

Supporting Information

Pentaquinone based probe for relay recognition of F⁻ and Cu²⁺ ions: Sequential logic operations at molecular level

Vandana Bhalla,* Roopa and Manoj Kumar*

Department of Chemistry, UGC Sponsored-Centre for Advanced Studies-I, Guru Nanak Dev
University, Amritsar-143005, Punjab, INDIA

Page no. Contents

- S3** ¹H NMR spectrum of receptor **2a**. (**Figure S1**)
- S4** IR spectrum of receptor **2a**. (**Figure S2**)
- S5** Mass spectrum of receptor **2a**. (**Figure S3**)
- S6** UV-vis spectra of **2a** in the presence of Bu₄NOH in DMSO. (**Figure S4**)
- S7** UV-vis spectra of **2a** in the presence of different anions in DMSO. (**Figure S5**)
- S8** Fluorescence response of **2b** (5 μM) in the presence of OH⁻ ions. (**Figure S6**)
- S9** Partial ¹H NMR spectra of **2a** in DMSO (A) **2a** (B) **2a** + 1.0 equiv F⁻. (**Figure S7**)
- S10** Fluorescence response of **2b** (5 μM) in the presence of F⁻ ions. (**Figure S8**)
- S10** UV-vis spectra of **2a** in the presence of F⁻ ions in DMSO/H₂O. (**Figure S9**)
- S10** UV-vis spectra of **3** in the presence of Cu²⁺ ions in DMSO/H₂O. (**Figure S10**)
- S11** Fluorescence response of **2a** towards F⁻ ions in DMSO/H₂O. (**Figure S11**)
- S11** Fluorescence response of **3** towards Cu²⁺ ions in DMSO/H₂O. (**Figure S12**)
- S11** Fluorescence response of **2a** (5 μM) in the presence of various anions. (**Figure S13**)
- S12** UV-vis response of **2a** towards in the presence of various metal ions. (**Figure S14**)
- S12** Fluorescence response of **2a** (5 μM) in the presence of various metal ions. (**Figure S15**)
- S12** Mass spectrum of **2a**-Cu²⁺ complex. (**Figure S16**)
- S13** Job's Plot of **3** with Cu²⁺ ions in DMSO. (**Figure S17**)

S14 Fluorescence response of **3** towards various metal ions (10 equiv each) in DMSO. (**Figure S18**)

S15 Fluorescence response of receptor **2a** on addition of OH⁻ ions in DMSO (**Figure S19**)

S16 Fluorescence response of receptor **3** on addition of Cu²⁺ ions in DMSO (**Figure S20**)

S17 Fluorescence response of receptor **3** + Cu²⁺ on addition of OH⁻ ions in DMSO (**Figure S21**)

S18 UV-vis spectra showing reusability of the receptor **2a** for the sensing of F⁻ and Cu²⁺ ions sequentially in DMSO (**Figure S22-S25**)

S19 UV-vis response of **3** on addition of Cu²⁺ ions in DMSO (**Figure S26**)

S20 Fluorescence response of **2a** on addition of ClO₄⁻ ions in DMSO (**Figure S27**)

Figure S1. ^1H NMR (DMSO, 300 MHz, ppm) spectrum of **2a**.

