Electronic Supplementary Information

Solvent Dependent Competition between Fluorescence Resonance Energy Transfer and Through Bond Energy Transfer in Rhodamine Appended Hexaphenylbenzene Derivatives for Sensing of Hg^{2+} Ions

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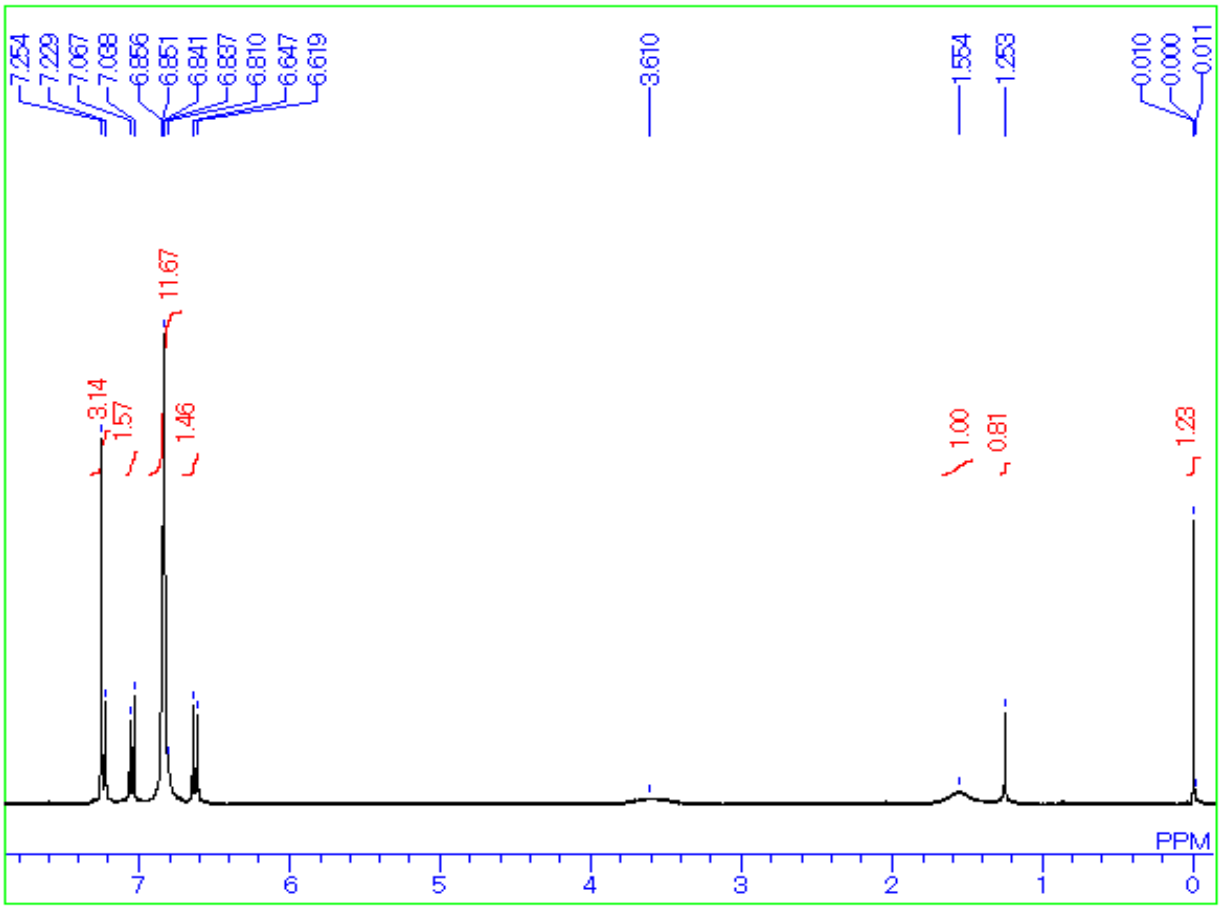
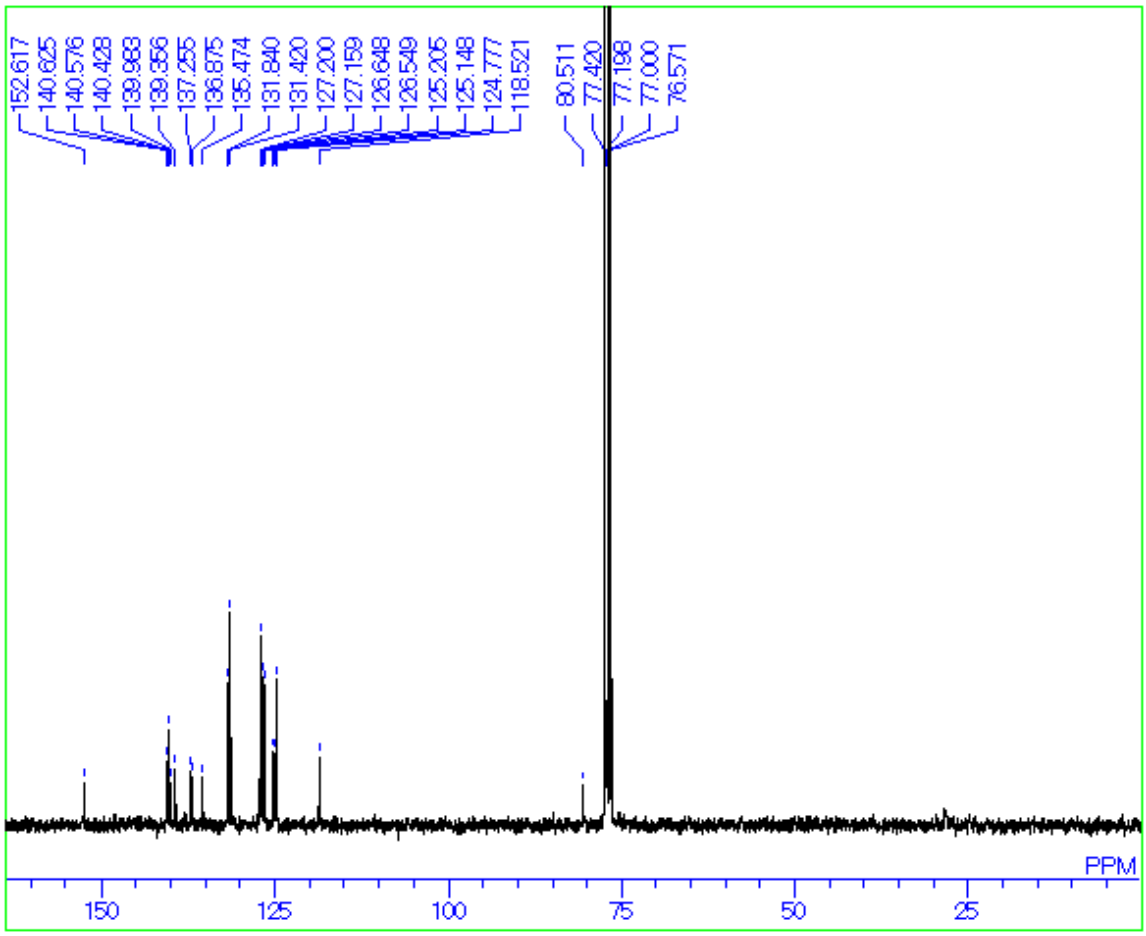
