Supporting Information

How stereochemistry decides the selectivity: an approach towards metal ion detection

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NMR Study:

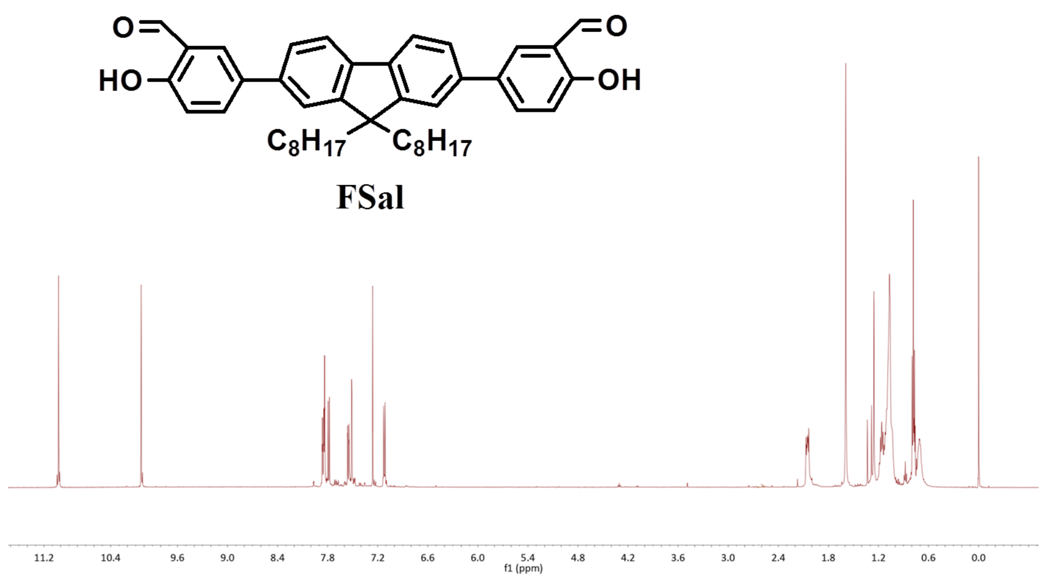


Figure S1. ^{1}H-NMR of Fsal

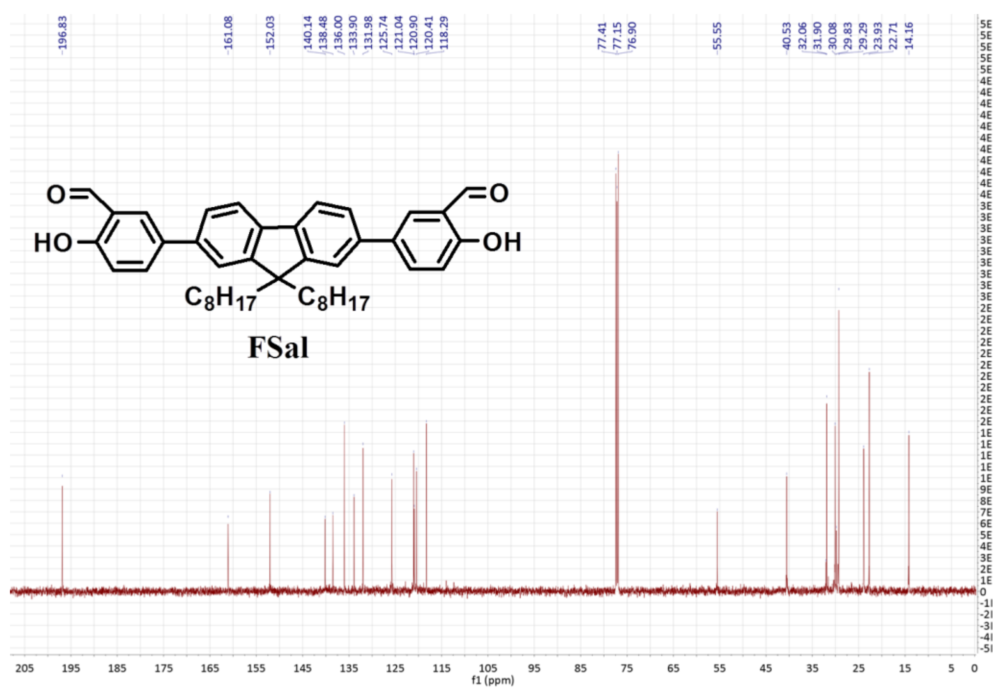


Figure S2. ^{13}C-NMR of Fsal

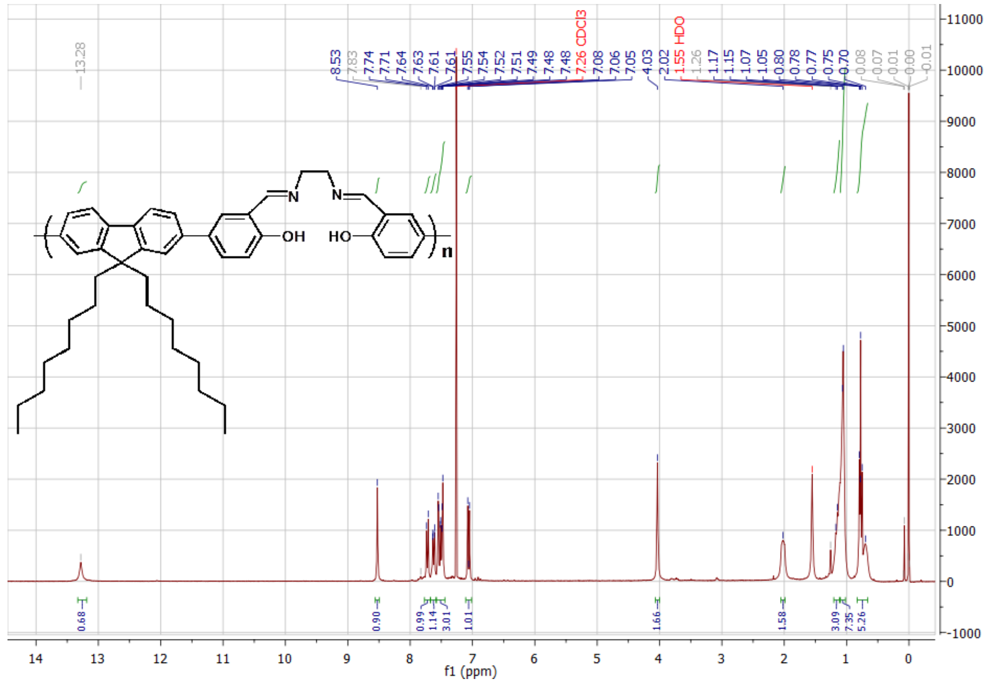


Figure S3. ^{1}H-NMR of FSP1

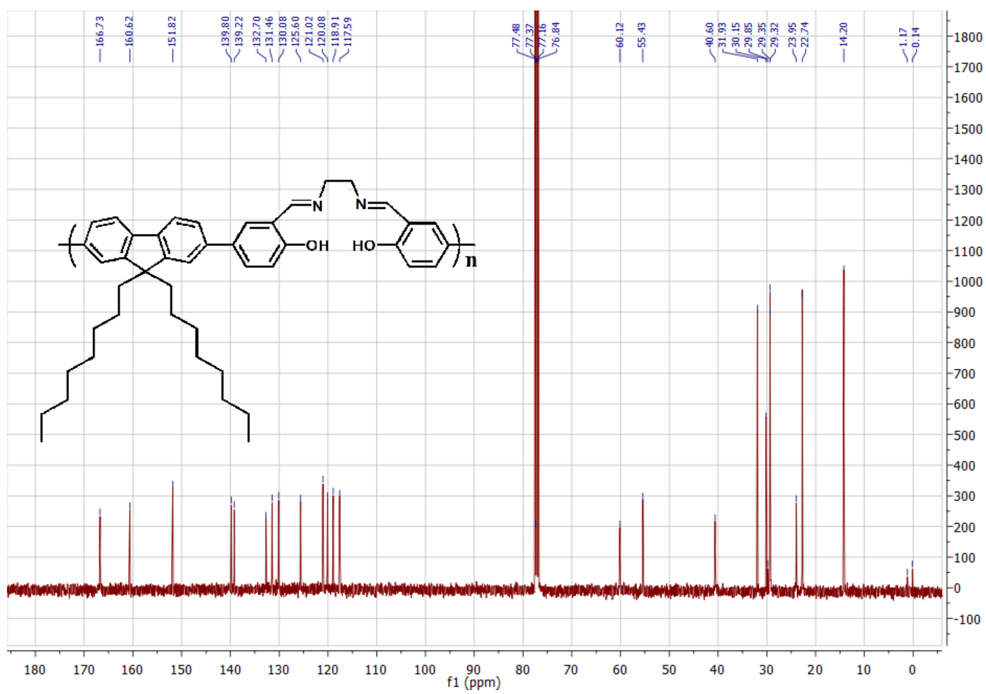


Figure S4. ^{13}C-NMR of FSP1

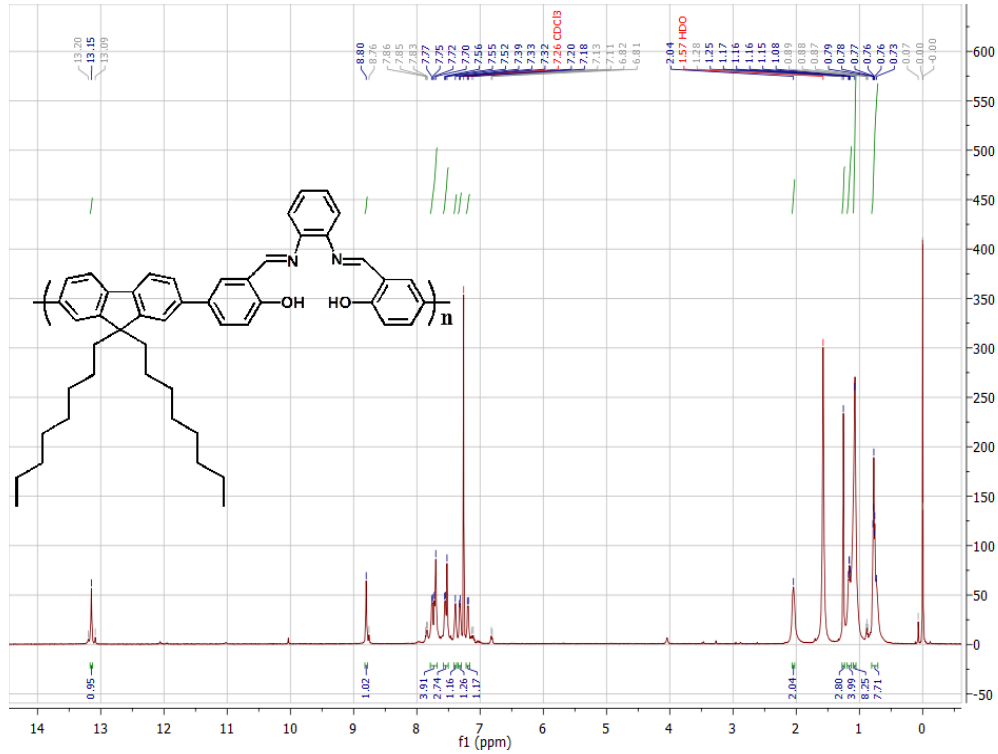


Figure S5. [1]H-NMR of FSP2

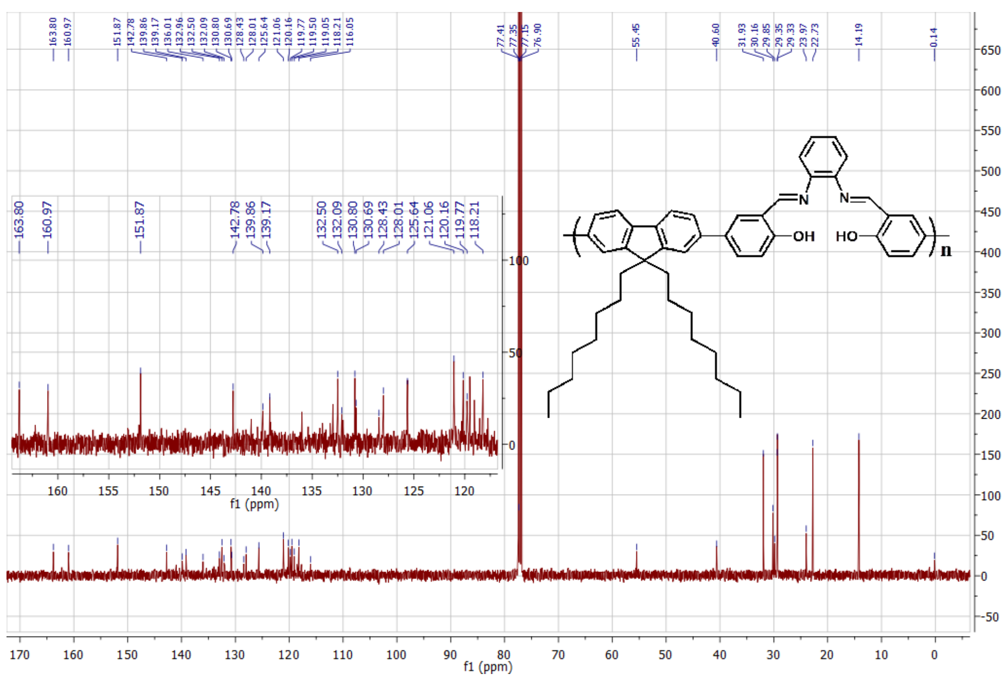


Figure S6. [13]C-NMR of FSP2

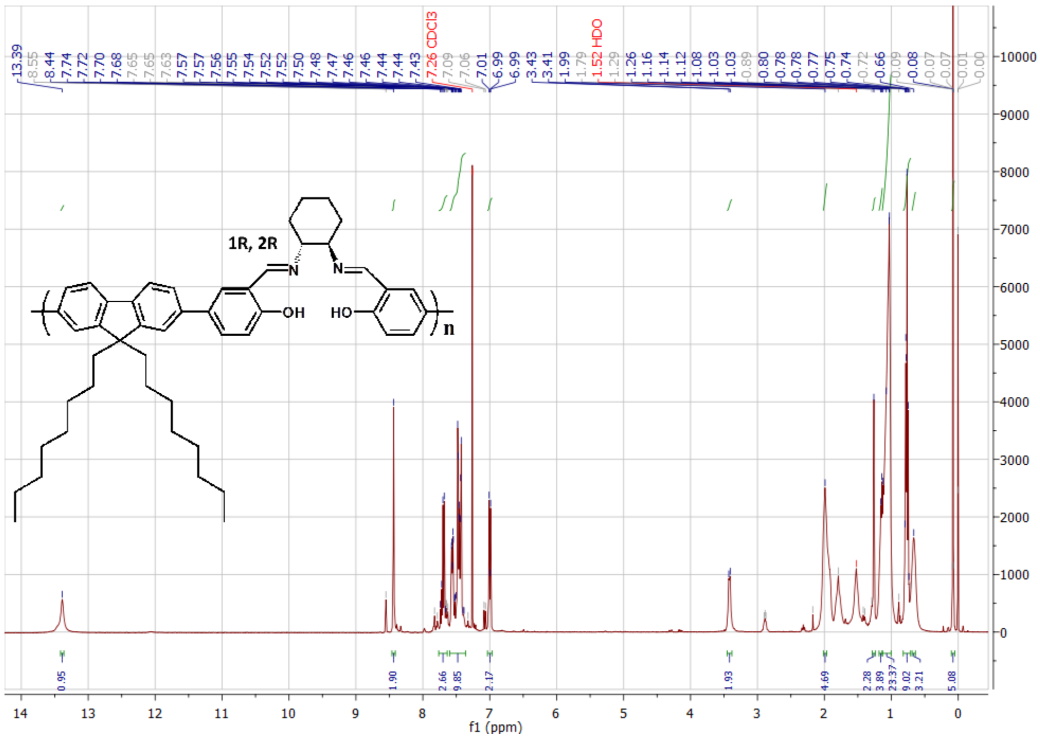


Figure S7. ^{1}H-NMR of FSP3

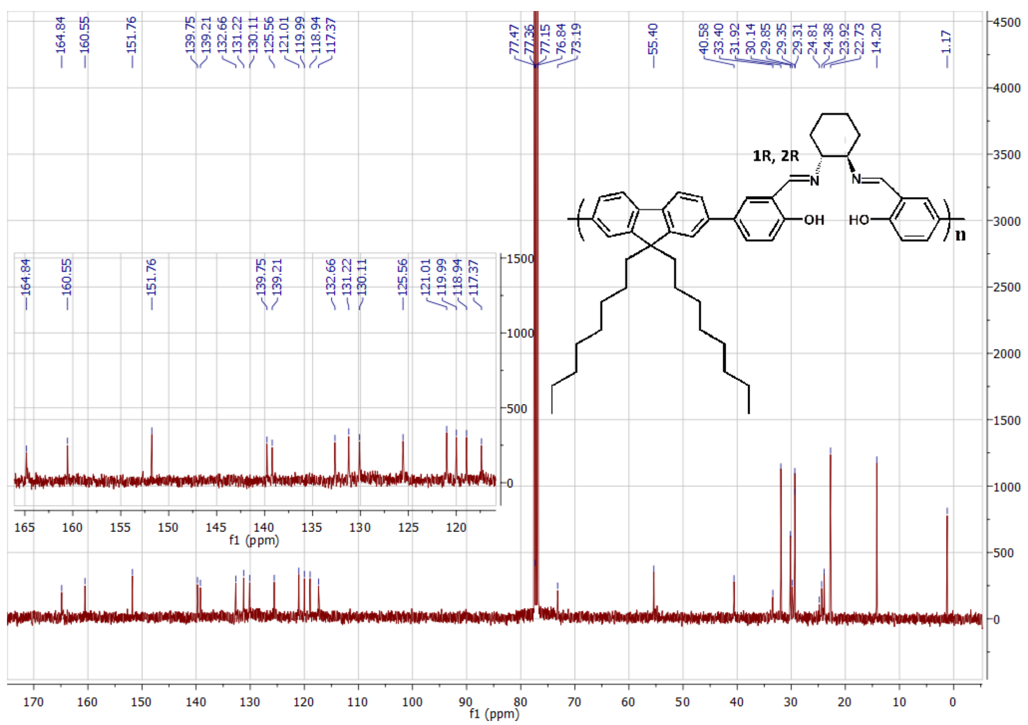


Figure S8. ^{13}C-NMR of FSP3

