

Supporting Information

“Turn-On” fluorescent chemosensor for Zinc (II) dipodal ratiometric receptor: Application in live cell imaging.

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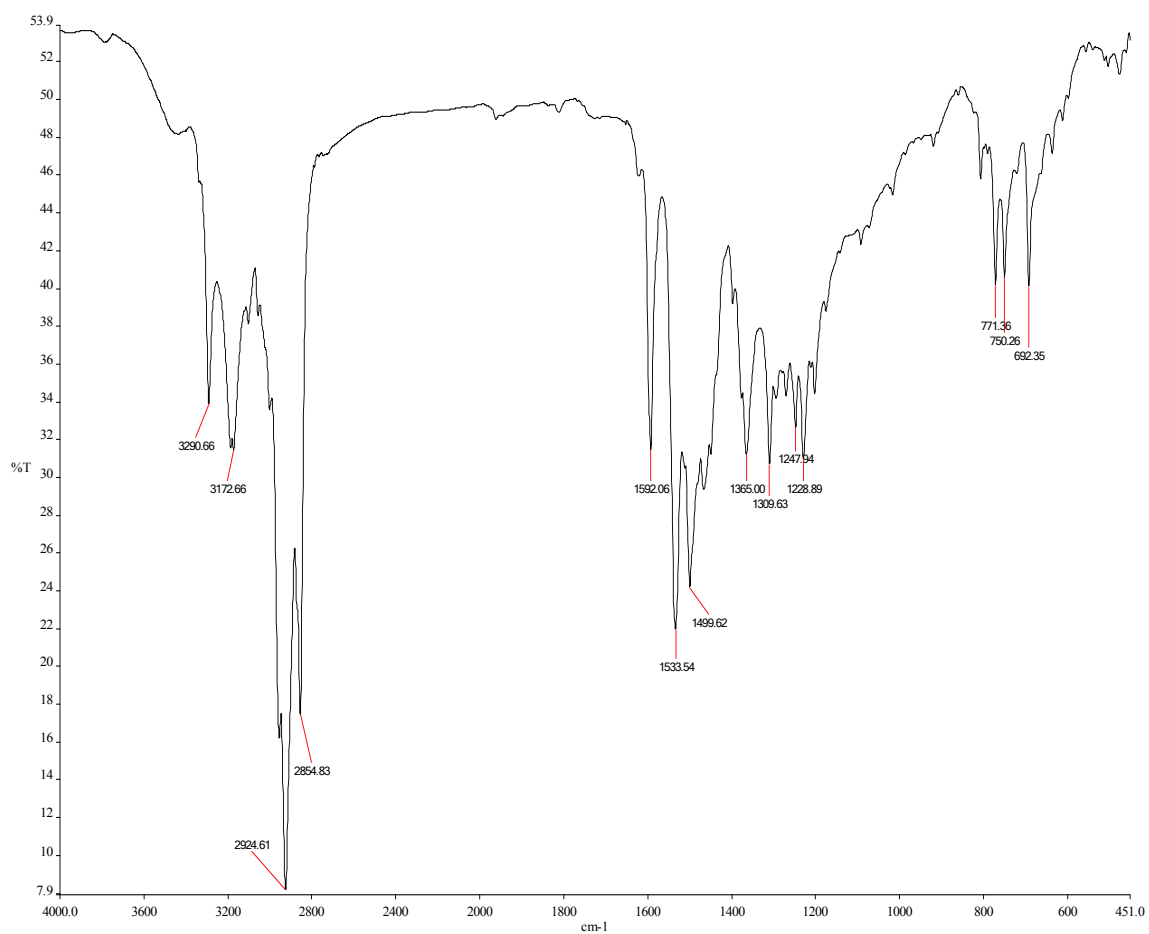