^{1}H NMR of compound 3 (300 MHz, $CDCl_3$)

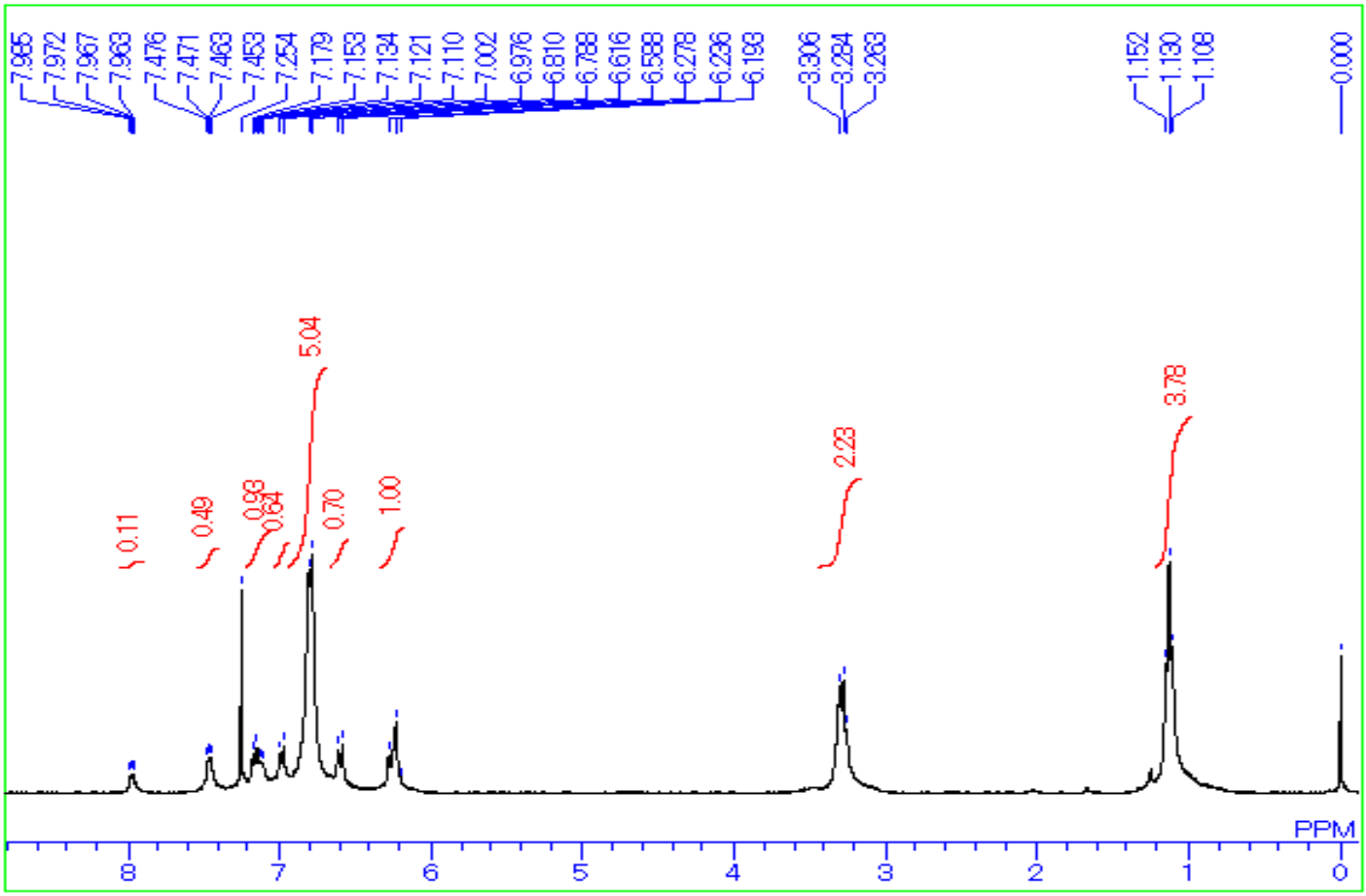


^{13}C NMR spectrum of compound 3 (75 MHz, $CDCl_3$)

