

Studies on the effect of fluorine on the interaction of different metal ions with a fluorinated azobenzene-Schiff base: intramolecular C–F activation under polar solvent

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Supporting Information

General Experimental process for UV-visible and Fluorescence Emission

For UV-vis and Fluorescence studies, the stock solution of probes **1-4** (1 mM) were prepared in EtOH and then diluted to make a final solution of 35 μ M. Added 1 mL of PBS buffer solution (pH = 7) for each 20 mL of stock solution. We dissolved metal ions in water (10 μ mol). Added metal ions solution to ethanolic solution of compounds **1-4** at volume (9:1, compound: metal ions) (Here we have fixed the concentration of ligand vs metal to 1:1). Then we recorded UV-visible and Fluorescence emission at 0-hr and 24-hrs for each compound and metal ions.

These metal salts have been used in the experiments. Sodium acetate, Potassium acetate, Lithium carbonate, Manganese sulphate, Magnesium Chloride Cobalt nitrate, Aluminium sulphate, Cerium chloride, Zinc acetate, Copper acetate, Nickel acetate, Mercuric chloride, Lead nitrate.

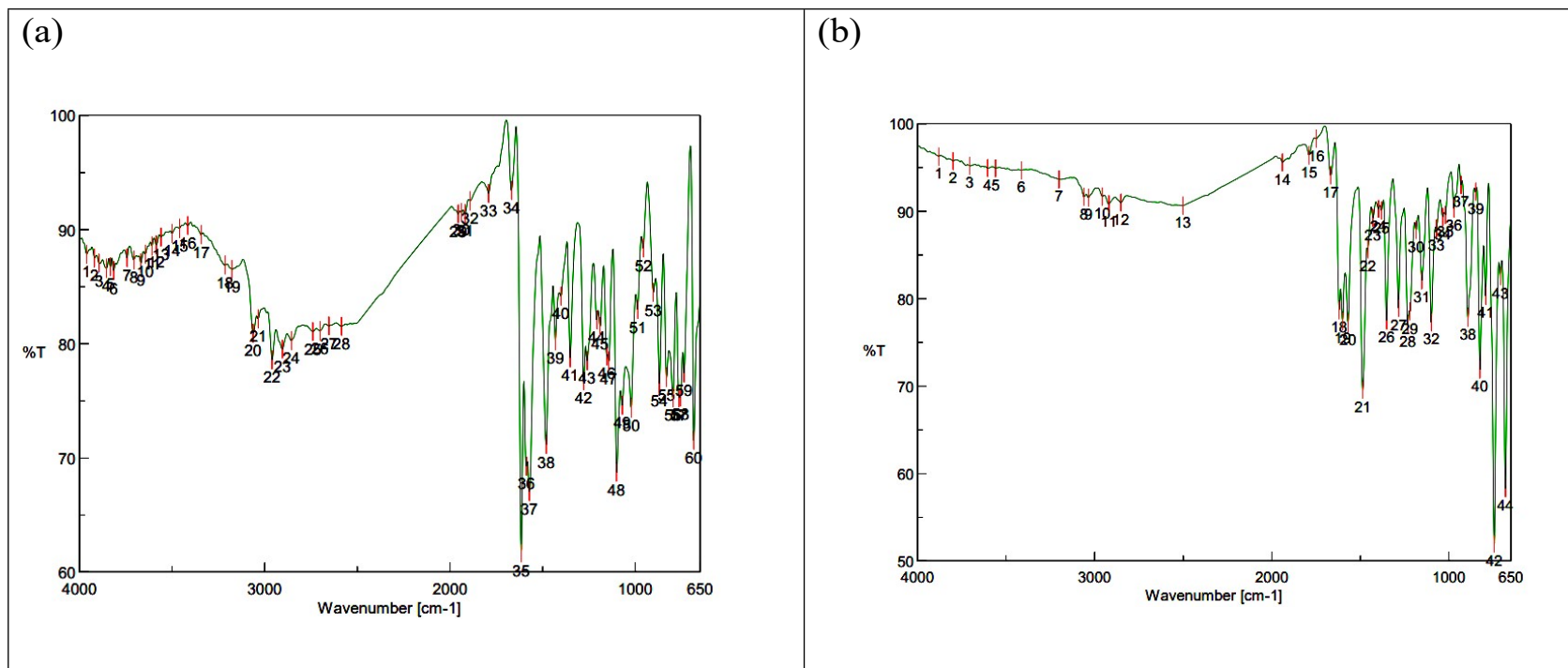
General Experimental process for NMR-Experiment

