Electronic Supplementary Material (ESI) for RSC Advances

Azaindole-1,2,3-triazole coujugate as selective fluorometric sensor for dihydrogenphosphate

Kumaresh Ghosh[*a], Debasis Kar[a], Soumen Joardar[a], Debashis Sahu[b,c], Bishwajit Ganguly[*b,c]

[a]*Department of Chemistry, University of Kalyani, Kalyani, Nadia-741235, India, Email: ghosh_k2003@yahoo.co.in,* [b]*Computation and Simulation Unit(Analytical Discipline and Centralized Instrument Facility), CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, 364002.* [c]*Academy of Scientific and Innovative Research; CSIR- Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, 364002, India.*

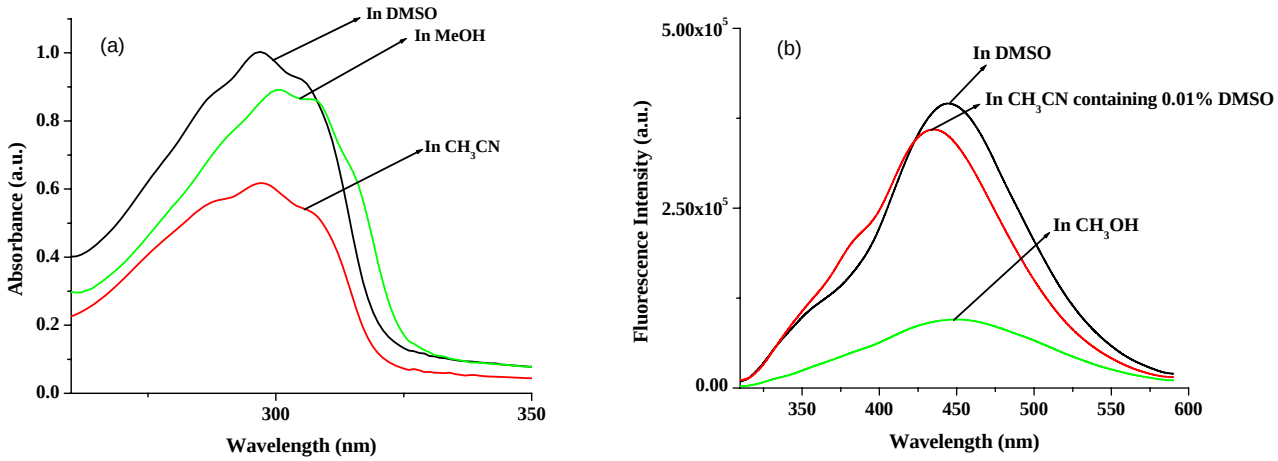


Figure 1S. (a) Absorption and (b) emission spectra of **3** (*c* = 3.09 x 10^{-5} M) in different solvents.

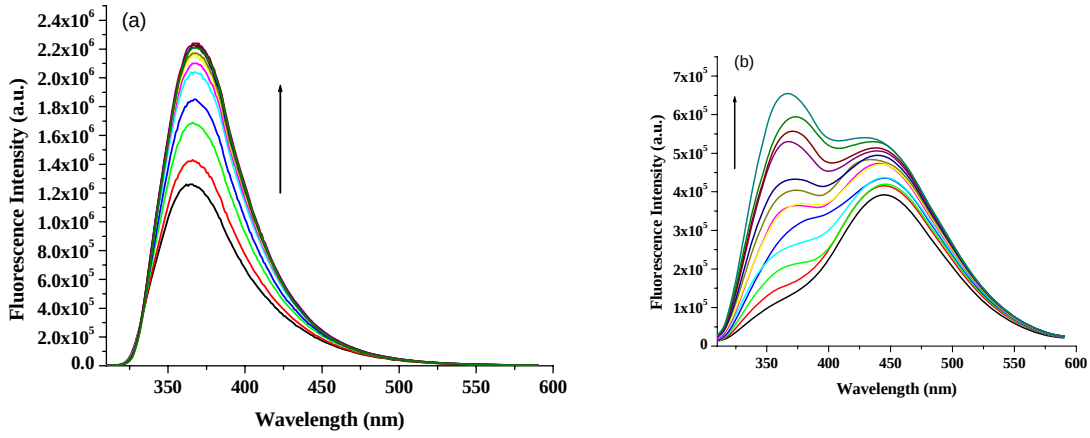


Figure 2S. Change in emission of (a) **1** (c = 3.23 x 10^{-5} M) and (b) **3** (c = 4.25 x 10^{-5} M) upon titration with DMSO in CH_3CN containing 0.01%DMSO.

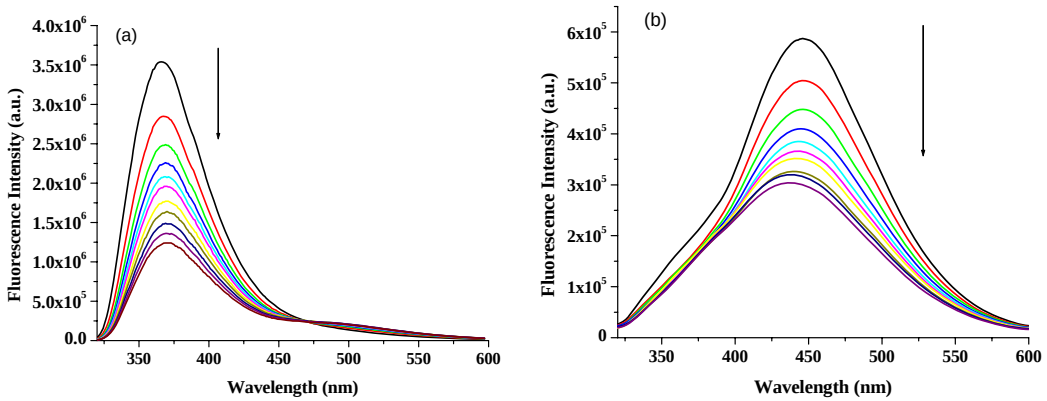


Figure 3S. Change in emission of (a) **1** (c = 3.25 x 10^{-5}M) and (b) **3** (c = 3.09 x 10^{-5} M) upon titration with CH_3OH in CH_3CN containing 0.01%DMSO.

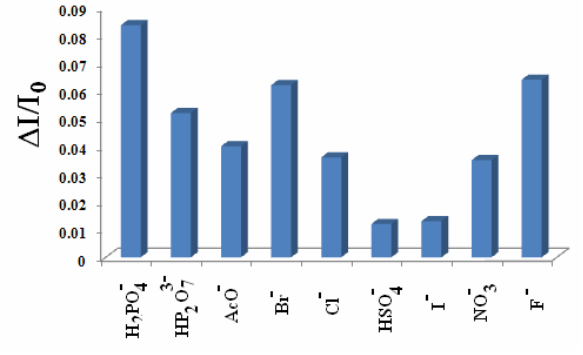


Figure 4S. Change in fluorescence ratio of **1** (*c* = 4.52 x 10^{-5} M) at 370 nm upon addition of 15 equiv. amounts of different guests in DMSO.

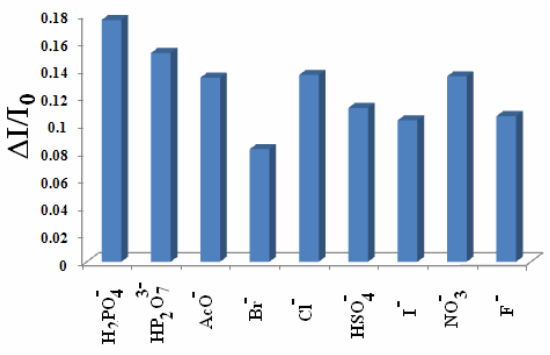


Figure 5S. Change in fluorescence ratio of **3** (*c* = 3.45 x 10^{-5} M) at 370 nm upon addition of 15 equiv. amounts of different guests in DMSO.

