Electronic Supplementary Material (ESI) for RSC Advances.

The maiden report of a fluorescent-colorimetric sensor for expeditious detection of bifluoride ion in aqueous media

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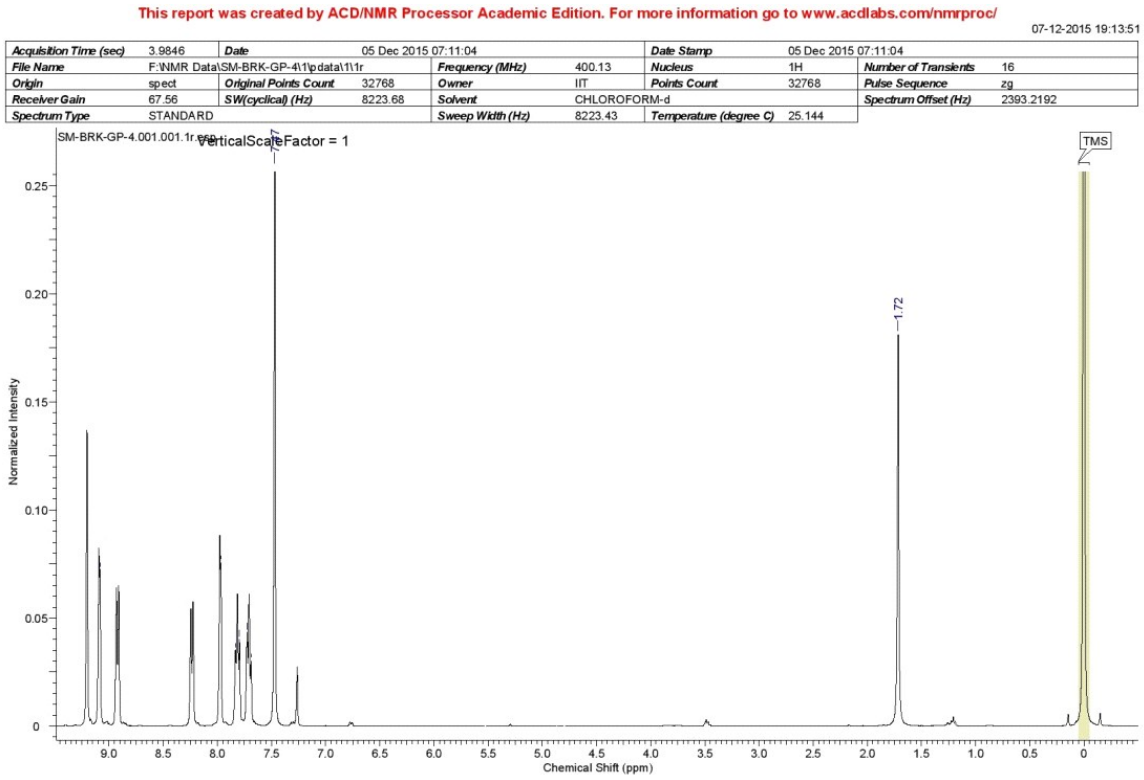


Fig. S1. ^{1}H NMR Spectra of **L** in $CDCl_3$.

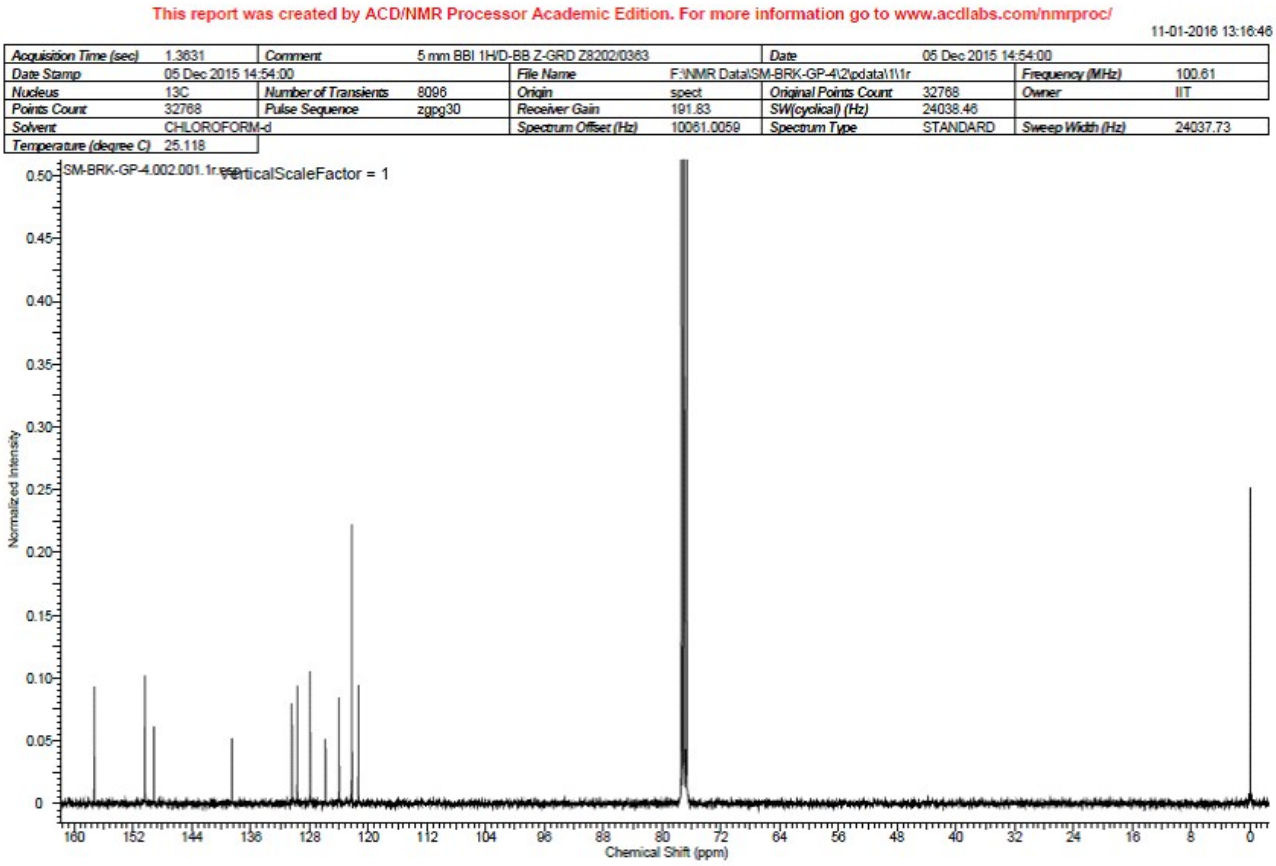


Fig. S2. ^{13}C NMR Spectra of **L** in $CDCl_3$.

