Electronic Supporting Information

Dual Colorimetric Receptor with Logic Gate Operations: Anion Induced Solvatochromism

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^{1}H NMR spectra:

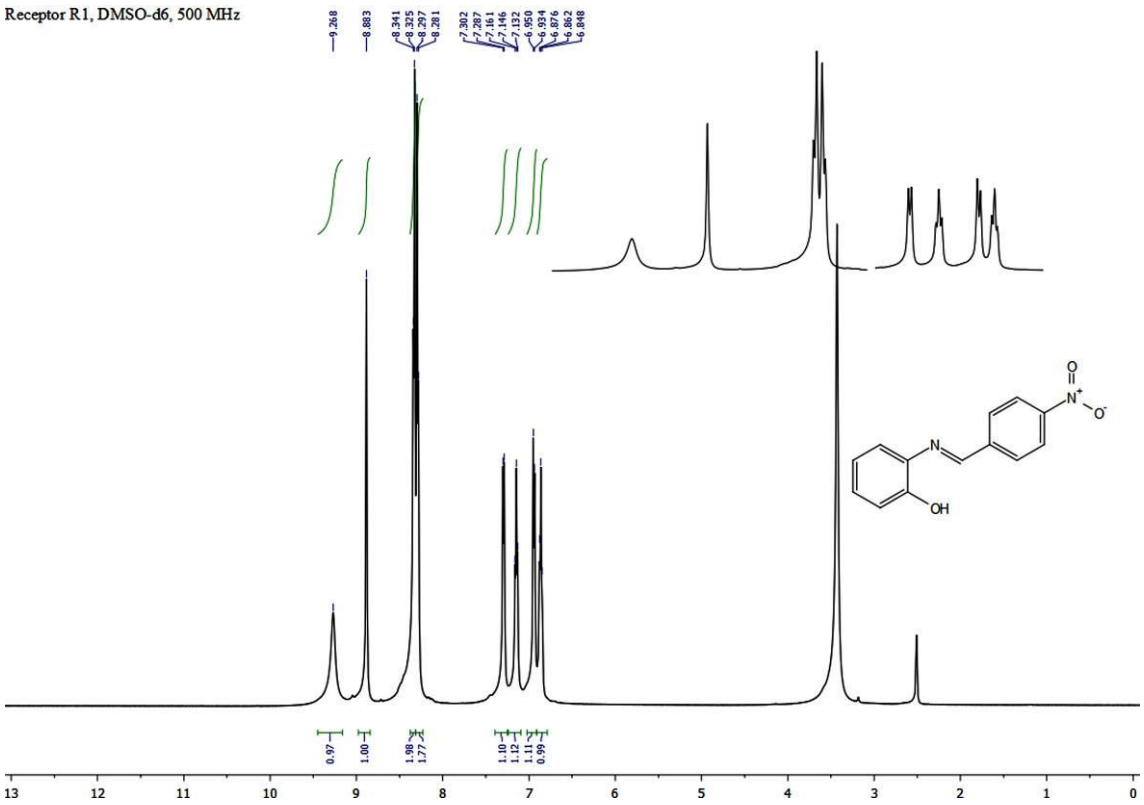

Fig. S1. ^{1}H NMR spectra of R1.

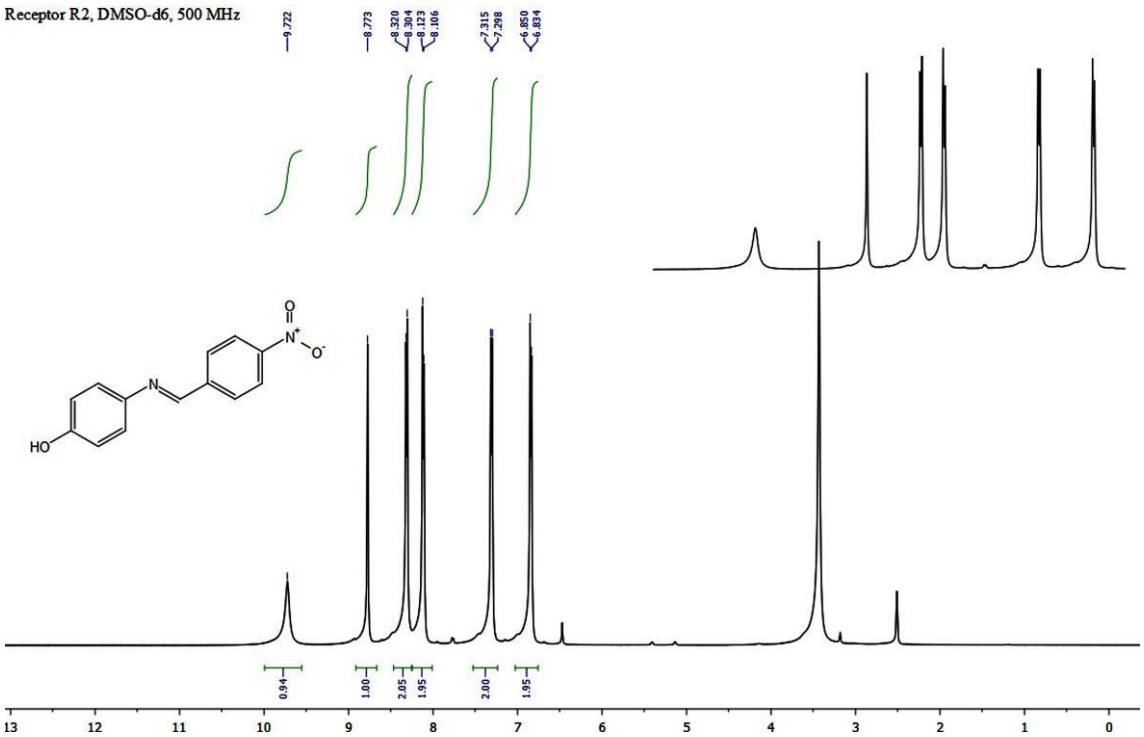

Fig. S2. ^{1}H NMR spectra of R2.