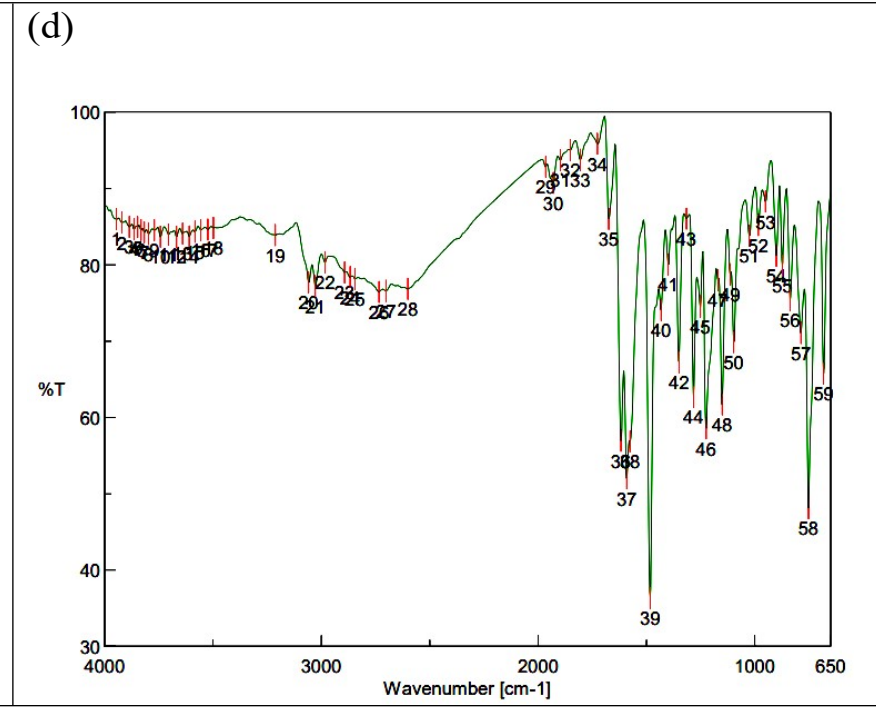
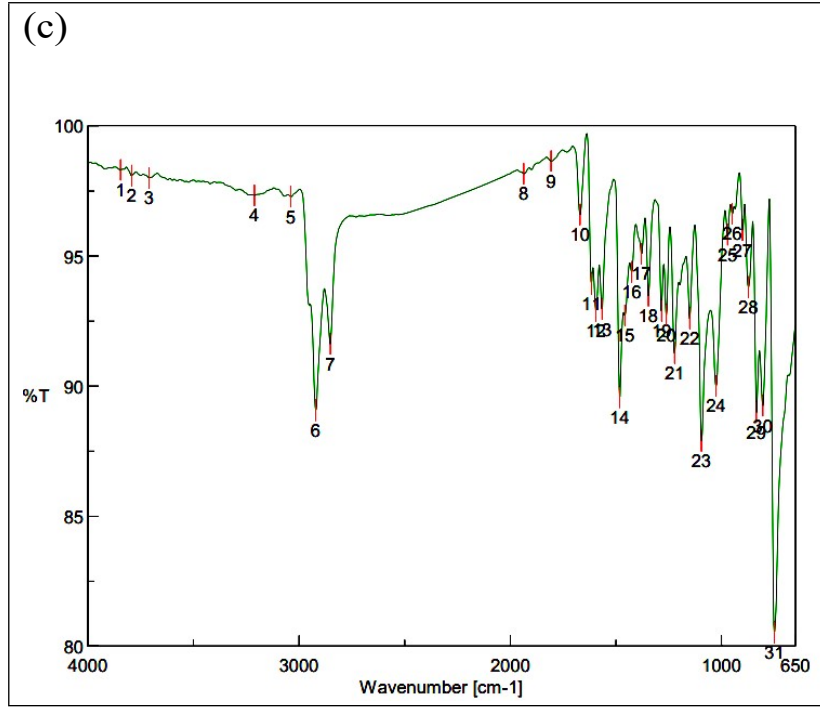
- For, ¹H and ¹⁹F NMR-experiment, we dissolved the compounds **1-4** in *d*₆-DMSO (5 mg in 0.35 mL), added 0.4 mg of buffer (pH = 7) in 0.05 mL of D₂O. We dissolved metal ions (0.4 mg in 0.1 mL) in D₂O.
- Added metal ions solution to DMSO solution of compounds **1-4** at volume (9:1, Compound: Metal ions) (Here we have fixed the concentration of ligand vs metal to 1:1). Then we recorded ¹H NMR and ¹⁹F NMR at 0-hr and 24-hrs for each compound and metal ions.

