Supporting Information

Hg^{2+} induced hydrolysis of pentaquinone based Schiff Base: A new chemodosimeter for Hg^{2+} ions in aqueous media

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Figure S1. ^{1}H NMR ($CDCl_3$, 300 MHz, ppm) spectrum of **3**.

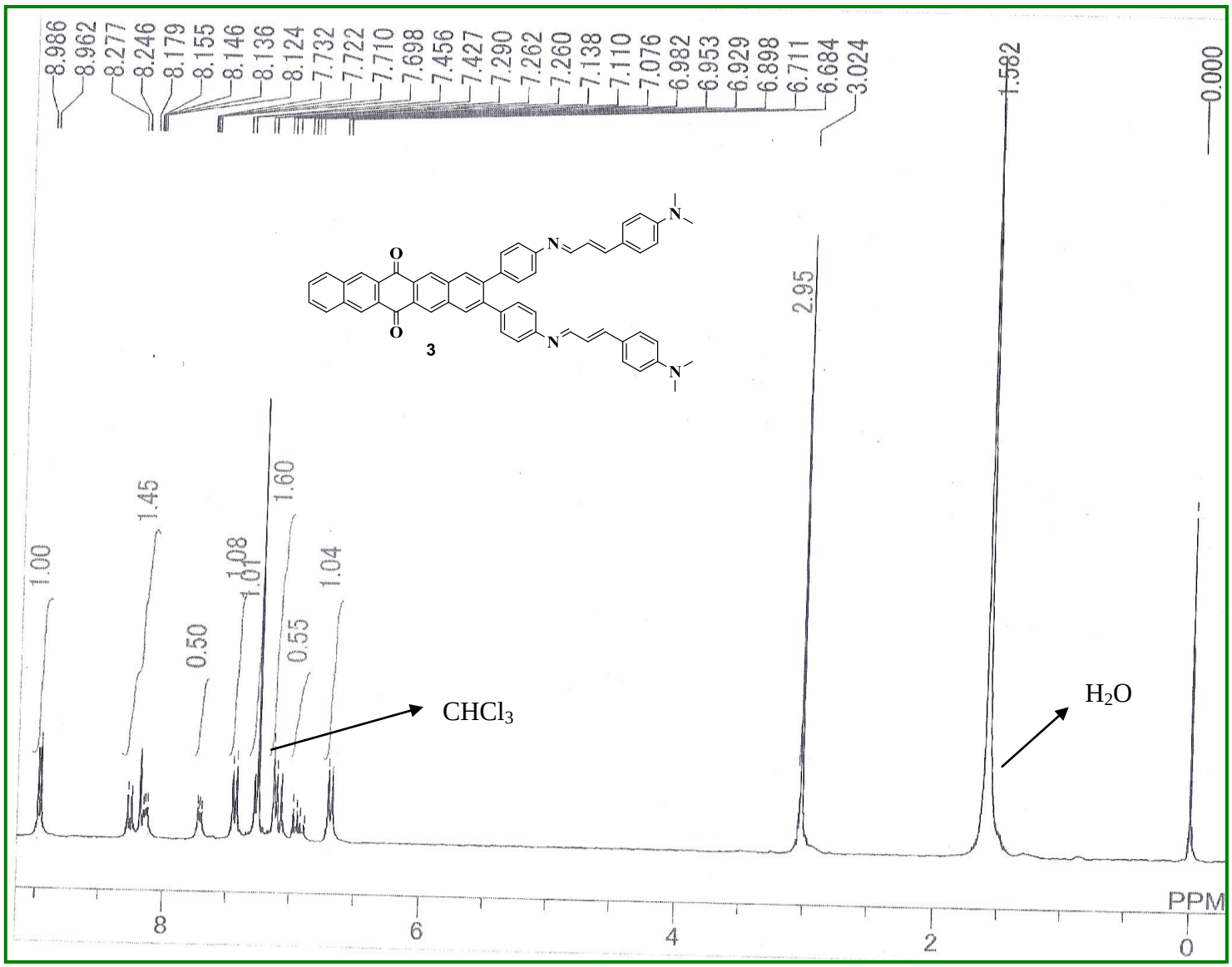


Figure S2. ^{13}C NMR (1,1,2,2-tetrachloroethane-d_2, 75.45 MHz, ppm) spectrum of **3**.