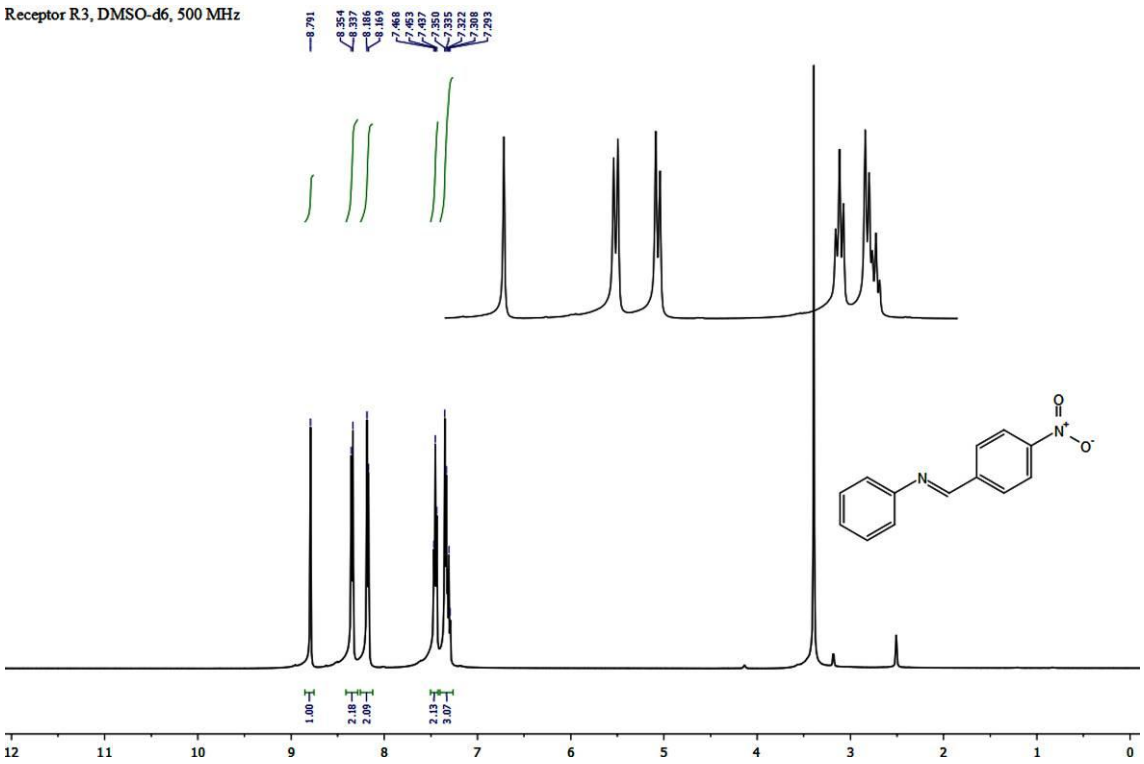

Fig. S3. ^{1}H NMR spectra of R3.

^{13}C NMR Spectra

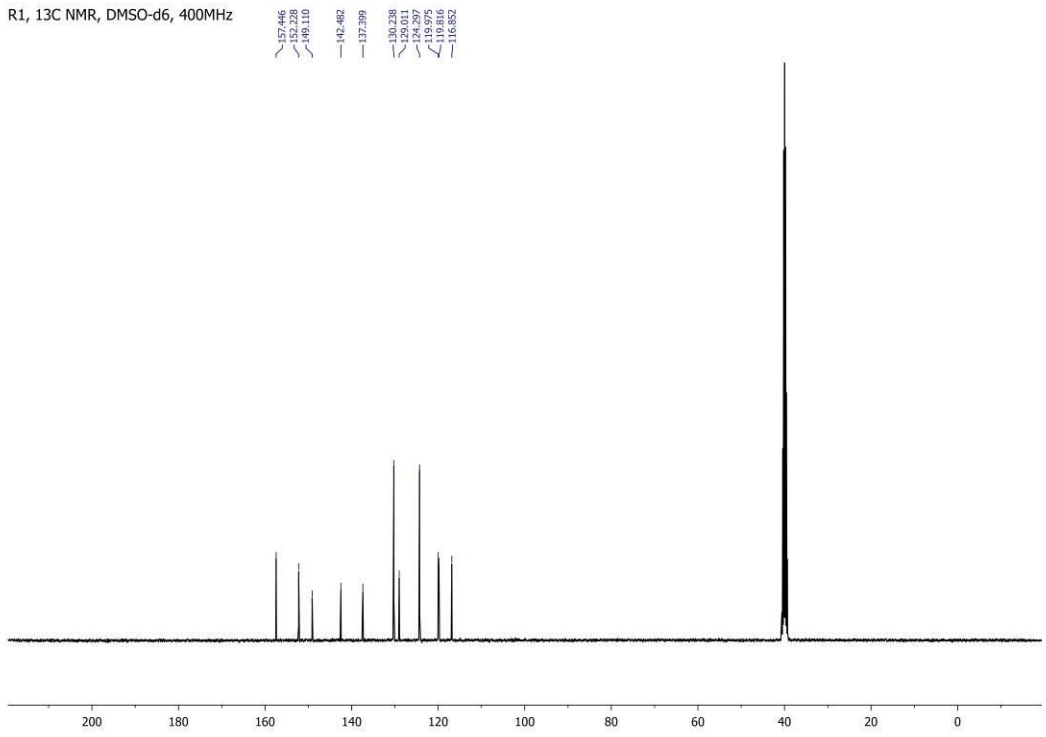

Fig. S4. ^{13}C NMR spectra of R1.

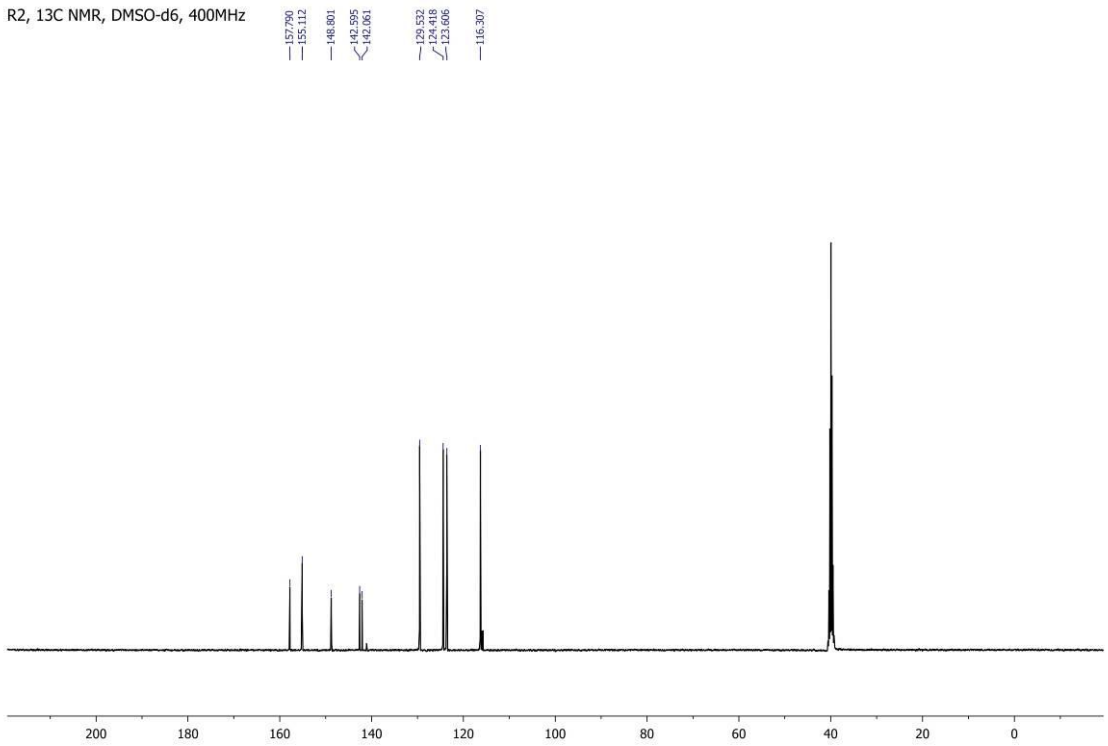

Fig. S5. ^{13}C NMR spectra of R2.