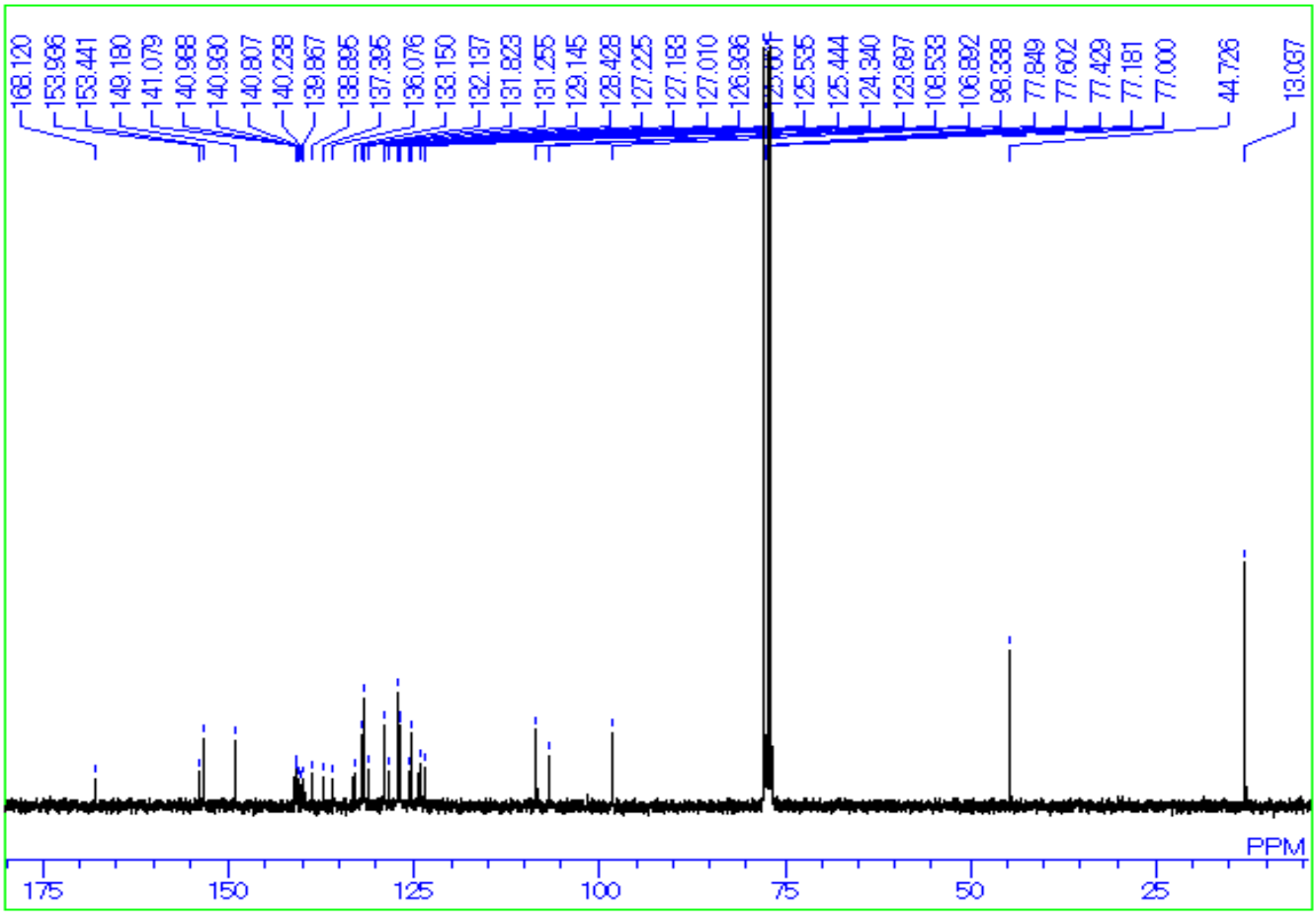


Mass spectrum of compound 3

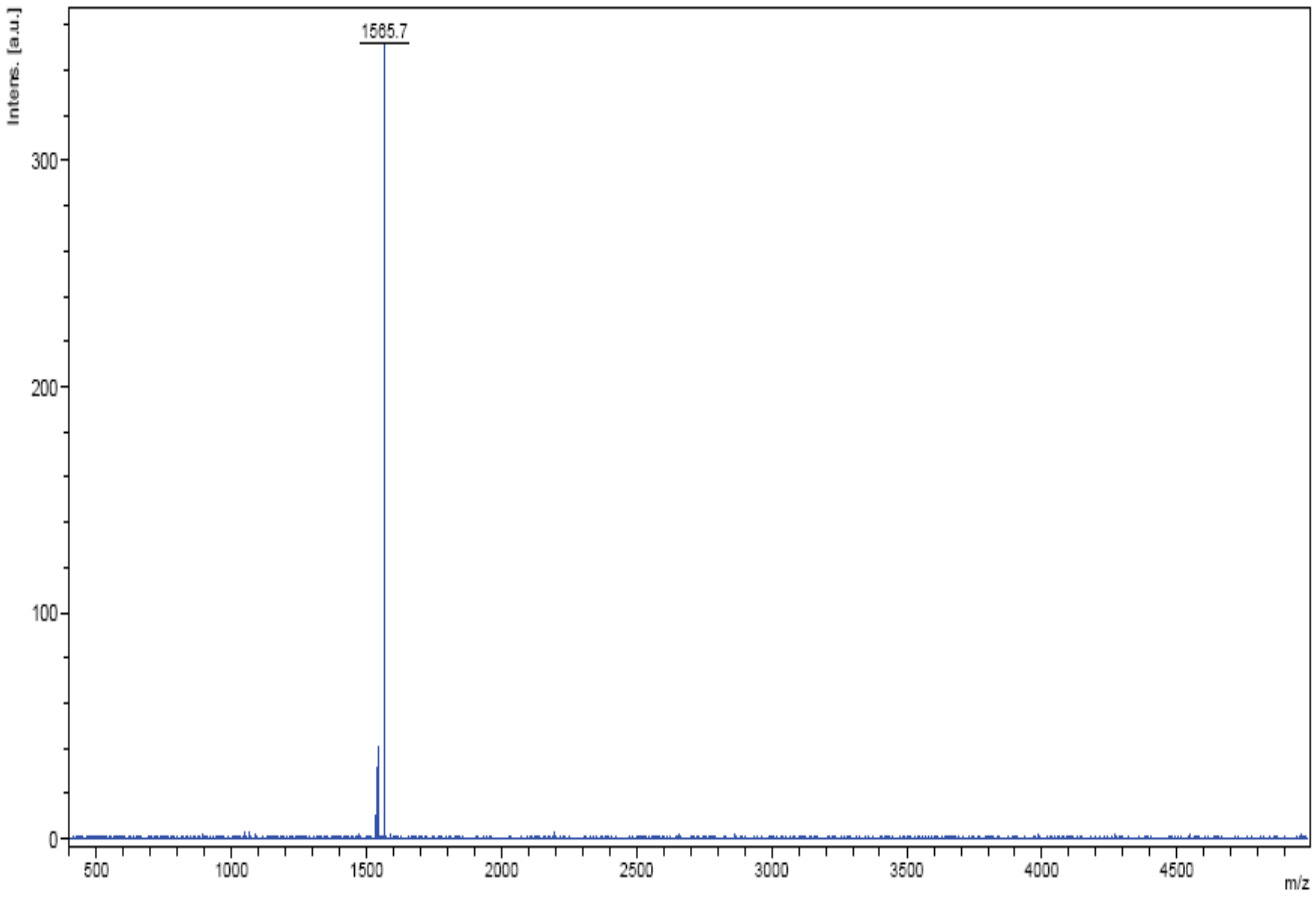