Figure S1. IR spectra of receptor 2

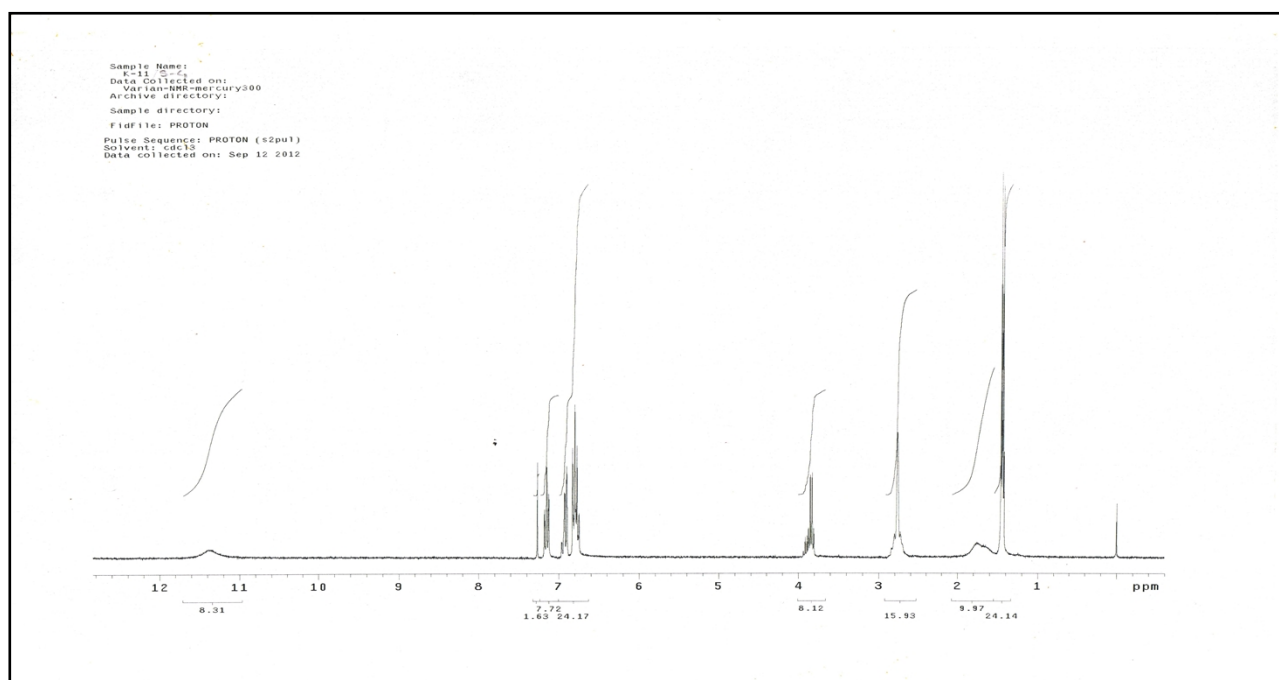


Figure S2. ¹H-NMR spectra of receptor 2

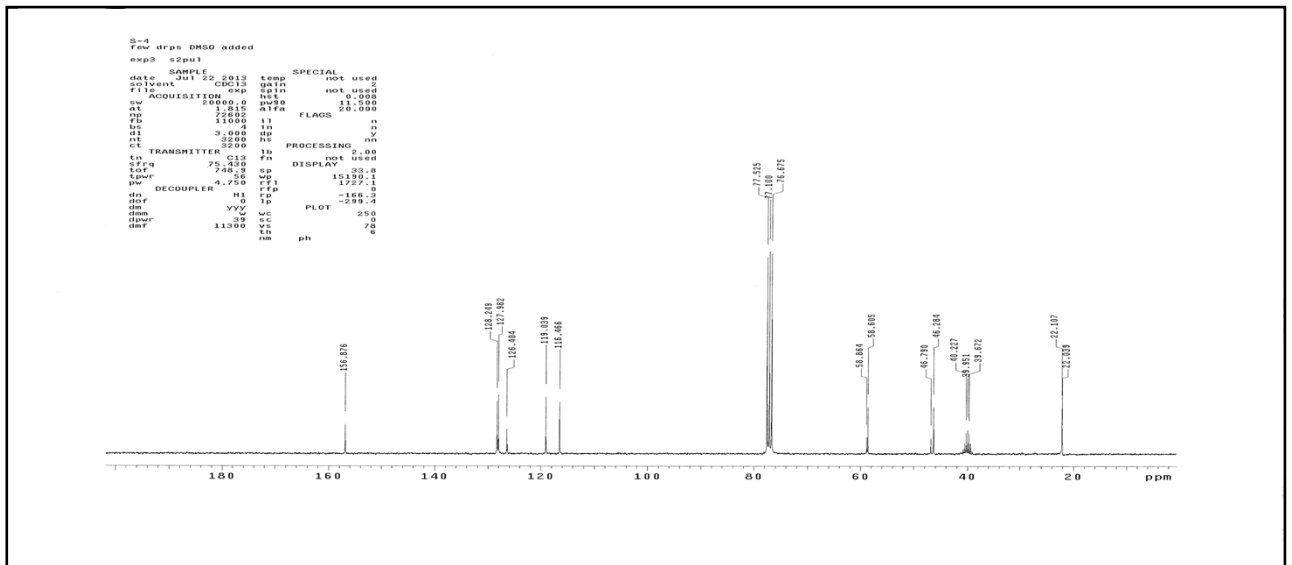


Figure S3. ¹³C-NMR spectra of receptor 2

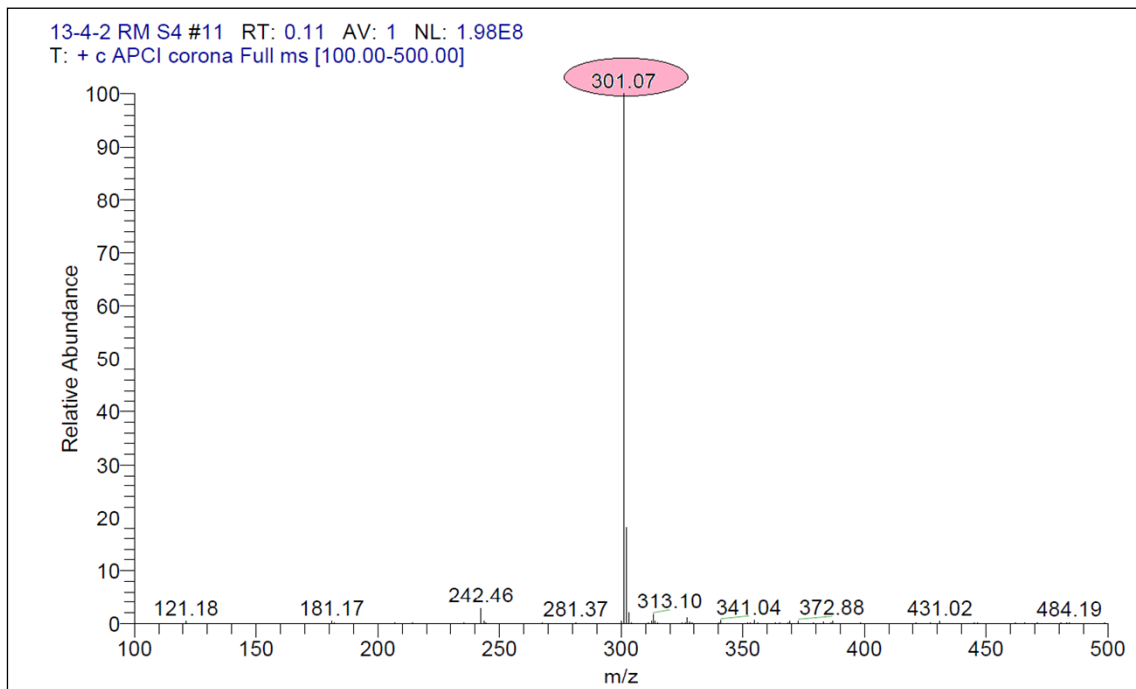


Figure S4. LC-MS spectra of receptor 2 ($M+H^+$)

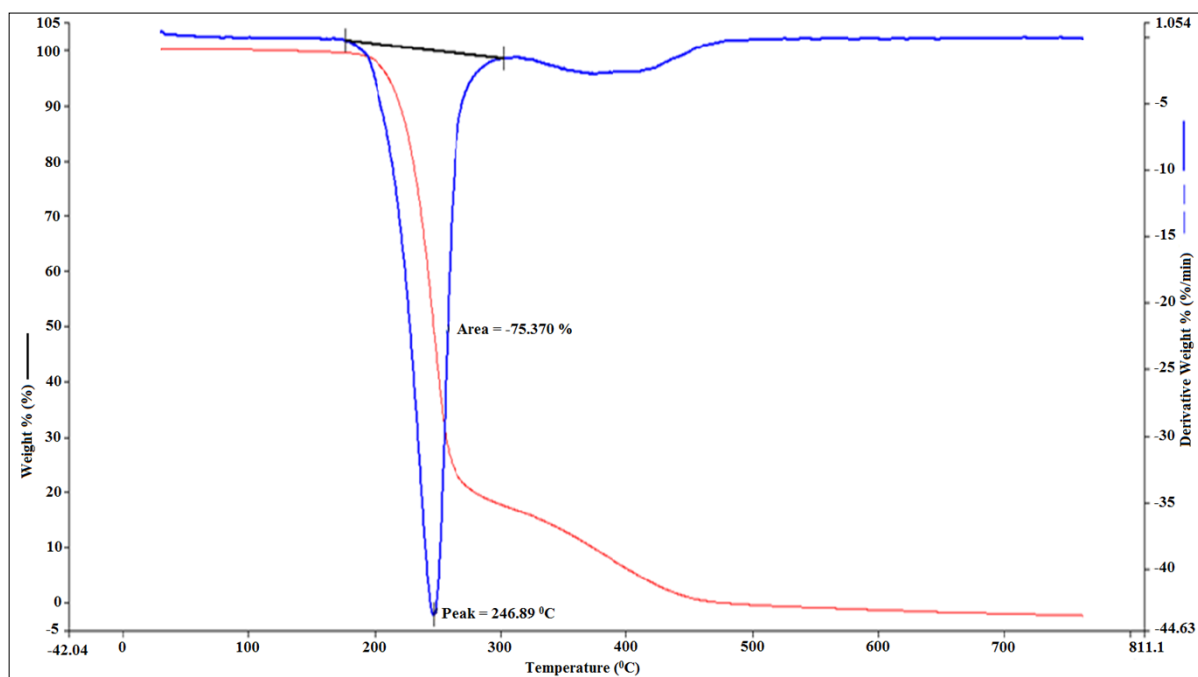


Figure S5a. TGA of receptor 2 (heating rate 10 °C per minute under nitrogen environment).