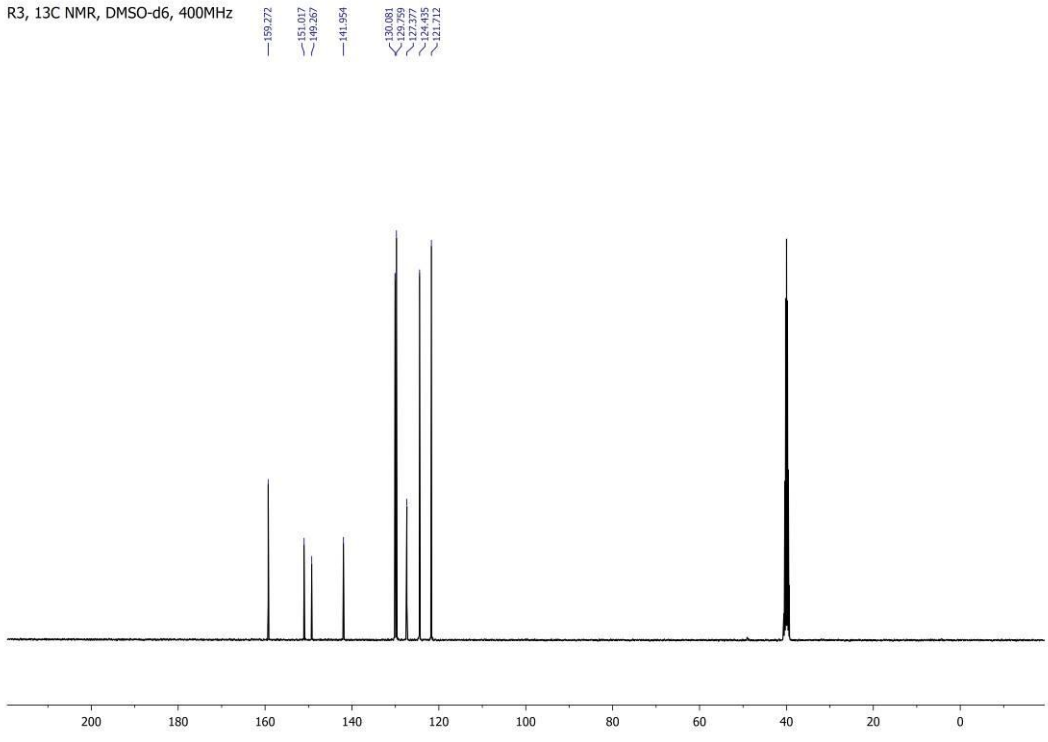

Fig. S6. ^{13}C NMR spectra of R3.

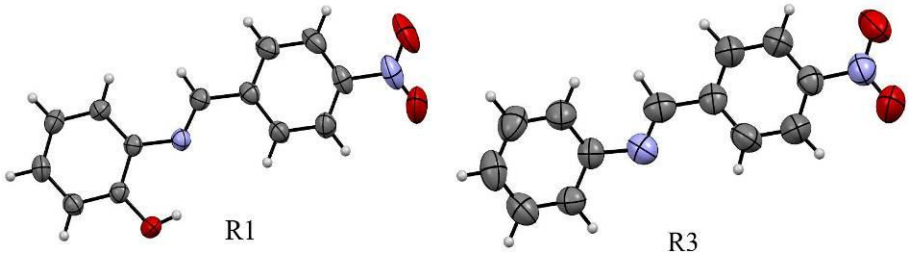

Fig. S7 The ORTEP diagrams (50% probability) of receptor R1 and R3

Table S1 Crystallographic data of receptor R1 and R3

Parameters	Receptor R1	Receptor R3
Chemical formula	$C_{13}H_{10}N_2O_3$	$C_{13}H_{10}N_2O_2$
Formula weight	242.23	226.23
Crystal System	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/n
a (Å)	11.9767(8)	14.6480(2)
b (Å)	5.9302(4)	10.8265(2)
c (Å)	16.1269(10)	14.7278(2)
Sβ (°)	96.635(2)	101.940 (2)
γ (°)	90.00	90.00
V $(Å)^3$	1137.73(13)	2285.10 (6)
Z	4	8
Crystal size	0.47 × 0.30 × 0.27	0.47 × 0.33 × 0.26
F (000)	504	944
R-factor (%)	5.23	6.85

Photographs:

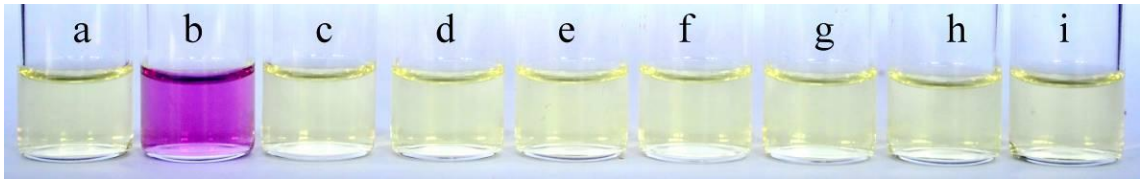

Fig. S8. Change in colour of R1 (5×10^{-5}M) in dry ACN with the addition of 1 equiv. of tetrabutylammonium anions. (a) Free Receptor R1, (b) F^-, (c) Cl^-, (d) Br^- (e) I^-, (f) NO_3^-, (g) HSO_4^-, (h) $H_2PO_4^-$ and (i) AcO^-.

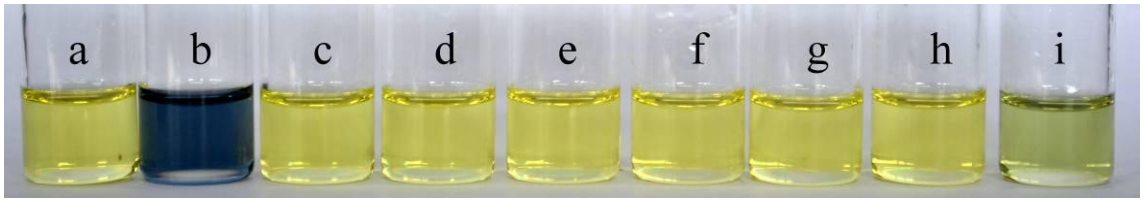

Fig. S9. Change in colour of R2 (5×10^{-5}M) in dry DMSO with the addition of 1 equiv. of tetrabutylammonium anions. (a) Free Receptor R2, (b) F^-, (c) Cl^-, (d) Br^- (e) I^-, (f) NO_3^-, (g) HSO_4^-, (h) $H_2PO_4^-$ and (i) AcO^-.

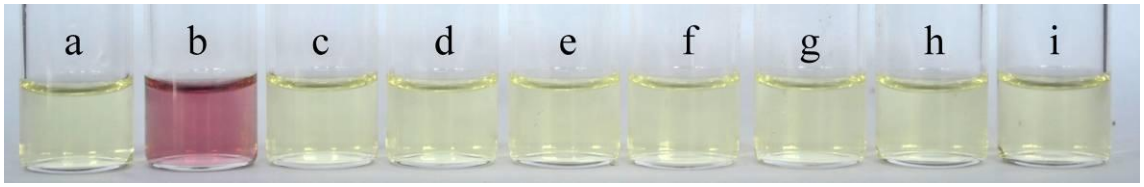

Fig. S10. Change in colour of R2 (5×10^{-5}M) in dry ACN with the addition of 1 equiv. of tetrabutylammonium anions. (a) Free Receptor R2, (b) F^-, (c) Cl^-, (d) Br^- (e) I^-, (f) NO_3^-, (g) HSO_4^-, (h) $H_2PO_4^-$ and (i) AcO^-.

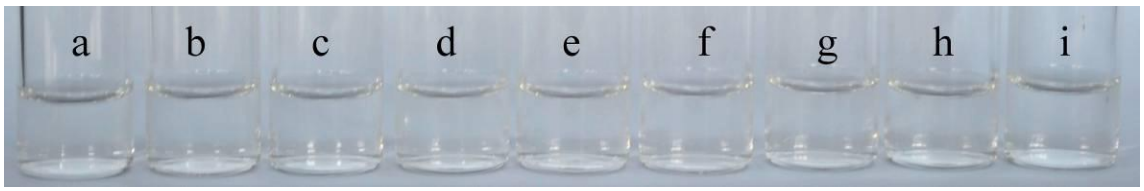

Fig. S11. Change in colour of R3 (5×10^{-5}M) in dry DMSO with the addition of 1 equiv. of tetrabutylammonium anions. (a) Free Receptor R3, (b) F^-, (c) Cl^-, (d) Br^- (e) I^-, (f) NO_3^-, (g) HSO_4^-, (h) $H_2PO_4^-$ and (i) AcO^-.