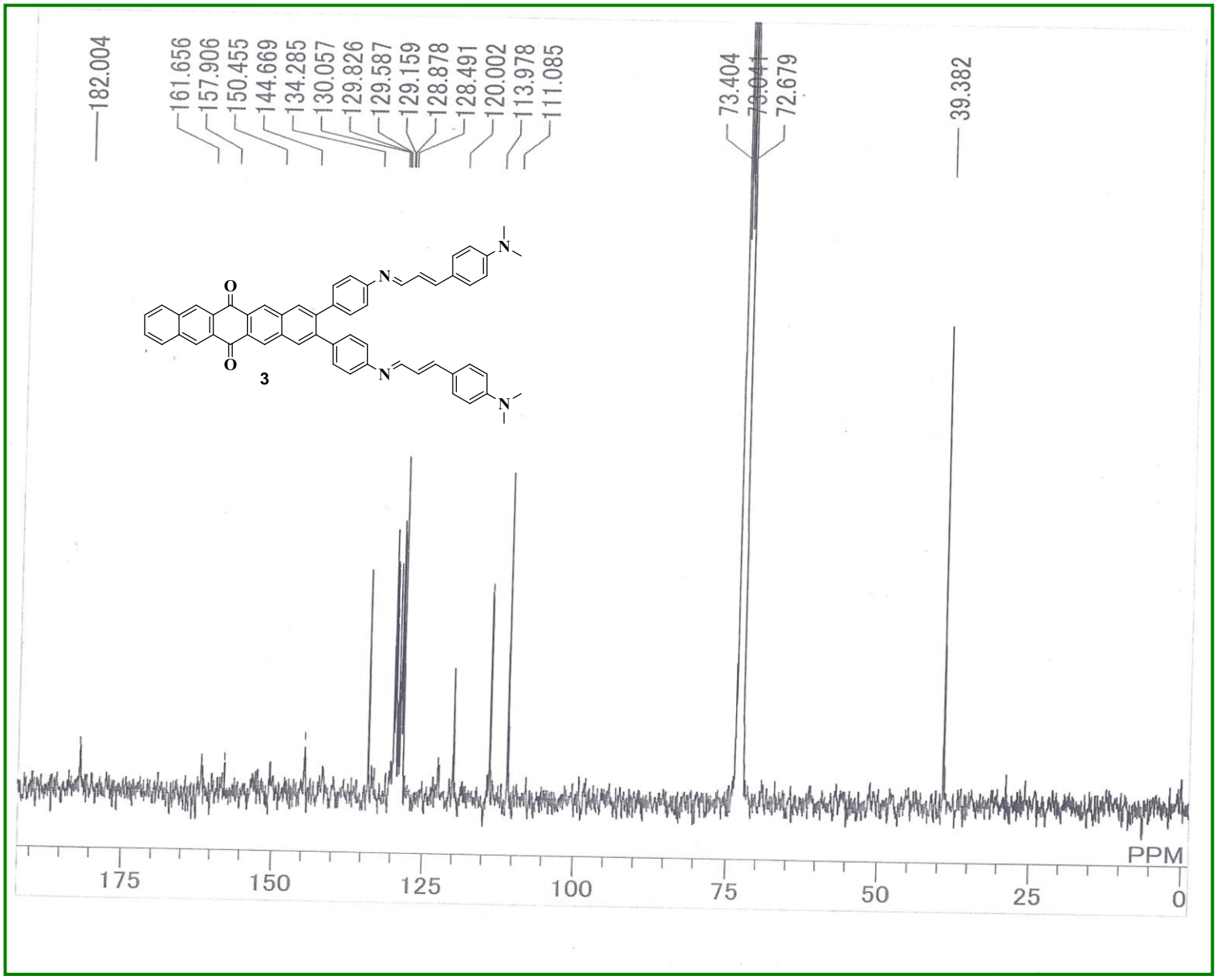


Figure S3. Mass spectrum of **3**.