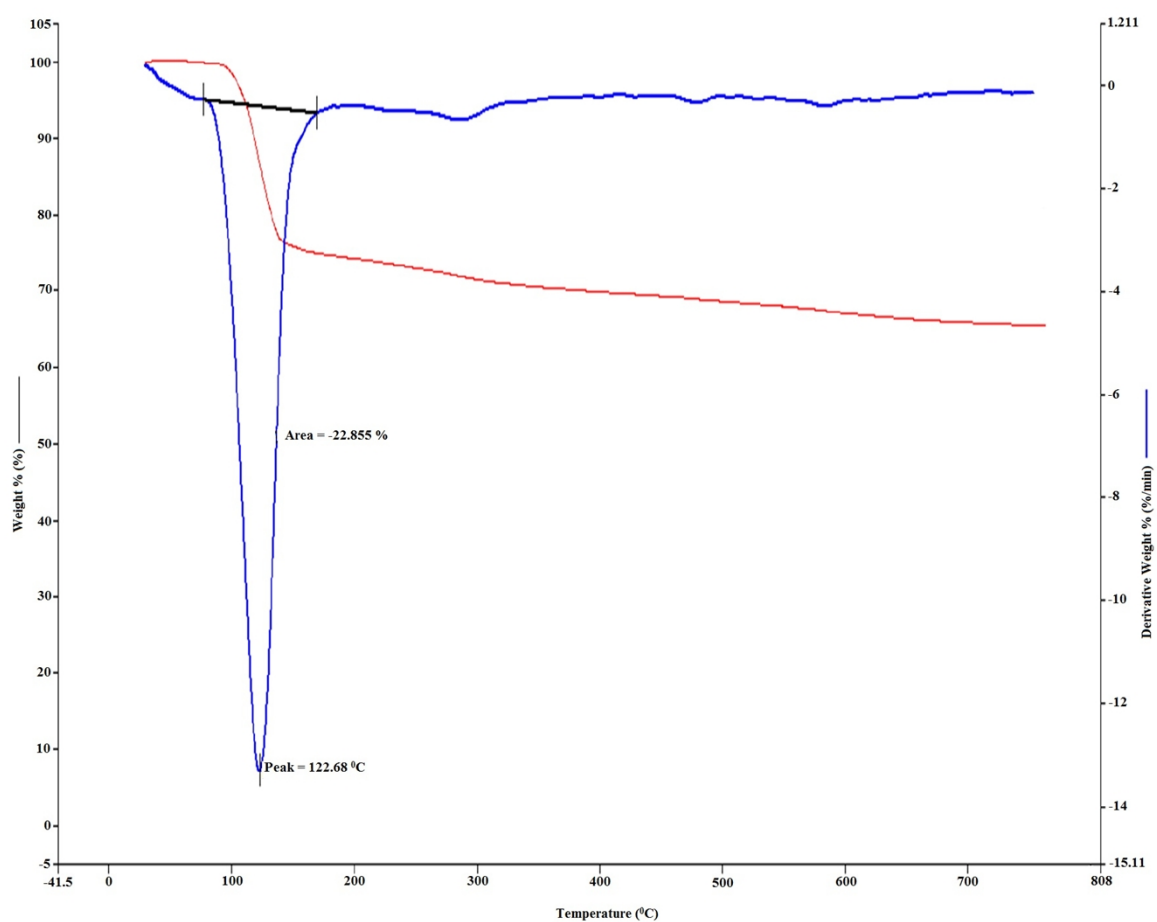


Figure S5b. TGA of receptor 2.Zn²⁺ (heating rate 10 °C per minute under nitrogen environment).

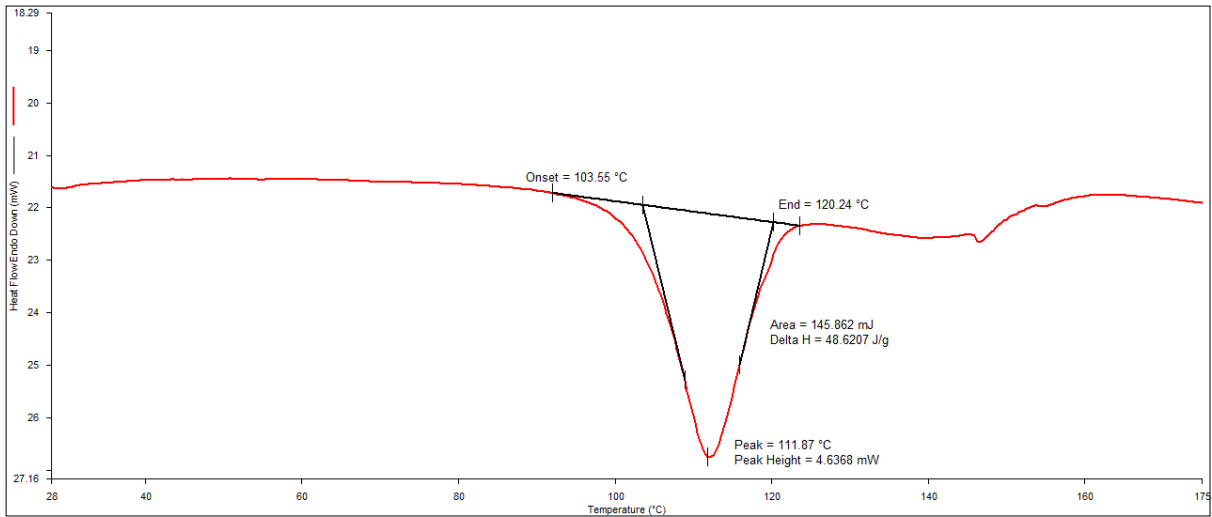


Figure S6a. DSC of receptor **2**.