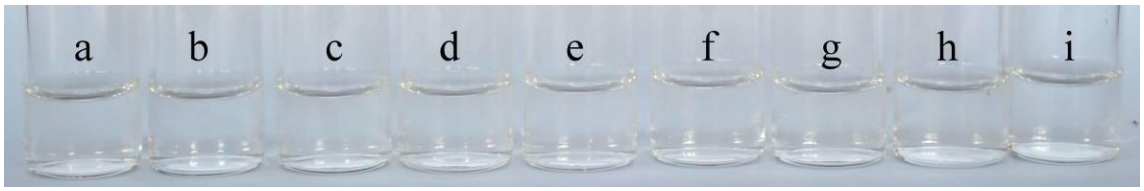

Fig. S12. Receptor R3 (5×10^{-5}M) in dry ACN after the addition of 1 equiv. of tetrabutylammonium anions. (a) Free Receptor R3, (b) F^-, (c) Cl^-, (d) Br^- (e) I^-, (f) NO_3^-, (g) HSO_4^-, (h) $H_2PO_4^-$ and (i) AcO^-.

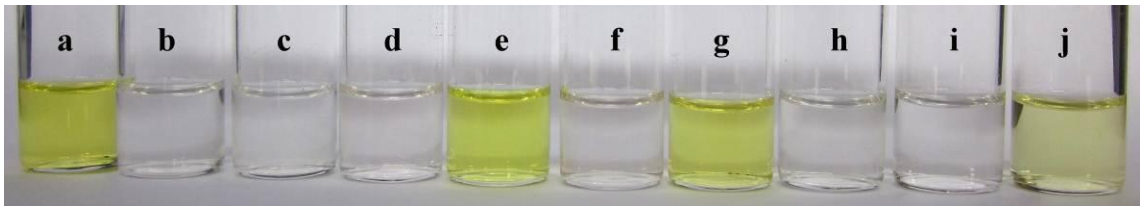

Fig. S13. Change in color after addition of 3 equiv. of different cations (as nitrate salts) to the receptor solution in ACN (5×10^{-5} M). (a) Receptor R2, (b) Mg^{2+}, (c) Ca^{2+}, (d) Co^{2+}, (e) Ni^{2+}, (f) Cu^{2+}, (g) Zn^{2+}, (h) Cd^{2+}, (i) Hg^{2+} and (j) Pb^{2+}.

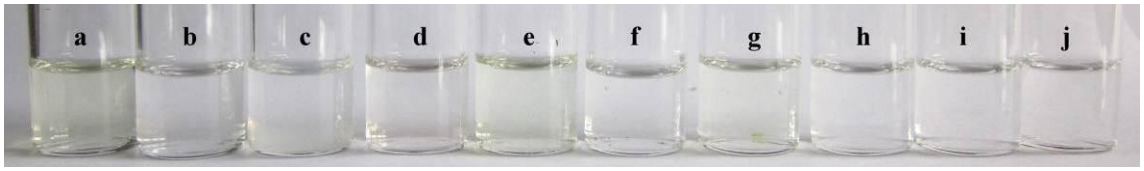

Fig. S14. Change in color after addition of 3 equiv. of different cations (as nitrate salts) to the receptor solution in ACN (5×10^{-5} M). (a) Receptor R3, (b) Mg^{2+}, (c) Ca^{2+}, (d) Co^{2+}, (e) Ni^{2+}, (f) Cu^{2+}, (g) Zn^{2+}, (h) Cd^{2+}, (i) Hg^{2+} and (j) Pb^{2+}.

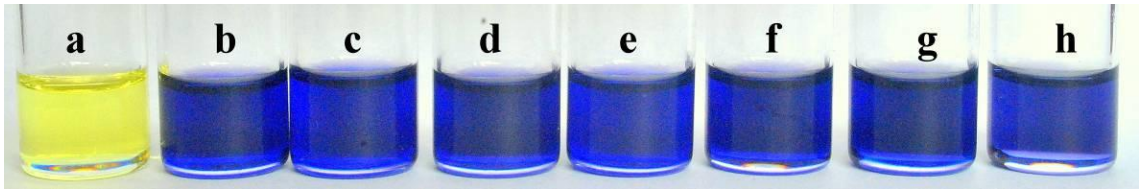

Fig. S15. Competitive study of receptor R1 (5×10^{-5}M) in DMSO by adding 1 equiv. F^- ion and 1 equiv. of other anions. (a) Receptor R1, (b) R1 + F^-, (c) R1 + Cl^- + F^-, (d) R1 + Br^- + F^-, (e) R1 + I^- + F^-, (f) R1 + NO_3^- + F^-, (g) R1 + HSO_4^- + F^- and (h) R1 + $H_2PO_4^-$ + F^-.

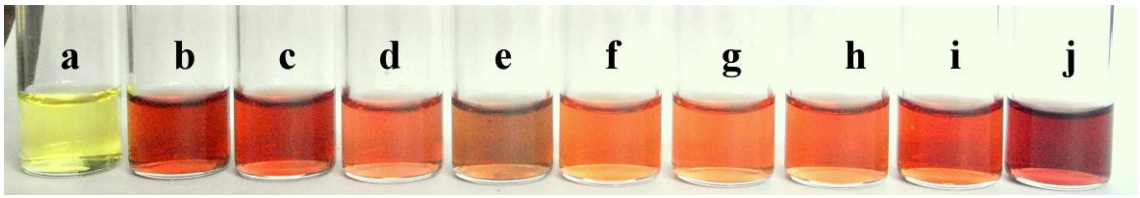

Fig. S16 Competitive study of receptor R1 (5×10^{-5}M) in ACN by adding 3 equiv. Cu^{2+} ion and 3 equiv. of other cations. (a) Receptor R1, (b) R1 + Mg^{2+} + Cu^{2+}, (c) R1 + Ca^{2+} + Cu^{2+}, (d) R1 + Co^{2+} +

Cu^{2+}, (e) R1 + Ni^{2+} + Cu^{2+}, (f) R1 + Cu^{2+}, (g) R1 + Zn^{2+} + Cu^{2+}, (h) R1 + Cd^{2+} + Cu^{2+}, (i) R1 + Hg^{2+} + Cu^{2+} and (j) R1 + Pb^{2+} + Cu^{2+}

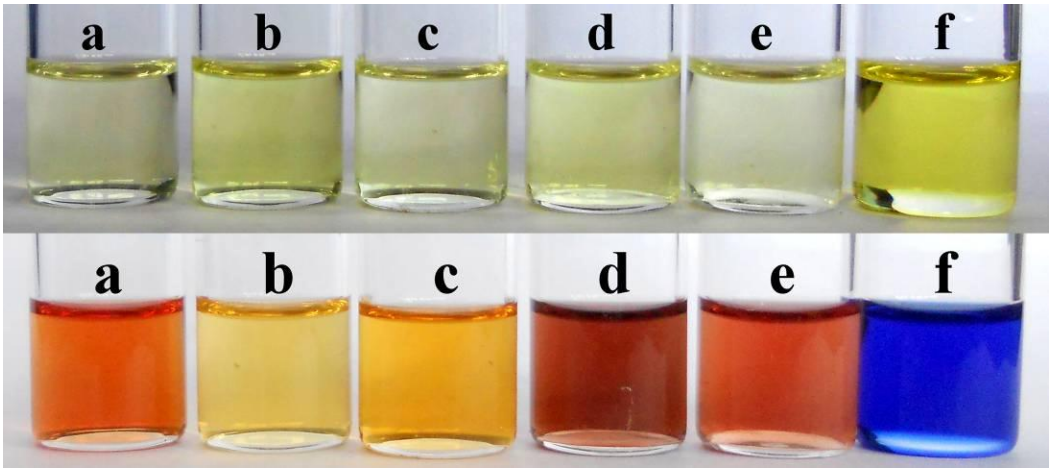

Fig. S17: Solvatochromic effect of the receptor R2 upon addition of 1 equiv. of F^- ions in different solvents. Top row: R2 solution (5×10^{-5}M) in different solvents. Bottom row: R2+F^- ions; (a) 1,4-Dioxane, (b) THF, (c) DCM, (d) Acetone, (e) ACN and (f) DMSO.

