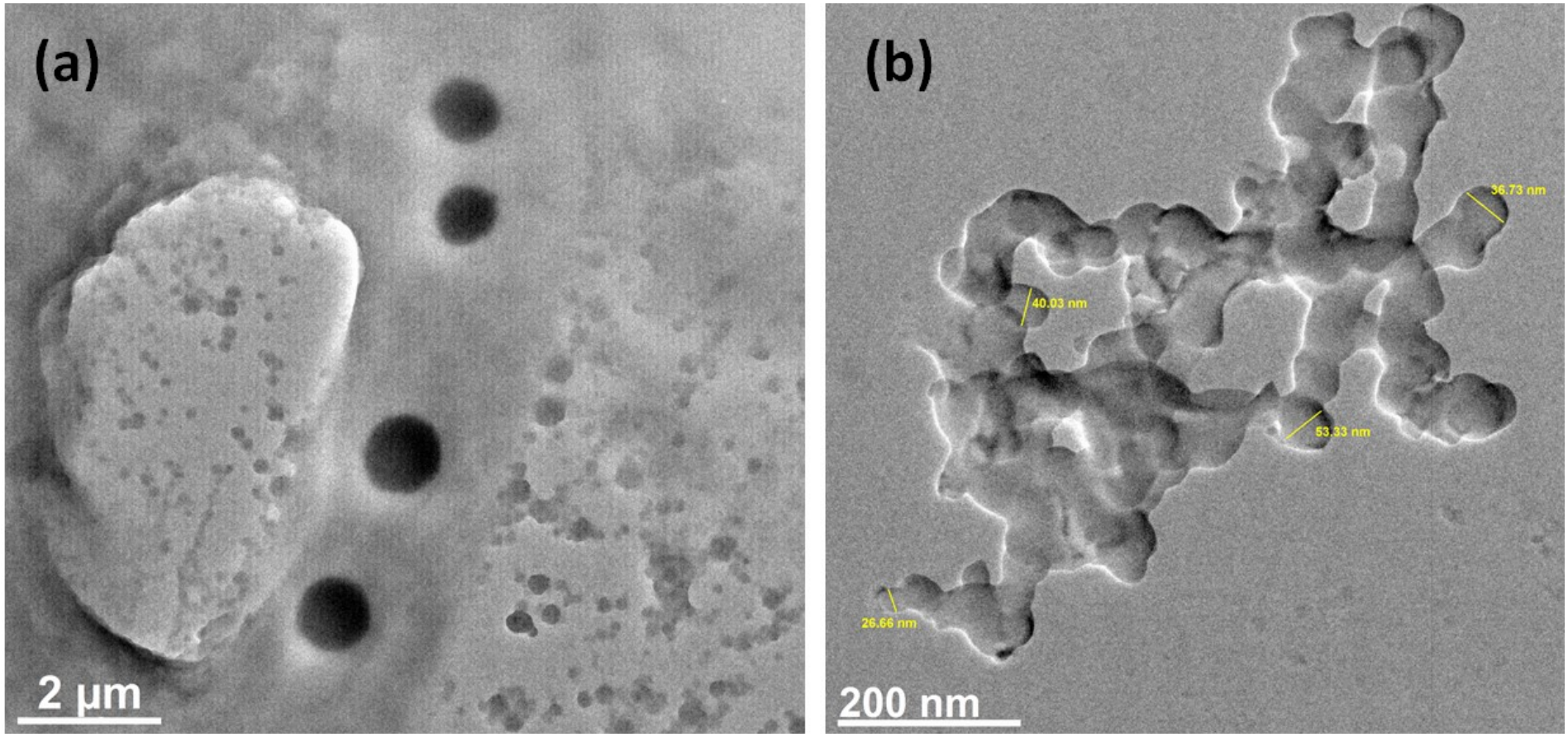


Fig. S40 UHR-FEG-TEM figure of **6** (a) at 0% water and (b) 100% water fraction at 298 K.

2.4 NMR spectra:

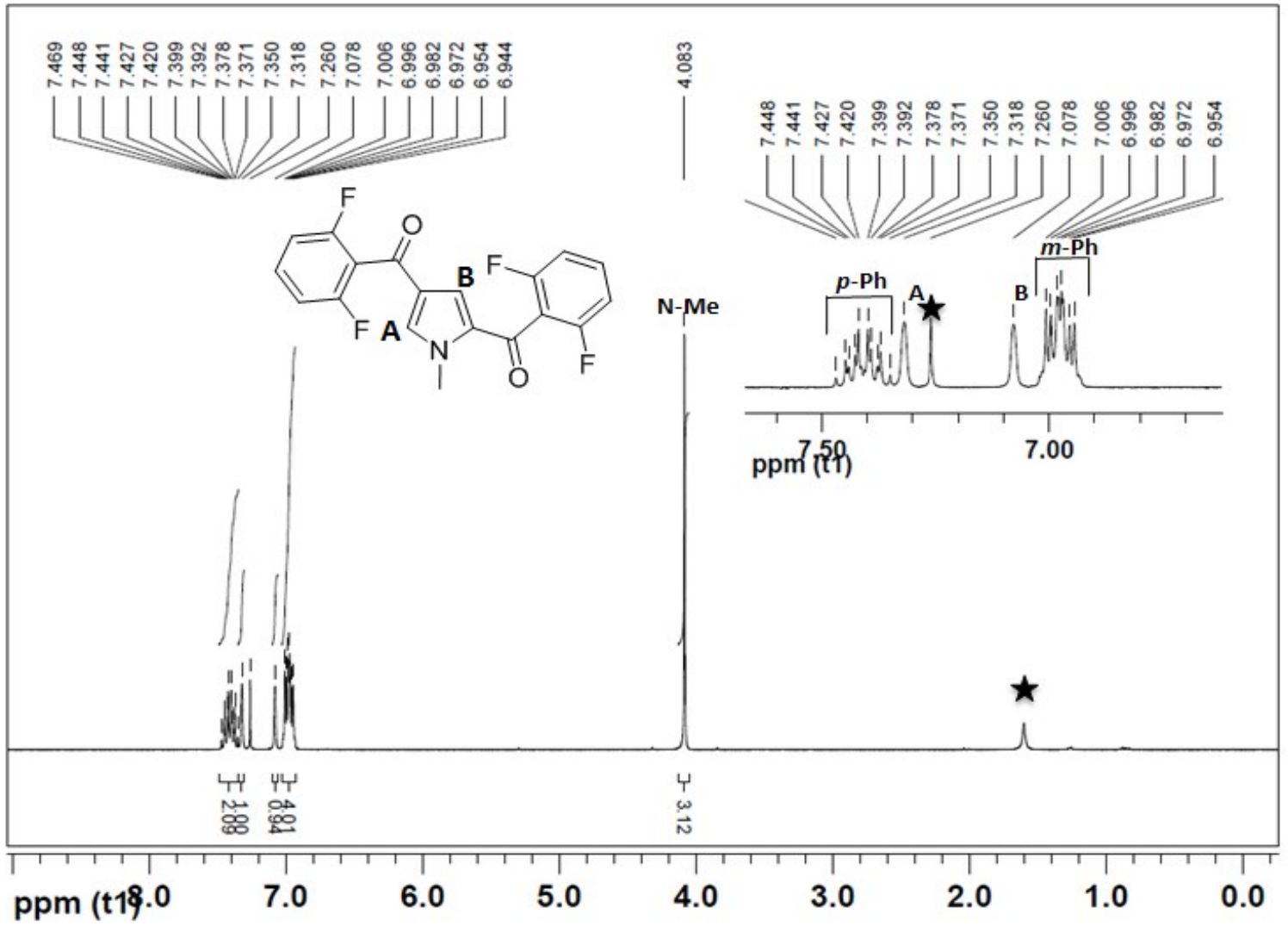


Fig. S41 ^{1}H NMR spectrum of **2** in $CDCl_3$ (* indicates residual solvent peak and solvent impurity)

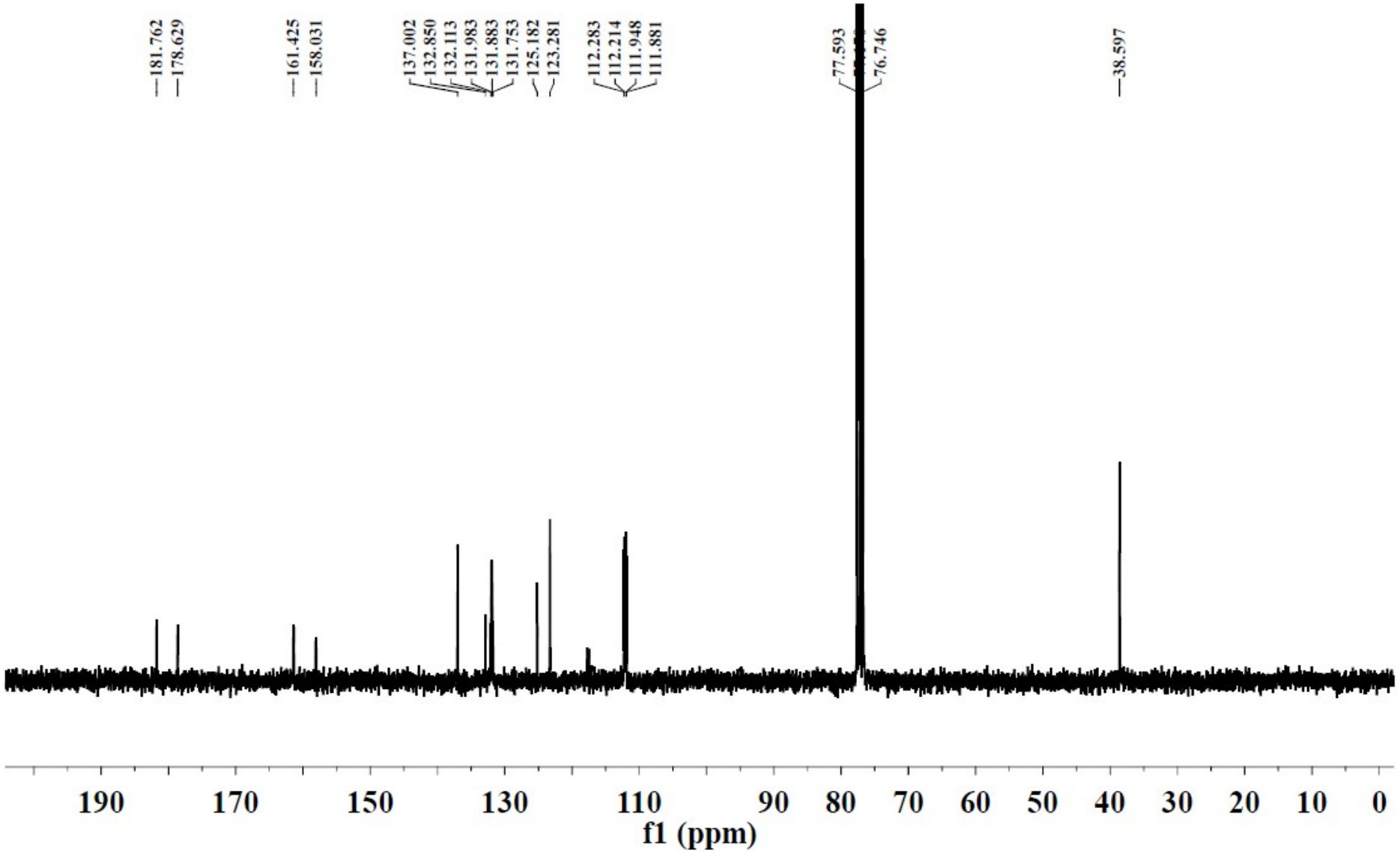


Fig. S42 ^{13}C NMR spectrum of **2** in $CDCl_3$

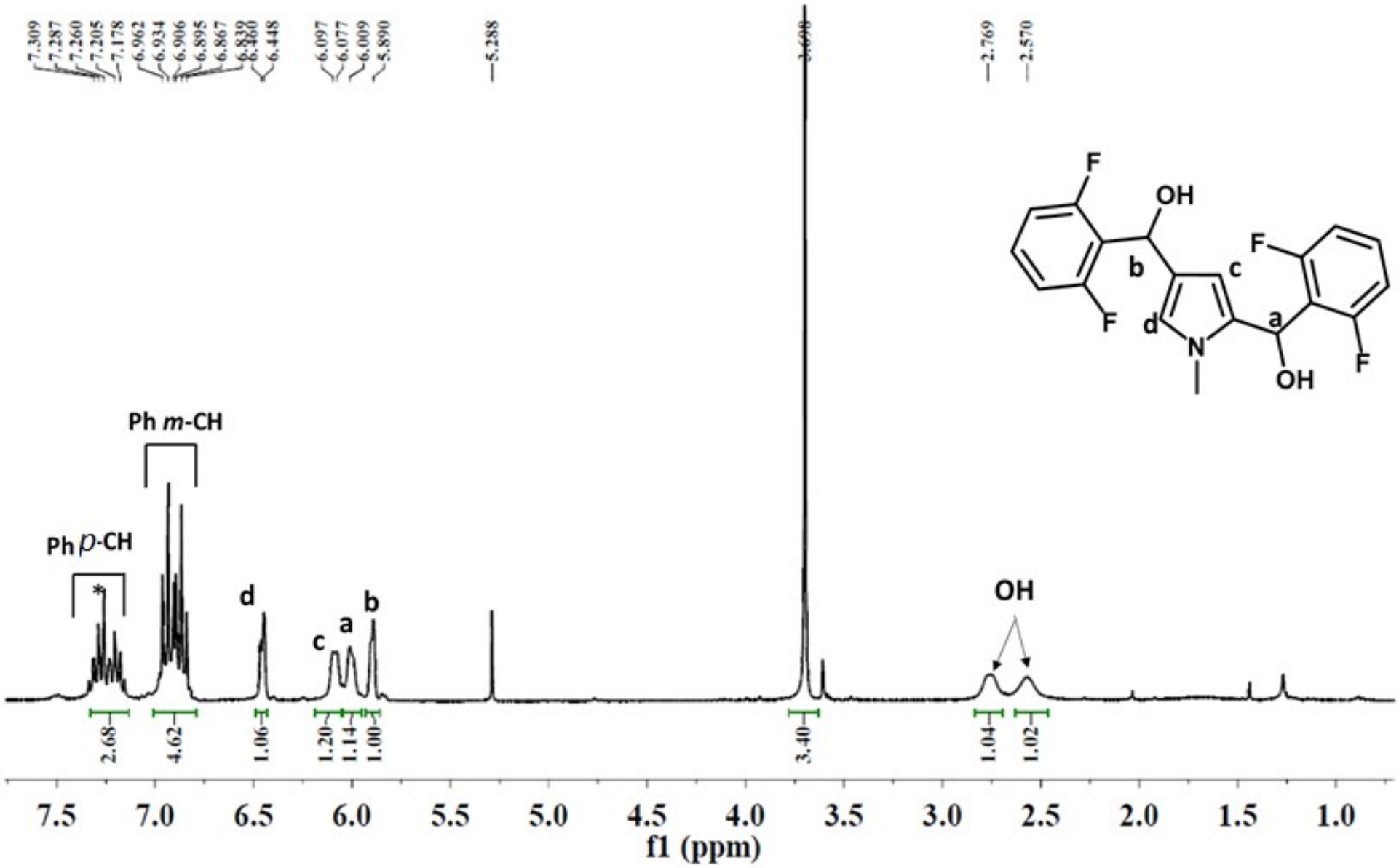


Fig. S43 ^{1}H NMR spectrum of **3** in $CDCl_3$

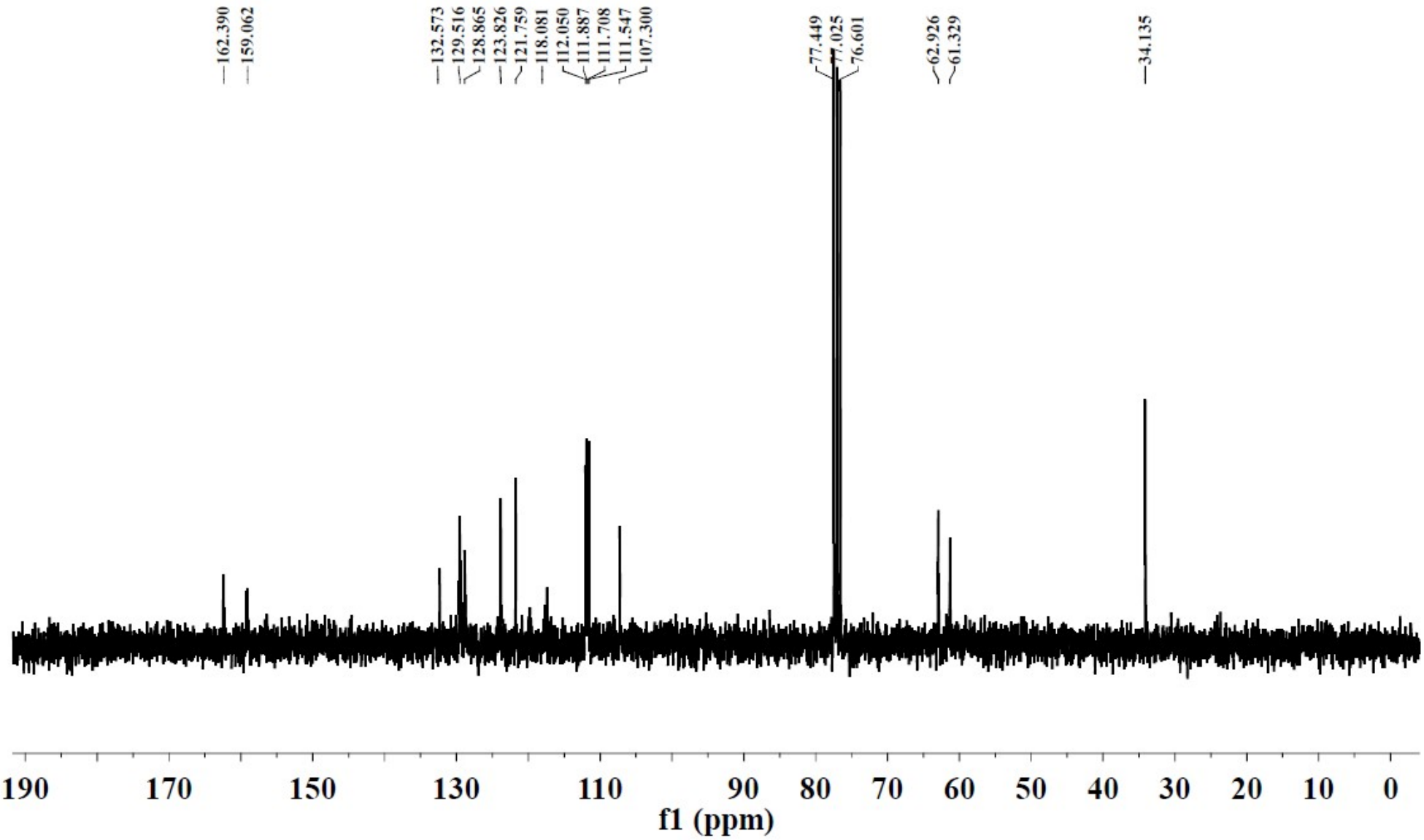


Fig. S44 ^{13}C NMR spectrum of **3** in $CDCl_3$

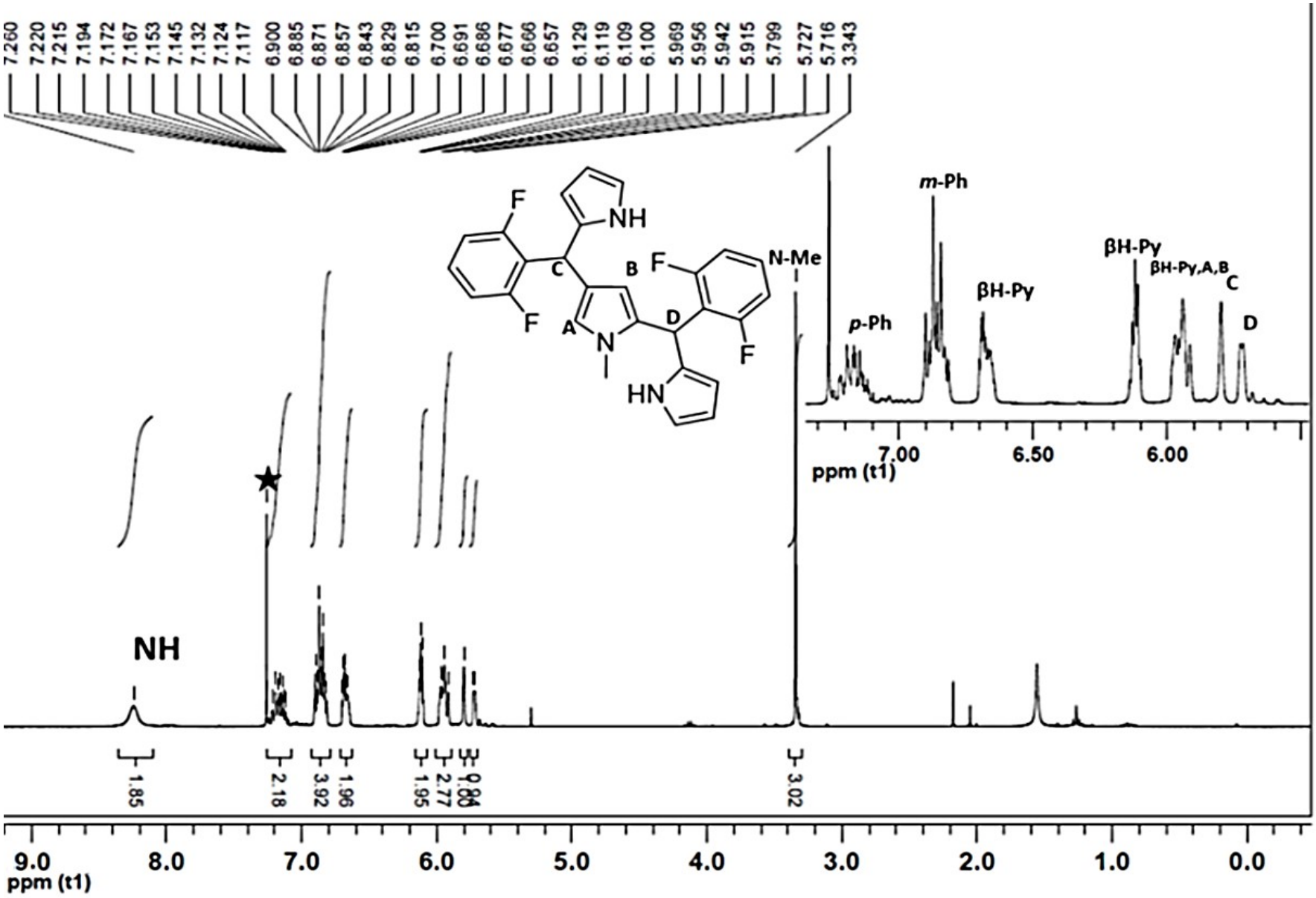


Fig. S45 ^{1}H NMR spectrum of **4** in $CDCl_3$ (* indicates residual solvent peak and solvent impurity)

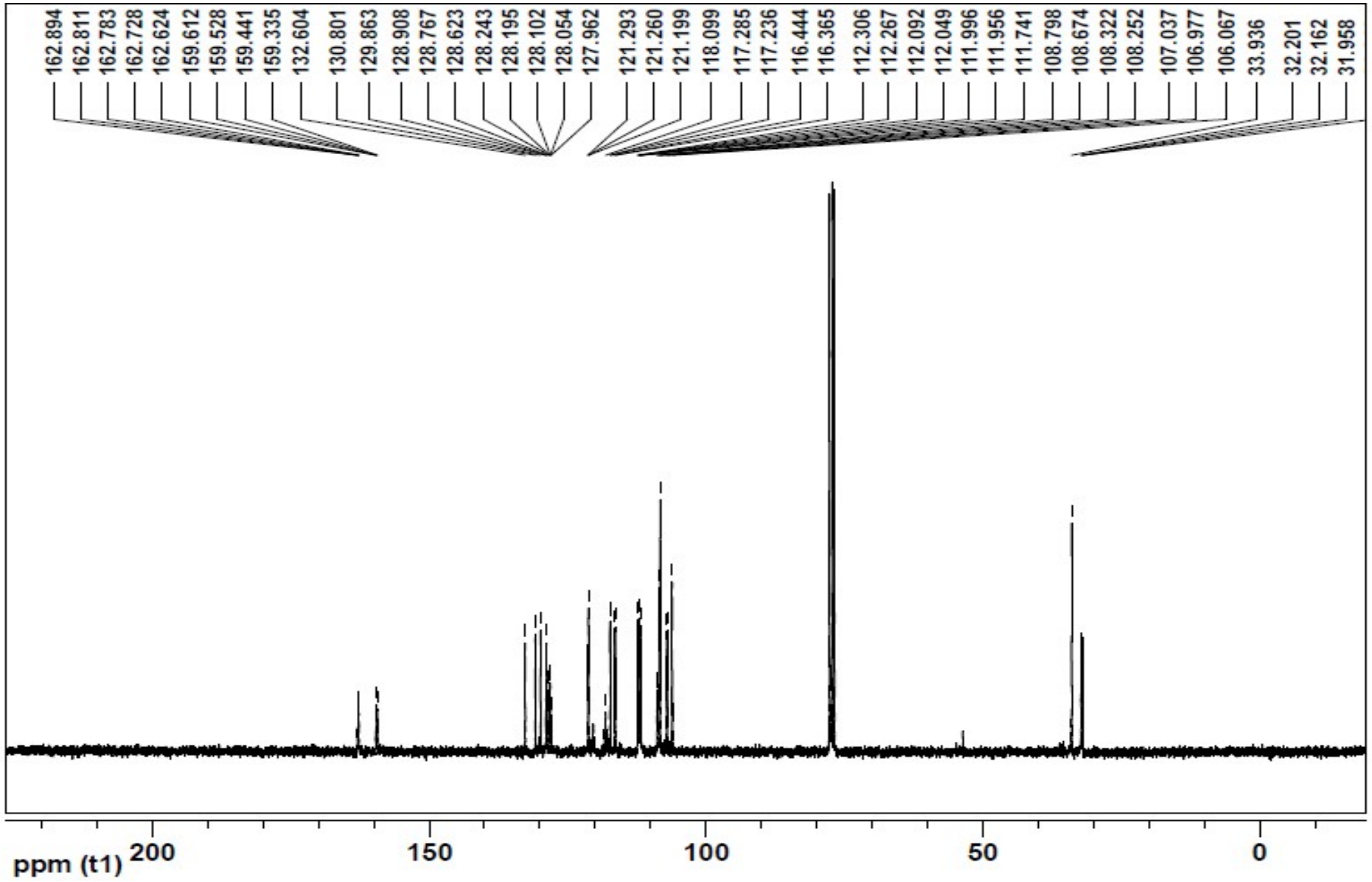


Fig. S46 ^{13}C NMR spectrum of **4** in $CDCl_3$

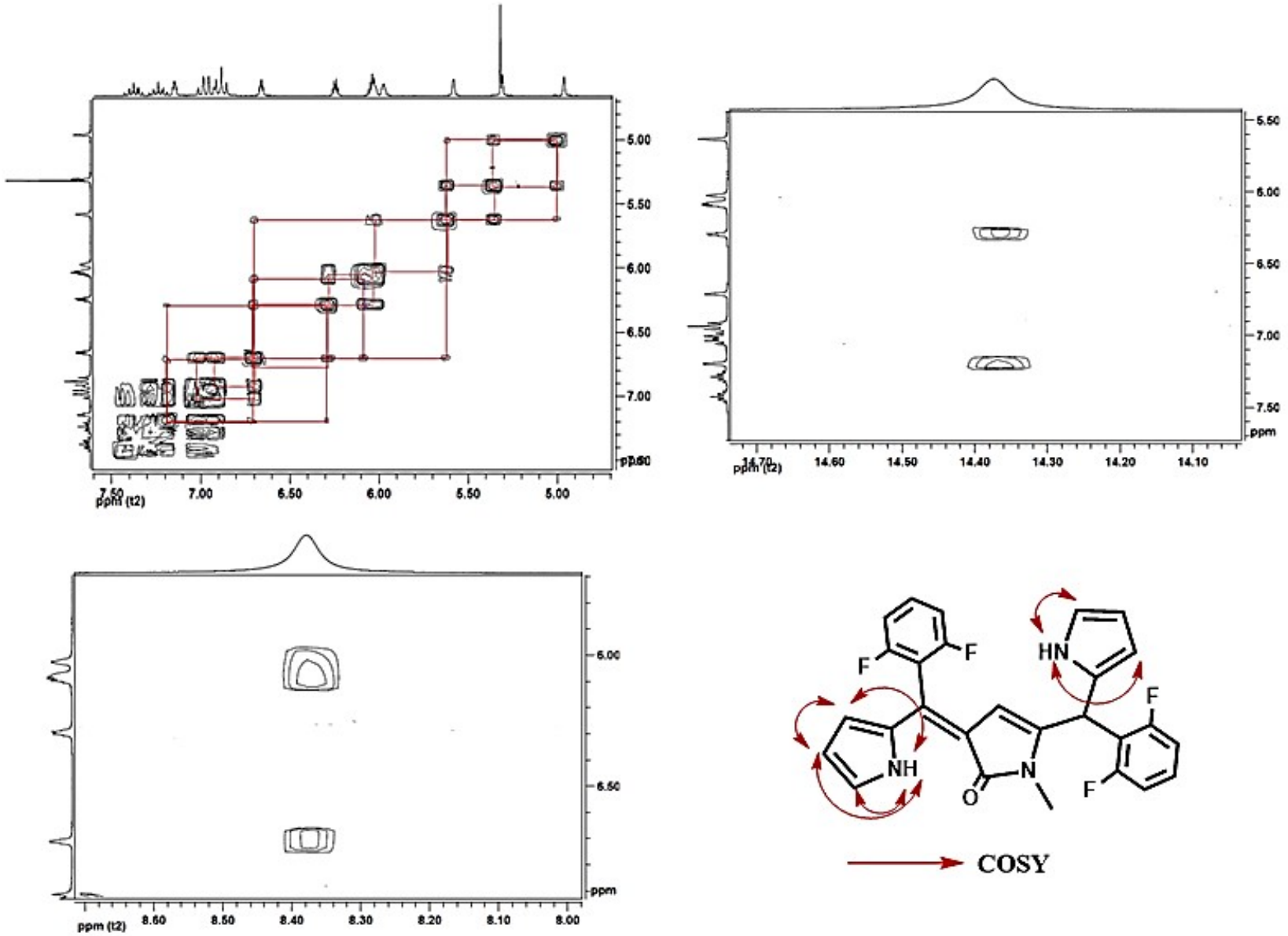


Fig. S47 ^{1}H -^{1}H 2D COSY NMR spectra of **5** in CD_2Cl_2 at 298 K

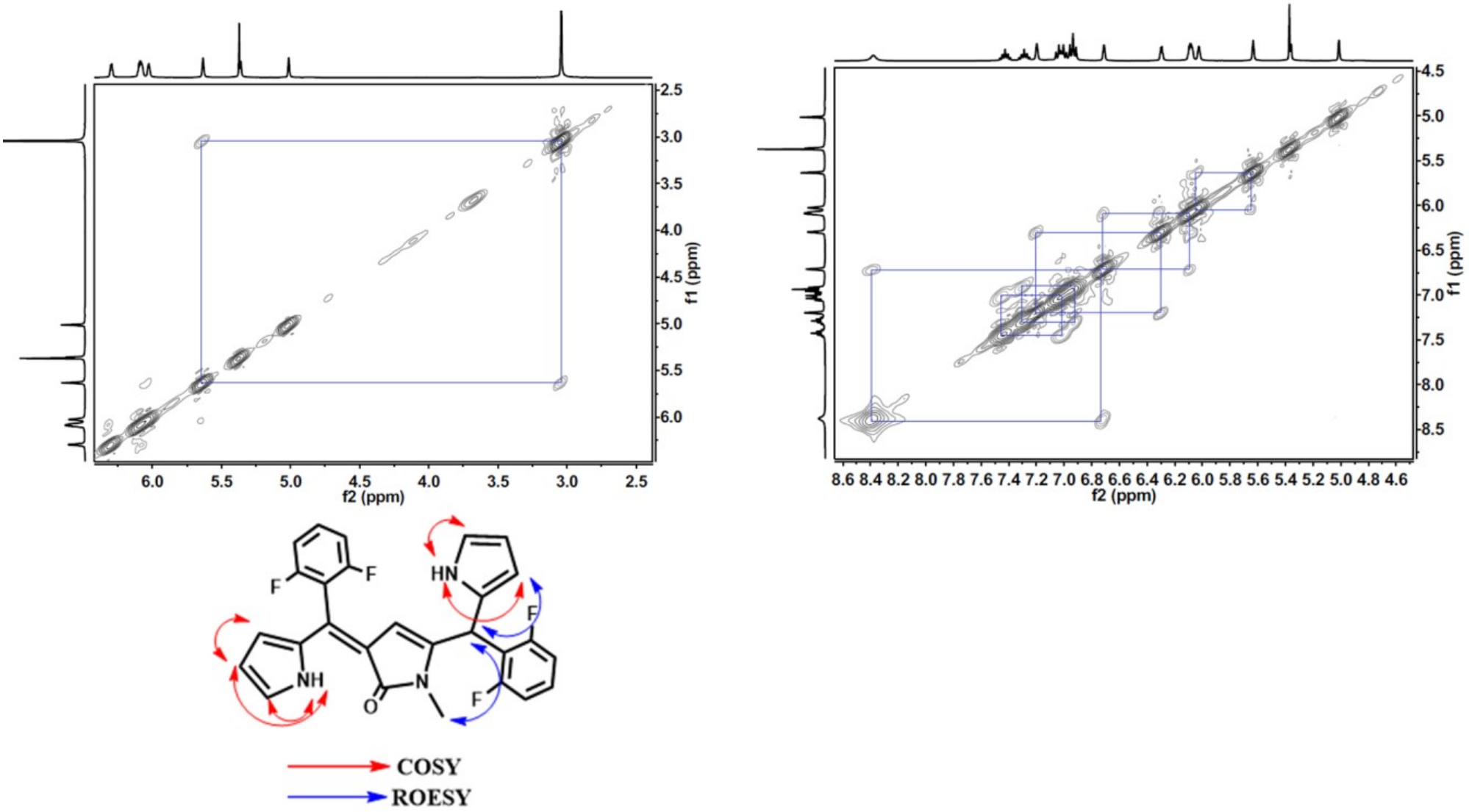


Fig. S48 ^{1}H -^{1}H 2D ROESY NMR spectra of **5** in CD_2Cl_2 at 298 K

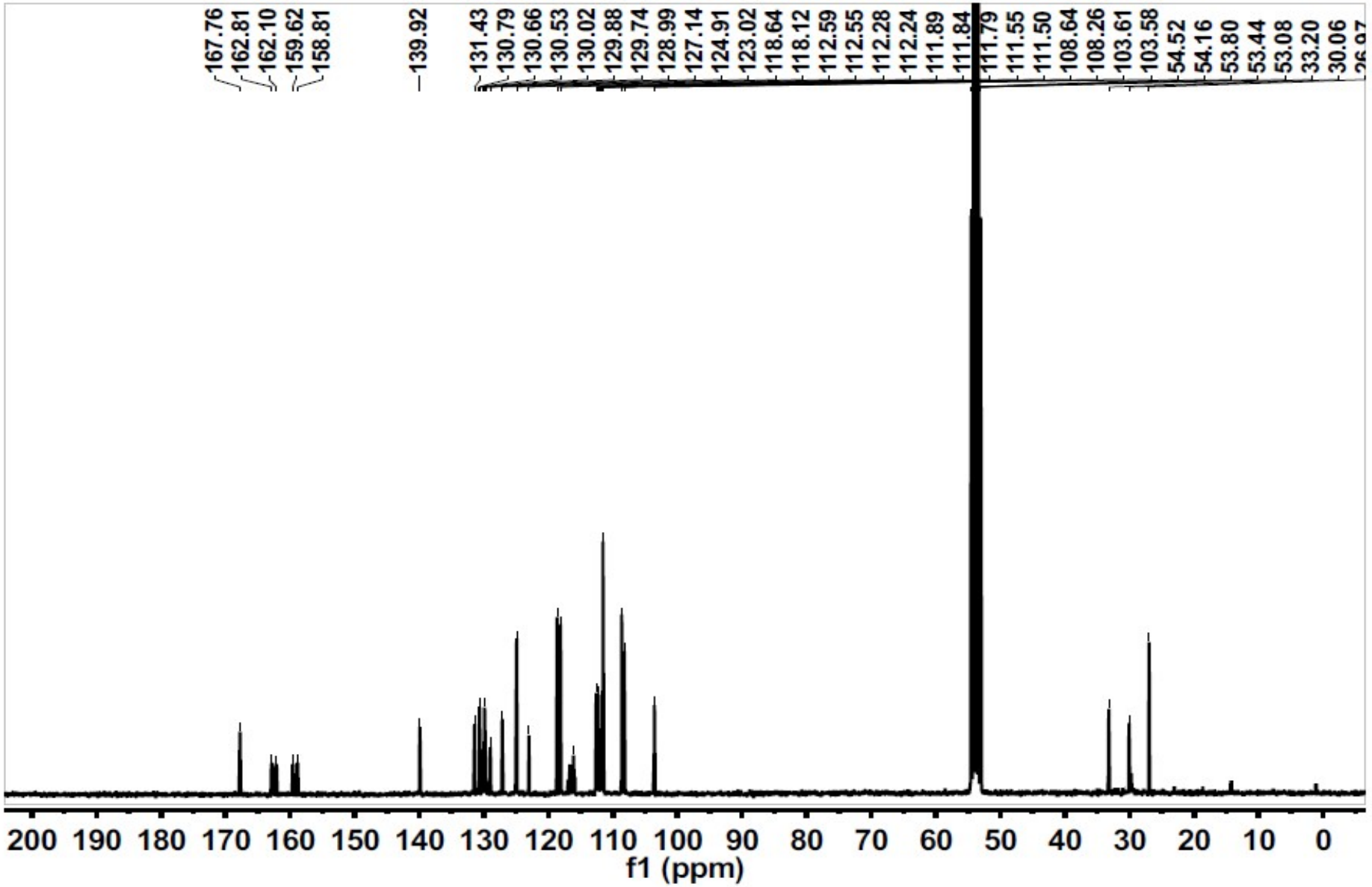
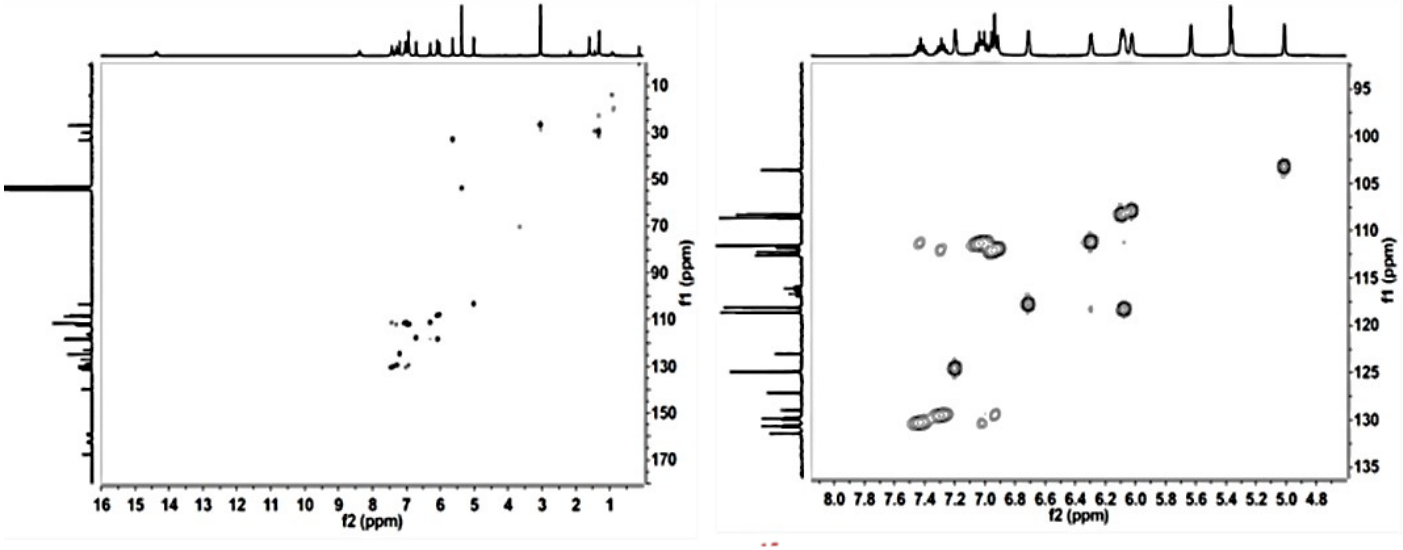