Sample Preparation for JOBs Experiment

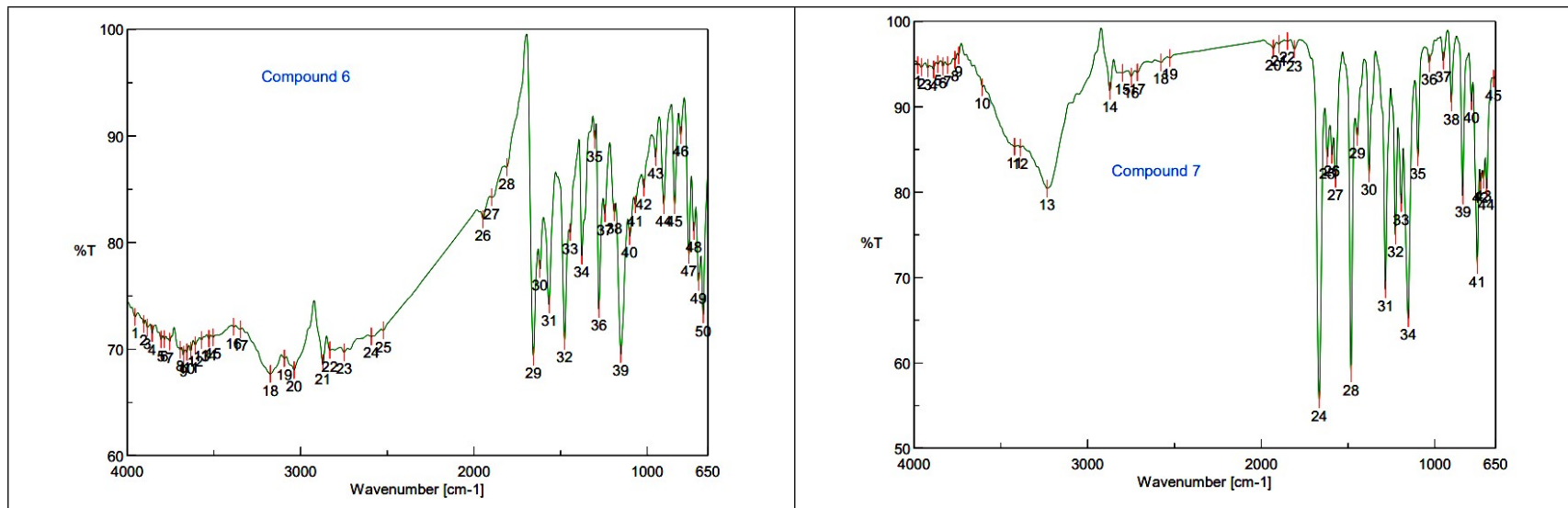
We dissolved compound **1-4** EtOH to 35 μ M, added 7 microliters of buffer for each metal ions in water at 35 μ M, mole then we mix the stock solution of compound and ligand in ratio 2.7 + 0.3, 2.4 + 0.6, 2.1 + 0.9, 1.8 + 1.2, 1.5 + 1.5, 1.2 + 1.8, 0.9 + 2.1, 0.6 + 2.4, 0.3 + 2.7 (Compound + Metal ions) to make overall volume 3 ml.

SI-1: IR of compound 1(a), 2(b), 3(c) and 4(d).





SI-2: IR of compound 6 and 7.



SI-3: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions where change was not found at 0-hours.