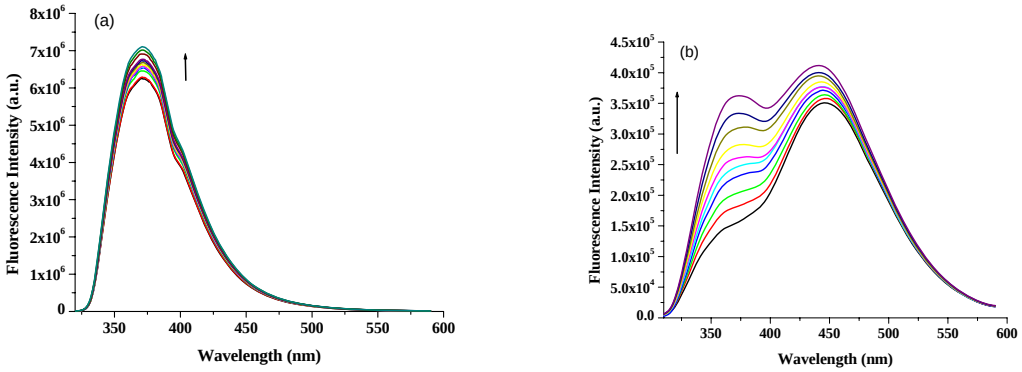


Figure 6S. Change in emission of (a) **1** (c = 4.52 x 10^{-5} M) and (b) **3** (c = 3.63 x 10^{-5} M) when titrated with $H_2PO_4^-$ (c = 1 x 10^{-3} M) in DMSO.

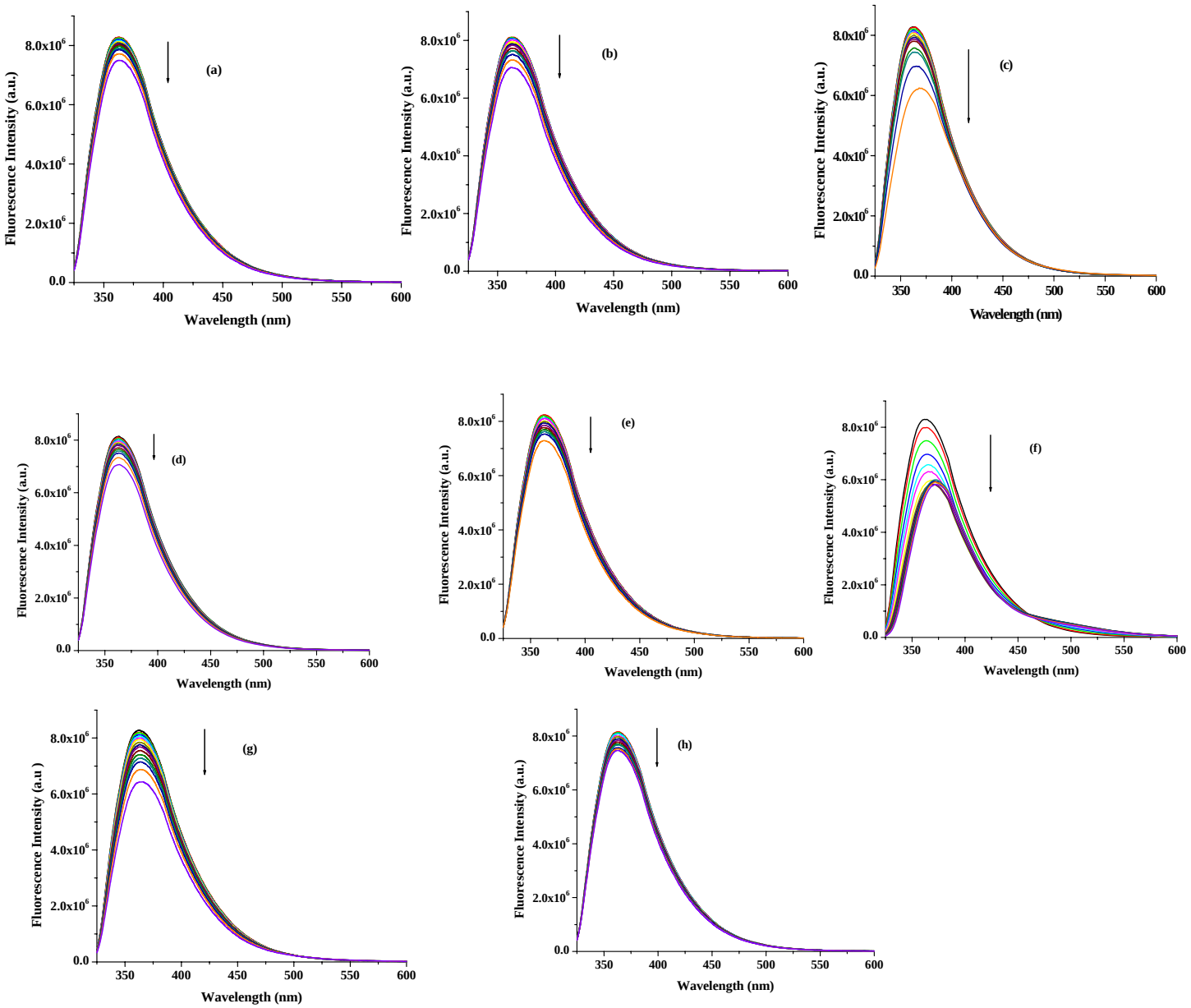


Figure 7S. Change in emission of **1** (c = 2.51 x 10^{-5} M) upon addition of a) Cl^-, b) Br^-, c) F^-, (d) I^-, e) HSO_4^-, (f) $HP_2O_7^{3-}$, (g)AcO^-, (h) NO_3^- in CH_3CN containing 0.01% DMSO.