Fig. S49 ^{13}C NMR spectra of **5** in CD_2Cl_2 at 298 K



^{1}H (ppm)	^{13}C (ppm)
14.32 (i)	-
8.34 (j)	-
7.14 (a)	124.91 (1)
6.25 (b)	111.55 (2)
6.66 (h)	118.24 (14)
6.04 (c)	108.64 (3)
5.97 (f)	108.26 (12)
5.58 (e)	33.20 (10)
2.99 (k)	26.97 (15)
4.96 (d)	103.58 (8)

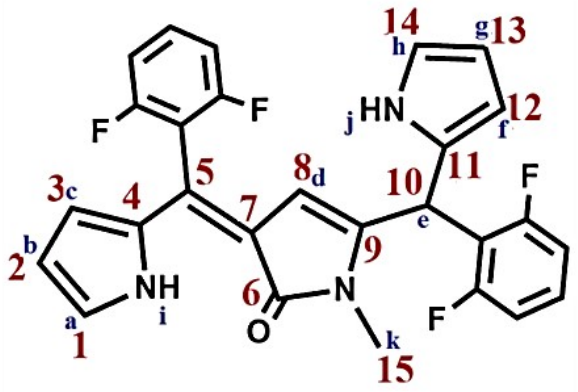
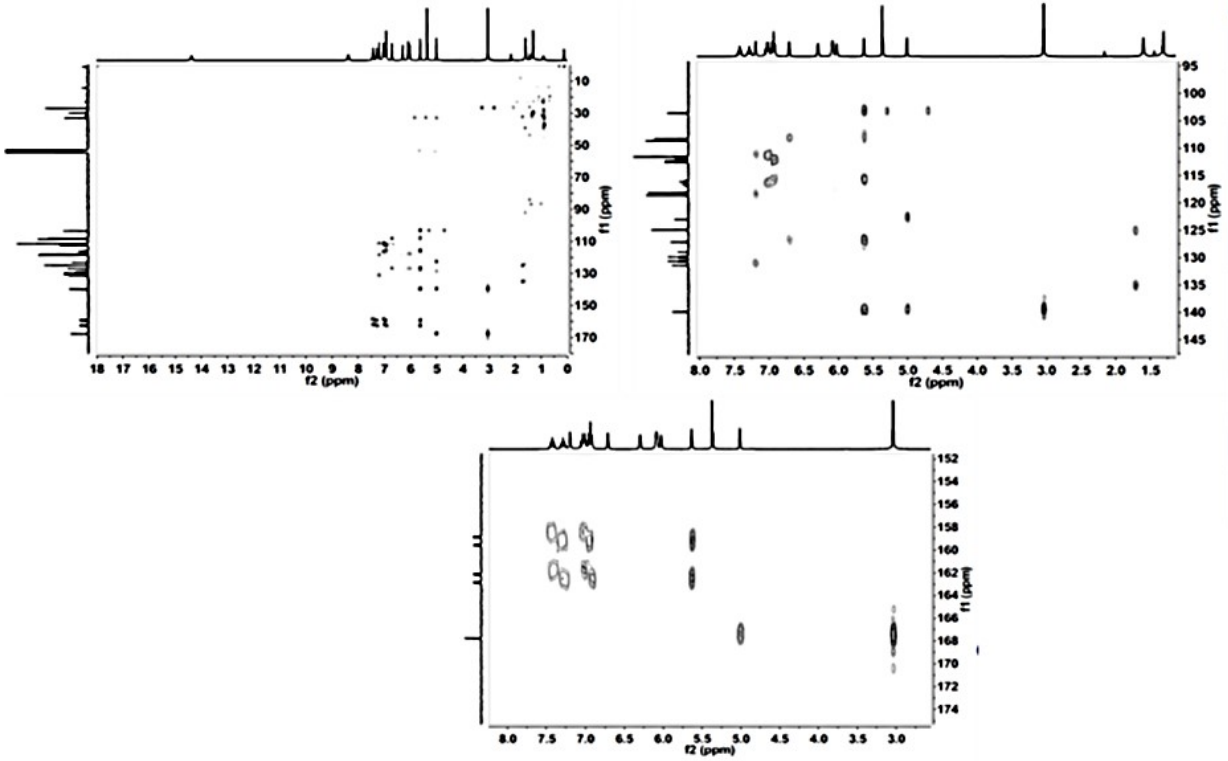


Fig. S50 HSQC NMR spectra of **5** in CD_2Cl_2 at 298 K



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
7.14 (a)	111.55 (2)	4.96 (d)	33.20 (10)
	118.12 (14)		123.02 (5)
	130.66 (4)		128.98 (7)
			139.92 (9)
6.65 (h)	108.26 (12)		167.75 (6)
	127.14 (11)	5.58 (e)	103.58 (8)
5.97 (f)	118.12 (14)		108.26 (12)
	127.14 (11)		116.10 (13)
2.99 (k)	139.92 (9)		127.14 (11)
	167.75 (6)		139.92 (9)

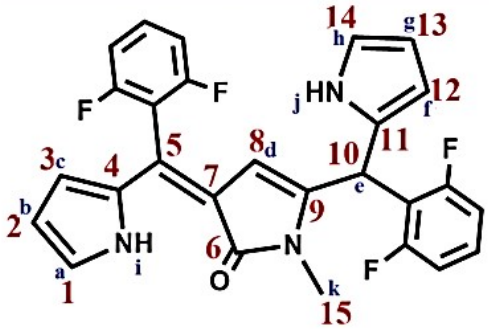


Fig. S51 HMBC NMR spectra of **5** in CD_2Cl_2 at 298 K

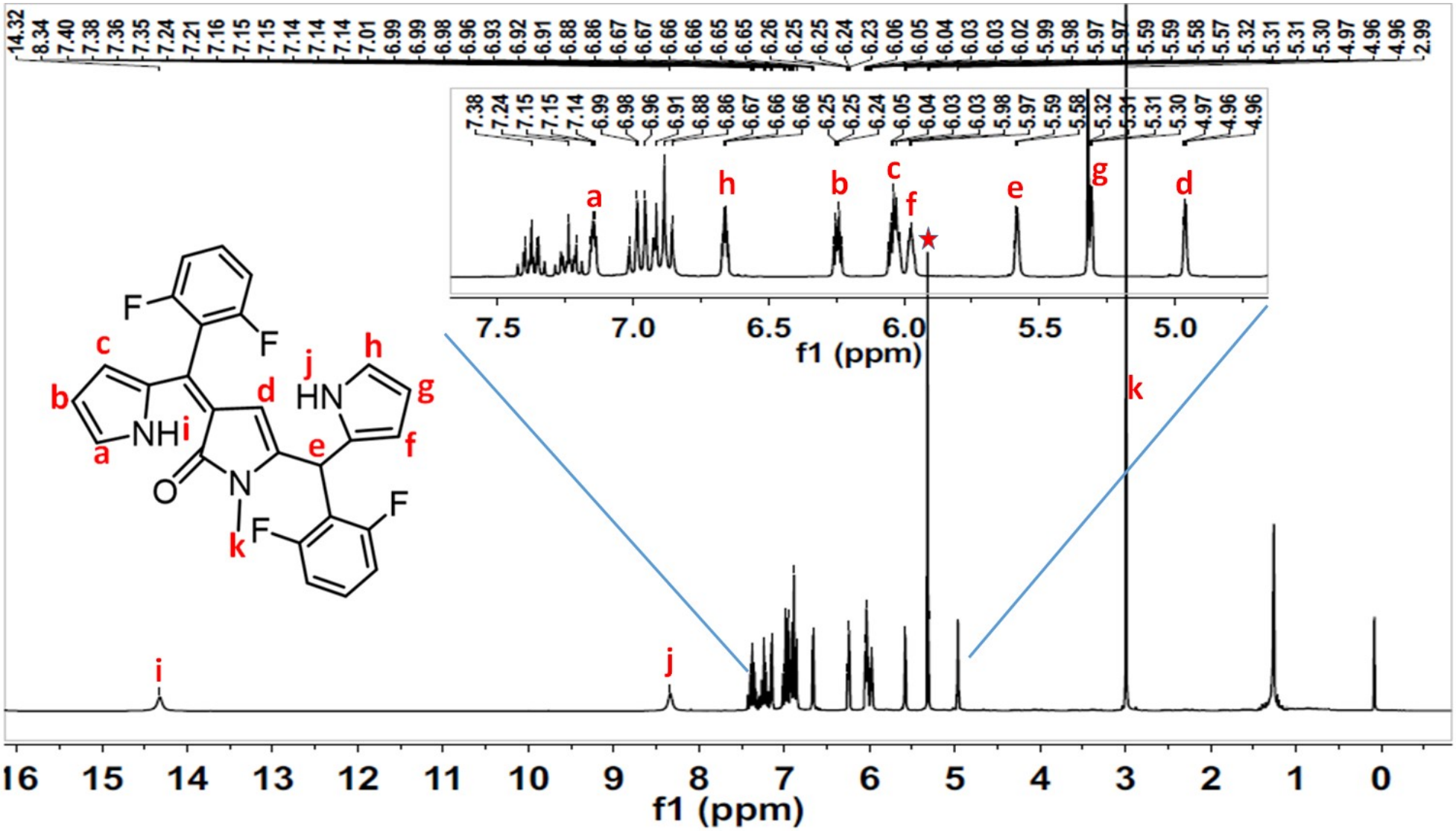


Fig. S52 Complete ^{1}H NMR spectral assignment of **5** in CD_2Cl_2 at 298 K

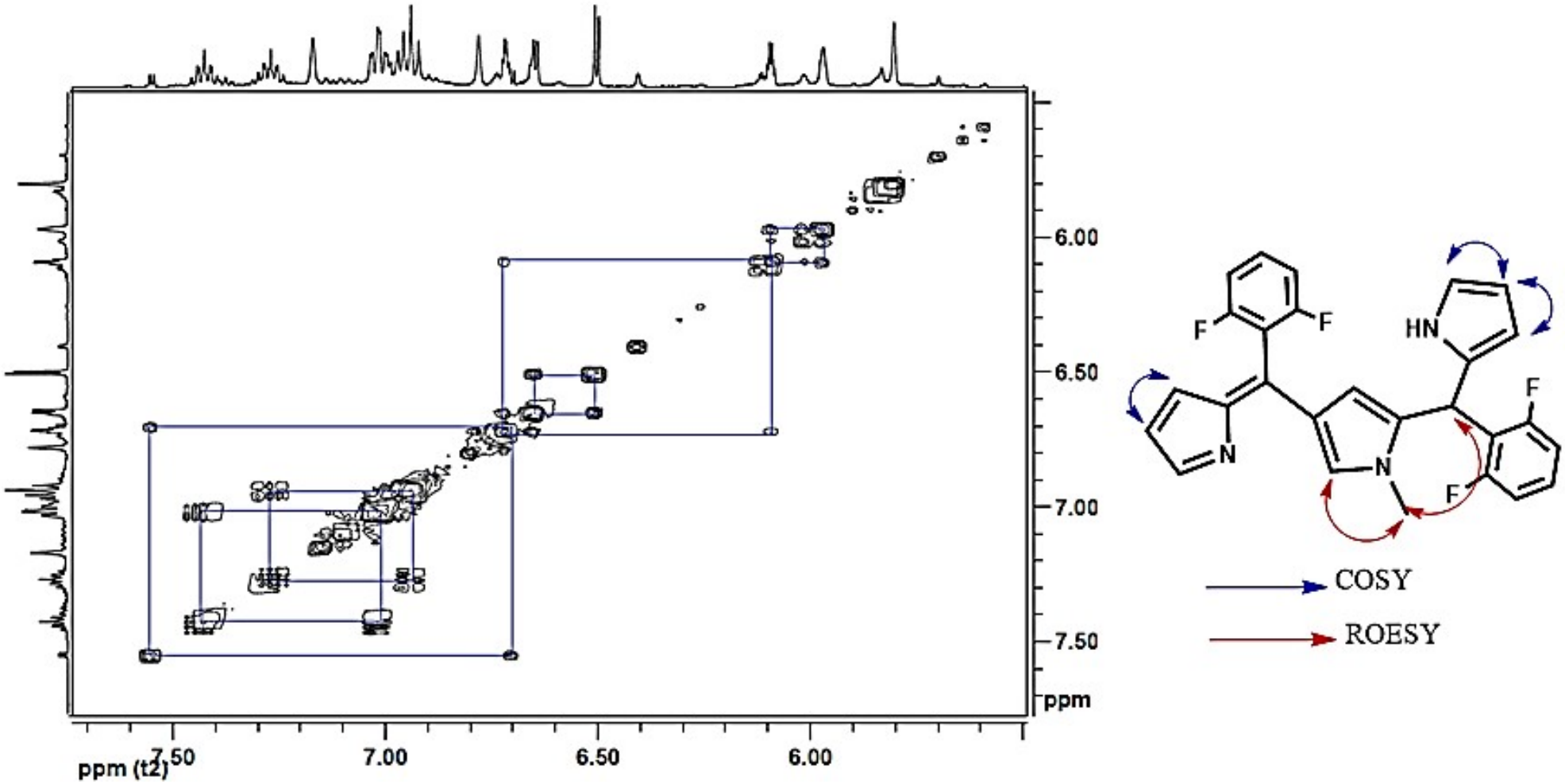


Fig. S53 ^{1}H-^{1}H 2D COSY spectra of **6** in CD_2Cl_2 at 298 K

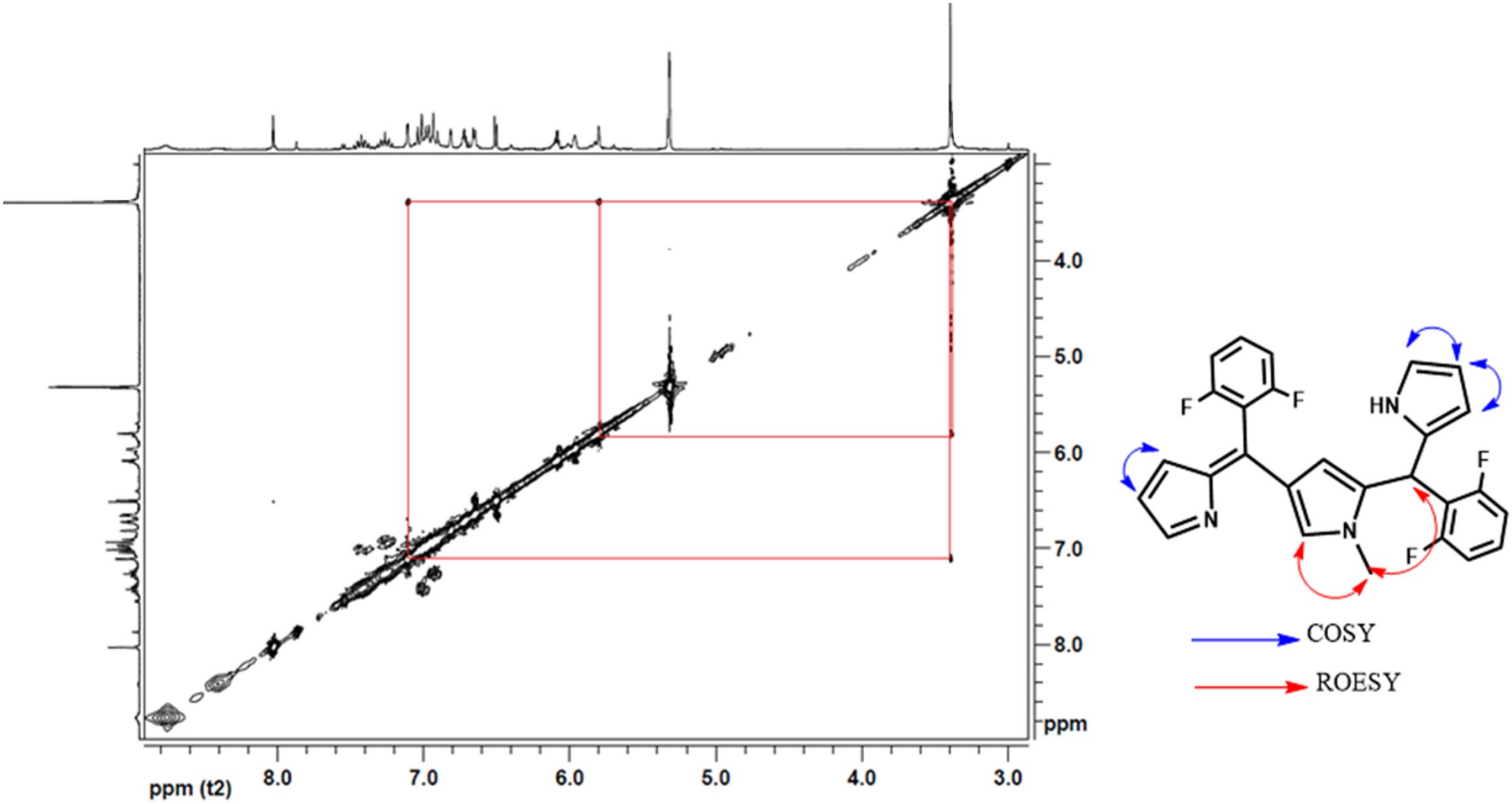


Fig. S54 ^{1}H-^{1}H 2D ROESY spectra of **6** in CD_2Cl_2 at 298 K

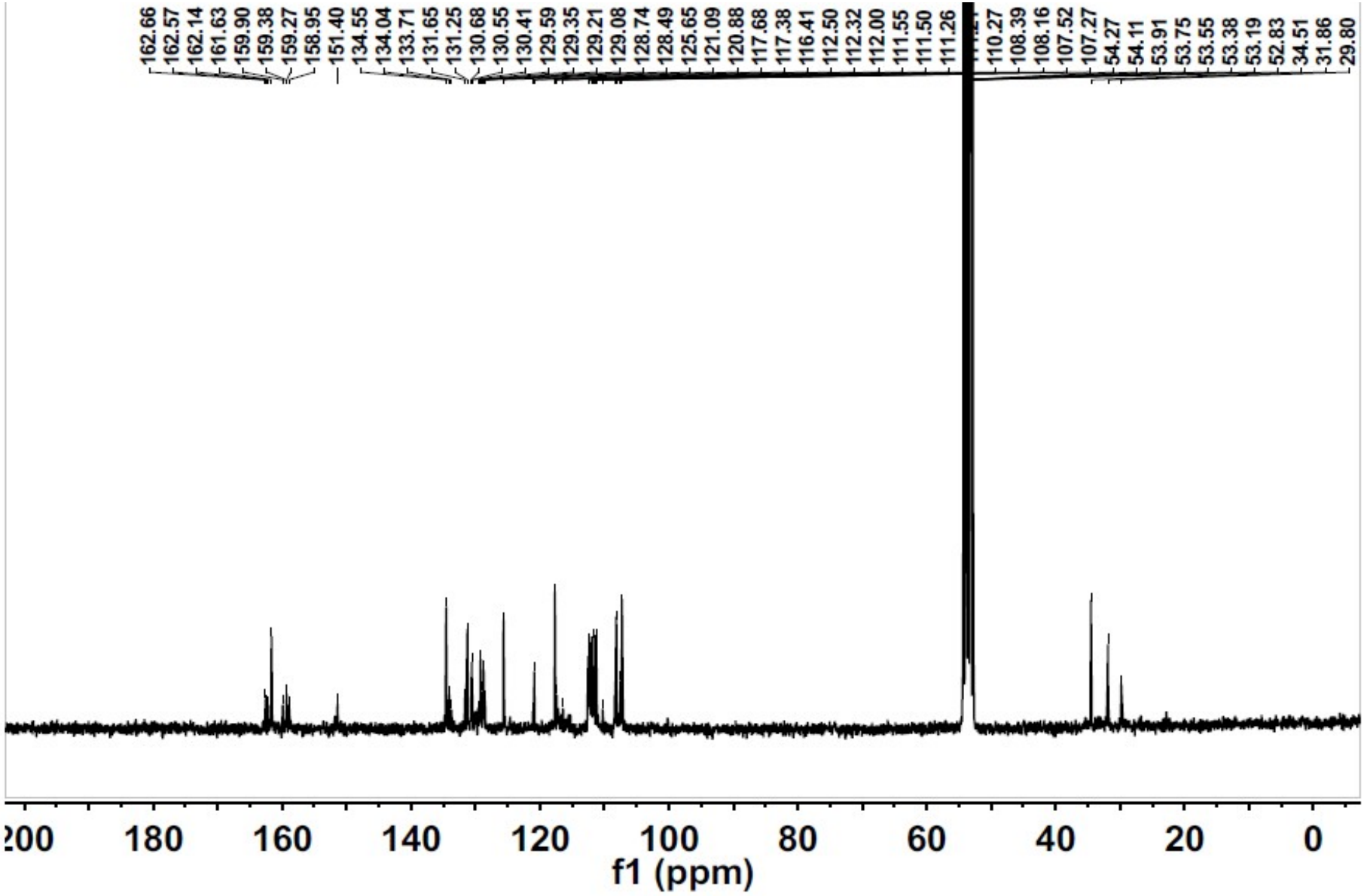
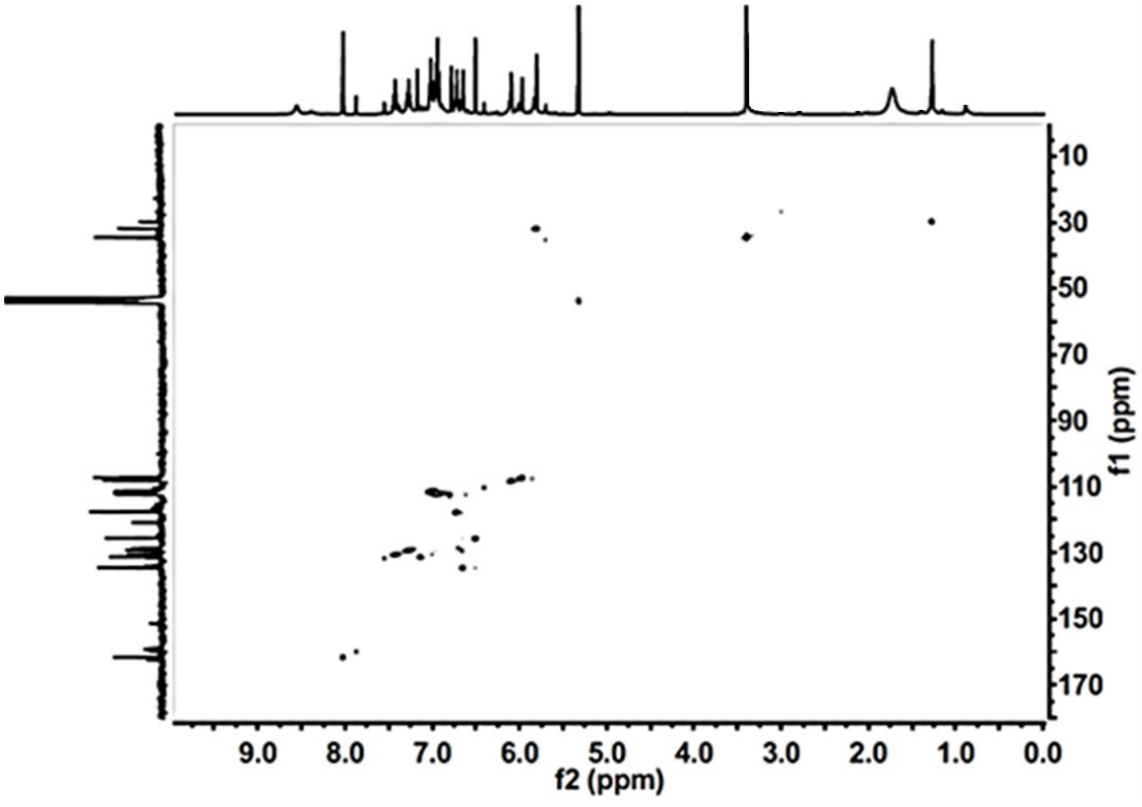


Fig. S55 ^{13}C NMR spectra of **6** in CD_2Cl_2 at 298 K



^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.02 (a)	161.63 (1)	6.50 (b)	125.6 (2)
7.17 (d)	131.30 (6)	6.09 (i)	108.0 (13)
6.78 (e)	112.3 (8)	5.97 (h)	107.0 (12)
6.71 (j)	117.6 (14)	5.80 (g)	31.8 (10)
6.65 (c)	134.5 (3)	3.39 (f)	34.5 (15)

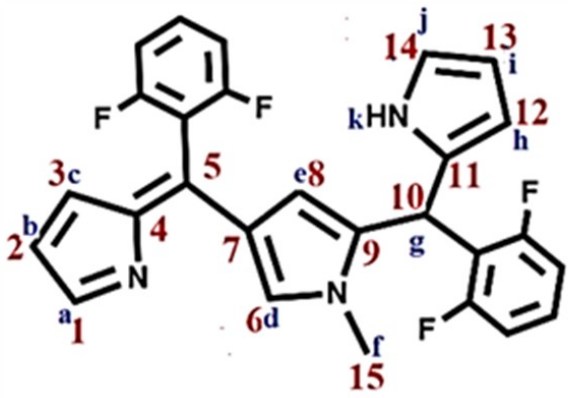
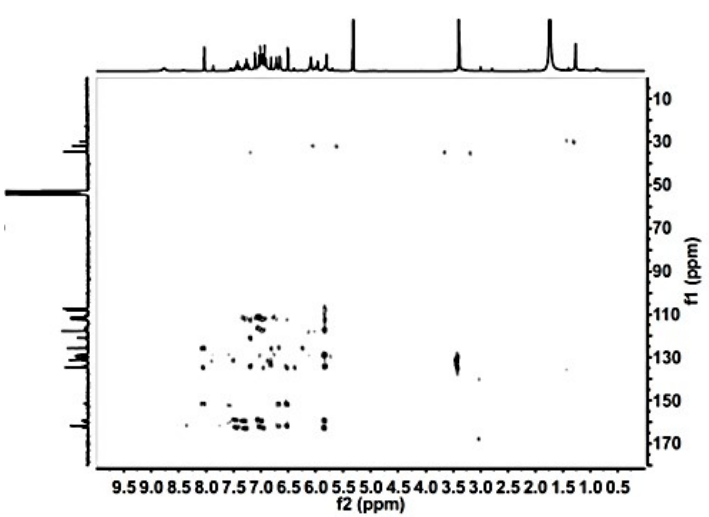
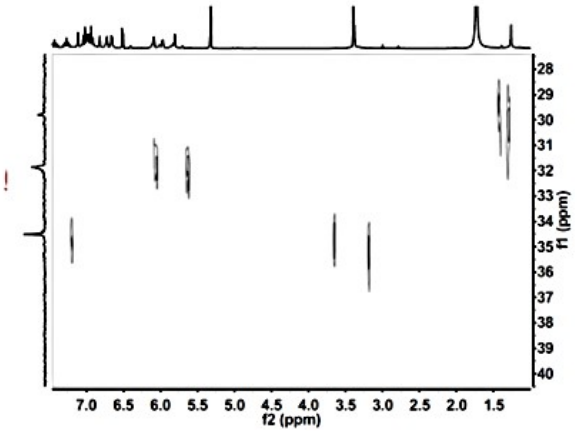
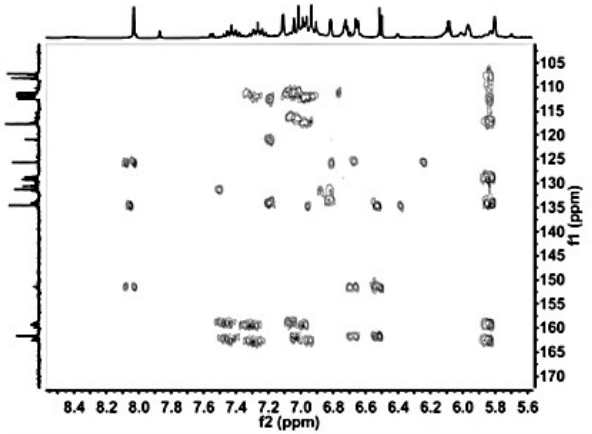


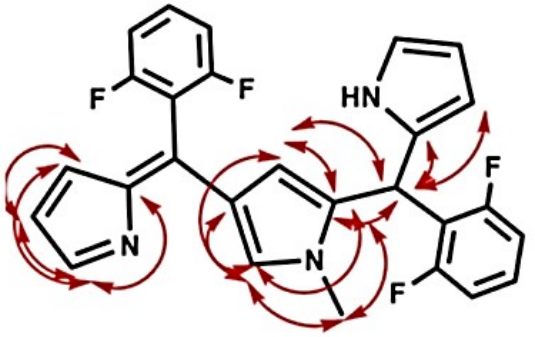
Fig. S56 HSQC NMR spectra of **6** in CD_2Cl_2 at 298 K







^{1}H (ppm)	^{13}C (ppm)	^{1}H (ppm)	^{13}C (ppm)
8.02 (a)	134.5 (3)	5.80 (g)	134.1 (9)
	125.6 (2)		129.2 (11)
	151.4 (4)		112.3 (8)
7.17 (d)	112.3 (8)		107.0 (12)
	120.8 (7)	3.39 (f)	131.3 (6)
	134.1 (9)		134.1 (8)
6.78 (e)	134.1 (9)	6.65 (c)	125.6 (2)
			161.6 (1)



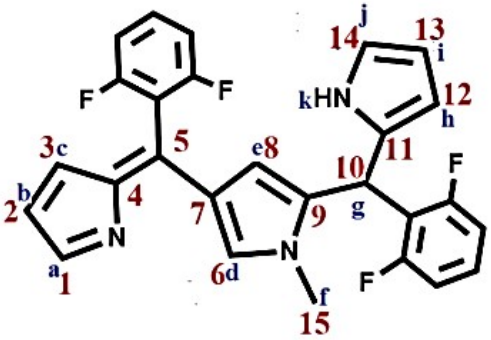


Fig. S57 HMBC NMR spectra of **6** in CD_2Cl_2 at 298 K

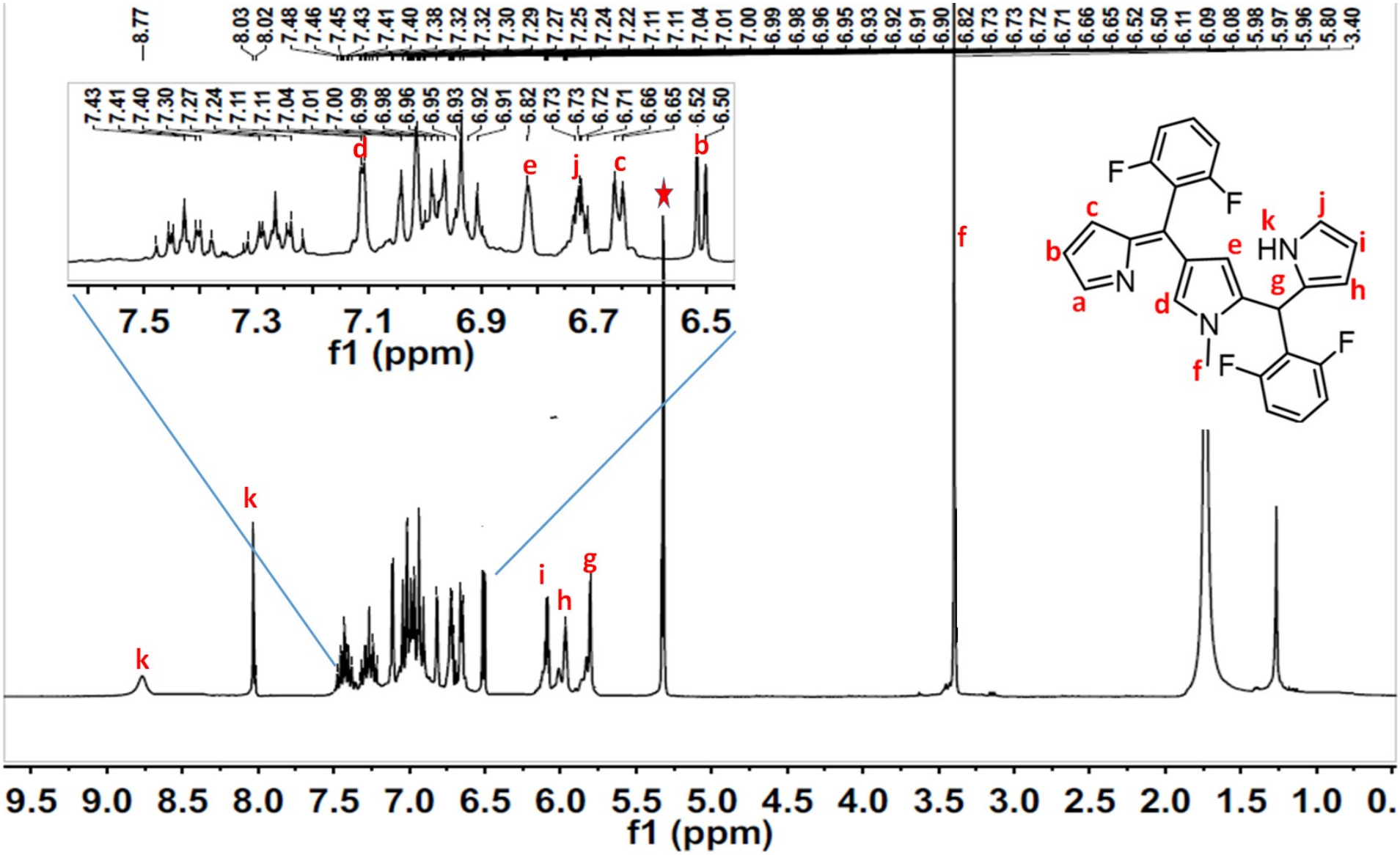


Fig. S58 Complete ^{1}H NMR spectral assignment of **6** in CD_2Cl_2 at 298 K

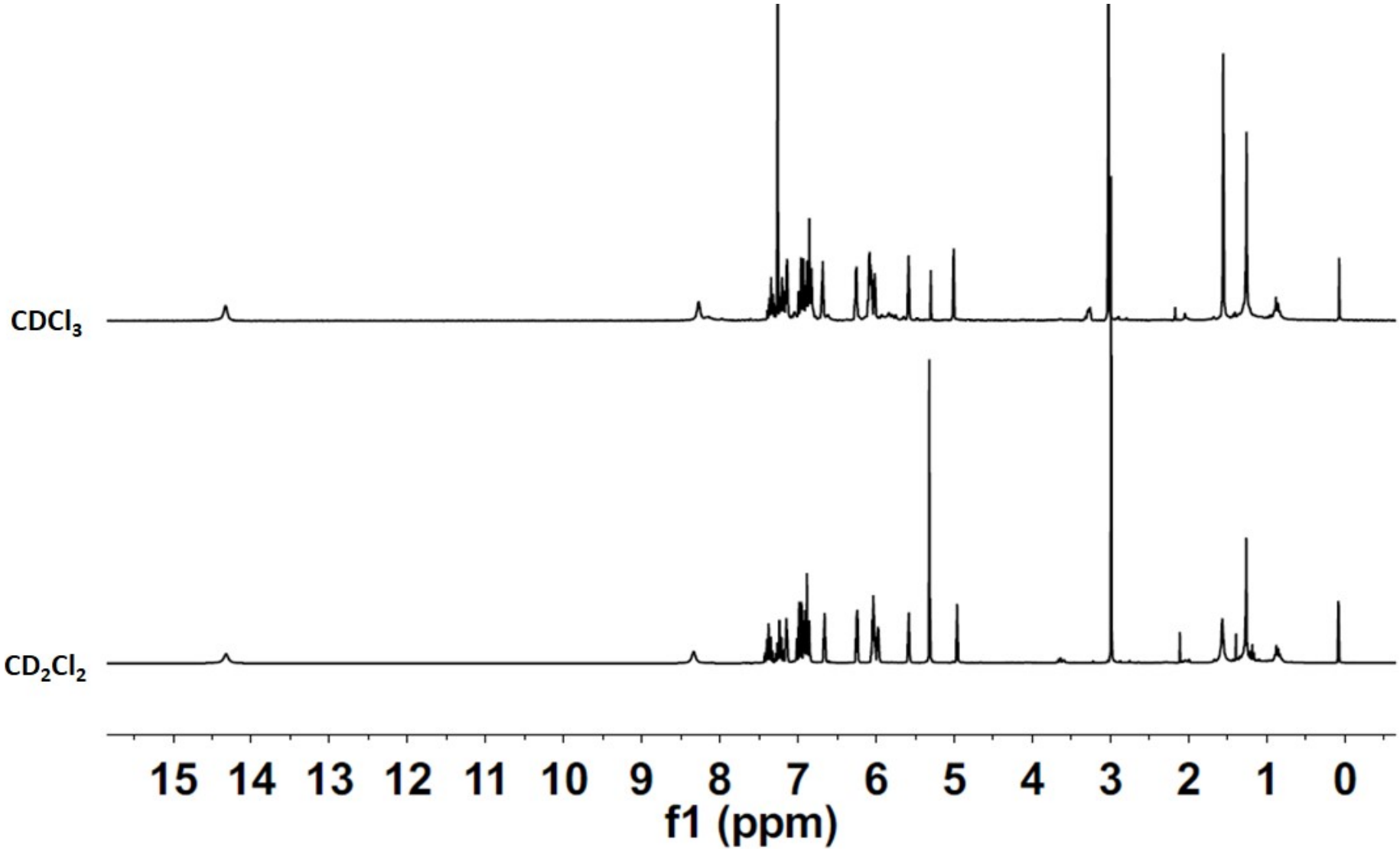


Fig. S59 Comparative ^{1}H NMR spectral assignment of **5** in (A) CD_2Cl_2 and (B) $CDCl_3$ at 298 K

