Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Cholesterol appended pyridinium ureas: A case of gel making and breaking for selective visual readout of F^-

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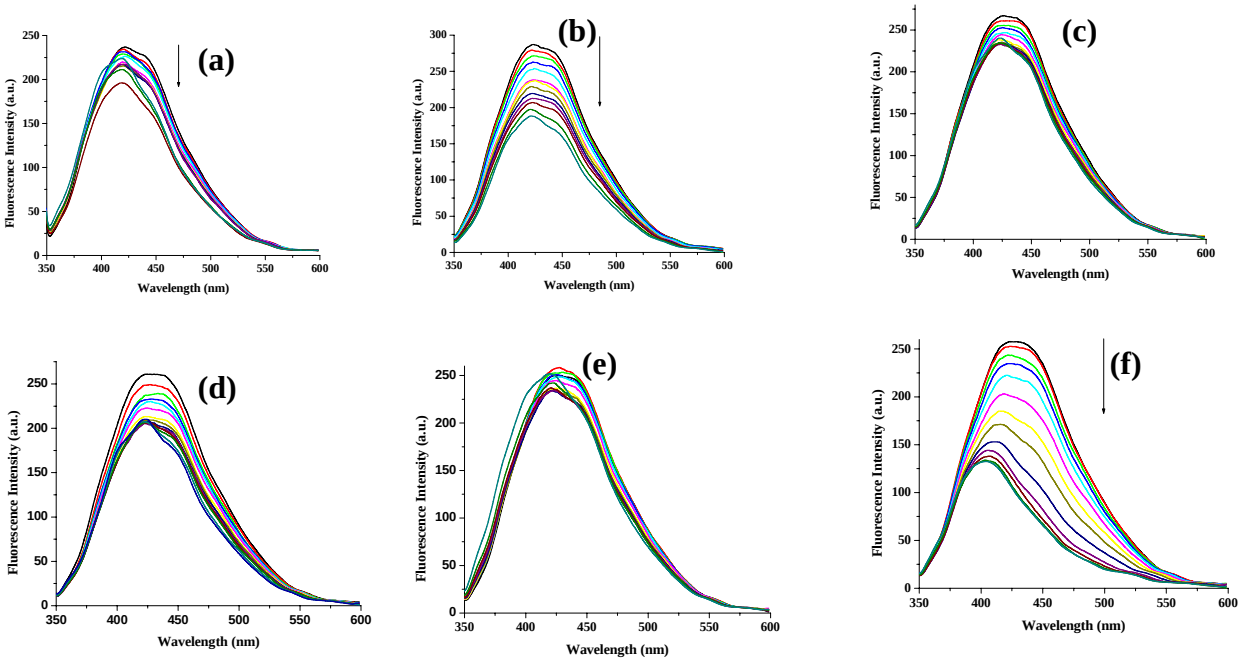
1. Change in emission of receptor **1** with HSO_4^-, Cl^-, Br^-, I^-, ClO_4^-, AcO^- , $H_2PO_4^-$in CH_3CN.
2. Change in of absorbance receptor **1** with HSO_4^-, Cl^-, Br^-, I^-, ClO_4^-, AcO^-, $H_2PO_4^-$ in CH_3CN.
3. Change of emission spectra of receptor **1** upon addition of 2 equivalent of different anions in CH_3CN.
4. Change in emission of receptor **1** with HSO_4^-, Cl^-, Br^-, I^-, ClO_4^- AcO^-, $H_2PO_4^-$ in DMSO.
5. Change in absorbance of receptor **1** with HSO_4^-, Cl^-, Br^-, I^-, ClO_4^- AcO^-, $H_2PO_4^-$ in DMSO.
6. Change of emission spectra of receptor **1** upon addition of 15 equivalent of different anion in DMSO.
7. Benesi–Hilderband plot for **1** with fluoride in CH_3CN.
8. Benesi–Hilderband plot for **1** with F^- in DMSO.
9. Photograph of formation of gel for receptor **1** with 5 equiv. amounts of Fluoride in DMSO.
10. Job Plot of **1** with TBAF in DMSO.
11. Comparision of IR Septra.
12. Characterization spectra
13. Comparative ^1H NMR and FTIR spectra
14. UV-vis titration spectra for 2 with the anions.

1. Change in emission of receptor 1 with various anions in CH_3CN.



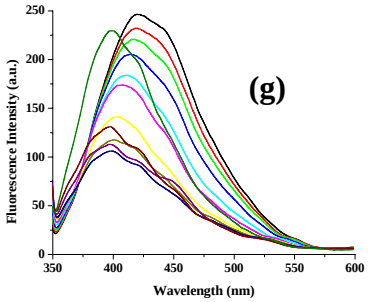


Figure 1S. Fluorescence titration spectra for **1** (c = 6.32 x 10^{-5} M) with (a) HSO_4^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) ClO_4^-, (f) AcO^- (g) $H_2P0_4^-$ in CH_3CN (in all cases [anion] = 1x 10^{-3} M).

2. Change in absorbance of receptor 1 with various anions in CH_3CN.

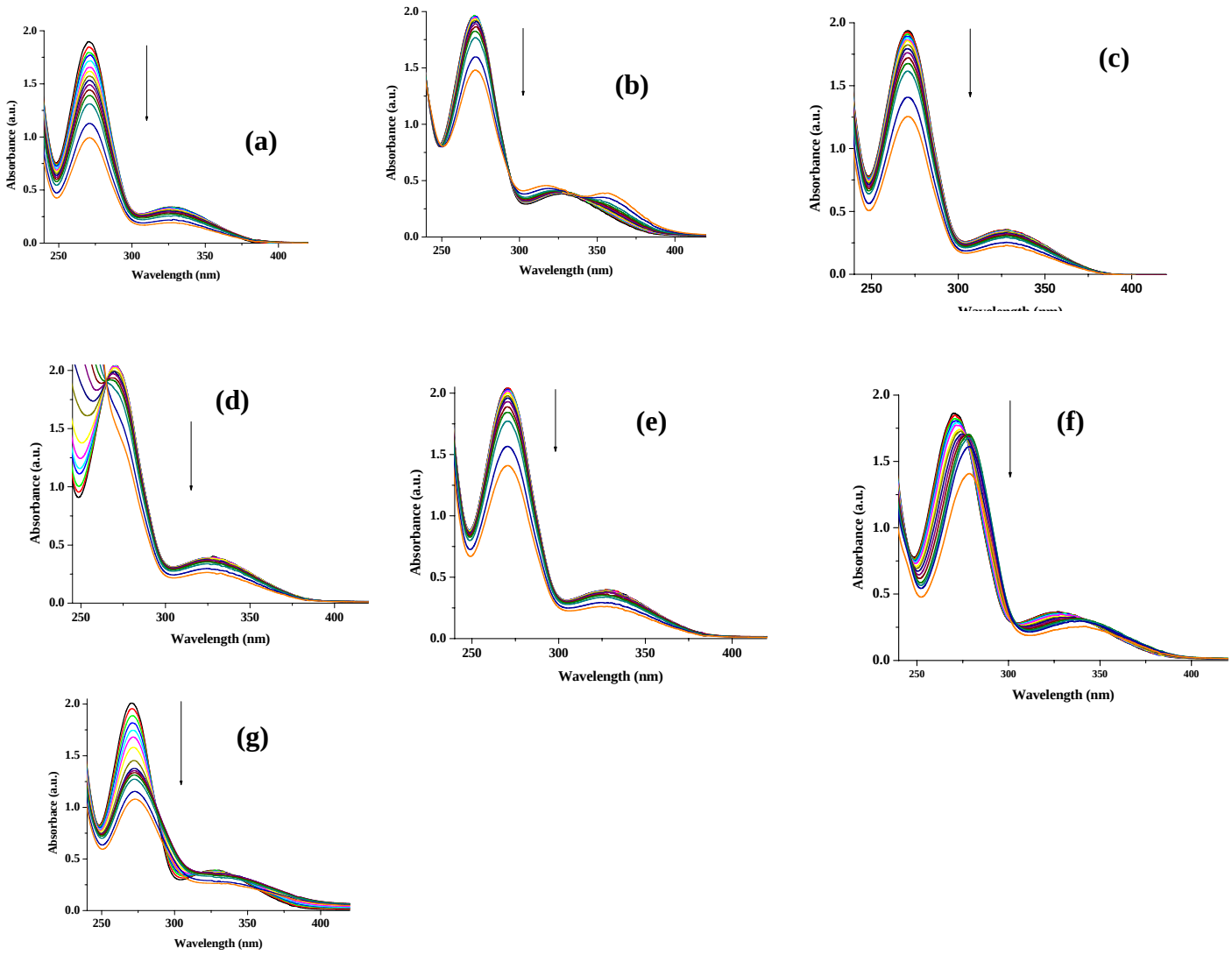


Figure 2S. Change in absorbance of receptor **1** (c = 6.32 x 10^{-5} M) with (a) HSO_4^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) ClO_4^- (f) AcO^- (g) $H_2P0_4^-$ in CH_3CN (in all cases [anion] = 1x 10^{-3} M).