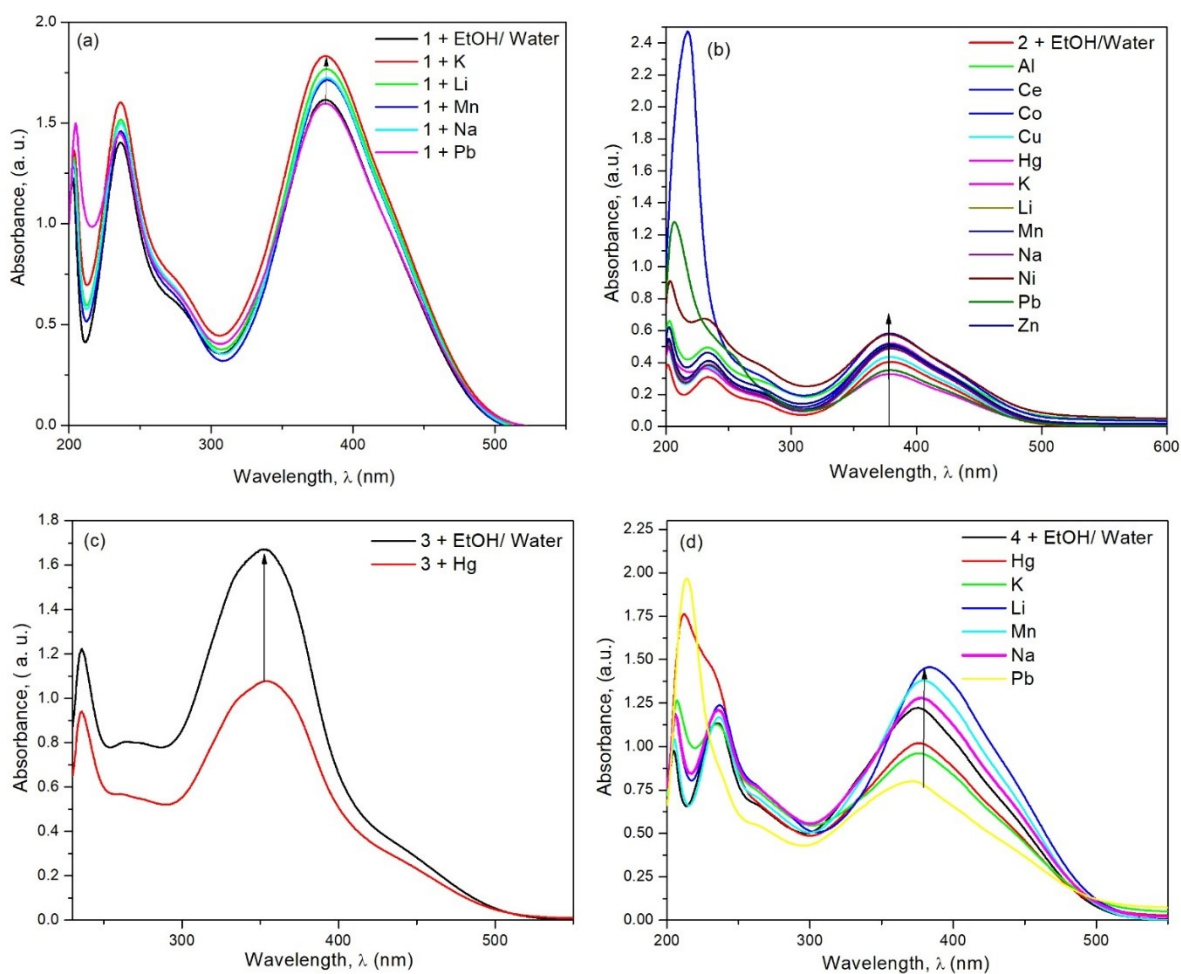


Figure3: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions at 0-hours.

SI-4: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions where mild change was found at 0-hours.

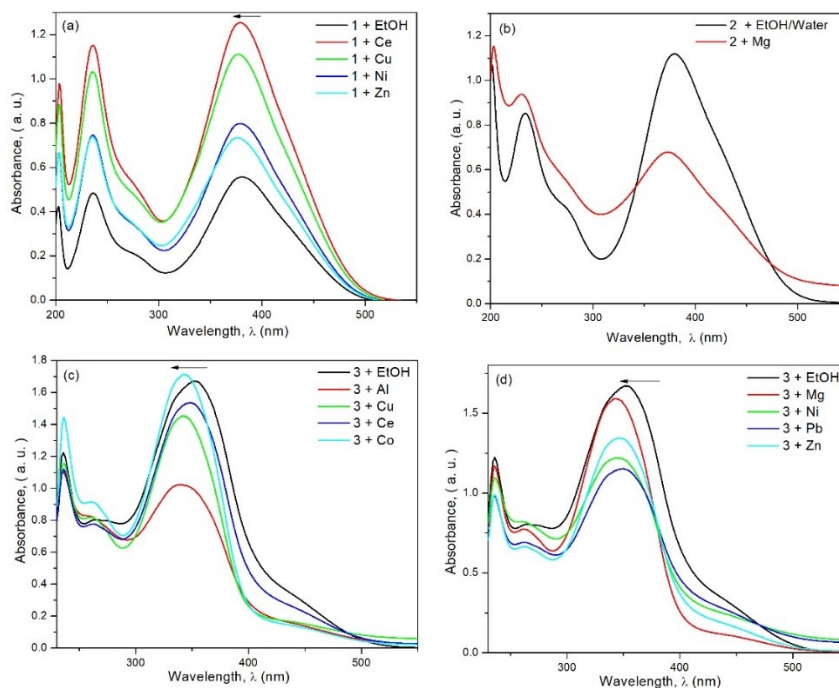


Figure4: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **3(d)** after addition of different metal ions at 0-hours with mild change.

SI-5: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions where change was not found at 24-hours.