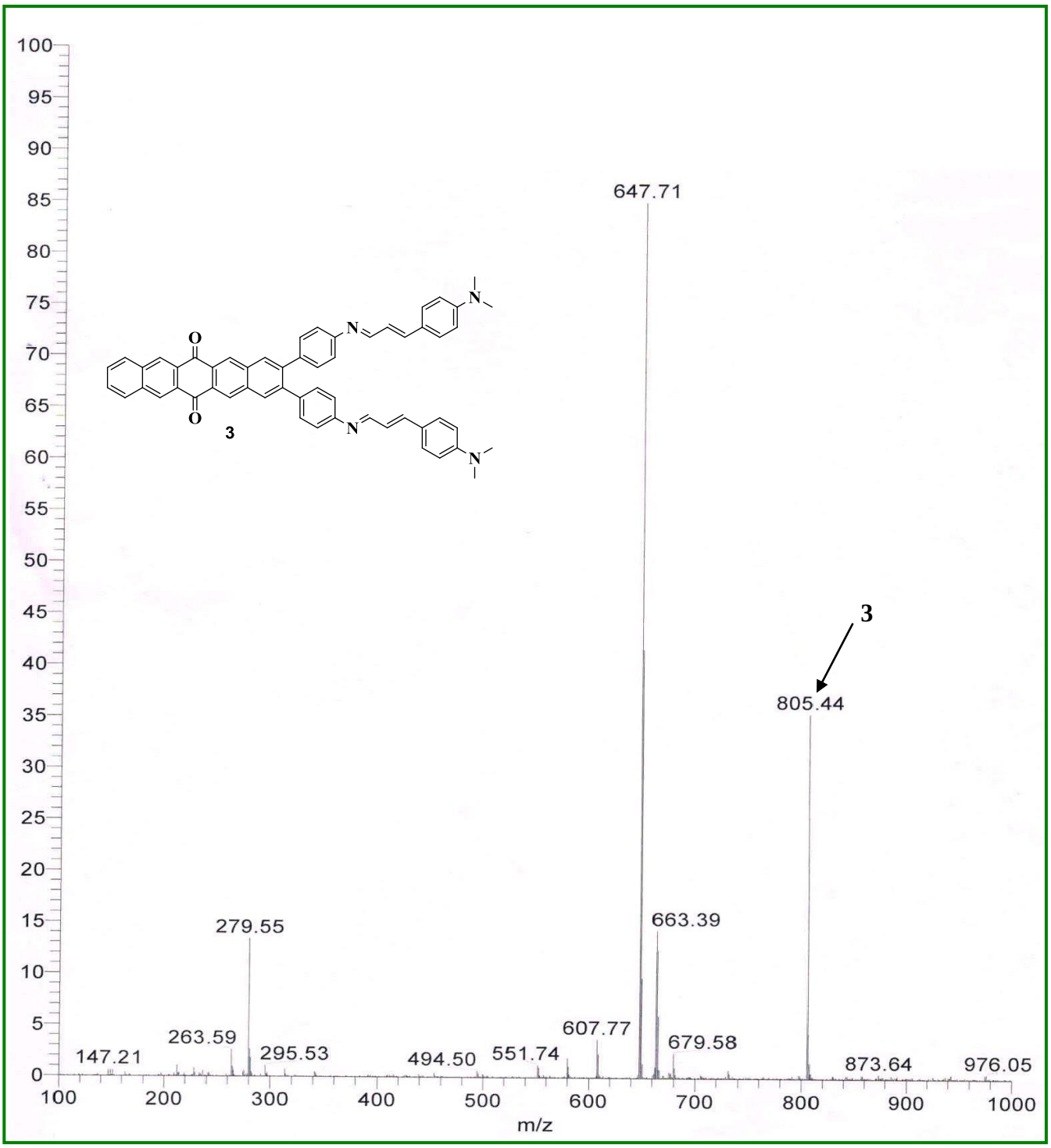
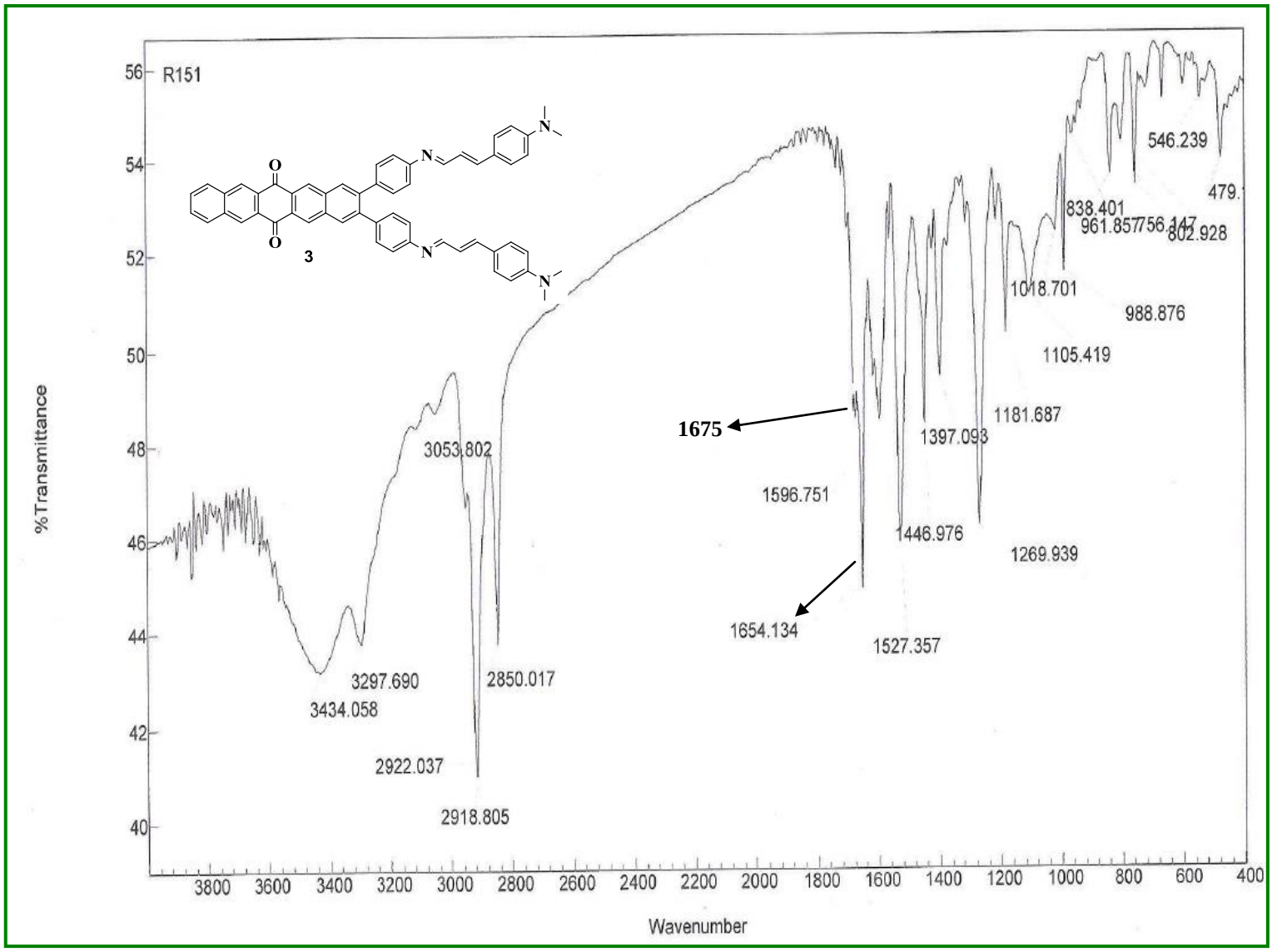