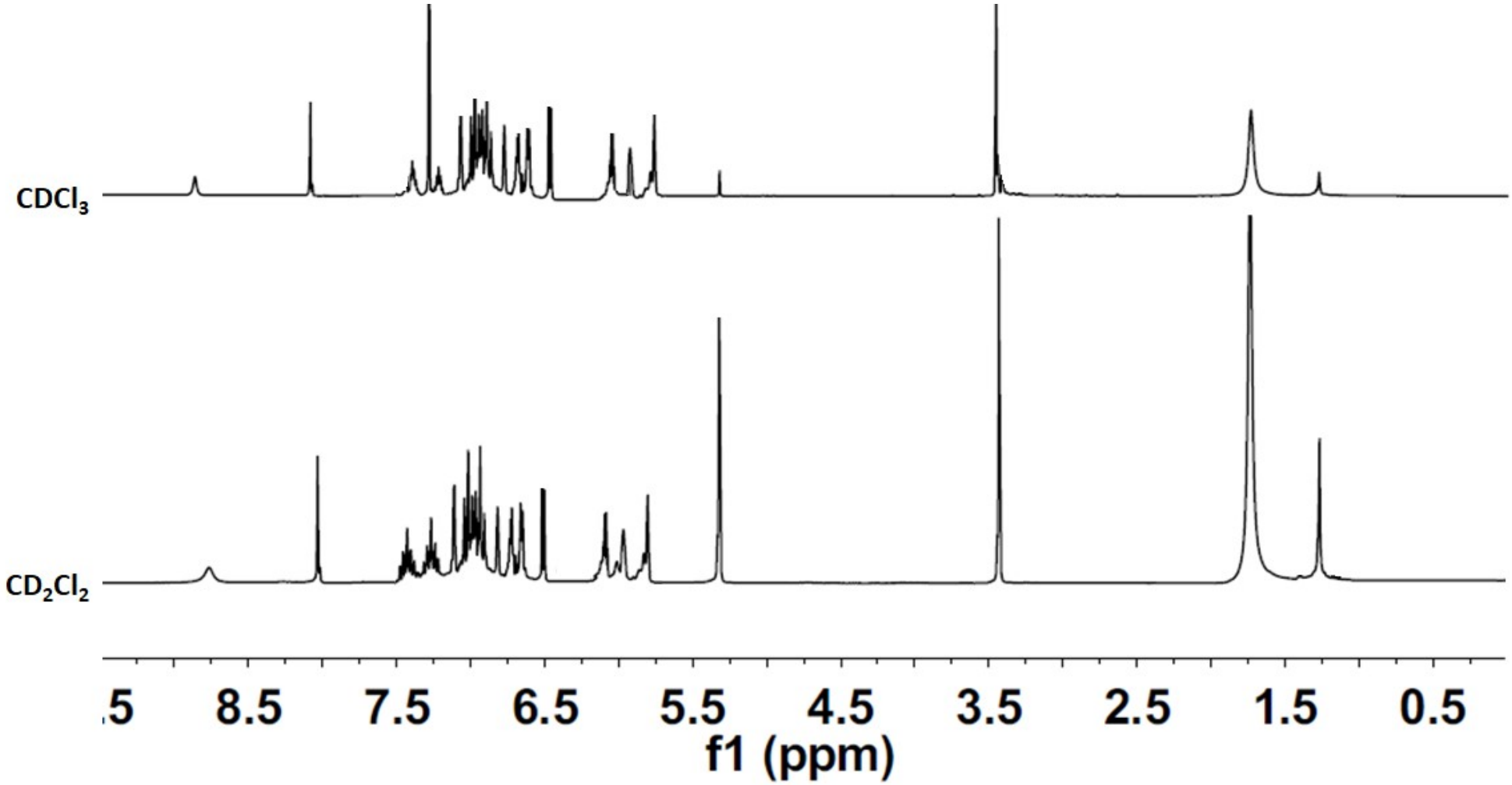


Fig. S60 Comparative ^{1}H NMR spectral assignment of **6** in (A) CD_2Cl_2 and (B) $CDCl_3$ at 298 K

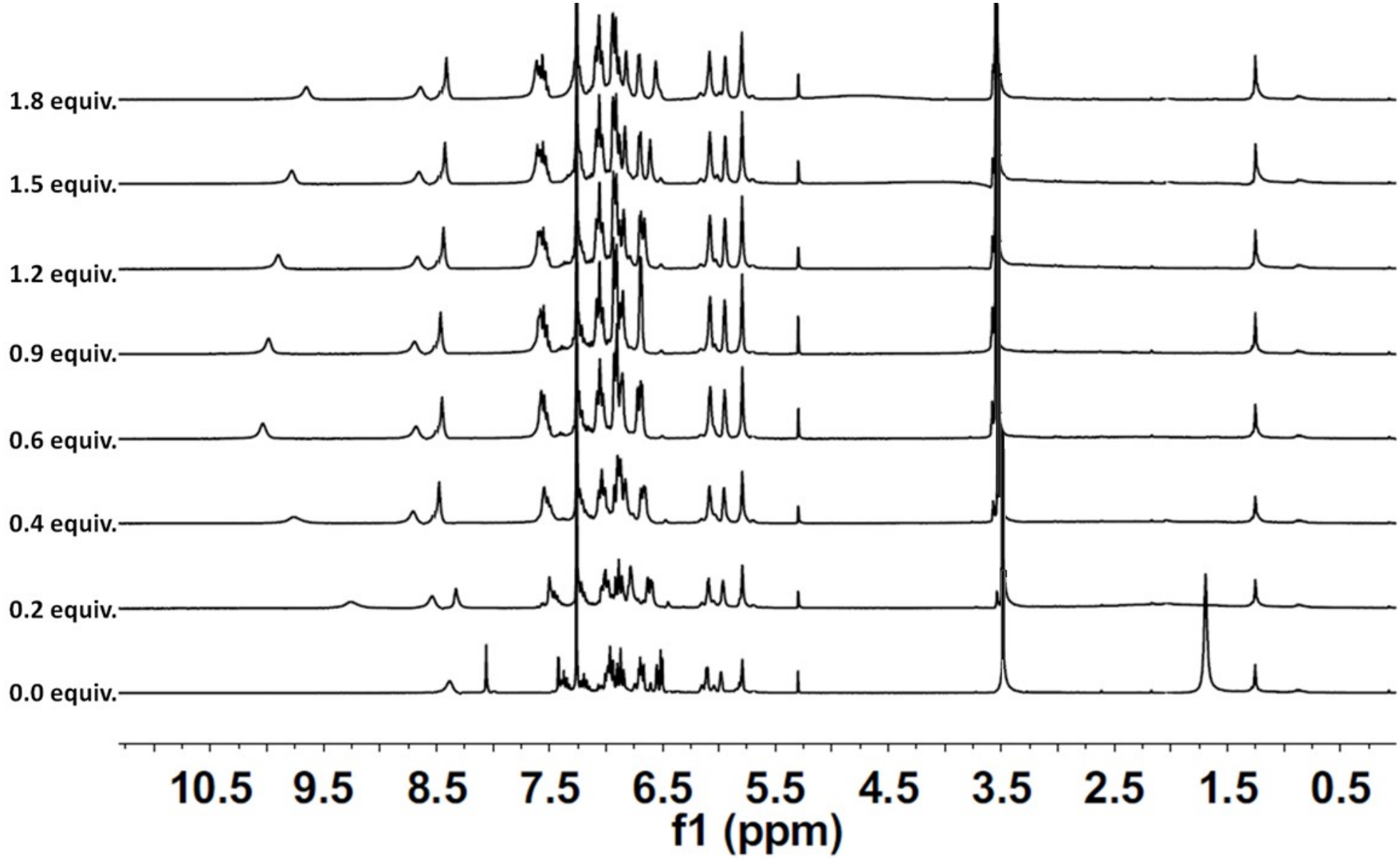


Fig. S61 Acid titration ^{1}H NMR spectra of **6** in $CDCl_3$ at 298 K

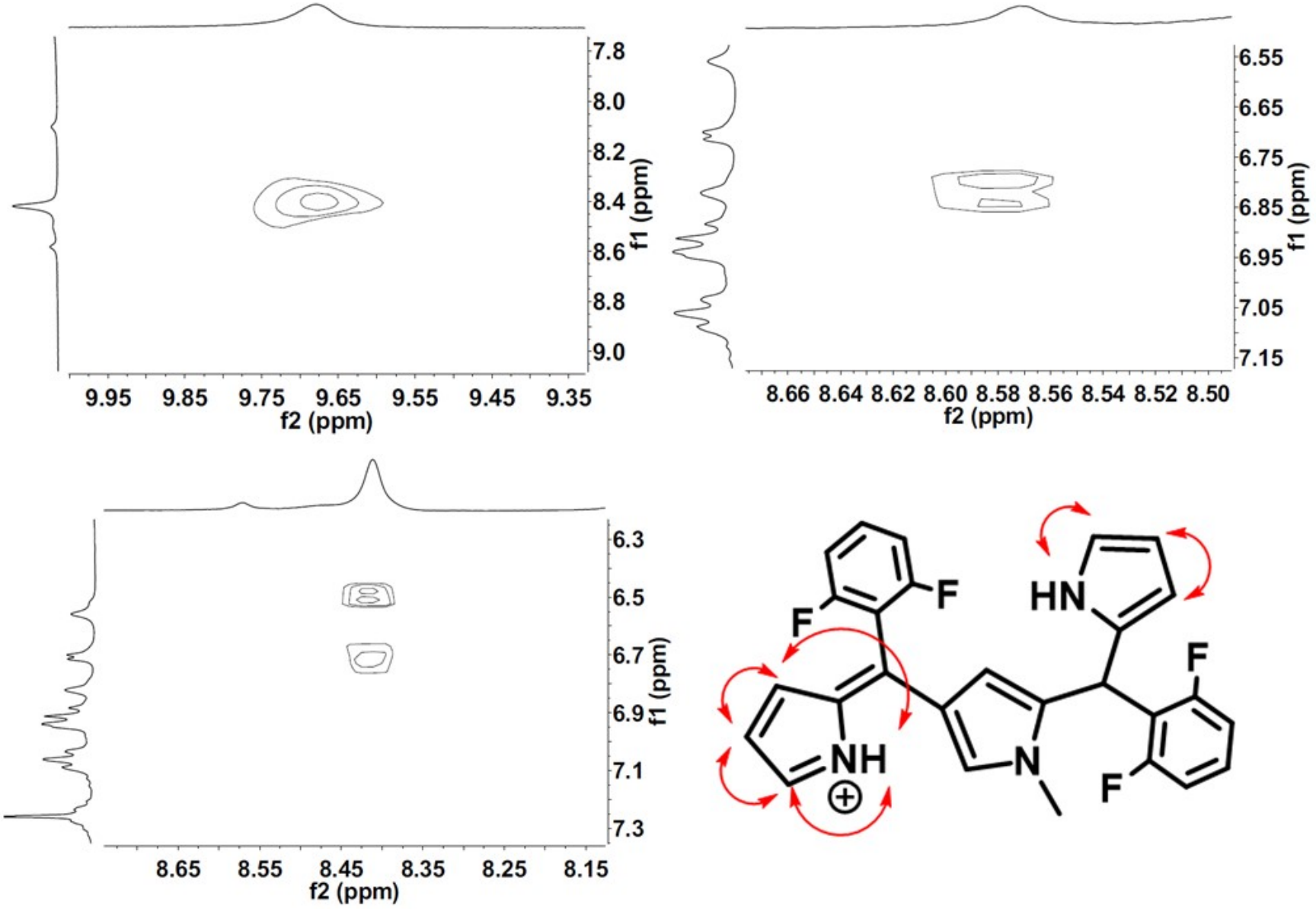


Fig. S62 ^{1}H-^{1}H 2D COSY spectra of protonated **6** in $CDCl_3$ at 298 K

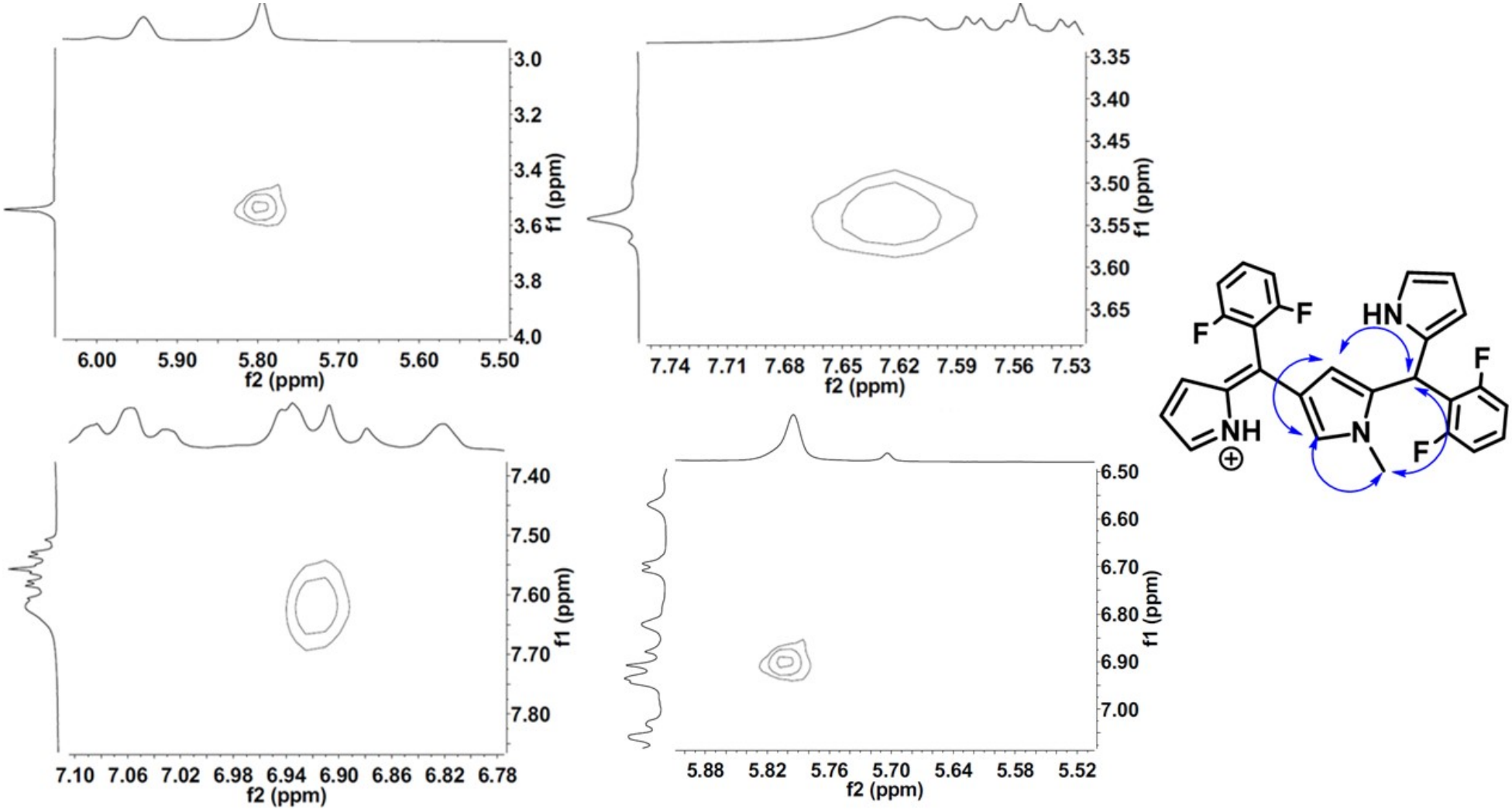


Fig. S63 ^{1}H-^{1}H 2D ROESY spectra of protonated **6** in $CDCl_3$ at 298 K

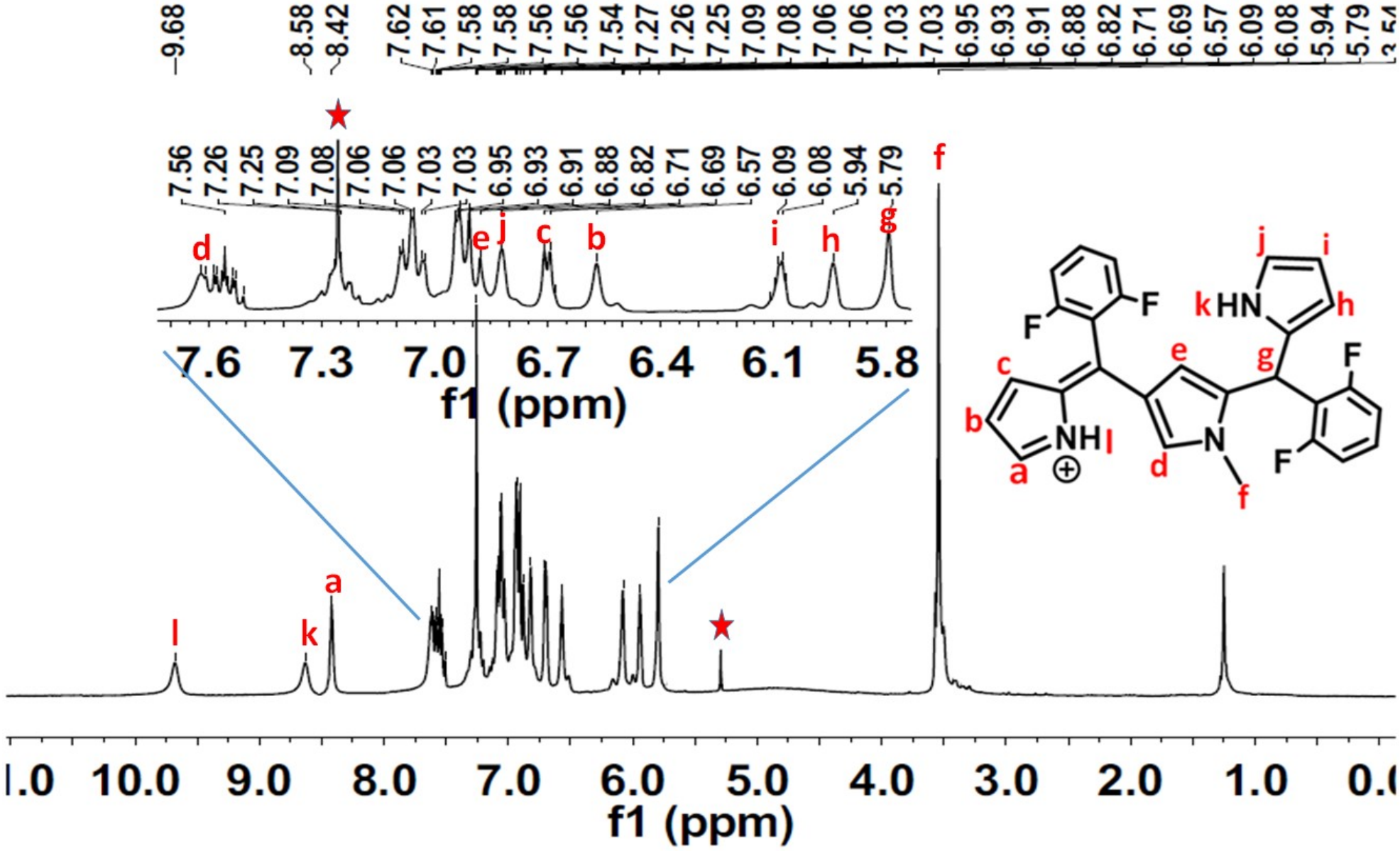


Fig. S64 Complete ^{1}H NMR spectral assignment of protonated **6** in $CDCl_3$ at 298 K

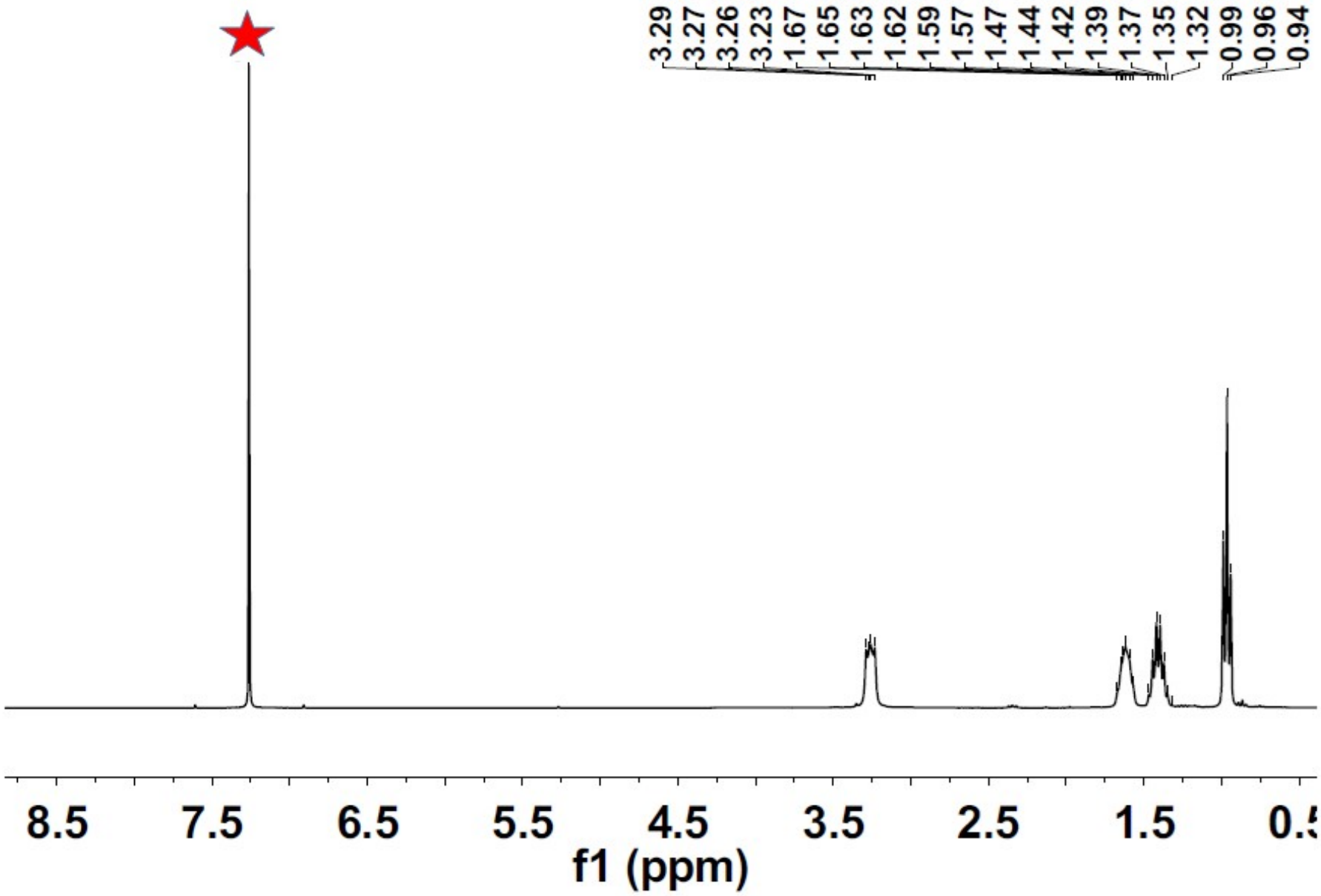


Fig. S65 ^{1}H NMR spectral pattern of TBAF in $CDCl_3$ at 298 K

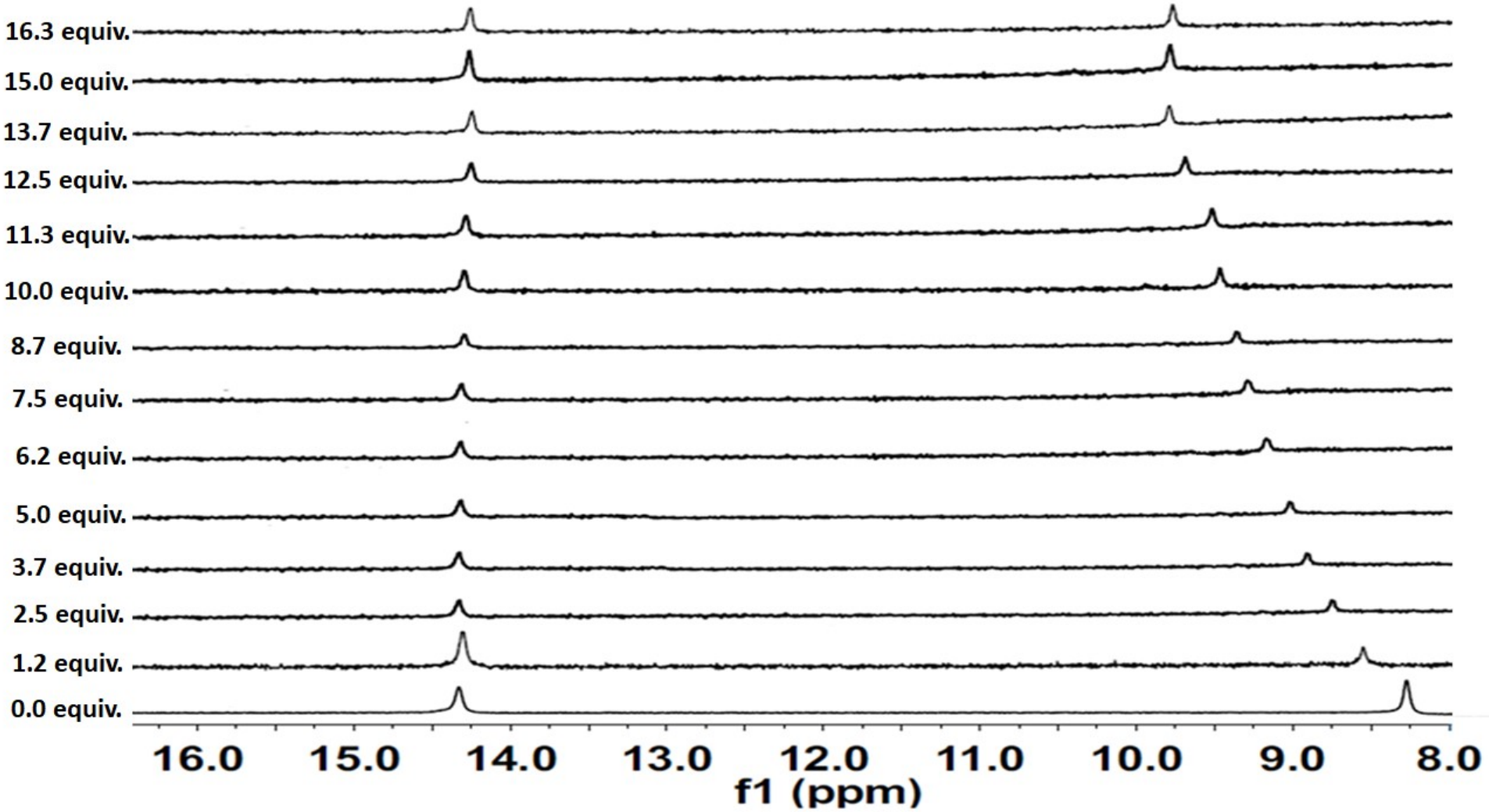


Fig. S66 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.58 M) to **5** (1×10^{-2} M) in $CDCl_3$ at 298 K

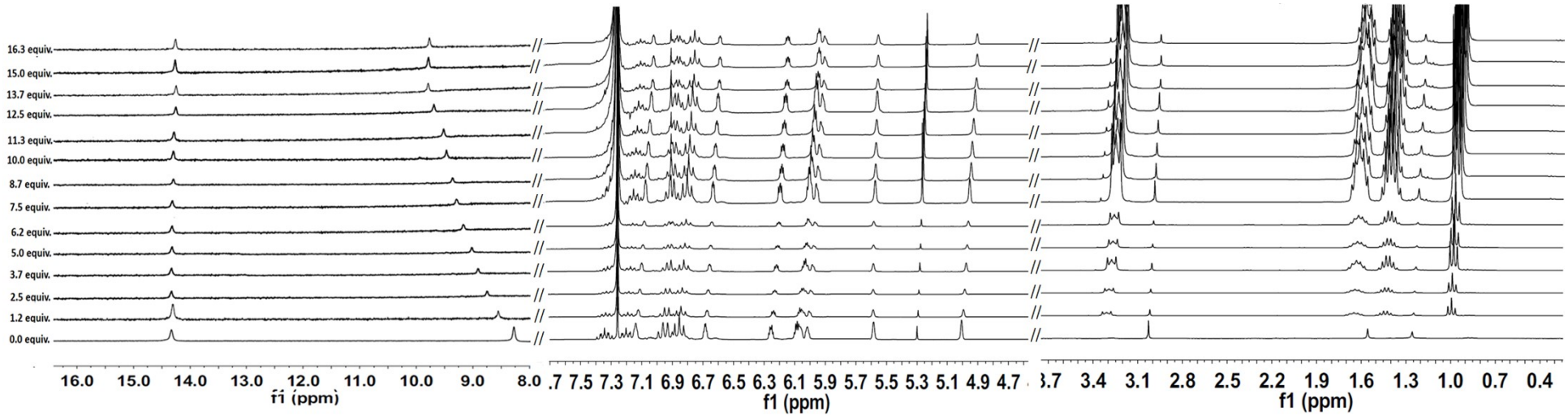


Fig. S66A ^{1}H NMR spectral pattern observed upon addition of TBAF (0.58 M) to **5** (1×10^{-2} M) in $CDCl_3$ at 298 K (full range)

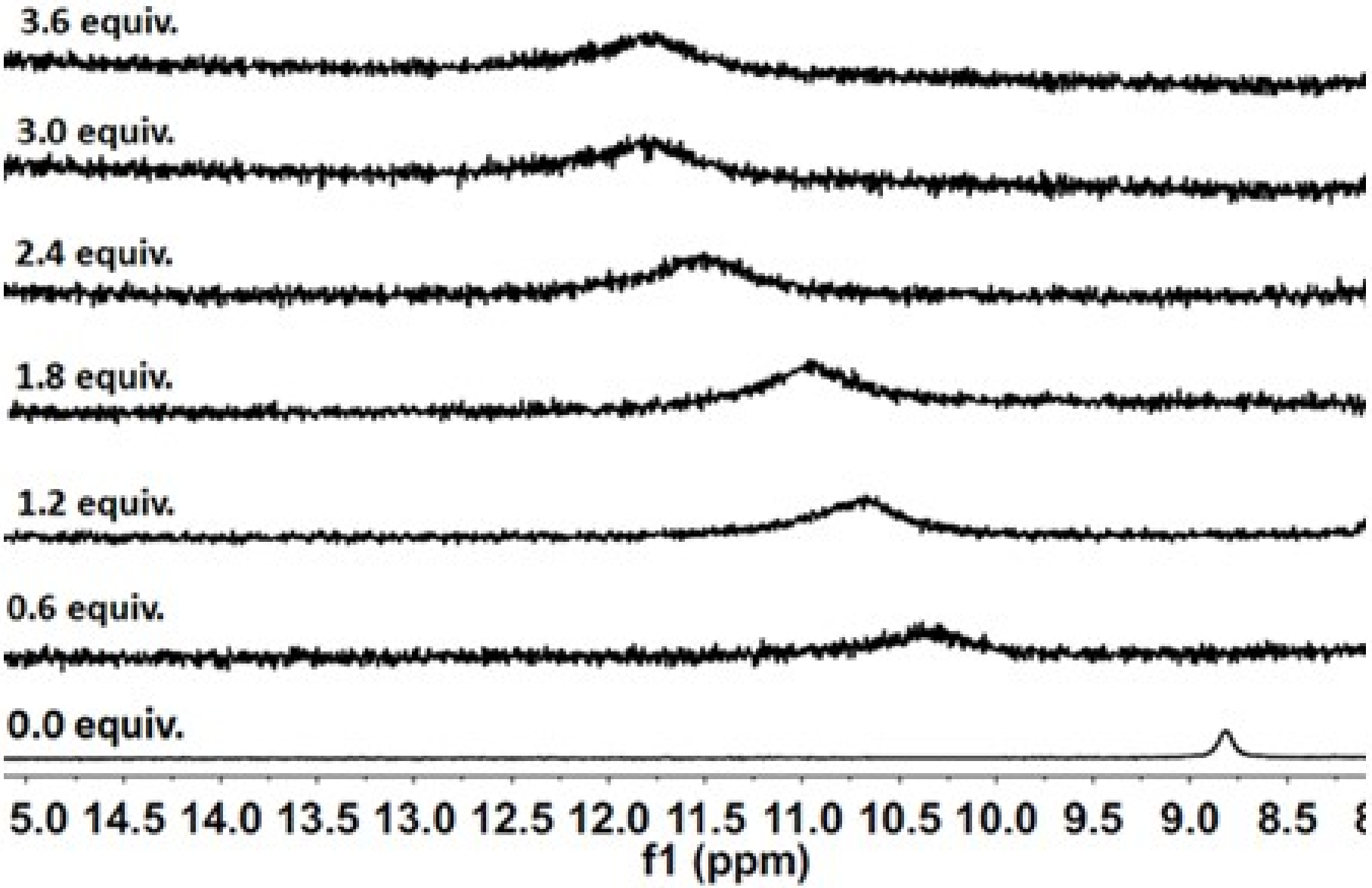


Fig. S67 ^{1}H NMR spectral pattern observed upon addition of TBAF (0.58 M) to **6** (1×10^{-2} M) in $CDCl_3$ at 298 K

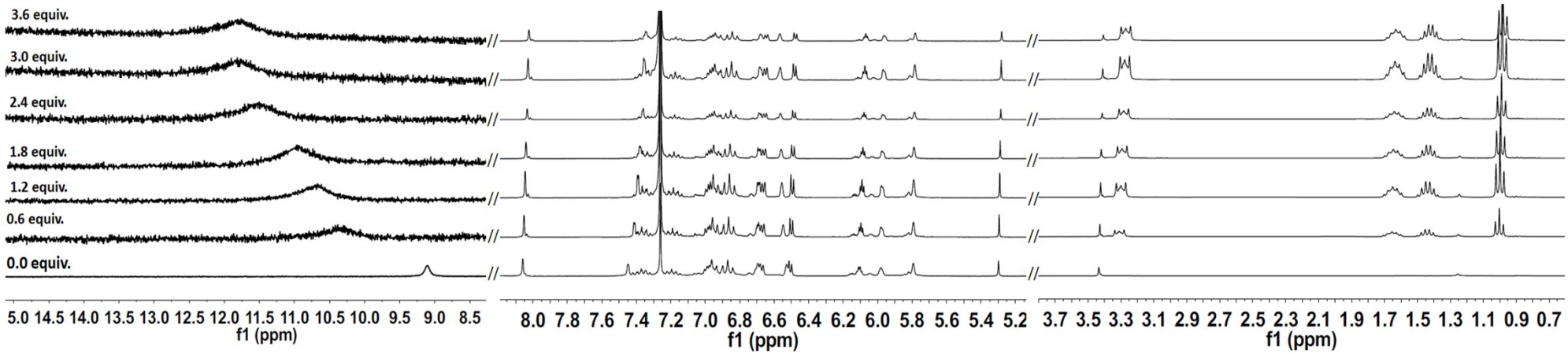


Fig. S67A ^{1}H NMR spectral pattern observed upon addition of TBAF (0.58 M) to **6** (1×10^{-2} M) in $CDCl_3$ at 298 K (full range)