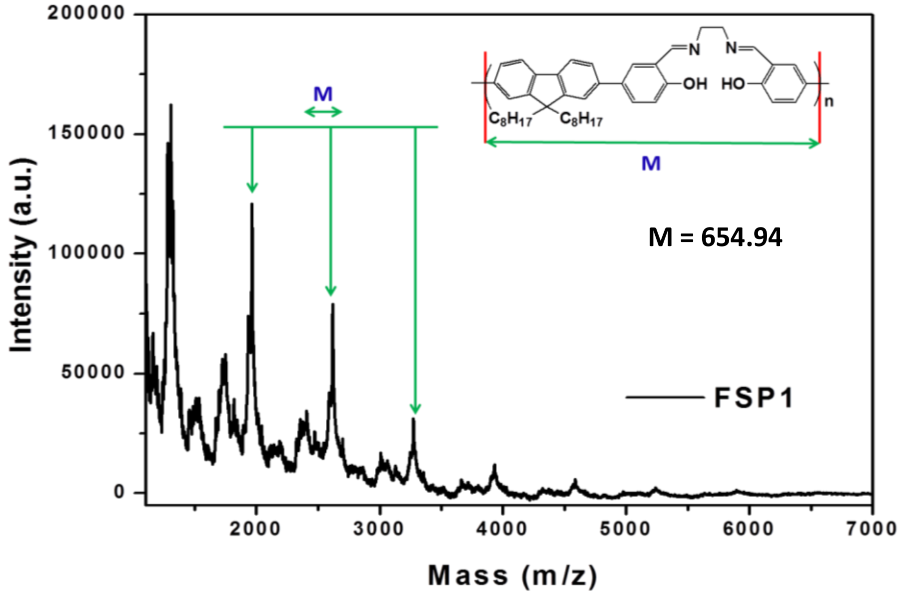


Figure S9. MALDI-TOF spectrum of FSP1 in ditranol matrix bearing repetitive monomeric units (with their corresponding mass fragments M) up to a degree of polymerization (DP) of 9 ($M_W \sim 5900$).

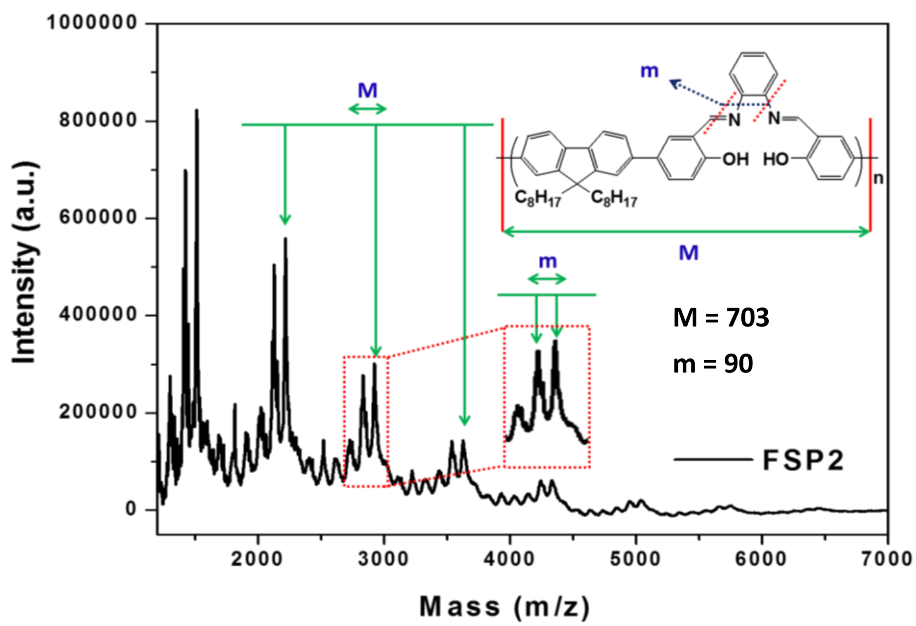


Figure S10. MALDI-TOF spectrum of FSP2 in ditranol matrix bearing repetitive monomeric units (with their corresponding mass fragments M and m) up to a degree of polymerization (DP) of 9 ($M_W \sim 6300$).

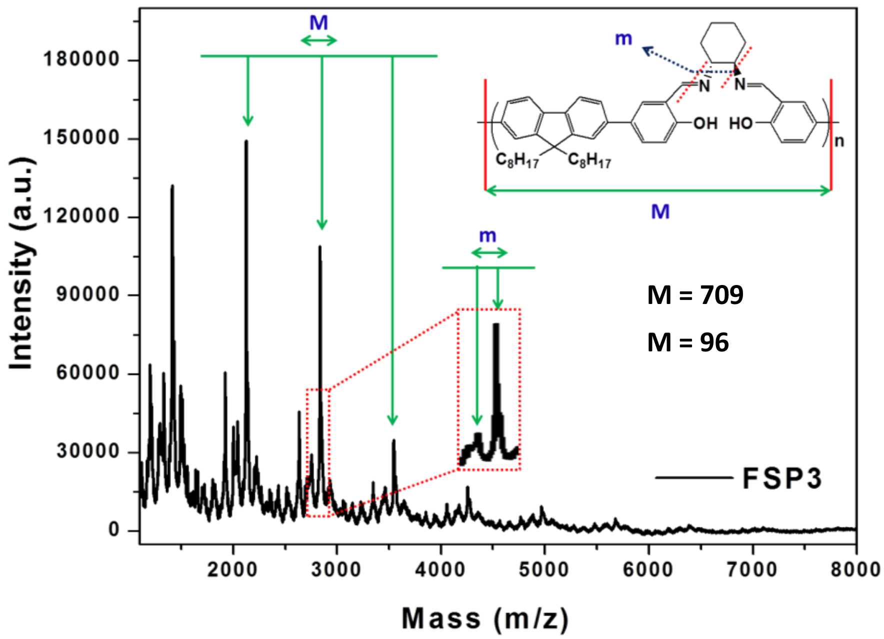


Figure S11. MALDI-TOF spectrum of FSP3 in ditranol matrix bearing repetitive monomeric units (with their corresponding mass fragments M and m) up to a degree of polymerization (DP) of 9 (M_W ~ 6400).