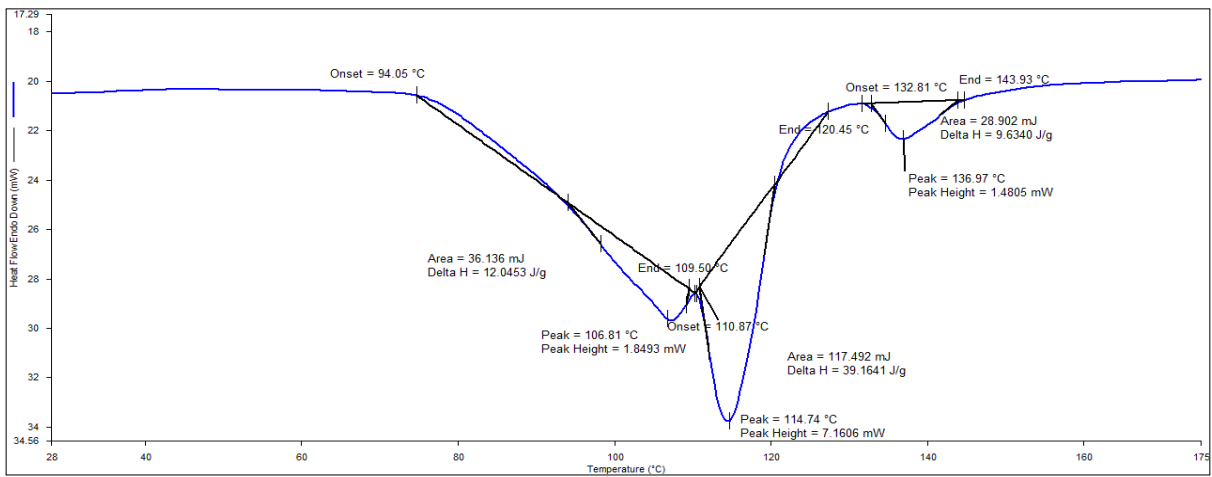


Figure S6b. DSC of receptor **2.Zn²⁺**.

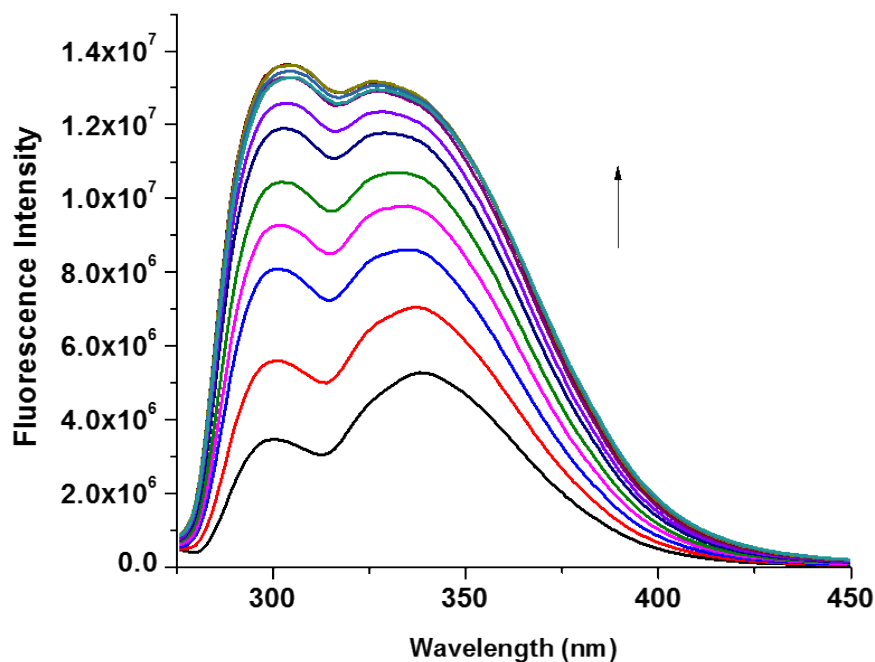


Figure S7a. Fluorescence titration spectra of receptor **2** (0.1 mM) in the presence of different concentrations of Zn^{2+} (1 mM) ($\lambda_{\text{ex}} = 278$ nm, $\lambda_{\text{em}} = 341$ nm, excitation and emission slit 5 nm) up to 10 μl (0.05 equiv.).

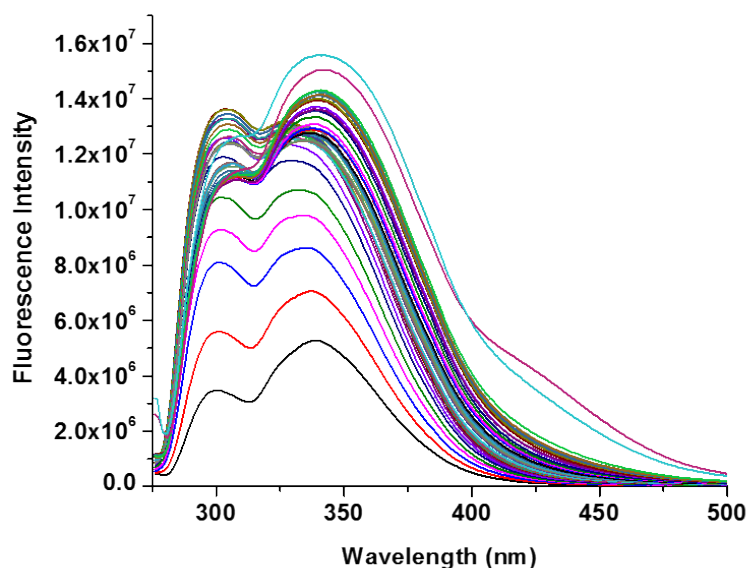


Figure S7b. Fluorescence titration spectra of receptor **2** (0.1 mM) in the presence of different concentrations of Zn^{2+} (1 mM) ($\lambda_{\text{ex}} = 278$ nm, $\lambda_{\text{em}} = 341$ nm, excitation and emission slit 5 nm) up to 400 μL (2 equiv.).

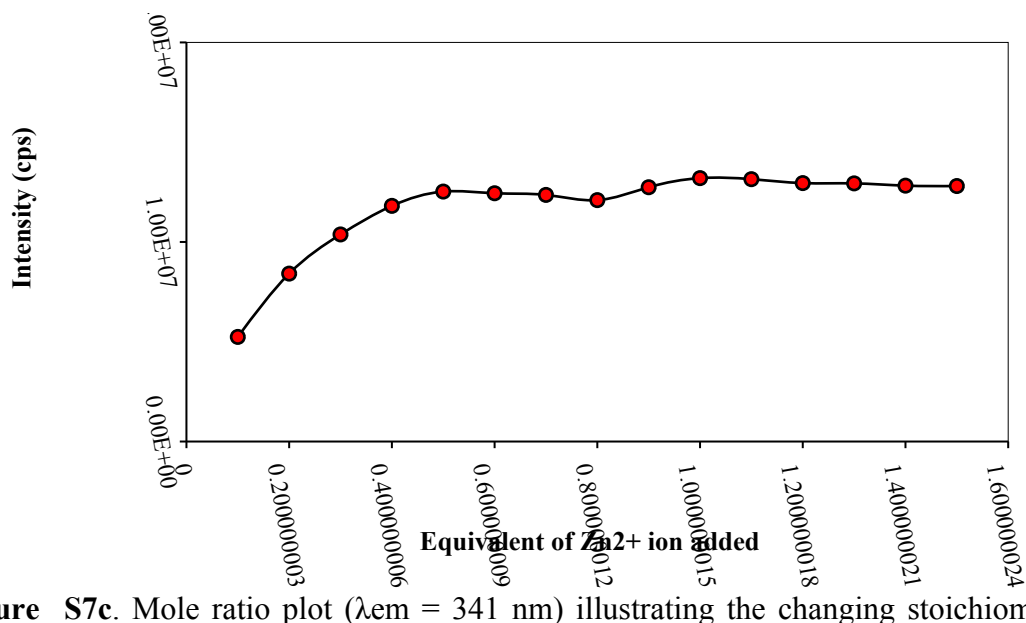


Figure S7c. Mole ratio plot ($\lambda_{em} = 341 \text{ nm}$) illustrating the changing stoichiometry from 2:1 to 1:1.

