

## Azaindole-1,2,3-triazole in a tripod for selective sensing of chloride, dihydrogenphosphate and ATP under different conditions

Kumaresh Ghosh,<sup>\*a</sup> Debasis Kar,<sup>b</sup> Soumen Joardar,<sup>b</sup> Asmita Samadder<sup>b</sup> and Anisur Rahaman Khuda-Bukhsh<sup>b</sup>

Departments of Chemistry<sup>a</sup> and Zoology<sup>b</sup>, University of Kalyani, Kalyani, Nadia-741235, India,

Email: [ghosh\\_k2003@yahoo.co.in](mailto:ghosh_k2003@yahoo.co.in)

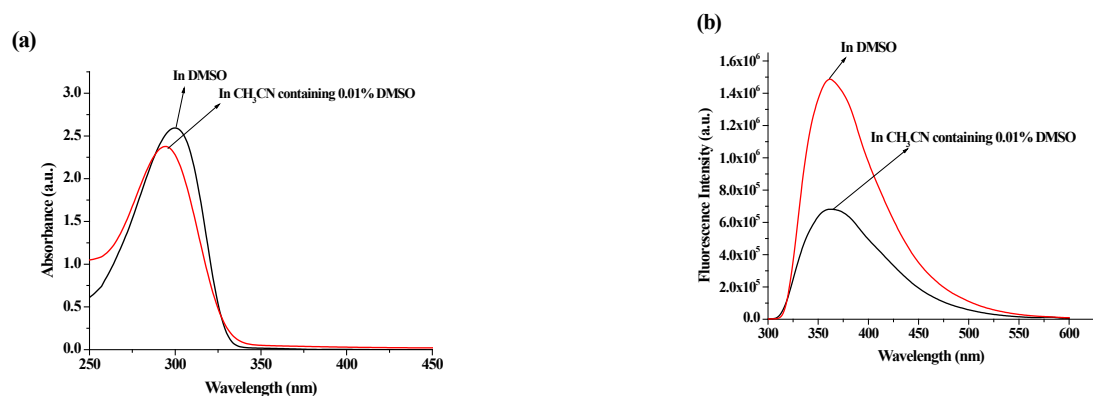
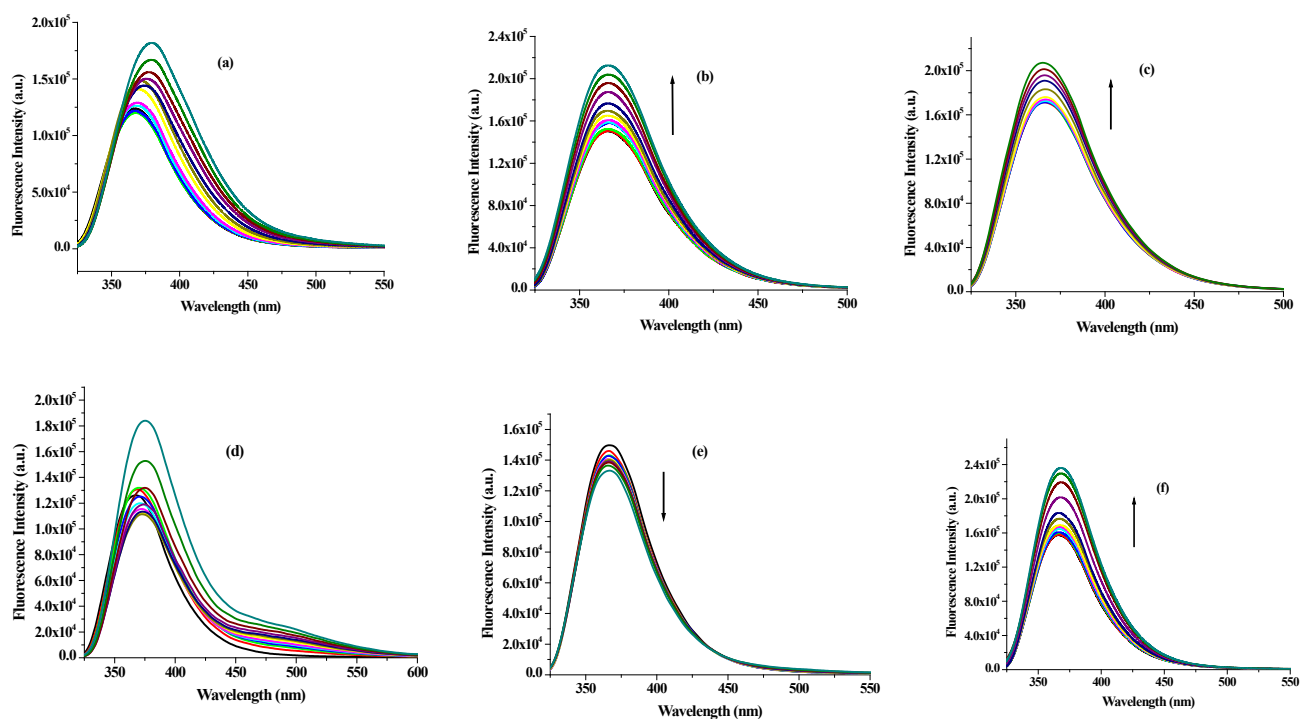
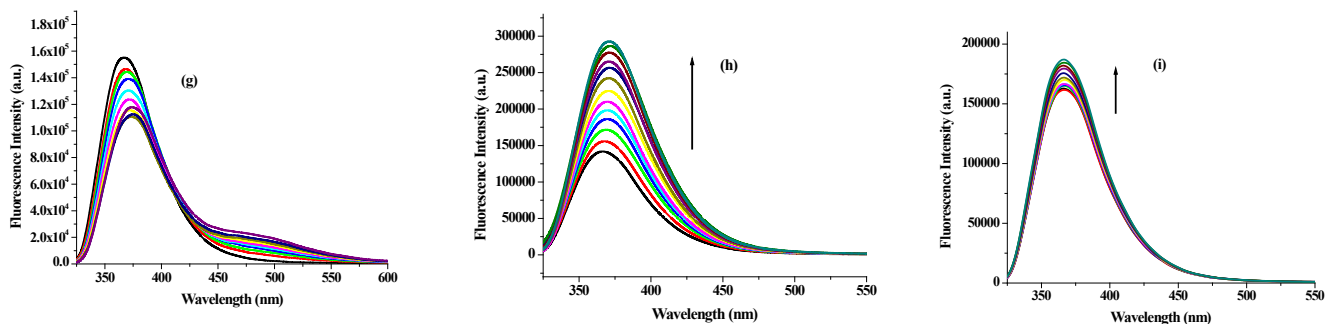
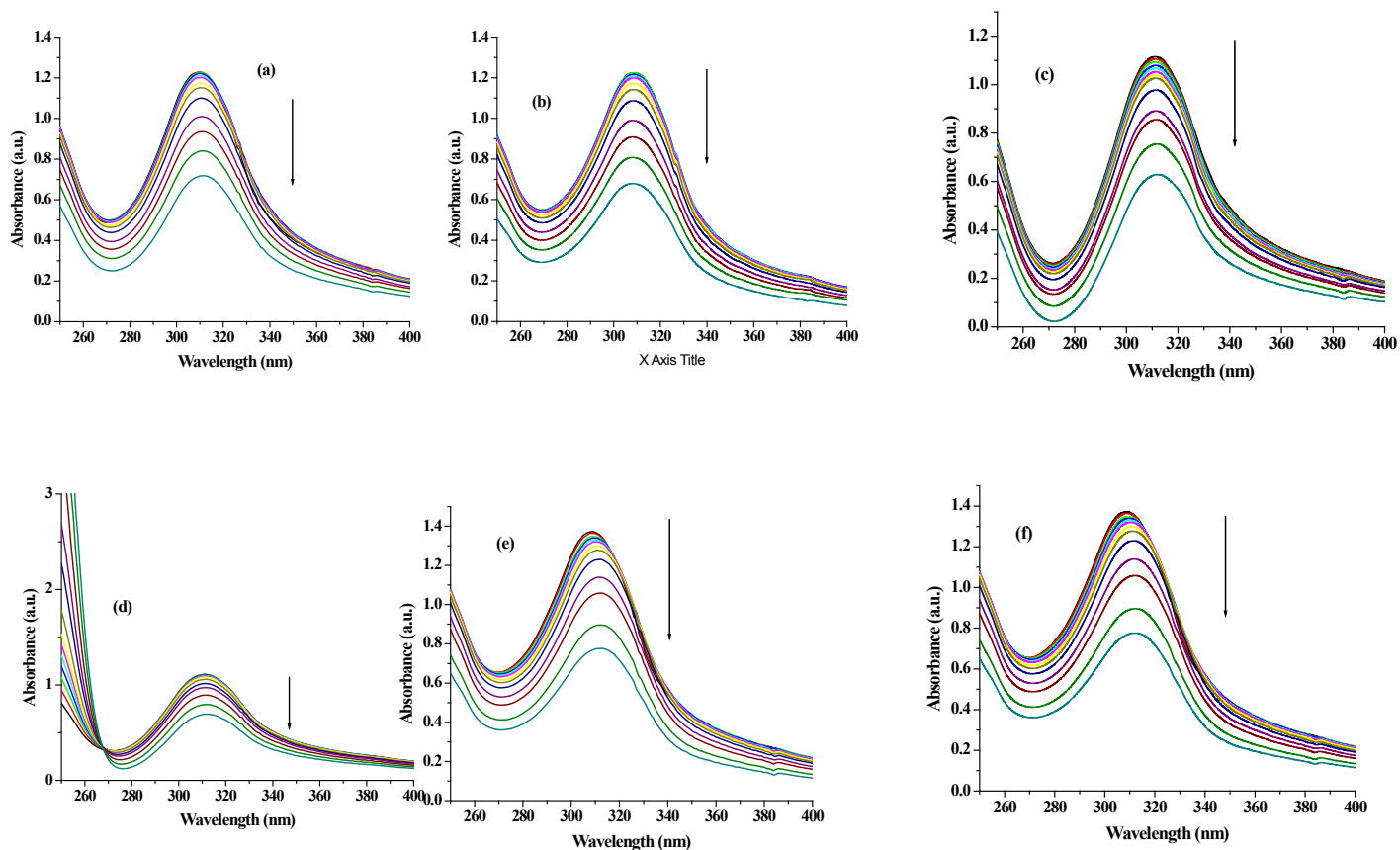


