

Supporting Information

Harvesting red fluorescence through design specific tuning of ICT and ESIPT: An efficient optical detection of cysteine and live cell imaging

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Figure S1: Effect of solvent polarity on absorption and emission spectrum of **R1**

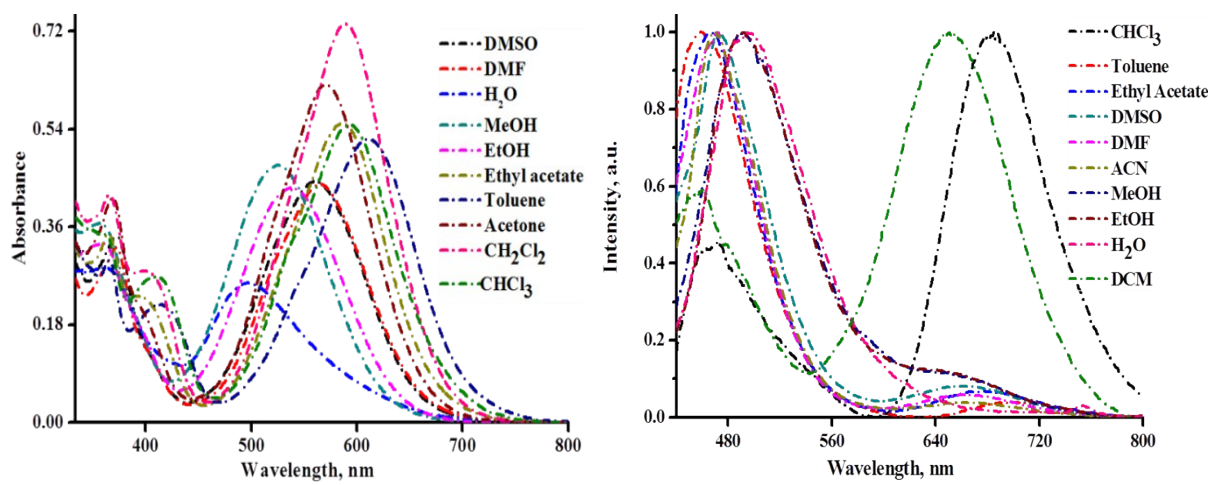


Figure S2: Naked eye colour changes of R1 ($10\mu\text{ M}$) towards different anions and neutral analytes in of $\text{H}_2\text{O}:\text{ACN}$ (7:3, v/v)

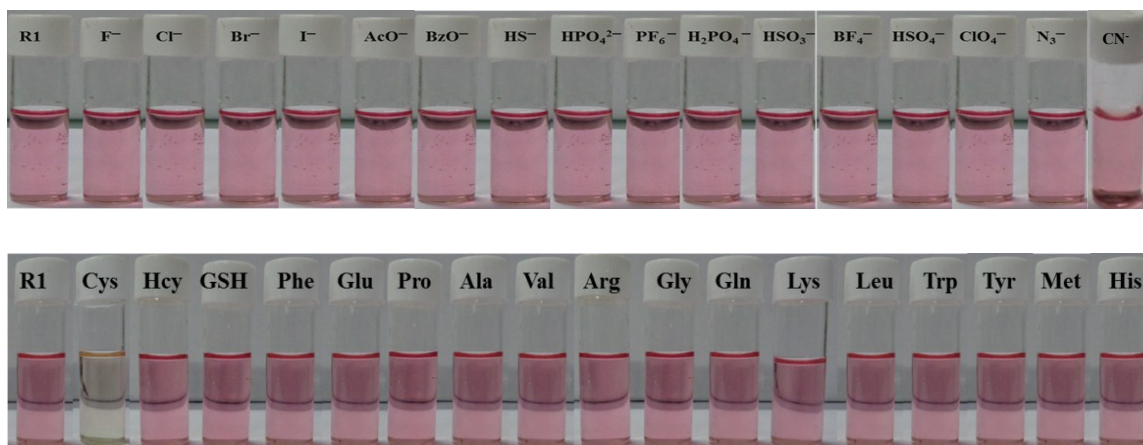


Figure S3: Detection limit and calibration curves for **R1** with Cys from UV-visible titration data

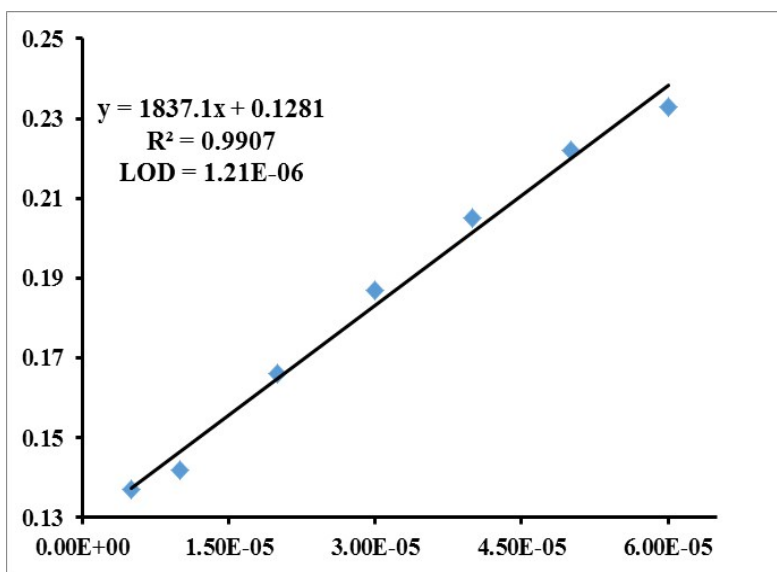


Figure S4: Non-linear curve fitting for **R1** with Cys from UV-visible titration data