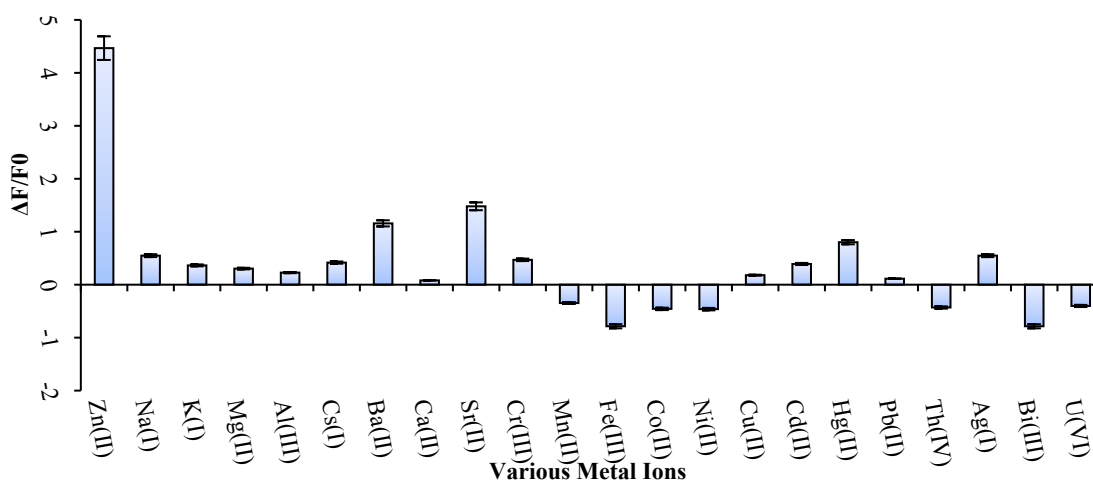


Figure S8. Fluorescence spectrometric response ($\Delta F = F - F_0$) of receptor **2** (0.1 mM) upon addition of 100 μL of respective cation salts (1 mM) in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$.

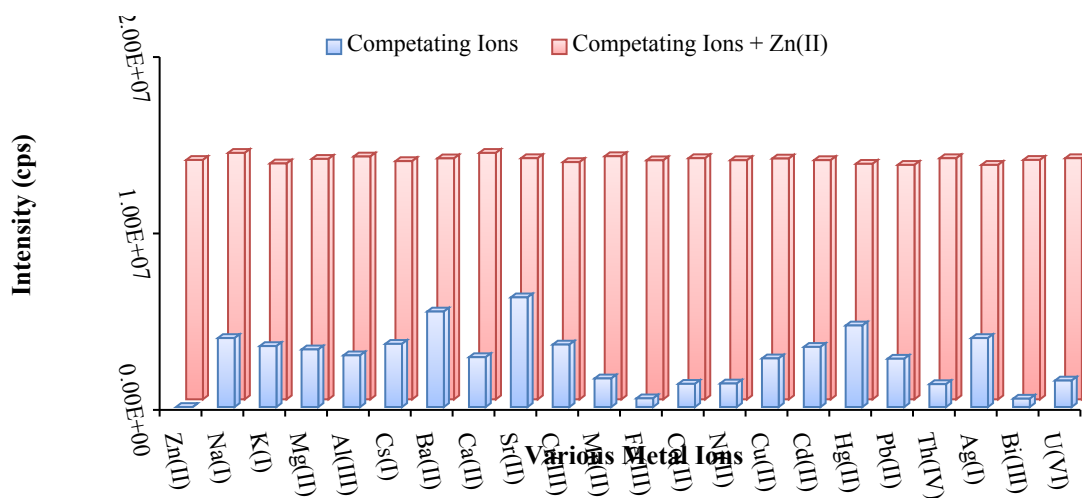


Figure S9. A fluorescence sensing of Zn^{2+} ion (1 mM, 1equiv) by receptor **2** (0.1 mM) in the presence of other competing cations (1mM, 2 equiv.).

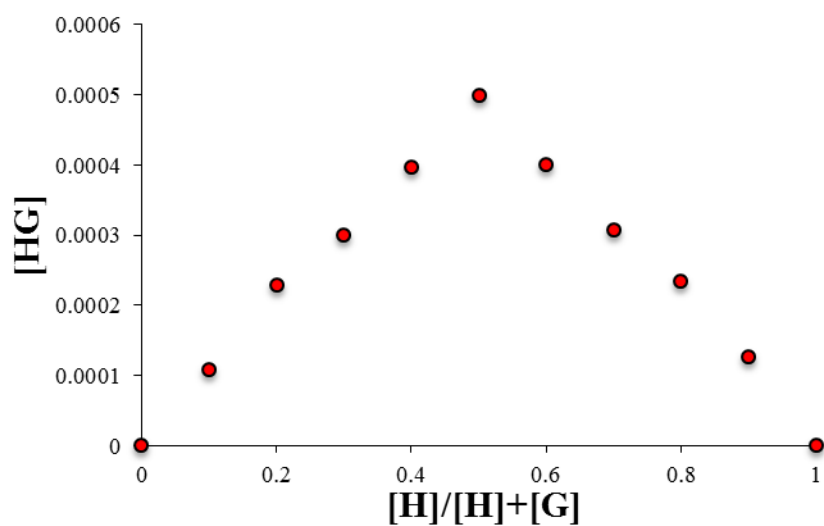


Figure S10a. Job's plot representing the stoichiometry of complex **2**. Zn^{2+} (host : guest; 1:1).

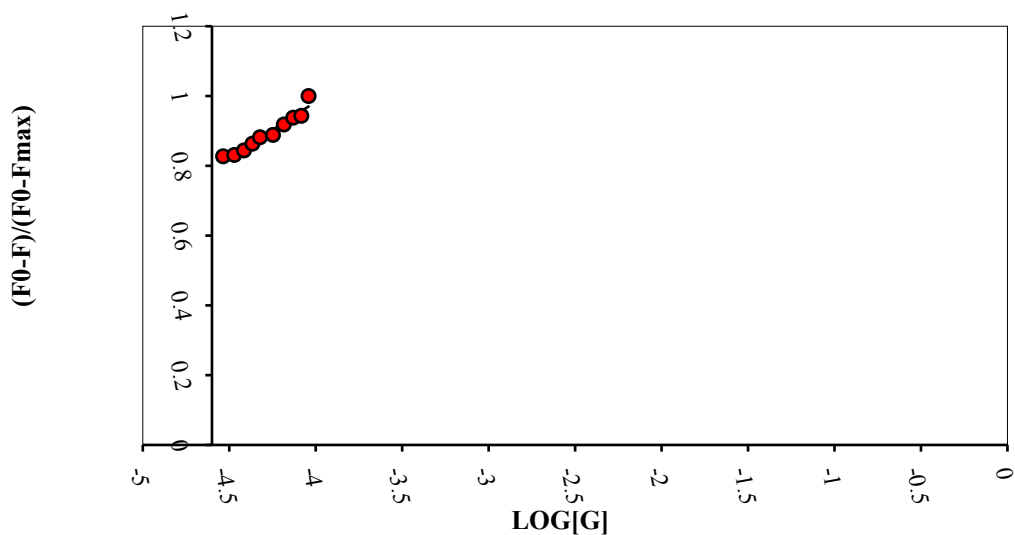


Figure S10b. Normalized plot obtained from fluorescence spectroscopy ($\lambda_{em} = 341$ nm).