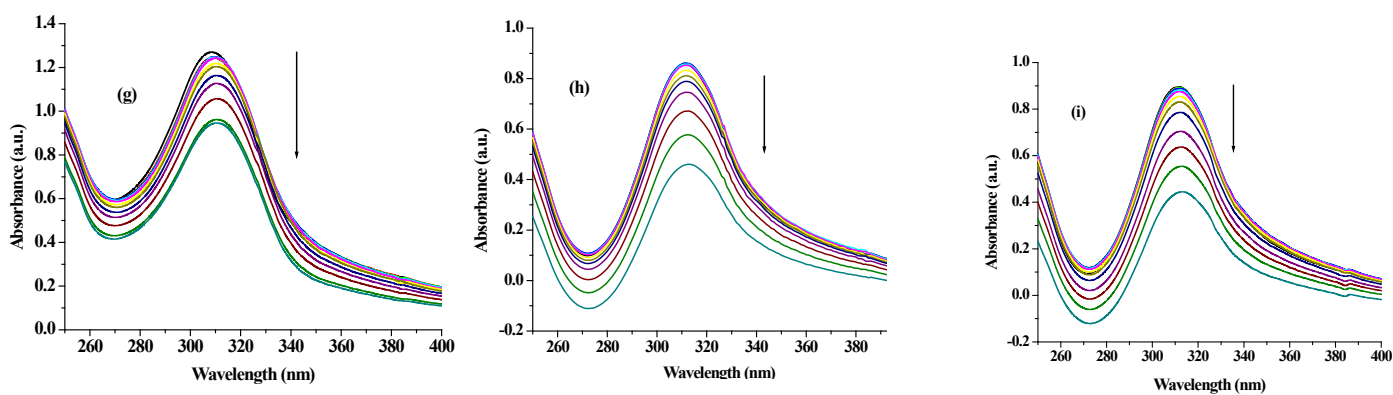
Figure 1S. Absorbance spectra (a) and emission spectra (b) of 2 ( $c = 5.73 \times 10^{-5}$  M) in different solvents.



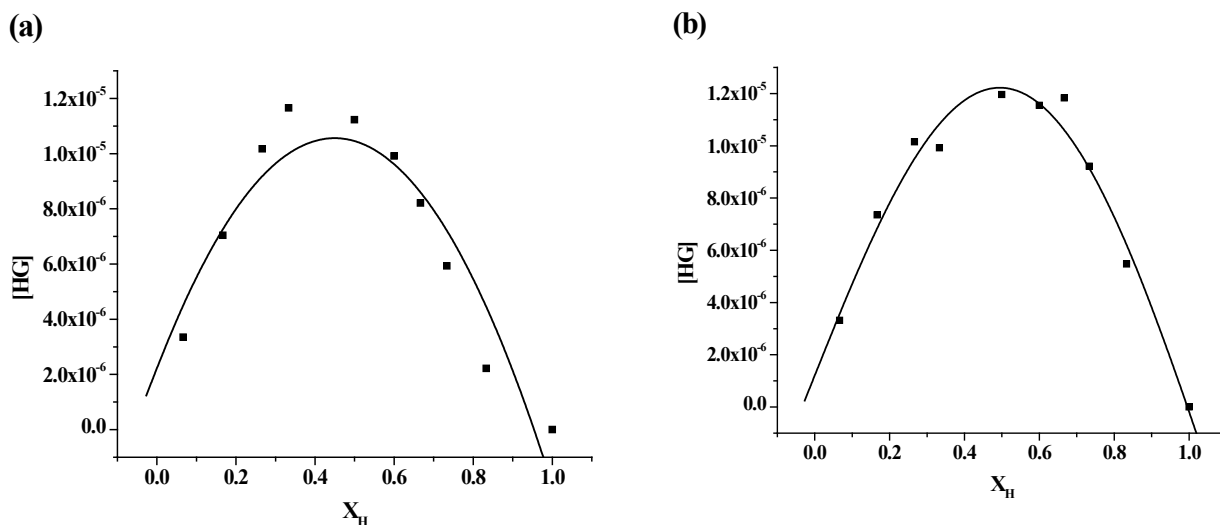


**Figure 2S.** Change in emission of **1** ( $c = 5.02 \times 10^{-5}$  M) upon addition of a)  $F^-$  (b)  $Br^-$  (c)  $I^-$  (d)  $P_2O_7^{4-}$  (e)  $HSO_4^-$  (f)  $ClO_4^-$  (g)  $HP_2O_7^{3-}$  (h)  $AcO^-$  (i)  $NO_3^-$  in  $CH_3CN$  containing 0.01% DMSO [changes in Figs. a, d and g are irregular].