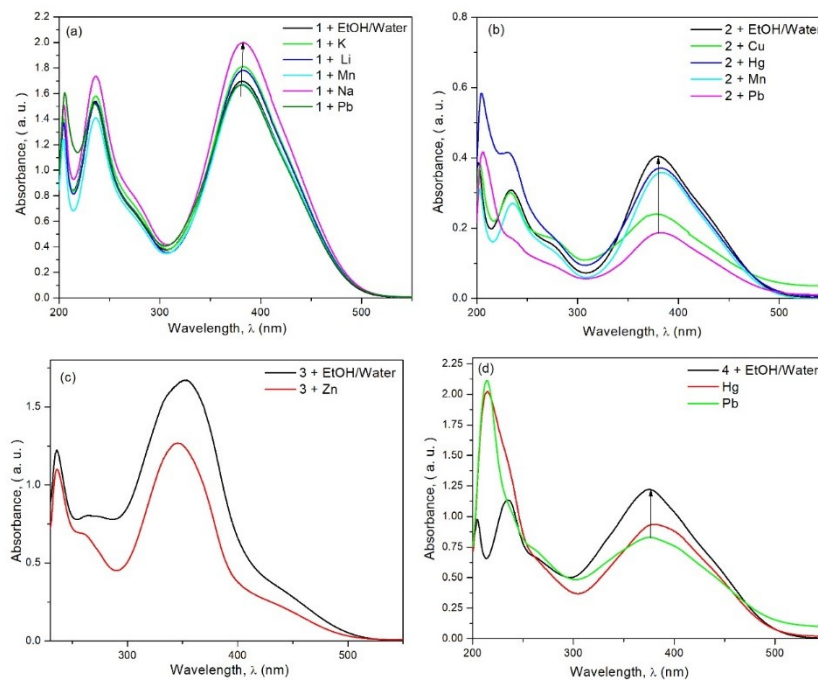
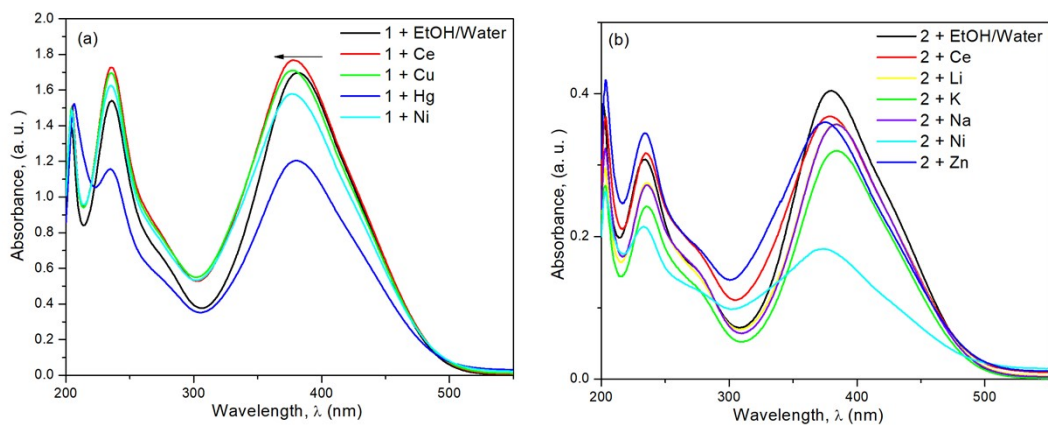
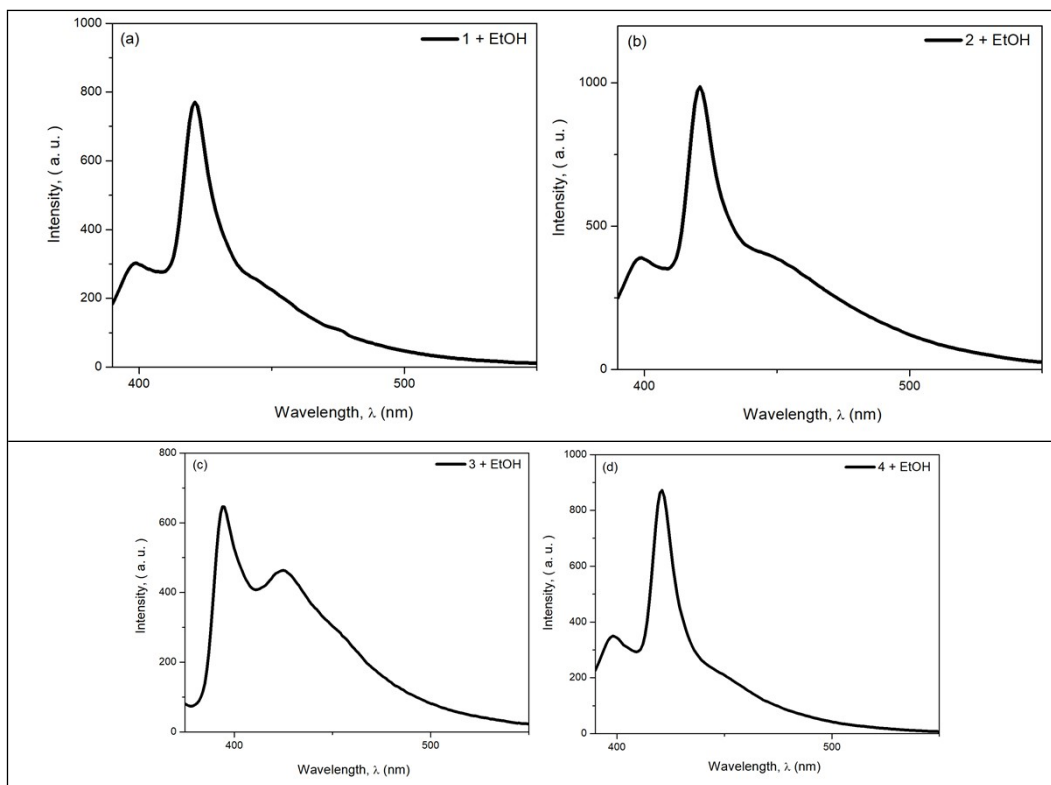


Figure5: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions at 0-hours with mild change.

SI-6: Uv-Visible absorption spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** after addition of different metal ions where mild change was found at 24-hours.