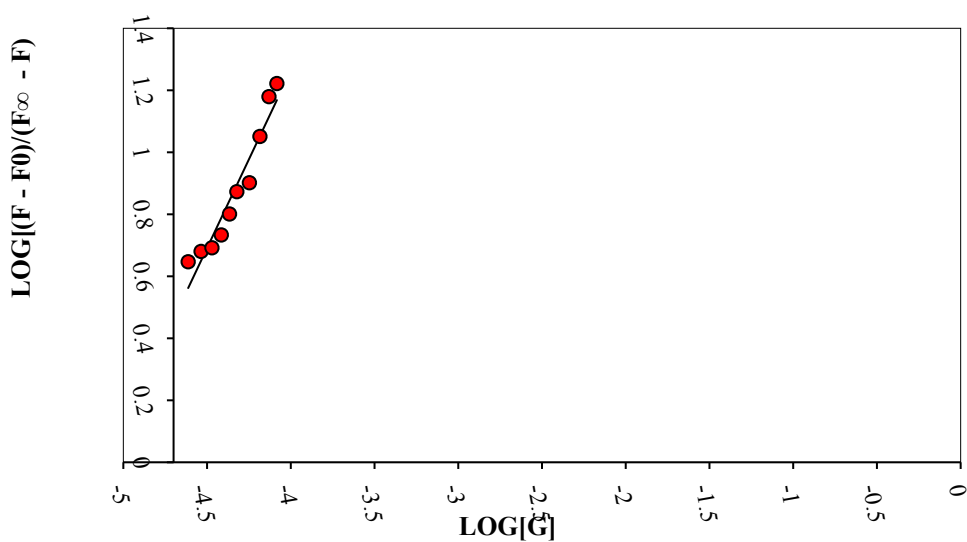


Figure S10c. Fluorescence intensity at 341nm of receptor **2** (0.1 mM) versus increasing concentration of $\text{Log}[\text{Zn}^{2+}]$. The fluorescence response fits to a Hill coefficient of 1.1446, which is in concordance with the 1:1 binding stoichiometry for the receptor **2**. Zn^{2+} complex.

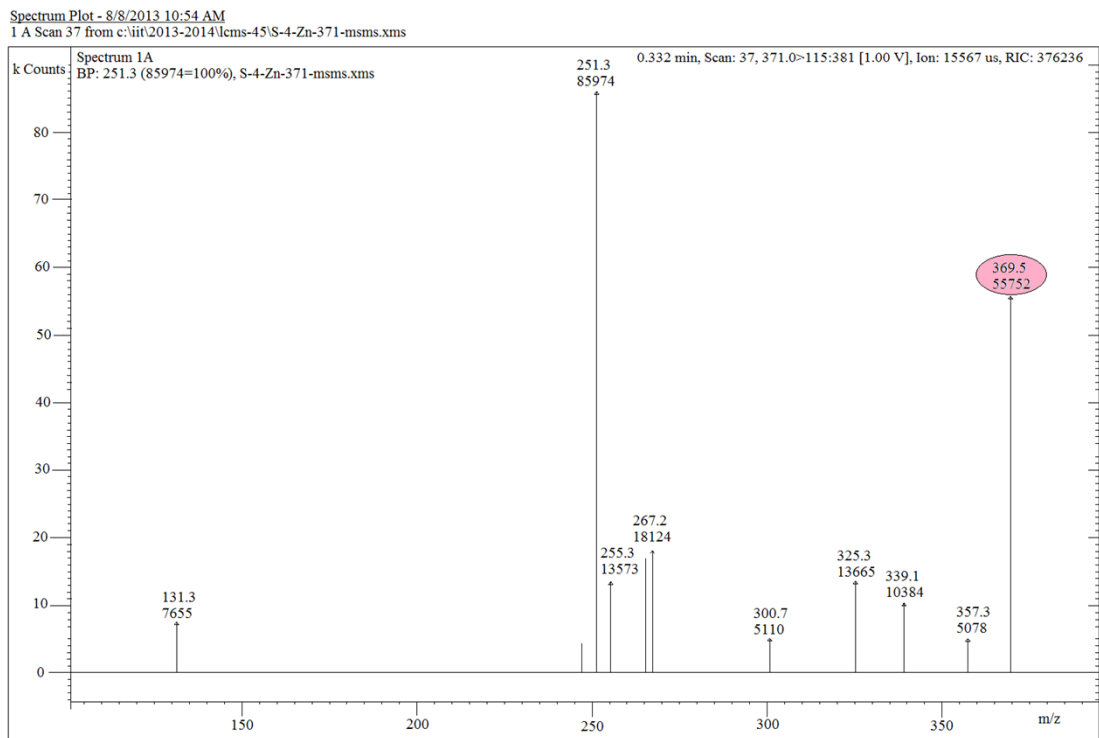


Figure S11. LC-MS spectra of **2**.Zn²⁺ complex (M+H⁺)

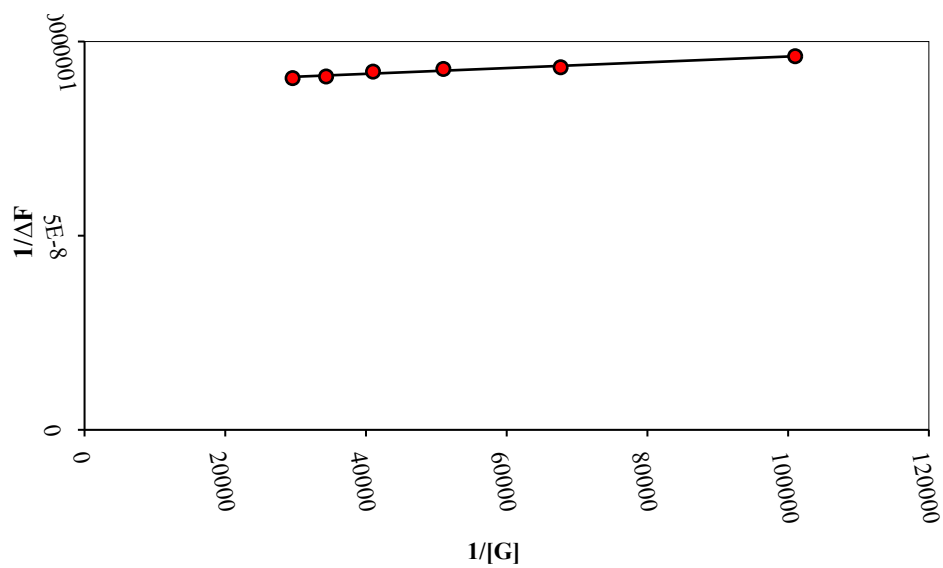


Figure S12a. A Benesi-Hildebrand methodology for receptor **2**, ($1/\Delta F$) vs $1/[G]$, $K_a = 1.29 \times 10^6 \text{ M}^{-1}$.