3. Change of emission spectra of receptor 1 upon addition of 2 equivalent of different anion in CH_3CN.

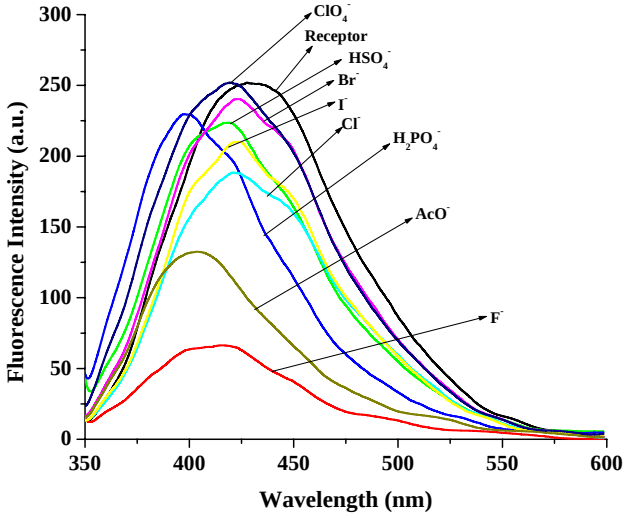
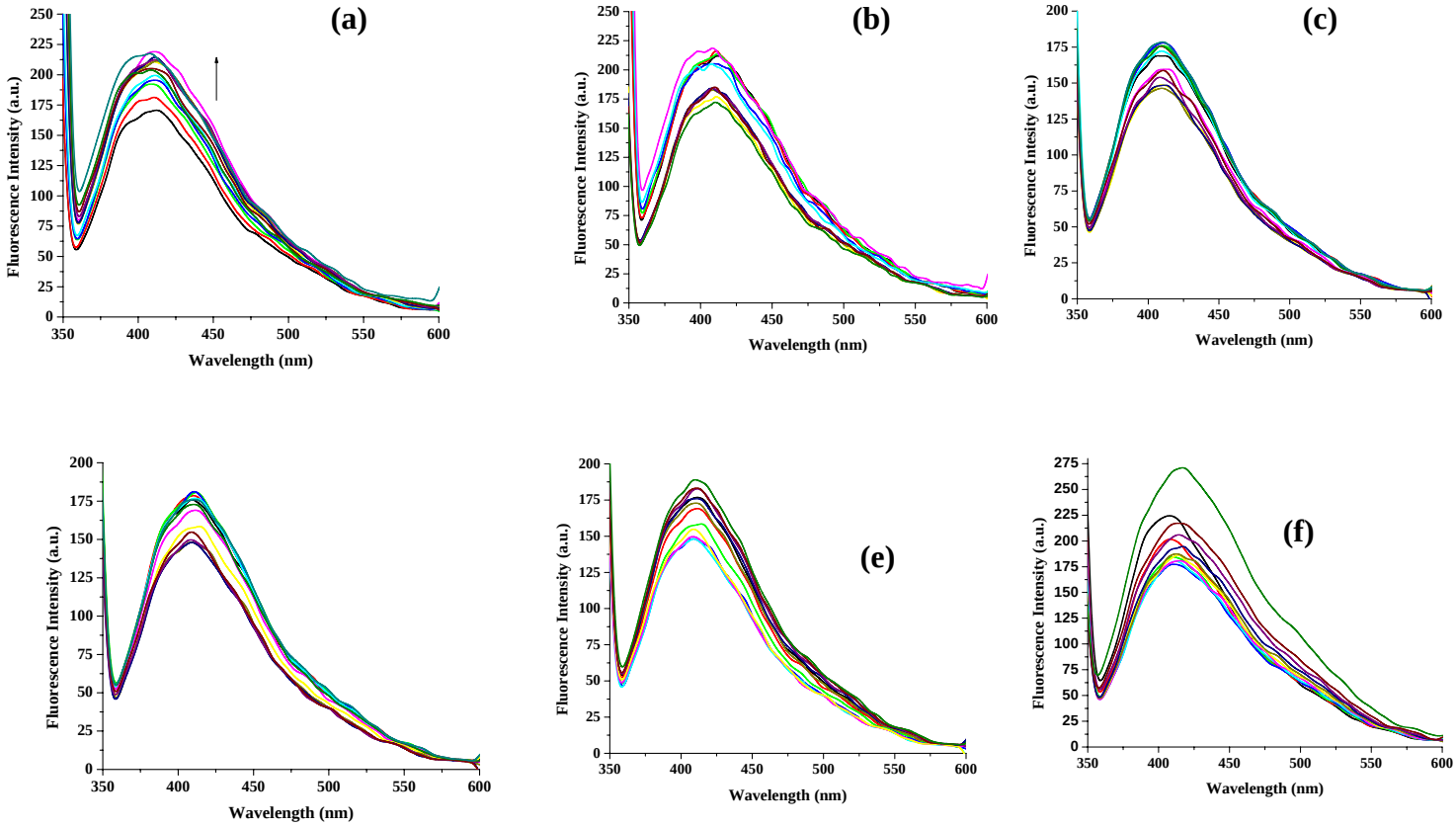


Figure 3S: Change in emission of receptor **1**(c = 6.32x 10^{-5} M)) upon addition of 2 eqv.of different Guests (c = 1x10^{-3}M) in CH_3CN.