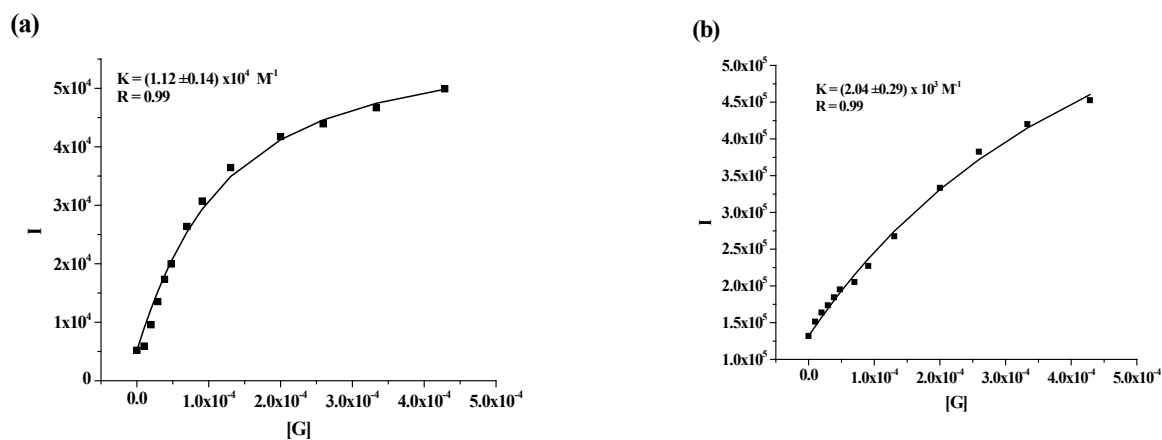




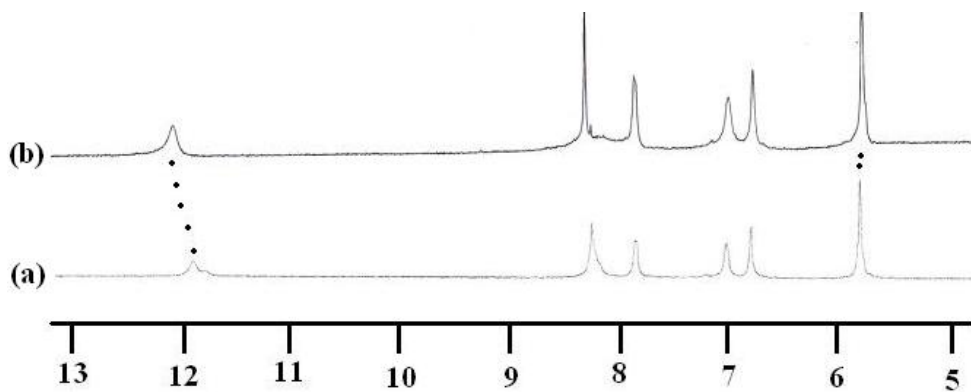
**Figure 3S.** Change in absorbance of **1** ( $c = 2.51 \times 10^{-5}$  M) upon addition of a)  $\text{F}^-$  (b)  $\text{Br}^-$  (c)  $\text{I}^-$  (d)  $\text{P}_2\text{O}_7^{4-}$  (e)  $\text{HSO}_4^-$  (f)  $\text{ClO}_4^-$  (g)  $\text{HP}_2\text{O}_7^{3-}$  (h)  $\text{AcO}^-$  (i)  $\text{NO}_3^-$  in  $\text{CH}_3\text{CN}$  containing 0.01% DMSO.



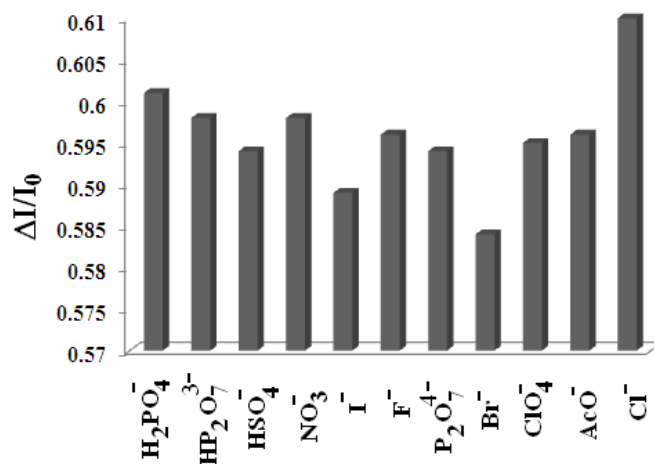
**Figure 4S.** UV-vis Job plots for **1** with (a)  $\text{H}_2\text{PO}_4^-$  and (b)  $\text{Cl}^-$  ions in  $\text{CH}_3\text{CN}$  containing 0.01% DMSO ( $[\text{H}] = [\text{G}] = 5.42 \times 10^{-5}$  M).