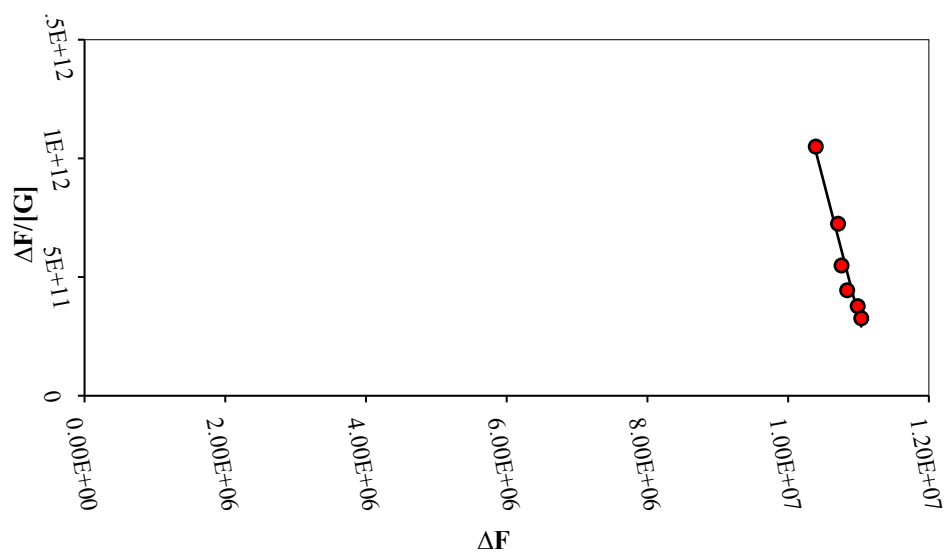


Figure S12b. A Scatchard methodology for receptor **2**, $\Delta F/[G]$ vs ΔF , $K_a = 1.00 \times 10^6$ M^{-1} .

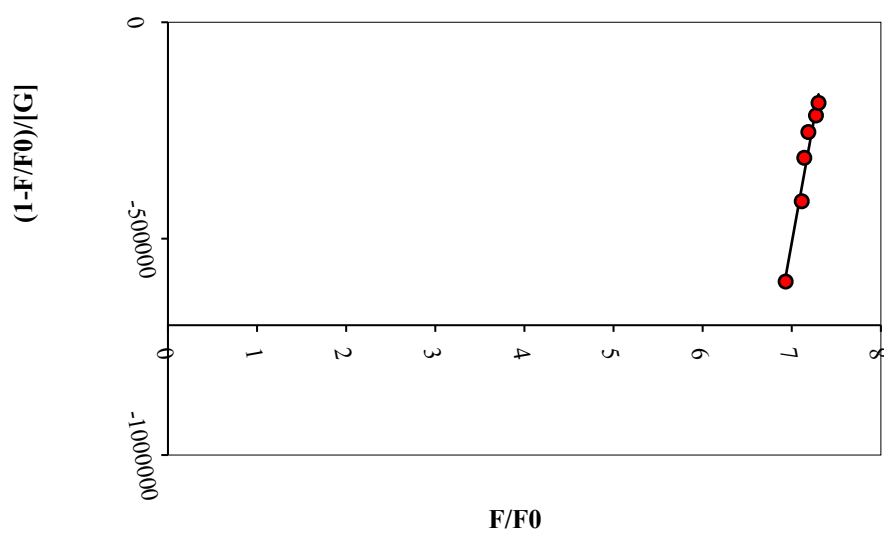


Figure S12c. Connor's fitting method for receptor **2**, $(1-F/F_0)/[G]$ vs F/F_0 , $K_a = 1.94 \times 10^6$ M^{-1} .

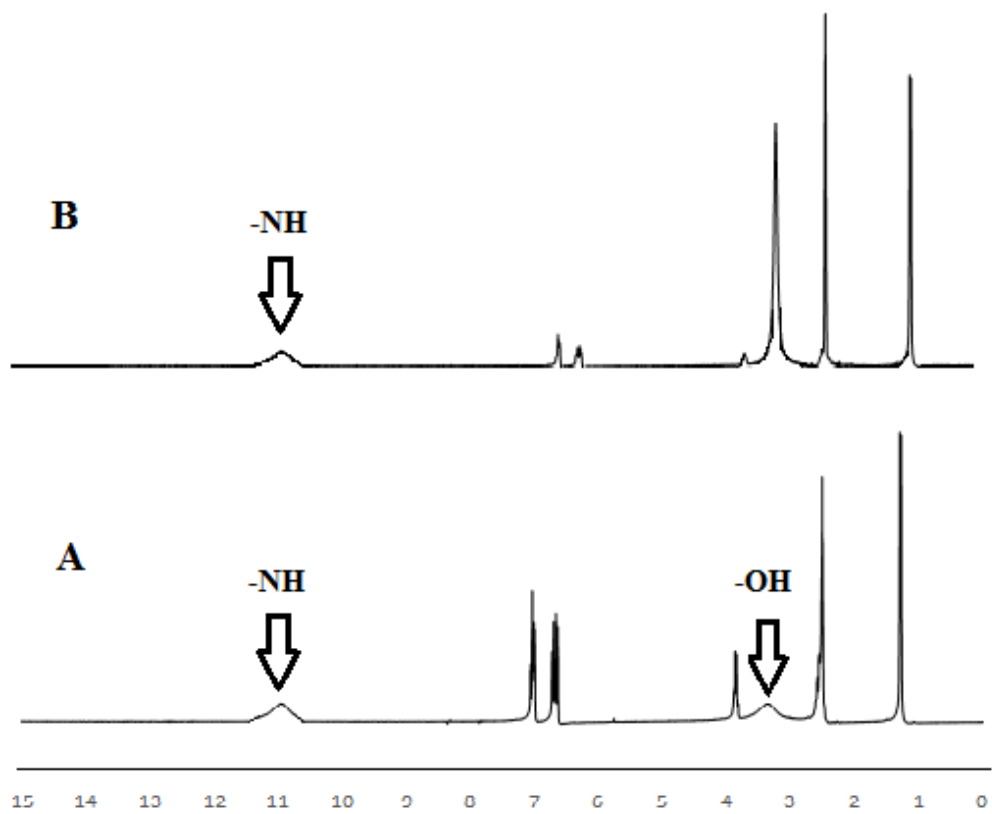


Figure S13. ¹H-NMR spectra (A) only receptor 2 (B) complex 3.