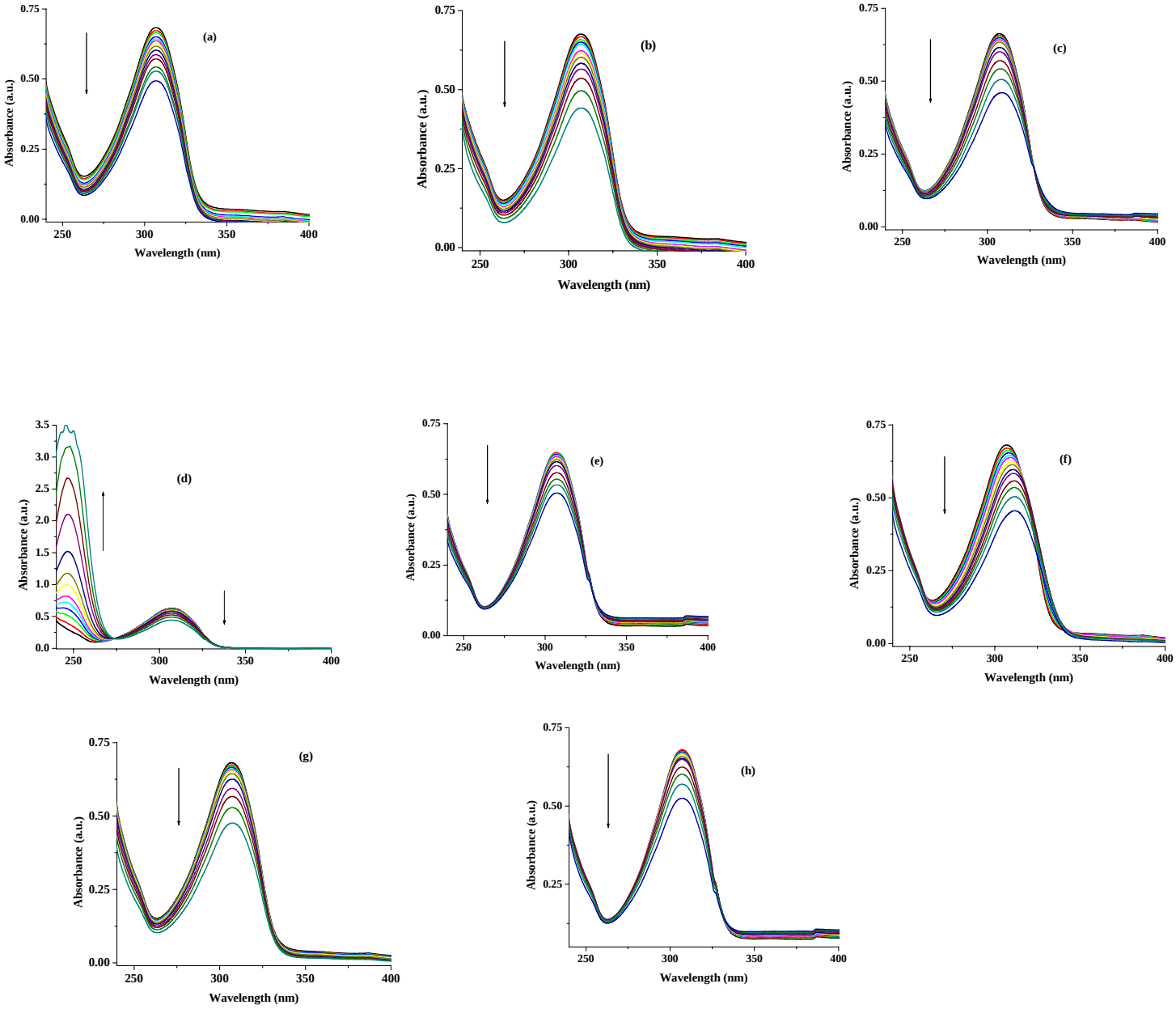


Figure 8S. Change in absorbance of 1 (c = 2.51 x 10^{-5} M) upon addition of a) Cl^-, b) Br^-, c) F^-, (d) I^-, e) HSO_4^-, (f) $HP_2O_7^{3-}$, (g)AcO^-, (h) NO_3^- in CH_3CN containing 0.01% DMSO.

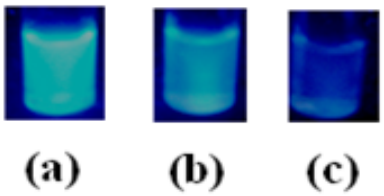


Figure 9S. Photographs of color change of (a) **1**(c = 2.5x10^{-5} M) and with 15 equiv. amounts of (b) $HP_2O_7^{3-}$ (*c* = 1 x 10^{-3} M) and (c) $H_2PO_4^-$ (*c* = 1 x 10^{-3} M) under UV illumination.

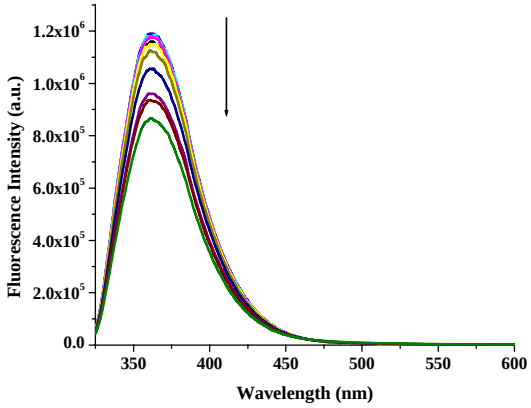


Figure 10S. Change in emission of receptor **2** (*c* = 2.21x 10^{-5} M) upon addition of 15 equiv. .amounts of $H_2PO_4^-$ (*c* = 1 x 10^{-3} M) in CH_3CN containing 0.01% DMSO.

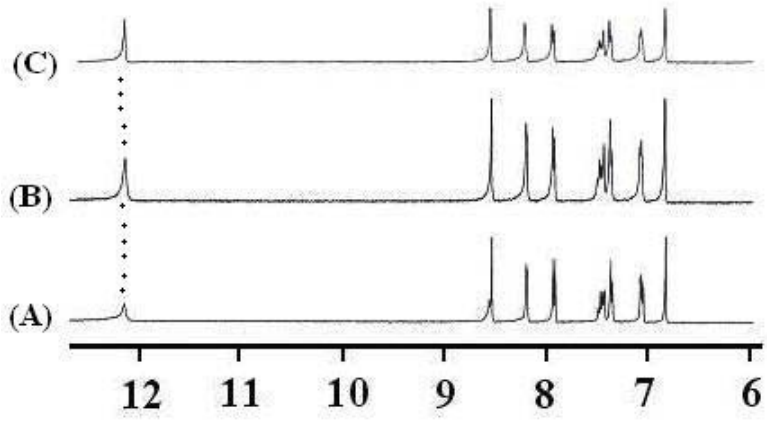


Figure 11S. Partial ^{1}H NMR (400 MHz) of **1** (*c* = 5.01 x 10^{-3} M) in the absence (A) and presence of 1 equiv (B) and 2 equiv (C) amounts of tetrabutylammonium dihydrogenphosphate in d_6-DMSO.