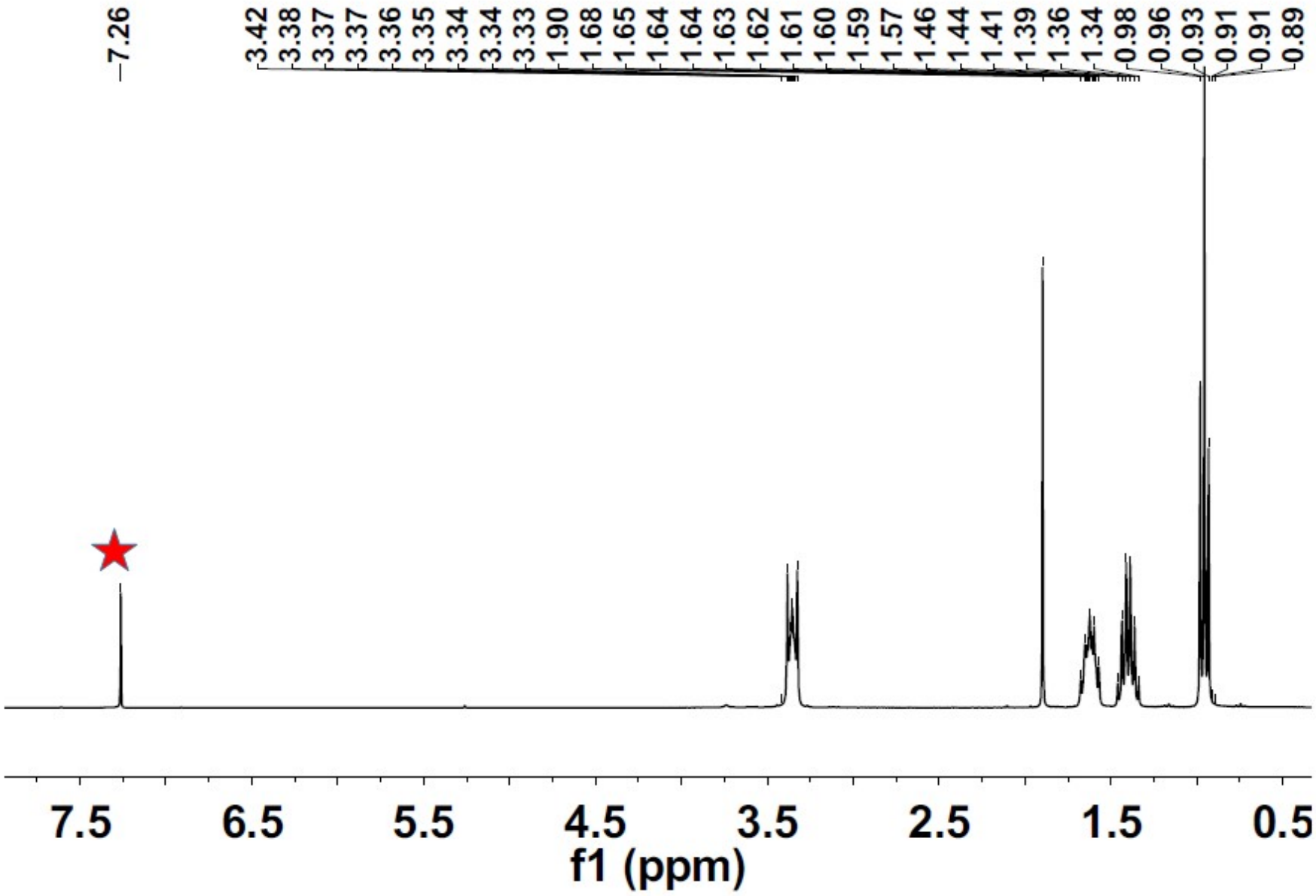


Fig. S68 ^{1}H NMR spectral pattern of TBAOAc in $CDCl_3$ at 298 K

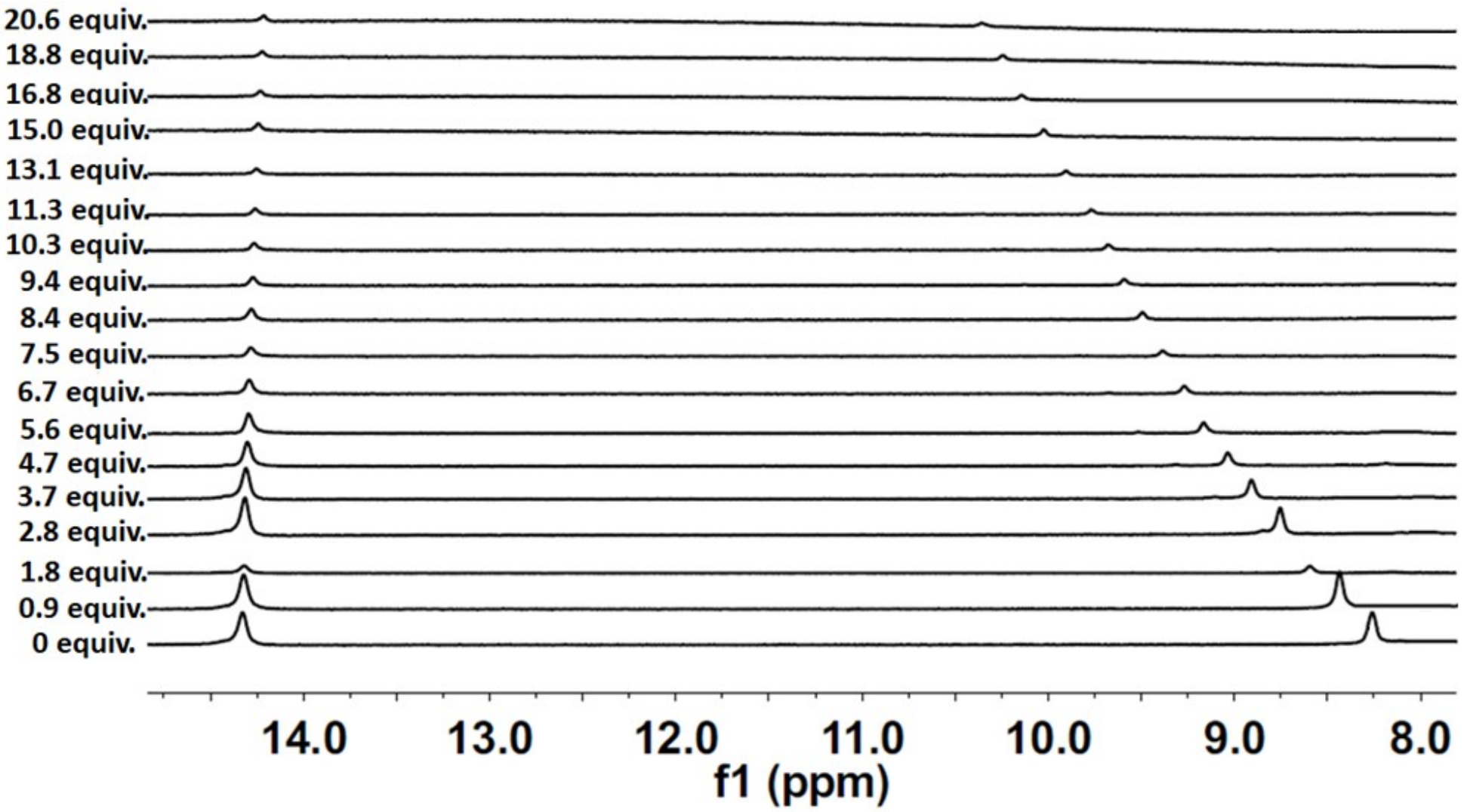


Fig. S69 ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.58 M) to **5** (1×10^{-2} M) in $CDCl_3$ at 298 K

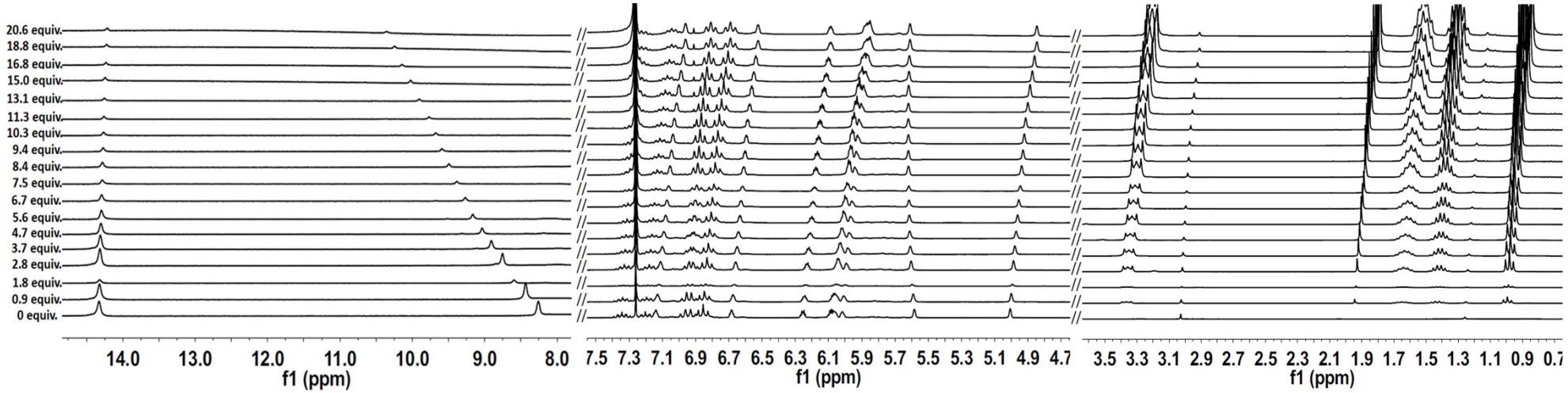


Fig. S69A ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.58 M) to **5** (1×10^{-2} M) in $CDCl_3$ at 298 K (full range)

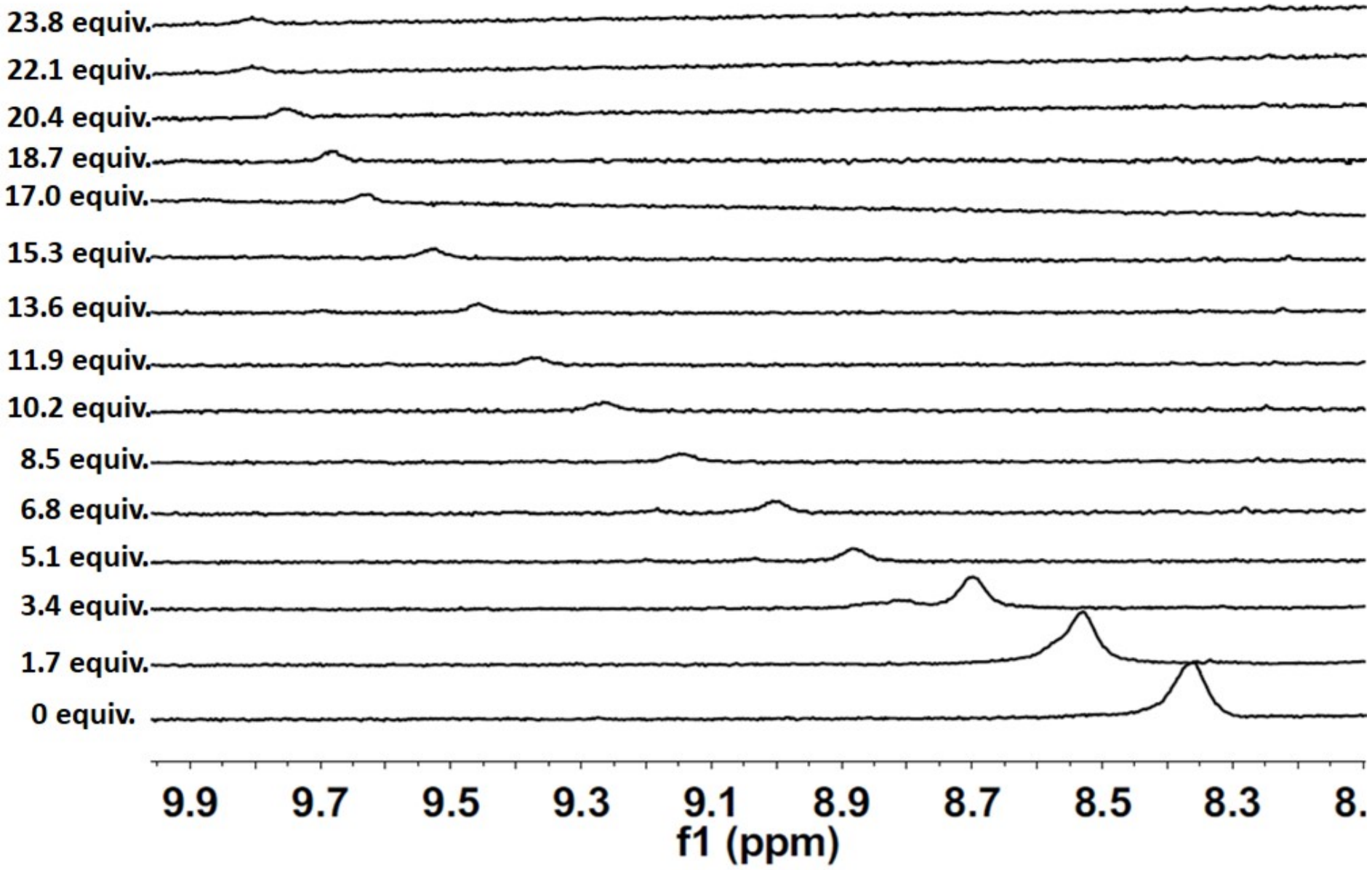


Fig. S70 ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.58 M) to **6** (1×10^{-2} M) in $CDCl_3$ at 298 K

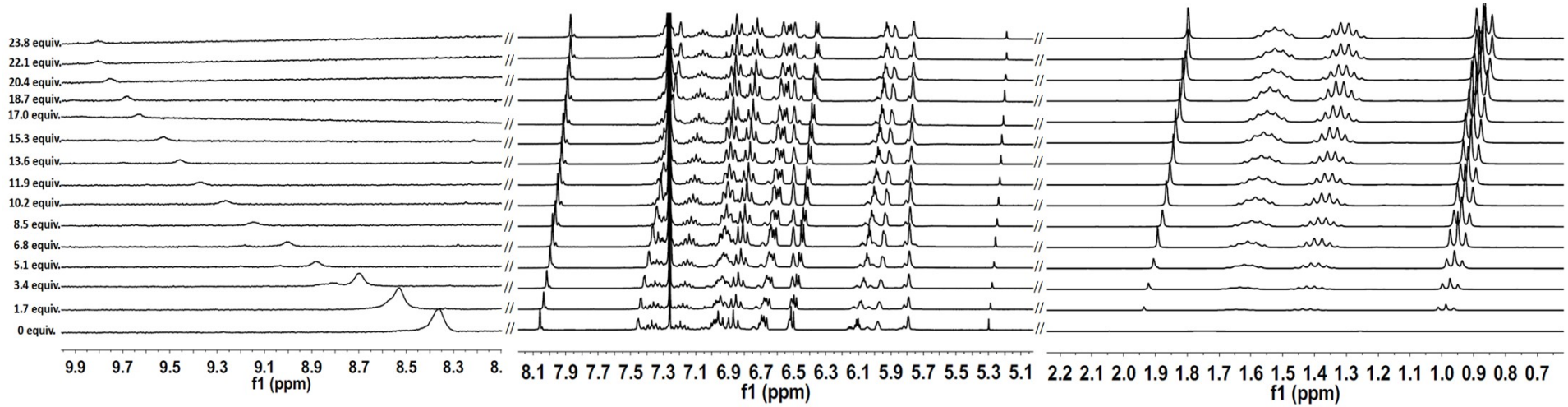


Fig. S70A ^{1}H NMR spectral pattern observed upon addition of TBAOAc (0.58 M) to **6** (1×10^{-2} M) in $CDCl_3$ at 298 K (full range)

2.5 Crystallographic Data

Parameters	5	6
Chemical formula	$C_{27}H_{19}F_4N_3O$	$C_{27}H_{19}F_4N_3$
Formula weight	477.46	461.47
Temperature	120 K(2)	115 K(2)
Crystal system	monoclinic	monoclinic
Space group	P 21/n	P 21/n
a (Å); α (°)	9.346(2); 90	9.2264(8); 90
b (Å); β(°)	12.355(4); 103.210(9)	12.9652(11); 99.768(3)
c (Å); γ (°)	20.062(4); 90	18.7337(18); 90
V (Å3); Z	2255.3(10); 4	2208.5(3); 4
ρ (calc.) g m-3	1.406	1.388
μ(Mo Kα) mm-1	0.110	0.106
2θmax (°)	25.000	27.100
R(int)	0.0952	0.0607
Completeness to θ	96.3	96.3
Data / param.	14118/1123	14118/1123
GOF	1.043	1.046
R1 [F>4σ(F)]	0.0952	0.0607
wR2 (all data)	0.2288	0.1442
max. peak/hole (e.Å-3)	1.209/-0.849	1.209/-0.849
CCDC	**2003102**	**2003103**

Table S2. Dihedral Angles of **5**

Planes	Dihedral Angle (°)
Py1-Py2	4.26
Py2-Py3	74.97
Py1-Ar1	84.58
Py2-Ar1	86.47
Py2-Ar2	86.06
Py3-Ar2	62.13

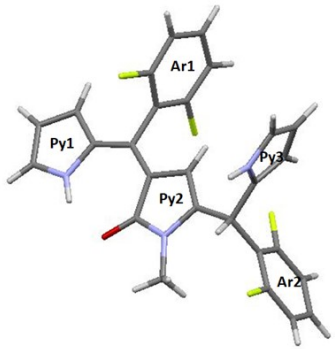
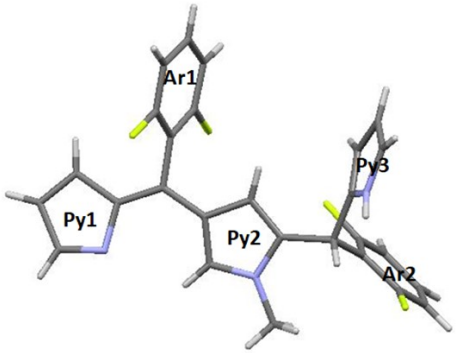


Table S3. Dihedral Angles of **6**

planes	Dihedral Angle (°)
Py1-Py2	10.05
Py2-Py3	65.37
Py1-Ar1	73.25
Py2-Ar1	72.60
Py2-Ar2	85.10
Py3-Ar2	67.98



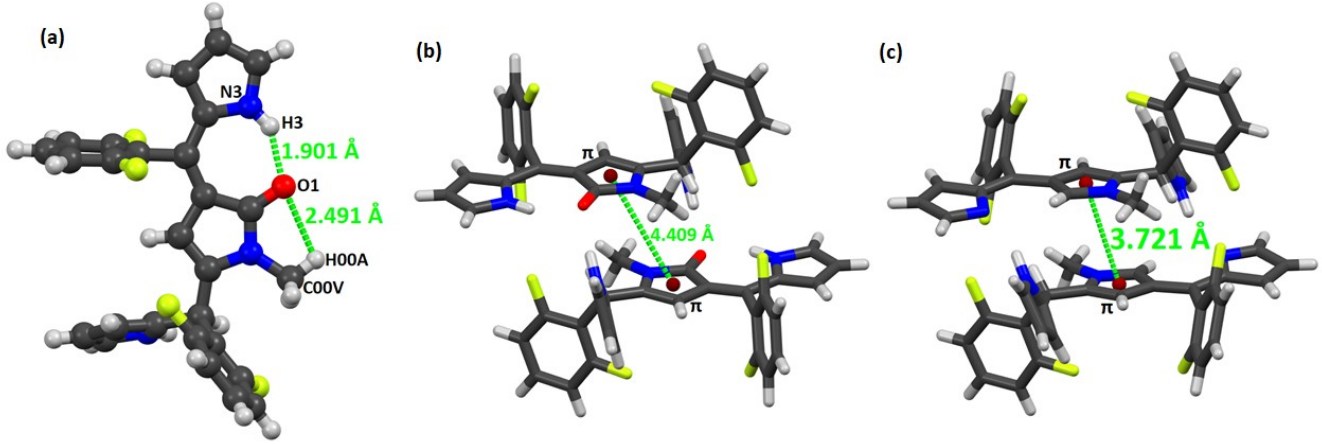


Fig. S71 Crystal structure of **5** showing (a) intra molecular H-bonding, (b) large π-π separation and (c) structure of **6** showing strong π-π stacking interaction.

2.6 Theoretical Data

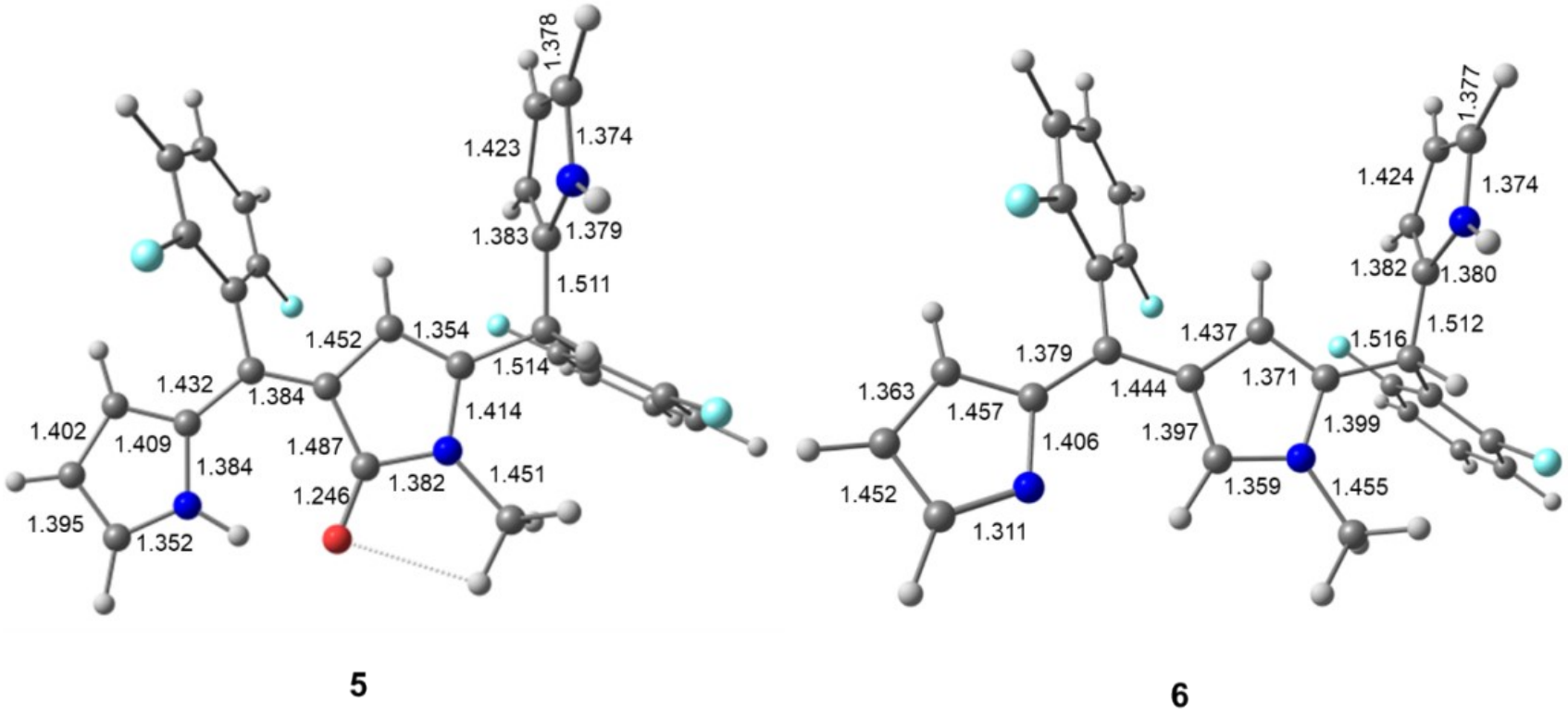


Fig. S72 A key bond lengths (Å) of gas phase optimised geometries of **5** and **6**, at B3LYP/ 6-31G (d, p) level of theory

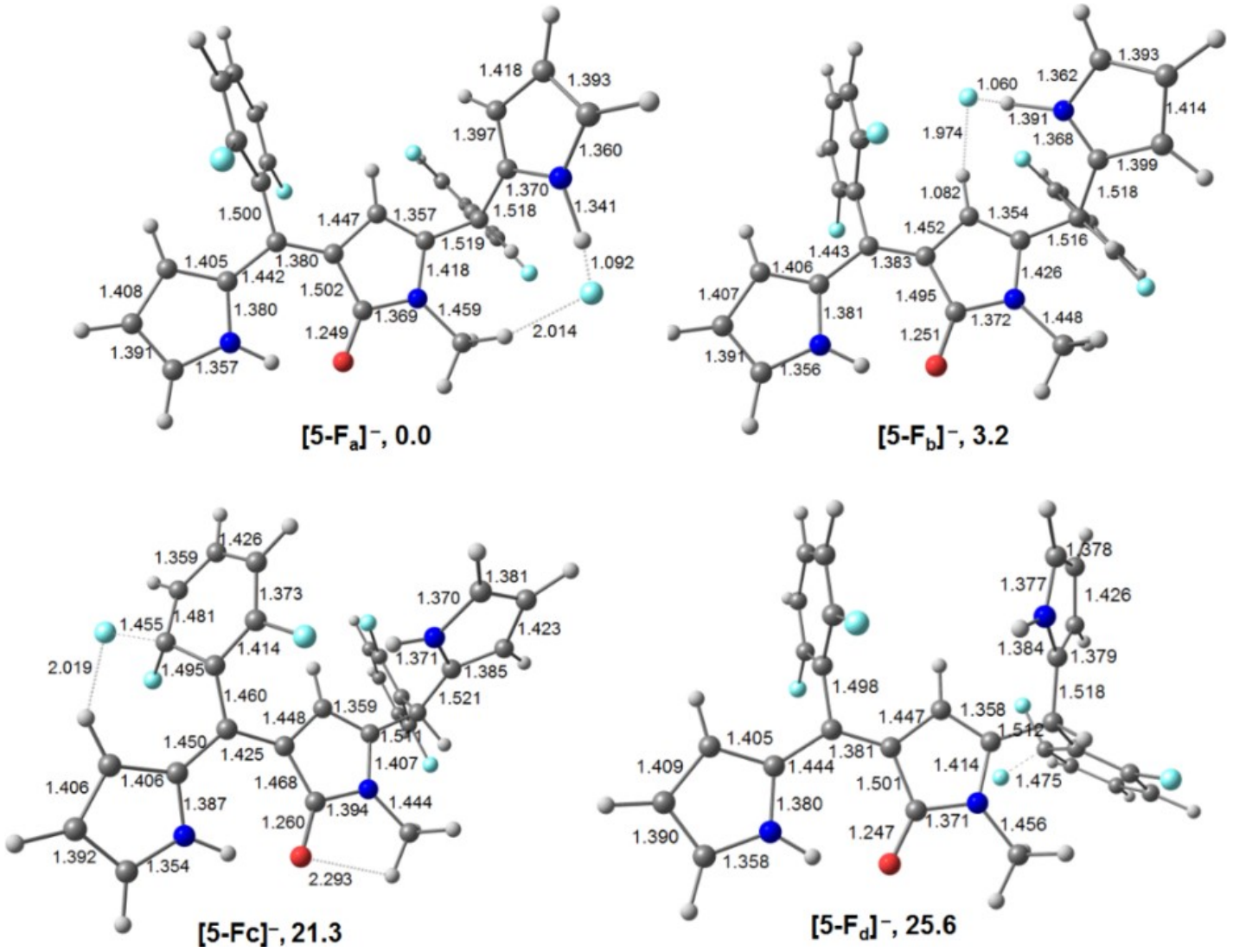


Fig. S73 A key bond lengths (Å) of gas phase optimised geometries of [**5**-F_a]$^-$, [**5**-F_b]$^-$, [**5**-F_c]$^-$ and [**5**-F_d]$^-$ at B3LYP/ 6-31G (d, p) level of theory.

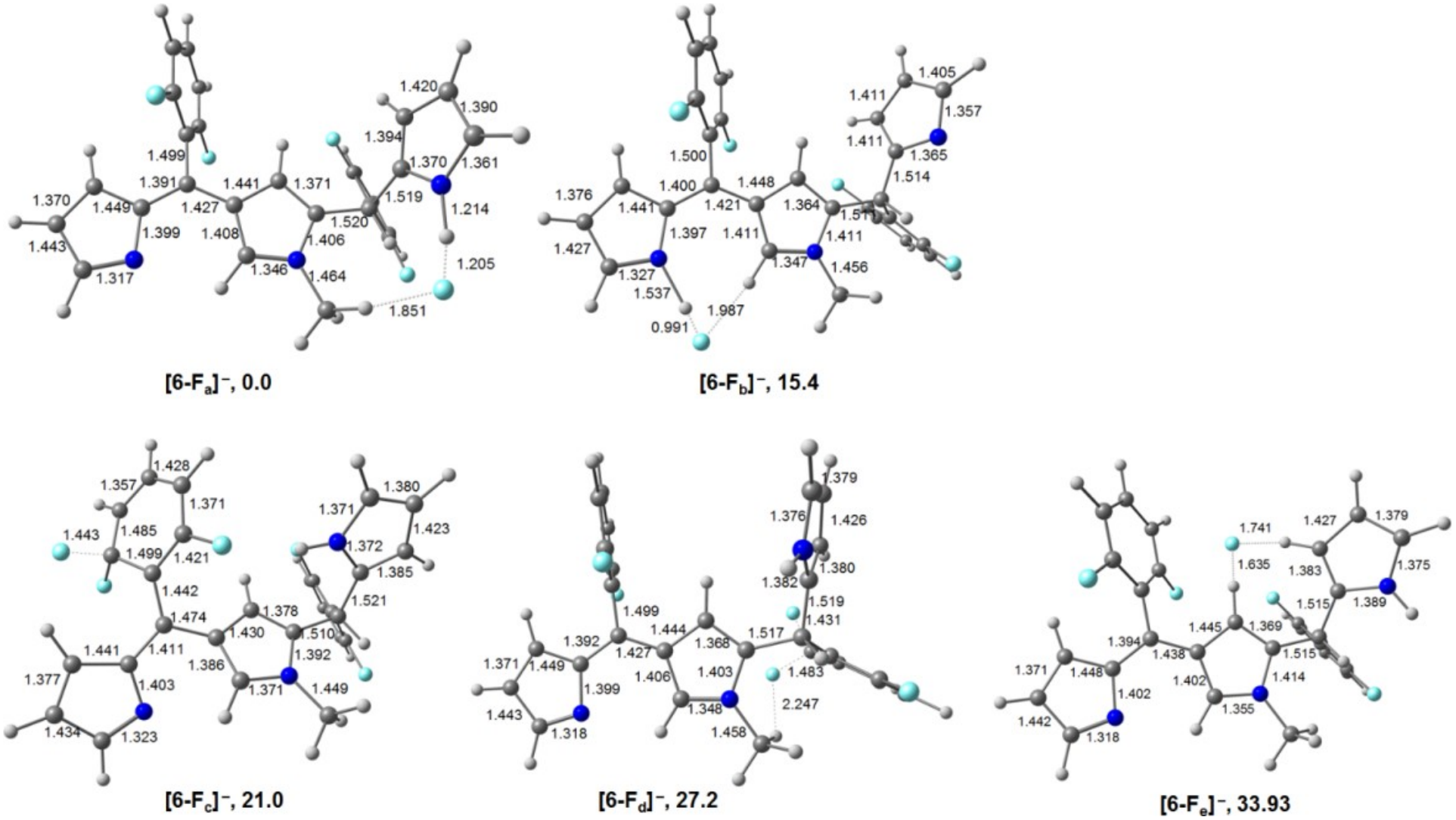


Fig. S74 A key bond lengths (Å) of gas phase optimised geometries of [**6**-F_a]$^-$, [**6**-F_b]$^-$, [**6**-F_c]$^-$ and [**6**-F_d]$^-$ at B3LYP/ 6-31G (d, p) level of theory.

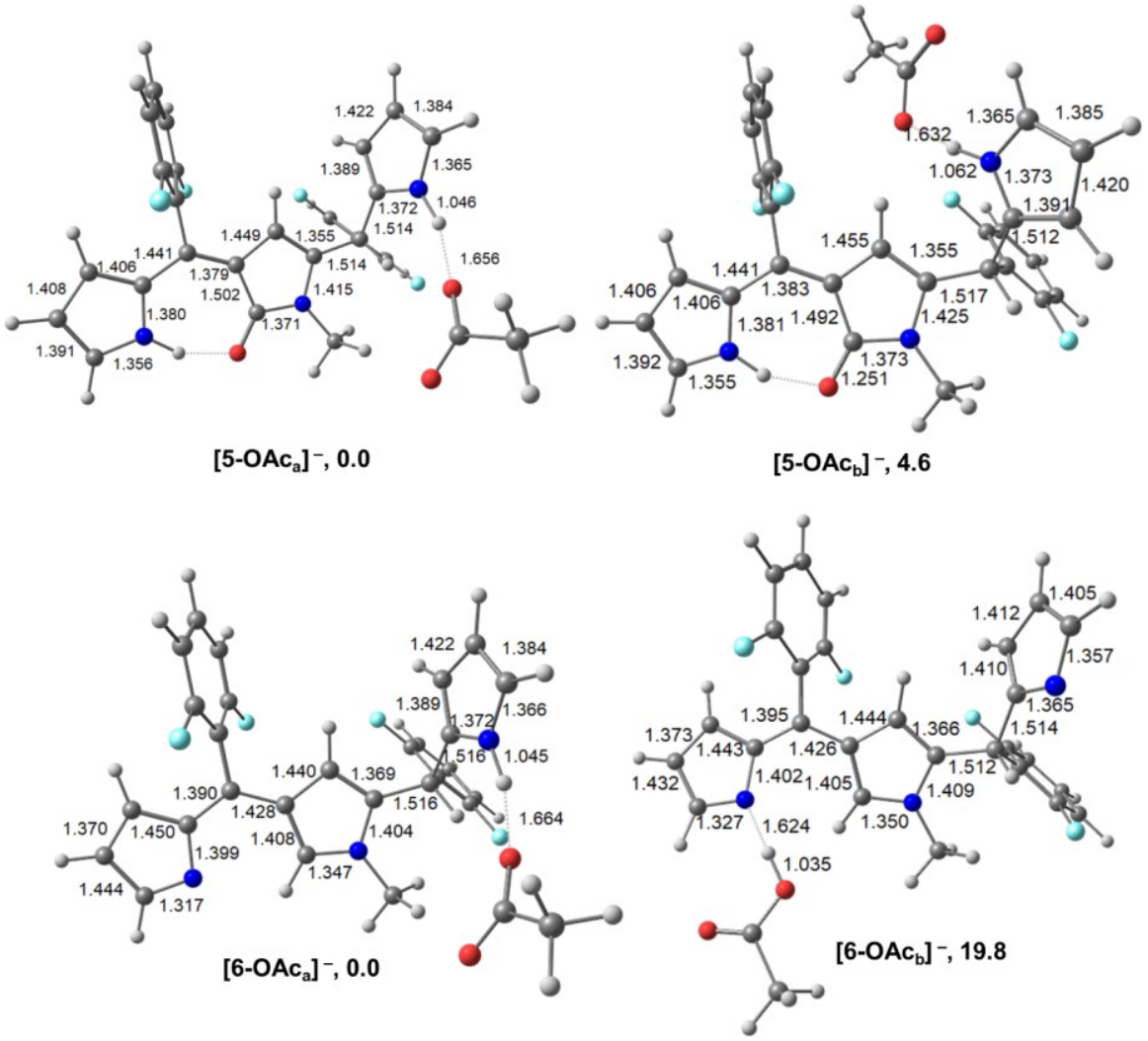
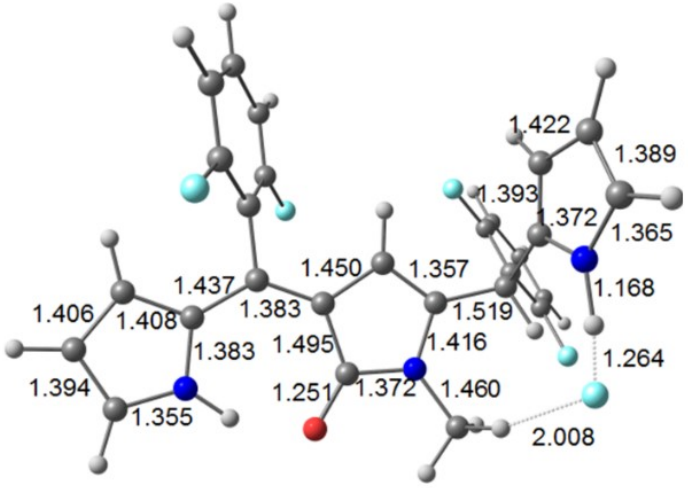
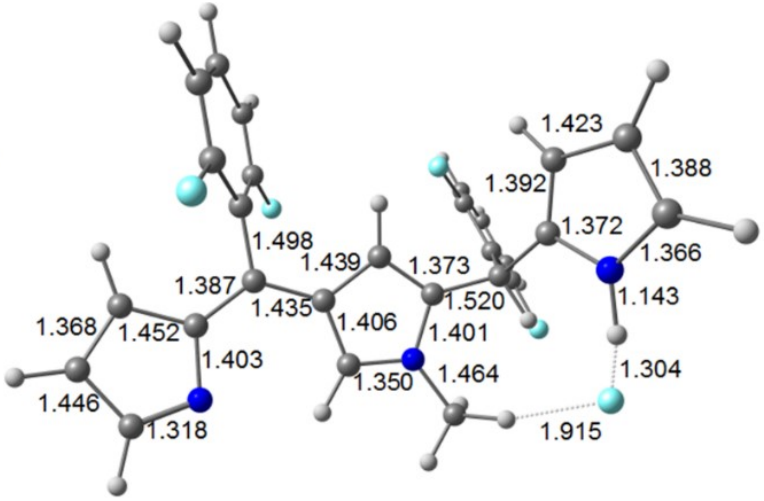


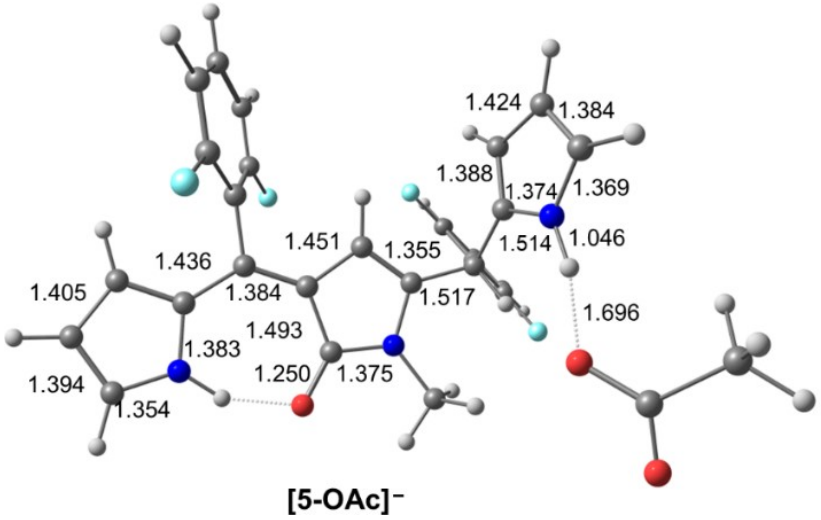
Fig. S75 A key bond lengths (Å) of gas phase optimised geometries of [**5**-OAc$_a$]$^-$, [**5**-OAc$_b$]$^-$ [**6**-OAc$_a$]$^-$ and [**6**-OAc$_b$]$^-$ at B3LYP/ 6-31G (d, p) level of theory.