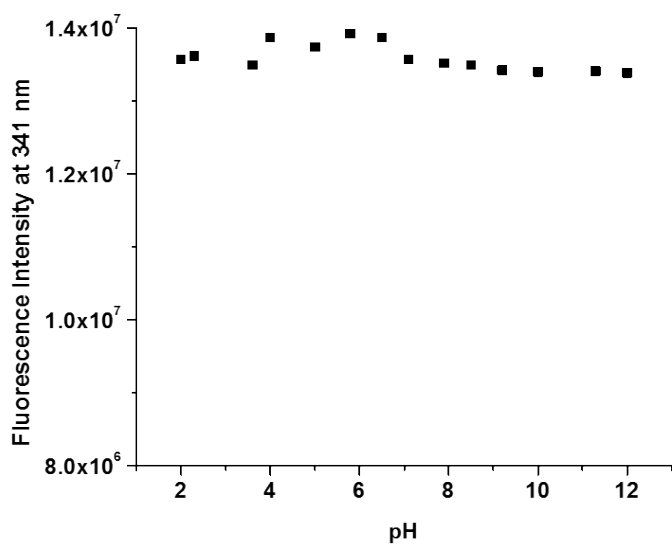


Figure S14: Change in fluorescence intensity of receptor **2** at 341 nm upon varying the pH of the solution.

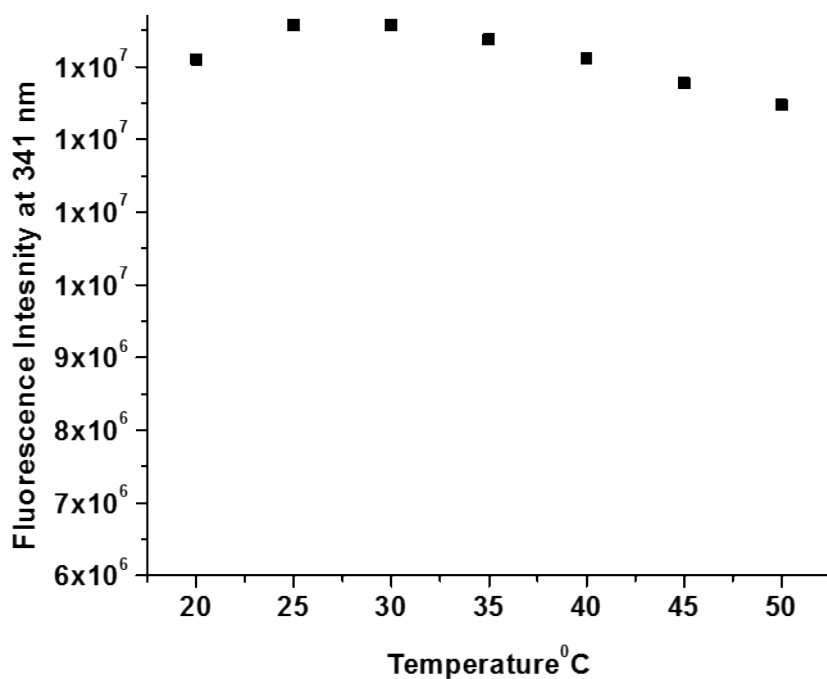


Figure S15: Change in fluorescence intensity of receptor **2** at 341 nm at various temperature.

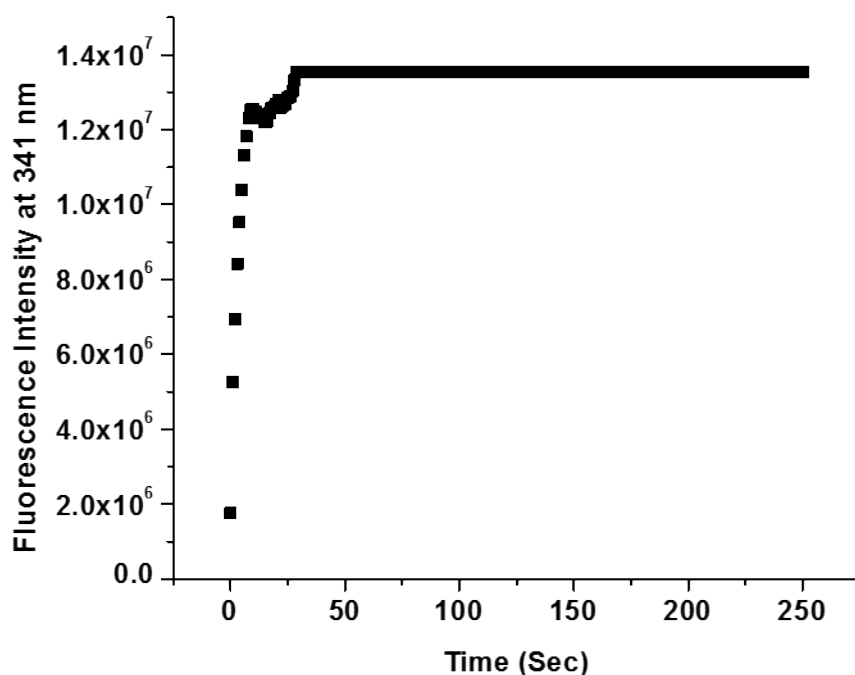


Figure S16: Fluorescence intensity of receptor **2** at 341 nm upon addition of Zn²⁺ ion (1 mM) over time.

Table S1: Comparison of literature reports with present work.

References	Detection Limit	Solvent
Zhou <i>et. al.</i> , (2012)	2.2×10^{-7} M	CH ₃ CN-H ₂ O
Dong <i>et. al.</i> ,(2014)	1×10^{-7} M	CH ₃ CN-Tris-HCl
Li <i>et. al.</i> , (2014)	4.9×10^{-8} M	CH ₃ CN-H ₂ O
Kaur <i>et. al.</i> , (2014)	1×10^{-6} M	DMF-H ₂ O
Sivaraman <i>et. al.</i> , (2012)	1.5×10^{-7} M	Phosphate buffer
Present work	6.5×10^{-7} M	CH ₃ CN-H ₂ O

Table S2: An optimized bond angles, dihedral angles, bond length and energy calculated at B3LYP/ LANL2DZ level.

Parameter	Receptor 2	3
Dihedral angles (°)		
N25-C29-C30-N26	61.09	55.65
C29-C30-N26-C24	-135.57	-158.35
C5-C4-C23-N25	33.34	115.51
O21-C3-C4-C23	-0.50	6.07
C27-C23-N25-C29	-66.67	-63.07
C3-C4-C23-N25	-147.43	-68.10
O22-C12-C11-C24	-2.34	6.08
C11-C24-N26-C30	157.50	169.33
Bond angles (°)		
C23-N25-C29	116.22	113.26
C5-C4-C23	121.38	123.03
C30-N26-C24	120.29	113.26
N26-C24-C28	113.49	110.98
N25-C29-C30	109.24	111.36
Bond Length (Å)		
N25-C29	1.46	1.52
C30-N26	1.46	1.52
C24-N26	1.47	1.54
C23-N25	1.47	1.54
C12-O22	1.39	1.46
C3-O21	1.40	1.46
O22-H45	0.97	0.97
O21-H44	0.97	0.97
N25-H42	1.01	1.02
N26-H43	1.01	1.02
C23-C27	1.54	1.53
Energy (a.u.)	-960.28	-1025.33