4. Change in emission of receptor 1 with various anions in DMSO.



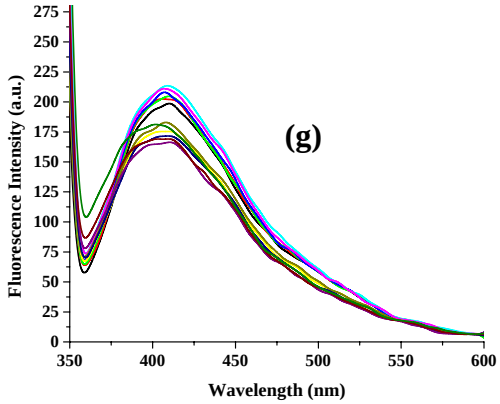
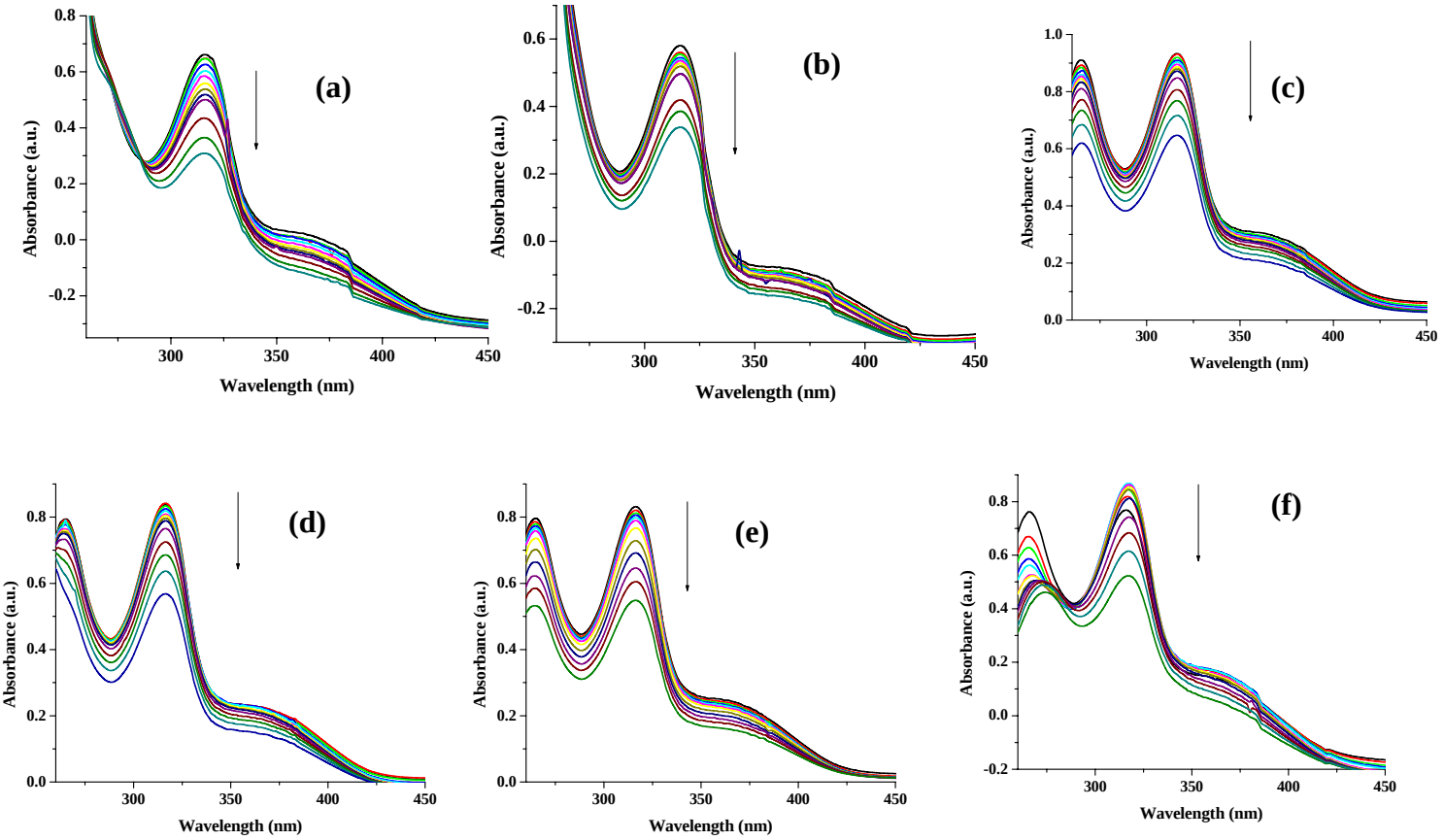


Figure 4S. Fluorescence titration spectra for **1** (c = 6.01 x 10^{-5} M) with (a) HSO_4^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) ClO_4^-, (f) AcO^- (g) $H_2P0_4^-$ in DMSO (in all cases [anion] = 1x 10^{-3} M)

5. Change in absorbance of receptor 1 with various anions in DMSO.



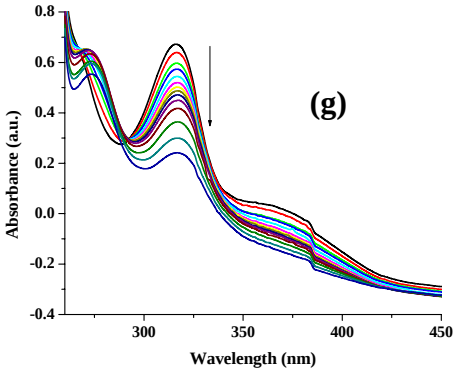


Figure 5S. Change in absorbance of receptor **1** (c = 6.01 x 10^{-5} M) with (a) HSO_4^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) ClO_4^- (f) AcO^- (g) $H_2P0_4^-$ in DMSO (in all cases [anion] = 1x 10^{-3} M).

6. Change of emission spectra of receptor 1 upon addition of 15 equivalent of different anion in DMSO.

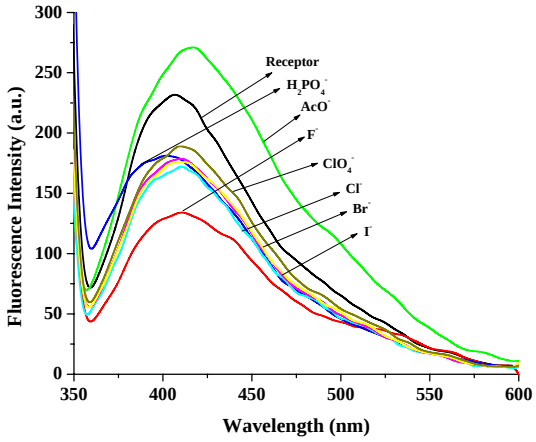


Figure 6S: Change in emission of receptor 1(*c* = 6.01x 10^{-5} M)) upon addition of 15eqv.of Different Guest (*c* = 1x10^{-3}M) in DMSO

7. Benesi–Hilderband plot for 1 with F^- in CH_3CN.

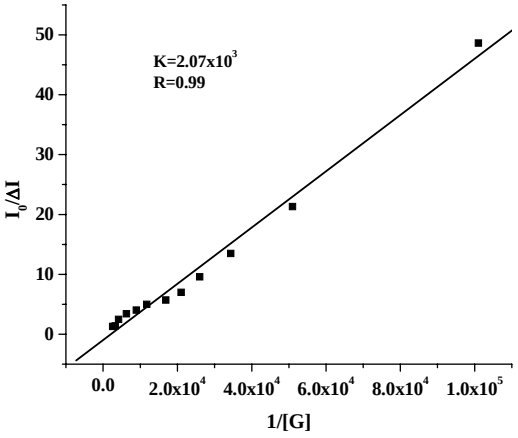


Figure 7S: Benesi–Hilderband plot for receptor **1** (c = 6.32x 10^{-5} M) with fluoride (c = 1x10^{-3} M) at 430 nm in CH_3CN

8. Benesi–Hilderband plot for 1 with F^- in DMSO.

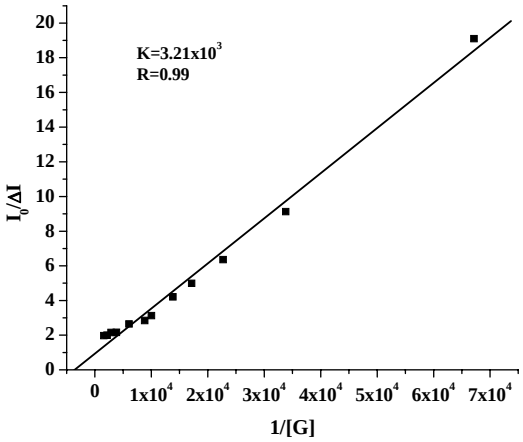


Figure 8S: Benesi–Hilderband plot for receptor **1** (c = 6.01x 10^{-5} M) with fluoride (c = 1x10^{-3} M) at 410 nm in DMSO.

9. Photograph of formation of gel for receptor 1 with 5 equiv. amounts of Fluoride in DMSO.

Fig 9S. Photograph of Receptor **1** (c = 3.58x10^{-3} M) with 5 equiv. amounts of Fluoride (c = 1.5x10^{-2} M) in DMSO.