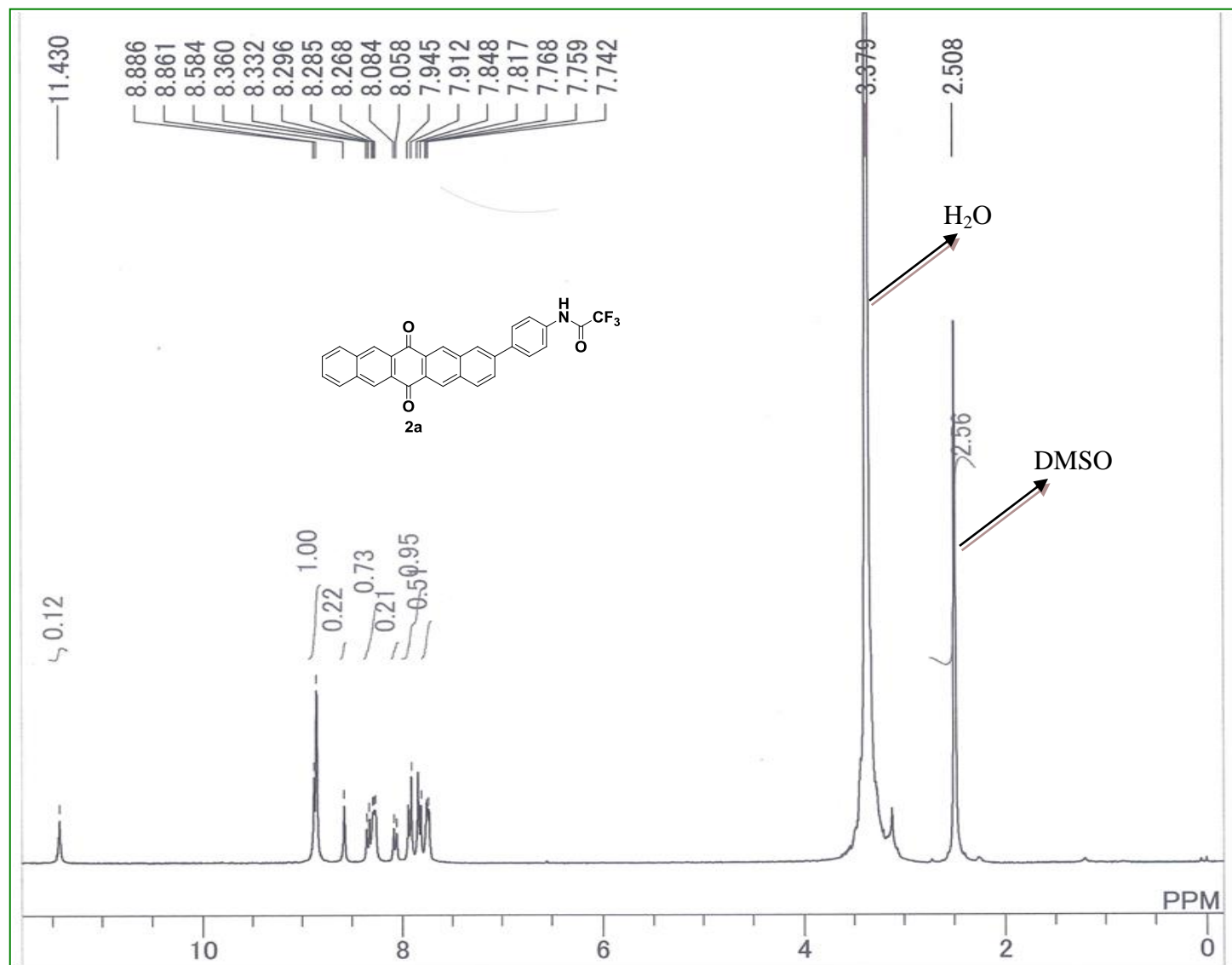


Figure S2. IR spectrum of **2a**.