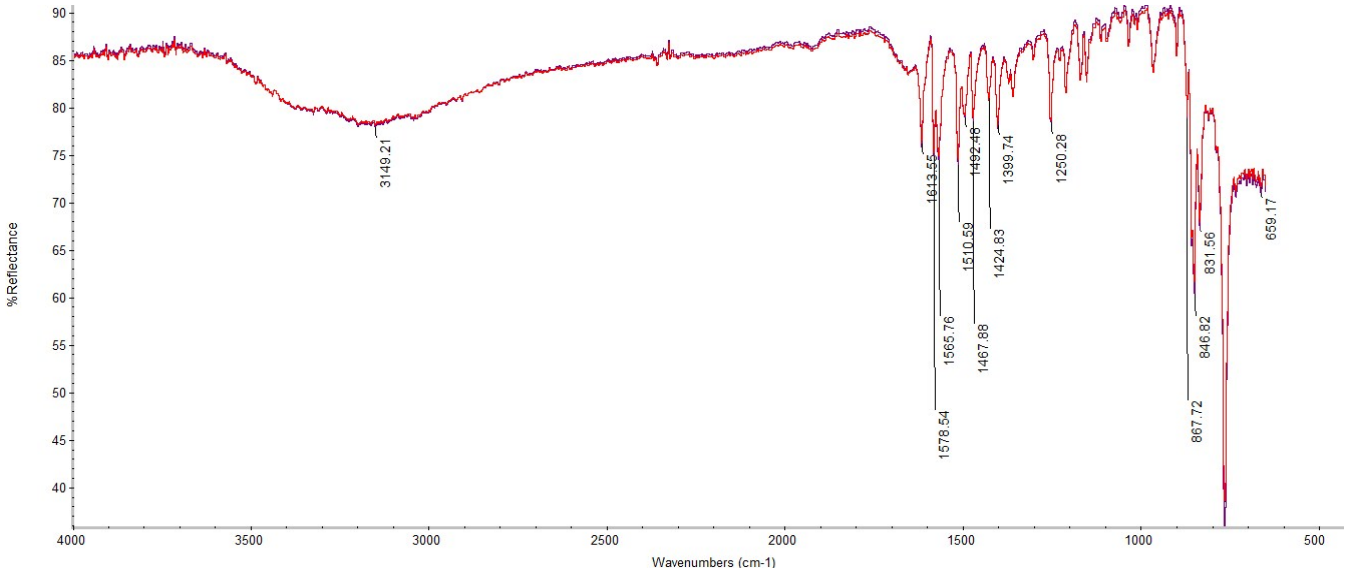


Fig. S3. IR Spectra of **L**.