10. Job plot of 1 with F^- in DMSO.

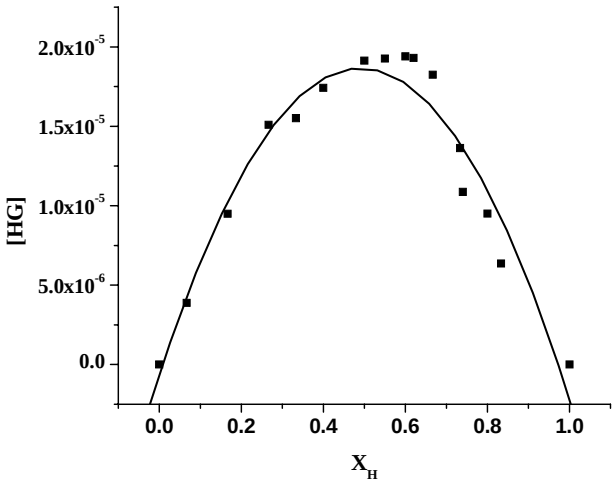


Fig 10S. Job plot for **1** (c = 5.96 x 10^{-5} M) with TBAF in DMSO.

11. Comparison of IR- Sepctra.

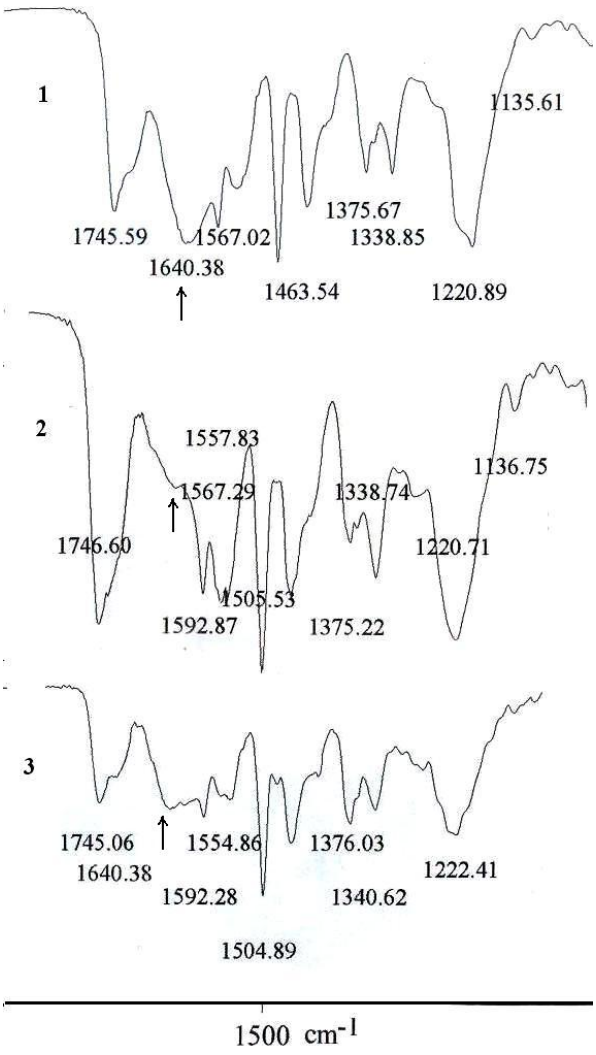
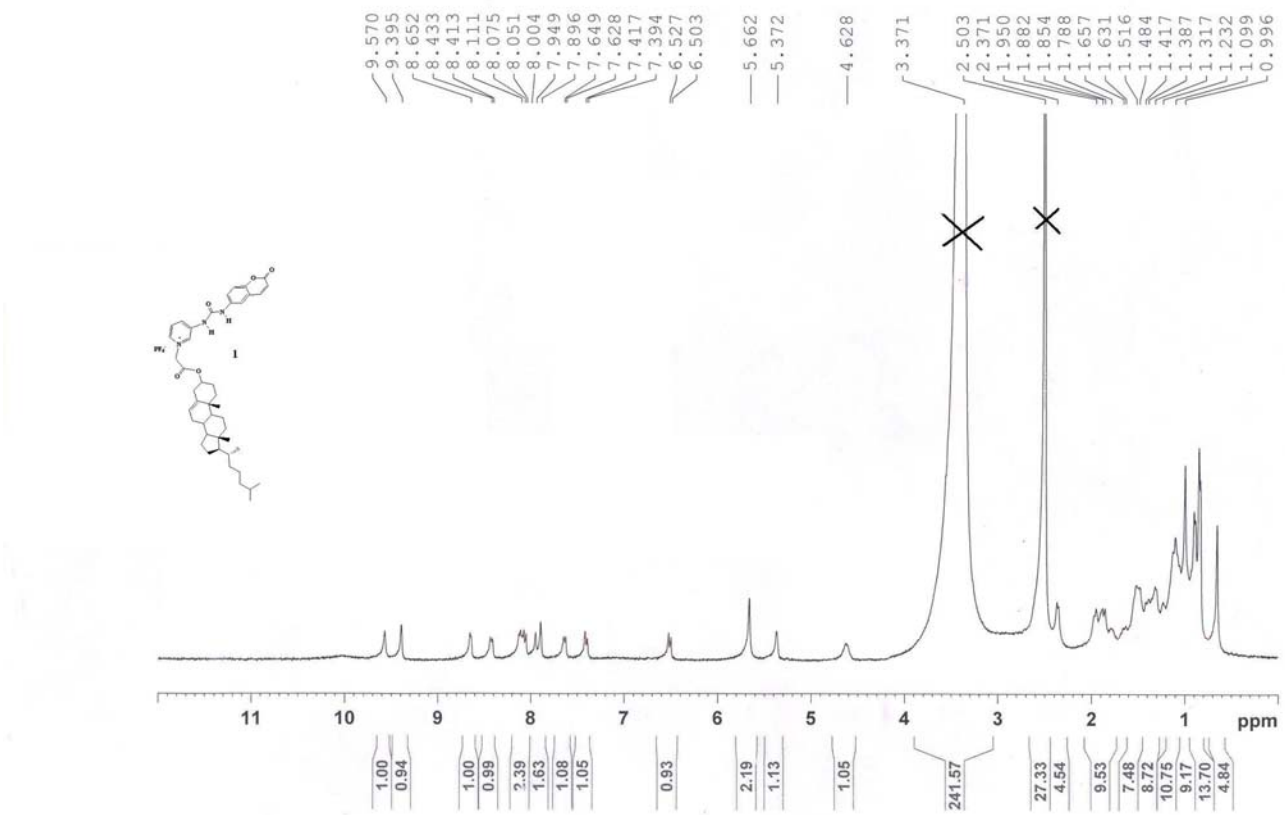