UV-vis titrations:

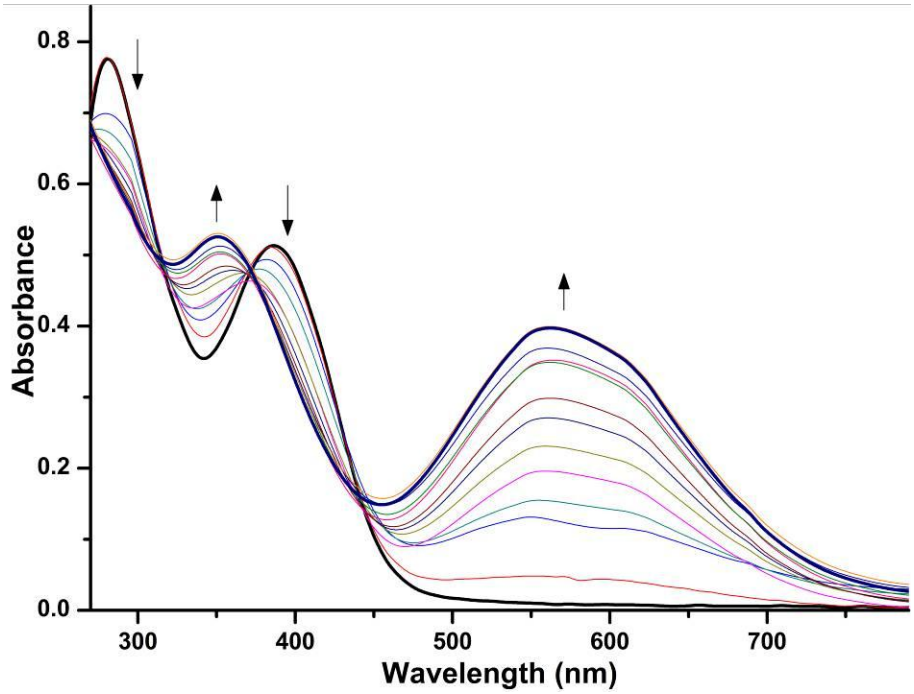

Fig. S18: UV-vis titration spectra of R1 (5×10^{-5}M) with the increasing concentration of TBAOH (0–25 equiv.) in dry DMSO.

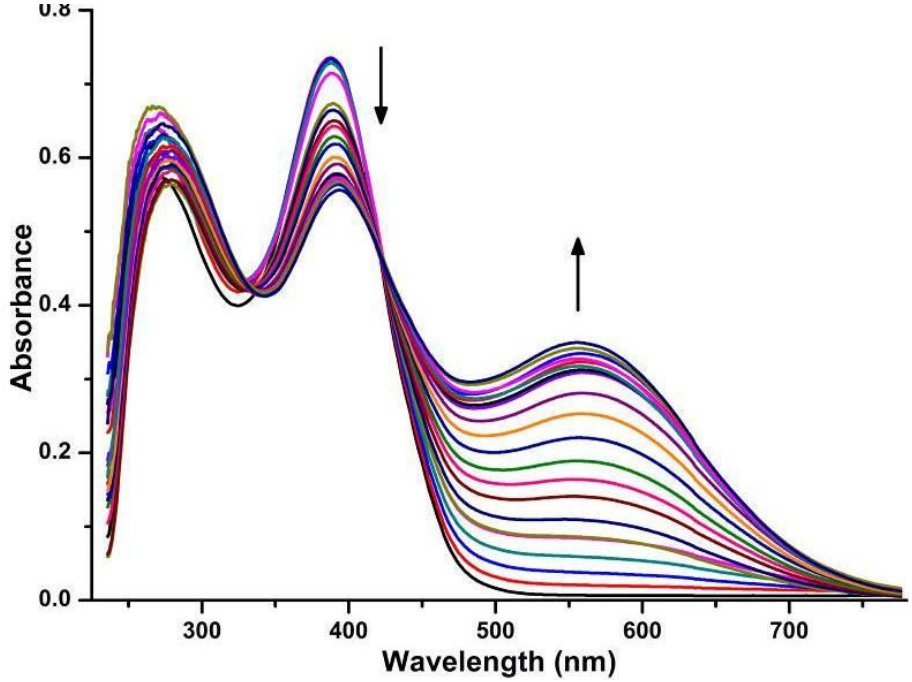

Fig. S19: UV-vis titration spectra of R2 (5×10^{-5}M) with the increasing concentration of TBAF (0–25 equiv.) in dry DMSO.

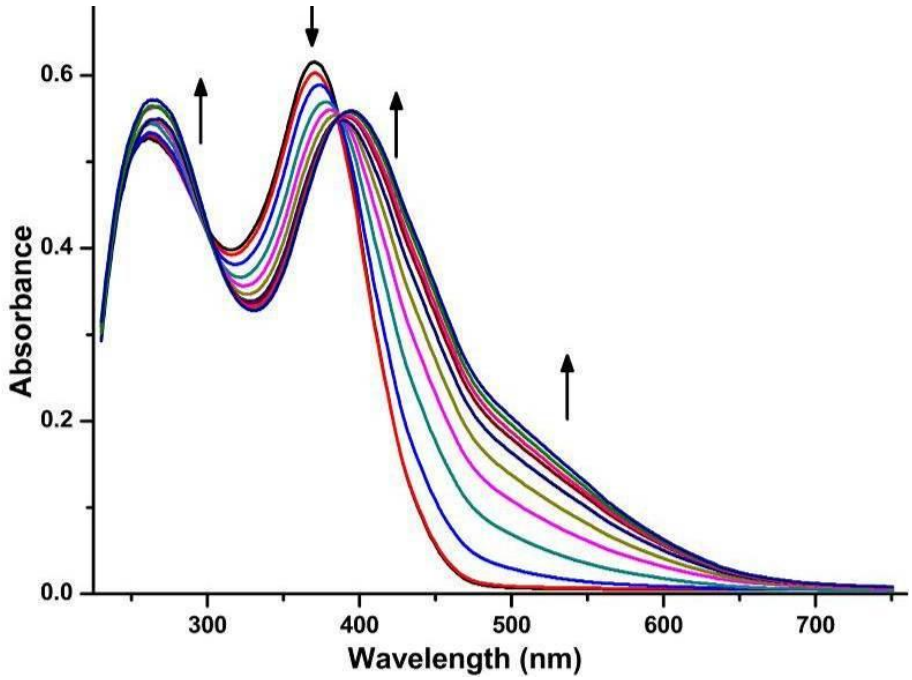

Fig. S20: UV-vis titration spectra of R2 (5×10^{-5}M) with the increasing concentration of TBAF (0–10 equiv.) in dry ACN.