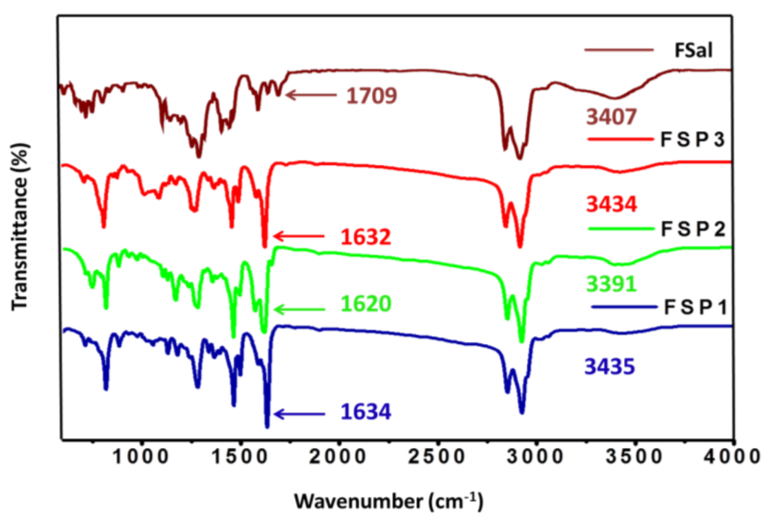


Figure S12. FTIR spectra of FSal, FSP1, FSP2, and FSP3.

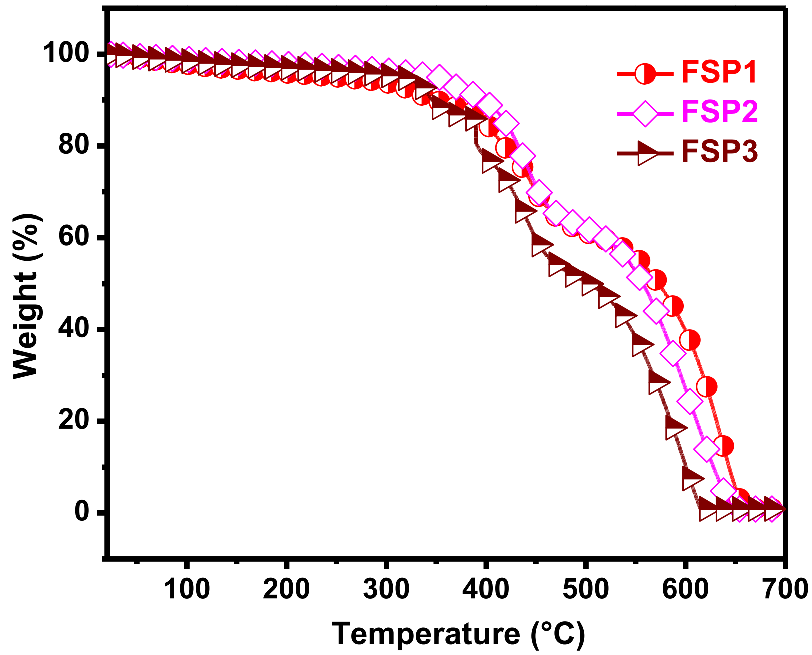


Figure S13. TGA thermograms of **FSP1**, **FSP2** and **FSP3**.

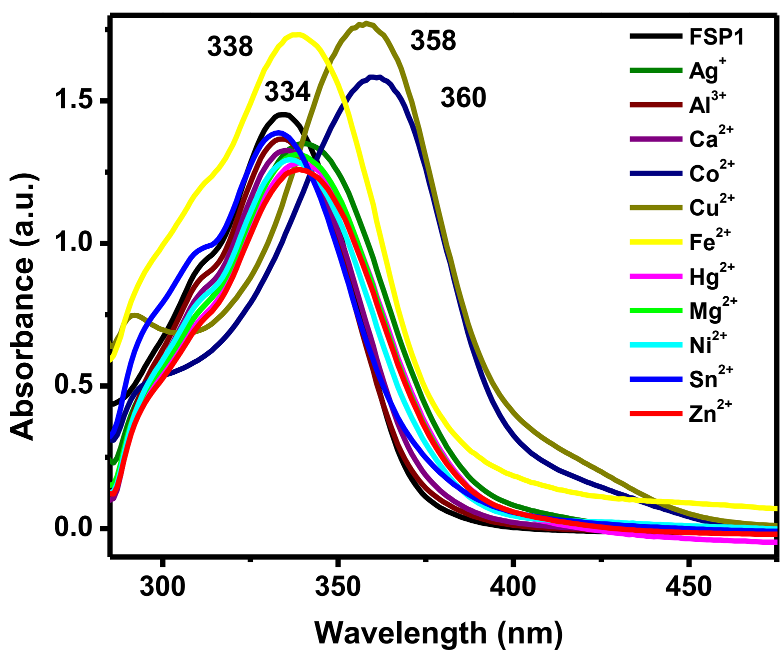


Figure S14. Absorption spectra of **FSP1** (15 μM in THF) upon addition of 22 equiv. of different cations in H_2O.

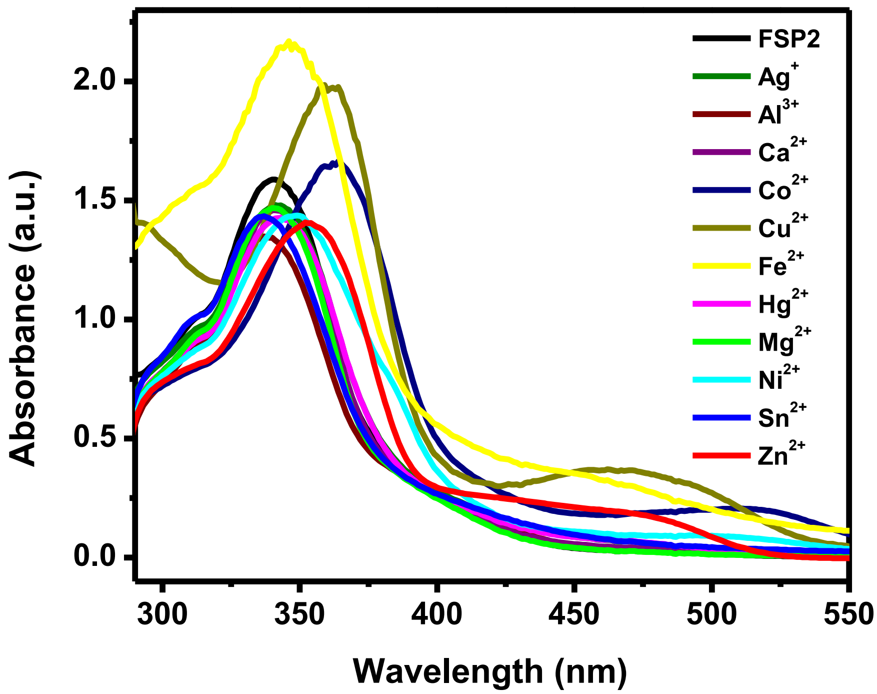


Figure S15. Absorption spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of different cations in H_2O.

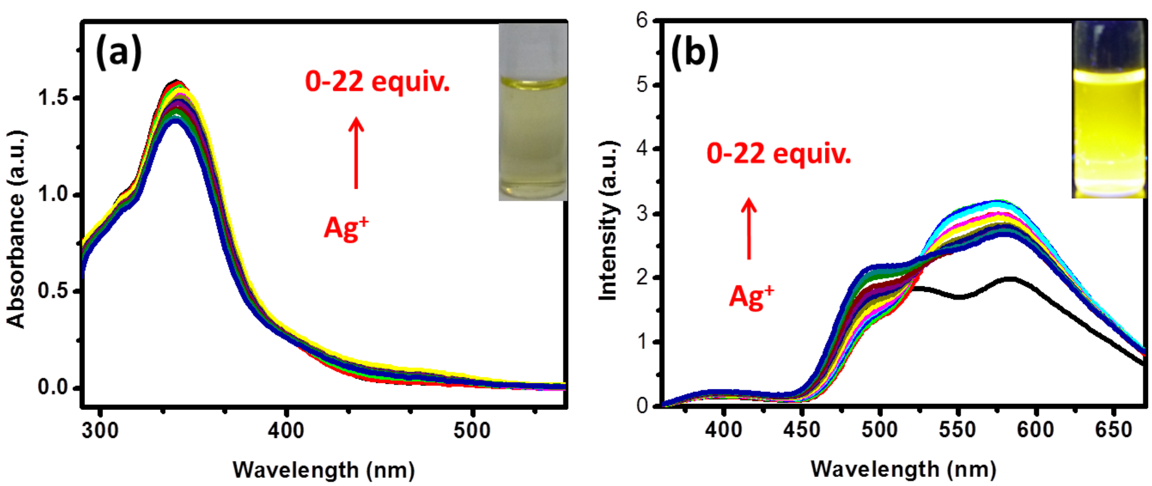


Figure S16. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Ag^+ in H_2O. Excitation at 340 nm (slit 5/5).

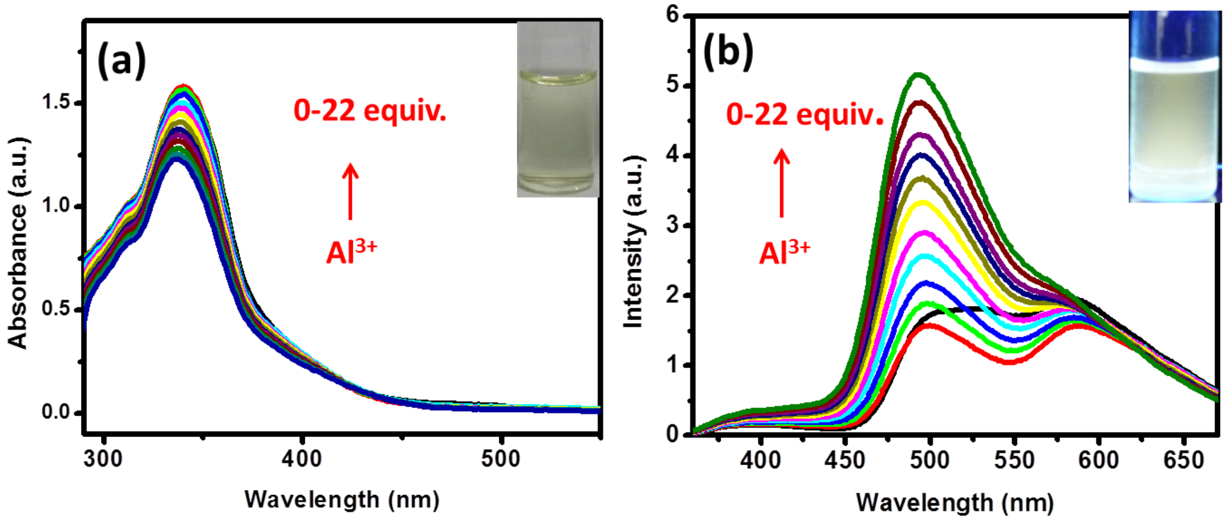


Figure S17. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Al^{3+} in H_2O. Excitation at 340 nm (slit 5/5).