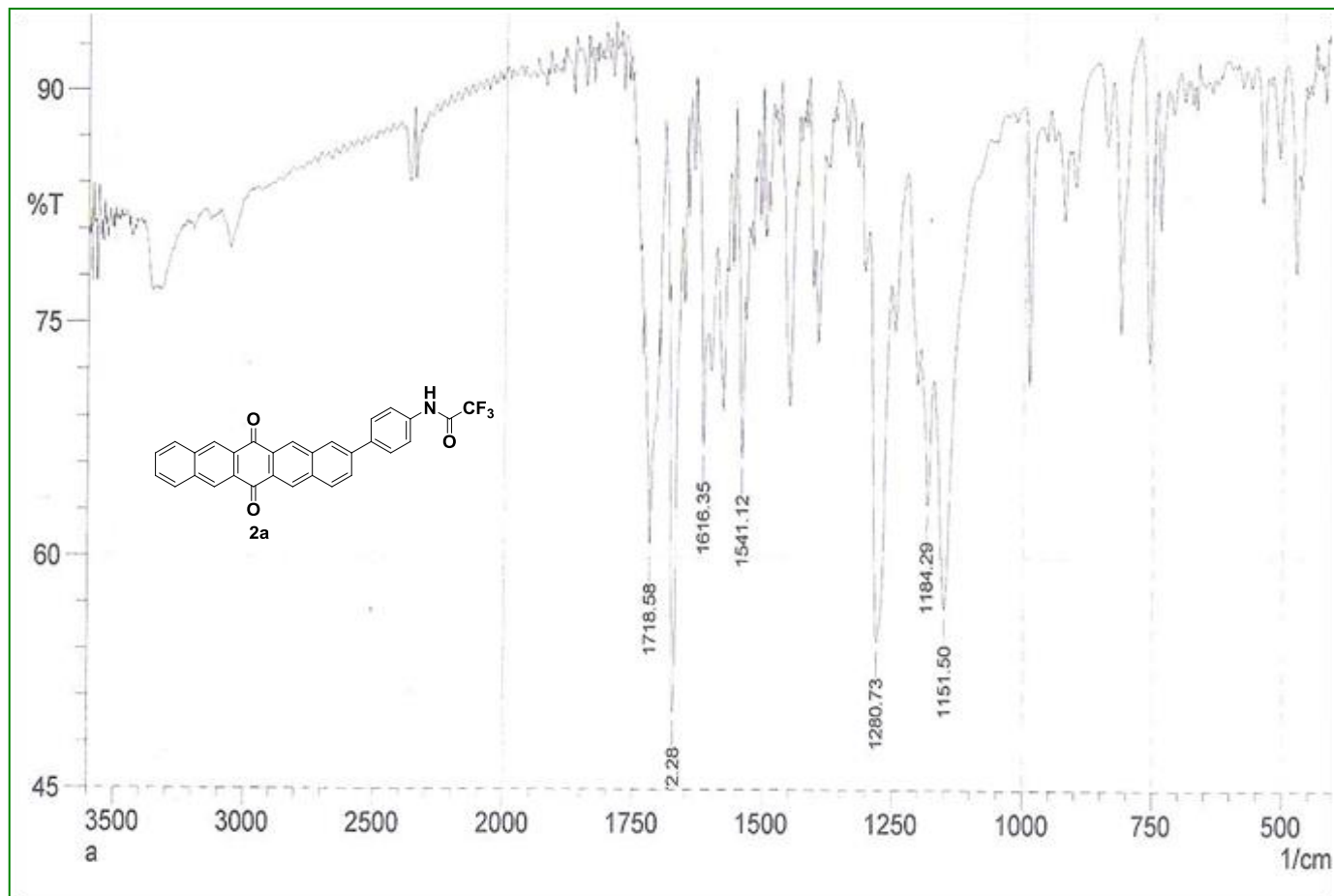
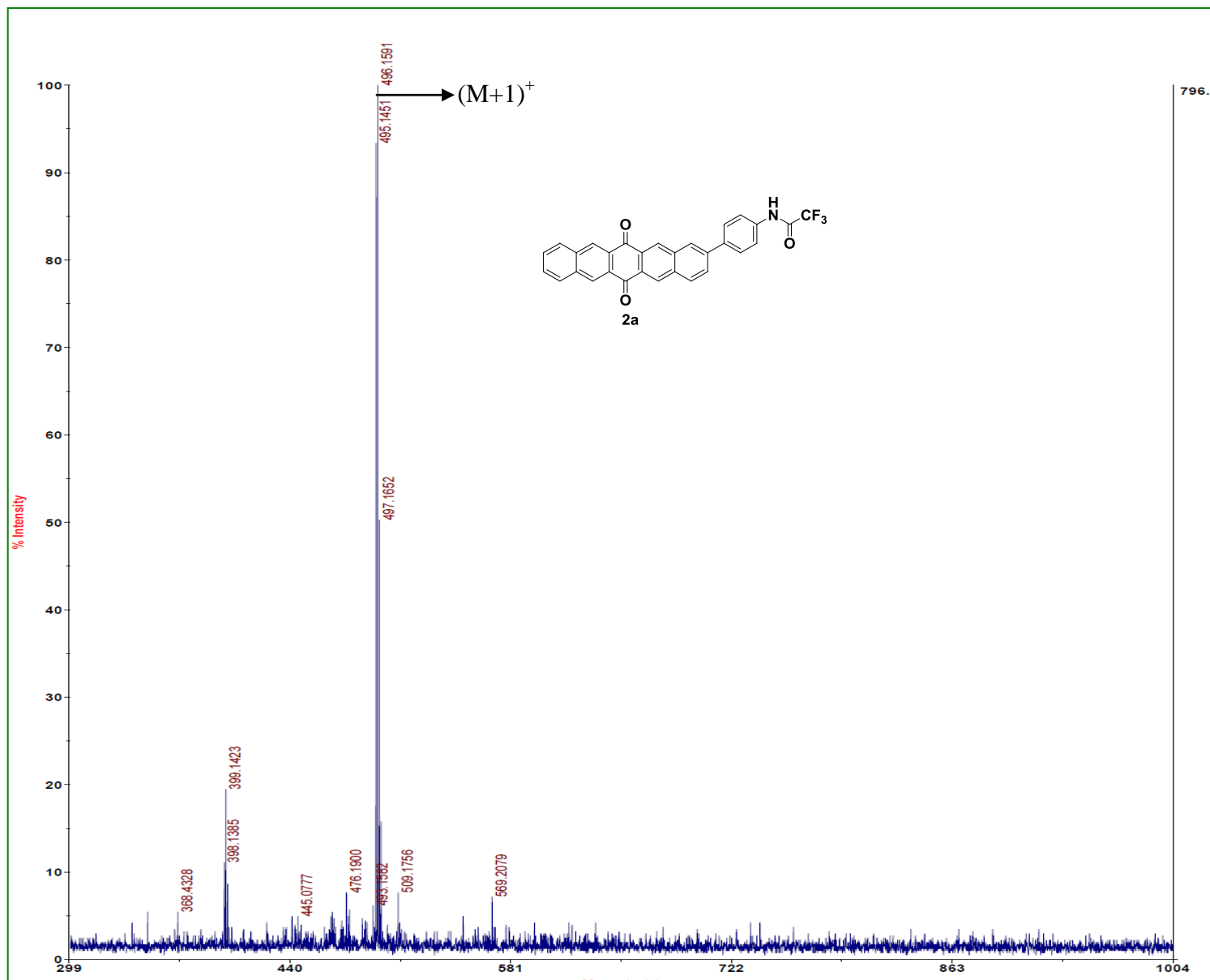


Figure S3. MALDI-TOF mass spectrum of **2a**.



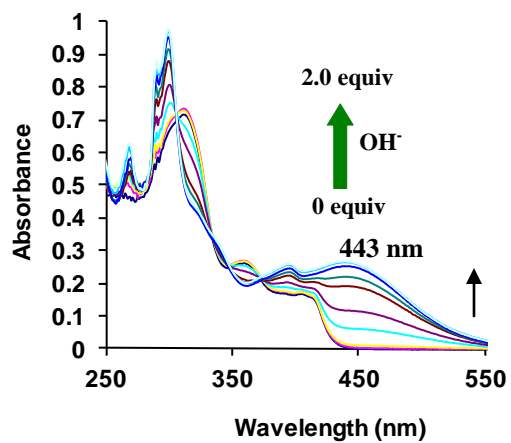


Figure S4. UV-vis response of receptor **2a** (5 μM) on addition of OH⁻ ions (0-2.0 equiv) in DMSO.