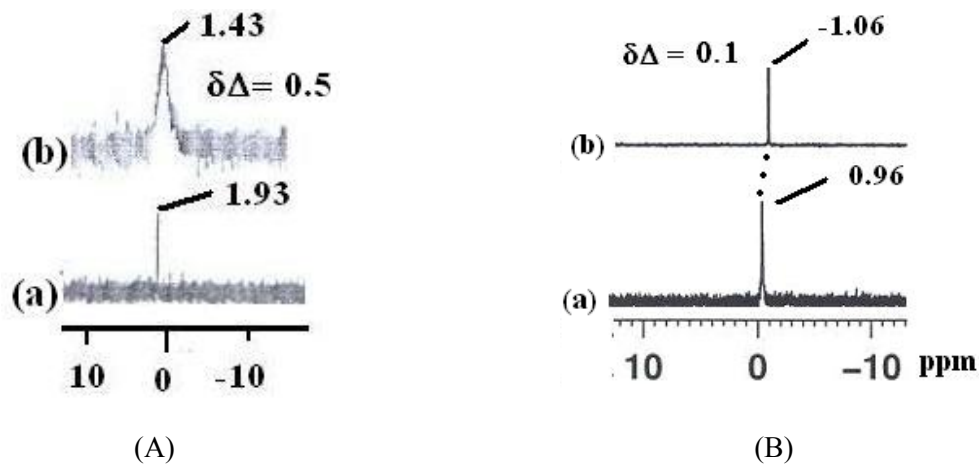
**Figure 5S.** Non linear plots for binding constants of **1** with (a)  $\text{H}_2\text{PO}_4^-$  and (b)  $\text{Cl}^-$  in  $\text{CH}_3\text{CN}$  containing 0.01% DMSO.



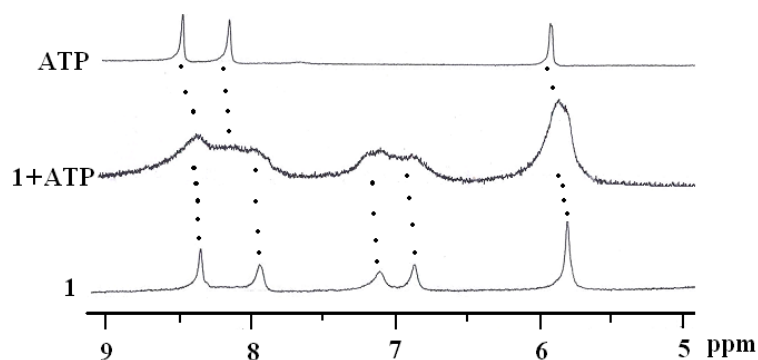
**Figure 6S.** Partial  $^1\text{H}$  NMR (400 MHz) of **1** ( $c = 4.63 \times 10^{-3} \text{ M}$ ) in (a)  $\text{CD}_3\text{CN}$  containing 2%  $\text{d}_6$ -DMSO and (b) in  $\text{d}_6$ -DMSO.



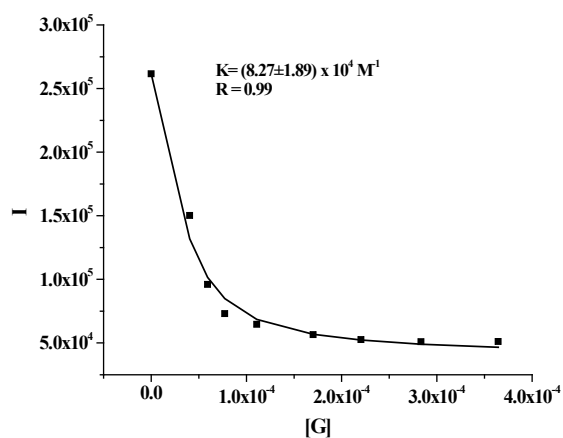
**Figure 7S.** Change in fluorescence ratio of **1** ( $c = 5.07 \times 10^{-5}$  M) at 370 nm upon addition of 15 equiv. amounts of different guests in DMSO.



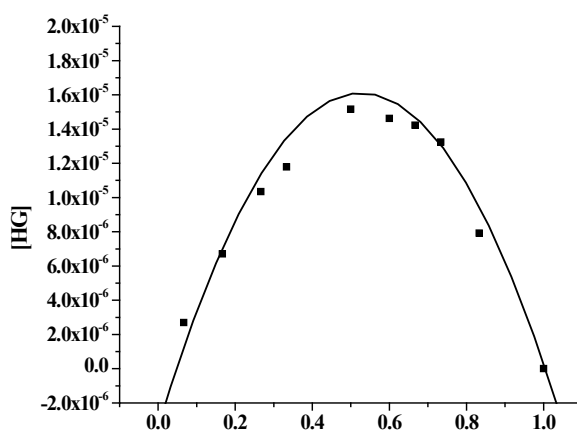
**Figure 8S.** Partial  $^{31}\text{P}$  NMR (400 MHz) of **1** ( $c = 4.68 \times 10^{-3}$  M) in (A) a. absence, b. presence of 1 equiv. amount of  $\text{TBAH}_2\text{PO}_4$  in  $\text{CD}_3\text{CN}$  containing 4%  $d_6$ -DMSO; (B) a. absence, b. presence of 1 equiv. amount of  $\text{TBAH}_2\text{PO}_4$  in  $d_6$ -DMSO.