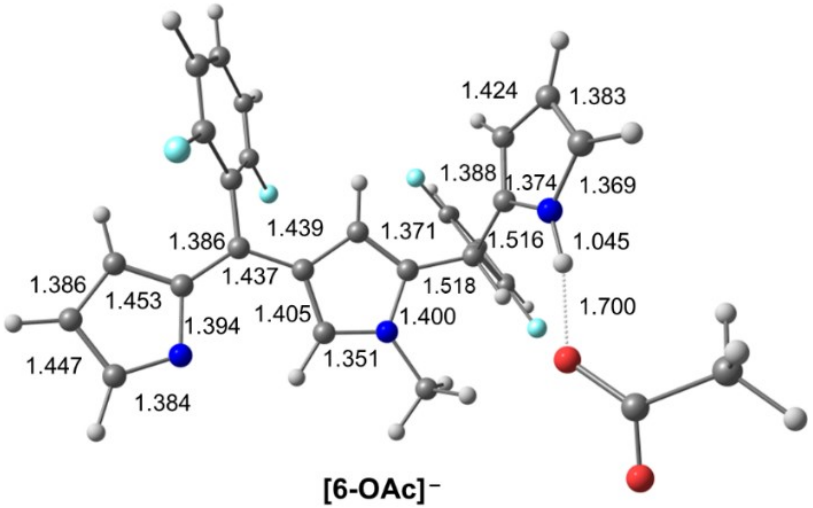
[5-F]⁻



[6-F]⁻



[5-OAc]⁻



[6-OAc]⁻

Fig. S76 A key bond lengths (Å) of solvent phase optimised geometries of [**5**-F_a]$^-$ [**6**-F_a]$^-$ [**5**-OAc_a]$^-$ [**6**-OAc_a]$^-$ at B3LYP/ 6-31G (d, p) level of theory.

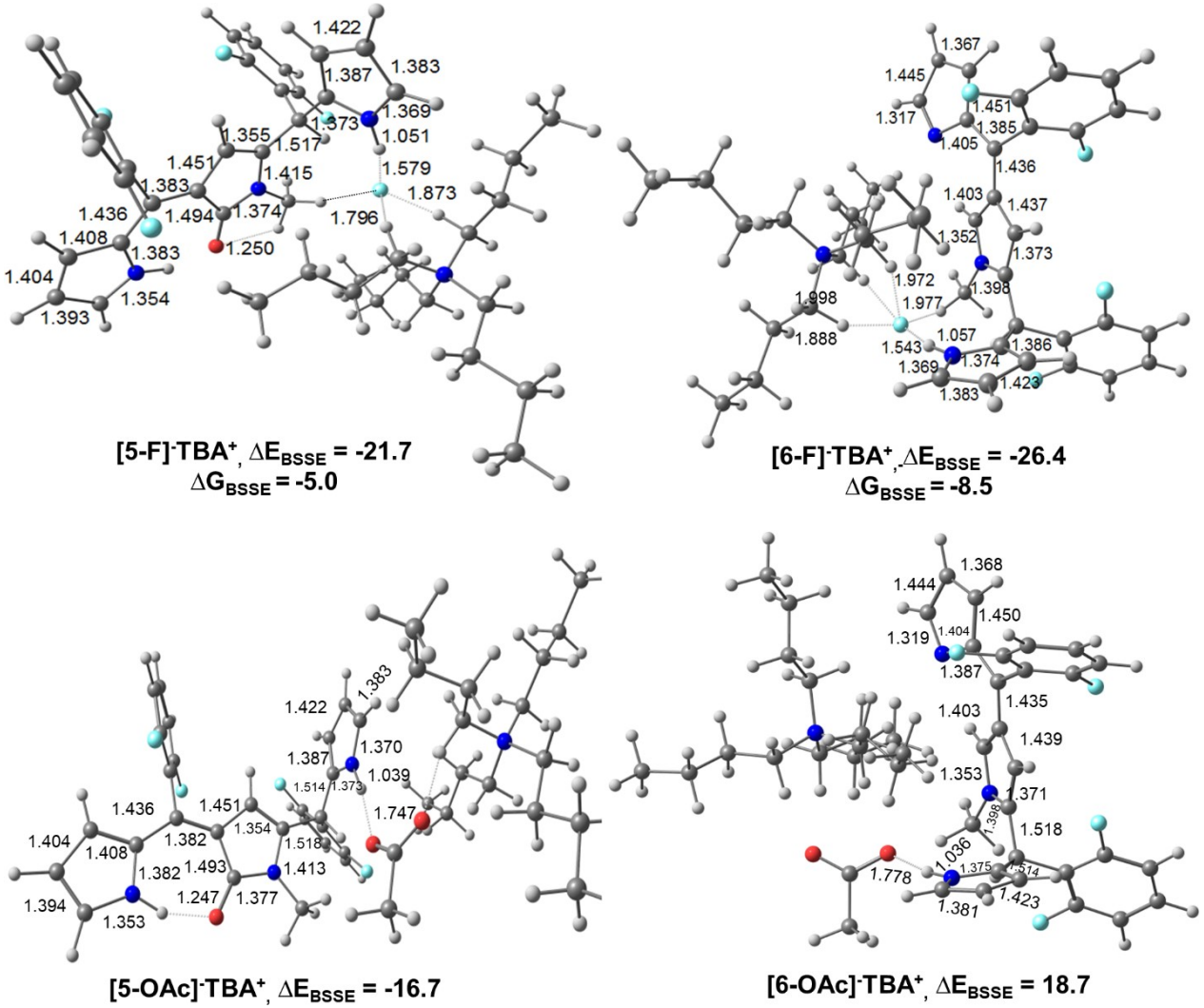
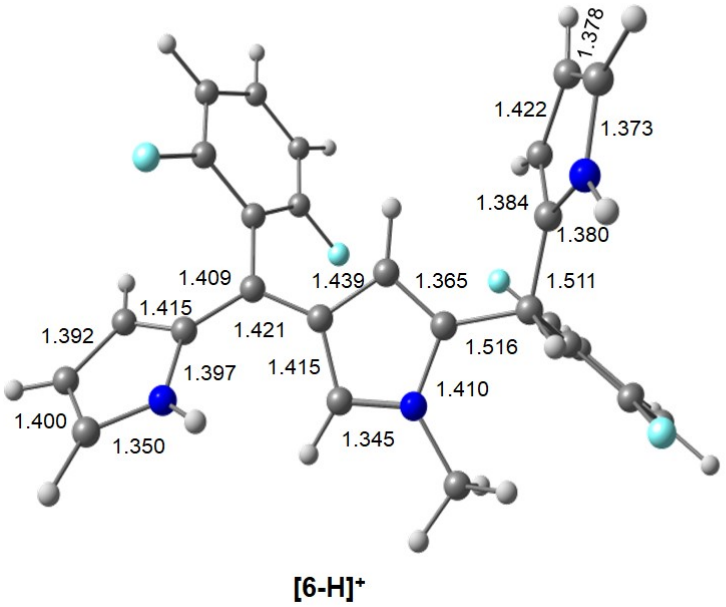


Fig. S77 A key bond lengths (Å) of DFT optimised geometries of [**5**-TBAF], [**6**-TBAF], [**5**-TBAOAc] and [**6**-TBAOAc] at B3LYP/ 6-31G (d, p) level of theory.



[6-H]⁺

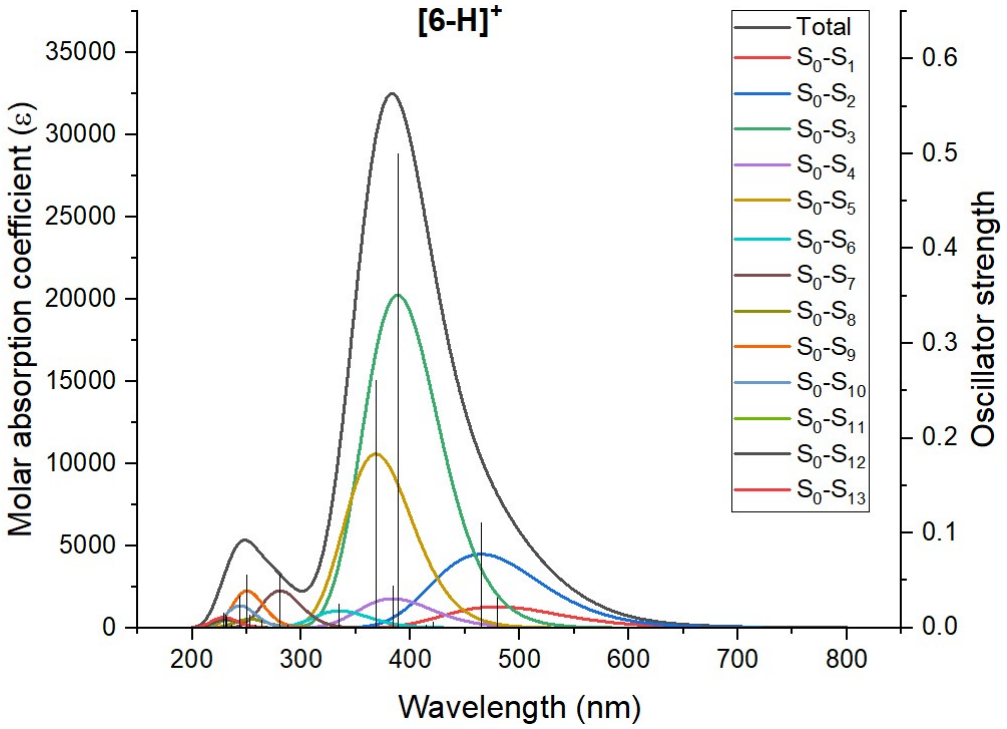


Fig.S78 A key bond lengths (Å) of optimised geometries of protonated **6** {[**6**-H] ⁺ } at B3LYP /6-31G (d, p) level for rest of atoms (b) UV-vis spectrum of most stable conformer of [**6**-H] ⁺ that is predicted from TD-DFT calculation in presence of dichloromethane solvent and at B3LYP / 6-31G (d,p) for rest of atoms

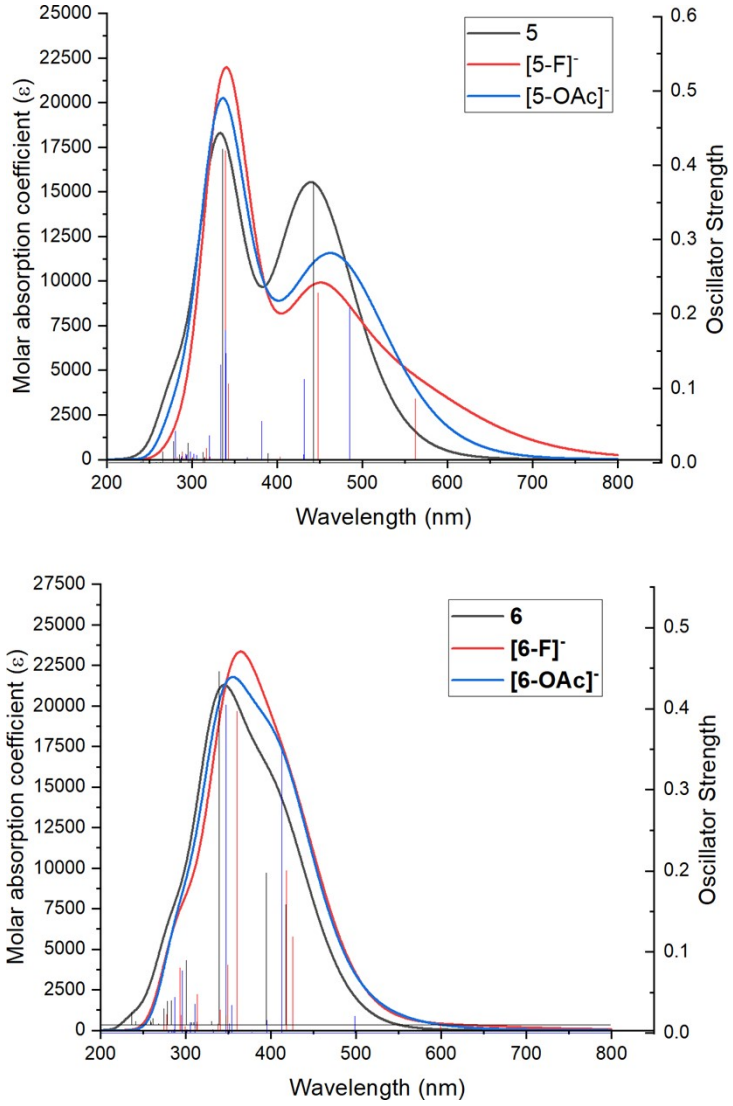


Fig. S79 Overlay of steady state absorption spectrum (total) of (a) **5**, [**5**-F]$^-$, [**5**-OAc]$^-$, (b) **6**, [**6**-F]$^-$, [**6**-OAc]$^-$, that is predicted from TD-DFT calculation in presence of chloroform and at B3LYP/6-31G (d, p) level of theory.

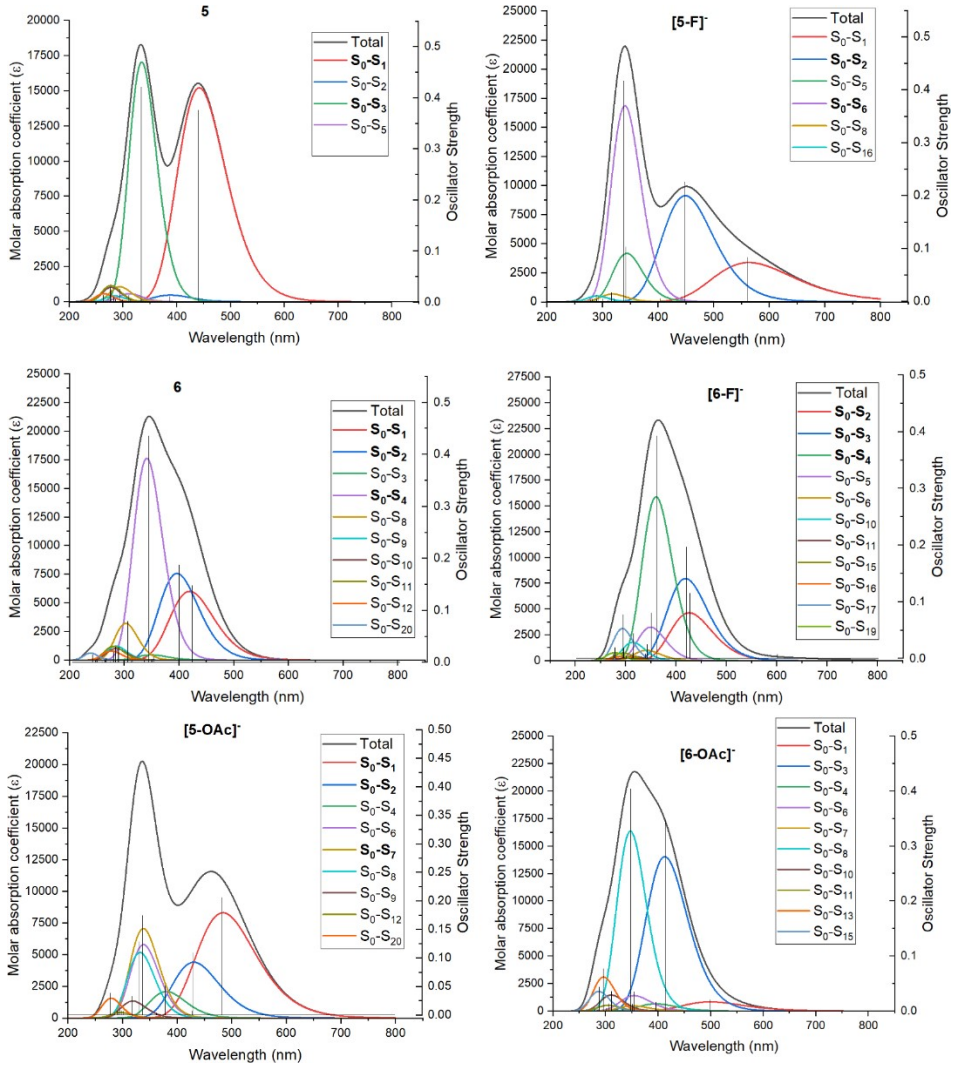


Fig. S80 Steady state absorption spectrum (total) and individual transitions of **5**, [**5**-F]$^-$, [**5**-OAc]$^-$, **6**, [**6**-F]$^-$, [**6**-OAc]$^-$, that is predicted from TD-DFT calculation in presence of chloroform and at B3LYP/6-31G (d, p) level of theory. The individual electronic transitions are represented with different colour where the major transition contributing to the total spectrum (shown in black) is labelled in bold.

Table S4. Summary of UV-vis spectral data of **5** that is predicted from TD-DFT calculation in presence of chloroform solvent and at B3LYP/6-31G (d,p) level of theory

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.8088**	**441.41**	**0.37650**	**Singlet-A**	**H -> L 94.3%**
2	3.1963	387.90	0.01180	Singlet-A	H-1 -> L 98.7%
3	**3.7065**	**334.50**	**0.42160**	**Singlet-A**	**H-2 -> L 91.2%, H -> L 5.2%**
4	3.9476	314.07	0.00660	Singlet-A	H -> L+2 53.1%, H -> L+1 46.2%
5	3.9803	311.49	0.01410	Singlet-A	H -> L+1 51.7%, H -> L+2 45.9%
6	4.1348	299.86	0.00570	Singlet-A	H-3 -> L 70.6%, H-7 -> L 15.6%, H-9 -> L 12.9%
7	4.1505	298.72	0.00410	Singlet-A	H-4 -> L 93.7%, H-5 -> L 5.4%
8	4.1809	296.55	0.00310	Singlet-A	H-7 -> L 52.4%, H-3 -> L 27.0%, H-9 -> L 17.3%
9	4.2171	294.00	0.02640	Singlet-A	H-5 -> L 90.9%
10	4.3287	286.42	0.00630	Singlet-A	H -> L+4 82.5%, H -> L+3 16.1%
11	4.3471	285.21	0.00200	Singlet-A	H -> L+3 81.8%, H -> L+4 16.7%
12	4.3701	283.71	0.01030	Singlet-A	H-9 -> L 56.9%, H-7 -> L 26.8%, H-8 -> L 12.6%
13	4.4689	277.44	0.02530	Singlet-A	H-1 -> L+1 54.2%, H-6 -> L 43.9%
14	4.4751	277.05	0.02850	Singlet-A	H-6 -> L 54.7%, H-1 -> L+1 44.2%
15	4.6937	264.15	0.01430	Singlet-A	H-8 -> L 85.7%, H-9 -> L 10.1%
16	4.7300	262.12	0.00030	Singlet-A	H-1 -> L+2 98.9%
17	4.8299	256.70	0.00060	Singlet-A	H-1 -> L+3 96.9%
18	5.0690	244.59	0.00010	Singlet-A	H-1 -> L+4 99.6%
19	5.1369	241.36	0.00260	Singlet-A	H-2 -> L+2 85.7%, H-2 -> L+1 12.2%
20	5.1923	238.78	0.00120	Singlet-A	H-2 -> L+1 85.4%, H-2 -> L+2 12.0%

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

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.9574**	**419.23**	**0.14860**	**Singlet-A**	**H -> L 82.9%, H-1 -> L 12.7%**
2	**3.1303**	**396.08**	**0.18740**	**Singlet-A**	**H-1 -> L 84.6%, H -> L 9.2%, H-2 -> L 5.0%**
3	3.5528	348.98	0.01140	Singlet-A	H-3 -> L 96.7%
4	**3.6383**	**340.78**	**0.43610**	**Singlet-A**	**H-2 -> L 88.1%, H -> L 7.2%**
5	3.7375	331.73	0.00440	Singlet-A	H-8 -> L 68.7%, H-7 -> L 27.7%
6	3.9900	310.74	0.00320	Singlet-A	H-5 -> L 97.5%
7	4.0227	308.21	0.00300	Singlet-A	H-4 -> L 97.4%
8	4.1034	302.15	0.07960	Singlet-A	H-7 -> L 69.3%, H-8 -> L 25.8%
9	4.3543	284.74	0.03020	Singlet-A	H -> L+1 50.0%, H-6 -> L 44.6%
10	4.3592	284.42	0.02510	Singlet-A	H-6 -> L 53.4%, H -> L+1 41.0%
11	4.4341	279.62	0.02960	Singlet-A	H -> L+2 79.7%, H-1 -> L+1 15.6%
12	4.4908	276.08	0.02000	Singlet-A	H-1 -> L+1 77.1%, H -> L+2 12.1%, H -> L+1 7.1%
13	4.5957	269.78	0.00180	Singlet-A	H-9 -> L 95.1%
14	4.7148	262.97	0.00840	Singlet-A	H -> L+3 87.9%, H-1 -> L+3 8.3%
15	4.7568	260.65	0.00320	Singlet-A	H-1 -> L+2 93.2%, H -> L+2 5.3%
16	4.7627	260.32	0.00530	Singlet-A	H -> L+4 94.2%
17	4.8619	255.01	0.00160	Singlet-A	H-1 -> L+3 88.9%, H -> L+3 8.5%
18	5.0584	245.11	0.00020	Singlet-A	H-1 -> L+4 94.4%
19	5.1080	242.73	0.00440	Singlet-A	H-2 -> L+1 95.8%
20	5.2140	237.79	0.01550	Singlet-A	H-2 -> L+2 96.0%

Table S6. Summary of UV-vis spectral data of [**5**-F_a]$^-$ that is predicted from TD-DFT calculation in presence of chloroform solvent and at B3LYP/6-31G (d,p) level of theory

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	2.2019	563.08	0.08330	Singlet-A	H -> L 97.8%
2	**2.7612**	**449.02**	**0.22550**	**Singlet-A**	**H-1 -> L 92.4%, H-3 -> L 5.9%**
3	3.0620	404.91	0.00530	Singlet-A	H-2 -> L 99.8%
4	3.4989	354.35	0.00060	Singlet-A	H -> L+1 92.5%, H-1 -> L+1 5.2%
5	3.6075	343.68	0.10290	Singlet-A	H -> L+2 81.8%, H-3 -> L 15.1%
6	**3.6415**	**340.48**	**0.41680**	**Singlet-A**	**H-3 -> L 74.0%, H -> L+2 16.1%**
7	**3.8470**	**322.29**	**0.00490**	**Singlet-A**	**H -> L+3 95.2%**
8	3.8994	317.96	0.01630	Singlet-A	H-1 -> L+1 93.0%, H -> L+1 5.1%
9	3.9303	315.46	0.00300	Singlet-A	H -> L+4 97.8%
10	3.9796	311.55	0.00160	Singlet-A	H-4 -> L 98.5%
11	4.1070	301.89	0.00420	Singlet-A	H-1 -> L+2 62.0%, H-12 -> L 12.0%,
12	4.1120	301.52	0.00350	Singlet-A	H-1 -> L+2 33.9%, H-12 -> L 22.3%,
13	4.2096	294.53	0.00640	Singlet-A	H-5 -> L 46.3%, H-6 -> L 44.4%
14	4.2163	294.06	0.00110	Singlet-A	H-5 -> L 50.8%, H-6 -> L 48.3%
15	4.2485	291.83	0.00380	Singlet-A	H-1 -> L+3 95.0%
16	4.2758	289.97	0.01210	Singlet-A	H-8 -> L 96.1%
17	4.3736	283.48	0.00430	Singlet-A	H-10 -> L 96.5%
18	4.3875	282.59	0.00200	Singlet-A	H-7 -> L 95.7%
19	4.4254	280.16	0.00240	Singlet-A	H-1 -> L+4 96.1%
20	4.4449	278.94	0.00020	Singlet-A	H-2 -> L+1 88.5%, H-2 -> L+2 11.3%

Table S7. Summary of UV-vis spectral data of [**5**-OAc_a]$^-$ that is predicted from TD-DFT calculation in presence of chloroform solvent and at B3LYP/6-31G (d,p) level of theory

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**2.5621**	**483.92**	**0.20540**	**Singlet-A**	**H -> L 91.0%, H-2 -> L 6.5%**
2	**2.8804**	**430.44**	**0.10890**	**Singlet-A**	**H-2 -> L 86.4%**
3	2.8857	429.65	0.00720	Singlet-A	H-1 -> L 95.2%
4	3.2615	380.14	0.05180	Singlet-A	H-3 -> L 98.3%
5	3.4093	363.66	0.00330	Singlet-A	H-4 -> L 99.6%
6	**3.6638**	**338.40**	**0.14320**	**Singlet-A**	**H-5 -> L 62.8%, H-6 -> L 27.3%,**
7	**3.6663**	**338.17**	**0.17450**	**Singlet-A**	**H-6 -> L 53.0%, H-5 -> L 36.4%,**
8	**3.7331**	**332.12**	**0.12800**	**Singlet-A**	**H -> L+1 85.9%, H-6 -> L 10.1%**
9	3.8916	318.59	0.03300	Singlet-A	H -> L+2 95.2%
10	4.0780	304.03	0.00670	Singlet-A	H -> L+3 97.2%
11	4.1257	300.52	0.00760	Singlet-A	H-12 -> L 44.4%, H-10 -> L 30.8%,
12	4.1848	296.27	0.01070	Singlet-A	H-2 -> L+2 50.1%, H-2 -> L+1 45.2%
13	4.2205	293.77	0.00310	Singlet-A	H -> L+4 92.8%
14	4.2366	292.65	0.00720	Singlet-A	H-8 -> L 74.9%, H-2 -> L+1 11.1%,
15	4.2537	291.47	0.00800	Singlet-A	H-2 -> L+1 40.1%, H-2 -> L+2 38.0%,
16	4.3257	286.62	0.00020	Singlet-A	H-1 -> L+2 59.8%, H-1 -> L+1 39.8%
17	4.3273	286.52	0.00450	Singlet-A	H-9 -> L 97.8%
18	4.3843	282.79	0.00000	Singlet-A	H-1 -> L+1 60.0%, H-1 -> L+2 39.7%
19	4.4106	281.11	0.00160	Singlet-A	H-7 -> L 97.7%
20	4.4412	279.17	0.03870	Singlet-A	H-11 -> L 66.6%, H-12 -> L 31.2%

Table S8. Summary of UV-vis spectral data of [**6**-F_a]$^-$ that is predicted from TD-DFT calculation in presence of chloroform solvent and at B3LYP/6-31G (d,p) level of theory

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	2.0677	599.62	0.00730	Singlet-A	H -> L 99.7%
2	**2.9110**	**425.92**	**0.11490**	**Singlet-A**	**H-1 -> L 53.3%, H-2 -> L 43.9%**
3	**2.9618**	**418.61**	**0.19710**	**Singlet-A**	**H-2 -> L 54.2%, H-1 -> L 35.7%, H-3 -> L 9.0%**
4	**3.4443**	**359.97**	**0.39320**	**Singlet-A**	**H-3 -> L 83.4%, H-1 -> L 8.1%, H-5 -> L 6.1%**
5	3.5506	349.19	0.08050	Singlet-A	H-5 -> L 91.7%
6	3.6373	340.87	0.02500	Singlet-A	H -> L+2 74.1%, H -> L+1 25.0%
7	3.6678	338.03	0.00820	Singlet-A	H -> L+1 74.1%, H -> L+2 24.8%
8	3.7388	331.61	0.00060	Singlet-A	H-11 -> L 83.3%, H-4 -> L 7.5%
9	3.7817	327.85	0.00030	Singlet-A	H-4 -> L 92.3%, H-11 -> L 6.8%
10	3.9500	313.88	0.04430	Singlet-A	H-6 -> L 91.9%, H-7 -> L 5.5%
11	3.9606	313.04	0.01050	Singlet-A	H-7 -> L 90.7%, H-6 -> L 6.4%
12	3.9620	312.93	0.00070	Singlet-A	H -> L+3 90.4%, H -> L+4 6.9%
13	3.9902	310.72	0.00240	Singlet-A	H -> L+4 92.0%, H -> L+3 7.3%
14	4.1382	299.61	0.00450	Singlet-A	H-10 -> L 98.5%
15	4.2076	294.67	0.01850	Singlet-A	H-8 -> L 46.8%, H-12 -> L 33.6%, H-1 -> L+1 15.3%
16	4.2116	294.39	0.01090	Singlet-A	H-8 -> L 50.8%, H-1 -> L+1 27.0%, H-12 -> L 19.1%
17	4.2268	293.33	0.07720	Singlet-A	H-1 -> L+1 52.1%, H-12 -> L 39.7%
18	4.3295	286.37	0.00110	Singlet-A	H-9 -> L 94.7%
19	4.4619	277.87	0.01960	Singlet-A	H-1 -> L+2 88.6%, H-2 -> L+2 8.0%
20	4.5150	274.61	0.00830	Singlet-A	H-2 -> L+1 57.8%, H-2 -> L+2 31.9%, H-1 -> L+2 5.7%

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

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	2.4864	498.65	0.02060	Singlet-A	H -> L 98.8%
2	2.7555	449.95	0.00040	Singlet-A	H-1 -> L 99.7%
3	**3.0058**	**412.48**	**0.34720**	**Singlet-A**	**H-2 -> L 89.0%, H-6 -> L 8.3%**
4	3.1365	395.29	0.01620	Singlet-A	H-3 -> L 97.4%
5	3.2852	377.40	0.00090	Singlet-A	H-4 -> L 99.6%
6	3.5011	354.13	0.03460	Singlet-A	H-5 -> L 88.2%, H-7 -> L 9.6%
7	3.5335	350.88	0.01190	Singlet-A	H-7 -> L 77.2%, H-6 -> L 11.3%, H-5 -> L 10.7%
8	**3.5732**	**346.98**	**0.40450**	**Singlet-A**	**H-6 -> L 77.0%, H-7 -> L 11.6%, H-2 -> L 8.2%**
9	3.7321	332.21	0.00340	Singlet-A	H-11 -> L 59.2%, H-10 -> L 33.0%, H-12 -> L 6.9%
10	3.9910	310.66	0.03600	Singlet-A	H -> L+2 84.0%, H -> L+1 14.6%
11	4.0628	305.17	0.01310	Singlet-A	H -> L+1 79.6%, H -> L+2 14.1%, H-2 -> L+1 5.6%
12	4.1132	301.43	0.00480	Singlet-A	H-9 -> L 98.7%
13	4.1891	295.97	0.07670	Singlet-A	H-12 -> L 85.6%, H-11 -> L 10.7%
14	4.2616	290.93	0.00030	Singlet-A	H-8 -> L 99.4%
15	4.3238	286.75	0.04420	Singlet-A	H-2 -> L+1 91.7%, H -> L+1 5.2%
16	4.3443	285.40	0.00300	Singlet-A	H -> L+4 76.0%, H -> L+3 22.0%
17	4.3658	283.99	0.00010	Singlet-A	H-1 -> L+2 86.7%, H-1 -> L+1 12.1%
18	4.3698	283.73	0.00240	Singlet-A	H -> L+3 73.7%, H -> L+4 22.1%
19	4.4289	279.94	0.00220	Singlet-A	H-10 -> L 64.4%, H-11 -> L 28.2%
20	4.4368	279.45	0.00040	Singlet-A	H-1 -> L+1 86.6%, H-1 -> L+2 12.0%

Table S10. Summary of UV-vis spectral data of [**6**-H]$^{+}$ that is predicted from TD-DFT calculation in presence of chloroform solvent and at B3LYP/6-31G (d,p) level of theory

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	1.6633	745.41	0.00090	Singlet-A	H -> L 99.9%
2	2.5870	479.26	0.03200	Singlet-A	H-1 -> L 93.0%
3	**2.6686**	**464.60**	**0.11090**	**Singlet-A**	**H-2 -> L 85.9%, H-4 -> L 10.5%**
4	2.9463	420.81	0.00620	Singlet-A	H-3 -> L 99.4%
5	2.9903	414.62	0.00350	Singlet-A	H-5 -> L 99.1%
6	**3.1934**	**388.25**	**0.50080**	**Singlet-A**	**H-4 -> L 46.7%, H-6 -> L 36.1%, H-2 -> L 10.4%,**
7	3.2319	383.63	0.04410	Singlet-A	H-6 -> L 59.1%, H-4 -> L 38.6%
8	**3.3675**	**368.18**	**0.26170**	**Singlet-A**	H-7 -> L 96.8%
9	3.7038	334.75	0.02570	Singlet-A	H-8 -> L 98.5%
10	4.3069	287.87	0.00250	Singlet-A	H -> L+1 98.8%
11	4.4204	280.48	0.05600	Singlet-A	H -> L+2 97.1%
12	4.6926	264.21	0.00830	Singlet-A	H -> L+3 89.5%, H -> L+4 7.9%
13	4.8029	258.14	0.00290	Singlet-A	H -> L+4 56.7%, H -> L+5 32.6%, H -> L+3 8.0%
14	4.9042	252.81	0.01320	Singlet-A	H -> L+5 62.6%, H -> L+4 32.2%
15	4.9540	250.27	0.05570	Singlet-A	H-9 -> L 87.8%
16	5.0839	243.88	0.03340	Singlet-A	H-1 -> L+1 53.3%, H-2 -> L+1 41.5%
17	5.2388	236.67	0.00370	Singlet-A	H-2 -> L+1 54.8%, H-1 -> L+1 43.9%
18	5.3453	231.95	0.01140	Singlet-A	H-1 -> L+2 64.4%, H-3 -> L+2 17.8%
19	5.3714	230.82	0.01280	Singlet-A	H-3 -> L+2 38.6%, H-1 -> L+2 31.7%,
20	5.4170	228.88	0.01590	Singlet-A	H-5 -> L+1 68.3%, H-7 -> L+3 18.1%,

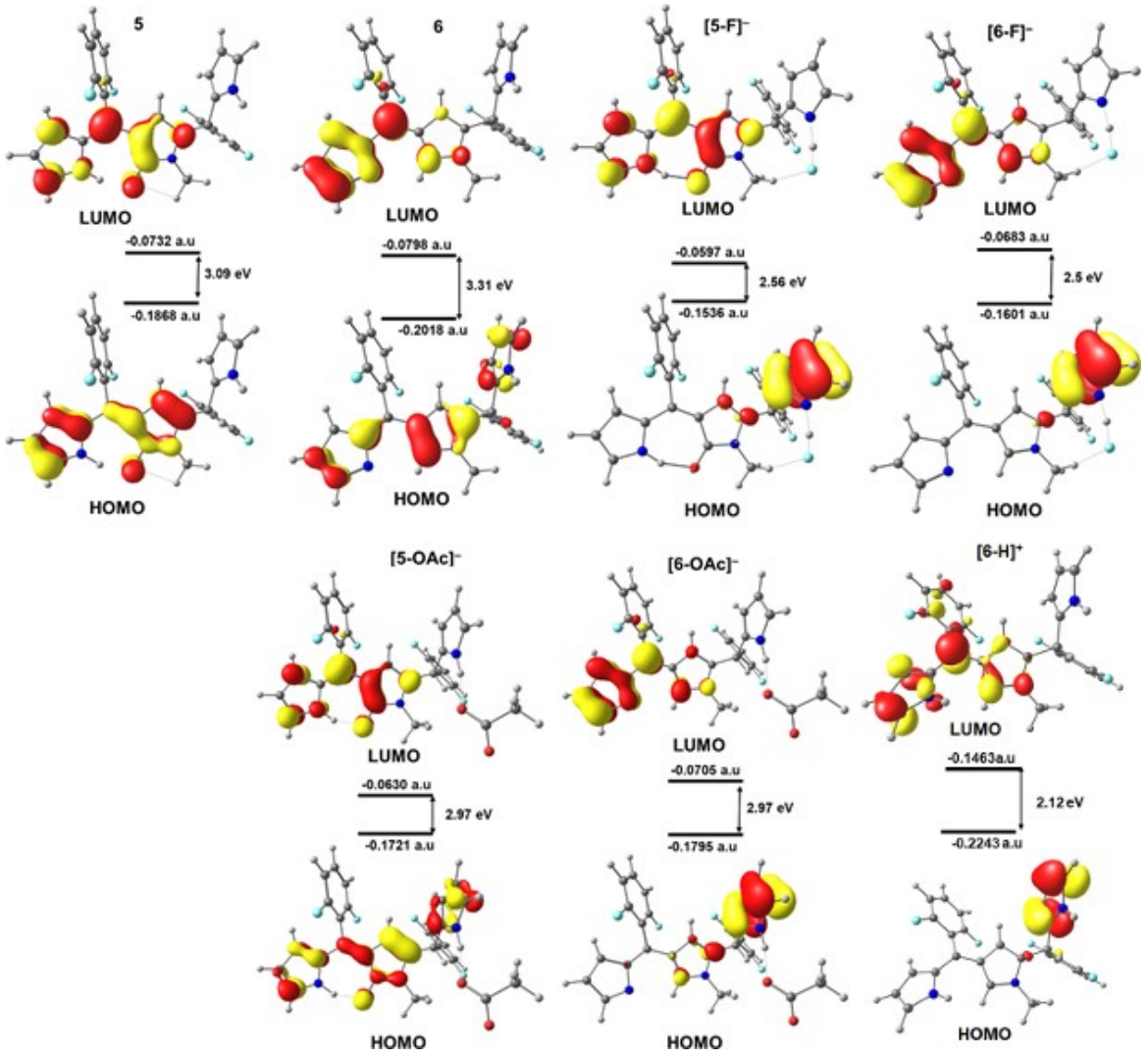


Fig. S81 FMO energy diagram for DFT optimised structures of **5**, **6**, [**5**-F_a]$^-$, [**6**-F_a]$^-$ and [**6**-H]$^+$at B3LYP/6-31G (d.p) level of theory in presence of solvent.