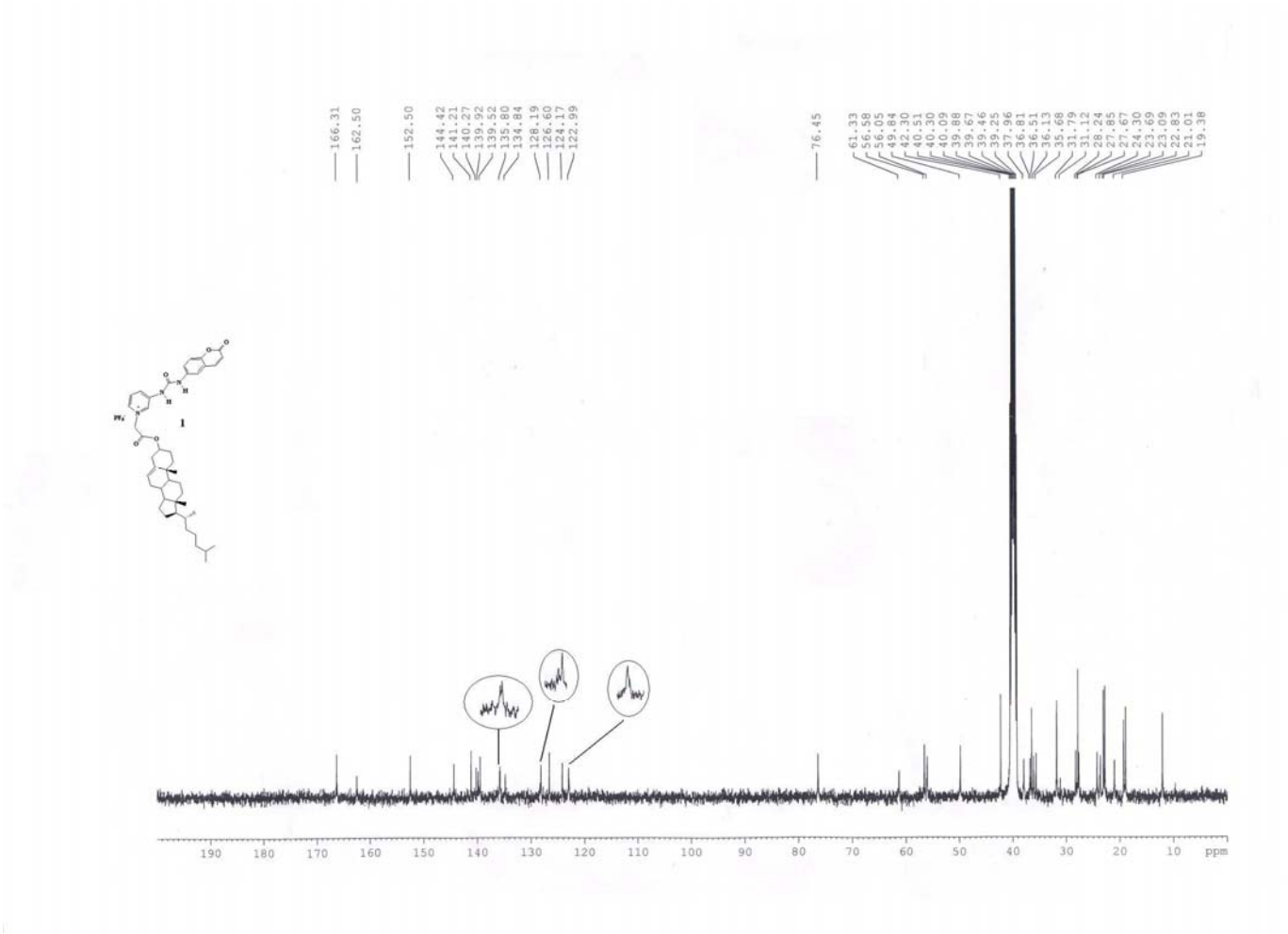
Fig 11S. 1 Partial IR spectrum of **2a**. 2 partial IR spectrum of **2a** in gel state. 3 Partial IR spectrum of **2a** after breaking the gel with fluoride**.**

12. Characterization spectra

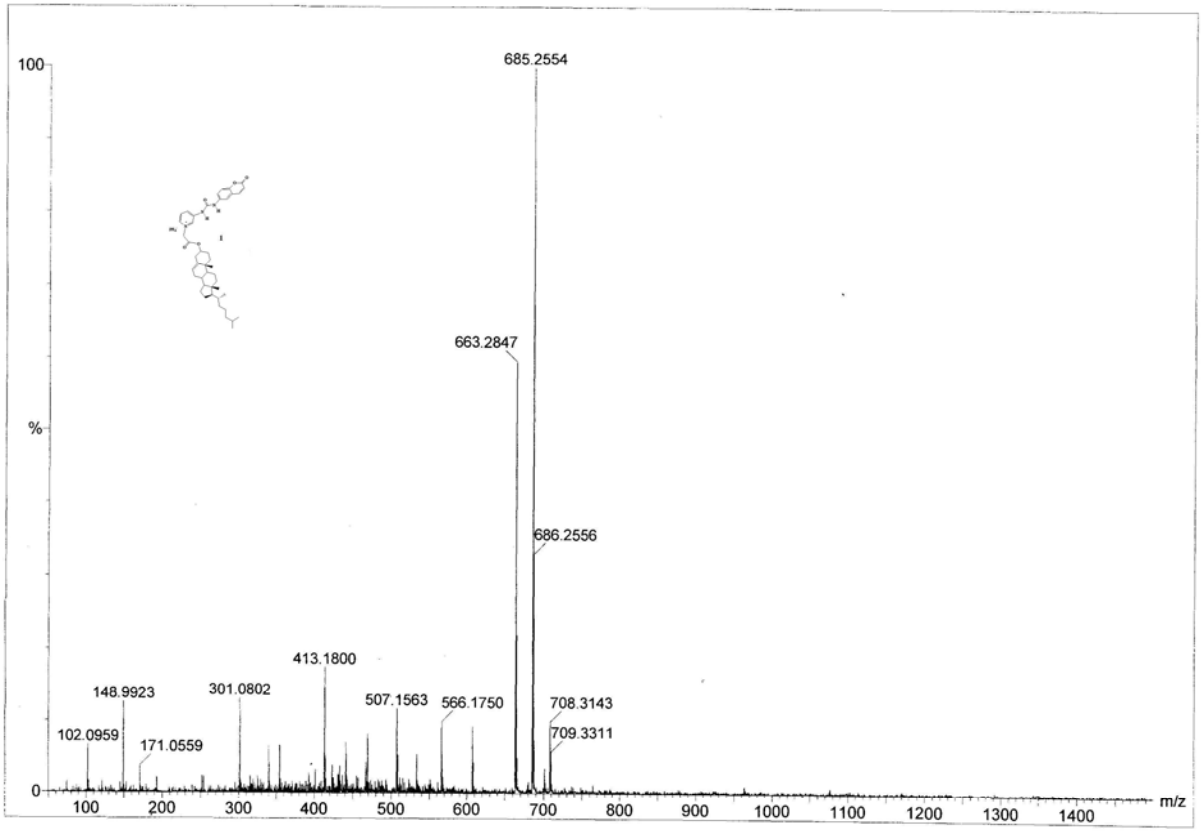
^{1}H NMR (400 MHz, d_6-DMSO)