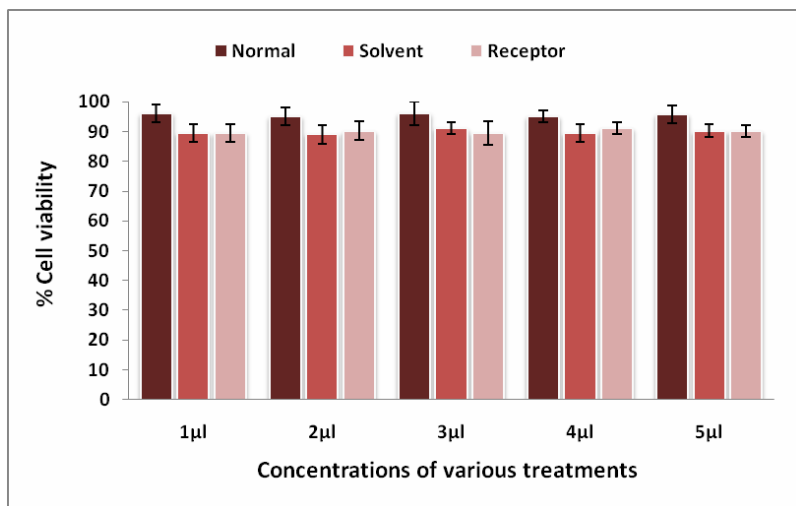
**Figure 9S.** Partial <sup>1</sup>H NMR (400 MHz) of **1** ( $c = 5.96 \times 10^{-3}$  M) in presence and absence of 1 equiv. amount of ATP in  $d_6$ -DMSO:  $D_2O$  (1:1, v/v).



**Figure 10S.** Non linear binding constant plot for **1** with ATP in  $CH_3CN$ :  $H_2O$  (1:1, v/v) at pH = 7.3 containing 10mM HEPPEs buffer.

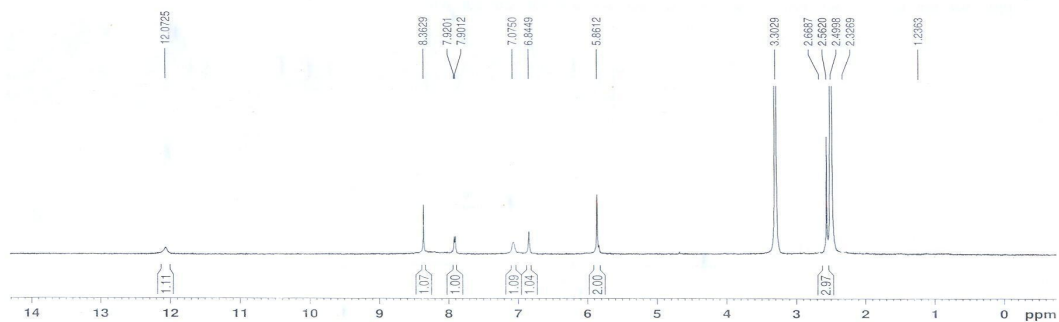
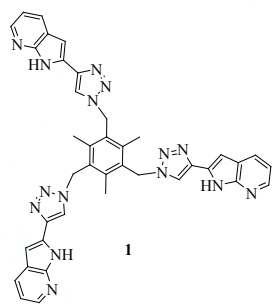


**Figure 11S.** UV-VIS Job plot for **1** with ATP in  $CH_3CN$ :  $H_2O$  (1:1, v/v) at pH = 7.3 containing 10mM HEPPEs buffer ( $[H] = [G] = 4.25 \times 10^{-5}$  M).



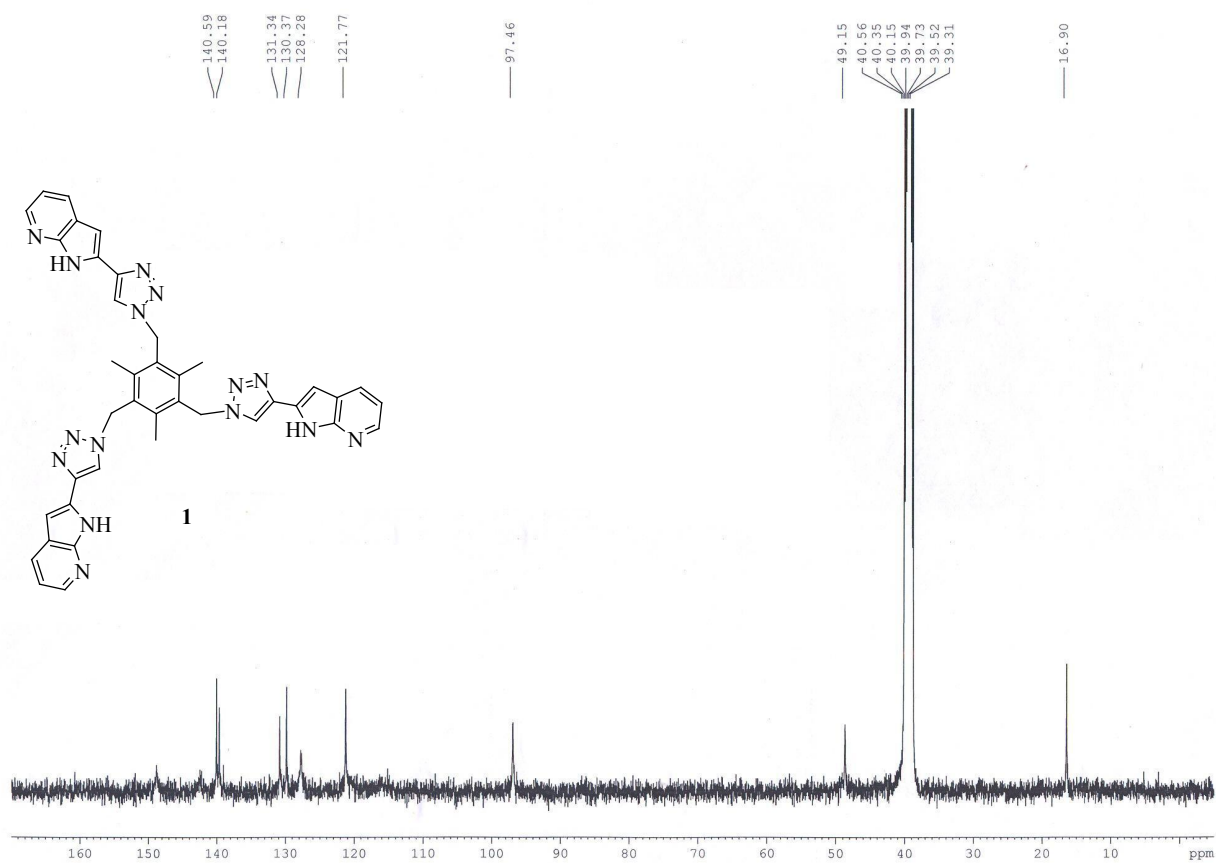
**Figure 12S.** MTT assay for receptor 1.