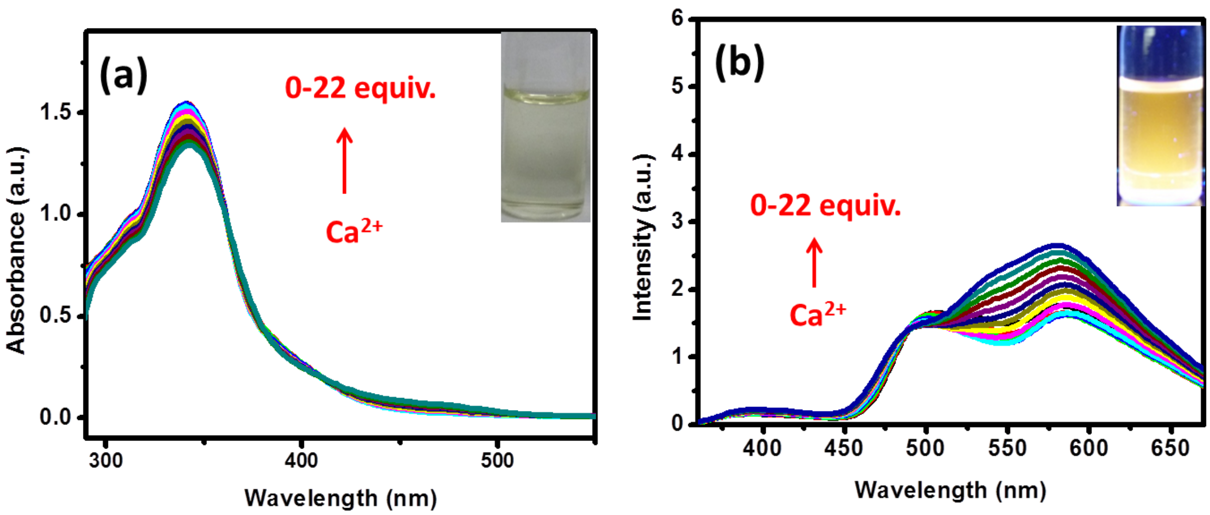


Figure S18.(a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Ca^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

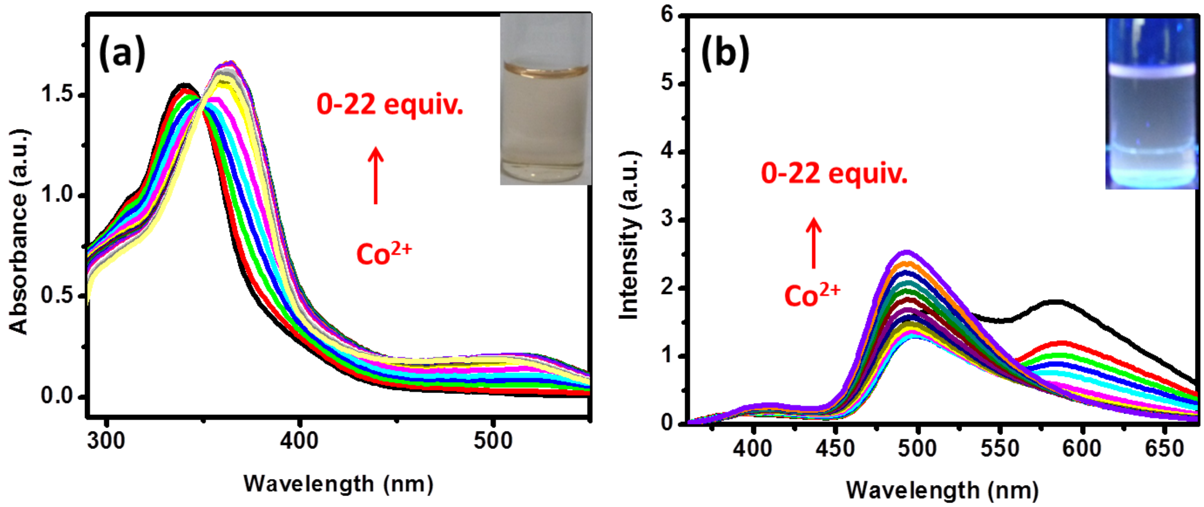


Figure S19. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Co^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

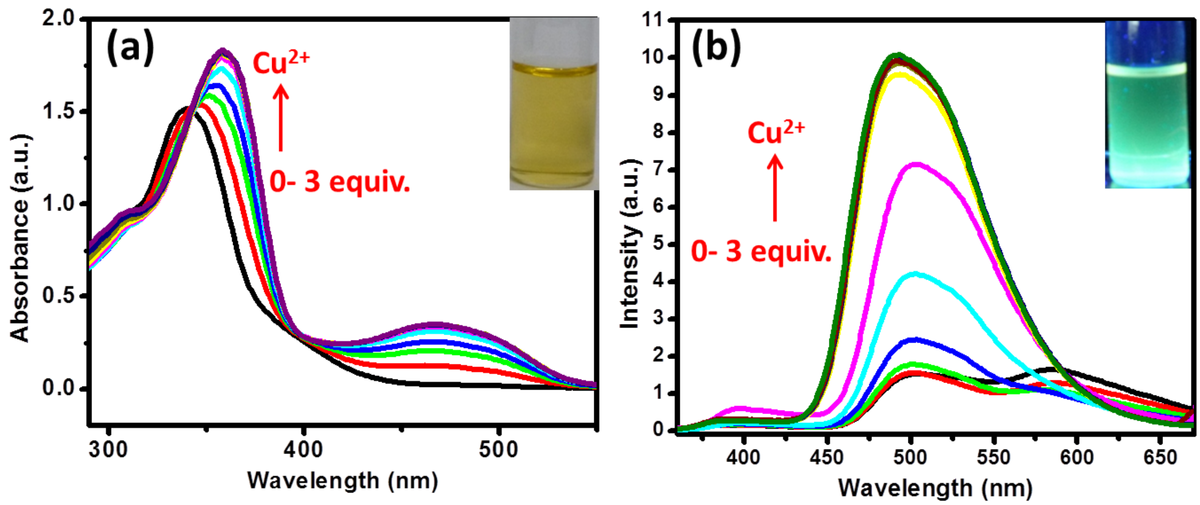


Figure S20. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 3 equiv. of Cu^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

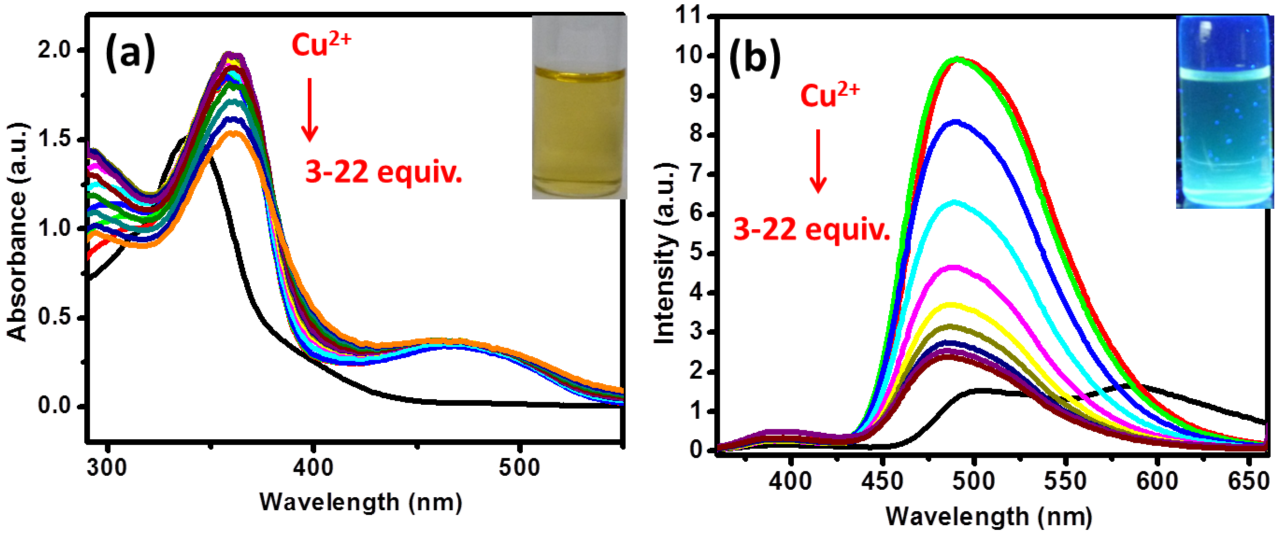


Figure S21. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 3-22 equiv. of Cu^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

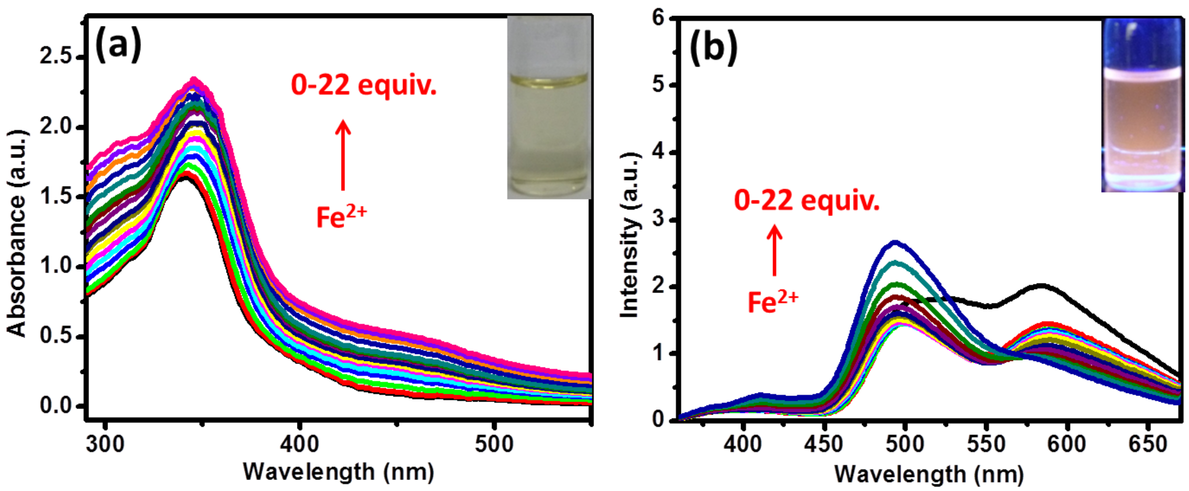


Figure S22. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Fe^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

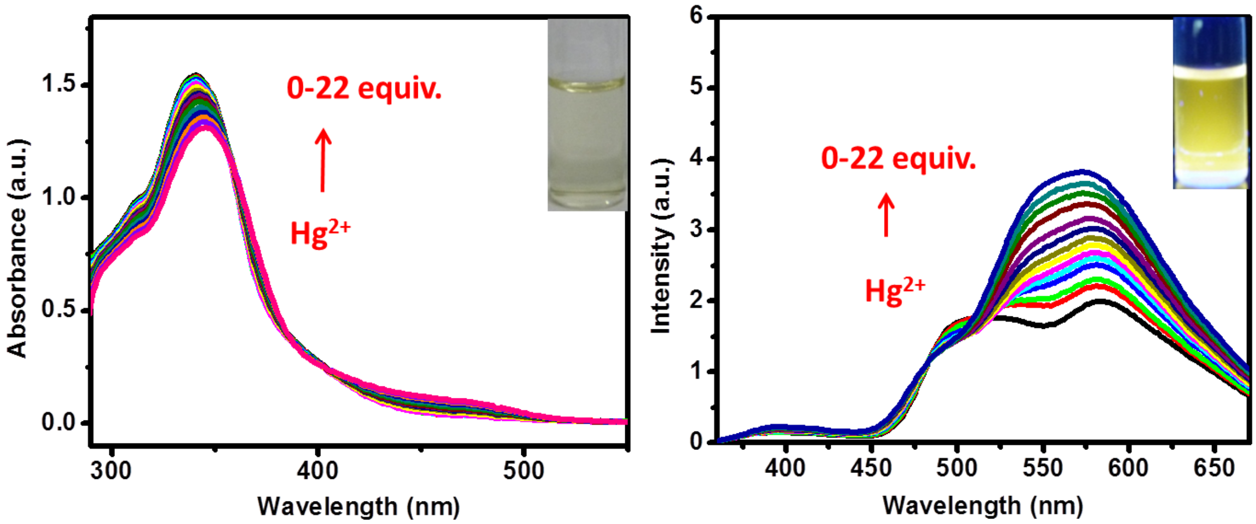


Figure S23. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Hg^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