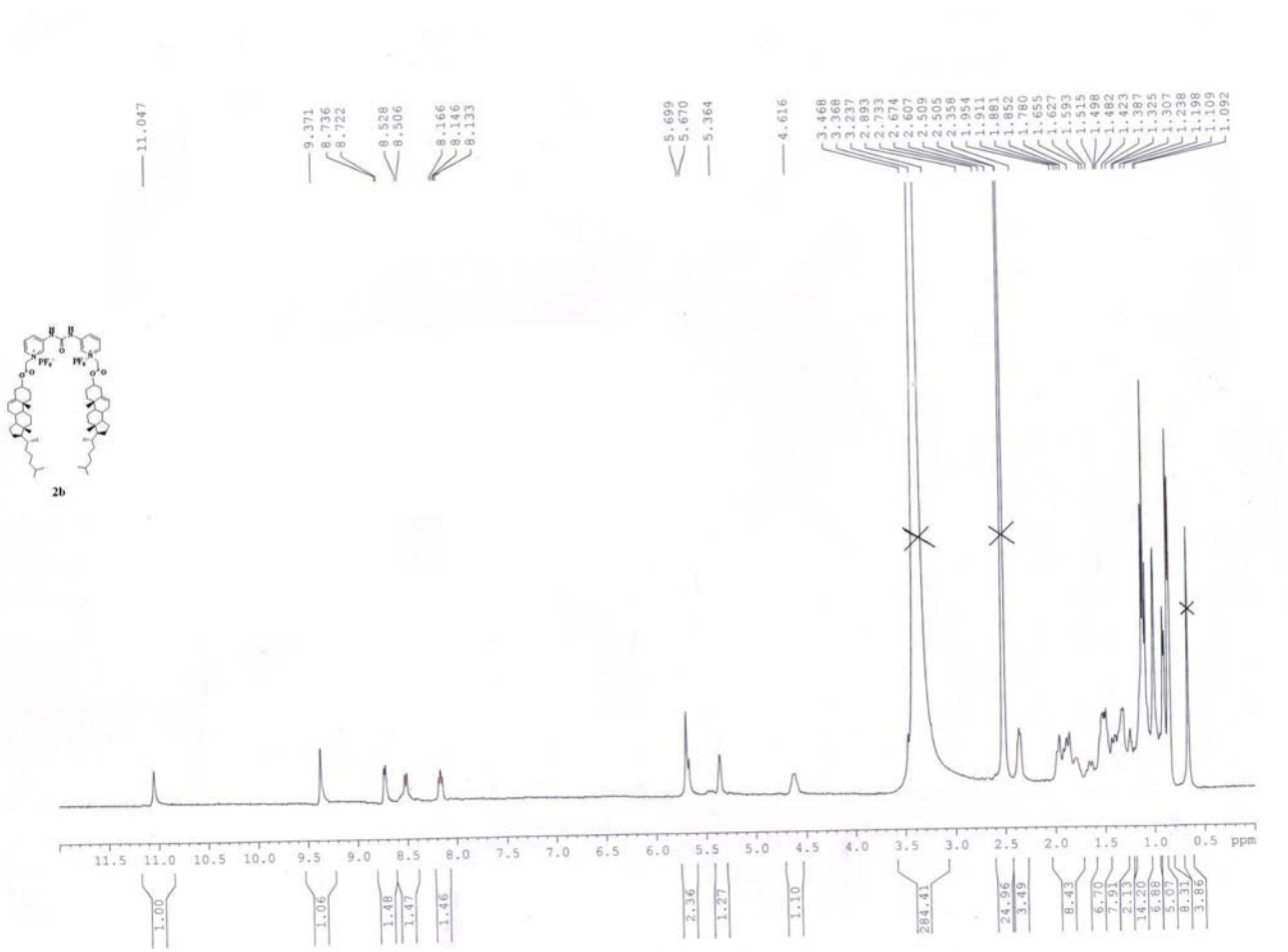
^{13}C NMR (100 MHz, d_6-DMSO)



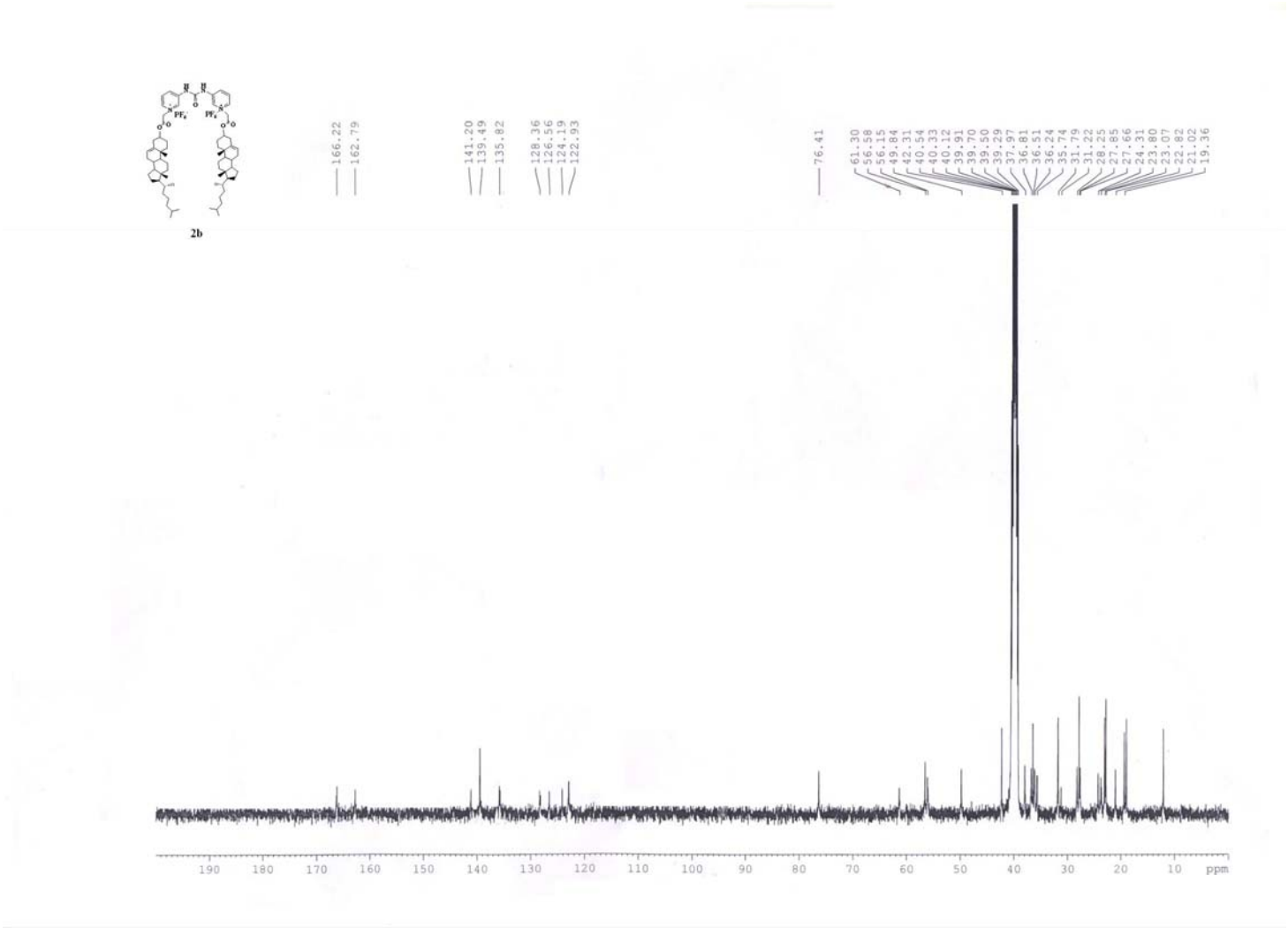
Mass



^{1}H NMR (400 MHz, d_6-DMSO)



^{13}C NMR (100 MHz, d_6-DMSO)



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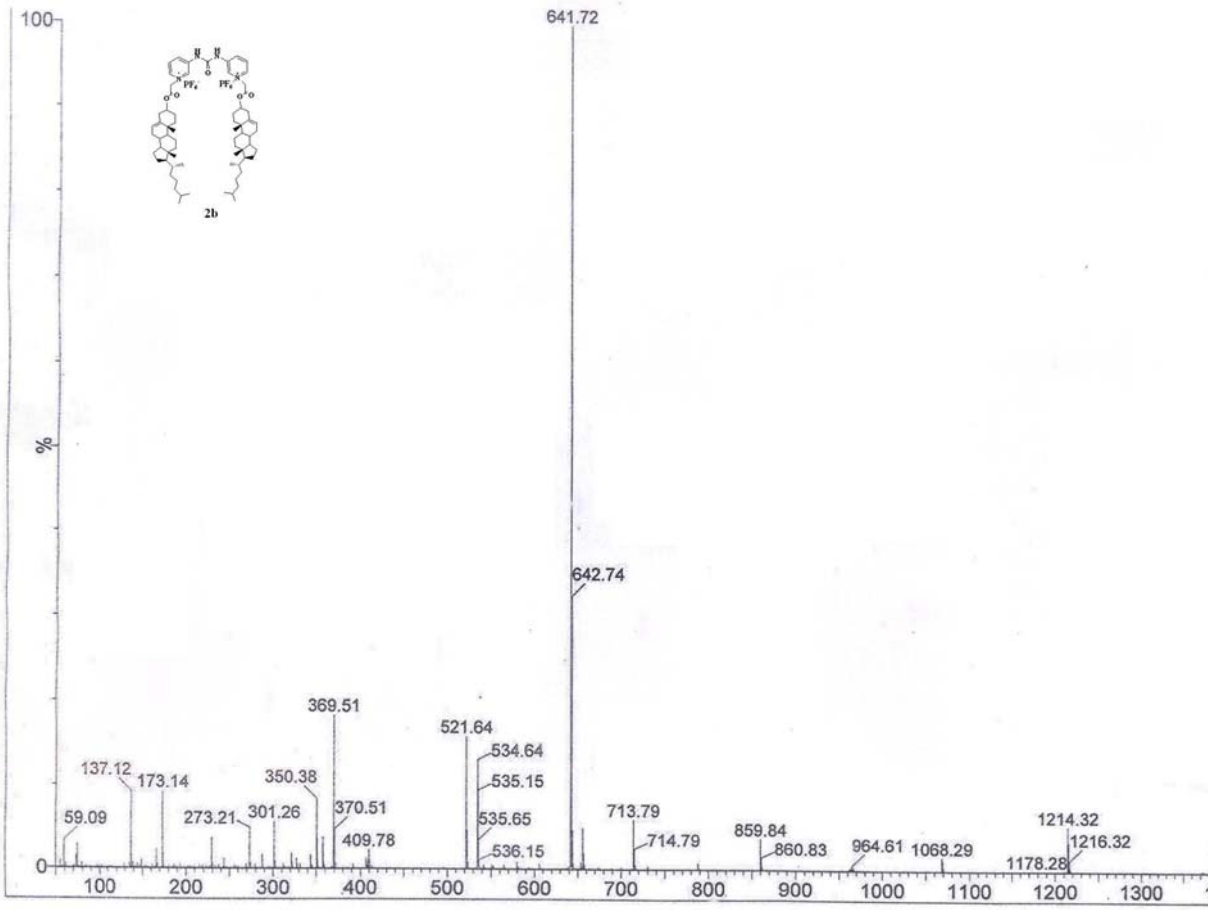