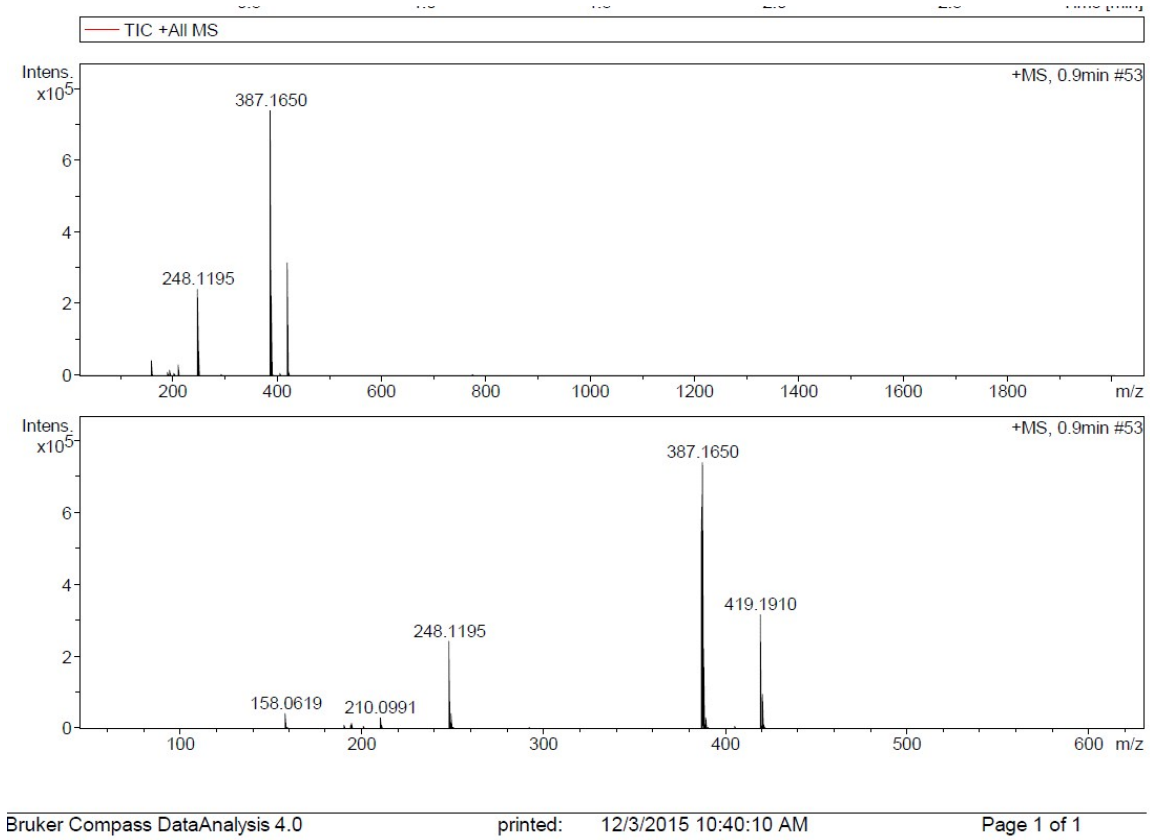


Fig. S4. Mass Spectra of **L.**

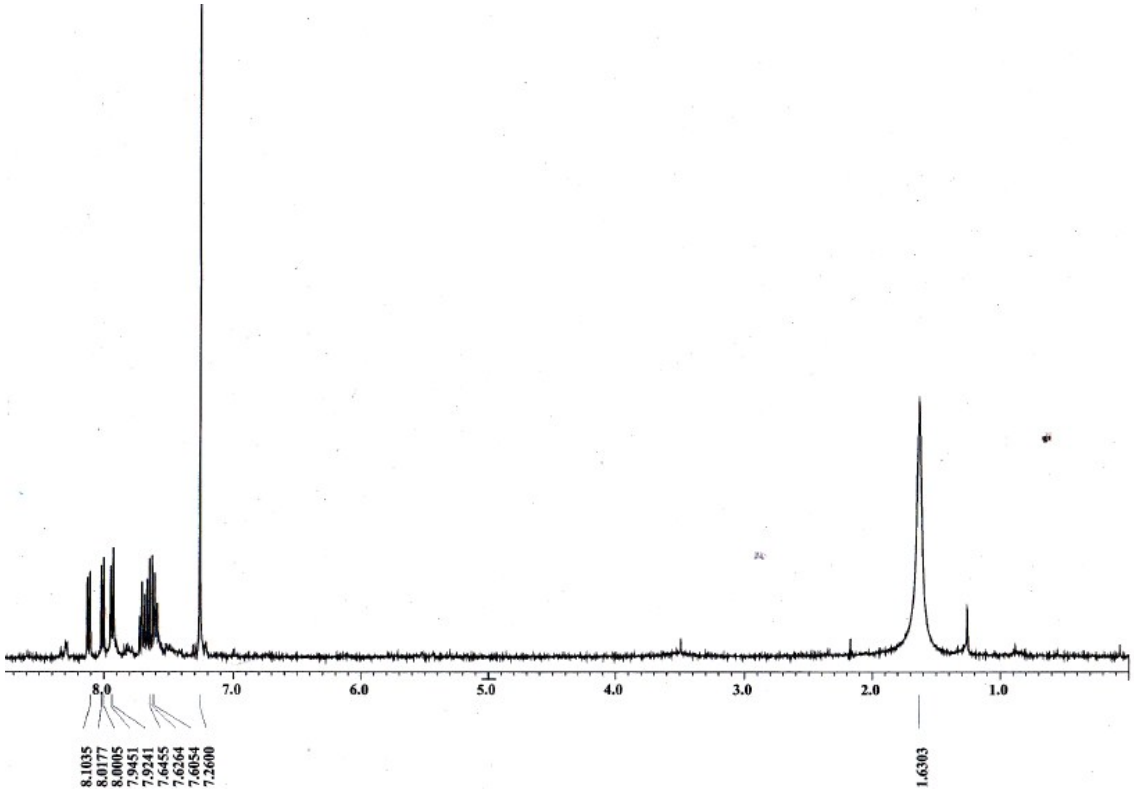


Fig. S5. ^{1}H NMR Spectra of $\mathbf{L_1}$ in $CDCl_3$.

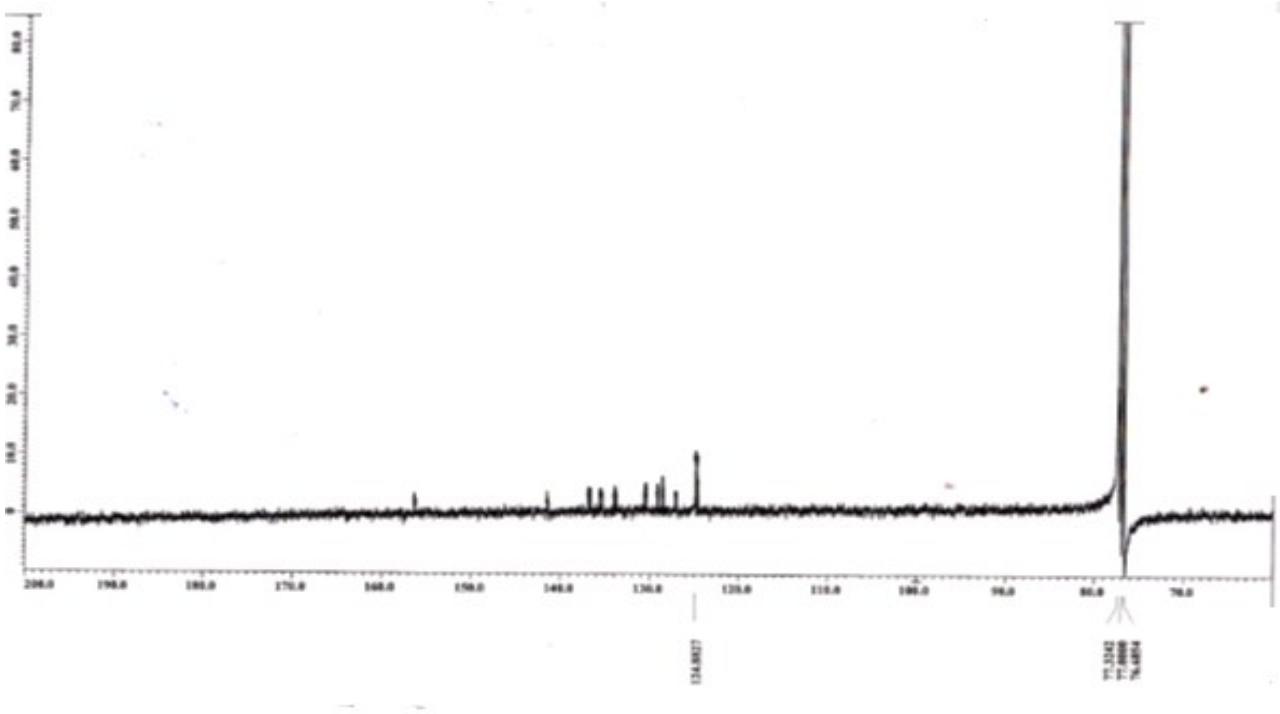


Fig. S6. ^{13}C NMR Spectra of $\mathbf{L_1}$ in $CDCl_3$.