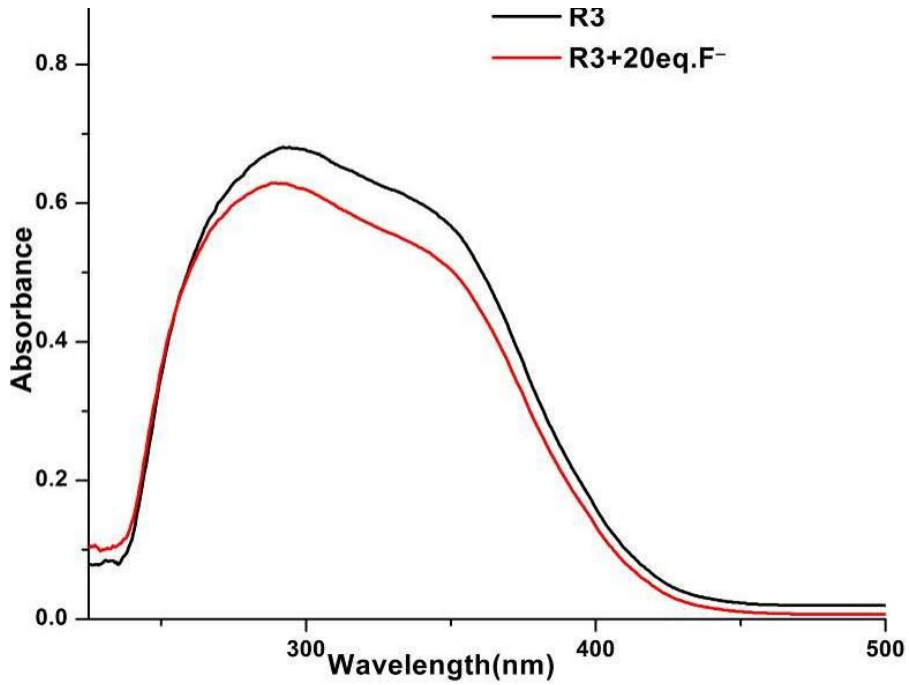

Fig. S21: UV-vis spectra of R3 (5×10^{-5}M) with the addition TBAF (20 equiv.) in dry DMSO.

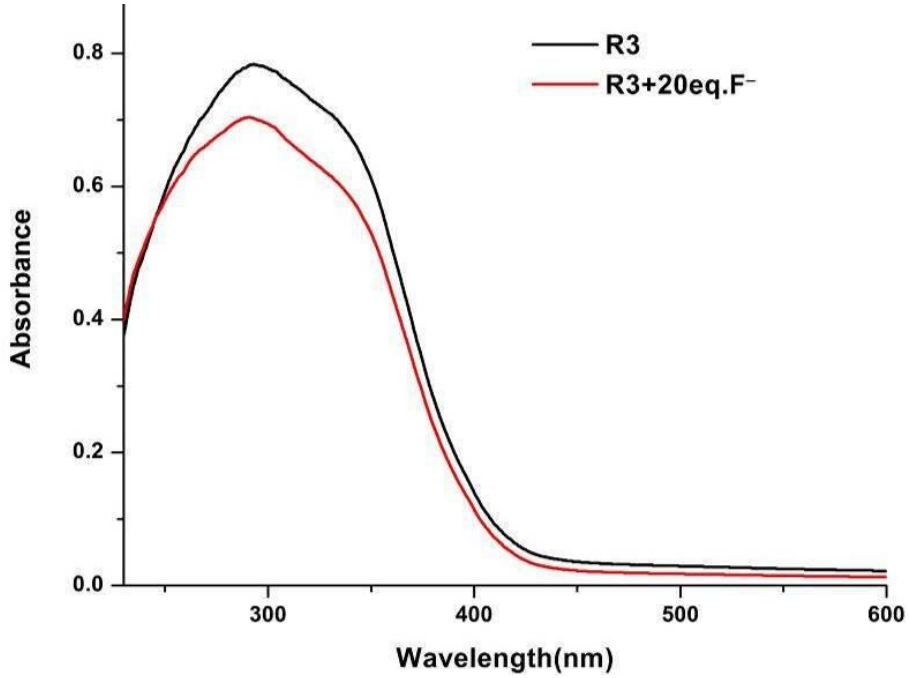

Fig. S22: UV-vis spectra of R3 (5×10^{-5}M) with the addition TBAF (20 equiv.) in dry ACN.

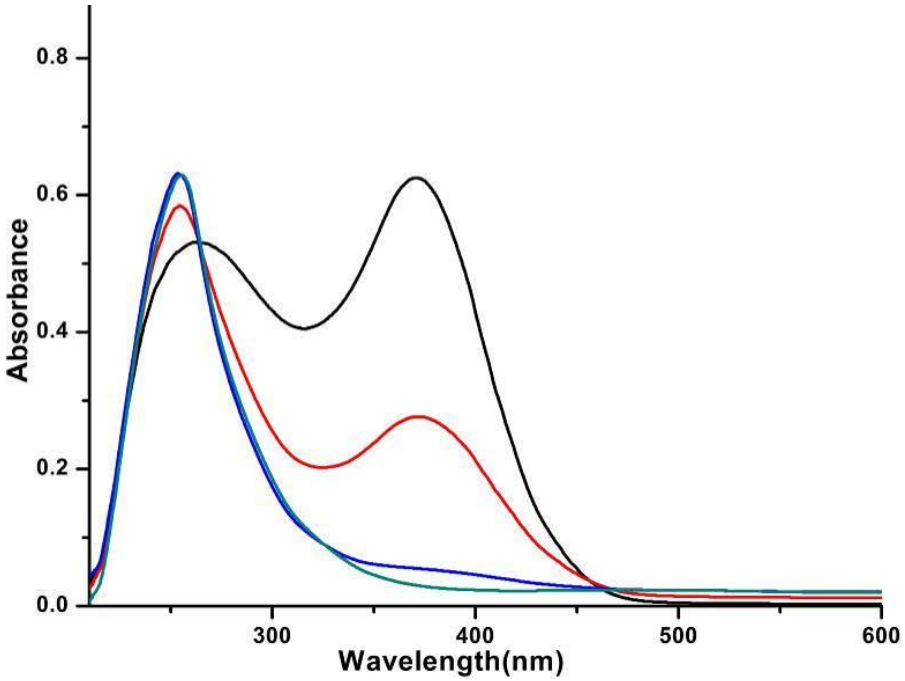

Fig. S23: UV-vis titration spectra of R2 (5×10^{-5}M) with the increasing concentration of Cu^{2+} ions (0–4 equiv.) in ACN.

The receptor did not show any new peak even after addition of 20 equiv. of Cu^{2+} solution. However, the peak corresponding to –OH disappeared in UV-vis spectra as shown in Fig. S23 (showed addition of Cu^{2+} ions only upto 4 equiv. for clarity).

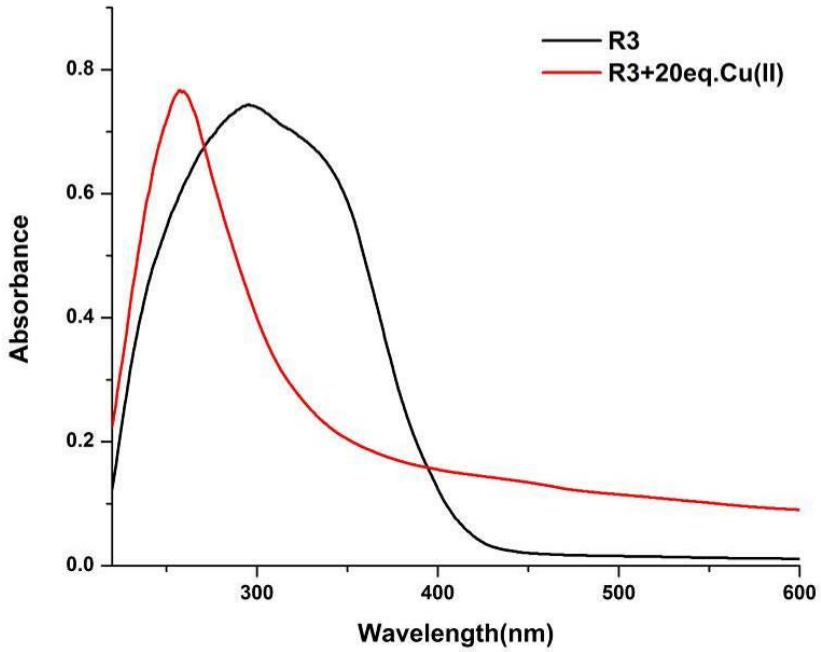

Fig. S24: UV-vis titration spectra of R3 (5×10^{-5}M) with 20 equiv. of Cu^{2+} ions in ACN.