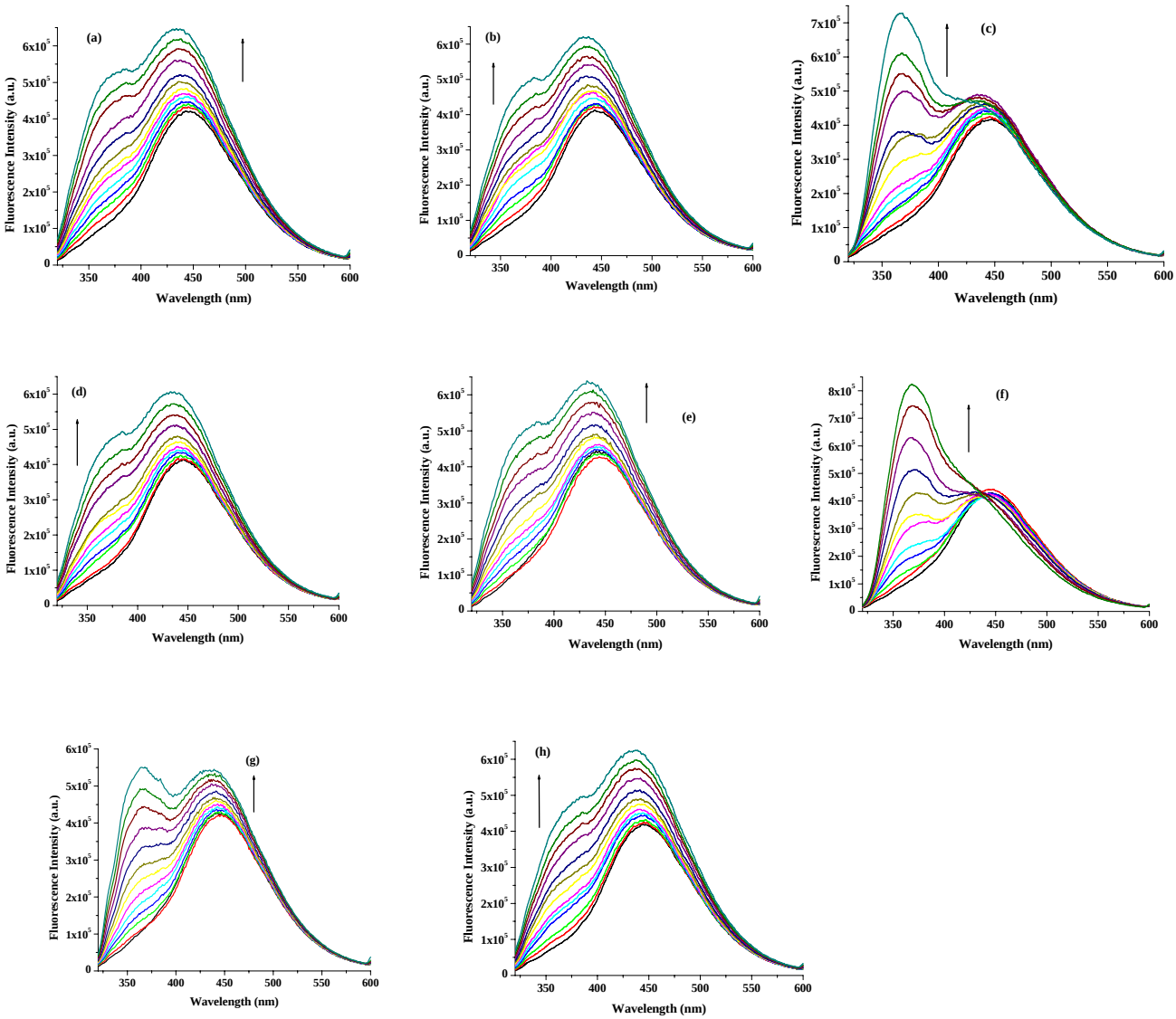


Figure 12S. Change in emission of **3** (c = 5.01 x 10^{-5} M) upon addition of (a) Cl^-, (b) Br^-, (c) F^-, (d) I^-, (e) HSO_4^-, (f) $HP_2O_7^{3-}$, (g) AcO^-, (h) NO_3^- in CH_3CN containing 0.01% DMSO.

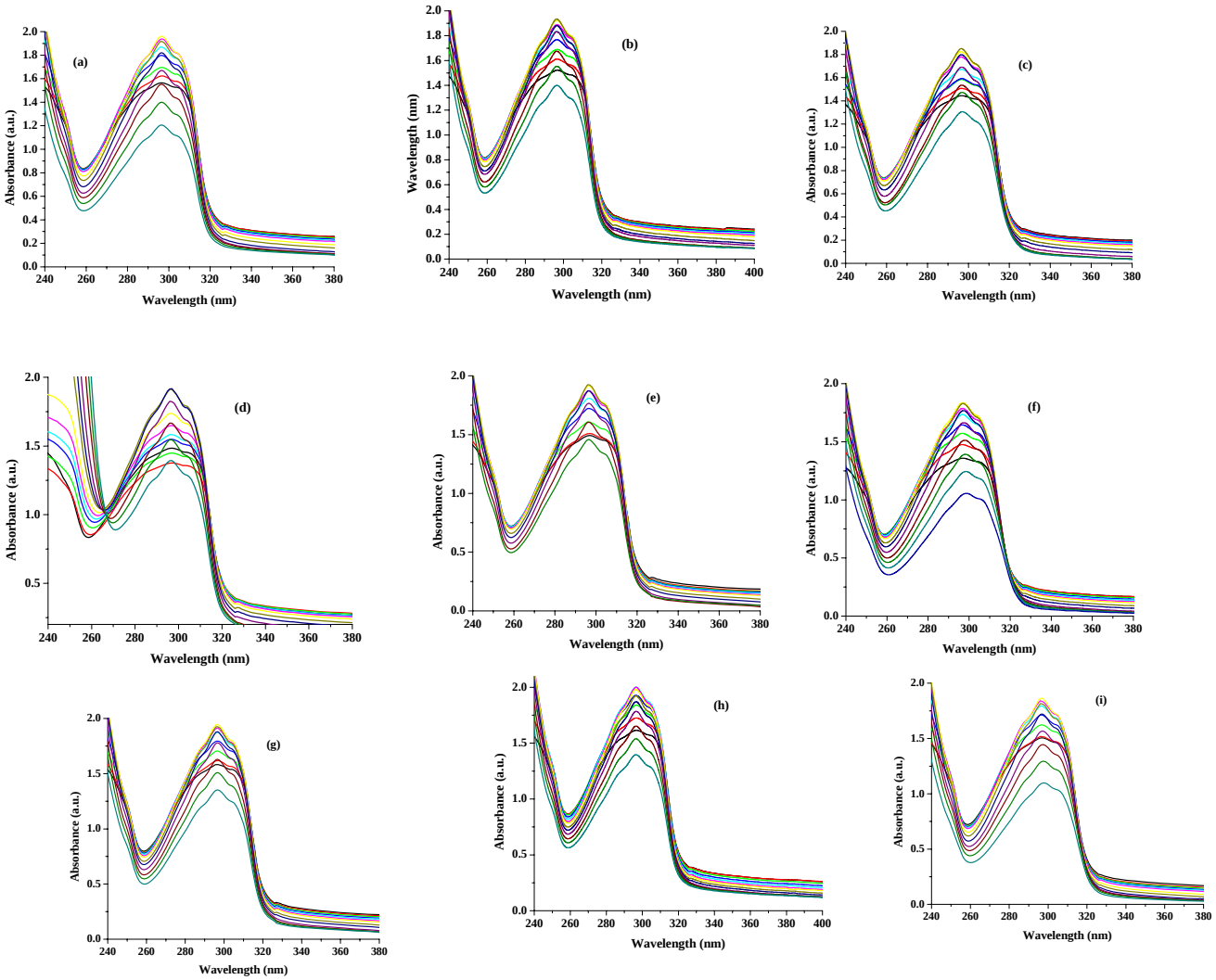


Figure 13S. Change in absorbance of **3** (c = 5.01 x 10^{-5} M) upon addition of (a) Cl^-, (b) Br^-, (c) F^-, (d) I^-, (e) HSO_4^-, (f) $HP_2O_7^{3-}$, (g)AcO^-, (h) NO_3^-, (i) $H_2PO_4^-$ in CH_3CN containing 0.01% DMSO.

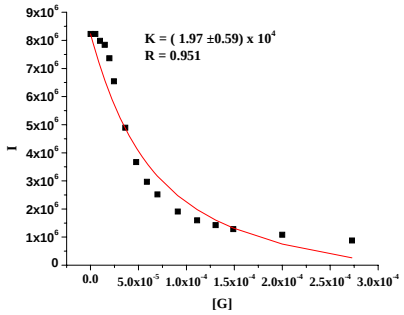


Figure 14S. Nonlinear binding constant curve for tetrabutylammonium dihydrogenphosphate (c=1x10^{-3}M) with receptor **1** (c=2.25x10^{-5} M) at 363 nm in CH_3CN containing 0.01% DMSO.