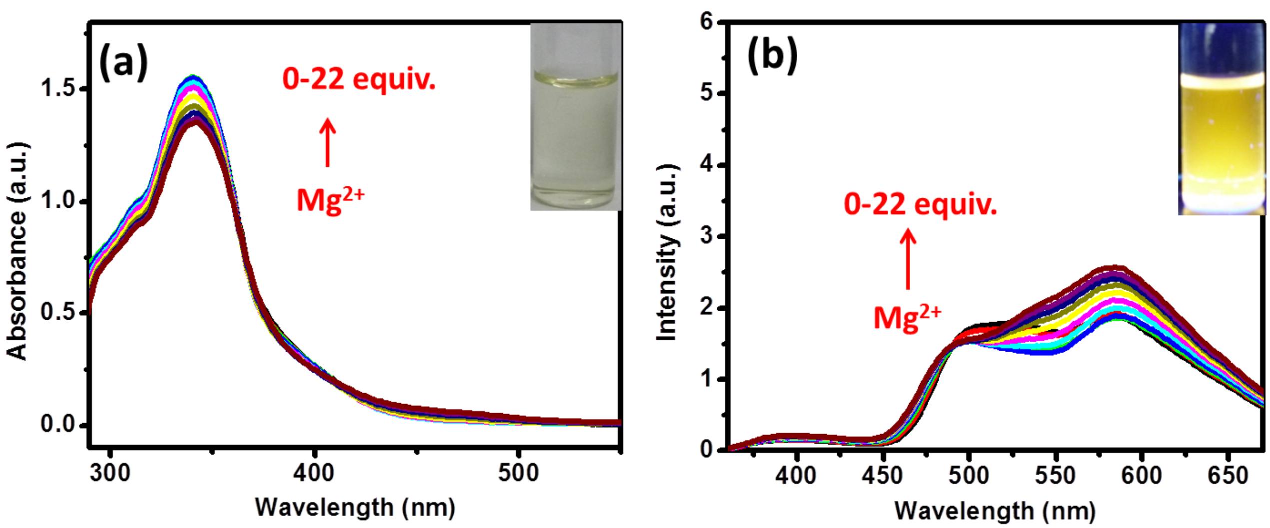


Figure S24. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Mg^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

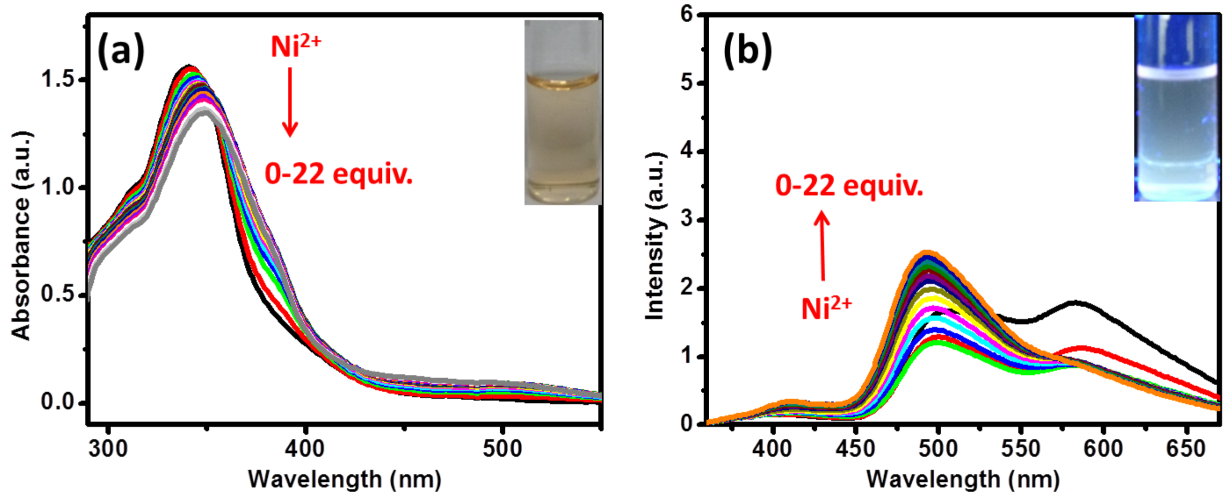


Figure S25. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Ni^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

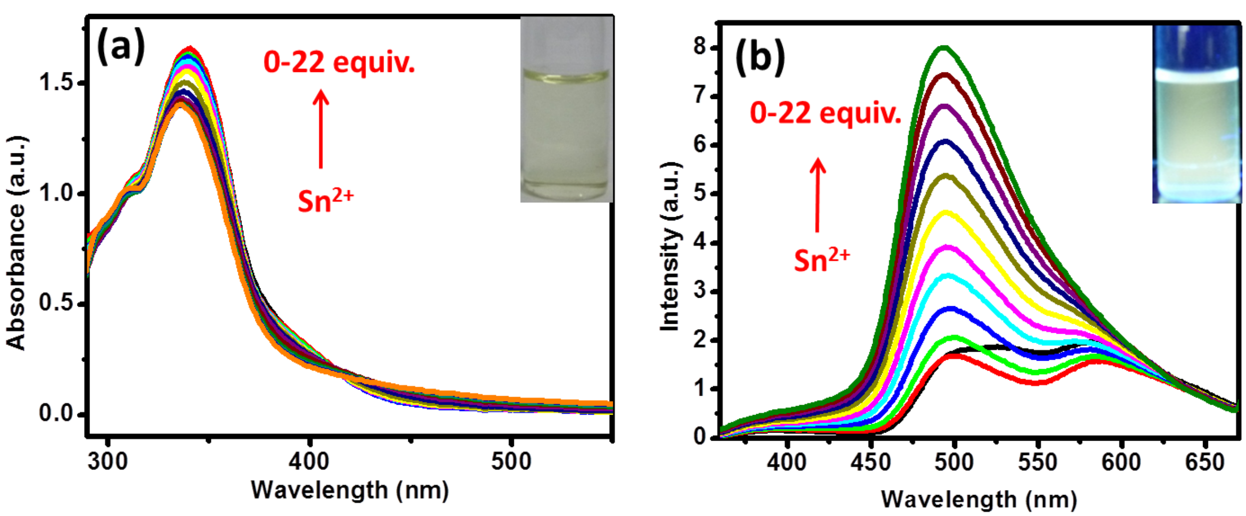


Figure S26. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Sn^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

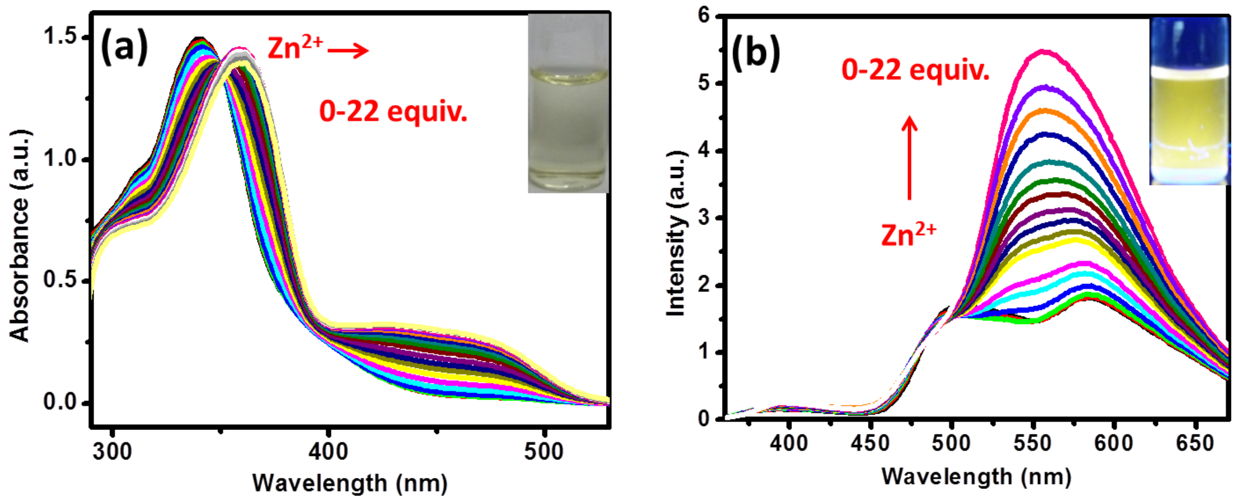


Figure S27. (a) Absorption and (b) emission titration spectra of FSP2 (15 μM in THF) upon addition of 22 equiv. of Zn^{2+} in H_2O. Excitation at 340 nm (slit 5/5).

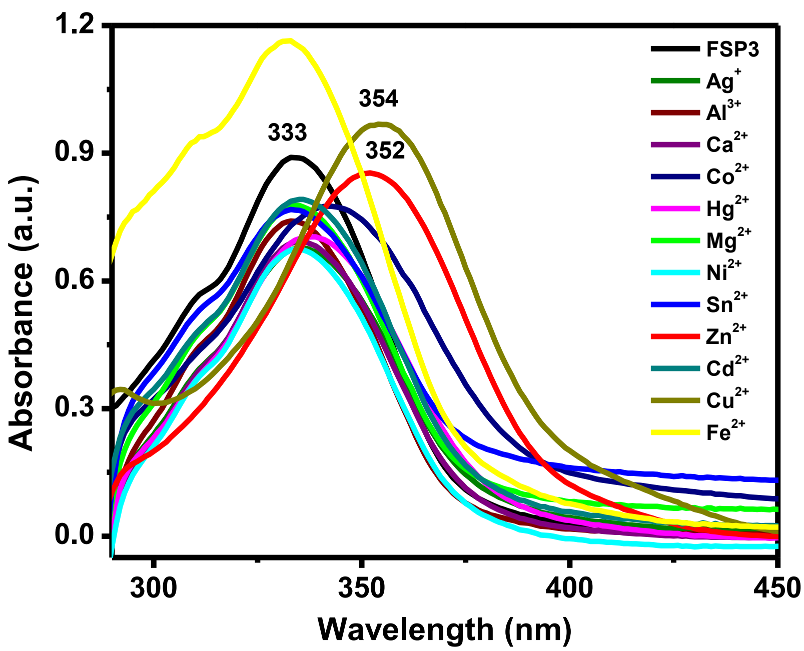


Figure S28. Absorption spectra of FSP3 (15 μM in THF) upon addition of 22 equiv. of different cations in H_2O.

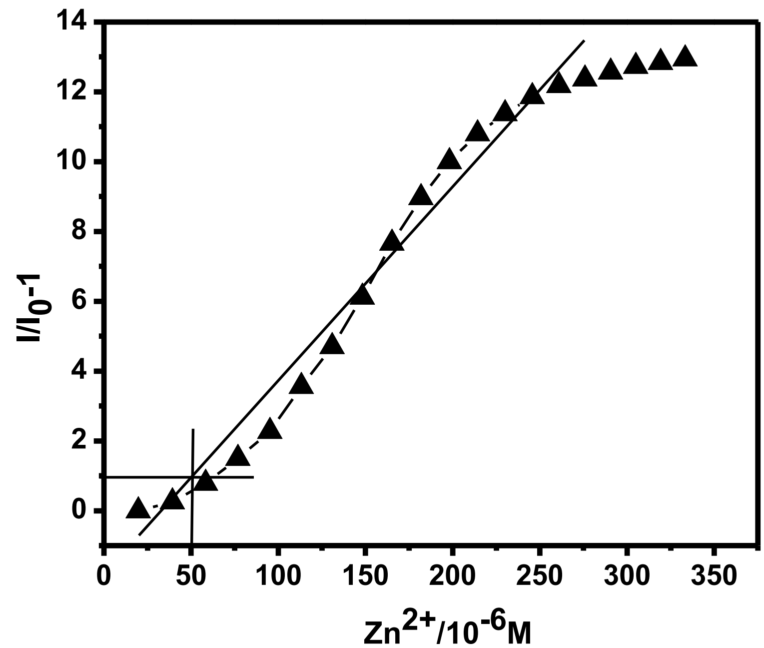


Figure S29. Plot of *I/I_0-1*vs [Zn^{2+}] in FSP3-Zn^{2+} complex for lower detection limit measurement.