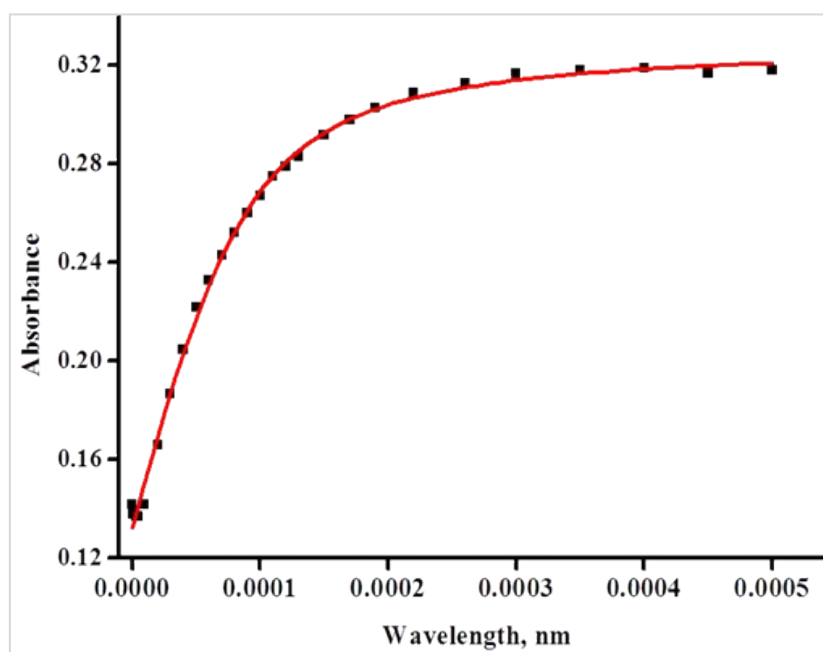


Figure S5: Fluorescence response of **R1** in the presence of different analytes under the UV lamp

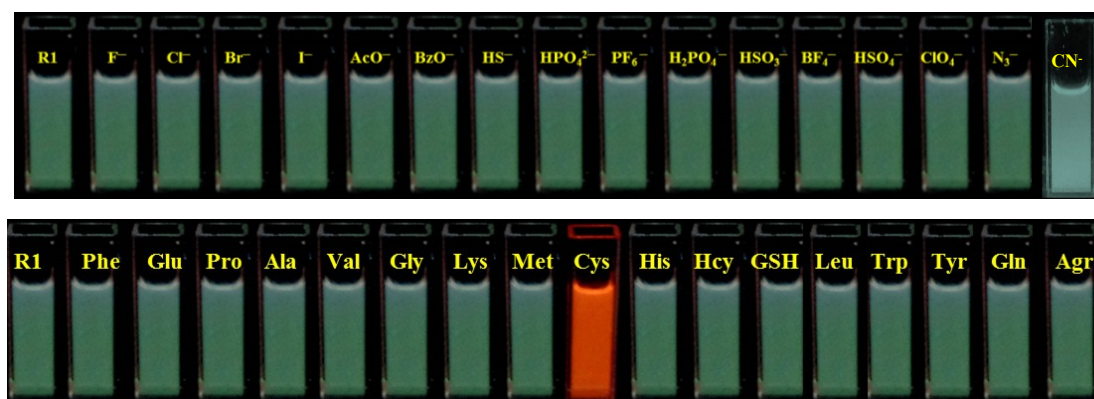


Figure S6: Non-linear curve fitting for **R1** with Cys from fluorescence titration data

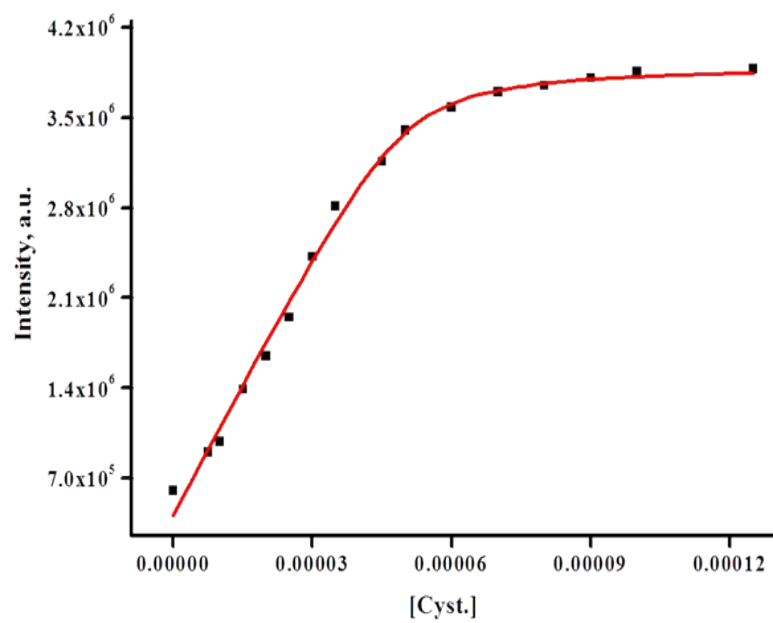


Figure S7: Detection limit and calibration curves for **R1** with Cys from fluorescence titration data