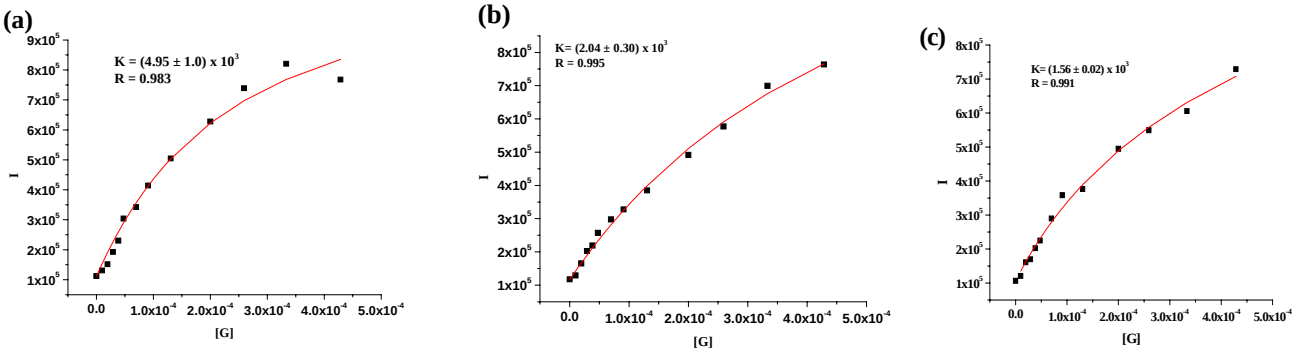


Figure 15S. Nonlinear binding constant curves for (a) tetrabutylammonium hydrogenpyrophosphate (b) tetrabutyl ammonium dihydrogenphosphate, (c) tetrabutylammonium fluoride (c = 1 x 10^{-3} M) with receptor **3** (c = 5.01 x 10^{-5} M) at 366 nm in CH_3CN containing 0.01% DMSO.

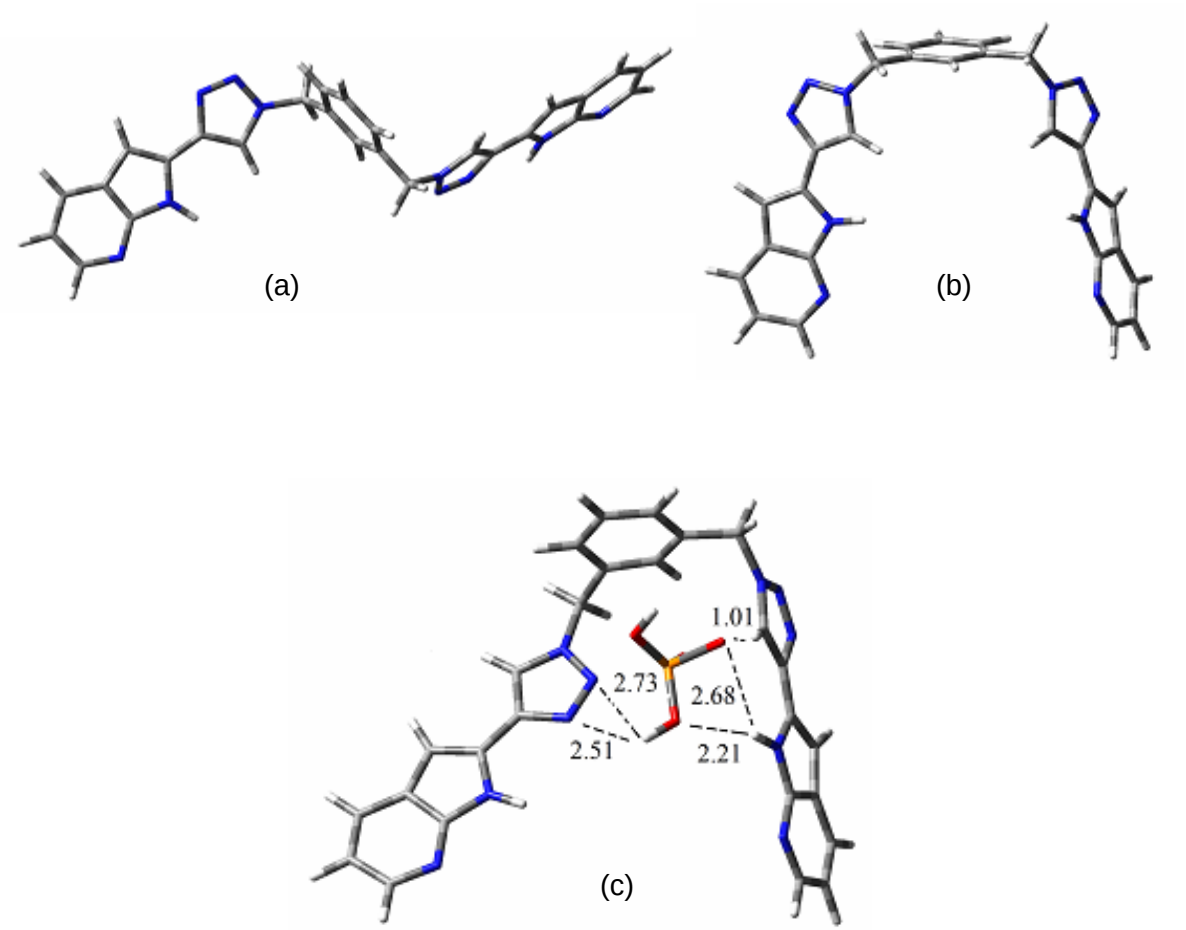
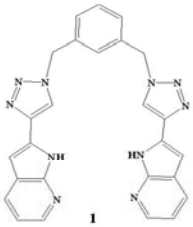
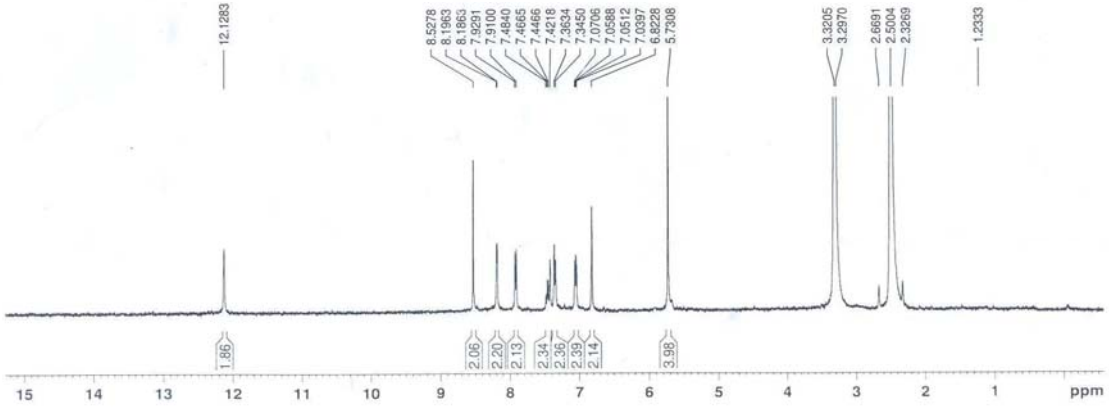


Figure 16S. PM6 optimized geometries of the (a) *anti*, (b) *syn* and (c) $H_2PO_4^-$- complexed forms of **1**. Numerical values in the complex (c) indicate the hydrogen bond distances in Å and the *anti* form is stable by 3.01 kcal/mol over the *syn* form.