**<sup>1</sup>H NMR (400 MHz, d<sub>6</sub>-DMSO)**

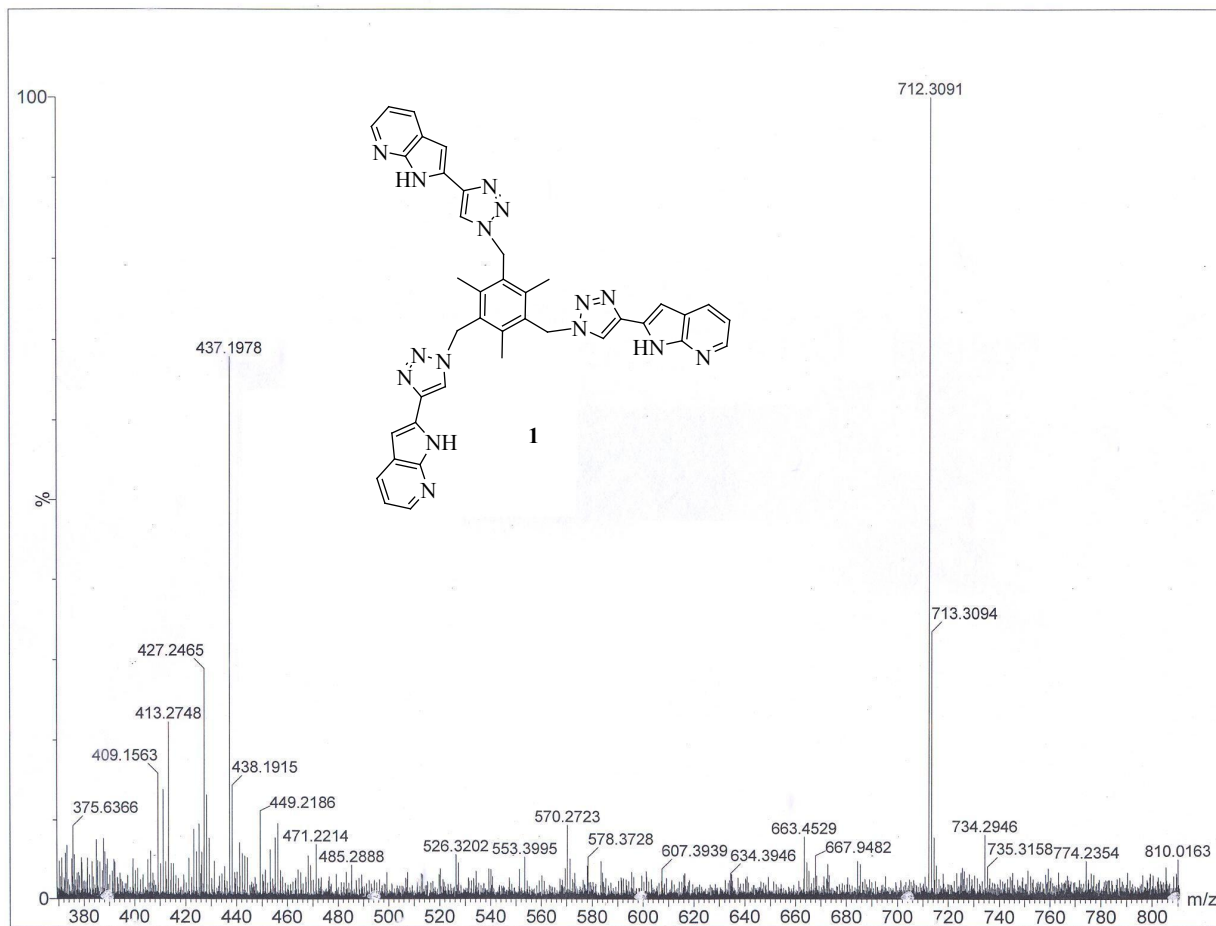




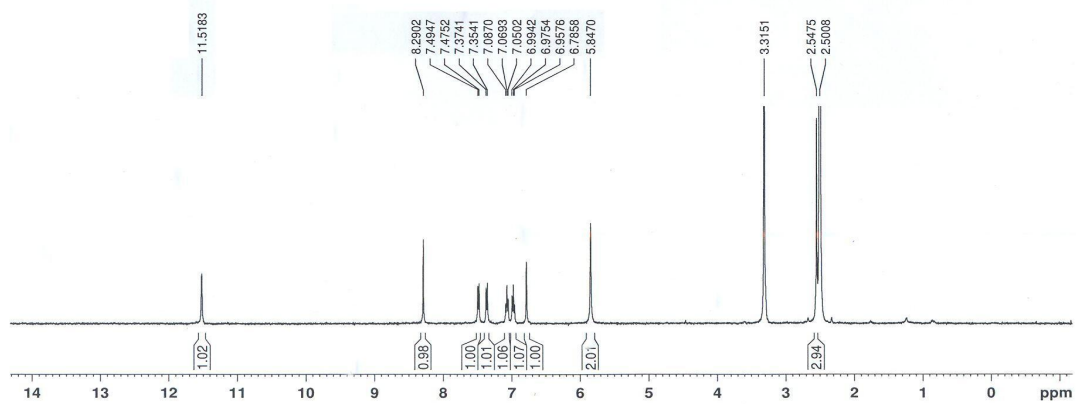
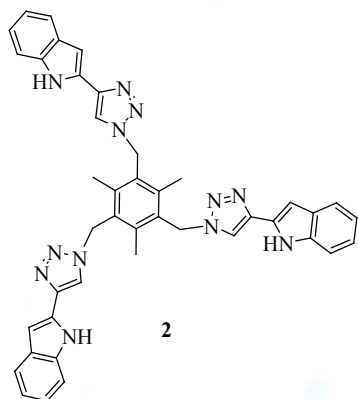
$^{13}\text{C}$  NMR (100 MHz,  $\text{d}_6\text{-DMSO}$ )