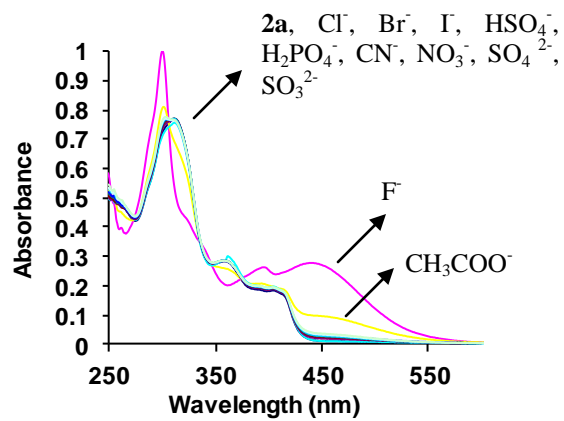


Figure S5. UV-vis spectra of **2a** (5 μM) in response to the presence of different anions (3.0 equiv each) in DMSO.

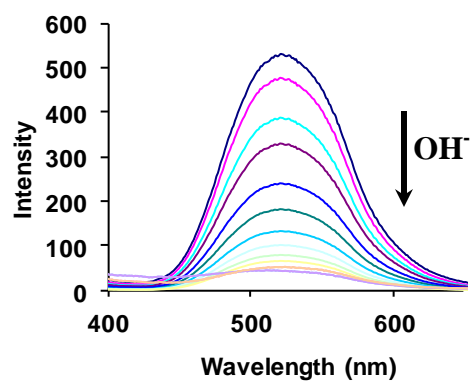
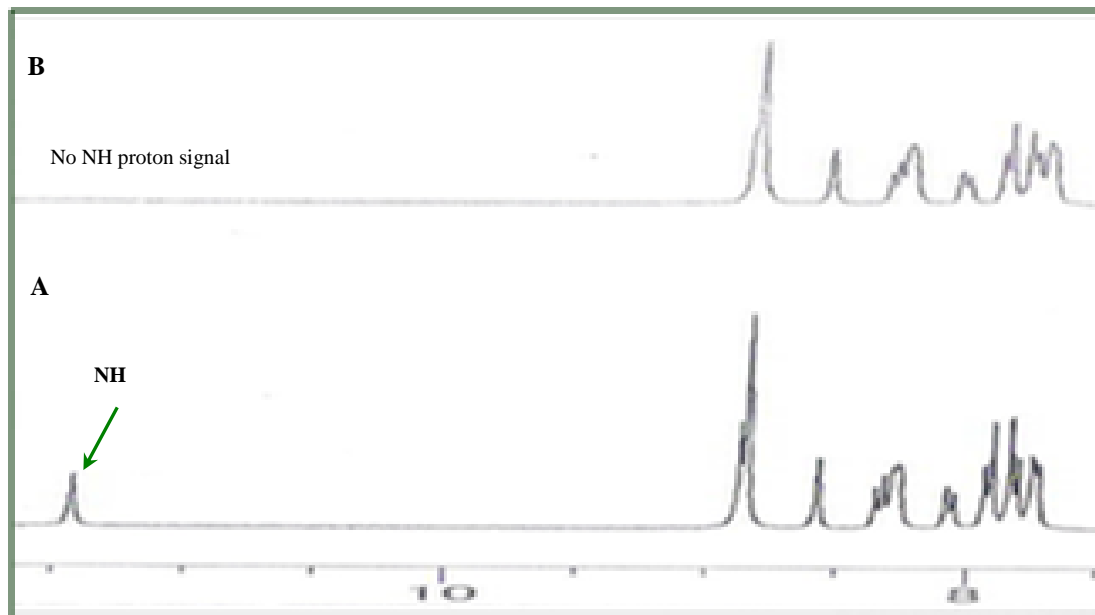


Figure S6. Fluorescence response of **2a** (5 μM) in the presence of OH⁻ ions (0-7.5 equiv) in DMSO.

Figure S7. Partial ^1H NMR spectra of **2a** in DMSO (A) **2a** (B) **2a** + 1.0 equiv F^-



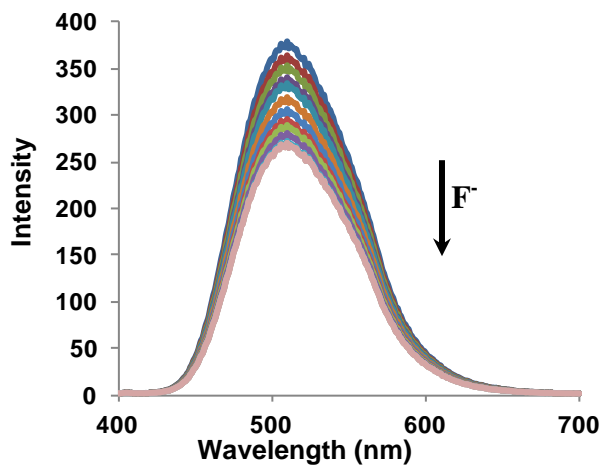


Figure S8. Fluorescence response of **2b** (5 μM) in the presence of F⁻ ions (0-100 equiv) in DMSO.

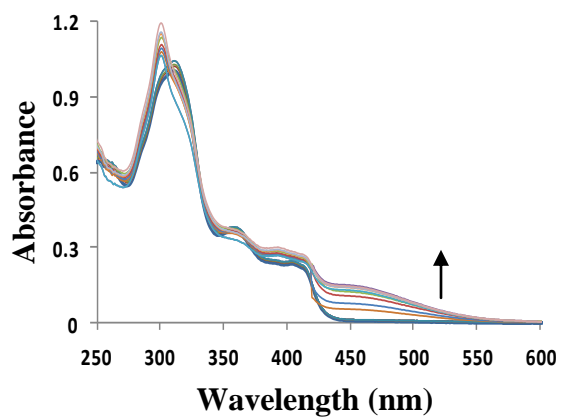


Figure S9. UV-vis response of receptor **2a** (10 μ M) on addition of F^- ions (0-350 equiv) in DMSO/ H_2O (9.5:0.5, v:v).