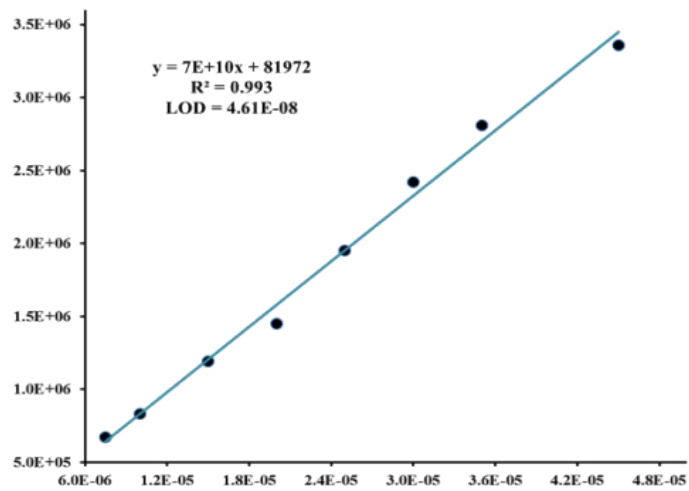


Figure S8: UV-vis. absorption spectrum of **R1** towards different anions

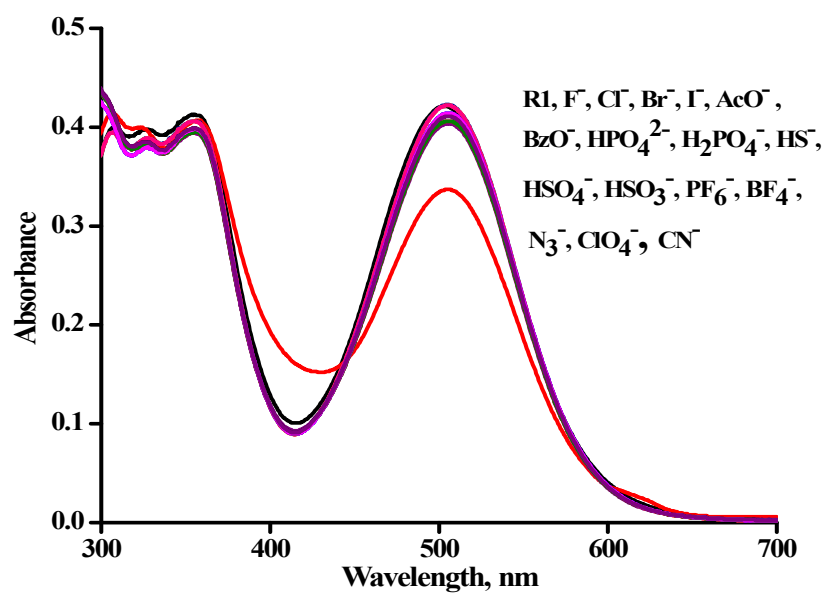


Figure S9: Emission spectrum of **R1** in the presence of different anions

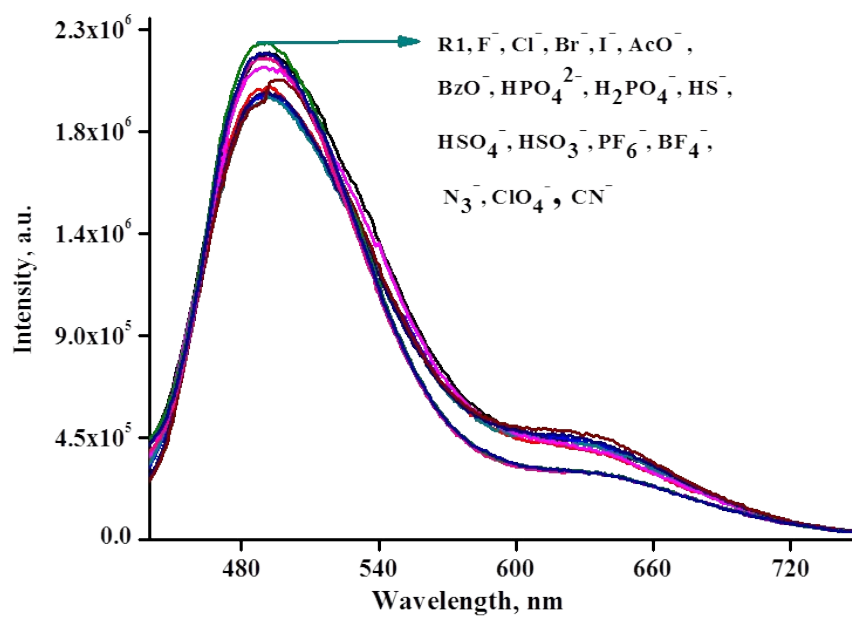


Figure S10: A plausible mechanism for selective response of R1 towards Cysteine

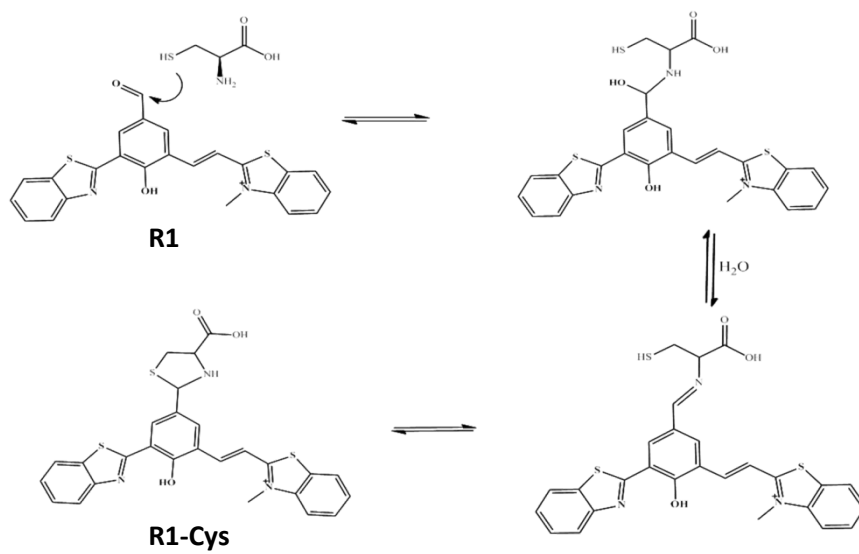