Figure S4. IR spectrum of **3**.



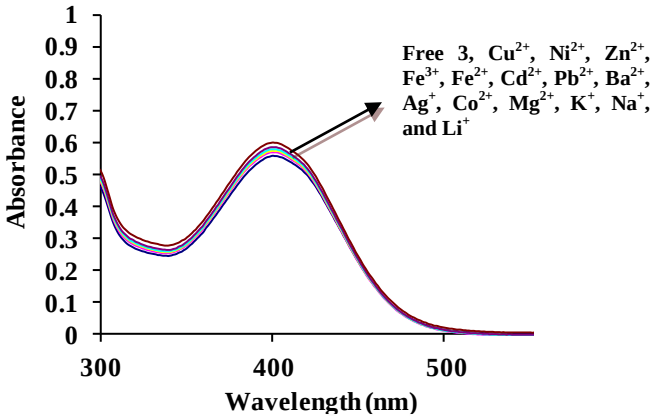


Figure S5. UV-vis spectra of **3** (5 μM) in the presence of various metal ions (0-200 equiv) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7.

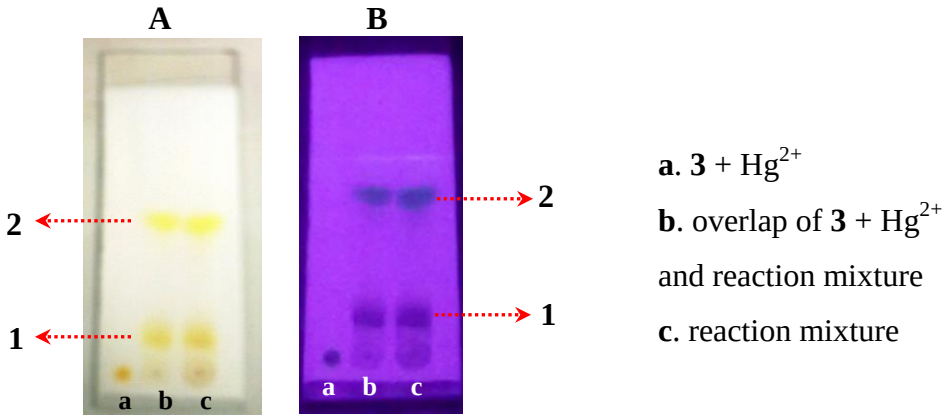


Figure S6. **TLC** showing the formation of pentaquinone diamine (**1**) and *N*,*N*-dimethylaminocinnamaldehyde (**2**). (**A**) naked eye (**B)** under UV lamp (excited at 365 nm).