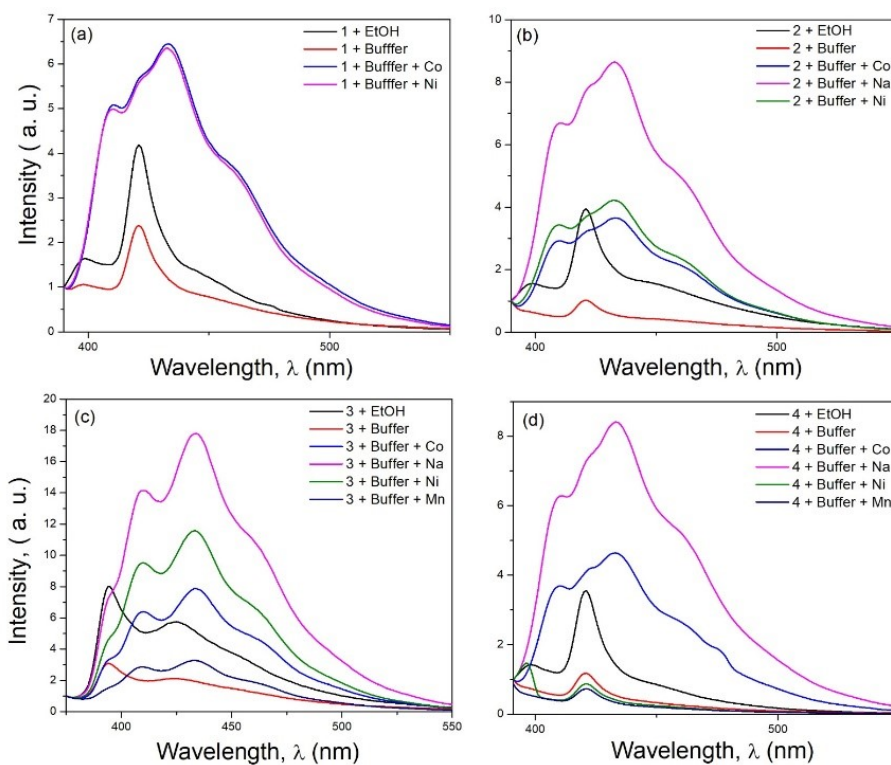


SI-7: Fluorescence emission spectra of compounds **1(a)**, **2(b)**, **3(c)** and **4(d)** in Ethanol.



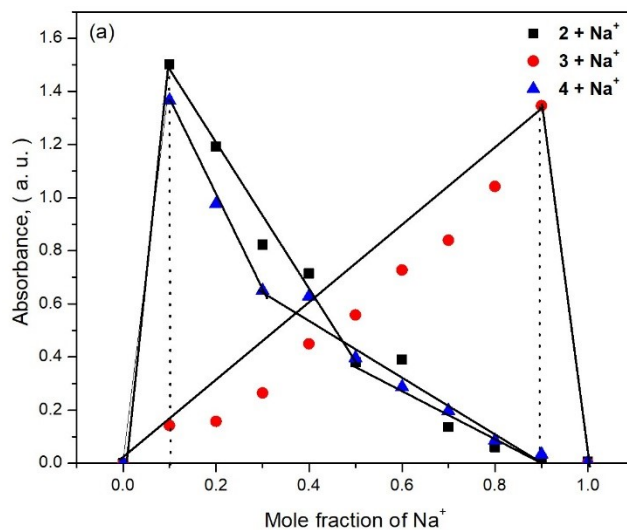
Fluorescence emission spectra of compounds **1-4** in EtOH (10 mM).

SI-8:

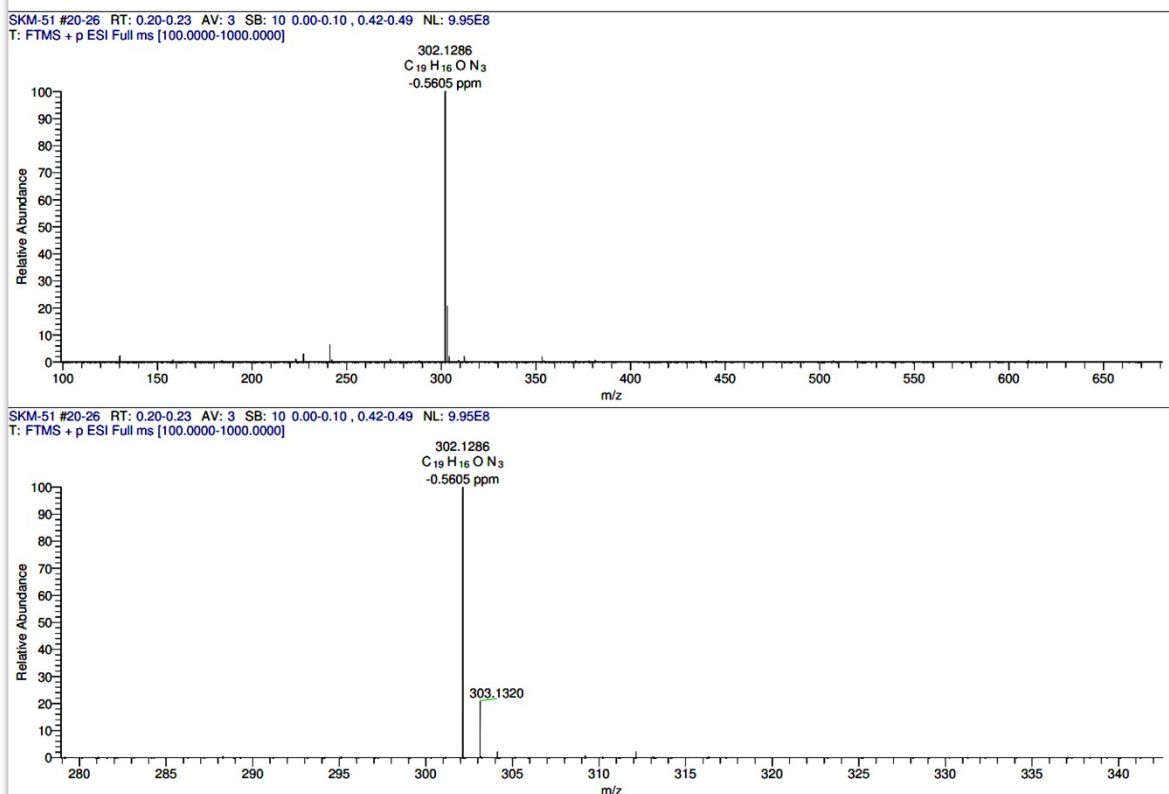


Change of fluorescence emission (normalised) band when ligands 1-4 interacted with metal ions Mn, Ni, Co, Na (10 mM).

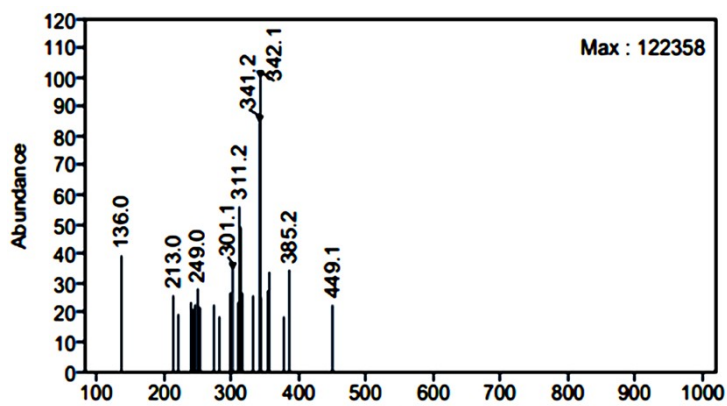
SI-9: Jobs plot of compounds 2, 3 and 4 with Na^+ .



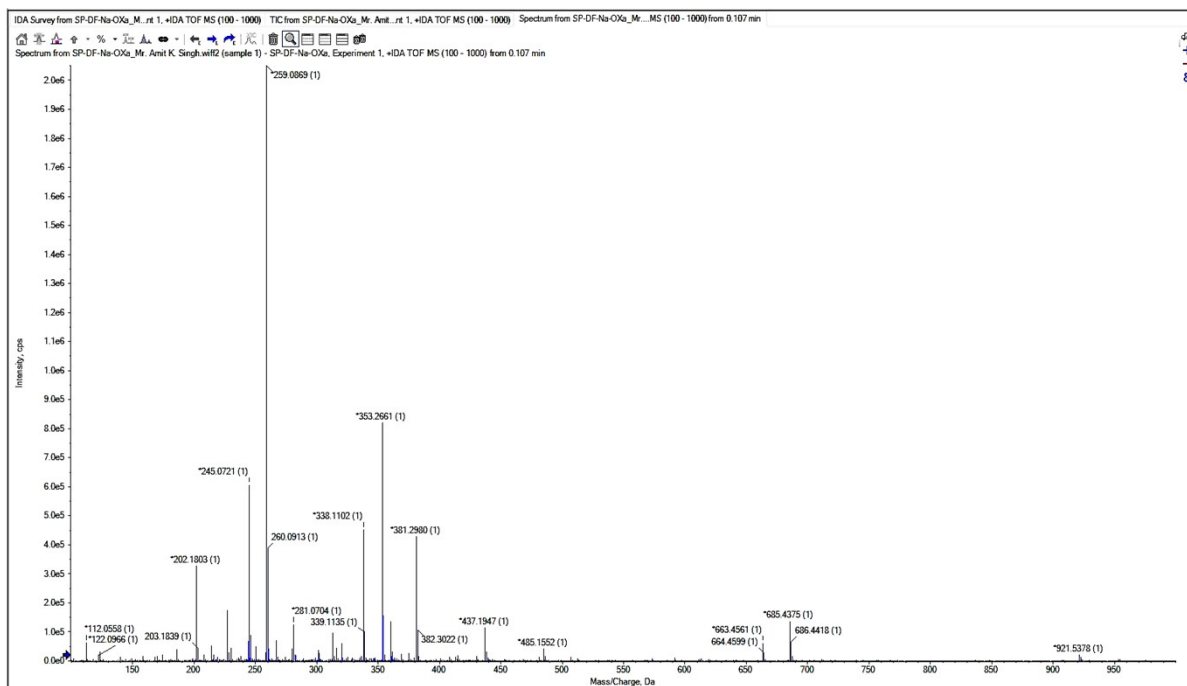
SI-10: HRMS of Compound 1.