Figure S11: HRMS spectrum of R1-Cys

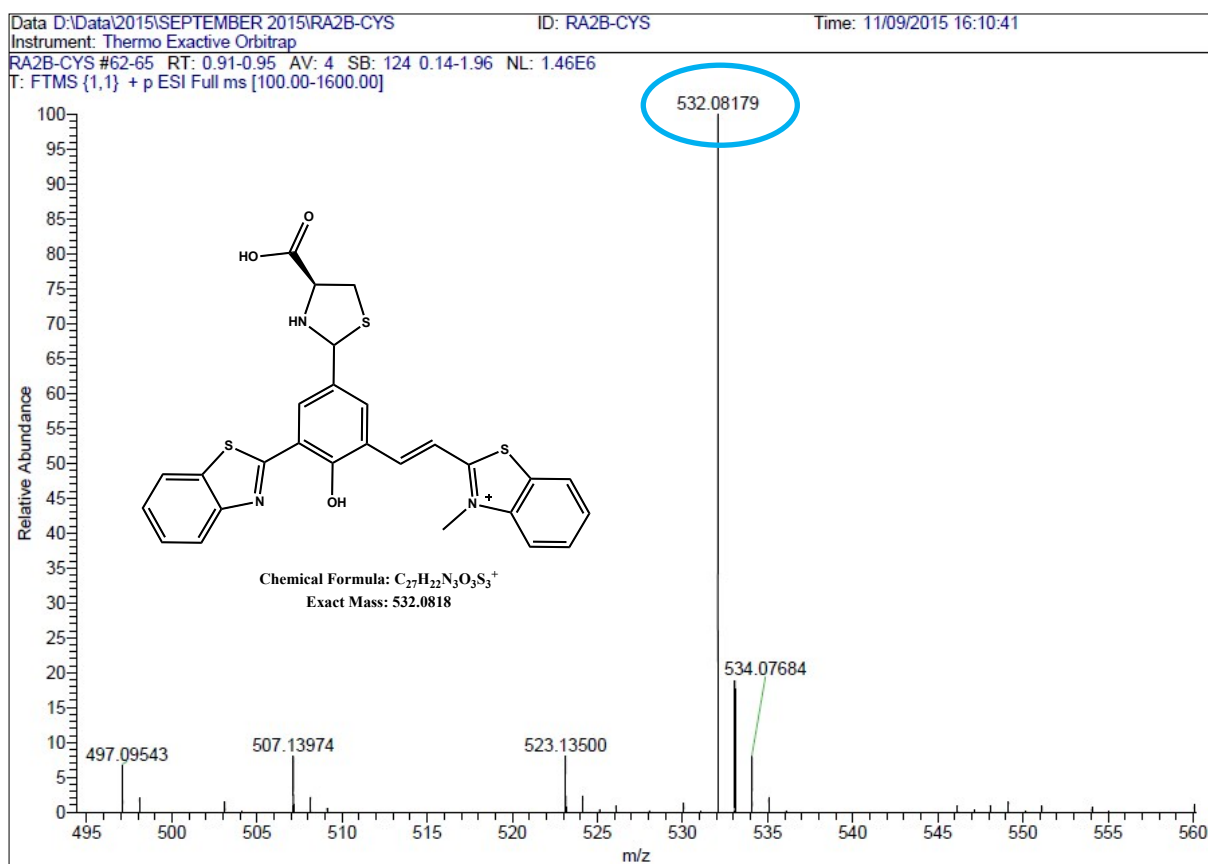


Figure S12: Optimised structure of **R1** and **R1-Cys**

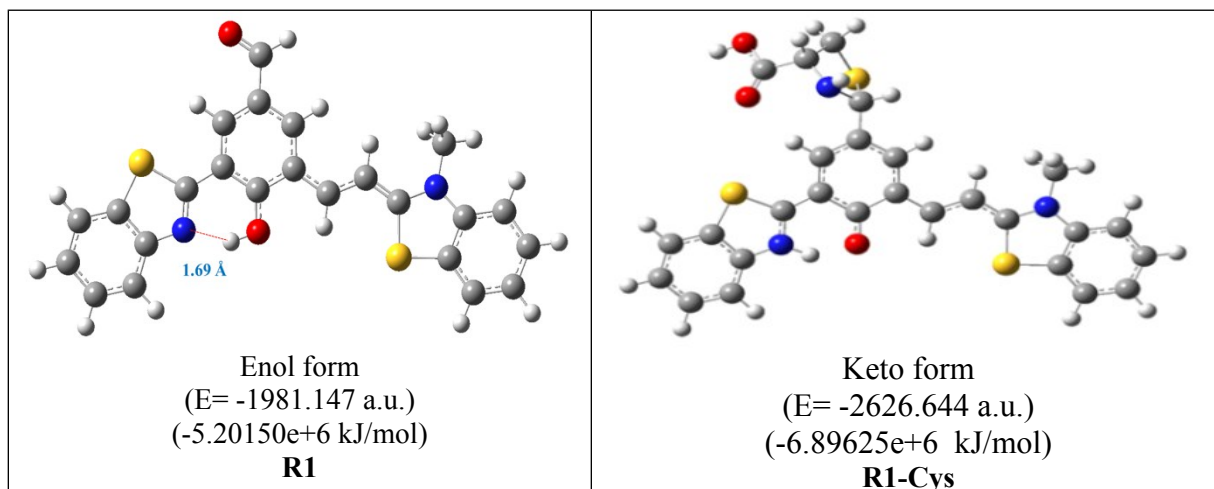


Figure S13. Cytotoxicity profile of R1 on HeLa cells after 24 hr treatment

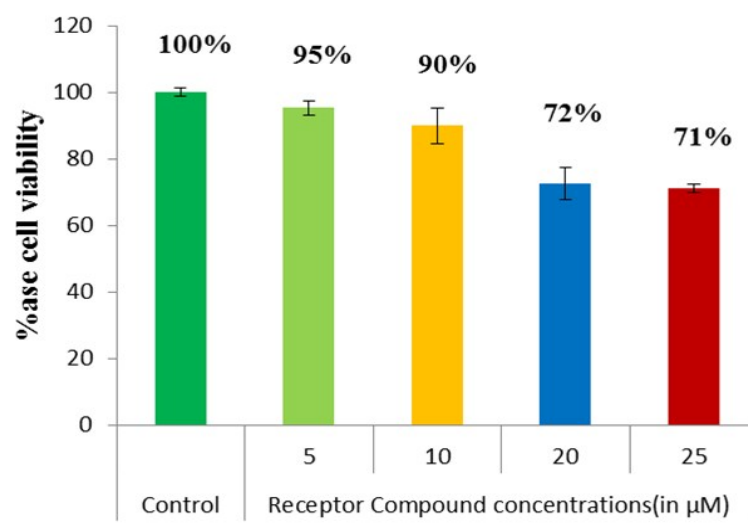


Figure S14: ¹H NMR spectrum of R1

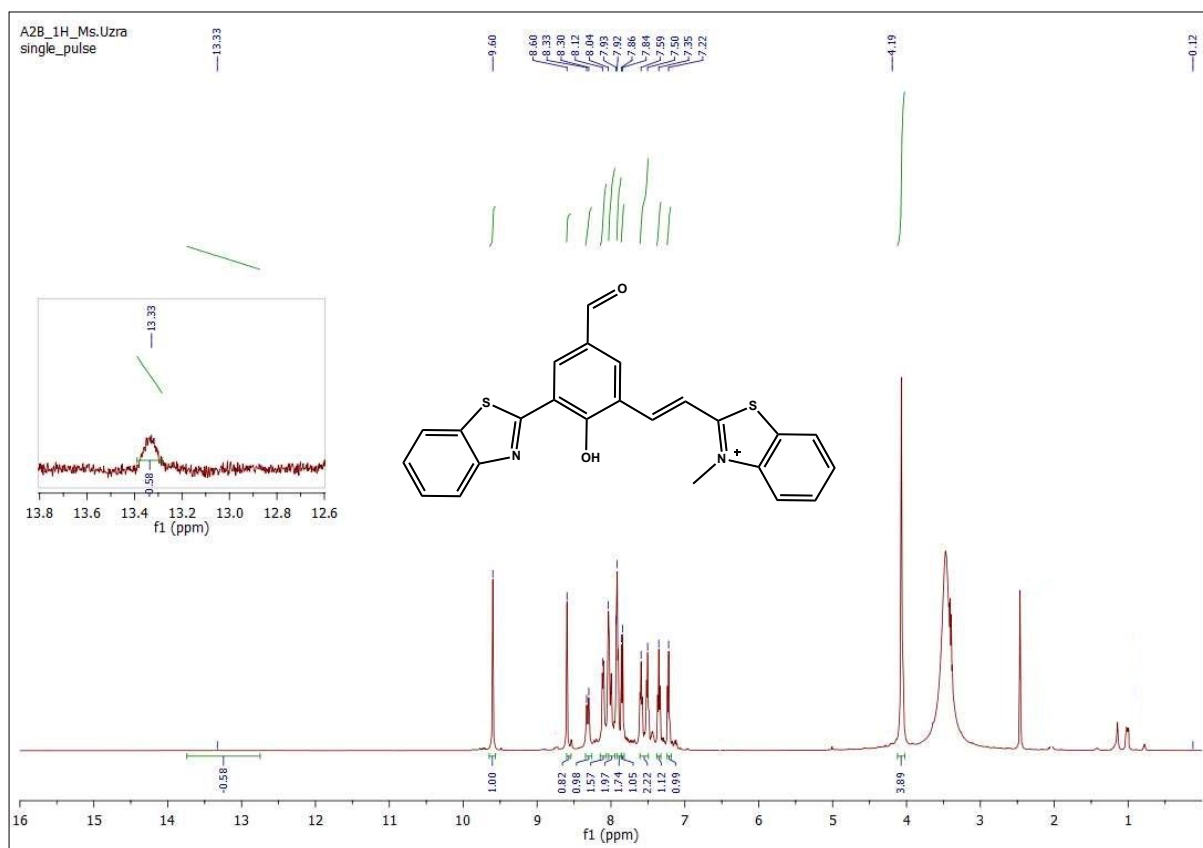


Figure S15: ¹³C NMR spectrum of R1