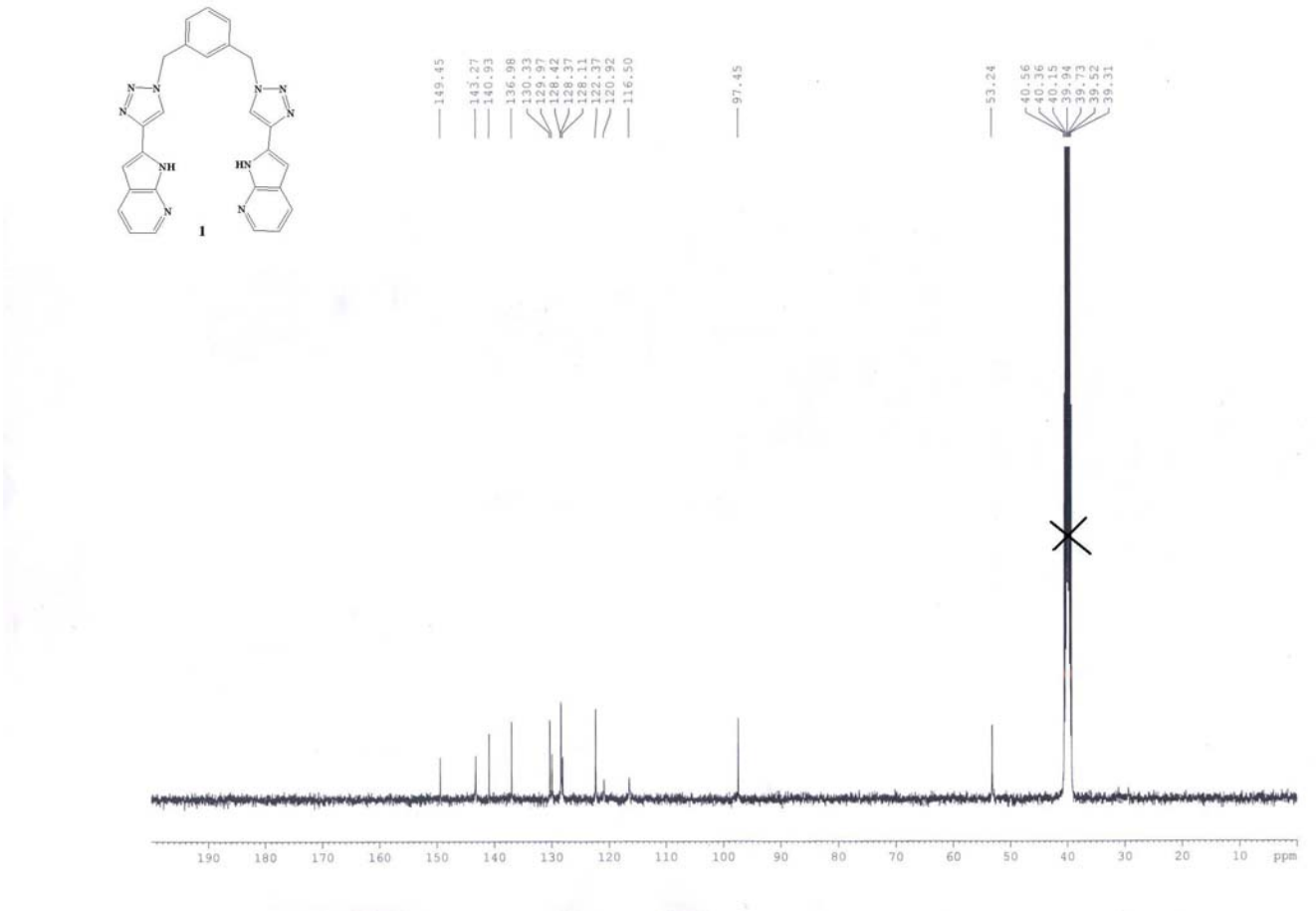
^{1}H NMR (400 MHz, d_6-DMSO)



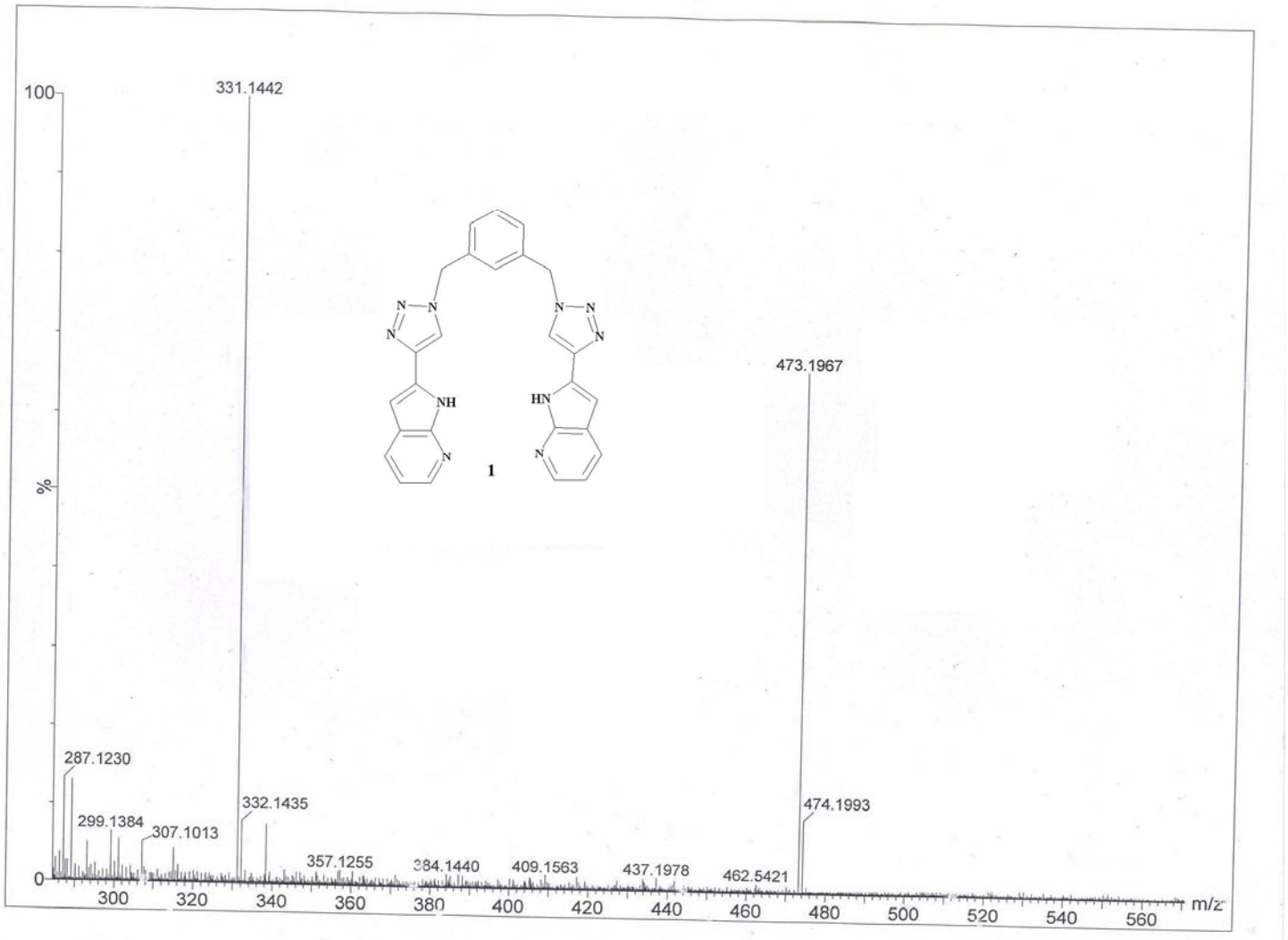
1



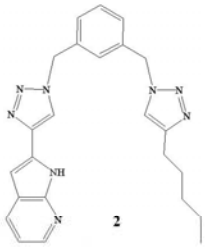
^{13}C NMR (100 MHz, d_6-DMSO)