UV–Vis changes with different anions:

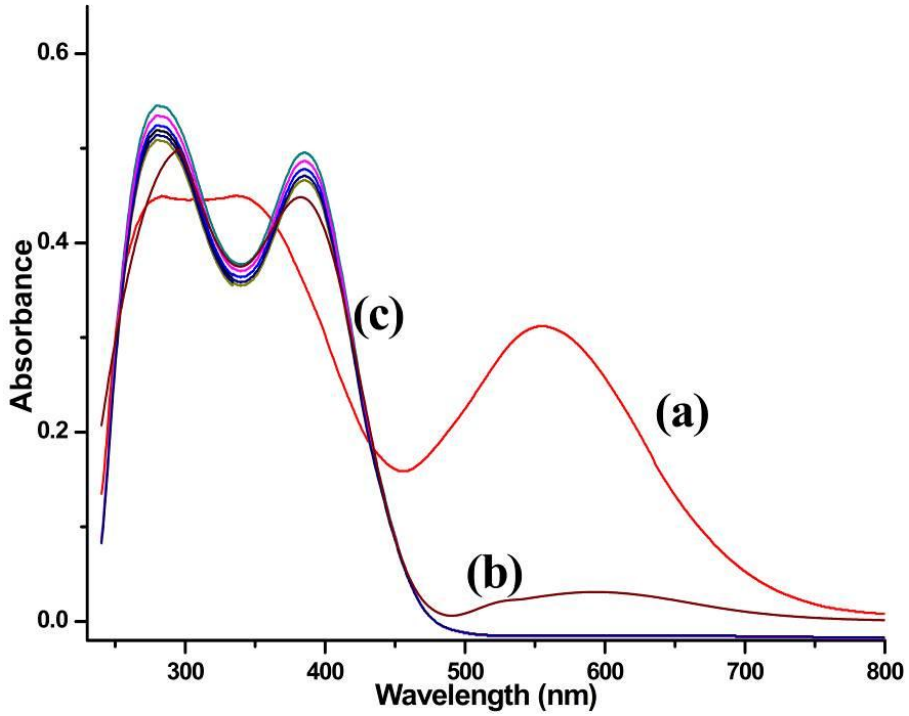

Fig. S25: UV–Vis changes of R1 in DMSO (5×10^{-5}M) after addition of 20 equiv. of (a) F^- ion, (b) AcO^- ion and (c) Cl^-, Br^-, I^-, NO_3^-, HSO_4^- and $H_2PO_4^-$ ions in the form of TBA salts.

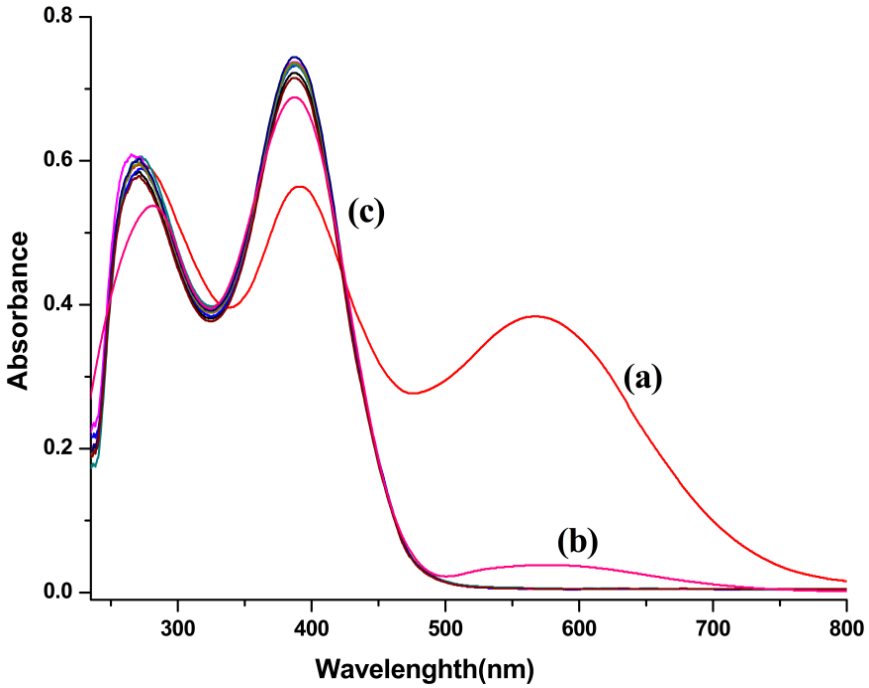

Fig. S26: UV–Vis changes of R2 in DMSO (5×10^{-5}M) after addition of 20 equiv. of (a) F^- ion, (b) AcO^- ion and (c) Cl^-, Br^-, I^-, NO_3^-, HSO_4^- and $H_2PO_4^-$ ions in the form of TBA salts.

UV–Vis changes with different cations:

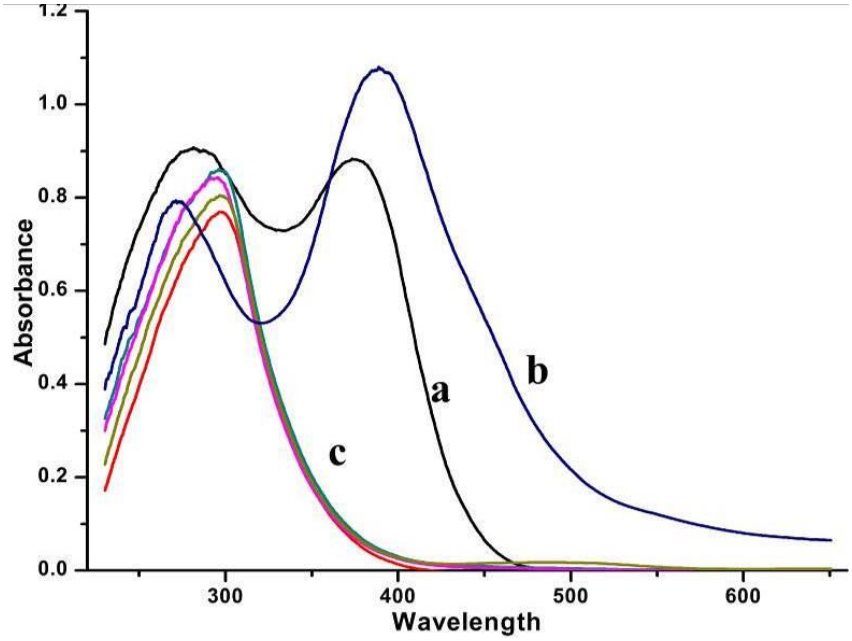

Fig. S27: UV–Vis changes of R1 in ACN (10×10^{-5}M) after addition of 40 equiv. of metal nitrates (a) Free receptor R1 (b) R1+ Cu^{2+} and (c) R1+ other metal salts (Mg^{2+}, Ca^{2+}, Co^{2+}, Cd^{2+}, Hg^{2+}). Ni^{2+} and Pb^{2+} are omitted for clarity.