S

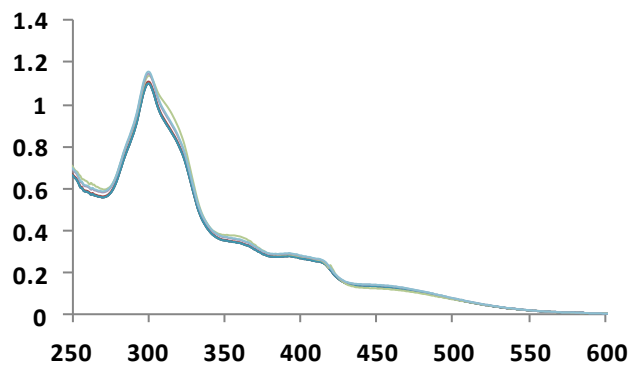


Figure S10. UV-vis response of **3** on addition of Cu^{2+} ions (0-350 equiv) in DMSO/ H_2O (9.5:0.5, v:v).

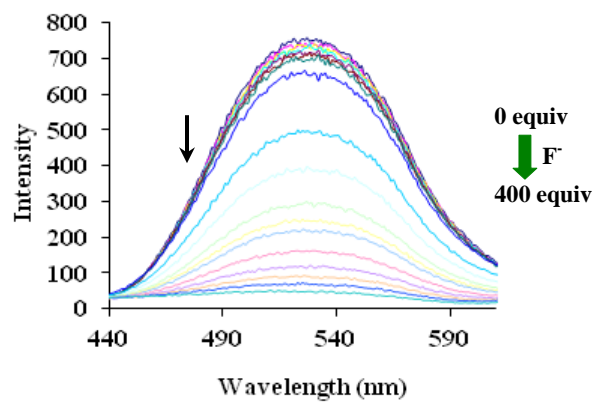


Figure S11. Fluorescence response of receptor **2a** (10 μM) on addition of F^- ions (0-400 equiv) in DMSO/ H_2O (9.5:0.5, v:v); $\lambda_{\text{ex}} = 310 \text{ nm}$.

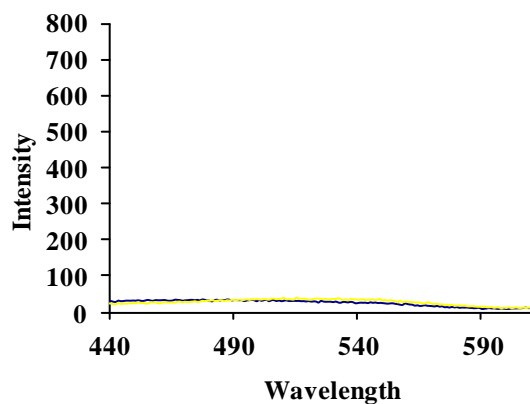


Figure S12. Fluorescence response of **3** on addition of Cu^{2+} ions (0-500 equiv) in DMSO/ H_2O (9.5:0.5, v:v); $\lambda_{\text{ex}} = 310 \text{ nm}$.

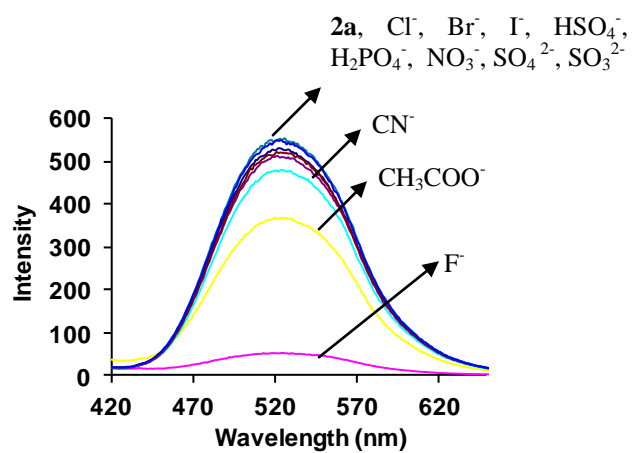


Figure S13. Fluorescence spectra of **2a** (5 μM) in response to the presence of different anions (12 equiv each) in DMSO.

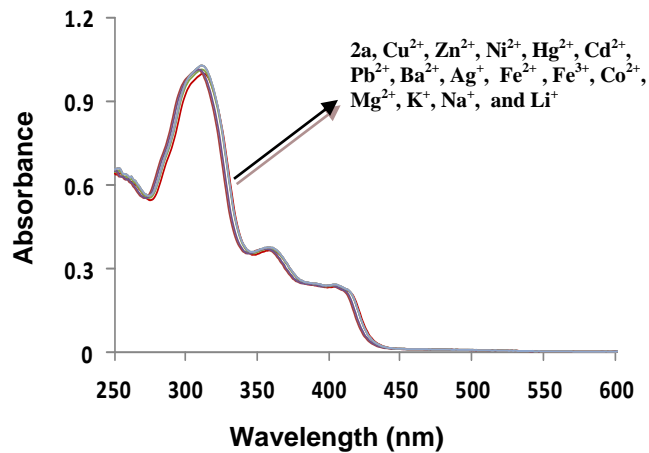


Figure S14. UV-vis response of **2a** (5 μM) in the presence of various metal ions (0-50 equiv) in DMSO.