13. Comparative ^{1}H NMR and FTIR spectra

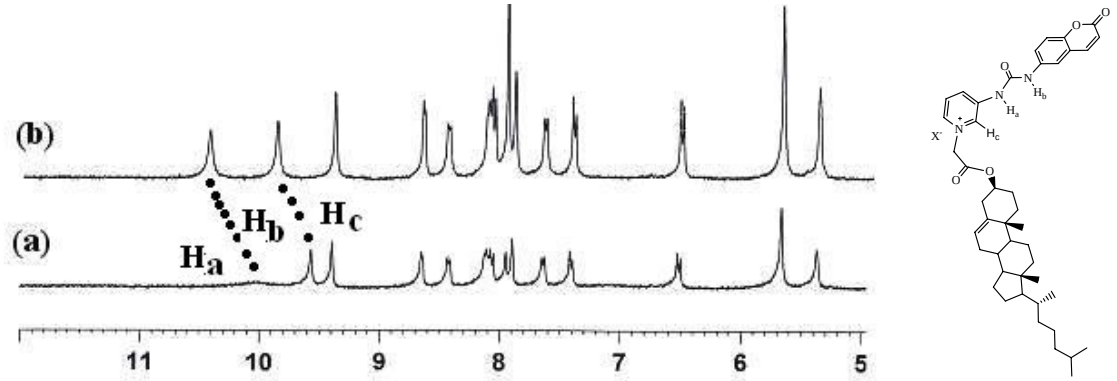

Fig 12S. Partial ^{1}H NMR (400 MHz, d_6DMSO) of (a) **1** (X = PF_6^- c = 4.8 x 10^{-3} M) and (b) X = Cl^- .

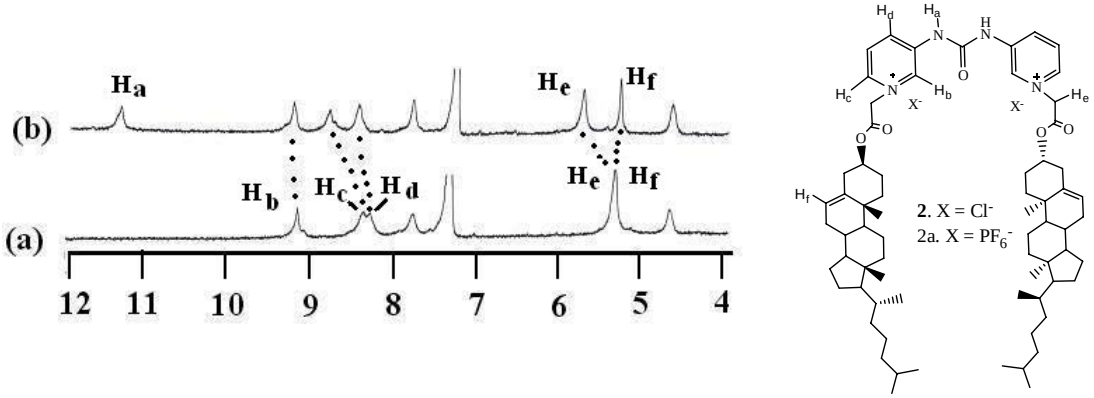

Fig 13S. Partial ^{1}H NMR (400 MHz $CDCl_3$ containing 5% d_6DMSO) of (a) **2a** and (b) **2**.

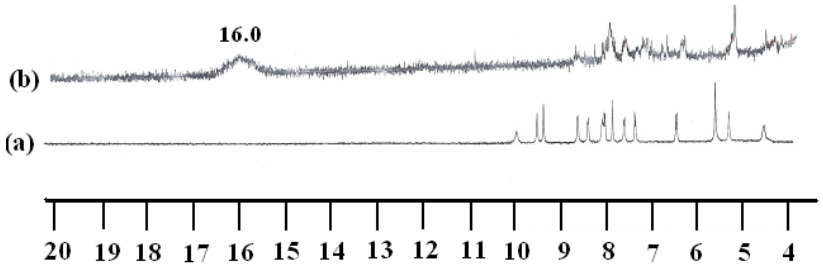

Fig 14S. Partial ^{1}H NMR (400 MHz, d_6DMSO) of (a) **1** and (b) after addition of 3 equivalent amounts of tetrabutylammonium fluoride.

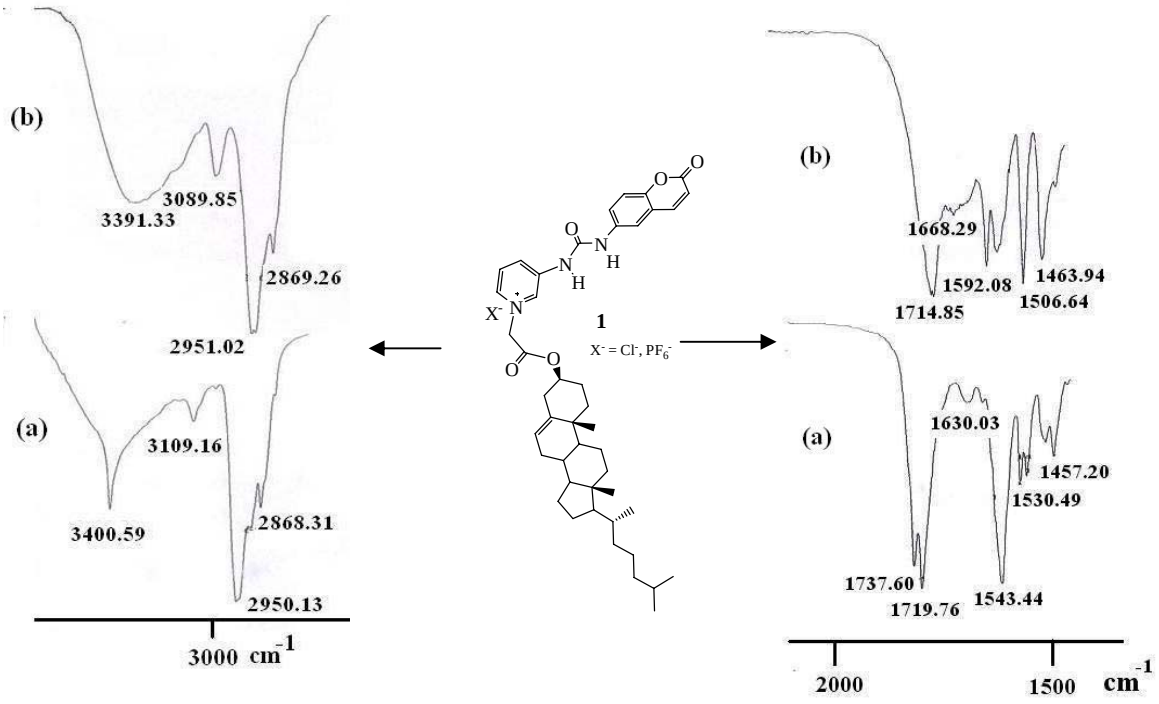

Fig 15S. Partial FT-IR (in KBr) of (a) **1** and (b) chloride salt of **1**.