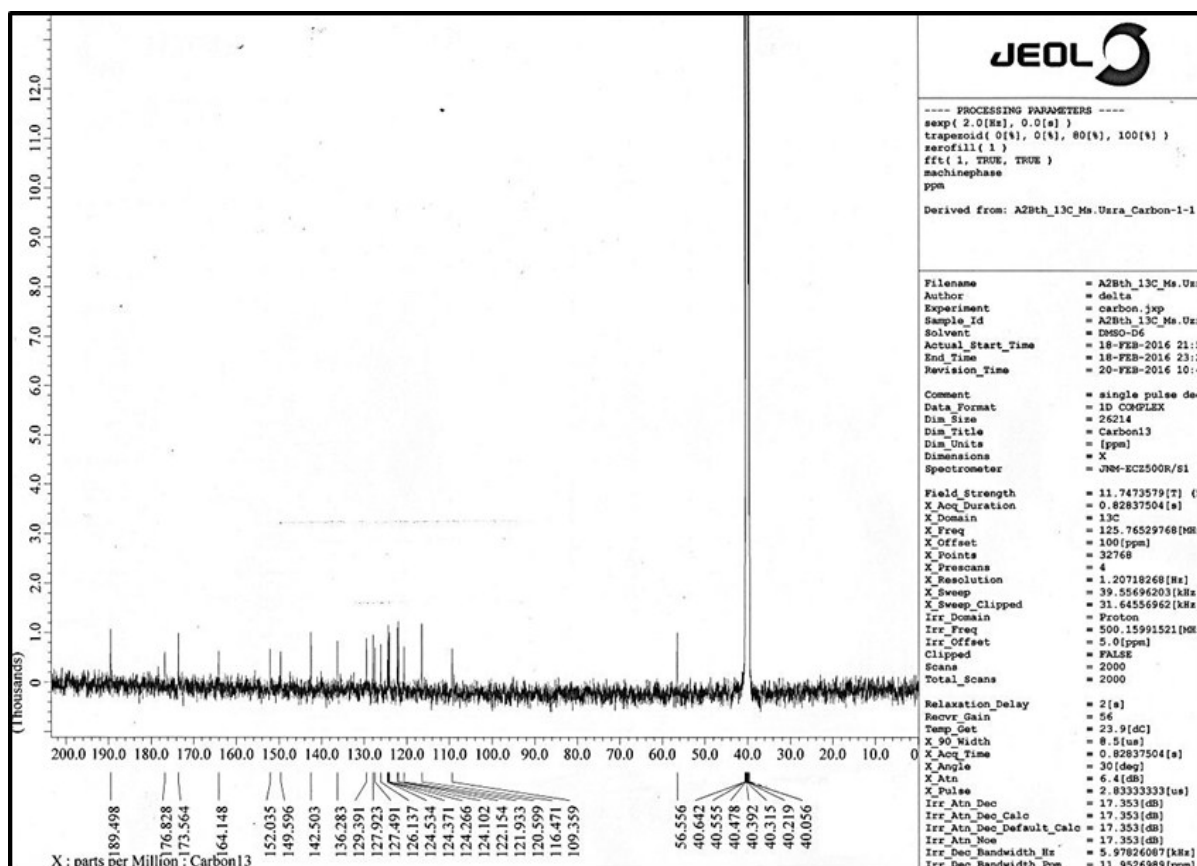


Figure S16: IR spectrum of R1

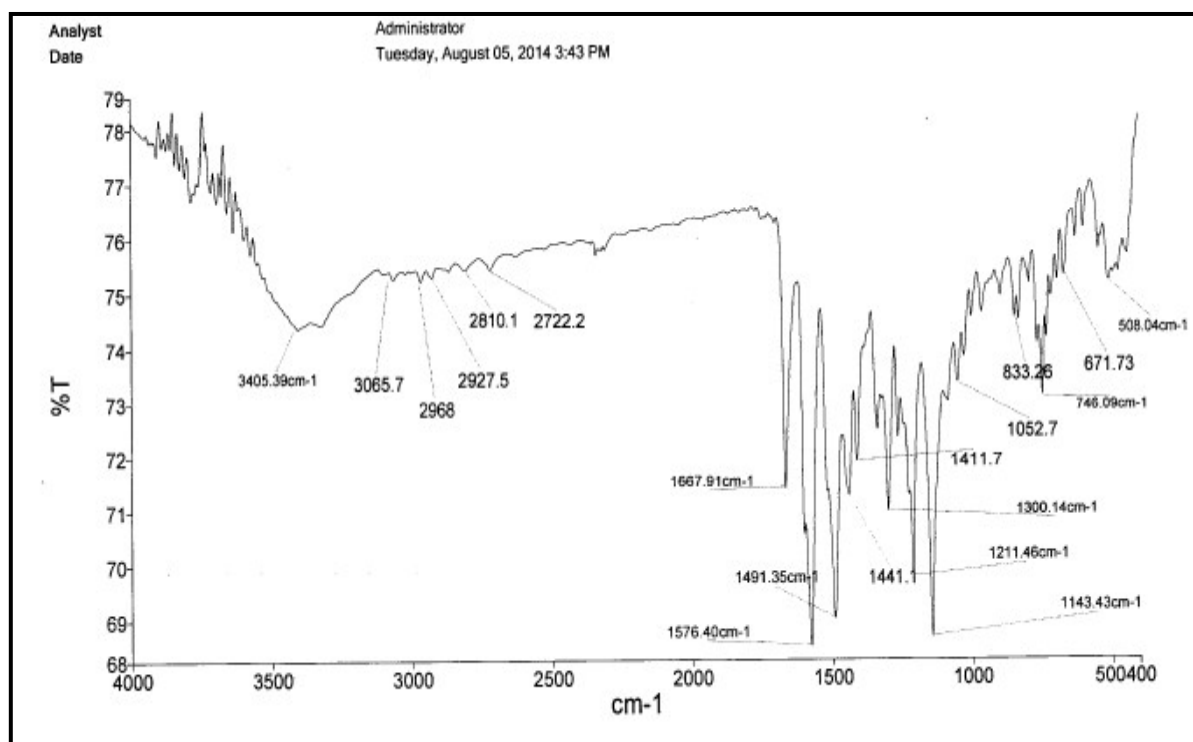


Figure S17: MASS spectrum of R1

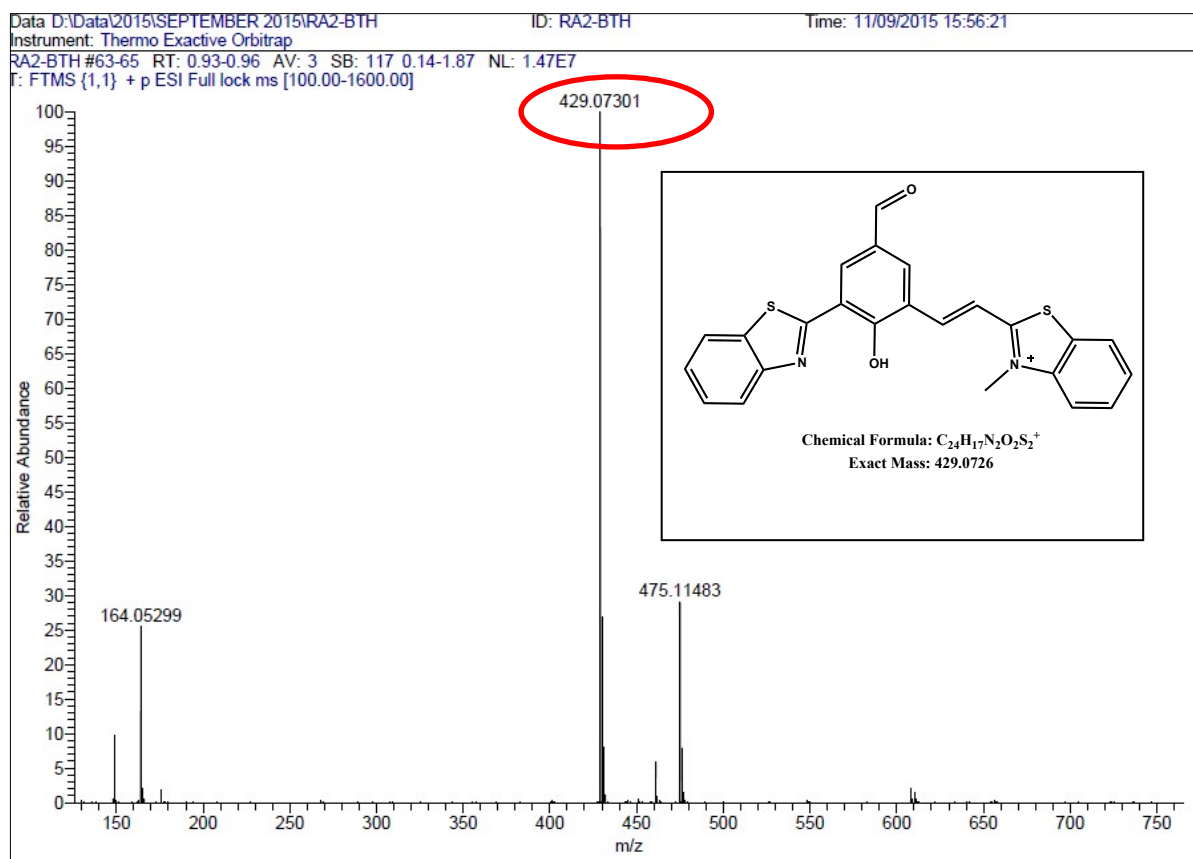


Figure S18: ^1H - ^1H COSY spectrum of R1

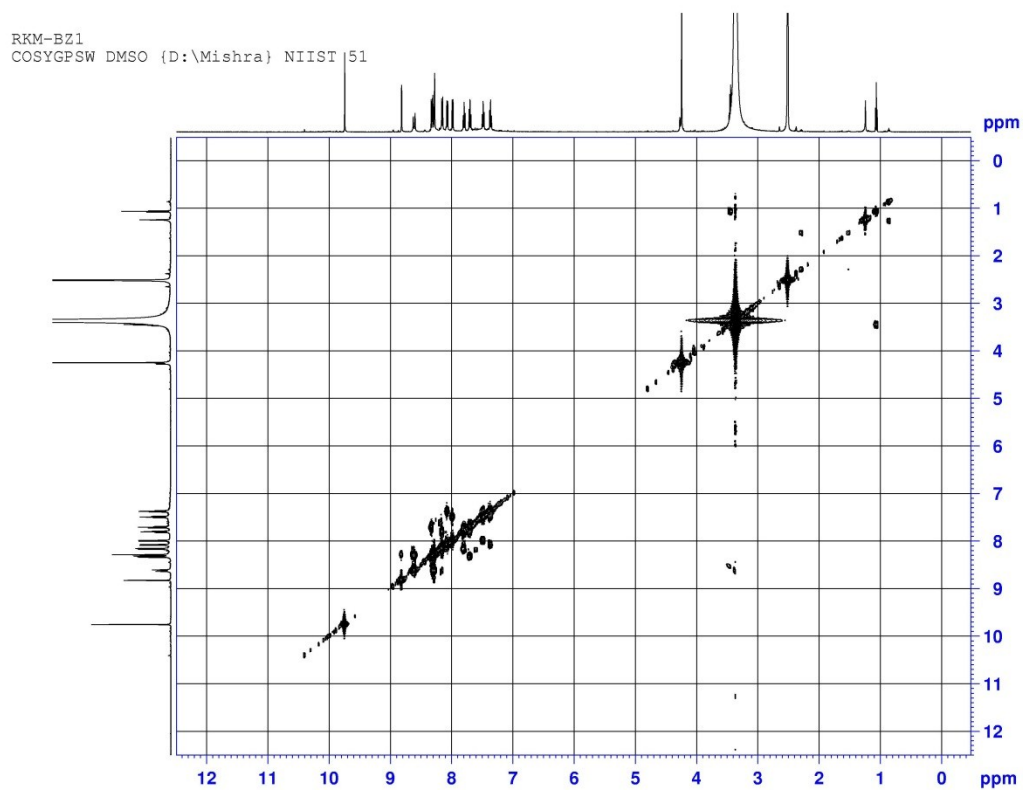
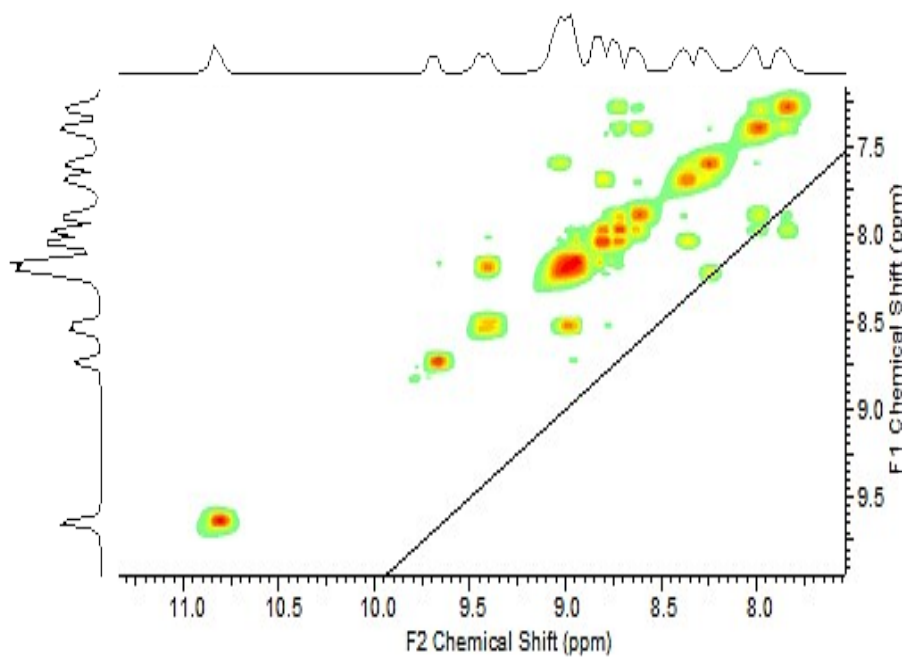
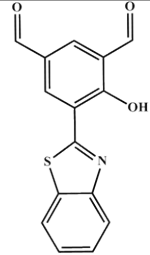
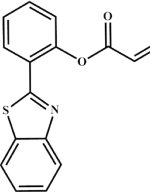