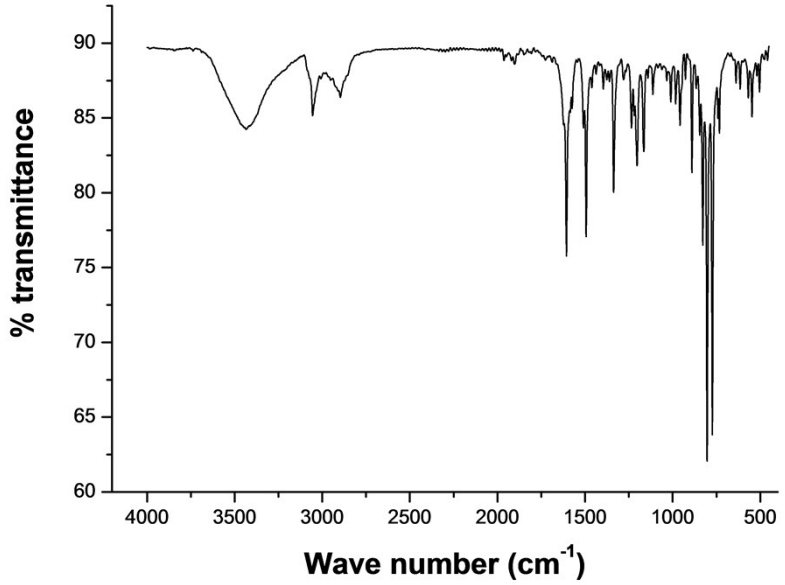


Fig. S7. IR Spectra of $\mathbf{L_1}$.

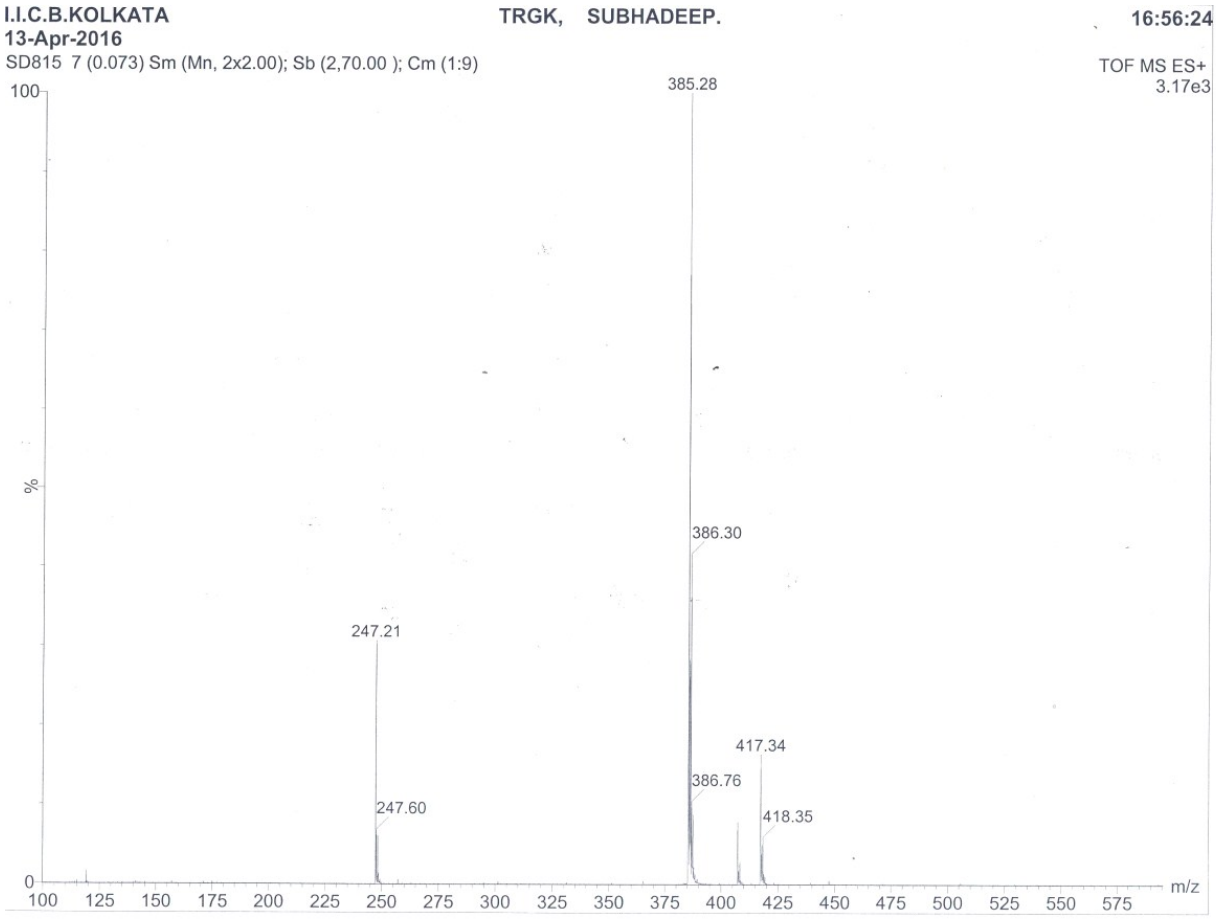


Fig. S8. Mass Spectra of $\mathbf{L_1}$.

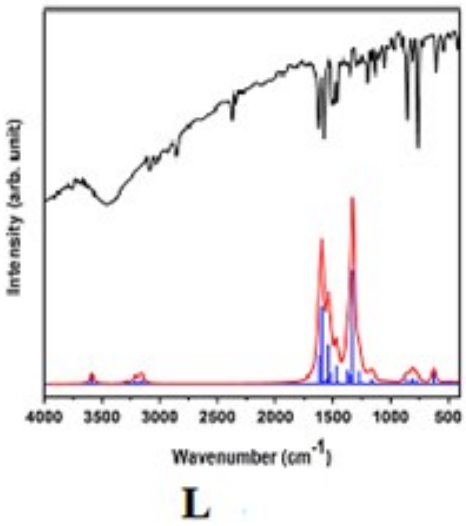


Fig. S9. The experimental (black) and calculated (red, non-scaled) vibrational spectra and calculated vibrational transition (blue) of for **L**.

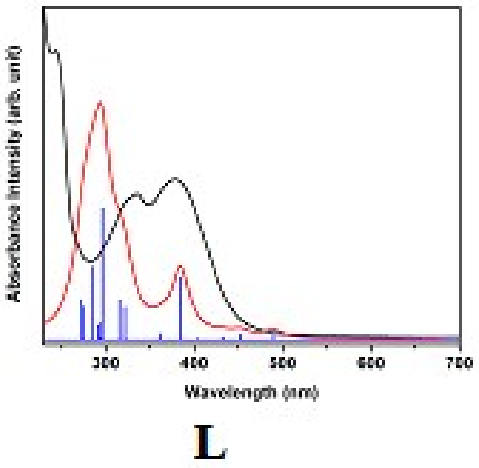


Fig. 10. The experimental (black), calculated (red) electronic absorption spectra and calculated electronic transition (blue) of **L**.