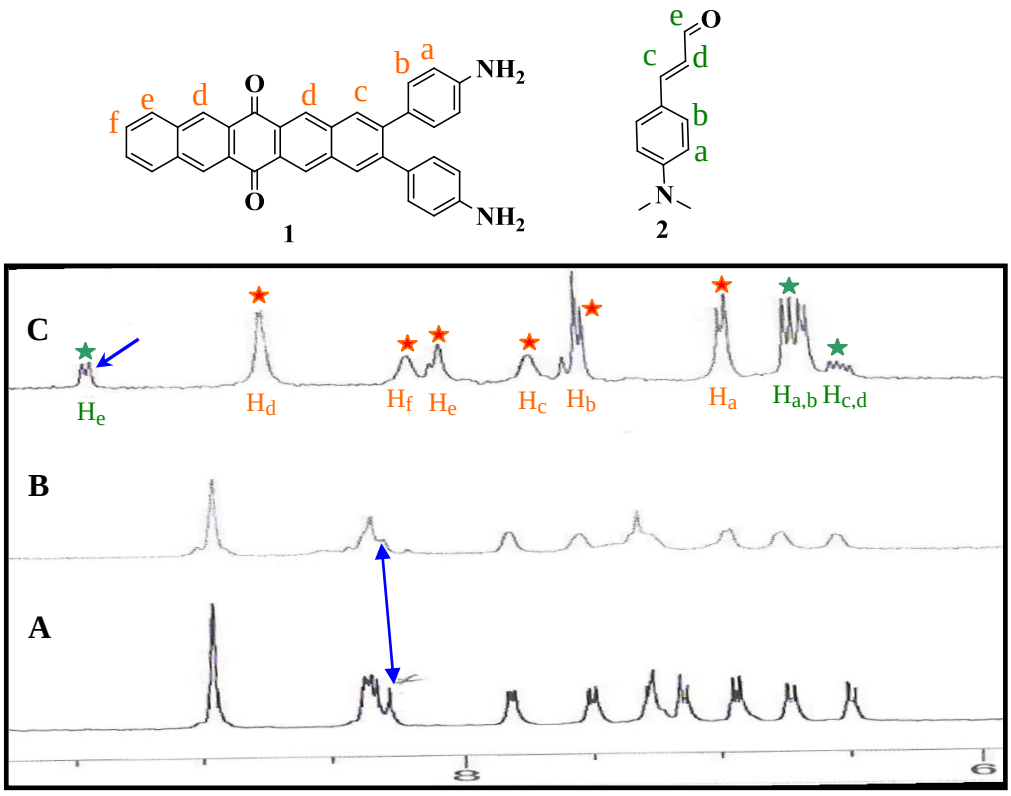
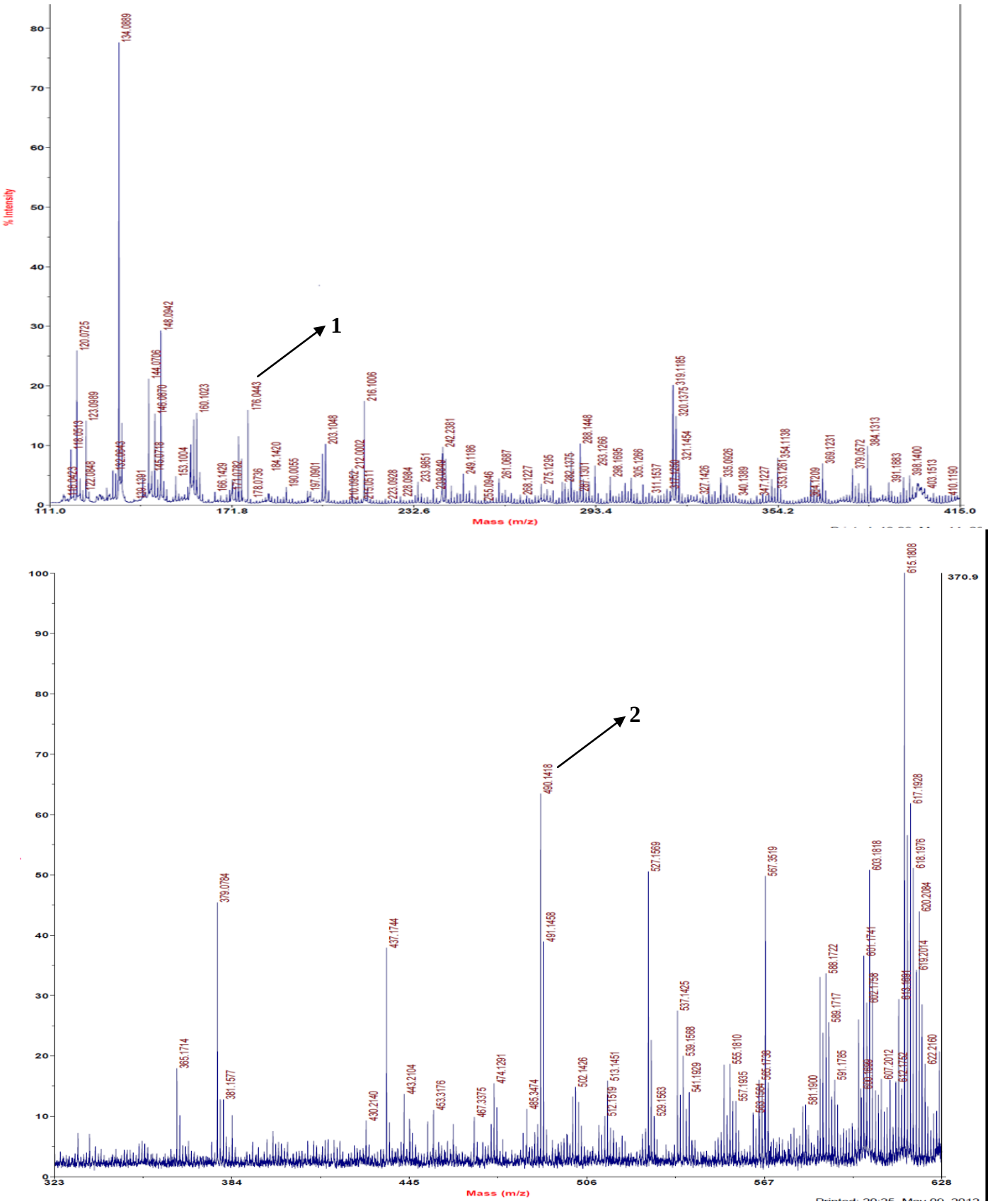