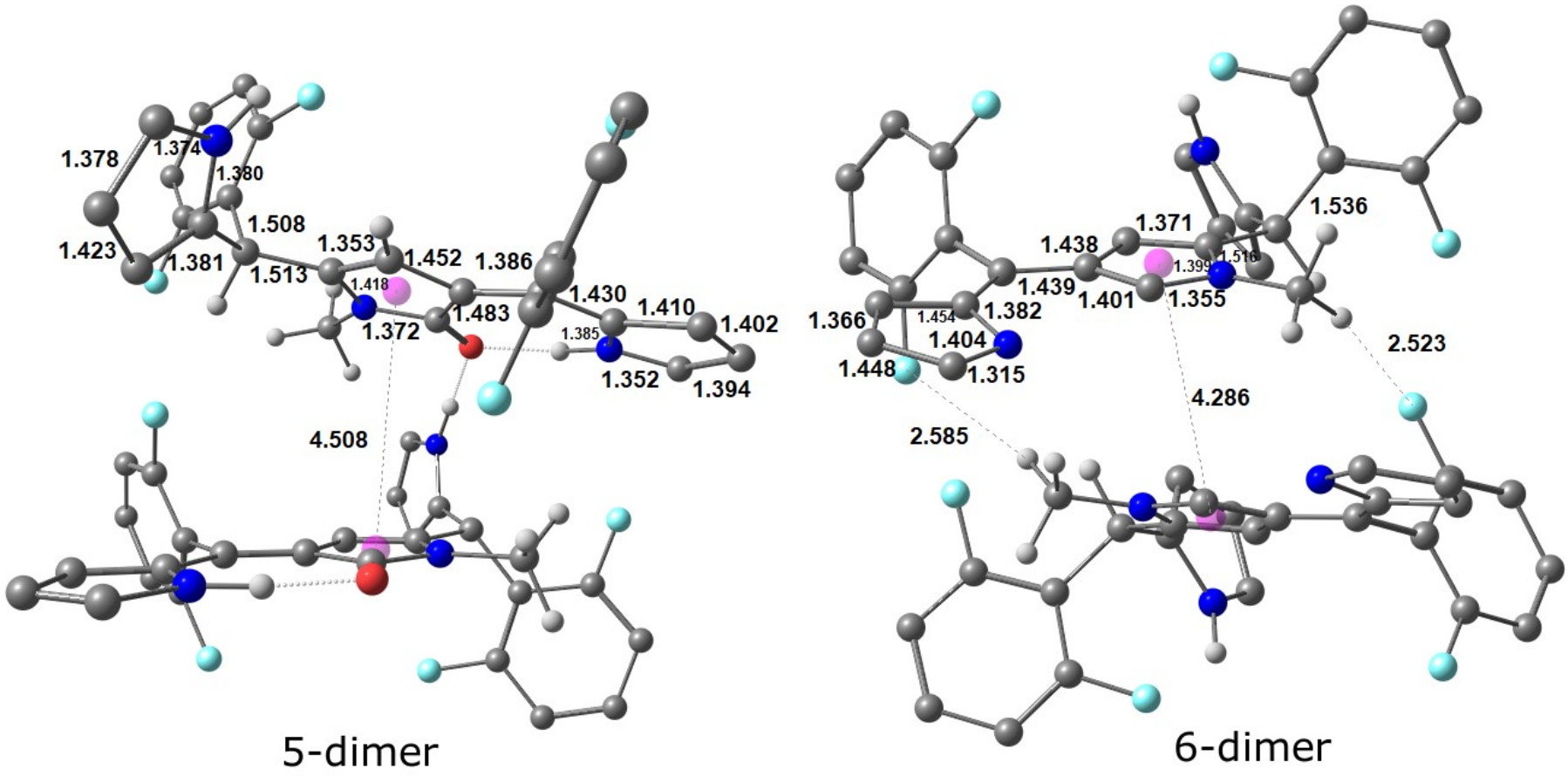


Fig.S82 A key bond lengths (Å) of optimised geometries of dimeric **5** (lateral overlap) and **6** (face to face overlap) at B3LYP /6-31G (d, p) level of theory. Note that except for pyrrole hydrogens, rest of the hydrogens are not shown for clarity.

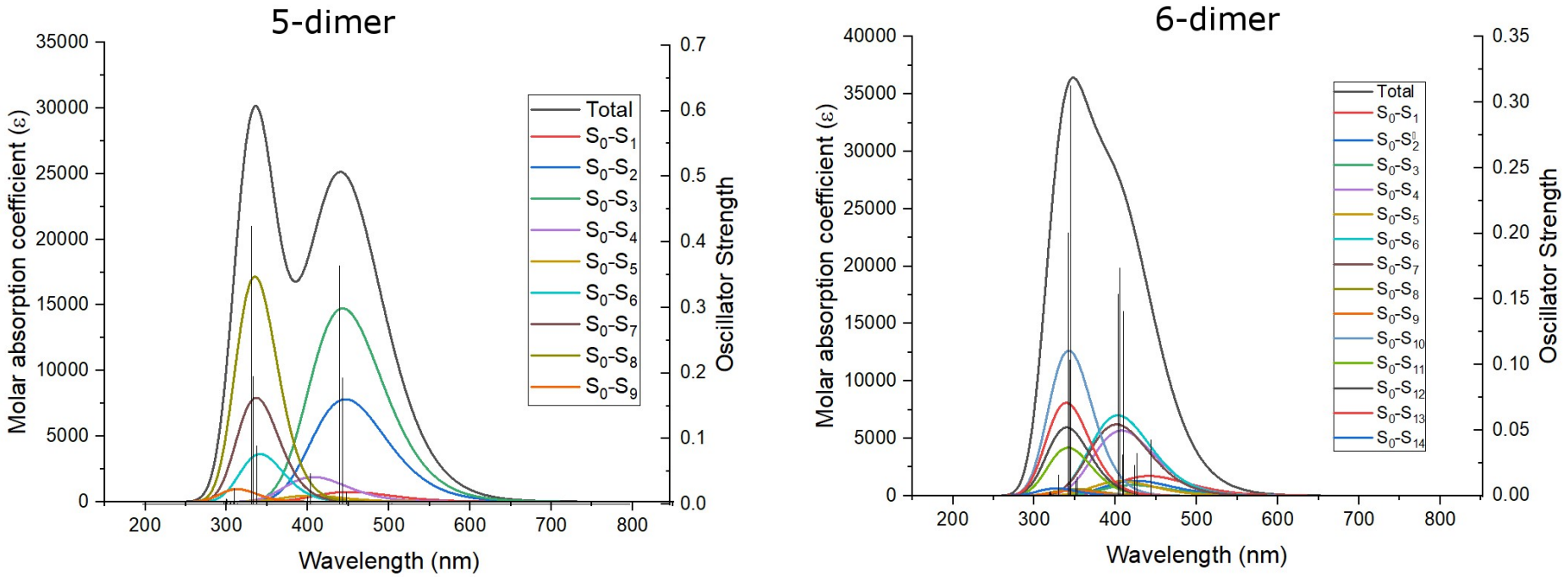


Fig. S83 UV-vis spectrum of most stable conformer of dimeric **5** (lateral overlap) **6** (face to face overlap) that is predicted from TD-DFT calculation in presence of water solvent and at B3LYP / 6-31G (d, p) level of theory.

Table S11. Summary of UV-vis spectral data of [**5-dimer**] that is predicted from TD-DFT calculation in presence of water solvent and at B3LYP/6-31G (d,p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	2.4444 eV	507.22 nm	0.00090	Singlet-A	H -> L 99.6%
2	2.7480 eV	451.18 nm	0.01860	Singlet-A	H-1 -> L+1 94.3%
3	2.7768 eV	446.50 nm	0.19330	Singlet-A	H-1 -> L 86.0%
4	**2.7983 eV**	**443.07 nm**	**0.36450**	**Singlet-A**	**H -> L+1 87.7%**
5	2.9555 eV	419.50 nm	0.00040	Singlet-A	H-2 -> L 99.9%
6	3.0466 eV	406.96 nm	0.04670	Singlet-A	H-3 -> L 95.0%
7	3.0732 eV	403.44 nm	0.01170	Singlet-A	H-2 -> L+1 98.1%
8	3.2169 eV	385.42 nm	0.00000	Singlet-A	H-3 -> L+1 99.9%
9	3.6315 eV	341.41 nm	0.08990	Singlet-A	H-4 -> L 88.9%, H-5 -> L 8.0%
10	**3.6828 eV**	**336.66 nm**	**0.19600**	**Singlet-A**	**H-5 -> L 79.1%, H-4 -> L 9.7%**
11	**3.7017 eV**	**334.94 nm**	**0.42440**	**Singlet-A**	**H-4 -> L+1 86.3%, H -> L+1 5.5%**
12	3.8834 eV	319.27 nm	0.00040	Singlet-A	H-6 -> L 97.2%
13	3.9143 eV	316.75 nm	0.00230	Singlet-A	H-5 -> L+1 97.5%
14	3.9587 eV	313.19 nm	0.02400	Singlet-A	H -> L+3 68.5%, H -> L+5 24.8%
15	3.9683 eV	312.44 nm	0.00340	Singlet-A	H-7 -> L 96.9%
16	4.0151 eV	308.79 nm	0.00490	Singlet-A	H-10 -> L 97.3%
17	4.0240 eV	308.11 nm	0.00210	Singlet-A	H-6 -> L+1 97.2%
18	4.0739 eV	304.34 nm	0.00710	Singlet-A	H -> L+5 70.5%, H -> L+3 26.6%
19	4.0857 eV	303.46 nm	0.00850	Singlet-A	H-1 -> L+4 54.7%, H-1 -> L+2 34.2%
20	4.1210 eV	300.86 nm	0.00250	Singlet-A	H-1 -> L+2 35.4%, H-13 -> L 29.8%,

Table S12. Summary of UV-vis spectral data of [**6-dimer**] that is predicted from TD-DFT calculation in presence of water solvent and at B3LYP/6-31G (d,p) level of theory.

No.	Energy (eV)	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	2.8104	441.16	0.04250	Singlet-A	H -> L 85.1%, H-1 -> L+1 9.7%
2	2.8414	436.35	0.00020	Singlet-A	H -> L+1 55.4%, H-1 -> L 40.3%
3	2.9206	424.52	0.03230	Singlet-A	H-1 -> L 31.7%, H -> L+1 19.9%, H-3 -> L 17.8%, H-1 -> L+1 11.9%, H
4	2.9413	421.53	0.02320	Singlet-A	H-2 -> L 36.9%, H-1 -> L+1 31.1%, H-2 -> L+1 12.6%, H-1 -> L 7.3%,
5	3.0425	407.51	0.14040	Singlet-A	H-2 -> L 52.9%, H-1 -> L+1 33.4%, H-3 -> L+1 6.6%
6	3.0491	406.63	0.03120	Singlet-A	H-3 -> L 65.9%, H-2 -> L+1 19.6%, H -> L+1 7.7%
7	**3.0767**	**402.98**	**0.17330**	**Singlet-A**	**H-2 -> L+1 58.6%, H-1 -> L 14.5%, H-3 -> L 8.1%, H -> L+1 7.2%**
8	**3.0894**	**401.32**	**0.15370**	**Singlet-A**	**H-3 -> L+1 82.4%**
9	3.5378	350.46	0.01440	Singlet-A	H-6 -> L 49.0%, H-6 -> L+1 21.4%, H-7 -> L 8.5%, H-7 -> L+1 7.3%,
10	3.5548	348.78	0.01140	Singlet-A	H-7 -> L+1 37.3%, H-7 -> L 34.5%, H-6 -> L+1 7.8%, H-6 -> L 5.3%
11	**3.6195**	**342.55**	**0.31270**	**Singlet-A**	**H-4 -> L 59.9%, H-5 -> L 22.6%**
12	3.6288	341.67	0.10360	Singlet-A	H-5 -> L 60.6%, H-4 -> L 22.1%,
13	3.6469	339.97	0.14710	Singlet-A	H-4 -> L+1 61.9%, H-5 -> L+1 23.0%,
14	3.6530	339.40	0.20020	Singlet-A	H-5 -> L+1 67.2%, H-4 -> L+1 21.9%
15	3.7815	327.87	0.00700	Singlet-A	H-18 -> L+1 48.7%, H-18 -> L 36.9%
16	3.7887	327.25	0.01590	Singlet-A	H-19 -> L 46.8%, H-19 -> L+1 27.1%, H-16 -> L 9.5%
17	3.8917	318.59	0.00130	Singlet-A	H-8 -> L 48.6%, H-6 -> L 23.8%, H-7 -> L+1 11.5%,
18	3.9030	317.66	0.00160	Singlet-A	H-6 -> L+1 45.9%, H-7 -> L 39.9%, H-7 -> L+1 8.0%
19	3.9083	317.23	0.00360	Singlet-A	H-8 -> L 31.2%, H-7 -> L+1 28.9%, H-6 -> L+1 16.6%, H-6 -> L 14.3%
20	3.9199	316.29	0.00260	Singlet-A	H-10 -> L 52.0%, H-10 -> L+1 26.8%, H-8 -> L+1 5.1%

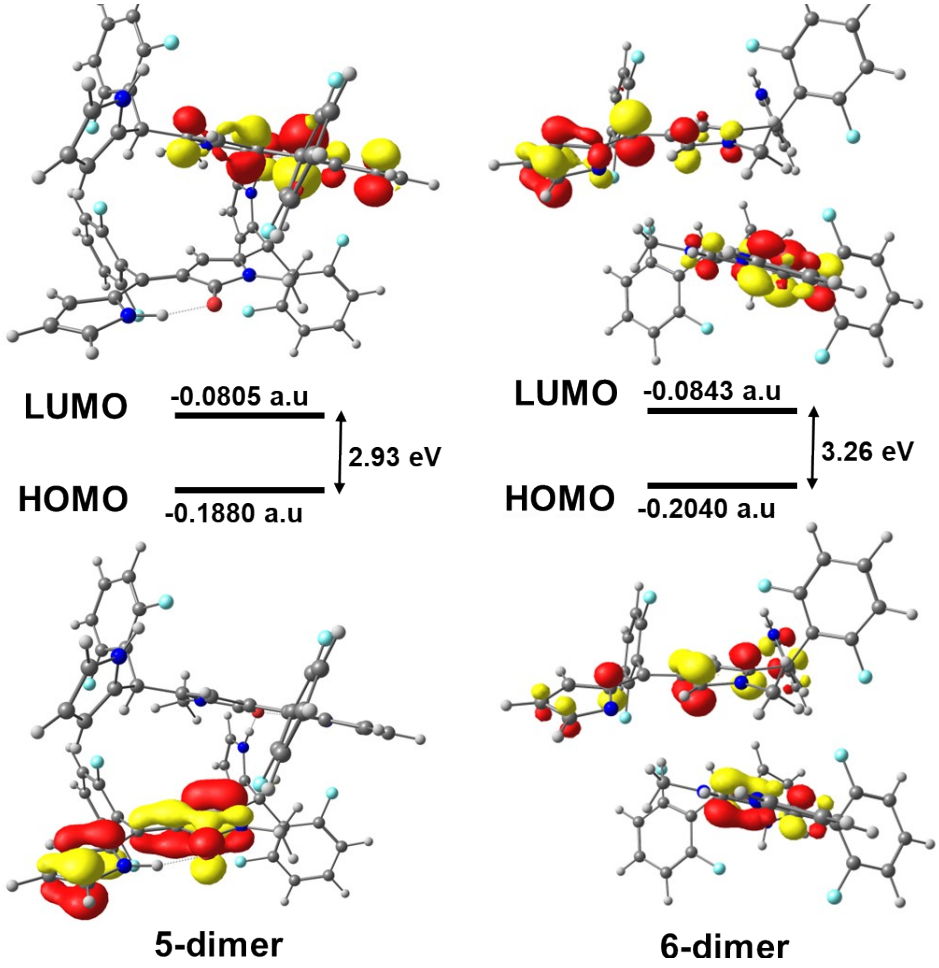


Fig. S84 FMO energy diagram for DFT optimised structures of dimeric **5** (lateral overlap) and **6** (face to face overlap) at B3LYP/6-31G (d.p) level of theory in presence of water.

Table S13 Complex reaction energies with basis set superimposition error (ΔE_{BSSE}) with zero-point energy correction (ΔE+ZPE+BSSE), free energy correction (ΔG+BSSE) in kcal/mol for [**5**-F_a]$^-$, [**6**-F_a]$^-$, and [**5**-TBAF], [**6**-TBAF], [**5**-OAc_a]$^-$, [**6**-OAc_a]$^-$, and [**5**-TBAOAc], [**6**-TBAOAc] at B3LYP/6-31G (d, p) level of theory.

	ΔE_{BSSE} (Ecom_corr)	ΔE+ZPE+BSSE	ΔG	ΔG+BSSE		Expt	
				kcal/mol	kJ/mol	kcal/mol	kJ/mol
[**5-F$_a$**]$^-$	-96.26	-59.55	-85.85	-50.93			
[**6-F$_a$**]$^-$	-79.42	-60.02	-87.76	-51.51			
[**5-OAc$_a$**]$^-$	-42.20	-28.38	-25.63	-16.10			
[**6-OAc$_a$**]$^-$	-35.01	-30.52	-27.70	-18.15			
[**5-TBAF**]	-21.70	-19.27	-21.66	-5.01	-20.96	-6.00	-25.09
[**6-TBAF**]	-26.40	-23.56	-26.91	-8.46	-35.44	-8.24	-34.49
[**5-TBAOAc**]$^-$	-16.70	-5.42	0.41		-	-	-
[**6-TBAOAc**]$^-$	-18.74	-11.48	-7.16	-	-	-	-

Table S14 Complexation energy with basis set superimposition error (ΔE_{BSSE}) for [**5**-F_a]$^-$, [**6**-F_a]$^-$ and [**5**-TBAF], [**6**-TBAF] at B3LYP/6-31G (d, p) level of theory.

Molecule	**Ecorr (a.u)**	**BSSE (a.u)**	**Efrag (a.u)**	**Ecom(raw) Kcal/mol**	**Ecom_corr (kcal/mol)**	**BSSE energy corr (kcal/mol**
[**5-F**]$^-$	-1779.00095	0.05564	-1778.84756	-131.18	-96.26	34.92
[**5-TBAF**]	-2465.15556	0.02653	-2465.12098	-38.35	-21.70	16.65
[**6-F**]$^-$	-1703.73462	0.05777	-1703.60805	-115.67	-79.42	36.25
[**6-TBAF**]	-2389.89600	0.02940	-2389.85392	-44.85	-26.40	18.45
[**5-OAc$_a$**]$^-$	-1907.70457	0.01519	-1907.65251	-42.20	-32.67	9.53
[**5-TBOAc$_a$**]	-2593.81636	0.01279	-2593.78976	-24.72	-16.70	8.02
[**6-OAc$_a$**]$^-$	-1832.44144	0.01521	-1832.38564	-44.56	-35.01	9.55
[**6-TBOAc$_a$**]	-2518.55932	0.01633	-2518.52945	-28.99	-18.74	10.25

Table S15. Total energies and with zero-point energy and free energy correction (a.u) for DFT optimised geometries at B3LYP/6-31G (d, p) level of theory.

Gas phase	E	E+ZPE	G	ΔE	ΔE+ZPE	ΔG
5	-1679.15559	-1678.75088	-1678.81526			
6	-1603.88883	-1603.48932	-1603.55248			
[6-H]$^+$	-1604.31112	-1603.89758	-1603.95947			
Ac-	-228.50220	-228.45414	-228.48194			
TBAOAc	-914.64984	-914.09323	-914.15651			
F$^-$	-99.75297	-99.75297	-99.76713			
TBAF	-785.96626	-785.45955	-785.43402			
[**5-F$_a$**]$^-$	-1779.05659	-1778.65439	-1778.71919	0.00	0.00	0.00
[**5-F$_b$**]$^-$	-1779.05156	-1778.64926	-1778.71264	3.16	3.22	4.12
[**5-F$_c$**]$^-$	-1779.01810	-1778.61384	-1778.67761	24.16	25.45	26.09
[**5-F$_d$**]$^-$	-1779.02565	-1778.62044	-1778.68338	19.42	21.30	22.48
[**5-OAc$_a$**]$^-$	-1907.71976	-1907.26542	-1907.33804	0.0	0.0	0.0
[**5-OAc$_b$**]$^-$	-1907.71271	-1907.25874	-1907.33075	4.42	4.19	4.58
[**6-F$_a$**]$^-$	-1703.79239	-1703.39570	-1703.45947	0.00	0.00	0.00
[**6-F$_b$**]$^-$	-1703.76848	-1703.37120	-1703.43667	15.00	15.37	14.31
[**6-F$_c$**]$^-$	-1703.76233	-1703.36221	-1703.42445	18.86	21.02	21.97
[**6-F$_d$**]$^-$	-1703.75124	-1703.35229	-1703.41634	25.82	27.24	27.06
[**6-F$_e$**]$^-$	-1703.73985	-1703.34163	-1703.40378	32.97	33.93	34.94
[**6-OAc$_a$**]$^-$	-1832.45664	-1832.00732	-1832.07857	0.00	0.00	0.00
[**6-OAc$_b$**]$^-$	-1832.42327	-1831.97565	-1832.04707	20.94	19.87	19.76
Solv	E	E+ZPE	G			
[**5-F$_a$**]$^-$	-1779.12613	-1778.72364	-1778.78796			
[**6-F$_a$**]$^-$	-1703.86262	-1703.46454	-1703.43396			
[**5-OAc$_a$**]$^-$	-1907.78958	-1907.33473	-1907.40508			
[**6-OAc$_a$**]$^-$	-1832.52574	-1832.07606	-1832.14673			
Counter ion	E	E+ZPE	G			
[**5-TBAF**]	-2465.18209	-2464.26767	-2464.36467			
[**6-TBAF**]	-2389.92539	-2389.01582	-2389.11027			
[**5-TBAOAc**]	-2593.82915	-2592.86561	-2592.97111			
[**6-TBAOAc**]	-2518.57565	-2517.61718	-2517.72039			

Cartesian Coordinates

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H, 3.889483, 4.863740, 9.276208
F, 2.145066, 2.024232, 12.798303
O, 4.013733, 7.174868, 12.188128
N, 3.078333, 5.336126, 11.163154
C, 3.066634, 6.373410, 12.077050
F, 3.198543, 2.408066, 8.214710
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C, 2.282430, 10.036930, 15.728366
H, 2.203020, 10.821267, 16.467388
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[**5-F$_a$**]$^-$
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H, 4.384462, 4.826349, 9.605794
H, 2.995774, 5.475482, 8.693867
F, 1.025090, 2.116583, 12.834237
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C, 1.831322, 4.649841, 11.114965
C, 1.664104, 3.401718, 10.265794
H, 2.174375, 3.592766, 9.319834
C, 2.384812, 2.205748, 10.891989
C, 2.052093, 1.611085, 12.114212
C, 2.715605, 0.514854, 12.654594
H, 2.382367, 0.119915, 13.607811
C, 3.788052, -0.037173, 11.955871
H, 4.318093, -0.894046, 12.360439
C, 4.179858, 0.517105, 10.739588
H, 5.012644, 0.125288, 10.166345
C, 3.478702, 1.614187, 10.248612
C, 0.229934, 3.144777, 9.841518
C, -0.864394, 2.535091, 10.458928
H, -0.884176, 2.069075, 11.433997
C, -1.941046, 2.645514, 9.543299
H, -2.951515, 2.275960, 9.679052
C, -1.441808, 3.316703, 8.428908
H, -1.953573, 3.590321, 7.512737
C, 1.338185, 7.025549, 13.795593
C, 0.233663, 6.430696, 14.616993
C, 0.441366, 5.348037, 15.476748
C, -0.569058, 4.774362, 16.241204
H, -0.333675, 3.931864, 16.881305
C, -1.857029, 5.300583, 16.151062
H, -2.660810, 4.862186, 16.734303
C, -2.120323, 6.382967, 15.312600
H, -3.112210, 6.809004, 15.214689
C, -1.075014, 6.920407, 14.568980
C, 1.844405, 8.274469, 14.308773
C, 1.465713, 8.965401, 15.472621
H, 0.711897, 8.641505, 16.175013
C, 2.246646, 10.134582, 15.549805
H, 2.210537, 10.892573, 16.320232
C, 3.083705, 10.136826, 14.438927
H, 3.831901, 10.851768, 14.127180
F, 1.737626, 4.581153, 7.400566

[5-F_d]$^-$ solvent optimised
Energy = -1779.126134, NImag =0.0
C, -1.553876, 3.198308, 0.389376
H, -0.934975, 4.092477, 0.466616
H, -2.230684, 3.307842, -0.464845
H, -2.146175, 3.044274, 1.300761
F, -1.693213, -1.979577, -1.253503
O, 1.273491, 3.319274, -0.016667
N, -0.651969, 2.067360, 0.194946
C, 0.706433, 2.207151, 0.058897
F, -4.516538, 1.789633, -0.802150
N, -3.040521, -0.186448, 2.763022
H, -3.212305, 0.965655, 2.843958
C, 1.268332, 0.822302, 0.045349
F, 2.077243, -1.297437, -2.293123
N, 3.796393, 2.596110, -0.261532
H, 2.923813, 3.141744, -0.163808
C, 0.122750, -0.053481, 0.201244
H, 0.150036, -1.129632, 0.241732
F, 3.623577, -0.971660, 2.145027
C, -1.003430, 0.698321, 0.282656
C, -2.459495, 0.289959, 0.427832
H, -2.999081, 1.174205, 0.775172

C, -3.073421, -0.082111, -0.921981
C, -2.685324, -1.173496, -1.706288
C, -3.256037, -1.494952, -2.931543
H, -2.895602, -2.363102, -3.471439
C, -4.276323, -0.684514, -3.429775
H, -4.736092, -0.917411, -4.384416
C, -4.703061, 0.425449, -2.702896
H, -5.489257, 1.080490, -3.060352
C, -4.093844, 0.694881, -1.482516
C, -2.692591, -0.711604, 1.543944
C, -2.618548, -2.098159, 1.649549
H, -2.366675, -2.789502, 0.858633
C, -2.939292, -2.418934, 2.997673
H, -2.983736, -3.408253, 3.437220
C, -3.190354, -1.216228, 3.646495
H, -3.472290, -1.031550, 4.675624
C, 2.583716, 0.417816, -0.090510
C, 2.837019, -1.060904, -0.074398
C, 2.574090, -1.876139, -1.178808
C, 2.800737, -3.247172, -1.187585
H, 2.574331, -3.819230, -2.079852
C, 3.316579, -3.845095, -0.037263
H, 3.498973, -4.914410, -0.022486
C, 3.598317, -3.079724, 1.094753
H, 3.995438, -3.520390, 2.001797
C, 3.353638, -1.712554, 1.049118
C, 3.769468, 1.213677, -0.249723
C, 5.099001, 0.782908, -0.422177
H, 5.422742, -0.246660, -0.464439
C, 5.908753, 1.926204, -0.535440
H, 6.980042, 1.955216, -0.676875
C, 5.067575, 3.032608, -0.431976
H, 5.293981, 4.088586, -0.469153
F, -3.385800, 2.200064, 2.636014

[**5-TBAF**]
Energy = -2465.182091, NImag =0.0
C, 1.612566, 5.986699, 7.298450
H, 2.303588, 6.824684, 7.197736
H, 2.161043, 5.051346, 7.150438
H, 0.802398, 6.052448, 6.563276
F, -0.527408, 2.751768, 10.916620
O, 2.219684, 7.942196, 9.286647
N, 1.056129, 6.058940, 8.642218
C, 1.365978, 7.062067, 9.527976
F, 1.073798, 2.695955, 6.469804
N, -2.724181, 4.646827, 7.359103
H, -2.217721, 5.172306, 6.603500
C, 0.467090, 6.867107, 10.705102
F, 0.696702, 5.273485, 13.517456
N, 2.211746, 9.288281, 11.547700
H, 2.421613, 8.942933, 10.595256
C, -0.372912, 5.735003, 10.360407
H, -1.156175, 5.313263, 10.968535
F, -2.002997, 8.970032, 12.389392
C, -0.005906, 5.269218, 9.141866
C, -0.530025, 4.099703, 8.329358
H, -0.290349, 4.317291, 7.286305
C, 0.207829, 2.803909, 8.667198
C, 0.194803, 2.187299, 9.922556
C, 0.878025, 1.013406, 10.215594
H, 0.811029, 0.601891, 11.216099
C, 1.630215, 0.404860, 9.211716
H, 2.170799, -0.512572, 9.420695
C, 1.690344, 0.974440, 7.941593
H, 2.267574, 0.533407, 7.137149
C, 0.985788, 2.149533, 7.706483
C, -2.039114, 3.993111, 8.353148
C, -2.964676, 3.391840, 9.192744
H, -2.740596, 2.803787, 10.069317

C, -4.254598, 3.699993, 8.679567
H, -5.205578, 3.384908, 9.087758
C, -4.068513, 4.476532, 7.550621
H, -4.791988, 4.914713, 6.877624
C, 0.423488, 7.579164, 11.889684
C, -0.597446, 7.141802, 12.897709
C, -0.426671, 5.995708, 13.680722
C, -1.358827, 5.569374, 14.620075
H, -1.160707, 4.669887, 15.191258
C, -2.522679, 6.317099, 14.794983
H, -3.263170, 5.998840, 15.521620
C, -2.743575, 7.469775, 14.041612
H, -3.640196, 8.068330, 14.153051
C, -1.780241, 7.853089, 13.116091
C, 1.227993, 8.690458, 12.313320
C, 1.203794, 9.372532, 13.544569
H, 0.549632, 9.144401, 14.372848
C, 2.183861, 10.376904, 13.497398
H, 2.431414, 11.083346, 14.276953
C, 2.789156, 10.294690, 12.245334
H, 3.585682, 10.885017, 11.815286
F, -1.161199, 5.939891, 5.715638
N, -2.551849, 8.656211, 4.397048
C, -3.683906, 9.583301, 3.987076
C, -3.611012, 11.046929, 4.421478
H, -4.597017, 9.137395, 4.382803
H, -3.734475, 9.521404, 2.894712
C, -4.788532, 11.837149, 3.825346
H, -3.649395, 11.122092, 5.512159
H, -2.672862, 11.511040, 4.098989
C, -4.784487, 13.308224, 4.250348
H, -4.754821, 11.770801, 2.729804
H, -5.733614, 11.369776, 4.131714
H, -5.629757, 13.846311, 3.811502
H, -4.855317, 13.407282, 5.338778
H, -3.866164, 13.811968, 3.929612
C, -1.238867, 9.189146, 3.830808
C, -0.061281, 8.207799, 3.847733
H, -0.997393, 10.083371, 4.403969
H, -1.464274, 9.505267, 2.807139
C, 1.274264, 8.964205, 3.785142
H, -0.110801, 7.553380, 4.725108
H, -0.133125, 7.538202, 2.983280
C, 2.475059, 8.021612, 3.668788
H, 1.271318, 9.658869, 2.932797
H, 1.382451, 9.585118, 4.684574
H, 3.415179, 8.580909, 3.641555
H, 2.517061, 7.333662, 4.518906
H, 2.417861, 7.417917, 2.756401
C, -2.801878, 7.273176, 3.760973
C, -4.171446, 6.644193, 4.012585
H, -2.038303, 6.621702, 4.207468
H, -2.636676, 7.408176, 2.687157
C, -4.152403, 5.188327, 3.511460
H, -4.402145, 6.643278, 5.083690
H, -4.977521, 7.187546, 3.504434
C, -5.506187, 4.489607, 3.659674
H, -3.847472, 5.173561, 2.456083
H, -3.383689, 4.638583, 4.065928
H, -5.460077, 3.465129, 3.278580
H, -5.811054, 4.434270, 4.709788
H, -6.293103, 5.016253, 3.107271
C, -2.482463, 8.466534, 5.933853
C, -1.659806, 9.473299, 6.738542
H, -2.040746, 7.465463, 6.069757
H, -3.522952, 8.467615, 6.267742
C, -1.885017, 9.224387, 8.241015
H, -0.594081, 9.340040, 6.521627
H, -1.905732, 10.516428, 6.511042
C, -0.989874, 10.097030, 9.124727

H, -2.940313, 9.412193, 8.481997
H, -1.703745, 8.166536, 8.464928
H, -1.203145, 9.919893, 10.181276
H, 0.068479, 9.870339, 8.959581
H, -1.144913, 11.163675, 8.921619

[**5-F$_b$**]$^-$
Energy = -1779.051560, NImag =0.0
C, 3.851813, 5.536464, 9.692498
H, 4.558088, 6.358437, 9.815954
H, 4.391212, 4.585984, 9.666508
H, 3.322460, 5.661880, 8.740246
F, 0.744697, 2.052832, 12.675761
O, 3.732141, 7.593475, 11.624869
N, 2.938408, 5.589748, 10.815278
C, 2.927733, 6.638169, 11.699973
F, 4.075392, 2.125319, 9.320055
N, -0.830730, 3.222925, 10.467159
H, -1.126328, 3.524379, 11.792884
C, 1.828410, 6.343930, 12.669923
F, 1.698463, 6.202900, 16.411530
N, 2.932392, 9.067294, 13.637019
H, 3.440124, 8.674503, 12.822896
C, 1.264948, 5.074125, 12.248204
H, 0.416336, 4.570177, 12.692763
F, -1.282041, 6.811711, 12.809700
C, 1.917107, 4.648669, 11.140813
C, 1.725074, 3.414069, 10.281468
H, 2.329604, 3.564667, 9.386390
C, 2.343914, 2.169656, 10.941994
C, 1.823864, 1.532608, 12.076747
C, 2.375602, 0.381805, 12.632456
H, 1.906399, -0.045871, 13.511461
C, 3.508476, -0.182678, 12.047807
H, 3.948698, -1.080886, 12.470212
C, 4.077942, 0.411752, 10.923520
H, 4.961746, 0.010820, 10.439761
C, 3.484055, 1.560139, 10.411584
C, 0.325148, 3.192877, 9.736914
C, 0.045714, 2.897126, 8.398360
H, 0.774750, 2.805833, 7.599661
C, -1.356911, 2.739206, 8.307577
H, -1.937489, 2.510249, 7.421025
C, -1.842737, 2.951794, 9.596122
H, -2.869232, 2.935241, 9.946500
C, 1.392516, 7.100838, 13.741951
C, 0.268417, 6.537294, 14.558055
C, 0.461038, 6.101435, 15.874387
C, -0.551439, 5.567201, 16.658775
H, -0.324964, 5.244865, 17.668867
C, -1.826370, 5.437886, 16.103240
H, -2.627336, 4.999826, 16.690940
C, -2.072336, 5.845874, 14.797111
H, -3.033859, 5.712532, 14.318553
C, -1.028568, 6.388030, 14.056351
C, 1.870062, 8.384439, 14.195428
C, 1.375999, 9.188988, 15.236646
H, 0.536258, 8.943156, 15.869176
C, 2.159396, 10.356795, 15.286442
H, 2.048932, 11.186975, 15.970597
C, 3.113855, 10.247428, 14.279857
H, 3.900210, 10.927326, 13.983479
F, -1.382774, 3.762956, 12.793418

[**5-F$_c$**]$^-$
Energy = -1779.018098, NImag =0.0
C, 4.342116, 4.882833, 10.561376
H, 5.023777, 5.731142, 10.634627
H, 4.787710, 3.989093, 11.002505
H, 4.108918, 4.682891, 9.513338

F, 3.656774, 2.534556, 12.541321
O, 4.079765, 7.009122, 12.424811
N, 3.135659, 5.237058, 11.295450
C, 3.122298, 6.231616, 12.239302
F, 2.972177, 2.509940, 8.059521
N, -0.792769, 3.925019, 10.089560
H, -0.636844, 4.920938, 10.095122
C, 1.786658, 6.147136, 12.919048
F, 0.590789, 6.061264, 16.463543
N, 3.099783, 8.614224, 14.256179
H, 3.720868, 8.116976, 13.592496
C, 1.135042, 5.005416, 12.314773
H, 0.161725, 4.620369, 12.570452
F, -1.075214, 7.254595, 12.212254
C, 1.941375, 4.482945, 11.354679
C, 1.662884, 3.393379, 10.343408
H, 1.836597, 3.870113, 9.366632
C, 2.636420, 2.225094, 10.378762
C, 3.002124, 1.570471, 11.636605
C, 3.841065, 0.383295, 11.490383
H, 4.052738, -0.167899, 12.401632
C, 4.384974, 0.018322, 10.282603
H, 5.033512, -0.856619, 10.244055
C, 4.126180, 0.728095, 9.090243
H, 4.547791, 0.459363, 8.129870
C, 3.251372, 1.799522, 9.209855
C, 0.198415, 2.994229, 10.347981
C, -0.422732, 1.769519, 10.469744
H, 0.095756, 0.847152, 10.678741
C, -1.823971, 1.969306, 10.298365
H, -2.594800, 1.210650, 10.331312
C, -2.026825, 3.314292, 10.076770
H, -2.930670, 3.883427, 9.912261
C, 1.238944, 6.996085, 13.859915
C, -0.154743, 6.684331, 14.313469
C, -0.433750, 6.226259, 15.606365
C, -1.716026, 5.926677, 16.053924
H, -1.849971, 5.567360, 17.067821
C, -2.786763, 6.084221, 15.175321
H, -3.794340, 5.848925, 15.503406
C, -2.568626, 6.535092, 13.874307
H, -3.378283, 6.662516, 13.164994
C, -1.267710, 6.821981, 13.476592
C, 1.811547, 8.171181, 14.473545
C, 1.217944, 9.077159, 15.368403
H, 0.205144, 9.019154, 15.738926
C, 2.174039, 10.064516, 15.677047
H, 2.046094, 10.910881, 16.337905
C, 3.327599, 9.746757, 14.969196
H, 4.284815, 10.246769, 14.927619
F, 1.859658, 1.296866, 12.443035