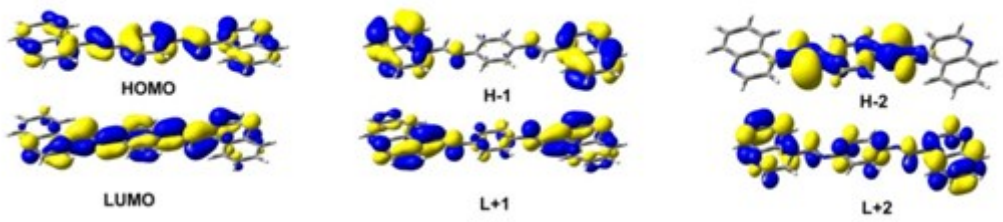


Fig. S11. Selected HOMOs and LUMOs of **L**.

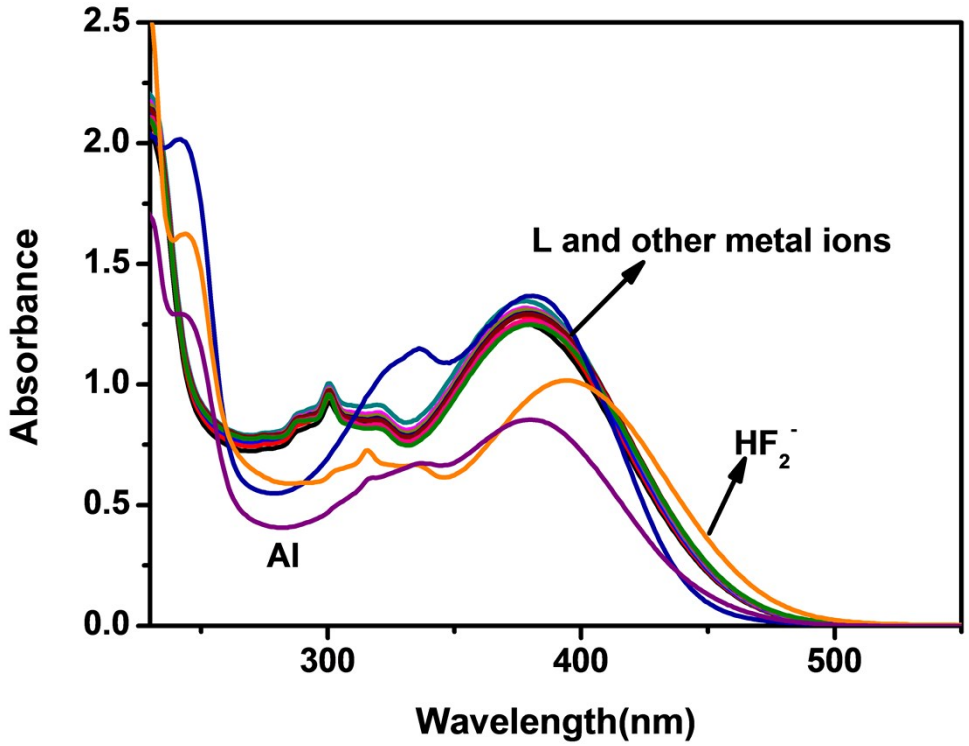


Fig. S12. Changes in the absorption spectra of **L** (50 μM) in the presence of 10 equiv. of different cations.