Figure S7. Partial ^{1}H NMR spectra of (**A**) **3** in DMSO-d_6 (**B**) **3** + Hg^{2+} in DMSO-d_6 (**C**) reaction of **3** with Hg^{2+} was carried out in DMSO-D_2O (9:1, v/v) for 5 min and then ^{1}H NMR spectrum of the resulting solution was recorded. ★ Protons of *N*,*N*-dimethylaminocinnamaldehyde (**2**) ★ Protons of pentaquinone diamine (**1**).

Figure S8. Mass spectrum of receptor **3** in THF-H_2O(9:1).



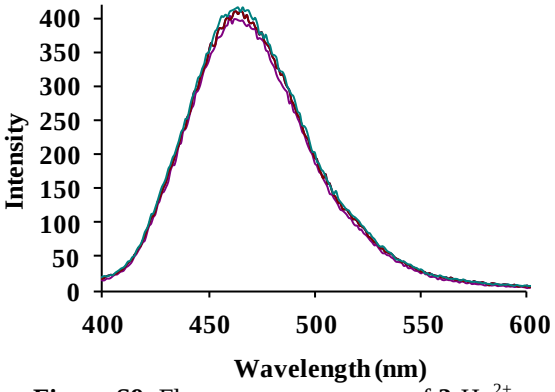


Figure S9. Fluorescence response of **3**-Hg^{2+} towards TBAI (400 equiv) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7.

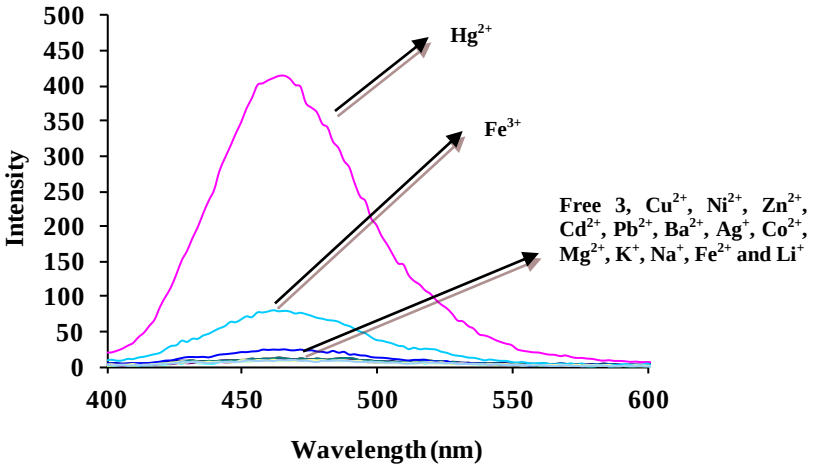


Figure S10. Fluorescence spectra of **3** (5 μM) in response to different metal ions (200 equiv each) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ_{ex} = 380 nm.

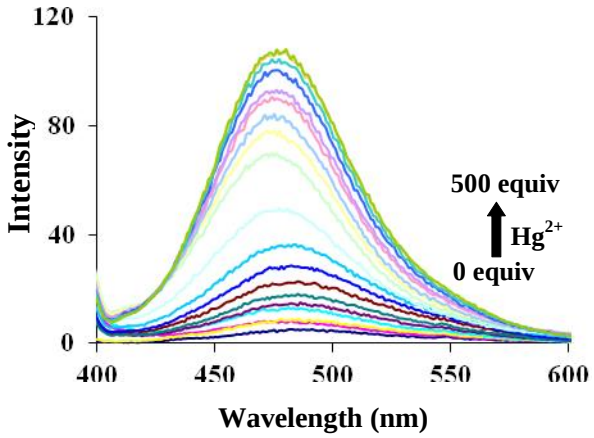


Figure S11. Fluorescence response of receptor **3** (5 μM) on addition of Hg^{2+} ions (0-500 equiv) in THF/H_2O (1:1, v:v) buffered with HEPES, pH = 7; λ_{ex} = 380 nm. Spectra were recorded at the interval of every 30 sec.