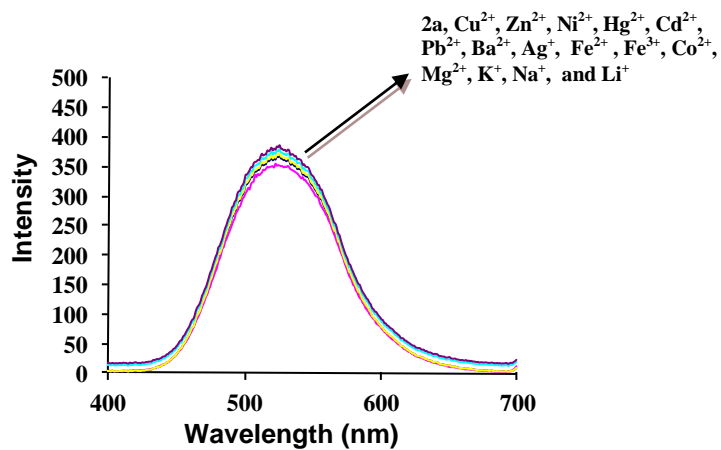
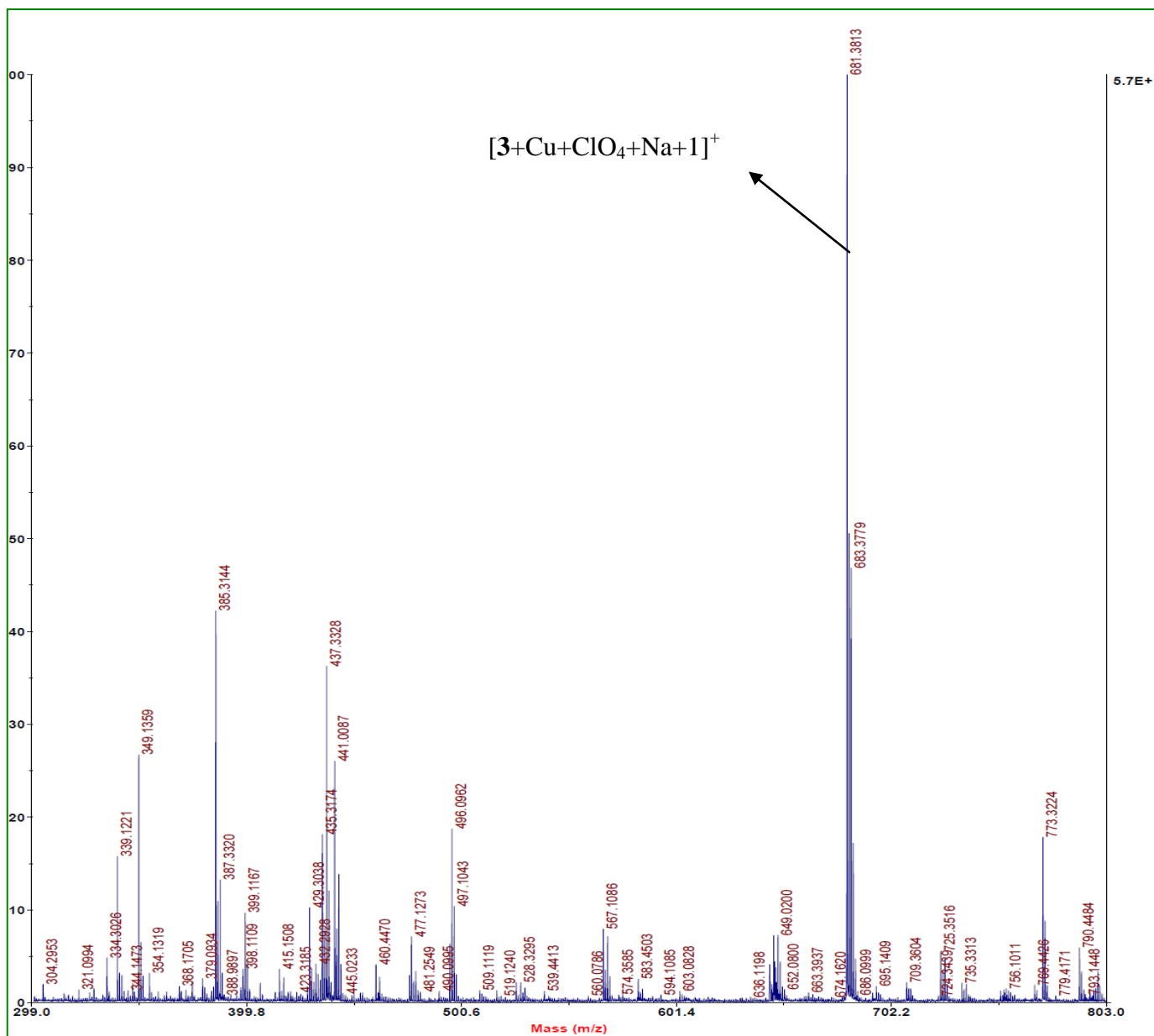


Figure S15. Fluorescence response of **2a** (5 μM) in the presence of various metal ions (0-50 equiv) in DMSO.

Figure S16. Mass spectrum of **2a**-Cu²⁺ complex.