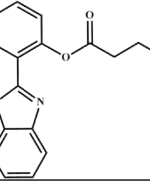
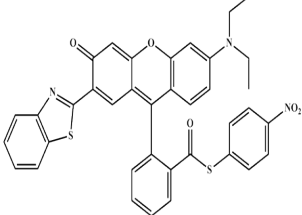
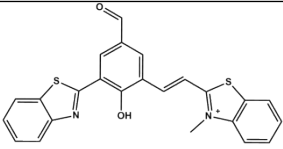


Table S1: Comparison of Fluorescent ES IPT Probes for Cysteine based on HBT derivative

S. No.	Probes	λ_{ex} and (λ_{em} / Keto λ_{em}) of probes in nm	Shift in (Enol λ_{em} / Keto λ_{em}) of probes in presence of cysteine	Solvent used for detection	Detection limit	Response time	Interference
ref 30		344 (436/ 521)	Enol (436) band decreases while keto. (521) one increases	HEPES buffer (at pH 7.4)	-----	~3 min to 5 min.	HCy
ref 31		304 (377/487)	Enol (377) band decreases while keto. (487) one increases	EtOH/phosphate buffer (20 mM, pH 7.4, 2:8 v/v)]	0.11 μ M	9 min.	HCy
ref 32		330 (380 /467)	Both the band increases (380 /467)	DMSO: 10 mM HEPES (v/v 8 : 2)	2.8 μ M	15 min	GSH
ref 33		305 (rhodol emission at 587 and HBT emission 454)	Rhodol emission at 587 decreases while HBT emission at 454 increases	DMF/ phosphate buffer (3 : 7 v/v, 20 mM, pH 7.4)	44 nM	5 min For Cys	Same response for Hcy , red fluorescent for GSH
R1	 Present Work	430 nm (492/625)	Enol. (492) band decreases while keto. (625) one increases	ACN/ H ₂ O (3:7 v/v)	49 nm	~ 1.0 min	No interference from Hcy/GSH