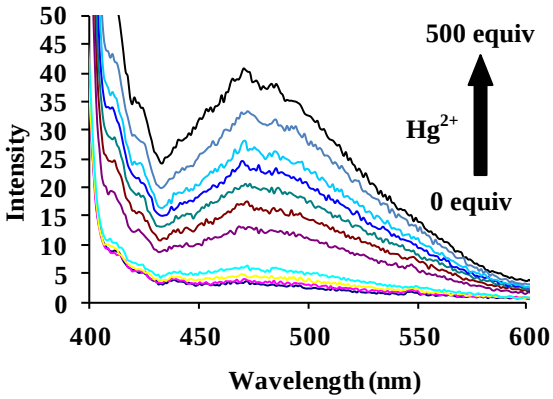


Figure S12. Fluorescence response of receptor **3** (5 μM) on addition of Hg^{2+} ions (0-500 equiv) in THF/H_2O (0.5:9.5, v:v) buffered with HEPES, pH = 7; λ_{ex} = 380 nm. Spectra were recorded at the interval of every 30 sec.

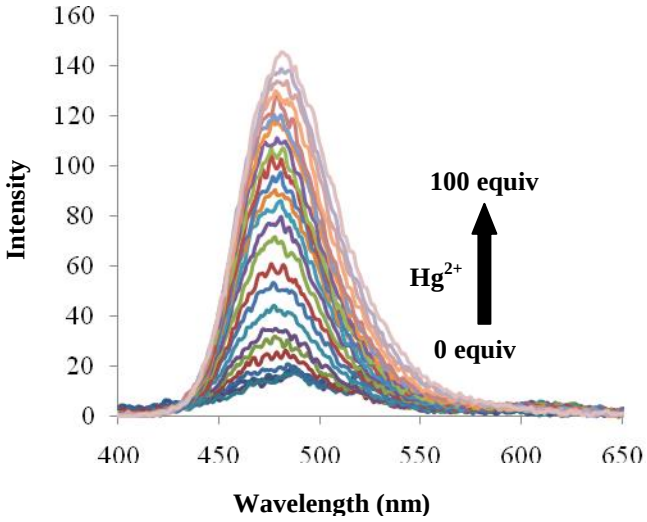


Figure S13. Fluorescence response of receptor **3** (5 μM) on addition of Hg^{2+} ions (0-100 equiv) in DMSO/H_2O (9.5: 0.5, v:v), λ_{ex} = 380 nm. Spectra were recorded at the interval of every 30 sec.

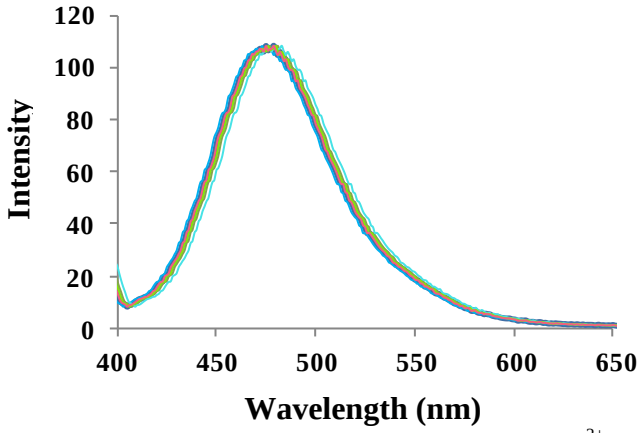


Figure S14. Fluorescence response of **3** + Hg^{2+} system on addition of human blood serum in THF/H_2O (1:1, v:v) buffered with HEPES, pH = 7; λ_{ex} = 380 nm.

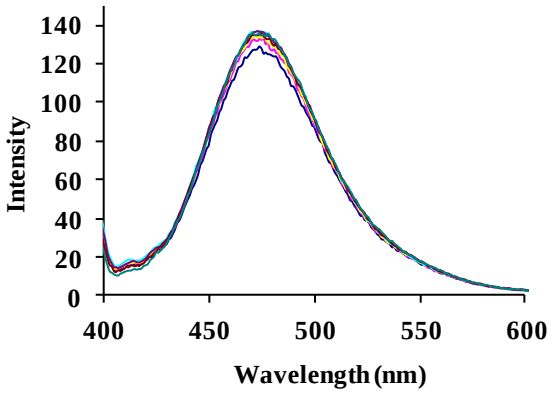


Figure S15. Fluorescence response of **3** + Hg^{2+} system on addition of cystein in THF/H_2O (1:1, v:v) buffered with HEPES, pH = 7; λ_{ex} = 380 nm.