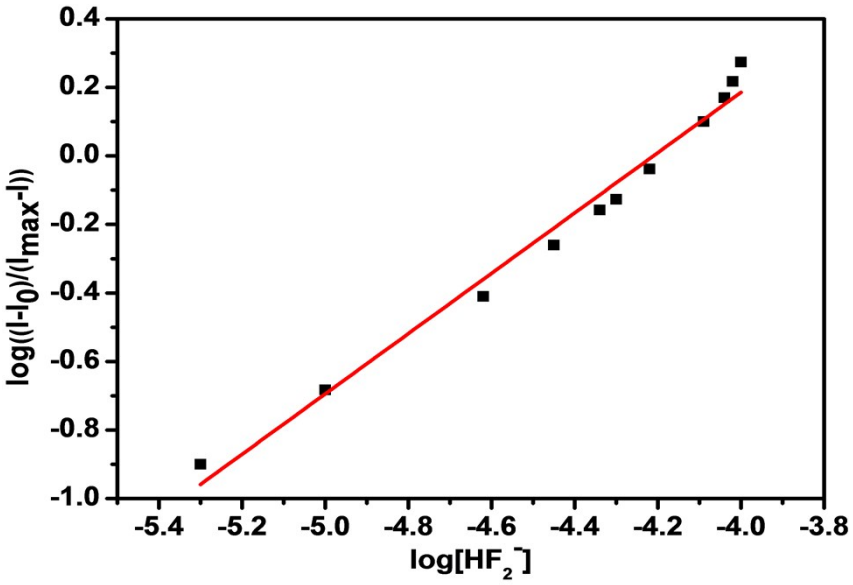


Fig. S13. Hill plot

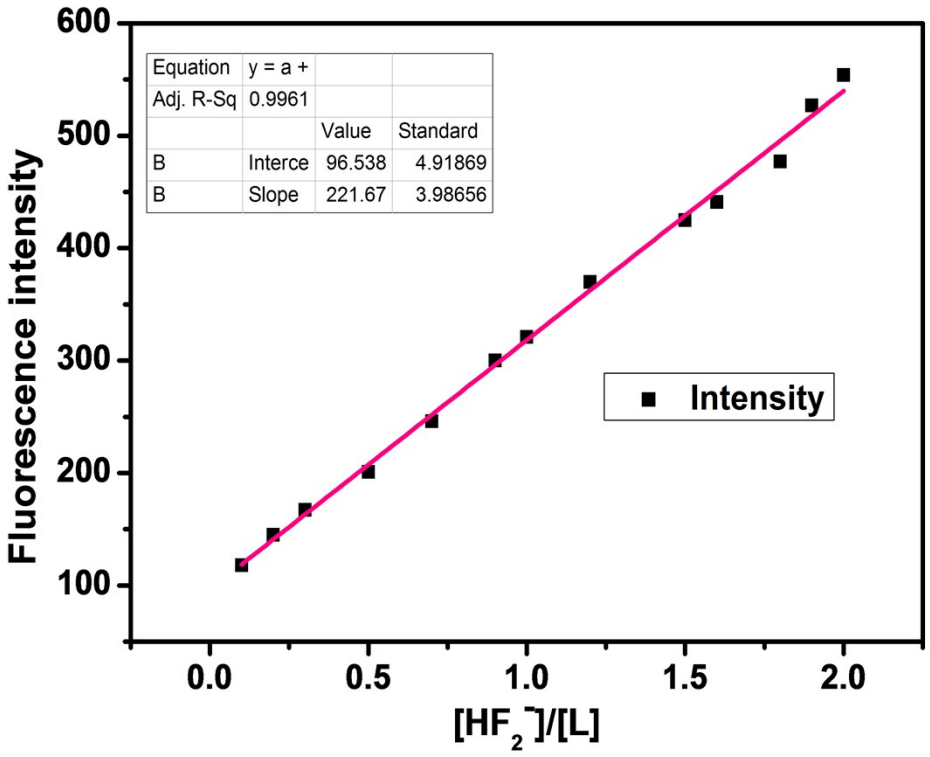


Fig. S14. Detection limit

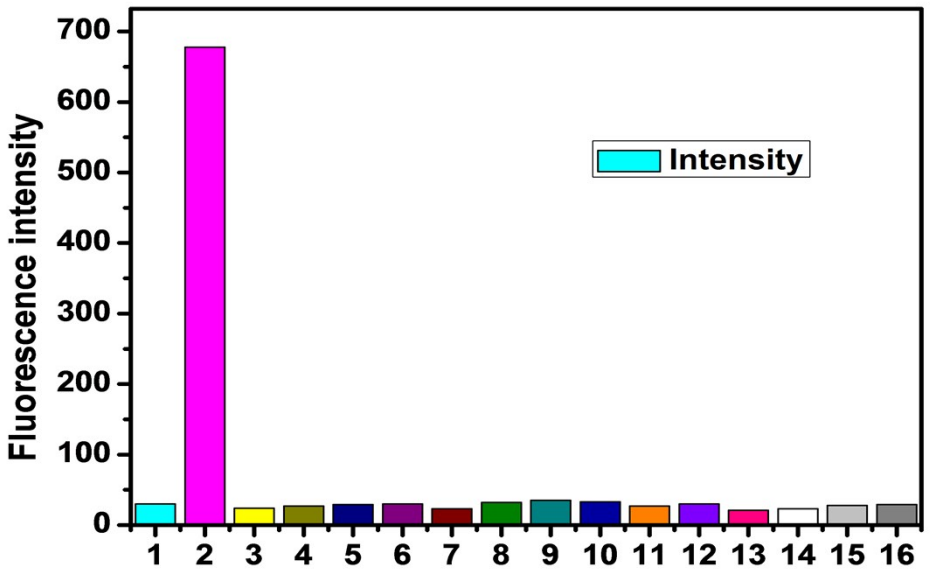


Fig. S15. The bar graph showing the relative absorption intensity of **L** upon treatment with various anions (1. **L**; 2. HF2-; 3. HSO_3^-; 4.F^-; 5.OAc^-; 6.Cl^-; 7. Br^-; 8.I^-; 9. $H_2PO_4^-$; 10. HCO_3^-; 11. N_3^-; 12. NO_3^-; 13. SO_4^{2-} 14.CO_3^{2-} ; 15. CN- and 16.SO_3^{2-}).

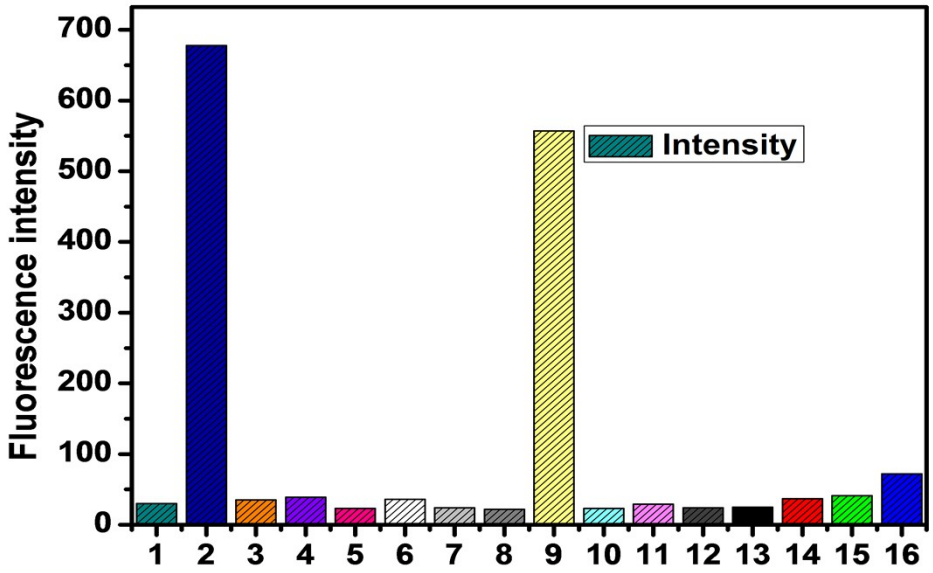


Fig. S16. The bar graph showing the relative absorption intensity of **L** upon treatment with various metal cations (1.L; 2.HF_2^-; 3.Mg^{2+}, 4. Mn^{2+}, 5. Fe^{3+}, 6. Ba^{2+}, 7.Co^{2+}, 8. K^+, 9. Al^{3+}, 10. Ni^{2+}, 11. Ca^{2+}, 12. Cu^{2+}, 13. Cr^{3+}, 14. Zn^{2+}, 15. Cd^{2+}, 16. Na^+.)

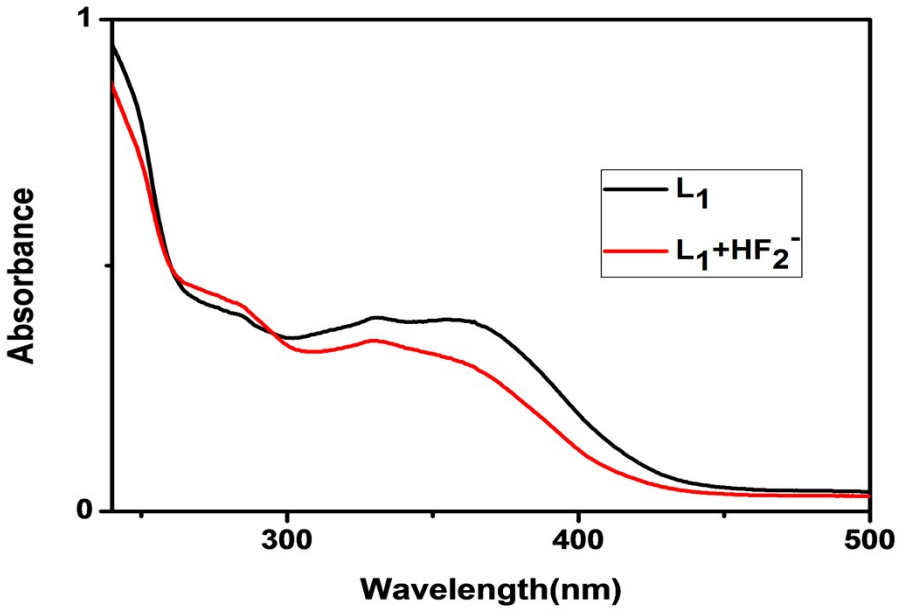


Fig. S17. Change in absorbance spectra of $\mathbf{L_1}$ in presence and absence of bifluoride ion.