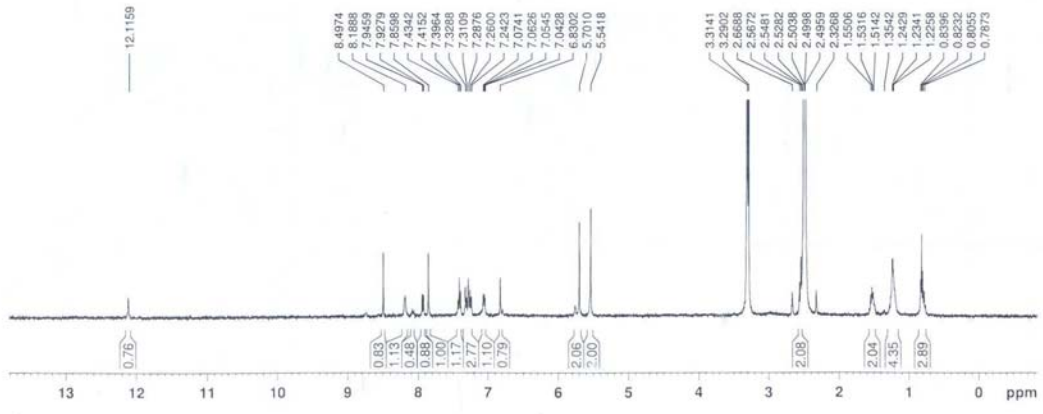


HRMS

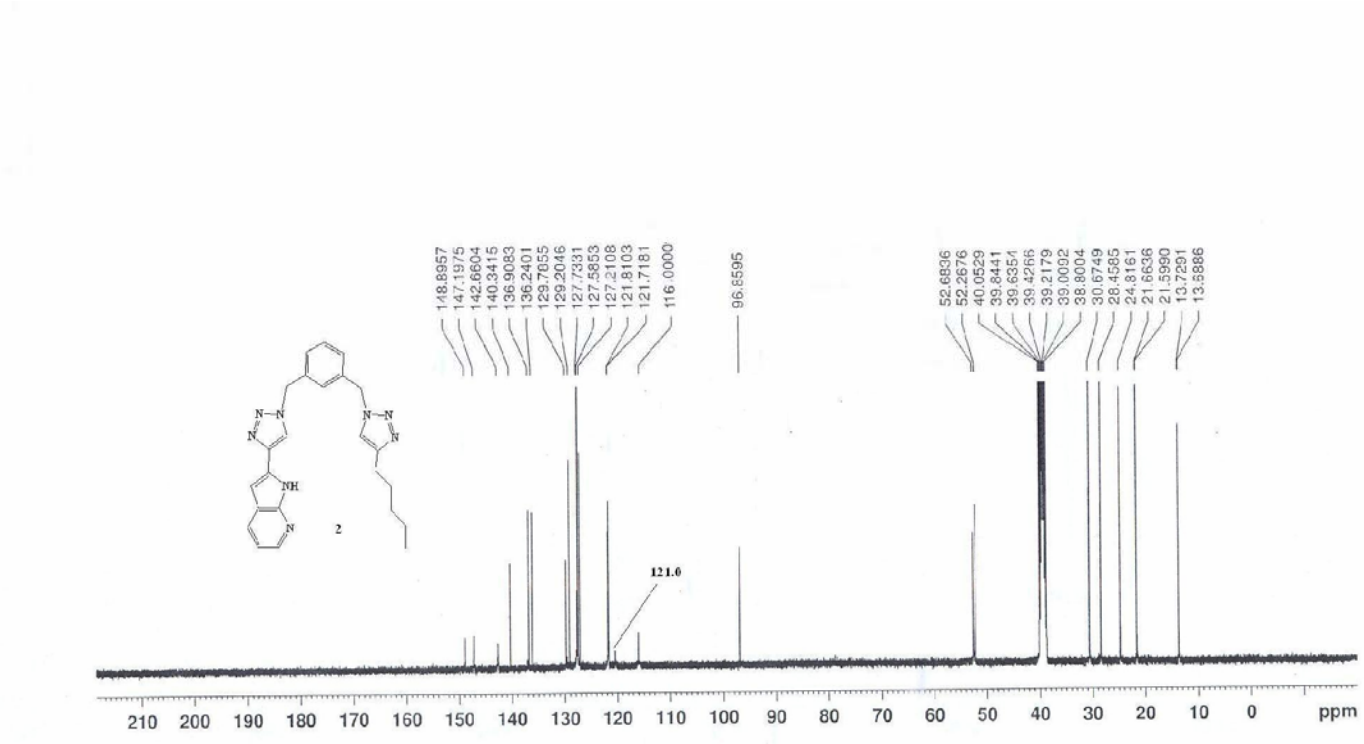


^{1}H NMR (400 MHz, d_6-DMSO)