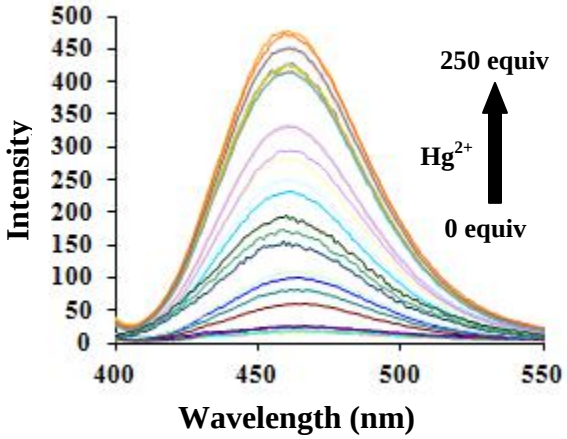


Figure S16. Fluorescence response of **3** upon addition of incremental amount of $Hg(NO_3)_2$ (250 equiv) in drinking water; λ_{ex} = 380 nm.

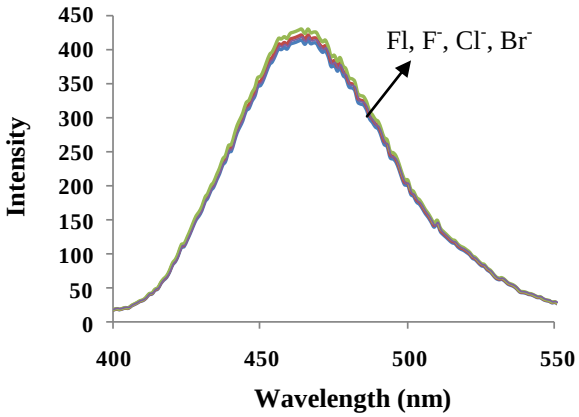
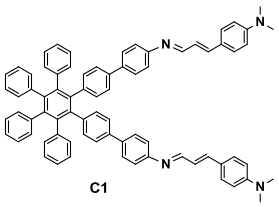


Figure S17. Fluorescence response of **3**-Hg^{2+} towards TBAX (400 equiv) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7. TBAX (X = F^-, Cl^- and Br^-)



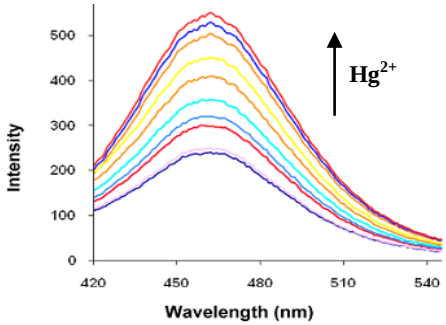
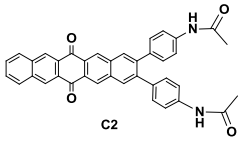


Figure S18. Fluorescence spectra of **C1** (5μM) in the presence of Hg^{2+} ions (0−150 μM) in THF:H_2O (6:4); λ_{Ex} = 380 nm.



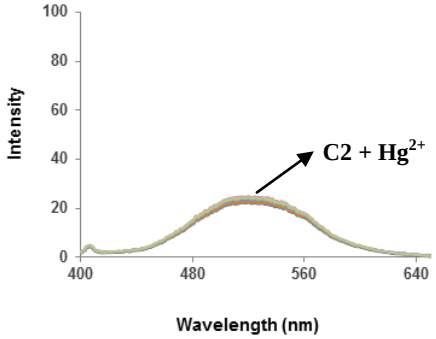
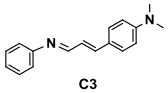


Figure S19. Fluorescence response of **C2** in the presence of Hg^{2+} ions (200 equiv) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ_{Ex} = 380 nm.



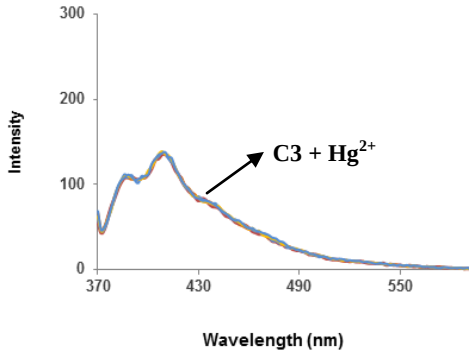


Figure S20. Fluorescence response of **C3** in the presence of Hg^{2+} ions (200 equiv) in THF/H_2O (9.5:0.5, v:v) buffered with HEPES, pH = 7; λ_{Ex} = 380 nm.