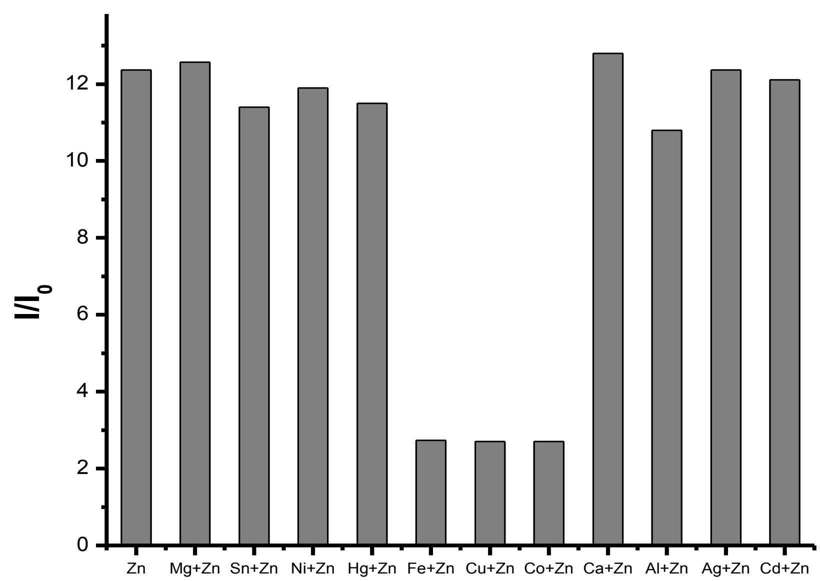


Figure S30. Fluorescence response of FSP3 (15 μM in THF) towards Zn^{2+} in presence of excess other cations (10 equiv. compare to [Zn^{2+}]).

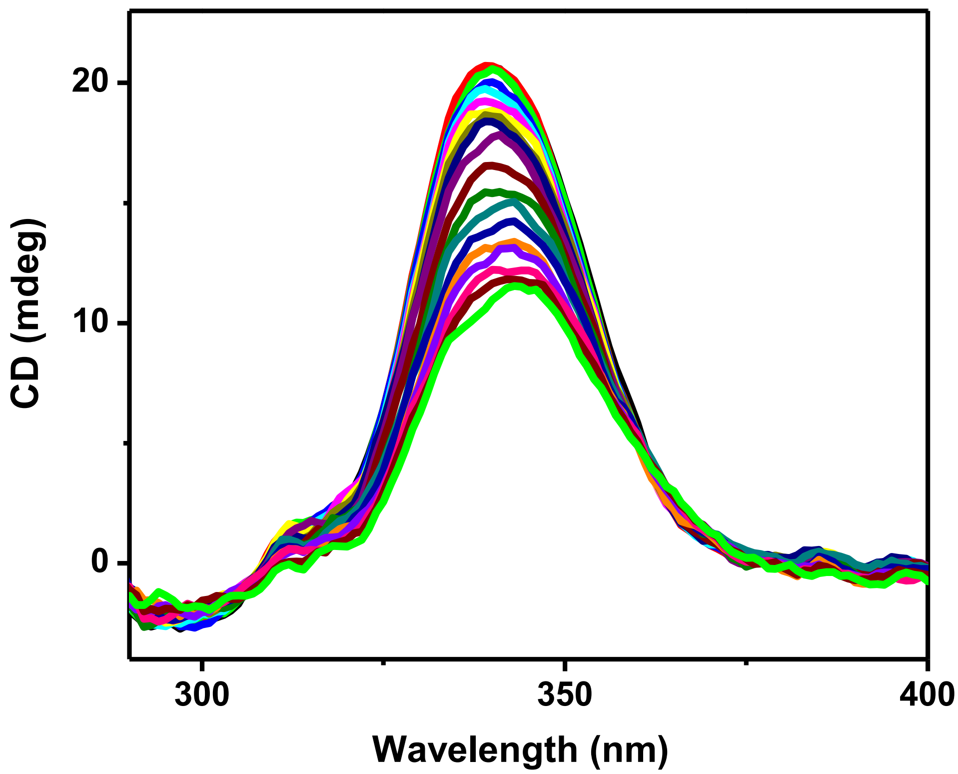
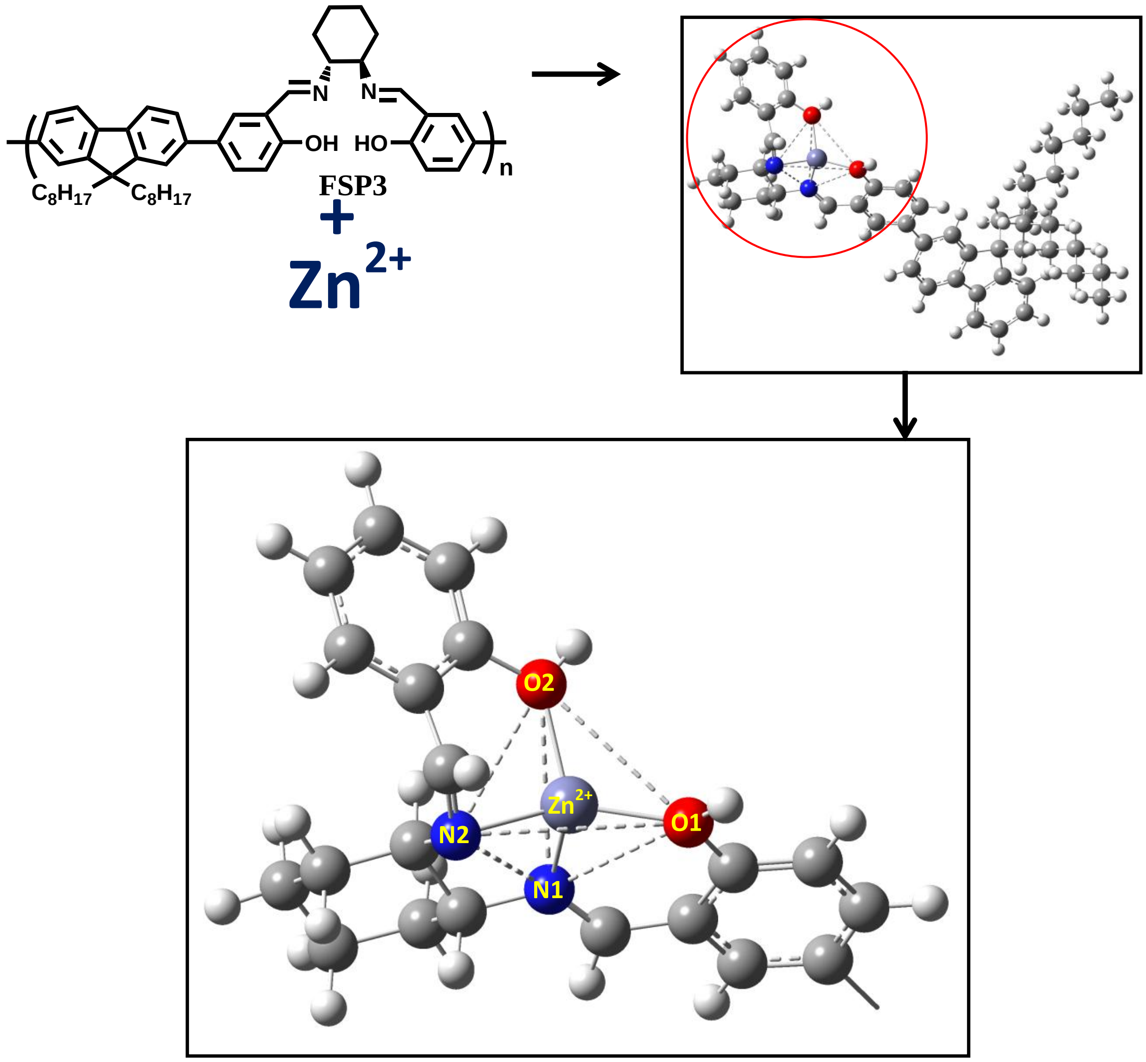


Figure S31. CD spectra of **FSP3** (15 μM) and **FSP3** with addition of 0-22 equiv. Zn^{2+} in THF.



Bond distances (Å)	
Zn-N1:	1.922
Zn-N2:	2.084
Zn-O1:	1.976
Zn-O2:	2.048

Bond angles (°)			
O1-Zn-O2:	117.70;	O1-Zn-N1:	96.08;
N1-Zn-N2:	86.33;	O2-Zn-N2:	94.94;
N1-Zn-O2:	124.32;	O1-Zn-N2:	145.01;

Figure S32. Theoretical bond distances and bond angles calculation of monomeric unit of FSP3-Zn^{2+} complex.

Low-lying transition calculation for FSP3

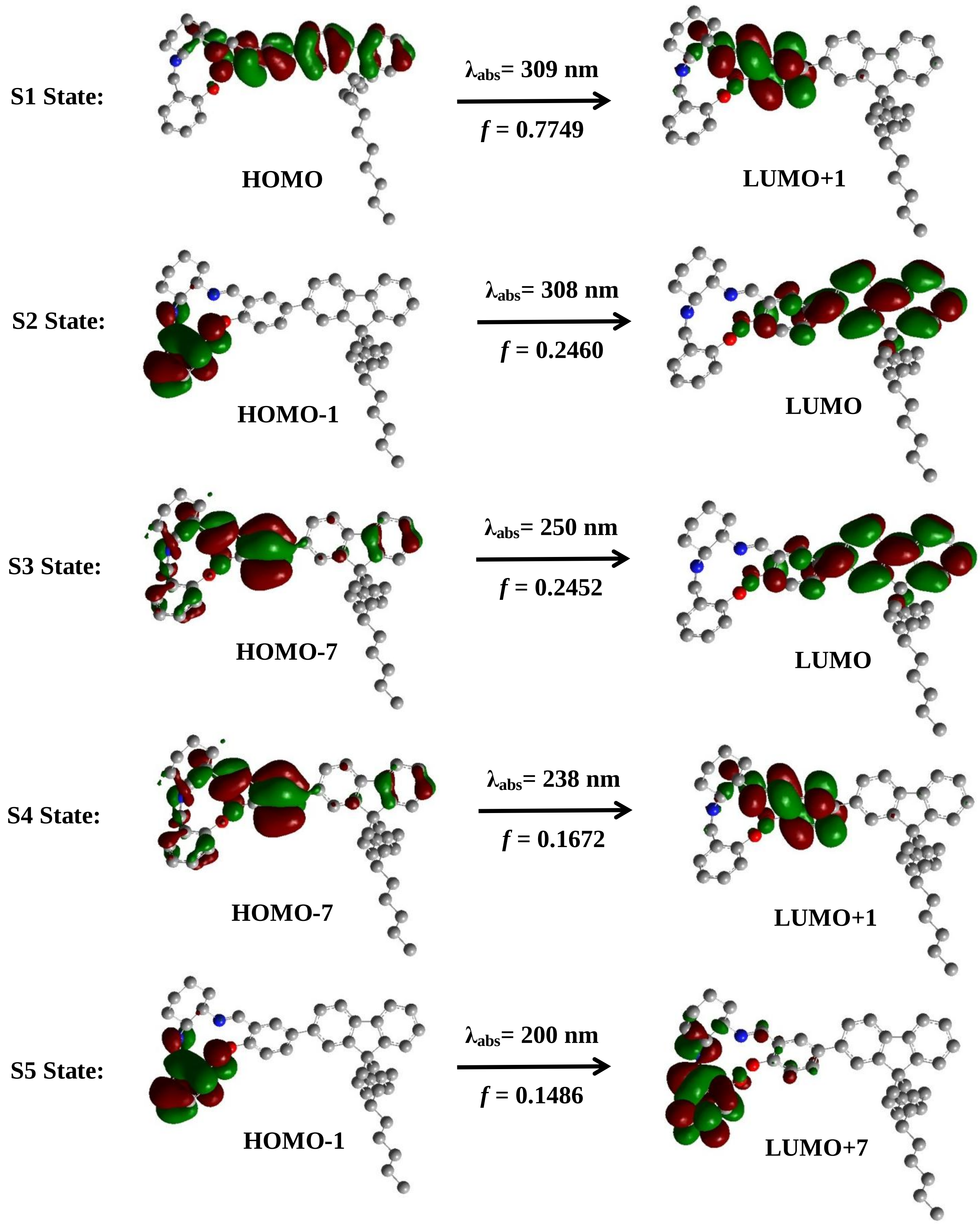


Figure S33. HOMO and LUMO of repeating unit of FSP2.