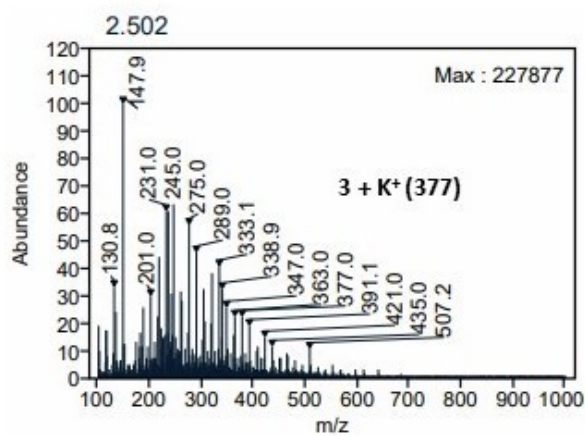
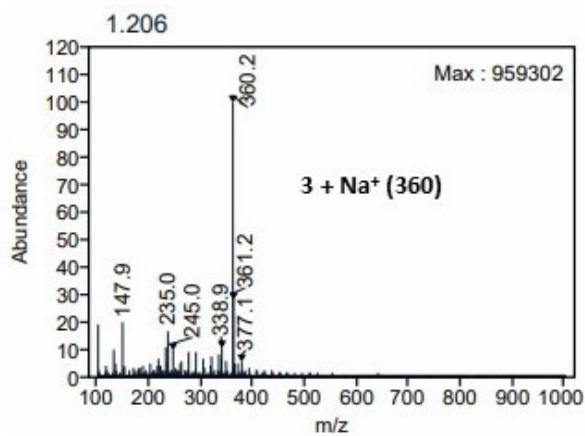
SI-11: HRMS of Compound 2.



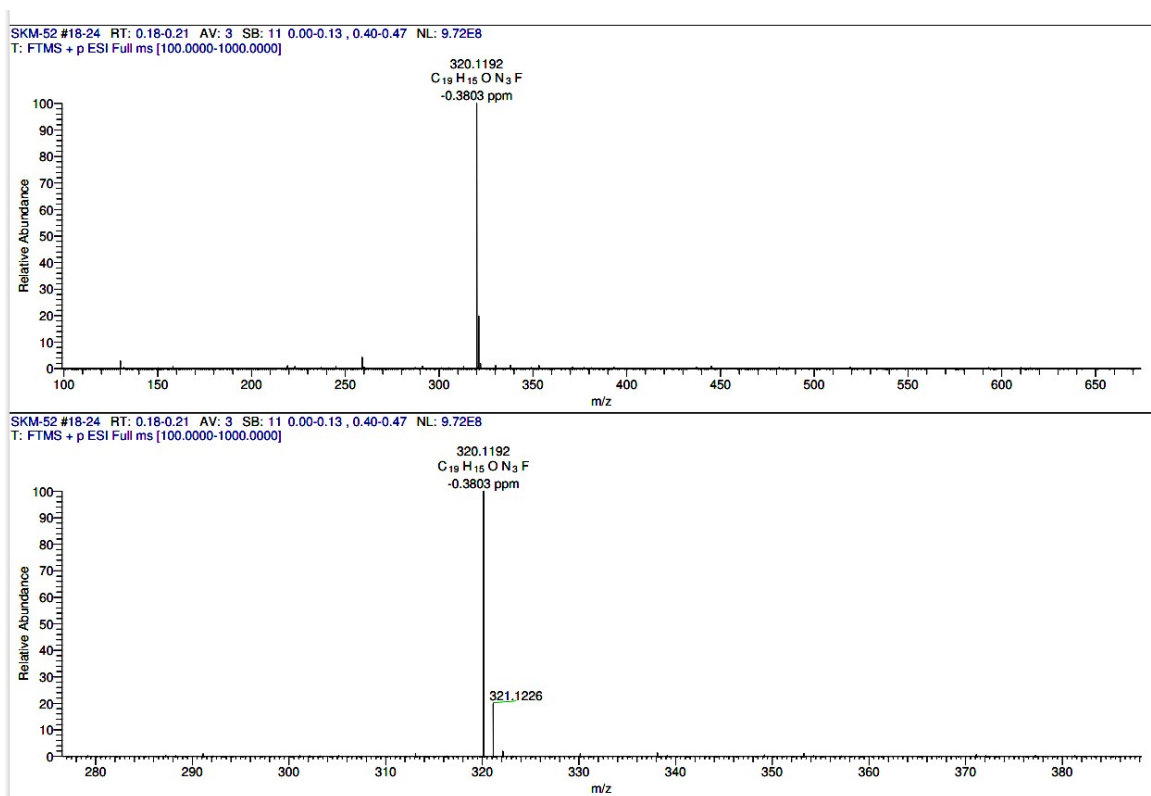
SI-12: HRMS of Compound 3.



SI-13: LC-MS of Compound 3 + Na⁺ and 3 + K⁺.



SI-14: HRMS of Compound 4.



SI-15: HRMS of Compound 7.