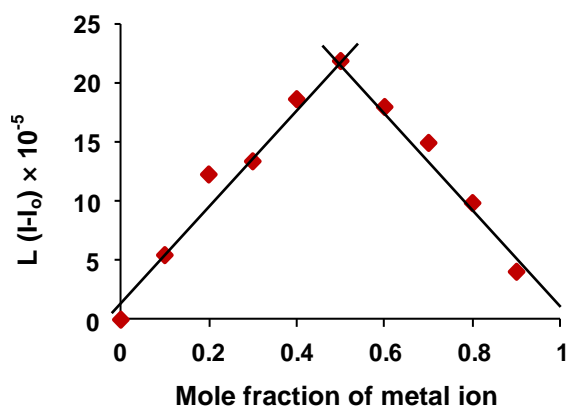


Figure S17. Job's plot of **3** with Cu^{2+} ions in DMSO representing stoichiometry 1:1.

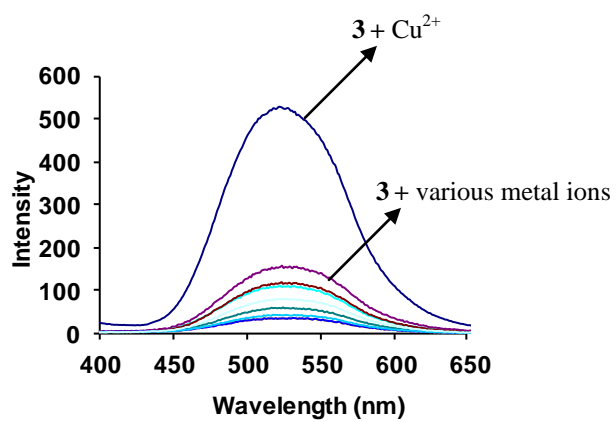


Figure S18. Fluorescence response of **3** towards various metal ions (10 equiv each) in DMSO.

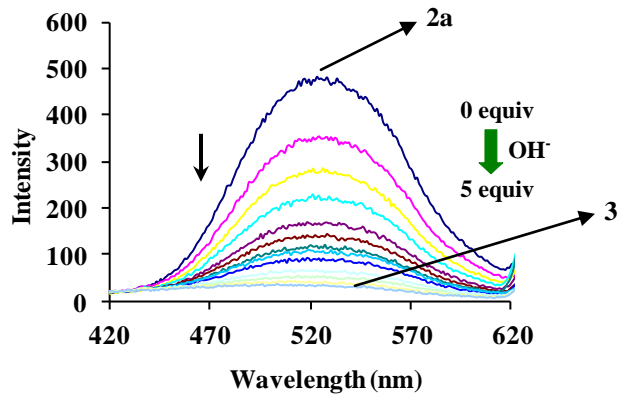


Figure S19. Fluorescence response of receptor **2a** (5 μM) on addition of OH⁻ ions (0-5.0 equiv) in DMSO; $\lambda_{\text{ex}} = 310$ nm.

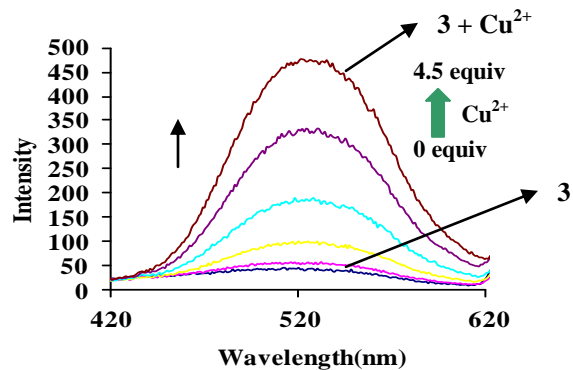


Figure S20. Fluorescence response of receptor **3** on addition of Cu²⁺ ions (0-4.5 equiv) in DMSO; $\lambda_{\text{ex}} = 310$ nm.

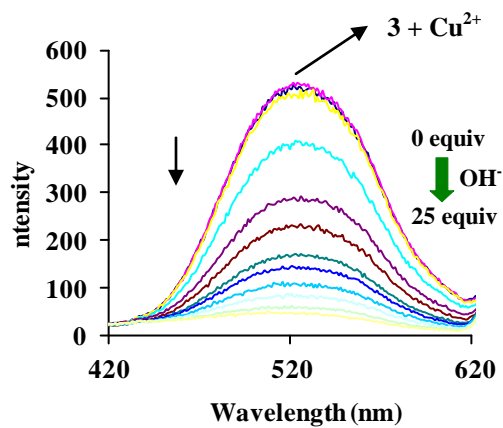


Figure S21. Fluorescence response of receptor **3 + Cu²⁺** on addition of OH⁻ ions (0-25 equiv) in DMSO; $\lambda_{\text{ex}} = 310$ nm.

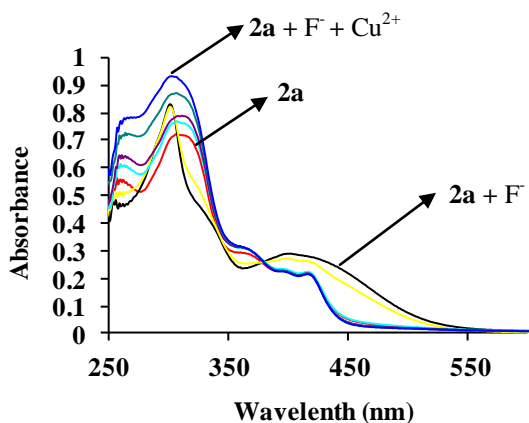


Figure S22. UV-vis response of receptor **2a** (5 μ M) on addition of F⁻ ions (0-3.0eq) and further addition of Cu²⁺ ions (0-8.0 equiv) to the solution of **2a** + F⁻ in DMSO.