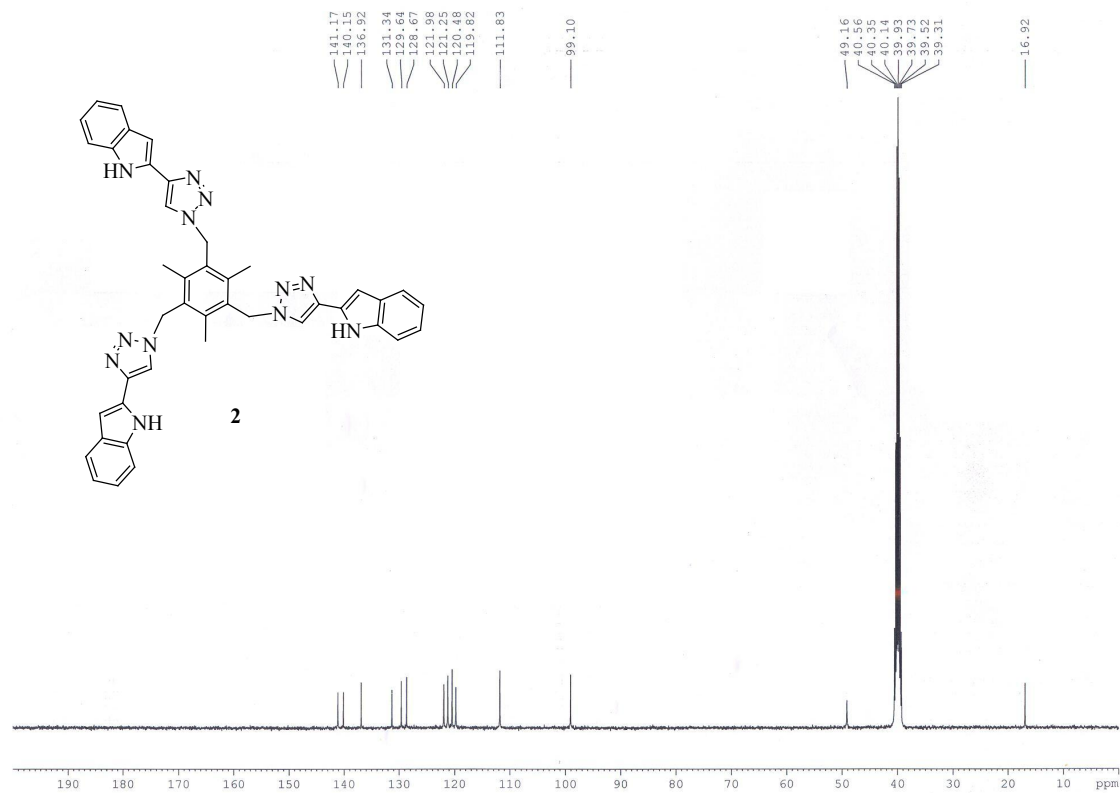
## Mass



**<sup>1</sup>H NMR (400 MHz, d<sub>6</sub>-DMSO)**



**$^{13}\text{C}$  NMR (100 MHz,  $\text{d}_6\text{-DMSO}$ )**



## Mass