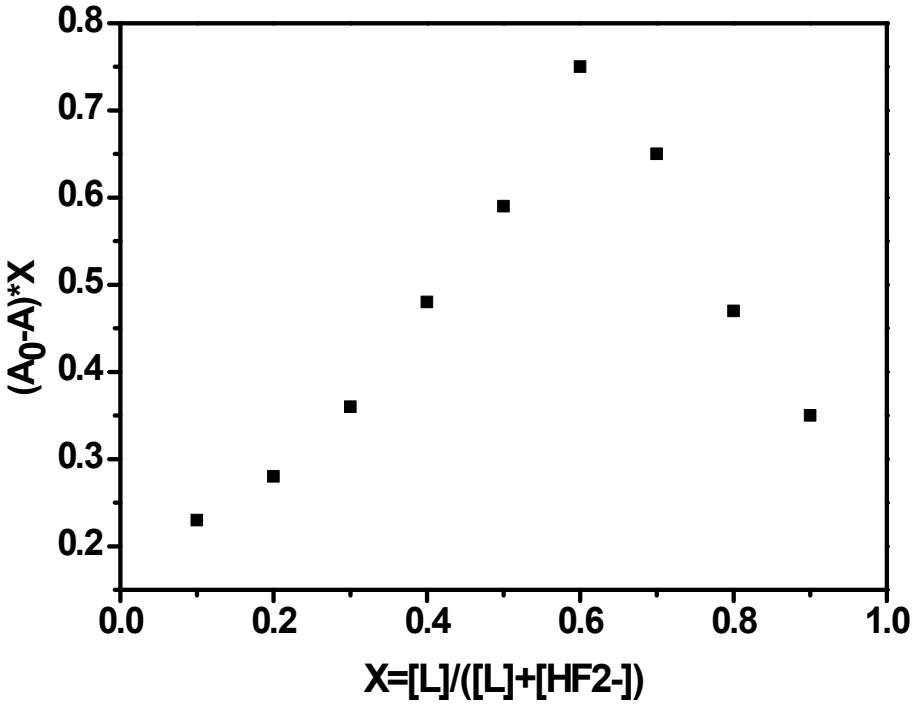


Fig. S18. Job's plot.

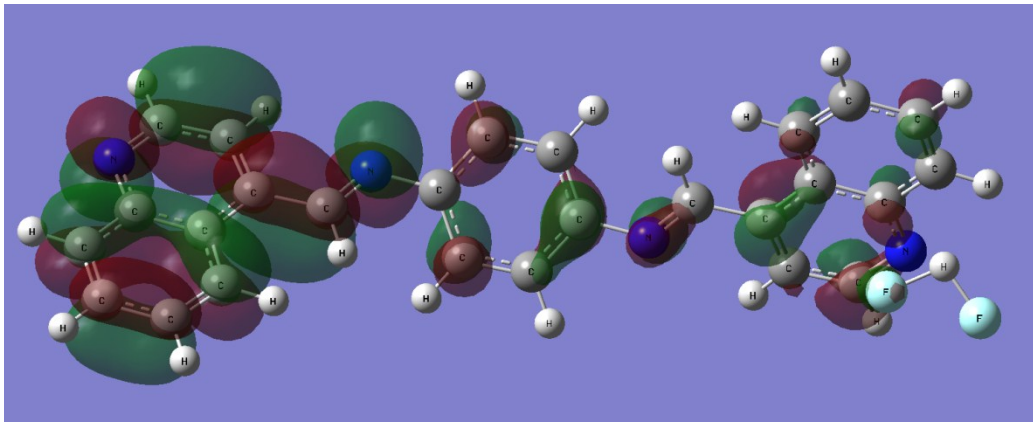
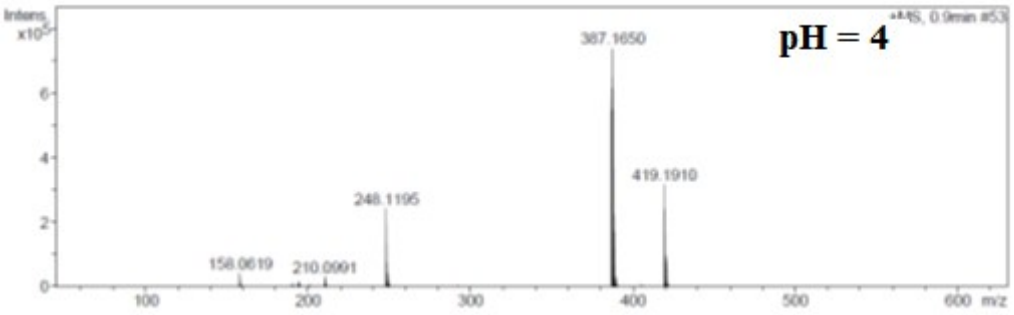
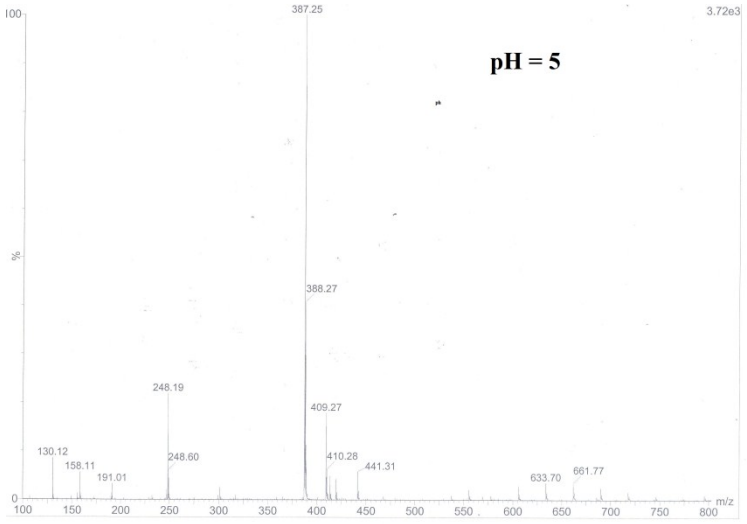