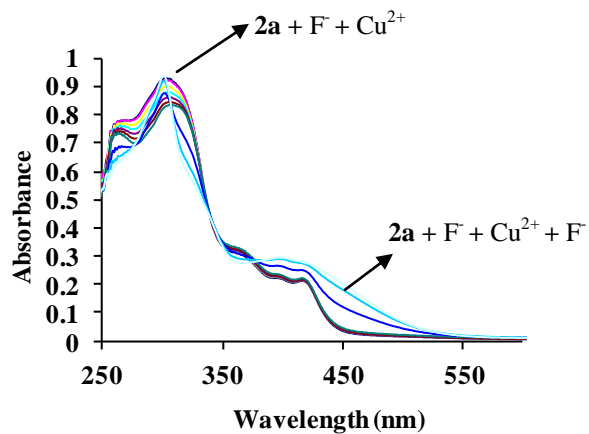


Figure S23. UV-vis response of **2a** + F⁻ + Cu²⁺ towards the addition of F⁻ ions (0-55 equiv) in DMSO.

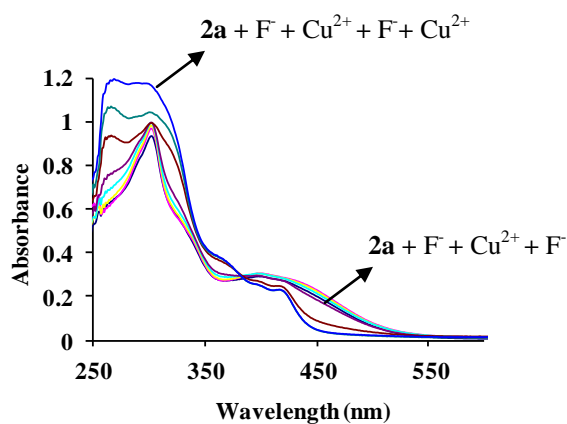


Figure S24. UV-vis response of **2a** + F⁻ + Cu²⁺ + F⁻ towards the addition of Cu²⁺ ions (0-50 equiv) in DMSO.

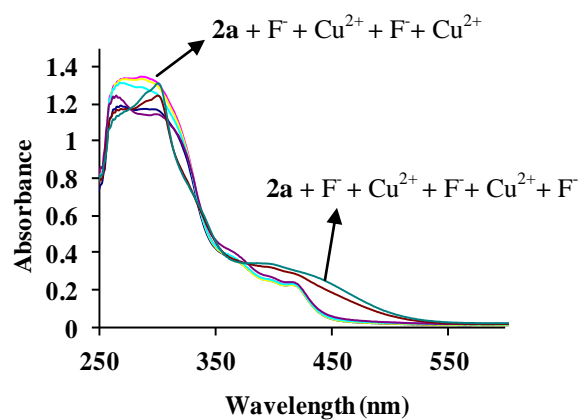


Figure S25. UV-vis response of **2a** + F⁻ + Cu²⁺ + F⁻ + Cu²⁺ towards the addition of F⁻ ions (0-200 equiv) in DMSO.

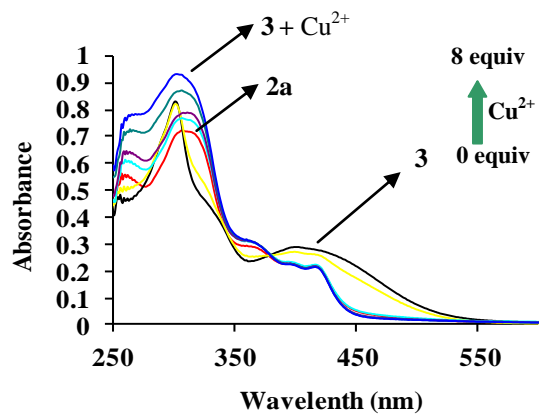


Figure S26. UV-vis response of **3** (15 μM) on addition of Cu²⁺ ions (0-8.0 equiv) in DMSO.

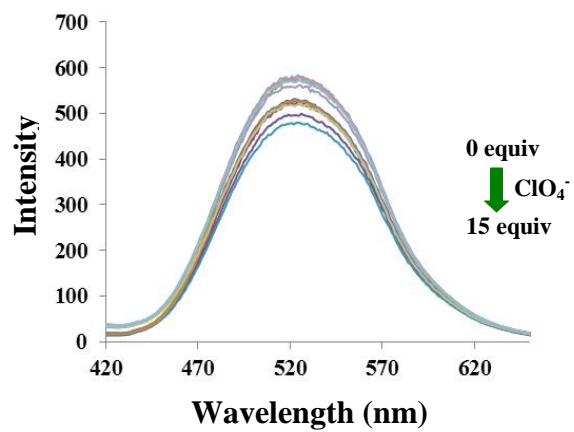


Figure S27. Fluorescence response of receptor **2a** (5 μM) on addition of ClO_4^- ions (15 equiv) in DMSO; $\lambda_{\text{ex}} = 310 \text{ nm}$.