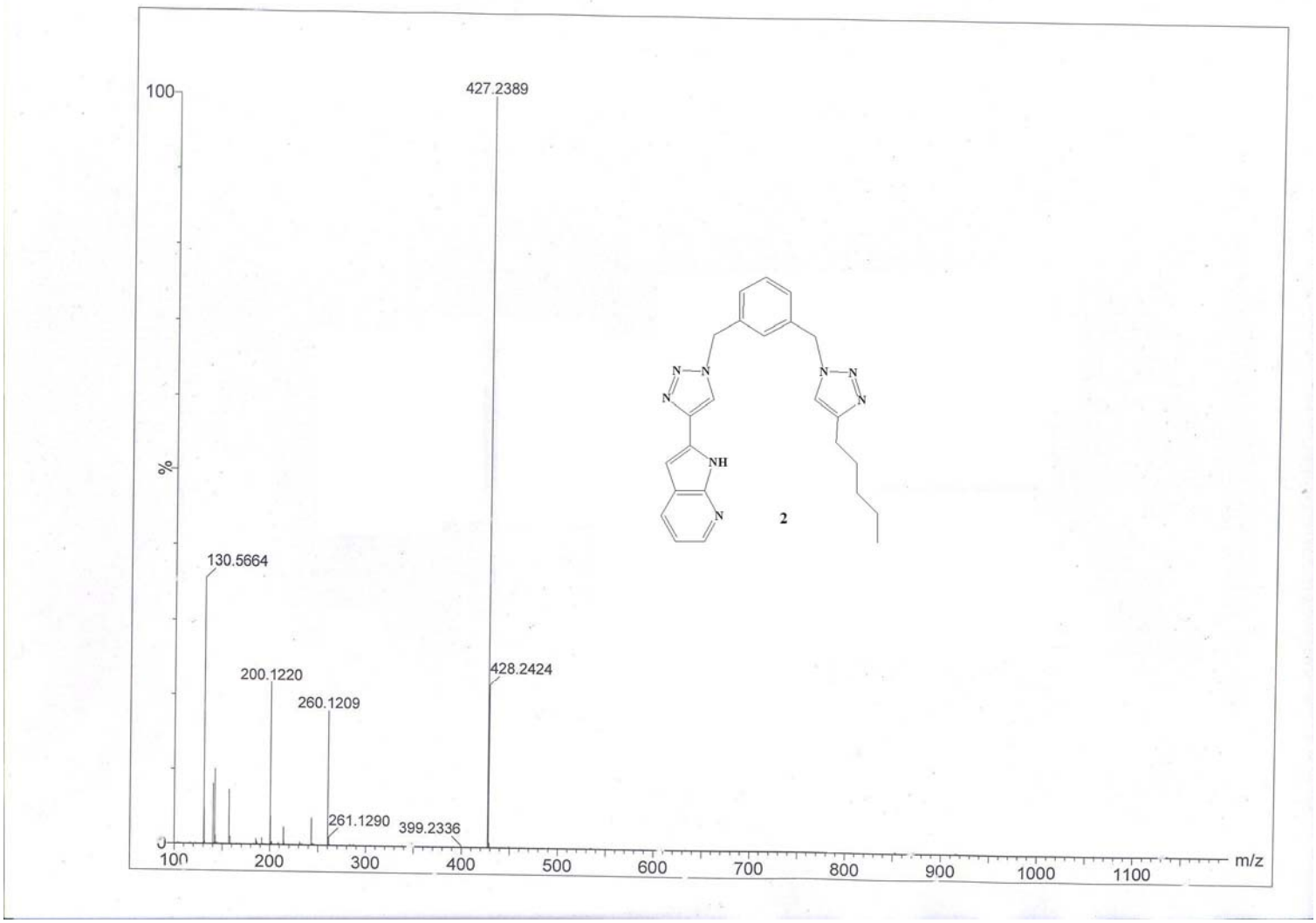




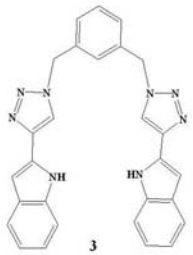
^{13}C NMR (100 MHz, d_6-DMSO)



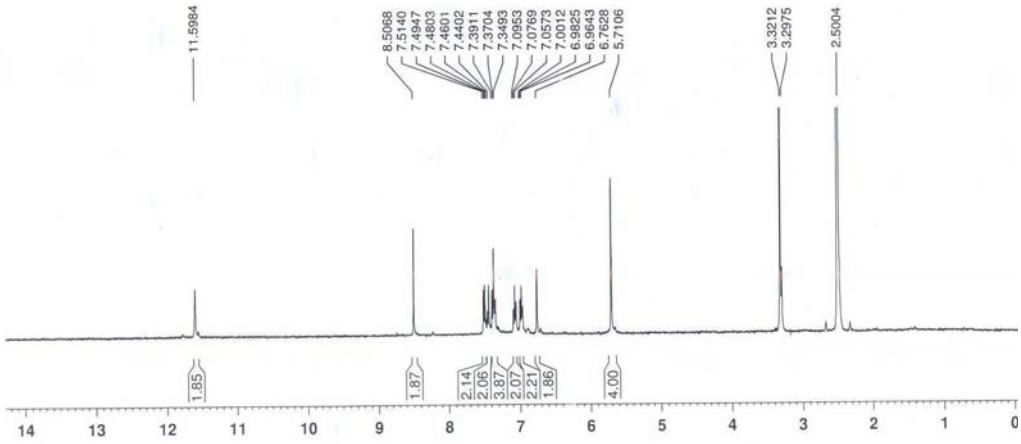
HRMS



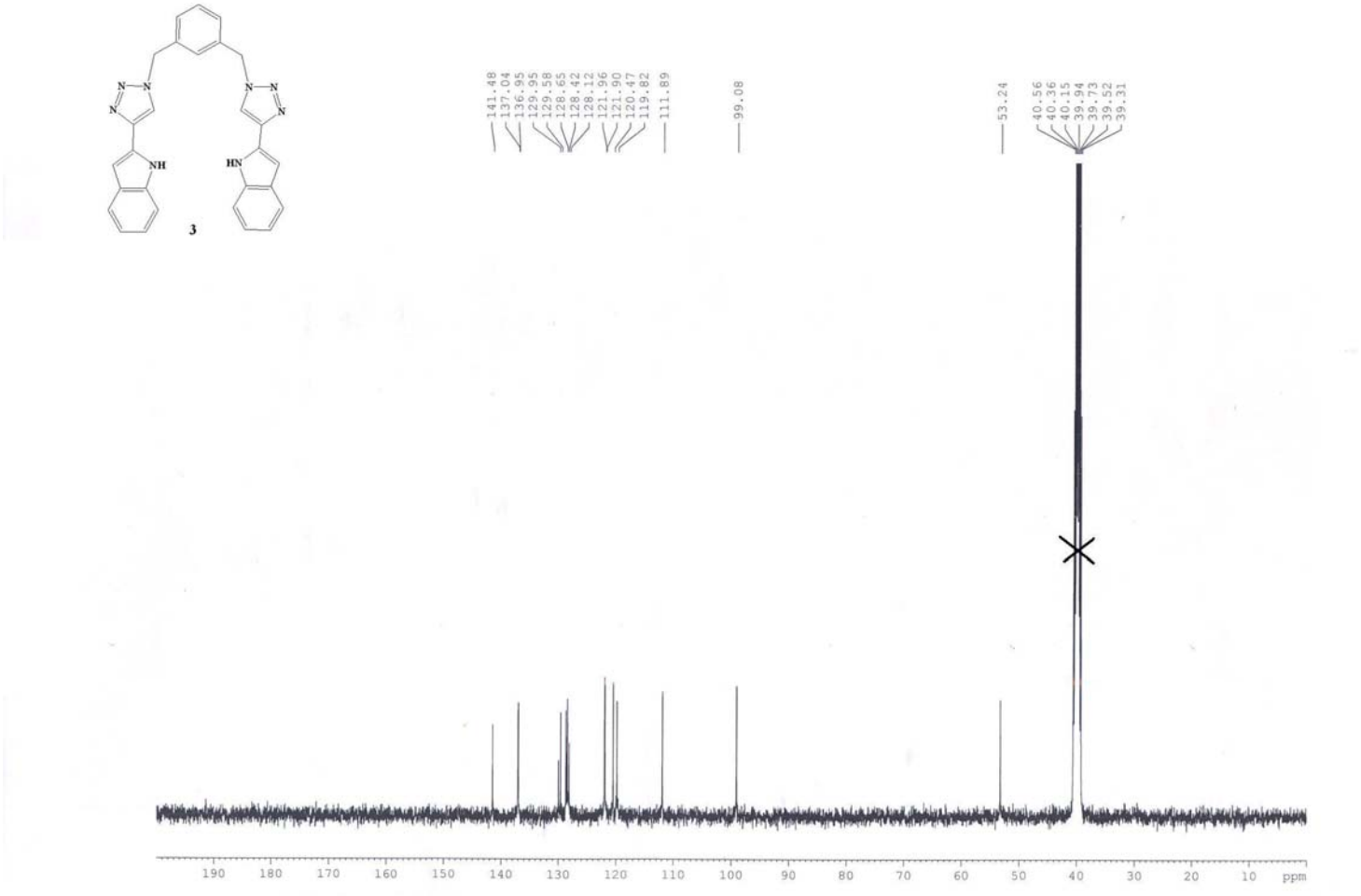
^{1}H NMR (400 MHz, d_6-DMSO)



3



^{13}C NMR (100 MHz, d_6-DMSO)



Electronic Supplementary Material (ESI) for RSC Advances

HRMS