Fig. S19. HOMO-LUMO of **L**-2(HF_2^-) adduct



(a)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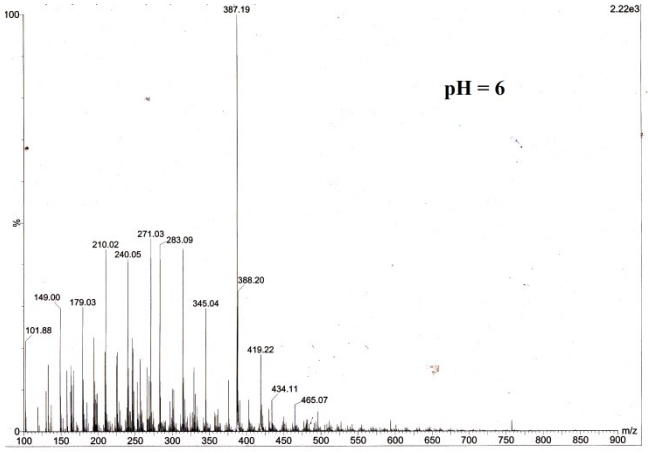
3.72e3
388.27
248.19
409.27
130.12
158.11
191.01
248.60
410.28
441.31
633.70
661.77
m/z

(b)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271.03
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149.00
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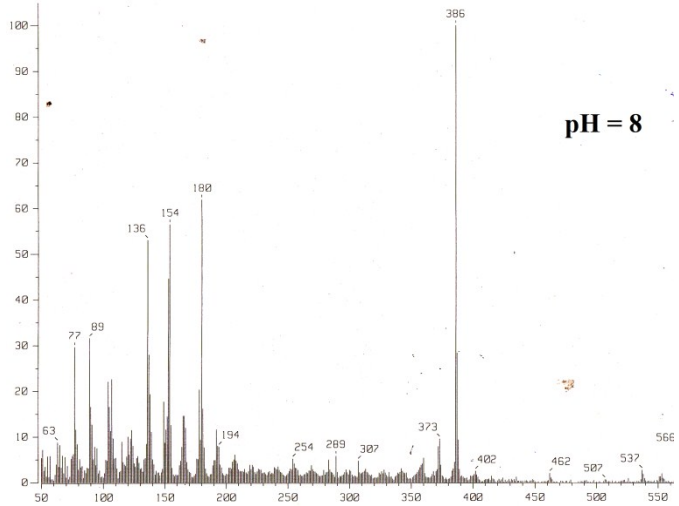
101.88
419.22
434.11
465.07
m/z

(c)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77
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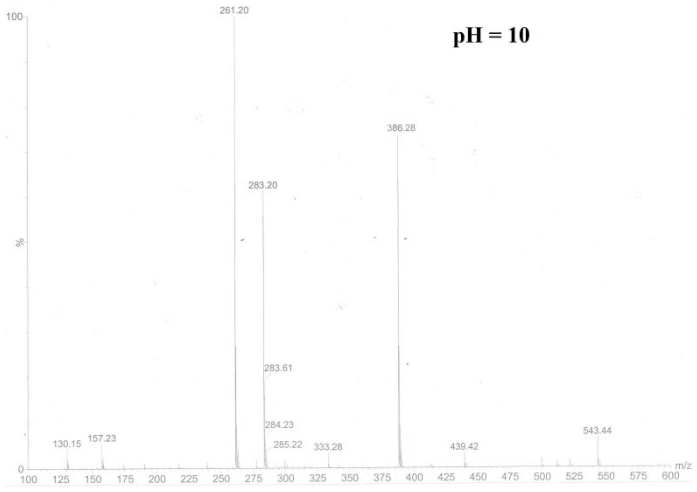
307
373
402
462
507
537
566

(d)



(e)

Fig. S20. ESI-MS of **L** at different pH, (a) pH = 4; (b) pH = 5; (c) pH = 6; (d) pH = 8 and (e) pH = 10

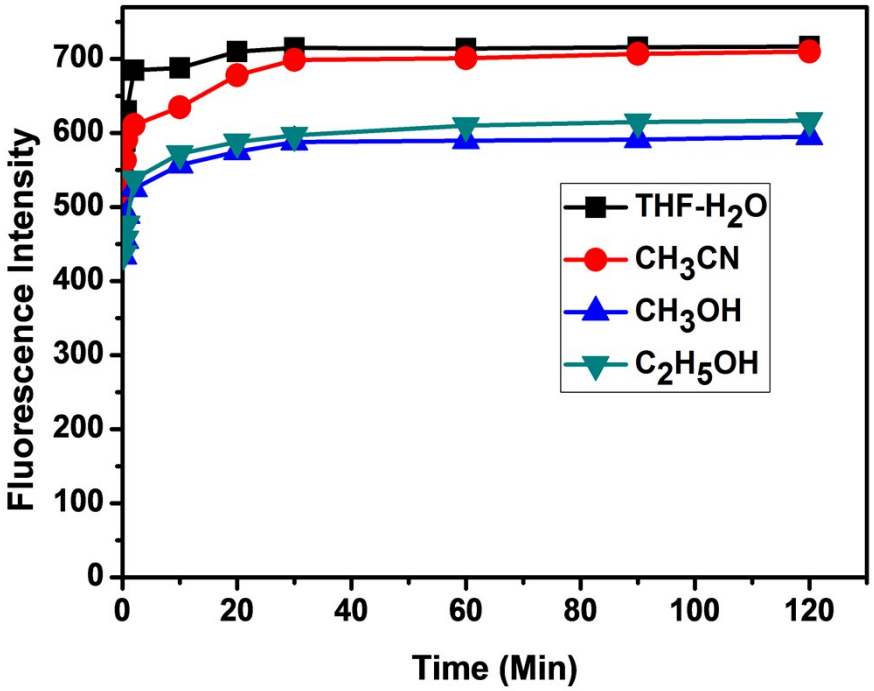


Fig. S21. Time evolution