[**5-F$_d$**]$^-$
Energy = -1779.025650, NImag=0.0
C, 3.539388, 5.876546, 9.470177
H, 4.079247, 6.824132, 9.506449
H, 4.257719, 5.049366, 9.421181
H, 2.919387, 5.854670, 8.564599
F, 0.421956, 2.017109, 12.389354
O, 3.406799, 7.885532, 11.424113
N, 2.739296, 5.812752, 10.670713
C, 2.727099, 6.840895, 11.611291
F, 4.269765, 2.281861, 9.664285
N, -0.695424, 4.058390, 10.269011
H, -0.614516, 4.747983, 11.009491
C, 1.849920, 6.394074, 12.699659
F, 1.435669, 6.260375, 16.561414
N, 3.070159, 8.882207, 13.805827
H, 3.445326, 8.570000, 12.887455
C, 1.468433, 5.043009, 12.346400

H, 0.862888, 4.392723, 12.957244
F, -1.043234, 6.257815, 12.509607
C, 1.982171, 4.719576, 11.130543
C, 1.781487, 3.483346, 10.284682
H, 2.409781, 3.591280, 9.397670
C, 2.305593, 2.225785, 10.981569
C, 1.621277, 1.546498, 11.994757
C, 2.113172, 0.410628, 12.627052
H, 1.520840, -0.051929, 13.408236
C, 3.356506, -0.090923, 12.242188
H, 3.758334, -0.974274, 12.728425
C, 4.086250, 0.544200, 11.238564
H, 5.056479, 0.185979, 10.913434
C, 3.544323, 1.676724, 10.641963
C, 0.356568, 3.330612, 9.775312
C, -0.142189, 2.509380, 8.777296
H, 0.439825, 1.809622, 8.191872
C, -1.540608, 2.753350, 8.677598
H, -2.236556, 2.281471, 7.996809
C, -1.850388, 3.718733, 9.614701
H, -2.787421, 4.193881, 9.864148
C, 1.345364, 7.081648, 13.841327
C, 0.209172, 6.483139, 14.535147
C, 0.155680, 6.305171, 16.018421
C, -0.625938, 5.129264, 16.465076
H, -0.447661, 4.806020, 17.485686
C, -1.601772, 4.593529, 15.685619
H, -2.232589, 3.799285, 16.080941
C, -1.806156, 5.036843, 14.345776
H, -2.638762, 4.702105, 13.739513
C, -0.878792, 5.911432, 13.835262
C, 1.917522, 8.319294, 14.334448
C, 1.481244, 9.187802, 15.350434
H, 0.618999, 9.018135, 15.971528
C, 2.385582, 10.261485, 15.420597
H, 2.347664, 11.099357, 16.104150
C, 3.346476, 10.047880, 14.436781
H, 4.188356, 10.655978, 14.134149
F, -0.408733, 7.449186, 16.718342

[**5-OAc$_a$**]$^-$
Energy = -1907.719757, NImag =0.0
C, -1.651210, 2.211377, -1.684072
H, -1.160818, 2.889883, -2.382726
H, -2.408580, 1.632879, -2.219331
H, -2.124314, 2.788874, -0.875614
F, -0.996750, -2.658709, -1.120962
O, 1.167991, 2.499701, -2.042808
N, -0.611262, 1.323373, -1.165809
C, 0.725749, 1.580427, -1.325086
F, -4.629274, 0.360901, -1.280307
N, -2.803411, -0.295957, 2.444491
H, -3.146719, 0.687576, 2.353703
C, 1.451537, 0.568011, -0.485635
F, 2.854526, -2.347237, -1.101259
N, 3.754160, 2.206623, -1.758168
H, 2.806341, 2.543004, -2.015274
C, 0.408449, -0.219092, 0.139492
H, 0.545295, -1.044513, 0.819146
F, 3.688784, 0.763732, 2.337437
C, -0.797211, 0.237682, -0.277938
C, -2.190726, -0.262021, 0.041122
H, -2.825954, 0.628254, 0.153448
C, -2.771035, -1.087783, -1.112486
C, -2.168536, -2.233469, -1.644228
C, -2.706414, -2.984084, -2.684004
H, -2.168306, -3.858648, -3.031962
C, -3.920257, -2.586643, -3.242429
H, -4.358048, -3.159332, -4.054319
C, -4.570425, -1.454292, -2.757518

H, -5.513923, -1.109385, -3.165258
C, -3.985078, -0.739016, -1.716497
C, -2.281138, -0.976304, 1.373532
C, -1.935682, -2.250895, 1.805606
H, -1.502962, -3.029860, 1.195674
C, -2.263219, -2.327890, 3.187255
H, -2.126195, -3.180349, 3.840071
C, -2.795766, -1.101862, 3.546391
H, -3.169965, -0.747569, 4.496578
C, 2.809845, 0.387449, -0.332923
C, 3.240946, -0.730017, 0.570244
C, 3.243336, -2.065111, 0.156621
C, 3.631697, -3.118420, 0.977900
H, 3.602080, -4.130074, 0.589758
C, 4.041334, -2.835140, 2.280223
H, 4.342218, -3.643978, 2.938768
C, 4.062865, -1.520353, 2.743746
H, 4.369977, -1.269260, 3.752495
C, 3.664838, -0.502980, 1.882743
C, 3.902922, 1.119772, -0.921515
C, 5.284255, 0.900240, -0.781944
H, 5.736650, 0.117400, -0.191099
C, 5.951559, 1.874034, -1.548727
H, 7.020128, 1.993909, -1.663156
C, 4.971696, 2.665872, -2.139483
H, 5.063224, 3.517503, -2.798577
O, -3.553902, 2.084120, 1.562713
C, -3.290476, 3.331531, 1.631398
O, -2.870234, 4.058069, 0.709763
C, -3.530433, 3.979658, 3.013986
H, -2.835087, 3.551927, 3.746615
H, -4.543360, 3.753875, 3.366092
H, -3.385039, 5.062232, 2.975202

[5-OAc$_b$]$^-$

Energy = -1907.712709, NImag =0.0
C, -1.364678, -3.712101, -1.040525
H, -0.752081, -4.600175, -0.881256
H, -2.265402, -3.770718, -0.426354
H, -1.666669, -3.676802, -2.094838
F, -1.988535, 0.671534, 1.646439
O, 1.405936, -3.767575, -0.545387
N, -0.551967, -2.567505, -0.681859
C, 0.804663, -2.671838, -0.500616
F, -4.540857, -2.761571, -0.347366
N, -2.316330, 1.655507, -1.229111
H, -1.609484, 1.995839, -0.513864
C, 1.296075, -1.281300, -0.276980
F, 3.355339, 0.438641, 2.320182
N, 3.866030, -3.001698, -0.099734
H, 3.002992, -3.555888, -0.249323
C, 0.115241, -0.432596, -0.337710
H, 0.101042, 0.636611, -0.169131
F, 2.298837, 0.977121, -2.242044
C, -0.966981, -1.206825, -0.591424
C, -2.437854, -0.878532, -0.760641
H, -2.850249, -1.661398, -1.400583
C, -3.215123, -1.018906, 0.559859
C, -2.975823, -0.230428, 1.691910
C, -3.710928, -0.334817, 2.869118
H, -3.461577, 0.318490, 3.697476
C, -4.743209, -1.268491, 2.943444
H, -5.327574, -1.360249, 3.853815
C, -5.024286, -2.086427, 1.850127
H, -5.815789, -2.827189, 1.868220
C, -4.258136, -1.937526, 0.699932
C, -2.763024, 0.389868, -1.516350
C, -3.623681, 0.477125, -2.605069
H, -4.145476, -0.358245, -3.057369
C, -3.685971, 1.842615, -2.988244

H, -4.258348, 2.265678, -3.803786
C, -2.861009, 2.536399, -2.118754
H, -2.582335, 3.577795, -2.033663
C, 2.596084, -0.846731, -0.095152
C, 2.812229, 0.630150, 0.031443
C, 3.196976, 1.227487, 1.235202
C, 3.432438, 2.589100, 1.368718
H, 3.717449, 2.985172, 2.336521
C, 3.260147, 3.408828, 0.253646
H, 3.412373, 4.479160, 0.343919
C, 2.869816, 2.868292, -0.968830
H, 2.703517, 3.484169, -1.844389
C, 2.657222, 1.498579, -1.053461
C, 3.808695, -1.623232, -0.030153
C, 5.133729, -1.171240, 0.104804
H, 5.435000, -0.137420, 0.181007
C, 5.973663, -2.298564, 0.113598
H, 7.051098, -2.307798, 0.203886
C, 5.153436, -3.415765, -0.017784
H, 5.403785, -4.466452, -0.060291
O, -1.161854, 4.679317, -0.460735
C, -0.574579, 3.984175, 0.392759
O, -0.507538, 2.710061, 0.455070
C, 0.114810, 4.738903, 1.554679
H, -0.653373, 5.072690, 2.263740
H, 0.617659, 5.637206, 1.180576
H, 0.824235, 4.102229, 2.088863

[5-OAc$_a$]$^-$ solvent optimised
Energy = -1907.789577, NImag =0.0
C, -1.596217, 2.278238, -1.572056
H, -1.123515, 3.126764, -2.066127
H, -2.216290, 1.743272, -2.296620
H, -2.227240, 2.623402, -0.745985
F, -0.663581, -2.798563, -0.799548
O, 1.207419, 2.782385, -1.761074
N, -0.525368, 1.424554, -1.071195
C, 0.803389, 1.768269, -1.153046
F, -4.265719, 0.099239, -1.784191
N, -2.782684, -0.109839, 2.283357
H, -3.087917, 0.871220, 2.084802
C, 1.550477, 0.726794, -0.386427
F, 2.917388, -2.081525, -1.157599
N, 3.814852, 2.579229, -1.416535
H, 2.870292, 2.909084, -1.674699
C, 0.532467, -0.167492, 0.131720
H, 0.702744, -1.039157, 0.742192
F, 3.860075, 0.786310, 2.460418
C, -0.683456, 0.256461, -0.288971
C, -2.060917, -0.340897, -0.073069
H, -2.770621, 0.488604, -0.126678
C, -2.445600, -1.292837, -1.208311
C, -1.748619, -2.460304, -1.537366
C, -2.107438, -3.310690, -2.575727
H, -1.513959, -4.198494, -2.761507
C, -3.223932, -2.991911, -3.349002
H, -3.521178, -3.642938, -4.164263
C, -3.957554, -1.838399, -3.076771
H, -4.827780, -1.557876, -3.658761
C, -3.550341, -1.026848, -2.024453
C, -2.247063, -0.921952, 1.312773
C, -1.976905, -2.154696, 1.890263
H, -1.549557, -3.009564, 1.388285
C, -2.366506, -2.072332, 3.257608
H, -2.297381, -2.857292, 3.999320
C, -2.857606, -0.795595, 3.465290
H, -3.257304, -0.329829, 4.354959
C, 2.914808, 0.590165, -0.201518
C, 3.367972, -0.587493, 0.609641
C, 3.354521, -1.891516, 0.105613

C, 3.769212, -2.997656, 0.837302
H, 3.733180, -3.980977, 0.382997
C, 4.221712, -2.802497, 2.142634
H, 4.548078, -3.653113, 2.731547
C, 4.256120, -1.522876, 2.697527
H, 4.598260, -1.344959, 3.710381
C, 3.831071, -0.451221, 1.921802
C, 3.984199, 1.417629, -0.685094
C, 5.372791, 1.236818, -0.532116
H, 5.843413, 0.415194, -0.012574
C, 6.018022, 2.302855, -1.180769
H, 7.082979, 2.471680, -1.256491
C, 5.021000, 3.115620, -1.718353
H, 5.097046, 4.029664, -2.289685
O, -3.454125, 2.329931, 1.301605
C, -4.581407, 2.933575, 1.392624
O, -4.989566, 3.838762, 0.638159
C, -5.478989, 2.486749, 2.564369
H, -4.988036, 2.717340, 3.517181
H, -5.626752, 1.401437, 2.537087
H, -6.450629, 2.985380, 2.537303

[**5-TBAOAc**]
Energy = -2593.829149, NImag =0.0
C, -1.895114, -0.974623, 3.124926
H, -2.391810, -0.533046, 3.989210
H, -1.877794, -2.062752, 3.238659
H, -0.867815, -0.602889, 3.047852
F, -3.221685, -2.898302, -1.542875
O, -4.170393, 0.735415, 3.094601
N, -2.662620, -0.582362, 1.952581
C, -3.715456, 0.303121, 2.017431
F, -0.251509, -3.837639, 2.014759
N, 0.600263, -0.492810, -0.783764
H, 0.911251, -0.155239, 0.148307
C, -4.104847, 0.586231, 0.603869
F, -6.316077, -0.663474, -1.431348
N, -6.116487, 2.283624, 2.238566
H, -5.433125, 1.776741, 2.827720
C, -3.175390, -0.174931, -0.209191
H, -3.148624, -0.206334, -1.286180
F, -4.281188, 3.584665, -1.445319
C, -2.335231, -0.856372, 0.605381
C, -1.208885, -1.817204, 0.271729
H, -0.502590, -1.766364, 1.103708
C, -1.702081, -3.265525, 0.234790
C, -2.688133, -3.744298, -0.635601
C, -3.148301, -5.055718, -0.636736
H, -3.915640, -5.341563, -1.346880
C, -2.611208, -5.959291, 0.278824
H, -2.959317, -6.986950, 0.293958
C, -1.626961, -5.544106, 1.173369
H, -1.187251, -6.215543, 1.901849
C, -1.206572, -4.220313, 1.128193
C, -0.423596, -1.392855, -0.951002
C, -0.523339, -1.677718, -2.305135
H, -1.242798, -2.339501, -2.761969
C, 0.475629, -0.915990, -2.971231
H, 0.668398, -0.892434, -4.035365
C, 1.148078, -0.193624, -2.003040
H, 1.942077, 0.533392, -2.091137
C, -5.128457, 1.385360, 0.129783
C, -5.289320, 1.456476, -1.359950
C, -5.879762, 0.423797, -2.094438
C, -6.041036, 0.466855, -3.474860
H, -6.508340, -0.370823, -3.979445
C, -5.593406, 1.592586, -4.165464
H, -5.708844, 1.644098, -5.243378
C, -4.997257, 2.651946, -3.482063
H, -4.636506, 3.537215, -3.992839

C, -4.859586, 2.560825, -2.101428
C, -6.083276, 2.167977, 0.861678
C, -7.143985, 2.948961, 0.364428
H, -7.397130, 3.067825, -0.678575
C, -7.802124, 3.525799, 1.462124
H, -8.660311, 4.182278, 1.436740
C, -7.138219, 3.090700, 2.607469
H, -7.330606, 3.304590, 3.649152
N, 5.748576, 0.131611, -0.125177
C, 6.536310, -0.540618, -1.240027
C, 7.390796, 0.349530, -2.141189
H, 5.803346, -1.071824, -1.847526
H, 7.163850, -1.291517, -0.748886
C, 8.150529, -0.506933, -3.168873
H, 6.759542, 1.066756, -2.674828
H, 8.114820, 0.928453, -1.557799
C, 9.009256, 0.335852, -4.115932
H, 8.786372, -1.230157, -2.641503
H, 7.432685, -1.097809, -3.752393
H, 9.538548, -0.297469, -4.833648
H, 8.396117, 1.042910, -4.684920
H, 9.759397, 0.913558, -3.564977
C, 6.726009, 0.839289, 0.810780
C, 6.167711, 1.298202, 2.160955
H, 7.121018, 1.689273, 0.255629
H, 7.549802, 0.133764, 0.959496
C, 7.111138, 2.327091, 2.804469
H, 5.156512, 1.708714, 2.063891
H, 6.071770, 0.437172, 2.831492
C, 6.648308, 2.743875, 4.203342
H, 8.130410, 1.919299, 2.861690
H, 7.173930, 3.214902, 2.160283
H, 7.320627, 3.491232, 4.635611
H, 5.641406, 3.172254, 4.172328
H, 6.621701, 1.885480, 4.883145

C, 5.025890, -0.965270, 0.682813
C, 4.152982, -1.933618, -0.113872
H, 4.405077, -0.421120, 1.397044
H, 5.814760, -1.508068, 1.213687
C, 3.300717, -2.774510, 0.854087
H, 3.474988, -1.395711, -0.784997
H, 4.764494, -2.605355, -0.728510
C, 2.514740, -3.871531, 0.131611
H, 3.950833, -3.229113, 1.615419
H, 2.608519, -2.106771, 1.379464
H, 1.900235, -4.430320, 0.841211
H, 1.844304, -3.443602, -0.620867
H, 3.183468, -4.579767, -0.372308
C, 4.668604, 1.084873, -0.690468
C, 5.046740, 2.551709, -0.895449
H, 3.840979, 1.046483, 0.028791
H, 4.353112, 0.634236, -1.633713
C, 3.825450, 3.308899, -1.447465
H, 5.322178, 3.007505, 0.060923
H, 5.896136, 2.682744, -1.575768
C, 4.098966, 4.802461, -1.643356
H, 3.517991, 2.864386, -2.403445
H, 2.988107, 3.171120, -0.753865
H, 3.213763, 5.314030, -2.032273
H, 4.369884, 5.282684, -0.696776
H, 4.919155, 4.971618, -2.350639
O, 1.143717, 0.044198, 1.868621
C, 1.982649, 0.851576, 2.363465
O, 3.016245, 1.295578, 1.782881
C, 1.708318, 1.328947, 3.794257
H, 2.515271, 1.962800, 4.167342
H, 1.578534, 0.466922, 4.456302
H, 0.768914, 1.891028, 3.815295

[**6**]

Energy = -1603.888827, NImag=0.0
C, -3.804104, 5.080634, 8.981017
H, -4.428710, 5.962245, 9.132447
H, -4.391173, 4.312469, 8.467255
H, -3.507737, 4.691578, 9.957395
C, -2.598149, 6.552960, 7.387408
H, -3.415766, 7.251008, 7.305622
C, -0.639381, 5.433084, 7.205191
H, 0.362497, 5.140830, 6.931083
C, -1.433099, 4.760382, 8.097313
C, -1.155979, 3.517046, 8.918404
H, -1.430168, 3.743296, 9.955954
C, -2.042936, 2.331127, 8.533905
C, -2.863032, 1.707824, 9.478629
C, -3.699935, 0.635631, 9.195914
H, -4.304378, 0.209055, 9.987898
C, -3.730716, 0.145816, 7.891038
H, -4.373657, -0.692396, 7.643658
C, -2.939608, 0.729440, 6.901797
H, -2.942008, 0.373757, 5.877979
C, -2.122225, 1.800494, 7.242356
C, 0.314222, 3.163462, 8.949664
C, 1.125469, 2.417807, 8.115287
H, 0.803176, 1.908445, 7.220566
C, 2.446593, 2.457316, 8.644490
H, 3.320682, 1.971214, 8.234838
C, 2.412079, 3.227314, 9.785804
H, 3.189199, 3.504041, 10.482299
C, -0.884610, 7.575044, 5.801310
C, 0.449156, 7.313326, 5.177390
C, 0.647203, 6.269210, 4.266336
C, 1.874565, 5.993679, 3.676151
H, 1.951248, 5.172851, 2.972636
C, 2.970071, 6.789943, 4.009695
H, 3.937523, 6.590175, 3.560549
C, 2.831649, 7.840407, 4.915782
H, 3.666218, 8.471978, 5.197368
C, 1.581946, 8.078027, 5.477468
C, -1.552636, 8.727210, 5.444509
C, -1.128583, 9.721177, 4.467375
H, -0.220221, 9.689465, 3.882247
C, -3.106270, 10.226433, 5.395339
H, -4.030912, 10.745811, 5.633845
C, -2.110061, 10.666404, 4.435222
H, -2.153518, 11.561586, 3.828473
C, -1.361490, 6.585014, 6.738744
F, -2.857971, 2.193166, 10.746770
F, -1.358606, 2.347712, 6.274244
F, -0.409930, 5.503035, 3.938150
F, 1.460275, 9.088861, 6.358798
N, -2.637193, 5.464894, 8.201129
N, 1.115454, 3.645543, 9.963981
H, 0.799013, 4.250210, 10.705278
N, -2.794079, 9.099332, 5.988722

[**6-H**]$^+$
Energy = -1604.3111253, NImag =0.0
C, -1.698046, -3.065103, -0.265952
H, -1.173956, -4.014361, -0.380130
H, -2.212566, -3.045092, 0.697440
H, -2.439088, -2.971089, -1.060810
C, 0.594656, -2.126447, -0.138932
H, 1.005423, -3.082703, 0.151475
C, 0.147764, 0.082182, -0.469824
H, 0.247741, 1.145654, -0.620005
C, -1.021165, -0.615040, -0.570995
C, -2.423833, -0.141557, -0.896969
H, -2.782147, -0.756530, -1.730787
C, -3.413603, -0.397571, 0.241919
C, -4.587398, -1.124026, 0.021673

C, -5.545186, -1.358971, 0.998536
H, -6.433342, -1.928080, 0.750466
C, -5.325531, -0.844894, 2.276524
H, -6.061063, -1.009775, 3.056413
C, -4.165361, -0.123324, 2.560878
H, -3.968566, 0.283557, 3.545848
C, -3.242359, 0.081239, 1.544179
C, -2.445274, 1.288655, -1.384896
C, -2.245278, 2.499179, -0.744307
H, -2.038646, 2.624466, 0.307514
C, -2.385033, 3.529592, -1.714474
H, -2.296418, 4.592847, -1.544162
C, -2.668559, 2.927051, -2.920401
H, -2.855980, 3.345996, -3.897429
C, 2.580479, -0.554693, 0.014626
C, 2.958448, 0.802611, 0.447895
C, 2.330489, 1.438099, 1.539548
C, 2.667698, 2.713657, 1.963891
H, 2.161802, 3.135787, 2.823952
C, 3.656563, 3.411945, 1.269396
H, 3.925262, 4.414308, 1.585343
C, 4.303935, 2.839799, 0.173335
H, 5.062388, 3.371546, -0.388699
C, 3.954461, 1.554404, -0.209558
C, 3.608231, -1.499176, -0.178382
C, 4.925483, -1.526034, 0.338368
H, 5.338178, -0.783437, 1.005308
C, 4.622554, -3.364284, -0.916950
H, 4.736330, -4.276629, -1.485294
C, 5.544234, -2.691653, -0.105540
H, 6.545749, -3.027731, 0.118411
C, 1.208128, -0.852704, -0.201970
F, -4.779965, -1.650373, -1.214561
F, -2.115915, 0.775013, 1.825694
F, 1.398130, 0.759901, 2.223253
F, 4.558655, 1.020135, -1.283023
N, -0.724944, -1.975297, -0.348327
N, -2.699006, 1.570346, -2.711773
H, -2.917854, 0.885624, -3.418470
N, 3.467872, -2.665270, -0.935222
H, 2.682177, -2.852509, -1.541113

[6-F$_a$]$^-$
Energy = -1703.792385, NImag =0.0
C, -3.204851, 5.587777, 9.823820
H, -3.706642, 6.542120, 9.995173
H, -3.959119, 4.814617, 9.641511
H, -2.600587, 5.288086, 10.697474
C, -2.325377, 6.820525, 7.850324
H, -2.970608, 7.671238, 7.998316
C, -0.760072, 5.344619, 7.126349
H, 0.044252, 4.875929, 6.583465
C, -1.385206, 4.803490, 8.219387
C, -1.192481, 3.482918, 8.947144
H, -1.781468, 3.537429, 9.866529
C, -1.772976, 2.312071, 8.150586
C, -2.889648, 1.611779, 8.622821
C, -3.473996, 0.531030, 7.969042
H, -4.335517, 0.048377, 8.416888
C, -2.932505, 0.109705, 6.756965
H, -3.369350, -0.731503, 6.227448
C, -1.830427, 0.775840, 6.223030
H, -1.382706, 0.487468, 5.278536
C, -1.289541, 1.848960, 6.922444
C, 0.217637, 3.263829, 9.468927
C, 1.409294, 2.813788, 8.902717
H, 1.557597, 2.483188, 7.884949
C, 2.386750, 2.875148, 9.930267
H, 3.431275, 2.596180, 9.850976
C, 1.742589, 3.360455, 11.062917

H, 2.139475, 3.549194, 12.053246
C, -0.988881, 7.535108, 5.810176
C, 0.093127, 7.072929, 4.881298
C, -0.123657, 6.073502, 3.927809
C, 0.864539, 5.612735, 3.064943
H, 0.621226, 4.834345, 2.350927
C, 2.141197, 6.166497, 3.153407
H, 2.928339, 5.815867, 2.493189
C, 2.413560, 7.165121, 4.086968
H, 3.397118, 7.609929, 4.185478
C, 1.389922, 7.593447, 4.926177
C, -1.542885, 8.786726, 5.562434
C, -1.203877, 9.684778, 4.476824
H, -0.467931, 9.502688, 3.705378
C, -2.807133, 10.522321, 5.796429
H, -3.560798, 11.183935, 6.217255
C, -2.006074, 10.785913, 4.625431
H, -2.041811, 11.671616, 4.002977
C, -1.341916, 6.635274, 6.859731
F, -3.458667, 2.008758, 9.784199
F, -0.229076, 2.472026, 6.356253
F, -1.355368, 5.538271, 3.830333
F, 1.666850, 8.555557, 5.825790
N, -2.345400, 5.736402, 8.648129
N, 0.430835, 3.592704, 10.781971
H, -0.513960, 3.971353, 11.443455
N, -2.547348, 9.356612, 6.352214
F, -1.595715, 4.276150, 11.877803

[6-F_a]$^-$ solvent optimised
Energy = -1703.862624, NImag =0.0
C, -1.504018, 3.212564, -0.656598
H, -0.903041, 4.106974, -0.826296
H, -2.116186, 3.022083, -1.544153
H, -2.166963, 3.339921, 0.212729
C, 0.747607, 2.152702, -0.566611
H, 1.253629, 3.047736, -0.888664
C, 0.182850, 0.077964, 0.151092
H, 0.228921, -0.944566, 0.488986
C, -0.968123, 0.814729, 0.020885
C, -2.425855, 0.465535, 0.272878
H, -2.985461, 1.403125, 0.232972
C, -3.003290, -0.413088, -0.837793
C, -3.998821, 0.079011, -1.689514
C, -4.576131, -0.648136, -2.724427
H, -5.345015, -0.187024, -3.333687
C, -4.139954, -1.953331, -2.944975
H, -4.574363, -2.542971, -3.745333
C, -3.141801, -2.500665, -2.138594
H, -2.773594, -3.509789, -2.284222
C, -2.603729, -1.722908, -1.120848
C, -2.696036, -0.025601, 1.685136
C, -2.593526, -1.252825, 2.333977
H, -2.285141, -2.188275, 1.890861
C, -2.973808, -1.031175, 3.686912
H, -3.015247, -1.769229, 4.478927
C, -3.286857, 0.316764, 3.800389
H, -3.623577, 0.880714, 4.661029
C, 2.680794, 0.521460, -0.230897
C, 2.973362, -0.906771, 0.111253
C, 2.642289, -1.958579, -0.749560
C, 2.893439, -3.293418, -0.459182
H, 2.616737, -4.056194, -1.177655
C, 3.499977, -3.608203, 0.757501
H, 3.702985, -4.644676, 1.005265
C, 3.846637, -2.600854, 1.657751
H, 4.313317, -2.818626, 2.611364
C, 3.577142, -1.280769, 1.316100
C, 3.760476, 1.340468, -0.526668
C, 5.156406, 0.946242, -0.596327

H, 5.545828, -0.048110, -0.426180
C, 4.868928, 3.119332, -1.061032
H, 5.070326, 4.156205, -1.318093
C, 5.856955, 2.071535, -0.935992
H, 6.924512, 2.172643, -1.084128
C, 1.298975, 0.907102, -0.220204
F, -4.428175, 1.352901, -1.506338
F, -1.629417, -2.284745, -0.361003
F, 2.060790, -1.654328, -1.929640
F, 3.907742, -0.310764, 2.194522
N, -0.593261, 2.090395, -0.422092
N, -3.117548, 0.919329, 2.586690
H, -3.319196, 1.985048, 2.225255
N, 3.640059, 2.705966, -0.825814
F, -3.521667, 3.075899, 1.540417

[**6-TBAF**]
Energy = -2389.925387, NImag =0.0
C, -2.687042, 4.543830, 10.682515
H, -3.643705, 5.041670, 10.852294
H, -2.876085, 3.576901, 10.209960
H, -2.144827, 4.420783, 11.629486
C, -2.182034, 6.675848, 9.498458
H, -3.103184, 7.142360, 9.805317
C, -0.161955, 6.162189, 8.608540
H, 0.787407, 6.221142, 8.100835
C, -0.627894, 5.063631, 9.286730
C, -0.002696, 3.705578, 9.554415
H, -0.626063, 3.230326, 10.313220
C, -0.089414, 2.779166, 8.343171
C, -0.891520, 1.633782, 8.377150
C, -1.040727, 0.751407, 7.313965
H, -1.682328, -0.114392, 7.429796
C, -0.356070, 1.016163, 6.129670
H, -0.453845, 0.342528, 5.284634
C, 0.451980, 2.147728, 6.028034
H, 0.995579, 2.388492, 5.121729
C, 0.560350, 2.994627, 7.124256
C, 1.373399, 3.795645, 10.185501
C, 2.664025, 3.624643, 9.709902
H, 2.943551, 3.378635, 8.696895
C, 3.545875, 3.835638, 10.806202
H, 4.625181, 3.764711, 10.791122
C, 2.760161, 4.129430, 11.905631
H, 3.035985, 4.333646, 12.930996
C, -1.024758, 8.549629, 8.224398
C, 0.003286, 8.771685, 7.163644
C, -0.074299, 8.143421, 5.913549
C, 0.872714, 8.318053, 4.911950
H, 0.740935, 7.806959, 3.965429
C, 1.964251, 9.149899, 5.159631
H, 2.716241, 9.295149, 4.390897
C, 2.098253, 9.793875, 6.389012
H, 2.939956, 10.438623, 6.613475
C, 1.119732, 9.593982, 7.355536
C, -1.775212, 9.636251, 8.643116
C, -1.801993, 10.957094, 8.042868
H, -1.236389, 11.271336, 7.176670
C, -3.192666, 10.798224, 9.790187
H, -3.911700, 11.052730, 10.564329
C, -2.706709, 11.688011, 8.761096
H, -3.001977, 12.718016, 8.608036
C, -1.129869, 7.215652, 8.744362
F, -1.583305, 1.367050, 9.514022
F, 1.350937, 4.084817, 6.993114
F, -1.129555, 7.348146, 5.663613
F, 1.271885, 10.208835, 8.548242
N, -1.883014, 5.394145, 9.806036
N, 1.445653, 4.098972, 11.523765
H, 0.607416, 4.345577, 12.119039

N, -2.659373, 9.595020, 9.734181
F, -0.646751, 4.896216, 12.829074
N, -0.326134, 7.735970, 14.145570
C, 0.254659, 7.712114, 12.714010
C, 1.747154, 7.993949, 12.552128
H, -0.320401, 8.447147, 12.149078
H, 0.003511, 6.701137, 12.370759
C, 2.146252, 7.869700, 11.070944
H, 2.005623, 9.002629, 12.894551
H, 2.347376, 7.283870, 13.131384
C, 3.652278, 8.046468, 10.860099
H, 1.840836, 6.887739, 10.696380
H, 1.602255, 8.618152, 10.483577
H, 3.901770, 8.004536, 9.795582
H, 4.005347, 9.010321, 11.246854
H, 4.212857, 7.249504, 11.359480
C, 0.342825, 6.609567, 14.940789
C, -0.210127, 6.347467, 16.343485
H, 1.400793, 6.865268, 14.998038
H, 0.197791, 5.728915, 14.297620
C, 0.727981, 5.398886, 17.108413
H, -0.331845, 7.272603, 16.921778
H, -1.198086, 5.880165, 16.281196
C, 0.190619, 5.020686, 18.491218
H, 0.881843, 4.491088, 16.512081
H, 1.715368, 5.868498, 17.212938
H, 0.880141, 4.349761, 19.012418
H, 0.049033, 5.906737, 19.120634
H, -0.775383, 4.509993, 18.414500
C, -1.814081, 7.362768, 14.015546
C, -2.705880, 8.330602, 13.238451
H, -2.183025, 7.286507, 15.040350
H, -1.785649, 6.363970, 13.563305
C, -4.161748, 7.832461, 13.292676
H, -2.667845, 9.339345, 13.669224
H, -2.409571, 8.420361, 12.188903
C, -5.126184, 8.747941, 12.533386
H, -4.208591, 6.819583, 12.872614
H, -4.483576, 7.742361, 14.339534
H, -6.149569, 8.361211, 12.571244
H, -5.137073, 9.755113, 12.966238
H, -4.832206, 8.839163, 11.483330
C, -0.204484, 9.100068, 14.807985
C, 1.097959, 9.432151, 15.542580
H, -1.034313, 9.173962, 15.516015
H, -0.387550, 9.833908, 14.019725
C, 1.066863, 10.884883, 16.046056
H, 1.235229, 8.763582, 16.398676
H, 1.966627, 9.296332, 14.894713
C, 2.326789, 11.263006, 16.830005
H, 0.948986, 11.563674, 15.191400
H, 0.182354, 11.034369, 16.679759
H, 2.280583, 12.300880, 17.172891
H, 2.452334, 10.625992, 17.712400
H, 3.225202, 11.156009, 16.212591

[6-F_b]$^-$
Energy = -1703.768482, NImag =0.0
C, -3.778212, 5.012200, 8.964473
H, -4.453159, 5.863267, 9.069099
H, -4.313678, 4.178746, 8.499842
H, -3.438325, 4.692760, 9.951508
C, -2.653215, 6.510243, 7.358103
H, -3.522975, 7.147808, 7.316350
C, -0.630128, 5.472006, 7.195901
H, 0.386733, 5.208716, 6.950438
C, -1.398558, 4.759844, 8.068787
C, -1.075144, 3.541070, 8.901966
H, -1.235222, 3.803715, 9.953373
C, -2.016186, 2.365915, 8.612630

C, -2.736042, 1.733208, 9.632088
C, -3.537773, 0.611770, 9.447965
H, -4.054637, 0.186418, 10.301263
C, -3.653502, 0.076063, 8.166133
H, -4.270423, -0.800875, 7.995534
C, -2.980800, 0.676624, 7.100963
H, -3.052833, 0.298768, 6.086998
C, -2.190628, 1.793824, 7.345975
C, 0.377043, 3.113980, 8.863424
C, 1.177624, 2.702586, 7.777427
H, 0.885435, 2.623807, 6.737171
C, 2.433700, 2.395176, 8.342351
H, 3.319948, 2.049802, 7.817654
C, 2.297522, 2.633918, 9.720170
H, 3.059139, 2.514390, 10.488521
C, -0.943890, 7.588597, 5.802219
C, 0.427506, 7.354585, 5.240435
C, 0.679298, 6.355453, 4.295253
C, 1.943469, 6.097016, 3.778713
H, 2.064786, 5.301910, 3.052390
C, 3.018448, 6.863442, 4.226942
H, 4.015327, 6.668471, 3.844625
C, 2.823448, 7.873079, 5.168242
H, 3.641064, 8.477736, 5.543206
C, 1.539107, 8.095081, 5.652476
C, -1.598506, 8.743215, 5.356036
C, -1.101019, 9.646639, 4.349096
H, -0.163980, 9.542353, 3.820833
C, -3.098974, 10.303891, 5.094490
H, -4.021447, 10.851903, 5.258238
C, -2.050521, 10.628223, 4.182541
H, -2.021547, 11.472741, 3.506678
C, -1.398693, 6.602121, 6.718588
F, -2.683091, 2.262520, 10.881418
F, -1.571876, 2.361668, 6.288716
F, -0.356667, 5.618724, 3.854040
F, 1.359961, 9.068709, 6.565809
N, -2.642826, 5.420205, 8.149309
N, 1.052590, 3.064396, 10.047939
N, -2.846761, 9.200256, 5.787131
H, -3.970684, 8.887479, 6.788539
F, -4.764410, 8.699259, 7.350665

[**6-F$_c$**]$^-$
Energy = -1703.762331, NImag =0.0
C, -2.915598, 5.916908, 10.008449
H, -3.450374, 6.863471, 10.101487
H, -3.646271, 5.101873, 10.034269
H, -2.244001, 5.812104, 10.869428
C, -2.081478, 7.007991, 7.924227
H, -2.573631, 7.940375, 8.144726
C, -0.983856, 5.284414, 6.990241
H, -0.402409, 4.686500, 6.304570
C, -1.503940, 4.850463, 8.190055
C, -1.317240, 3.542221, 8.921295
H, -1.908229, 3.593238, 9.839080
C, -1.907663, 2.362791, 8.146675
C, -3.148159, 1.822497, 8.491793
C, -3.749359, 0.760753, 7.826210
H, -4.716402, 0.402879, 8.160824
C, -3.081576, 0.195646, 6.740873
H, -3.530467, -0.631064, 6.199450
C, -1.840876, 0.694531, 6.344606
H, -1.297438, 0.285415, 5.500627
C, -1.287996, 1.757923, 7.048698
C, 0.121749, 3.305689, 9.354667
C, 0.646537, 2.337075, 10.194319
H, 0.081139, 1.547299, 10.671381
C, 2.046242, 2.571203, 10.299932
H, 2.759787, 1.998019, 10.876662