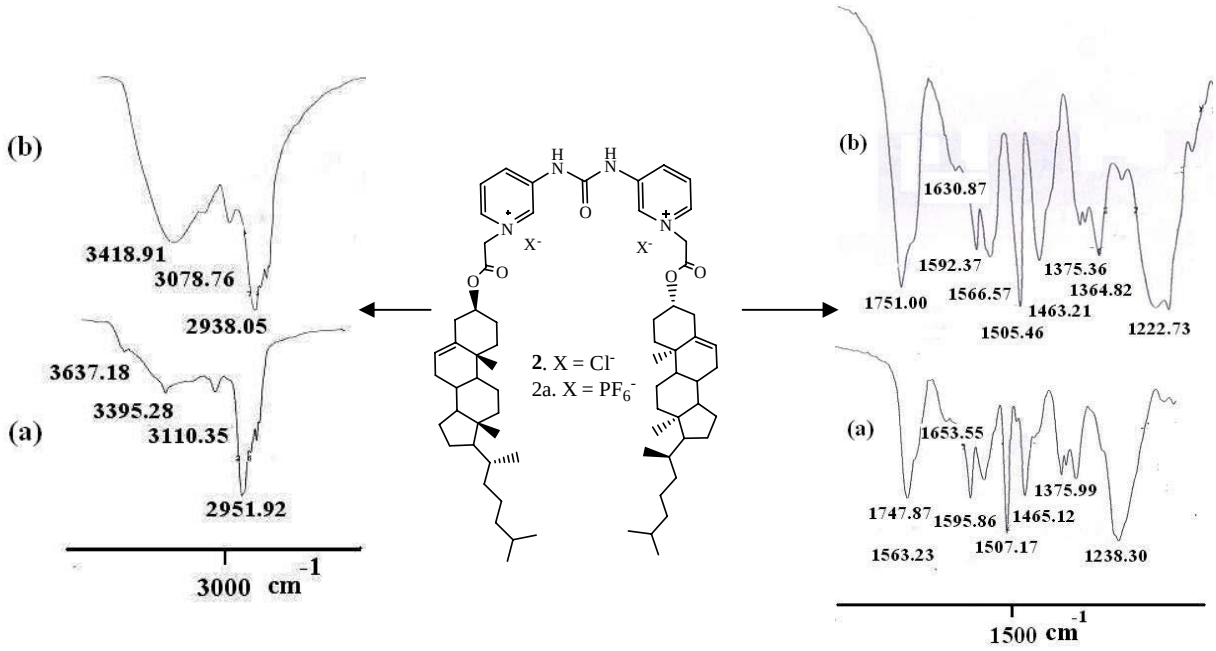

Fig 16S. Partial FT-IR (in KBr) of (a) **2a** and (b) **2**

14. UV-vis titration spectra for 2 with the anions.

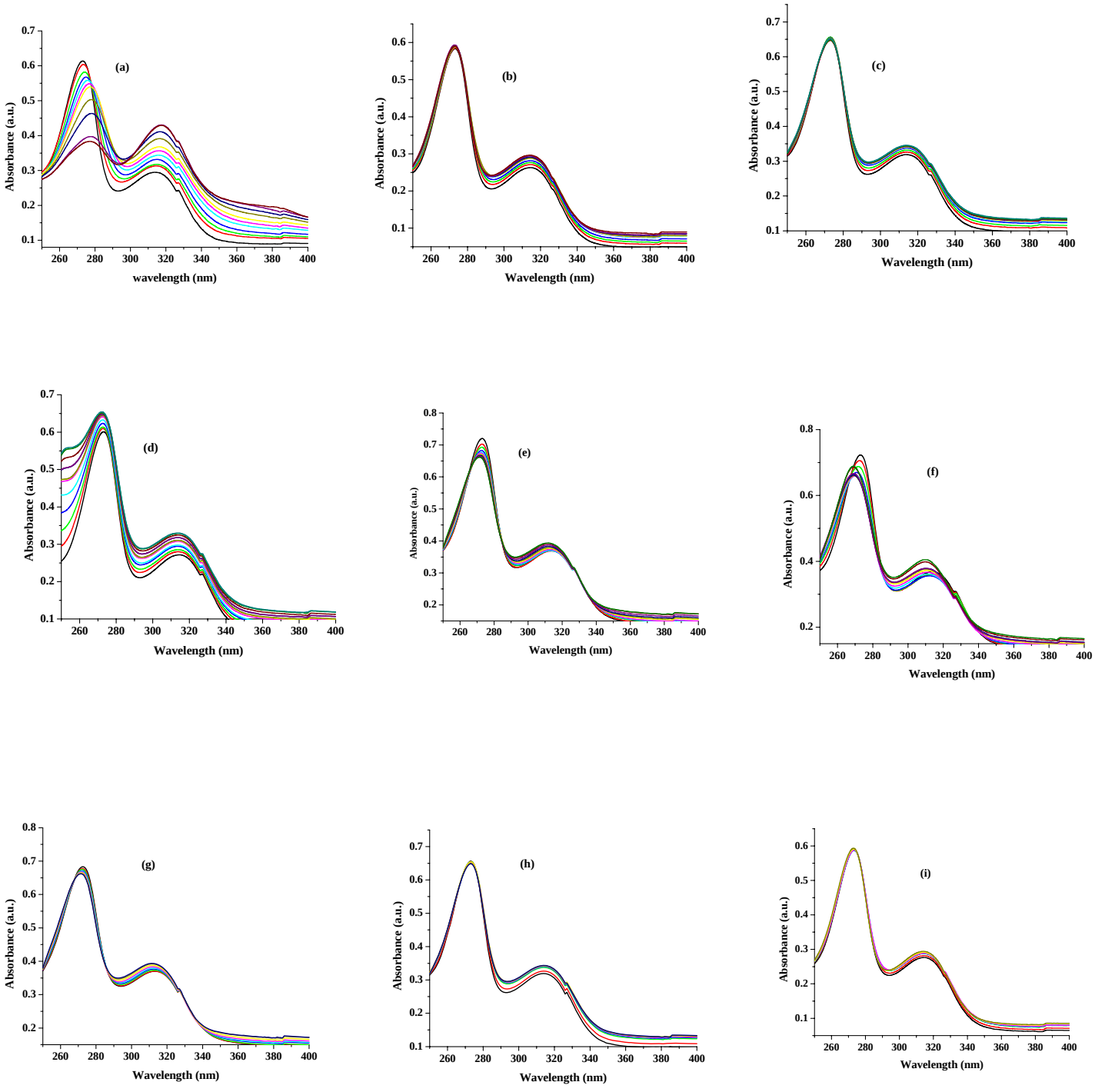

Fig 17S. Absorption titration spectra for **2** (c = 4.05 x 10^{-5} M) with (a) F^-, (b) Cl^-, (c) Br^-, (d) I^-, (e) $H_2PO_4^-$, (f) HSO_4^-, (g) AcO^-, (h) NO_3^-, (i) ClO_4^- in $CHCl_3$ (in all cases [anion] = 1x 10^{-3} M).