Low-lying transition calculation for repeating unit of FSP3-Zn^{2+}

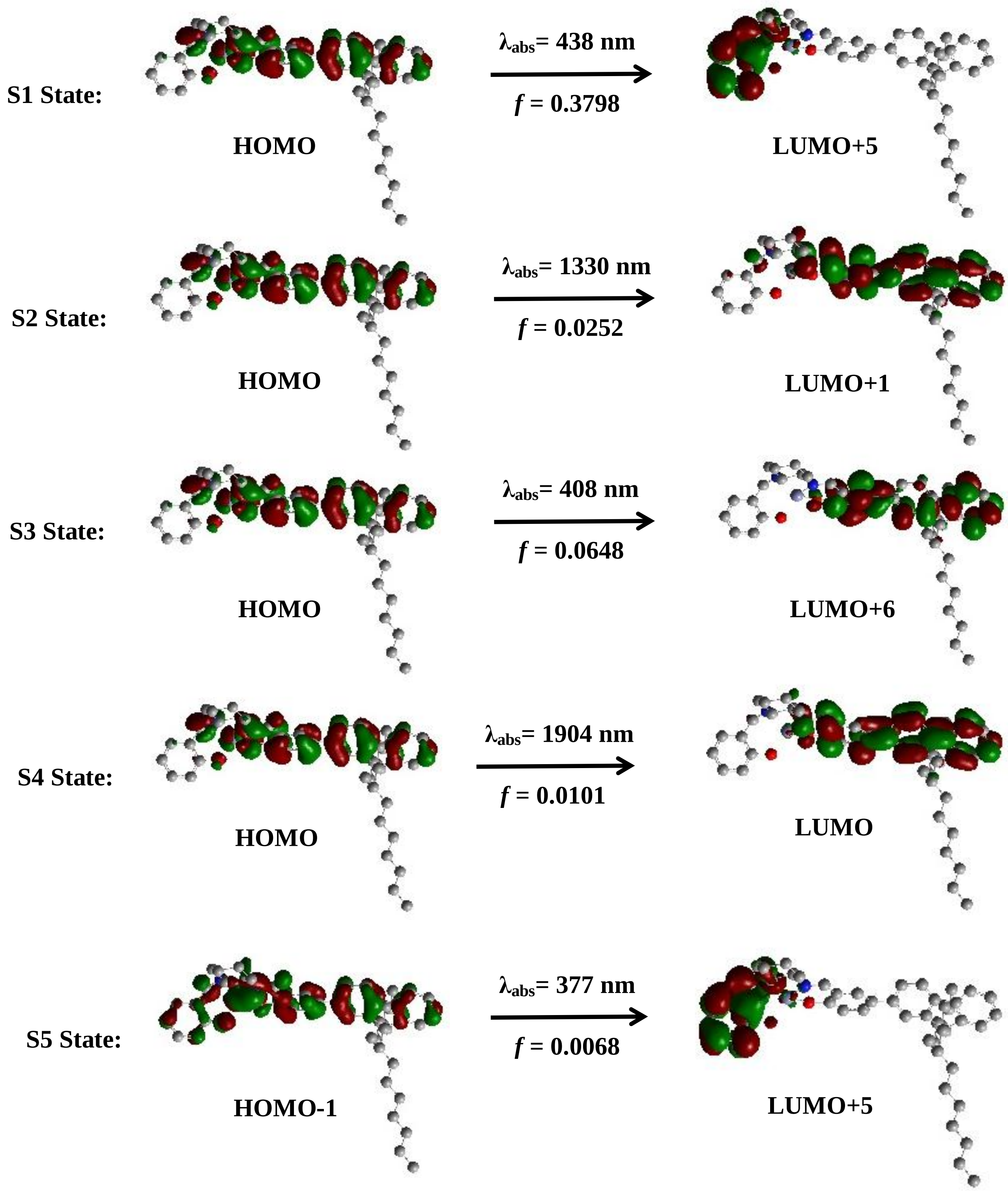


Figure S34. HOMO and LUMO of repeating unit of FSP3-Zn^{2+} complex.

NMR Titration: First polymers were solubilized in $CDCl_3$ (10 mM with respect to monomeric unit) and Zn salt was in DMSO-d^6. Then titrations were performed by addition of Zn^{2+} in to polymer solutions.

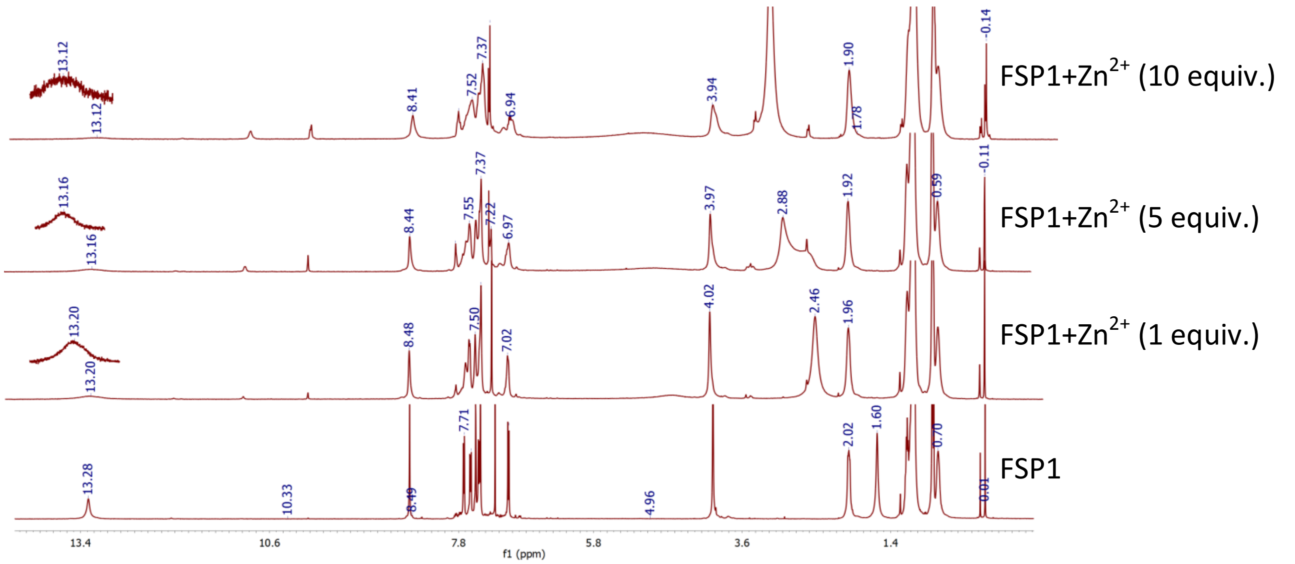


Figure S35. ^{1}H-NMR Titration of FSP1 with Zn^{2+}.

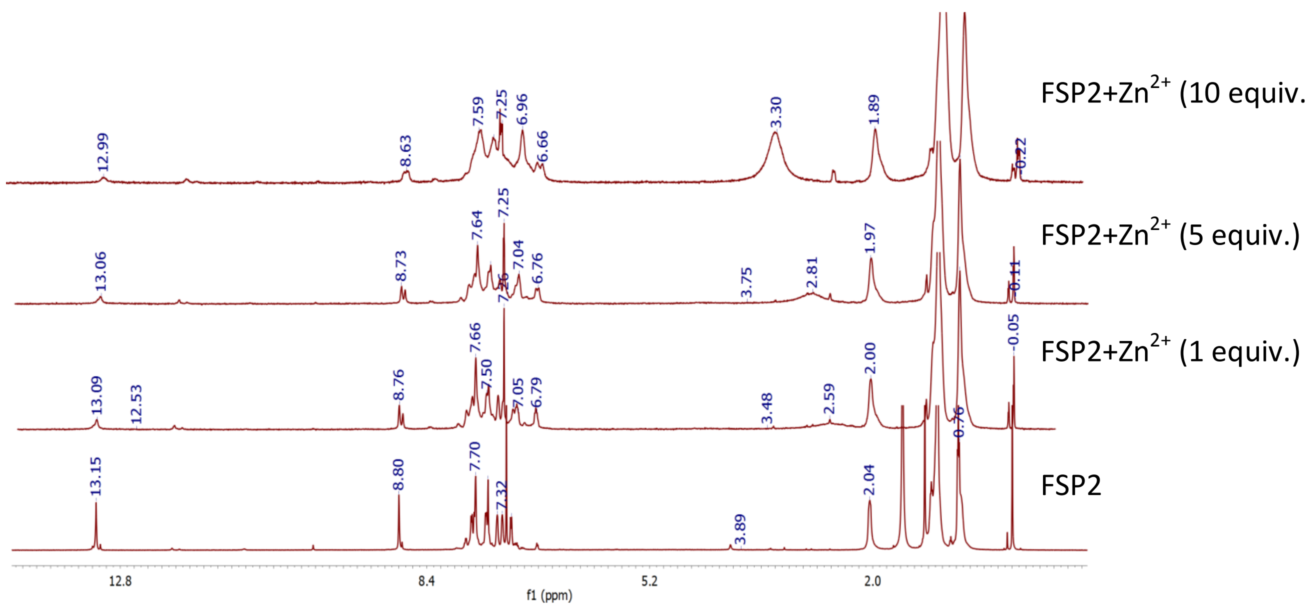


Figure S36. ^{1}H-NMR Titration of FSP2 with Zn^{2+}.

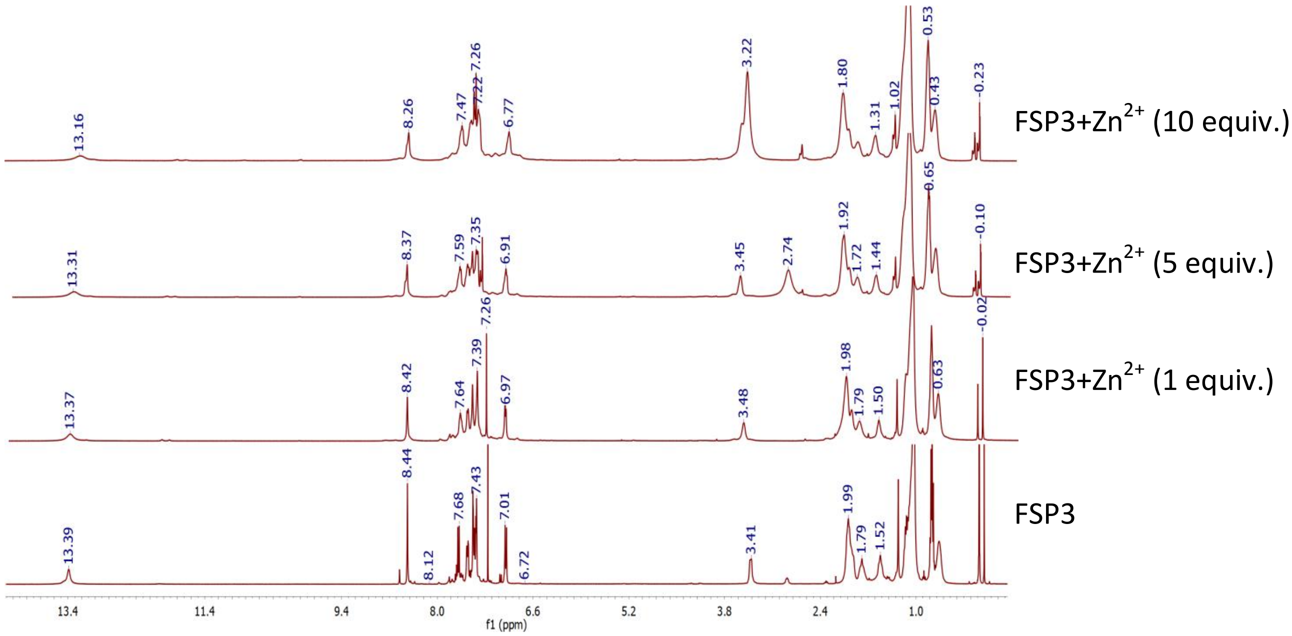


Figure S37. ^{1}H-NMR Titration of FSP3 with Zn^{2+}.