C, 2.331148, 3.677687, 9.525399
H, 3.261288, 4.190614, 9.331414
C, -0.904495, 7.533781, 5.703111
C, 0.349421, 7.212847, 5.067215
C, 0.597450, 7.402458, 3.600690
C, 1.604266, 6.479159, 3.018648
H, 1.594768, 6.400053, 1.936294
C, 2.547417, 5.881436, 3.789015
H, 3.330123, 5.286001, 3.322166
C, 2.525711, 6.004728, 5.211521
H, 3.324799, 5.632357, 5.840907
C, 1.437848, 6.625783, 5.768106
C, -1.771406, 8.581010, 5.325578
C, -1.497156, 9.725415, 4.494653
H, -0.566647, 9.920439, 3.986871
C, -3.566048, 9.800091, 5.350042
H, -4.581931, 10.112412, 5.587808
C, -2.633785, 10.501824, 4.515701
H, -2.796335, 11.447890, 4.010644
C, -1.322835, 6.662492, 6.816536
F, -3.813668, 2.364072, 9.547185
F, -0.093321, 2.230132, 6.642539
F, -0.579452, 7.309899, 2.870030
F, 1.432945, 6.691463, 7.147372
N, -2.187105, 5.923515, 8.755616
N, 1.159796, 4.112348, 8.962109
H, 1.063986, 4.908837, 8.340133
N, -3.075858, 8.671284, 5.835367
F, 1.037078, 8.740721, 3.285556

[6-F$_d$]$^-$
Energy = -1703.751239, NImag =0.0
C, -3.893646, 4.989843, 8.785818
H, -4.607333, 5.816432, 8.810433
H, -4.310611, 4.128216, 8.262472
H, -3.644161, 4.697157, 9.808161
C, -2.656443, 6.522096, 7.280954
H, -3.483641, 7.204816, 7.170747
C, -0.681853, 5.412960, 7.130334
H, 0.318695, 5.113858, 6.859450
C, -1.491264, 4.728172, 7.995162
C, -1.210310, 3.516900, 8.864787
H, -1.374814, 3.852092, 9.899659
C, -2.160840, 2.338304, 8.688830
C, -2.672491, 1.701979, 9.811375
C, -3.495779, 0.583421, 9.817225
H, -3.841468, 0.152626, 10.748548
C, -3.807827, 0.053692, 8.548187
H, -4.417457, -0.847600, 8.487845
C, -3.361369, 0.627888, 7.381474
H, -3.608641, 0.211337, 6.409706
C, -2.581131, 1.859816, 7.371863
C, 0.263135, 3.154923, 8.800950
C, 0.956476, 2.137454, 8.177881
H, 0.492147, 1.381047, 7.565593
C, 2.338875, 2.297106, 8.487435
H, 3.152224, 1.661763, 8.162221
C, 2.460475, 3.411123, 9.290372
H, 3.323785, 3.874254, 9.746342
C, -0.921933, 7.570597, 5.753992
C, 0.467143, 7.374314, 5.226242
C, 0.717541, 6.968033, 3.911853
C, 1.997787, 6.761441, 3.407927
H, 2.113546, 6.438483, 2.379701
C, 3.090632, 6.965095, 4.248703
H, 4.096851, 6.803528, 3.874897
C, 2.898586, 7.371205, 5.568731
H, 3.726975, 7.535861, 6.248080
C, 1.599290, 7.562114, 6.024778
C, -1.609652, 8.700272, 5.320609

C, -1.113480, 9.726843, 4.426759
H, -0.133405, 9.755159, 3.970149
C, -3.204081, 10.142643, 5.111474
H, -4.174160, 10.615042, 5.247947
C, -2.125655, 10.641638, 4.293625
H, -2.127292, 11.550583, 3.704576
C, -1.398556, 6.572240, 6.654683
F, -2.335666, 2.233408, 11.041052
F, -1.482407, 1.767221, 6.459526
F, -0.328374, 6.764376, 3.090264
F, 1.424128, 7.960030, 7.300802
N, -2.699806, 5.436533, 8.078306
N, 1.194647, 3.917412, 9.480105
H, 0.973624, 4.766406, 9.974867
N, -2.914311, 9.009806, 5.719044
F, -3.330036, 2.913765, 6.646324

[**6-F$_e$**]$^-$
Energy = -1703.739846, NImag =0.0
C, -3.395133, 5.535560, 9.579772
H, -4.252784, 6.184684, 9.393218
H, -3.744440, 4.502940, 9.644456
H, -2.957767, 5.809009, 10.548805
C, -2.453471, 6.755027, 7.645671
H, -3.223591, 7.509964, 7.656864
C, -0.592041, 5.489404, 7.229676
H, 0.319710, 5.067926, 6.737261
C, -1.293146, 4.916098, 8.256216
C, -1.093283, 3.620592, 9.015023
H, -1.516786, 3.767027, 10.015035
C, -1.912489, 2.468225, 8.407048
C, -2.892167, 1.792264, 9.133789
C, -3.650952, 0.735260, 8.643623
H, -4.394918, 0.271266, 9.281620
C, -3.418294, 0.310928, 7.336336
H, -3.993530, -0.512308, 6.923469
C, -2.449118, 0.942953, 6.557887
H, -2.240770, 0.638848, 5.538312
C, -1.717345, 1.997446, 7.098947
C, 0.344620, 3.202003, 9.242964
C, 1.466271, 3.128273, 8.436791
H, 1.531682, 3.460126, 7.380716
C, 2.505050, 2.571324, 9.241707
H, 3.524535, 2.390727, 8.925486
C, 1.999386, 2.308079, 10.497526
H, 2.457188, 1.899409, 11.387712
C, -0.952275, 7.566831, 5.762942
C, 0.324340, 7.272885, 5.043527
C, 0.536322, 6.080954, 4.340558
C, 1.731504, 5.792994, 3.683353
H, 1.831113, 4.826092, 3.210061
C, 2.763768, 6.715241, 3.730288
H, 3.707523, 6.495109, 3.239364
C, 2.614905, 7.918078, 4.434970
H, 3.413076, 8.648166, 4.510352
C, 1.414025, 8.159331, 5.078648
C, -1.678858, 8.689094, 5.369914
C, -1.390435, 9.554804, 4.245562
H, -0.561824, 9.444460, 3.560111
C, -3.240895, 10.185615, 5.333678
H, -4.136479, 10.730891, 5.625296
C, -2.381030, 10.502078, 4.220737
H, -2.505694, 11.316306, 3.516942
C, -1.321135, 6.669123, 6.824191
F, -3.142381, 2.199144, 10.416011
F, -0.791452, 2.578449, 6.338229
F, -0.507277, 5.258004, 4.170732
F, 1.289201, 9.314730, 5.778217
N, -2.441014, 5.704119, 8.500421
N, 0.680255, 2.696613, 10.491921

H, 0.040647, 2.604577, 11.264397
N, -2.845306, 9.127033, 6.011646
F, 1.348660, 4.195522, 5.813486

[**6-OAc$_a$**]$^-$
Energy = -1832.456646, NImag =0.0
C, -1.626407, 1.951111, -2.012236
H, -1.170793, 2.449277, -2.870485
H, -2.411355, 1.281944, -2.369869
H, -2.066960, 2.702618, -1.336037
C, 0.739836, 1.384061, -1.514268
H, 1.132404, 2.098717, -2.219376
C, 0.452841, -0.180735, 0.103872
H, 0.620407, -0.909847, 0.880871
C, -0.780707, 0.211402, -0.340817
C, -2.173084, -0.245893, 0.048916
H, -2.832529, 0.623300, -0.060516
C, -2.700162, -1.329974, -0.898499
C, -3.879158, -1.145737, -1.629826
C, -4.410608, -2.086806, -2.507033
H, -5.331019, -1.855410, -3.031217
C, -3.737025, -3.293018, -2.683626
H, -4.131960, -4.042701, -3.362391
C, -2.553291, -3.535471, -1.988162
H, -1.996779, -4.459407, -2.098437
C, -2.069974, -2.559094, -1.124212
C, -2.291439, -0.635530, 1.509262
C, -1.963676, -1.777127, 2.229778
H, -1.528750, -2.678486, 1.824921
C, -2.310939, -1.531096, 3.586854
H, -2.190992, -2.210905, 4.420585
C, -2.836544, -0.252527, 3.645223
H, -3.219653, 0.314577, 4.481890
C, 2.869168, 0.437641, -0.493640
C, 3.356260, -0.540955, 0.532366
C, 3.303714, -1.922416, 0.323515
C, 3.732371, -2.854242, 1.262417
H, 3.660793, -3.910373, 1.029196
C, 4.236661, -2.394906, 2.478614
H, 4.571018, -3.106383, 3.227226
C, 4.311143, -1.027753, 2.740105
H, 4.691782, -0.639767, 3.677947
C, 3.870932, -0.135759, 1.767325
C, 3.834174, 1.136506, -1.208989
C, 5.272424, 1.006086, -1.081385
H, 5.794588, 0.341348, -0.406589
C, 4.693777, 2.512291, -2.634495
H, 4.749223, 3.267629, -3.414877
C, 5.817514, 1.879385, -1.985133
H, 6.866411, 2.064574, -2.181741
C, 1.452648, 0.549090, -0.632519
F, -4.543931, 0.022178, -1.497643
F, -0.923718, -2.837016, -0.463170
F, 2.825036, -2.374032, -0.851031
F, 3.944553, 1.181613, 2.032951
N, -0.579369, 1.178363, -1.338918
N, -2.822594, 0.276458, 2.386269
H, -3.150134, 1.217139, 2.071872
N, 3.529789, 2.085312, -2.191345
O, -3.515205, 2.434809, 0.998850
C, -3.259926, 3.676764, 0.863838
O, -2.802007, 4.237592, -0.153464
C, -3.557625, 4.553641, 2.100183
H, -2.888289, 4.269744, 2.921384
H, -4.581926, 4.379527, 2.448358
H, -3.417428, 5.614415, 1.877621

[**6-OAc$_b$**]$^-$
Energy = -1832.423266, NImag =0.0
C, 1.105313, 2.890134, 0.089622

H, 0.298165, 3.619612, -0.000252
H, 1.626301, 3.034795, 1.041512
H, 1.820690, 3.046871, -0.719159
C, -0.758191, 1.276763, 0.276929
H, -1.438212, 2.046216, 0.598105
C, 0.305672, -0.637693, -0.331670
H, 0.541197, -1.656511, -0.597774
C, 1.212911, 0.382128, -0.383495
C, 2.662797, 0.392825, -0.811597
H, 2.762801, 1.105133, -1.637827
C, 3.594779, 0.896872, 0.296815
C, 4.478177, 1.961473, 0.087177
C, 5.407201, 2.408022, 1.020799
H, 6.055371, 3.239090, 0.764990
C, 5.468029, 1.771784, 2.259748
H, 6.186659, 2.097827, 3.005393
C, 4.595015, 0.719930, 2.541559
H, 4.601213, 0.205722, 3.496382
C, 3.689627, 0.314815, 1.567554
C, 3.159467, -0.907107, -1.408166
C, 3.238583, -2.197453, -0.845195
H, 2.938556, -2.500887, 0.150650
C, 3.812690, -3.003222, -1.852084
H, 4.025407, -4.067060, -1.796174
C, 4.044548, -2.143523, -2.938340
H, 4.473820, -2.402586, -3.904453
C, -2.183561, -0.824111, 0.256440
C, -2.055972, -2.315063, 0.252104
C, -1.353918, -3.002239, 1.249875
C, -1.192055, -4.382324, 1.255701
H, -0.633620, -4.844521, 2.061264
C, -1.745218, -5.125425, 0.213711
H, -1.618799, -6.203235, 0.194501
C, -2.453697, -4.493334, -0.806765
H, -2.884669, -5.042760, -1.635670
C, -2.594020, -3.110525, -0.766119
C, -3.464877, -0.301390, 0.431522
C, -4.630893, -1.054881, 0.826644
H, -4.651452, -2.117394, 1.025278
C, -5.115357, 1.117228, 0.599207
H, -5.626518, 2.071773, 0.535754
C, -5.663937, -0.158645, 0.946650
H, -6.687662, -0.359937, 1.234206
C, -0.969105, -0.098066, 0.079657
F, 4.405859, 2.635304, -1.090204
F, 2.845596, -0.690525, 1.883686
F, -0.830686, -2.294633, 2.266760
F, -3.270264, -2.511961, -1.764374
N, 0.533261, 1.555144, -0.000602
N, 3.657769, -0.868600, -2.678055
N, -3.824921, 1.047282, 0.299336
H, -3.287762, 2.436648, -0.347765
O, -2.926239, 3.334121, -0.715060
C, -3.822580, 4.311799, -0.670218
O, -4.962341, 4.209091, -0.243703
C, -3.264872, 5.610525, -1.224363
H, -2.943840, 5.464712, -2.260207
H, -2.381827, 5.913120, -0.652971
H, -4.023815, 6.391465, -1.175461

[6-OAc$_a$]$^-$ solvent optimised
Energy = -1832.525736, NImag =0.0
C, 1.595766, -1.990573, -1.927506
H, 1.157702, -2.766039, -2.556330
H, 2.177124, -1.311065, -2.555964
H, 2.256895, -2.439656, -1.177685
C, -0.801218, -1.582944, -1.390135
H, -1.146963, -2.376617, -2.031527
C, -0.592959, 0.122416, 0.088160
H, -0.804480, 0.895861, 0.809253

C, 0.659381, -0.218952, -0.353911
C, 2.027614, 0.351841, -0.027597
H, 2.753973, -0.428141, -0.266975
C, 2.383483, 1.538766, -0.926499
C, 3.472902, 1.476641, -1.802121
C, 3.847314, 2.505502, -2.658644
H, 4.707517, 2.373157, -3.304619
C, 3.094608, 3.678601, -2.657992
H, 3.366027, 4.497060, -3.316240
C, 1.991096, 3.801350, -1.813307
H, 1.381965, 4.697662, -1.789486
C, 1.665848, 2.738045, -0.980724
C, 2.226088, 0.615764, 1.451980
C, 1.951216, 1.688026, 2.288868
H, 1.510052, 2.627177, 1.991045
C, 2.353924, 1.311077, 3.602033
H, 2.285360, 1.913278, 4.498577
C, 2.856829, 0.025029, 3.520568
H, 3.267650, -0.621480, 4.283094
C, -2.976241, -0.701289, -0.384669
C, -3.510666, 0.388094, 0.492055
C, -3.475620, 1.733061, 0.107615
C, -3.952209, 2.768527, 0.901079
H, -3.900100, 3.787362, 0.535269
C, -4.487612, 2.457940, 2.151793
H, -4.863106, 3.251932, 2.788530
C, -4.543391, 1.134961, 2.589816
H, -4.948805, 0.867453, 3.558669
C, -4.056897, 0.135839, 1.754952
C, -3.890505, -1.577242, -0.947755
C, -5.337669, -1.517514, -0.831466
H, -5.901709, -0.774077, -0.285204
C, -4.662012, -3.236745, -2.100439
H, -4.673950, -4.122515, -2.730437
C, -5.825028, -2.565840, -1.562032
H, -6.858780, -2.847882, -1.715503
C, -1.550781, -0.733071, -0.560263
F, 4.206739, 0.336024, -1.831313
F, 0.589799, 2.886978, -0.169368
F, -2.963596, 2.033750, -1.105012
F, -4.105936, -1.141413, 2.188315
N, 0.507833, -1.271161, -1.264808
N, 2.776874, -0.384436, 2.216809
H, 3.088513, -1.295506, 1.810528
N, -3.526102, -2.669582, -1.750531
O, 3.464371, -2.560366, 0.737923
C, 4.569628, -3.209612, 0.712841
O, 4.975267, -3.925037, -0.224312
C, 5.440755, -3.083059, 1.978086
H, 4.903741, -3.490442, 2.842520
H, 5.641399, -2.028189, 2.196178
H, 6.387736, -3.615739, 1.864814

[**6-TBAOAc**]
Energy = -2518.575654, Nimag =0.0
C, -1.328087, -2.013866, 2.274632
H, -0.790779, -1.809127, 3.201711
H, -2.274865, -2.499126, 2.518490
H, -0.727314, -2.666950, 1.631583
C, -0.888961, 0.398225, 1.853647
H, -0.212100, 0.493227, 2.686174
C, -2.192151, 0.719328, 0.025901
H, -2.671036, 1.150726, -0.838769
C, -2.356384, -0.574016, 0.451125
C, -3.174472, -1.721083, -0.114764
H, -2.754119, -2.636165, 0.307816
C, -4.623021, -1.689360, 0.370100
C, -5.130976, -2.707958, 1.182215
C, -6.429275, -2.739406, 1.676206
H, -6.740527, -3.571074, 2.297540

C, -7.288231, -1.691045, 1.352161
H, -8.307913, -1.691897, 1.723079
C, -6.838852, -0.639136, 0.554983
H, -7.477532, 0.194602, 0.287102
C, -5.529175, -0.661505, 0.091376
C, -3.019498, -1.872890, -1.612960
C, -3.809077, -1.530487, -2.697515
H, -4.773917, -1.048707, -2.654827
C, -3.109567, -1.928299, -3.871312
H, -3.447043, -1.820941, -4.893065
C, -1.919083, -2.496272, -3.461801
H, -1.110037, -2.928204, -4.033063
C, -0.724147, 2.692835, 0.767834
C, -1.452564, 3.604505, -0.163635
C, -2.774066, 4.005900, 0.071280
C, -3.480479, 4.839727, -0.786309
H, -4.497578, 5.117149, -0.535438
C, -2.853019, 5.293148, -1.946450
H, -3.390703, 5.940981, -2.630995
C, -1.541898, 4.917408, -2.236383
H, -1.034202, 5.246051, -3.135643
C, -0.874191, 4.089206, -1.342692
C, 0.402215, 3.185884, 1.410206
C, 0.849841, 4.565023, 1.438161
H, 0.366882, 5.398418, 0.947248
C, 2.159776, 3.231454, 2.669680
H, 2.961356, 2.879142, 3.314424
C, 1.954191, 4.595984, 2.245209
H, 2.554642, 5.453810, 2.519027
C, -1.240448, 1.359516, 0.894315
F, -4.301794, -3.725694, 1.529159
F, -5.120936, 0.370999, -0.679862
F, -3.379364, 3.577405, 1.193205
F, 0.389200, 3.715724, -1.643682
N, -1.558917, -0.746124, 1.586866
N, -1.875814, -2.466495, -2.092708
H, -1.076903, -2.766660, -1.504517
N, 1.262952, 2.393385, 2.186152
N, 3.642708, -0.710344, 0.174604
C, 2.226054, -0.390542, -0.349286
C, 2.118080, 0.349520, -1.690051
H, 1.757353, 0.210244, 0.431602
H, 1.711197, -1.357809, -0.398745
C, 0.733540, 0.111723, -2.315063
H, 2.265593, 1.426611, -1.550508
H, 2.871263, 0.010950, -2.409027
C, 0.544819, 0.860476, -3.636186
H, 0.592361, -0.962616, -2.467073
H, -0.045202, 0.414696, -1.608146
H, -0.432895, 0.628638, -4.069026
H, 0.605083, 1.943813, -3.488471
H, 1.309082, 0.578018, -4.370824
C, 4.369764, -1.559866, -0.868222
C, 5.740672, -2.107423, -0.466206
H, 4.471032, -0.939927, -1.757358
H, 3.683674, -2.388448, -1.072792
C, 6.425500, -2.751409, -1.683207
H, 6.390373, -1.319374, -0.063724
H, 5.634864, -2.868541, 0.312476
C, 7.778525, -3.378552, -1.336580
H, 5.760980, -3.517500, -2.101105
H, 6.560606, -1.996423, -2.469453
H, 8.243396, -3.826379, -2.220106
H, 8.474237, -2.631854, -0.936952
H, 7.667869, -4.166632, -0.583983
C, 3.483117, -1.596387, 1.421082
C, 2.697613, -1.009737, 2.590740
H, 4.500960, -1.815239, 1.749612
H, 3.021432, -2.519030, 1.047478
C, 2.792774, -1.958757, 3.798133

H, 3.072174, -0.022487, 2.881557
H, 1.648590, -0.876282, 2.318407
C, 2.053713, -1.429354, 5.030366
H, 2.393679, -2.941932, 3.519062
H, 3.849099, -2.120258, 4.053220
H, 2.142880, -2.122460, 5.872596
H, 2.454398, -0.460956, 5.349400
H, 0.985914, -1.290164, 4.828711
C, 4.398244, 0.555780, 0.560221
C, 5.084422, 1.347041, -0.555222
H, 5.148673, 0.253810, 1.296150
H, 3.669127, 1.189213, 1.069655
C, 5.697909, 2.636425, 0.016966
H, 5.876935, 0.751572, -1.022180
H, 4.375572, 1.610685, -1.342887
C, 6.427134, 3.462637, -1.046186
H, 4.904386, 3.241419, 0.473628
H, 6.396371, 2.382190, 0.825858
H, 6.851210, 4.374088, -0.614275
H, 7.248155, 2.895170, -1.498400
H, 5.746596, 3.761426, -1.850753
O, 0.328900, -3.024466, -0.450333
C, 1.141440, -4.003472, -0.573570
O, 2.374908, -3.959302, -0.340424
C, 0.541402, -5.341825, -1.025805
H, -0.053481, -5.207395, -1.935186
H, -0.141578, -5.715591, -0.254765
H, 1.322066, -6.083806, -1.202096

TBAF

Energy = -785.966260, NImag =0.0
F, -1.527358, 0.203132, -2.647647
N, -0.274335, -0.001425, -0.010332
C, -0.430550, 1.457768, -0.482409
C, 0.830615, 2.304964, -0.639231
H, -1.087794, 1.933096, 0.248773
H, -0.953069, 1.305052, -1.457557
C, 0.460705, 3.635578, -1.319113
H, 1.305807, 2.525906, 0.325513
H, 1.578504, 1.799860, -1.259929
C, 1.664458, 4.564946, -1.500160
H, 0.004539, 3.418616, -2.291926
H, -0.309725, 4.146306, -0.725611
H, 1.372362, 5.500374, -1.987864
H, 2.121437, 4.821182, -0.537055
H, 2.437633, 4.096033, -2.119330
C, 0.513474, -0.745090, -1.100712
C, 0.641413, -2.257630, -0.919398
H, 1.504657, -0.289937, -1.123370
H, -0.079623, -0.485740, -2.010684
C, 1.655667, -2.820729, -1.929150
H, 0.958810, -2.537491, 0.095308
H, -0.323797, -2.743797, -1.094837
C, 1.773106, -4.346508, -1.867746
H, 1.358627, -2.513291, -2.939274
H, 2.640676, -2.368872, -1.747997
H, 2.503629, -4.717579, -2.593627
H, 2.091386, -4.683003, -0.874030
H, 0.812998, -4.826055, -2.088082
C, -1.699860, -0.596428, -0.032311
C, -2.713694, 0.025271, 0.926521
H, -1.575694, -1.652536, 0.217204
H, -1.978724, -0.460290, -1.103497
C, -4.031074, -0.767721, 0.866293
H, -2.356806, 0.034160, 1.965713
H, -2.926963, 1.063416, 0.651360
C, -5.121637, -0.176370, 1.764488
H, -4.381441, -0.796455, -0.172488
H, -3.842795, -1.810367, 1.156285
H, -6.044933, -0.761224, 1.703800

H, -4.807941, -0.158287, 2.814797
H, -5.360641, 0.852233, 1.472242
C, 0.320064, -0.132110, 1.376197
C, 1.845376, -0.082271, 1.508588
H, -0.036880, -1.084489, 1.779163
H, -0.131012, 0.660596, 1.978854
C, 2.257436, -0.139259, 2.988912
H, 2.299659, -0.926943, 0.980440
H, 2.252219, 0.826046, 1.057649
C, 3.777389, -0.134297, 3.179438
H, 1.818315, 0.713876, 3.523113
H, 1.833489, -1.040360, 3.452358
H, 4.043133, -0.172911, 4.240319
H, 4.241779, -0.996469, 2.688139
H, 4.227419, 0.770455, 2.756025

TBAOAc

Energy = -914.649837, NImag =0.0
N, 0.795739, 0.422079, -0.411530
C, 2.188062, 1.033356, -0.405841
C, 3.388165, 0.120530, -0.153549
H, 2.168176, 1.816764, 0.352573
H, 2.295135, 1.523213, -1.379176
C, 4.697983, 0.912160, -0.309133
H, 3.344181, -0.296641, 0.856498
H, 3.400300, -0.724322, -0.850180
C, 5.938570, 0.056812, -0.036992
H, 4.753961, 1.328336, -1.323670
H, 4.688407, 1.771673, 0.374065
H, 6.854561, 0.642737, -0.157112
H, 5.929866, -0.342427, 0.982948
H, 5.994024, -0.792993, -0.726021
C, 0.716837, -0.635938, -1.508167
C, -0.676451, -1.200903, -1.790739
H, 1.394940, -1.436288, -1.211194
H, 1.136885, -0.162889, -2.402372
C, -0.572016, -2.475958, -2.641807
H, -1.215682, -1.407809, -0.857319
H, -1.285286, -0.461080, -2.318379
C, -1.949783, -3.043798, -2.995180
H, -0.009891, -2.272348, -3.564936
H, 0.005455, -3.234897, -2.095119
H, -1.861587, -3.965221, -3.579620
H, -2.522123, -3.267260, -2.089425
H, -2.532305, -2.327004, -3.583585
C, -0.208370, 1.536003, -0.769722
C, -0.239504, 2.751994, 0.155569
H, -1.210701, 1.078466, -0.744761
H, 0.045839, 1.836963, -1.791949
C, -1.410133, 3.665085, -0.254602
H, -0.401819, 2.433943, 1.191056
H, 0.695342, 3.326917, 0.130183
C, -1.524972, 4.903269, 0.638057
H, -1.276633, 3.979026, -1.299224
H, -2.331184, 3.073738, -0.215443
H, -2.362656, 5.534683, 0.326181
H, -1.695940, 4.622382, 1.683348
H, -0.615949, 5.515962, 0.602677
C, 0.396401, -0.147641, 0.964008
C, 0.827059, -1.573207, 1.312068
H, -0.703414, -0.148589, 0.984831
H, 0.789396, 0.561787, 1.696014
C, 0.262102, -1.927840, 2.699946
H, 0.402475, -2.278499, 0.591315
H, 1.913786, -1.712411, 1.306519
C, 0.601276, -3.360103, 3.120695
H, 0.655888, -1.224240, 3.446851
H, -0.823979, -1.789895, 2.664810
H, 0.187893, -3.587070, 4.108273
H, 0.184937, -4.086832, 2.414532

H, 1.684684, -3.523837, 3.168378
O, -3.066302, 0.767219, -0.272677
C, -3.303031, -0.183898, 0.522217
O, -2.461830, -1.031746, 0.951826
C, -4.750741, -0.359092, 1.010860
H, -5.388160, 0.461189, 0.674109
H, -4.771116, -0.422489, 2.103800
H, -5.151541, -1.306056, 0.631924

Acetate
Energy = -228.502197, NImag =0.0
O, 1.159703, 0.706684, 0.000000
O, -1.115797, 0.798016, 0.000000
C, 0.000000, 0.220086, 0.000000
C, -0.042986, -1.354494, 0.000000
H, 0.487757, -1.744734, 0.879498
H, -1.068845, -1.741685, 0.000000
H, 0.487757, -1.744734, -0.879498

5-dimer
Energy = -3358.319699, NImag =0.0
C, 4.786983, 2.516799, 15.178445
H, 3.909552, 2.024518, 15.595787
H, 5.431444, 2.870154, 15.987313
H, 4.458690, 3.371707, 14.580424
F, 9.862916, 1.648528, 13.111815
O, 3.932111, -0.144284, 14.651981
N, 5.478765, 1.540858, 14.353413
C, 4.988115, 0.272214, 14.129729
F, 7.495456, 4.231669, 16.284159
N, 7.006358, 3.375248, 11.217021
H, 6.216195, 2.747805, 11.201763
C, 5.941091, -0.381708, 13.193066
F, 8.002854, -3.460980, 13.282312
N, 3.861753, -2.608669, 13.741730
H, 3.671765, -1.734755, 14.261520
C, 6.961000, 0.616159, 12.925576
H, 7.825879, 0.483876, 12.297146
F, 4.718358, 1.142994, 10.476799
C, 6.664391, 1.746946, 13.614196
C, 7.409789, 3.066289, 13.688043
H, 6.733680, 3.793244, 14.147903
C, 8.613466, 2.966740, 14.624636
C, 9.784585, 2.267991, 14.305584
C, 10.876642, 2.172412, 15.159156
H, 11.748266, 1.615025, 14.836279
C, 10.814617, 2.793496, 16.406341
H, 11.657658, 2.726852, 17.086050
C, 9.670905, 3.493735, 16.785081
H, 9.584809, 3.983597, 17.747922
C, 8.611347, 3.558343, 15.889179
C, 7.784776, 3.613940, 12.325135
C, 8.780272, 4.494086, 11.946587
H, 9.550899, 4.888279, 12.593722
C, 8.596418, 4.784940, 10.565000
H, 9.208248, 5.433342, 9.953652
C, 7.492210, 4.078580, 10.141338
H, 7.022249, 4.007930, 9.171830
C, 5.904502, -1.661874, 12.659622
C, 6.995831, -2.023339, 11.694615
C, 8.007502, -2.921430, 12.045460
C, 9.028296, -3.279860, 11.172928
H, 9.786478, -3.979025, 11.508496
C, 9.048522, -2.724085, 9.894110
H, 9.841092, -2.994893, 9.203346
C, 8.055867, -1.820922, 9.509878
H, 8.070698, -1.383406, 8.516699
C, 7.043188, -1.475287, 10.404674
C, 4.943509, -2.701064, 12.883405

C, 4.888317, -3.984927, 12.303748
H, 5.590353, -4.374601, 11.582064
C, 3.768908, -4.645105, 12.829003
H, 3.434481, -5.646635, 12.599071
C, 3.155364, -3.760544, 13.716221
H, 2.267199, -3.883008, 14.319663
C, 0.593630, 5.117565, 9.718841
H, 0.563560, 5.984840, 9.058628
H, 1.128033, 4.306079, 9.214283
H, -0.428412, 4.788126, 9.928793
F, 3.637974, 2.933454, 12.119787
O, 1.945492, 7.568275, 10.088707
N, 1.271676, 5.533154, 10.932406
C, 1.910912, 6.757079, 11.032854
F, -0.686344, 1.734692, 10.599405
N, -0.039256, 3.740020, 14.665316
H, -0.430454, 4.650626, 14.482584
C, 2.452581, 6.825451, 12.414875
F, 5.190302, 5.981632, 13.869424
N, 3.359566, 9.509410, 11.168181
H, 2.795096, 8.933688, 10.522002
C, 2.058297, 5.579341, 13.045524
H, 2.287879, 5.280738, 14.055795
F, 2.025496, 9.224762, 15.170158
C, 1.372546, 4.827120, 12.150233
C, 0.758657, 3.452381, 12.304550
H, -0.272356, 3.519532, 11.931080
C, 1.424720, 2.402594, 11.417658
C, 2.805040, 2.202853, 11.359756
C, 3.369224, 1.258040, 10.504254
H, 6.273867, -0.766970, 10.116257
C, 2.579743, 0.455599, 9.698371
H, 3.046996, -0.278358, 9.052217
C, 1.194520, 0.616686, 9.741618
H, 0.533811, 0.013320, 9.130835
C, 0.656203, 1.575666, 10.588351
C, 0.682190, 3.004931, 13.745950
C, 1.156924, 1.885304, 14.398736
H, 1.759944, 1.097966, 13.971311
C, 0.720167, 1.958780, 15.753788
H, 0.921339, 1.236283, 16.531689
C, -0.010886, 3.117082, 15.890955
H, -0.507349, 3.549366, 16.746931
C, 3.194969, 7.833268, 13.010595
C, 3.599599, 7.628777, 14.440887
C, 4.600820, 6.731229, 14.825874
C, 5.016230, 6.567320, 16.142105
H, 5.816181, 5.871710, 16.362712
C, 4.394958, 7.323997, 17.135162
H, 4.704495, 7.210631, 18.169019
C, 3.378129, 8.222213, 16.812242
H, 2.873803, 8.817554, 17.564534
C, 3.007442, 8.355899, 15.479681
C, 3.643972, 9.071163, 12.449841
C, 4.446262, 10.066138, 13.046224
H, 4.850101, 10.026957, 14.046660
C, 4.629881, 11.088876, 12.107085
H, 5.195419, 12.000310, 12.237037
C, 3.942065, 10.709132, 10.953896
H, 3.837517, 11.217765, 10.006167

6-dimer
Energy = -3207.800456, NImag =0.0
C, -1.973348, 7.414644, 8.053486
H, -1.997196, 8.158647, 7.256089
H, -2.651361, 6.606002, 7.778020
H, -2.320189, 7.864814, 8.988665
C, 0.480271, 7.578419, 7.732722
H, 0.408803, 8.528117, 7.228244
C, 1.156695, 5.652977, 8.714771

H, 1.761644, 4.839963, 9.084198
C, -0.209332, 5.723984, 8.804580
C, -1.205141, 4.719848, 9.349620
C, -0.552418, 3.425877, 9.772066
C, -0.650785, 2.166078, 9.213562
H, -1.227938, 1.914853, 8.334541
C, 0.153615, 1.284027, 9.989849
H, 0.298058, 0.225477, 9.825965
C, 0.717371, 2.028567, 11.003354
H, 1.383191, 1.747139, 11.805608
C, 2.993569, 7.141970, 7.715050
C, 4.021853, 6.158025, 8.180997
C, 4.181122, 4.915887, 7.559973
C, 5.113955, 3.969603, 7.963173
H, 5.182673, 3.029952, 7.427759
C, 5.935297, 4.269083, 9.050436
H, 6.671520, 3.545002, 9.383827
C, 5.818502, 5.491478, 9.711085
H, 6.442110, 5.748912, 10.559398
C, 4.868322, 6.404463, 9.266031
C, 3.435327, 8.246817, 7.012646
C, 4.813110, 8.601279, 6.710793
H, 5.691780, 8.041192, 6.998884
C, 3.353989, 10.090186, 5.886771
H, 2.938432, 10.952729, 5.372578
C, 4.761480, 9.769861, 6.006665
H, 5.587821, 10.345463, 5.610266
C, 1.625384, 6.827472, 8.029055
F, 3.388108, 4.626290, 6.503202
F, 4.756667, 7.580840, 9.910906
N, -0.608266, 6.916505, 8.192335
N, 0.285082, 3.325056, 10.862988
H, 0.525004, 4.099647, 11.461794
N, 2.569667, 9.209540, 6.468016
C, 1.545087, 6.608966, 4.138069
H, 1.616151, 7.616020, 4.551060
H, 2.199518, 5.960709, 4.721479
H, 1.879924, 6.611763, 3.096063
C, -0.896355, 6.992938, 4.367126
H, -0.783863, 8.064022, 4.407979
C, -1.652078, 4.857928, 4.345962
H, -2.290439, 3.989478, 4.392524
C, -0.286849, 4.831137, 4.222405
C, 0.670488, 3.659802, 4.127528
C, 0.011323, 2.338589, 4.441208
C, 0.183713, 1.509692, 5.532886
H, 0.839027, 1.705997, 6.369981
C, -0.665619, 0.380085, 5.358301
H, -0.771631, -0.460794, 6.029080
C, -1.329994, 0.548278, 4.162542
H, -2.055144, -0.073909, 3.659404
C, -3.419870, 6.703369, 4.594653
C, -4.498940, 5.670557, 4.516030
C, -5.220636, 5.265744, 5.643927
C, -6.214531, 4.294806, 5.606591
H, -6.726414, 4.026098, 6.523179
C, -6.513524, 3.692666, 4.385094
H, -7.288121, 2.934414, 4.334342
C, -5.823537, 4.055576, 3.228243
H, -6.038294, 3.607169, 2.265137
C, -4.833294, 5.026346, 3.319812
C, -3.798773, 8.011345, 4.830414
C, -5.153856, 8.535709, 4.879138
H, -6.060930, 7.965382, 4.734320
C, -3.614541, 10.133022, 5.201365
H, -3.152028, 11.096999, 5.395679
C, -5.036521, 9.877654, 5.103059
H, -5.828745, 10.609417, 5.193592
C, -2.069288, 6.230813, 4.442867
F, -4.930522, 5.835512, 6.832638

F, -4.168884, 5.375131, 2.202116
N, 0.161057, 6.156004, 4.238403
N, -0.914807, 1.737784, 3.614589
H, -1.219592, 2.125616, 2.735490
N, -2.881118, 9.053058, 5.043039
C, 1.441136, 3.624346, 2.799603
C, 2.839151, 3.587900, 2.769958
C, 0.832541, 3.615788, 1.541665
C, 3.589220, 3.552605, 1.600030
C, 1.526652, 3.581226, 0.340128
H, 4.670800, 3.529931, 1.665947
H, 0.973230, 3.578002, -0.591726
C, 2.920715, 3.549718, 0.377241
H, 3.485547, 3.521675, -0.548615
H, 1.427712, 3.785060, 4.907195
F, 3.502911, 3.604269, 3.947159
F, -0.527065, 3.630836, 1.481410
H, -1.875276, 4.441591, 8.530003
C, -2.113485, 5.289112, 10.447050
C, -3.506423, 5.217953, 10.342887
C, -1.645803, 5.895182, 11.615328
C, -4.380858, 5.706622, 11.306233
C, -2.468206, 6.401476, 12.612432
H, -5.448905, 5.617186, 11.145608
H, -2.021308, 6.857547, 13.488174
C, -3.850111, 6.302053, 12.449308
H, -4.513556, 6.690064, 13.215014
F, -4.033985, 4.659382, 9.230359
F, -0.300375, 5.992413, 11.797554