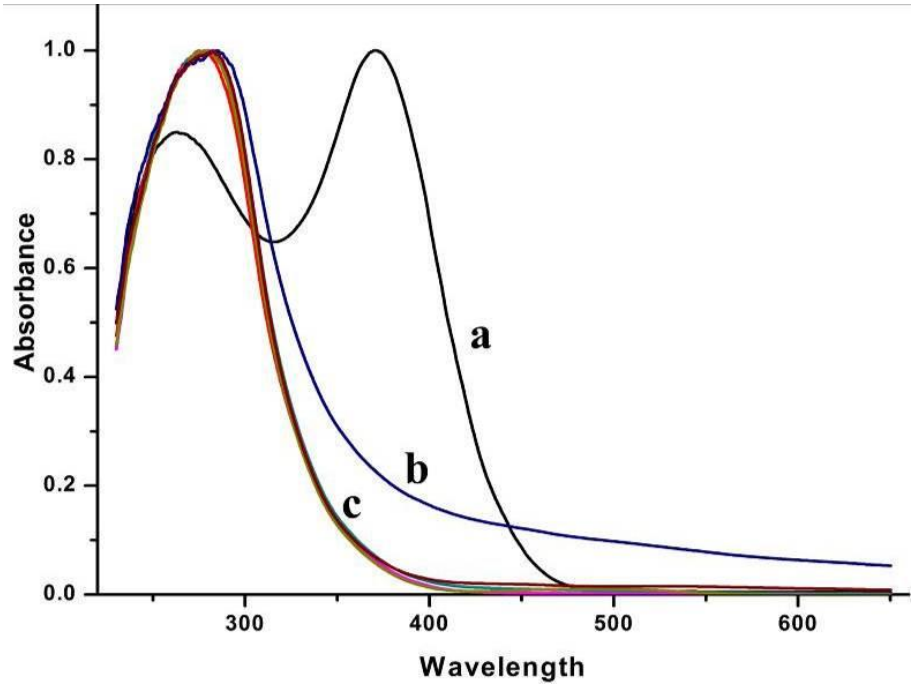

Fig. S28: UV–Vis changes of R2 in ACN (10×10^{-5}M) after addition of 40 equiv. of metal nitrates (a) Free receptor R2 (b) R2+ Cu^{2+} and (c) R2+ other metal salts (Mg^{2+}, Ca^{2+}, Co^{2+}, Zn^{2+}, Cd^{2+}, Hg^{2+}). Ni^{2+}, Zn^{2+} and Pb^{2+} are omitted for clarity.

Jobs plots:

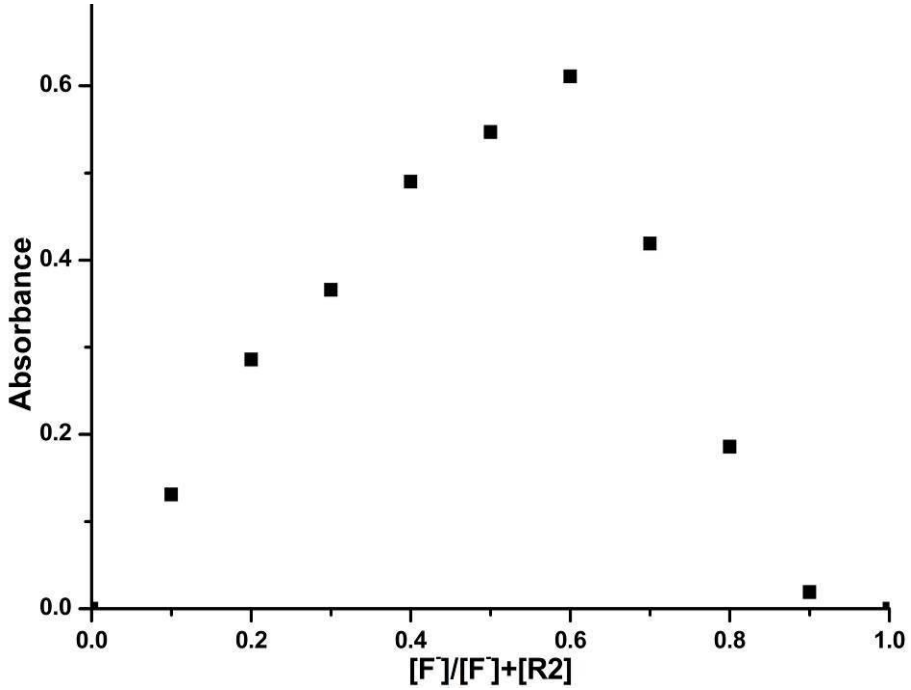

Fig. S29: Jobs plot for R2 with F^- ion at 500 nm in dry ACN.

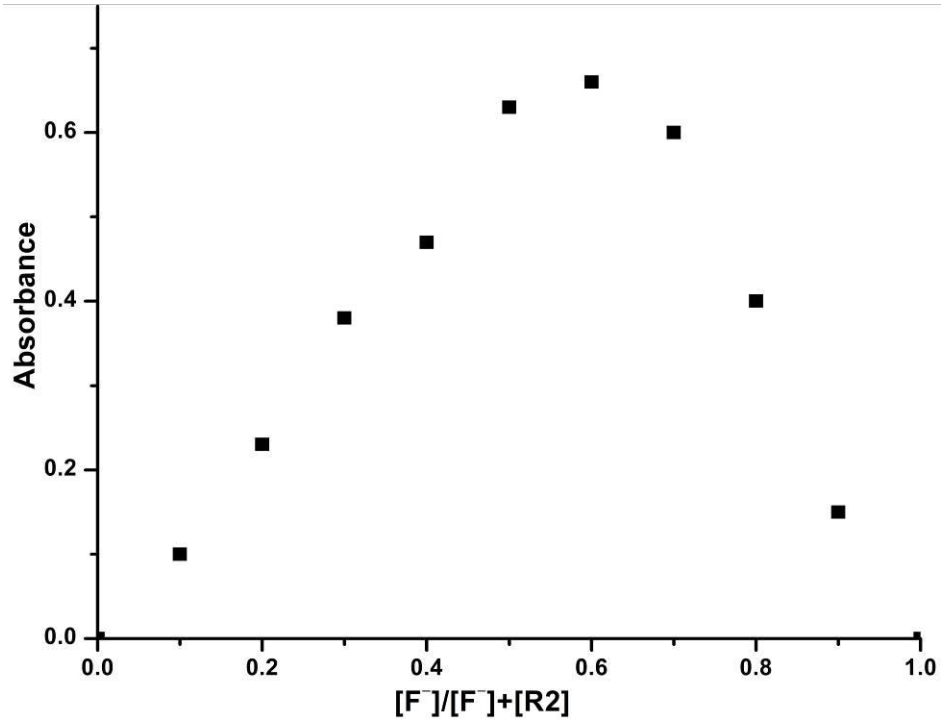

Fig. S30: Jobs plot for R2 with F^- ion at 558 nm in dry DMSO.

Binding constant:

Binding constant was calculated using equation (1).

$$\frac{1}{(A - A_0)} = \frac{1}{(A_{max} - A_0)} + \frac{1}{K[F^-]^n(A_{max} - A_0)} \quad \ldots\ldots\ldots\ldots (1)$$

Where, A_0, A, A_{max} are the absorption considered in the absence of F^-, at an intermediate, and at a concentration of saturation. K is binding constant, $[F^-]$ is concentration of F^- ion and n is the stoichiometric ratio.