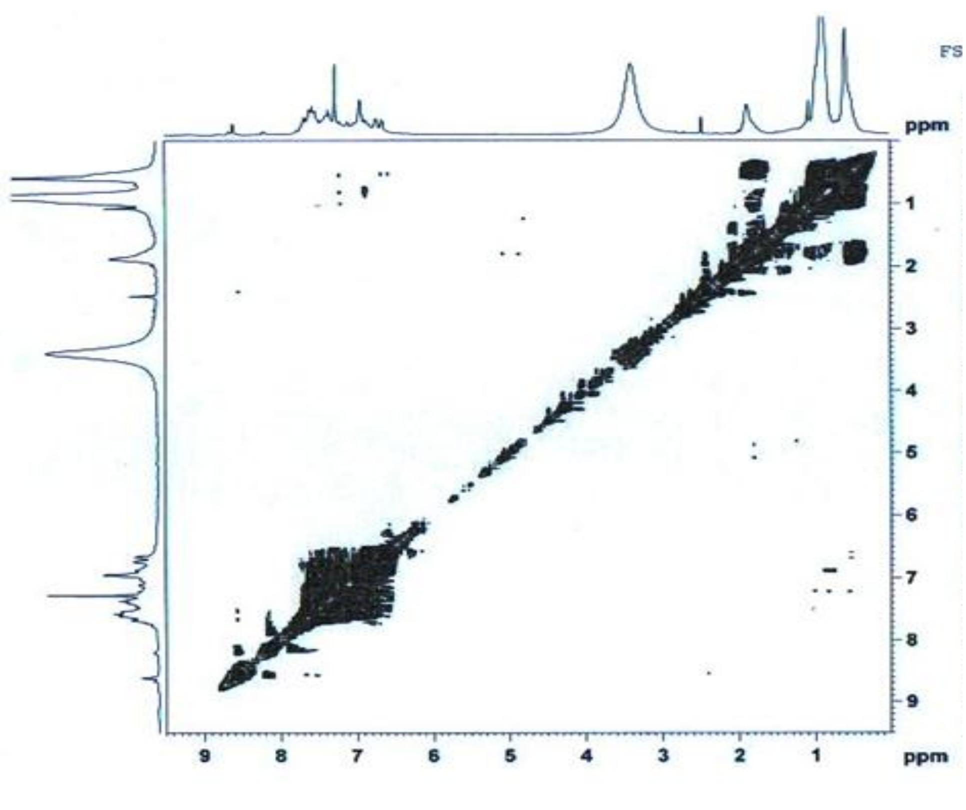


Figure S38. COSY NMR of FSP2 with Zn^{2+}.

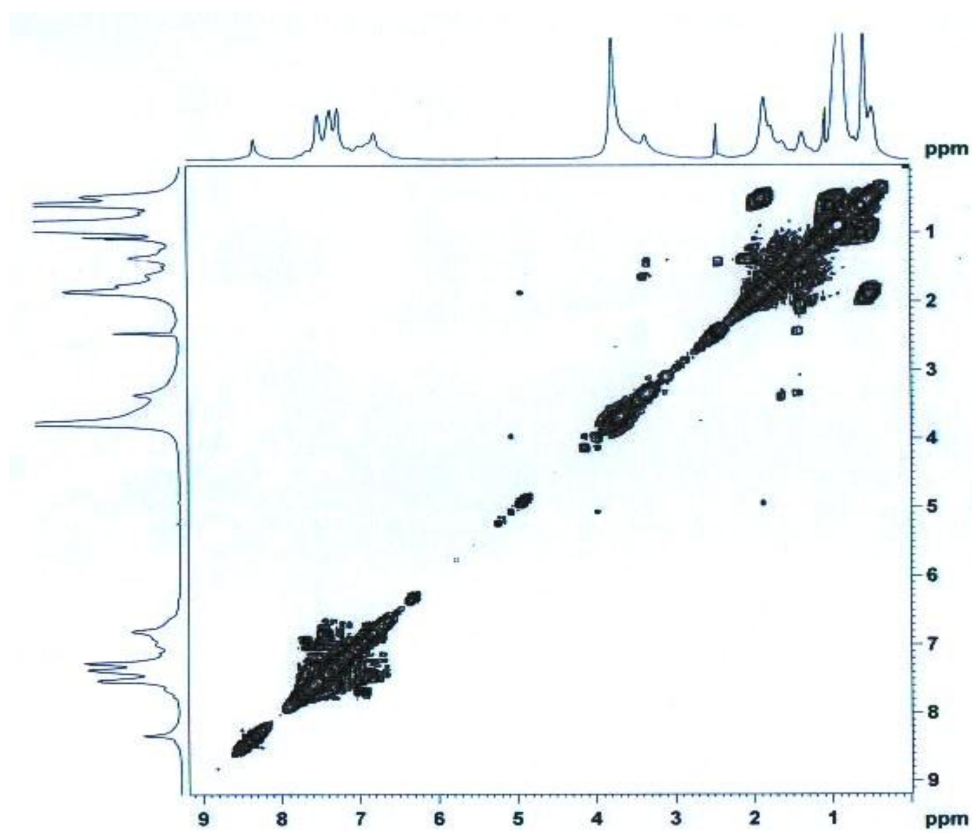


Figure S39. COSY NMR of FSP3 with Zn^{2+}.

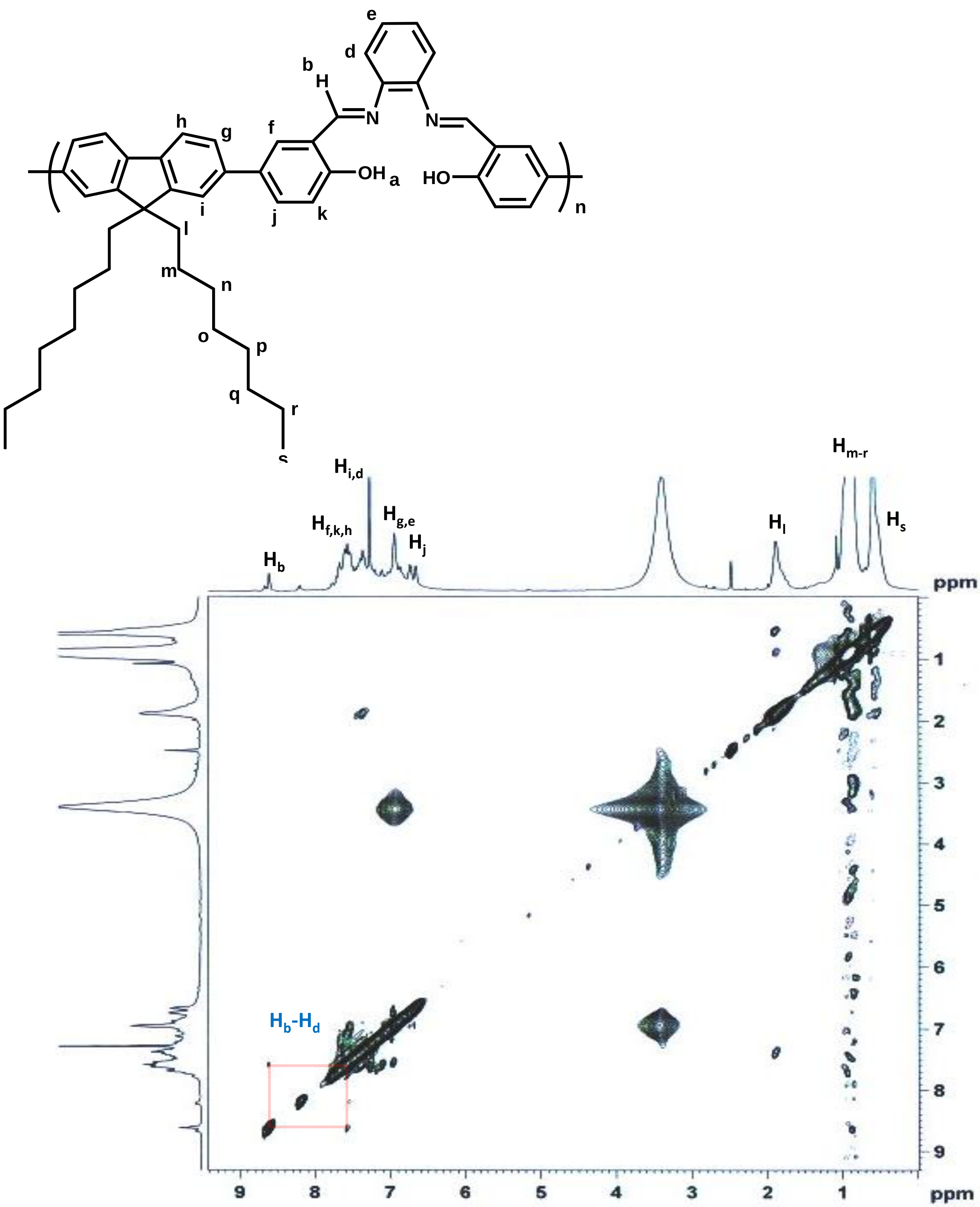


Figure S40. NOESY NMR of FSP2 with Zn^{2+}.

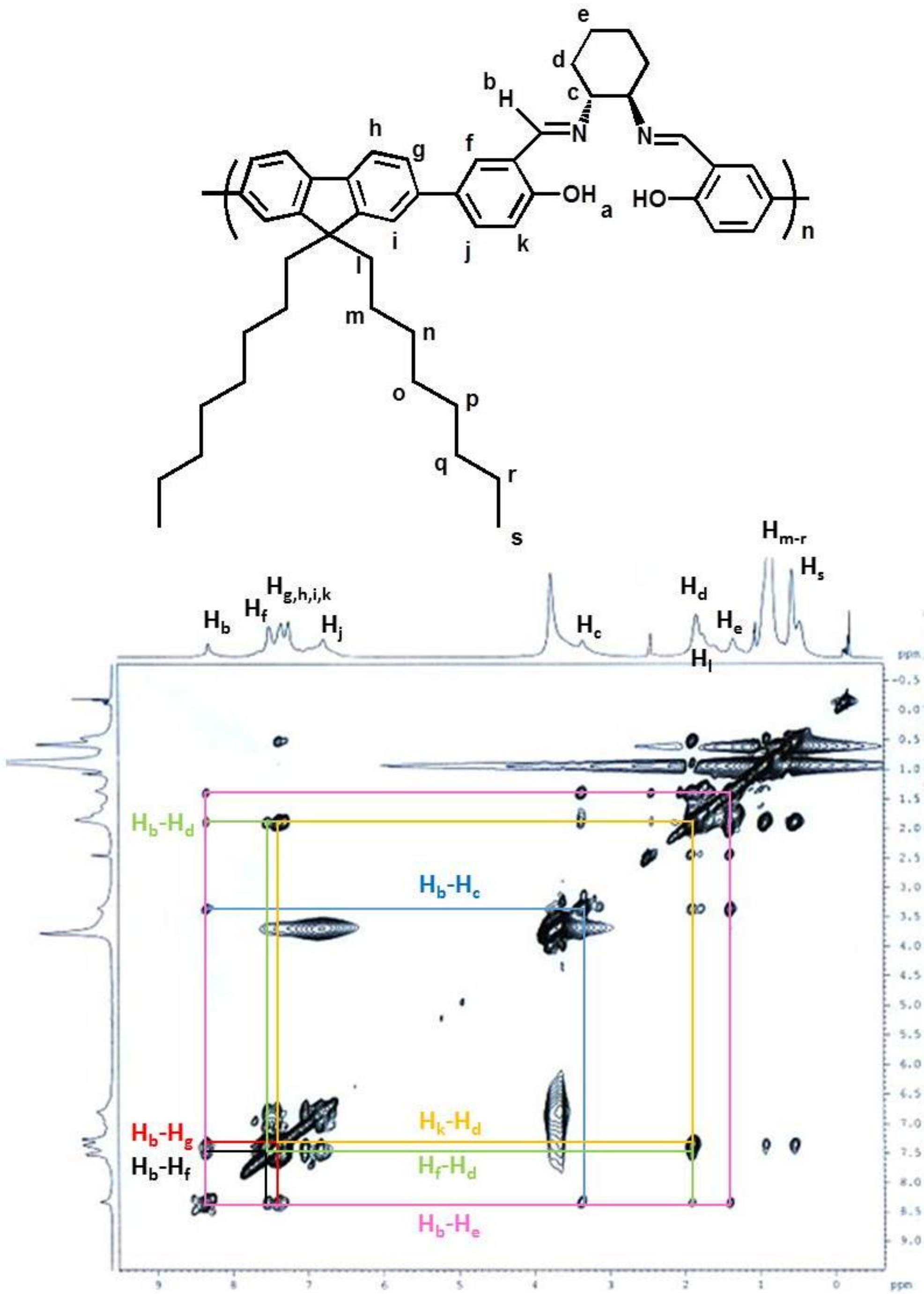


Figure S41. NOESY NMR of FSP3 with Zn^{2+}.