^{1}H NMR spectrum of compound 5 (300MHz, $CDCl_3$)



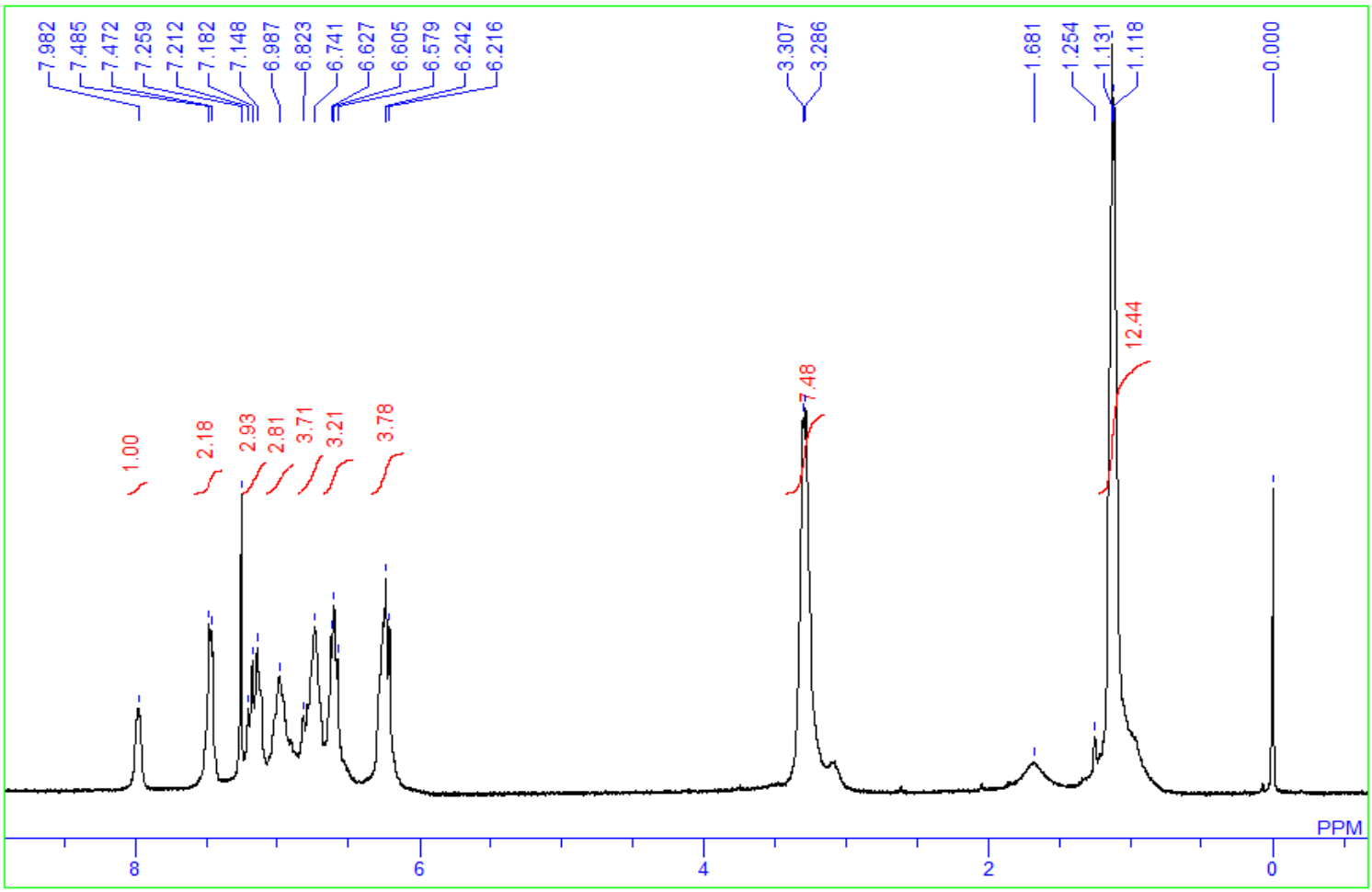
^{13}C NMR of compound 5 (75 MHz, $CDCl_3$)



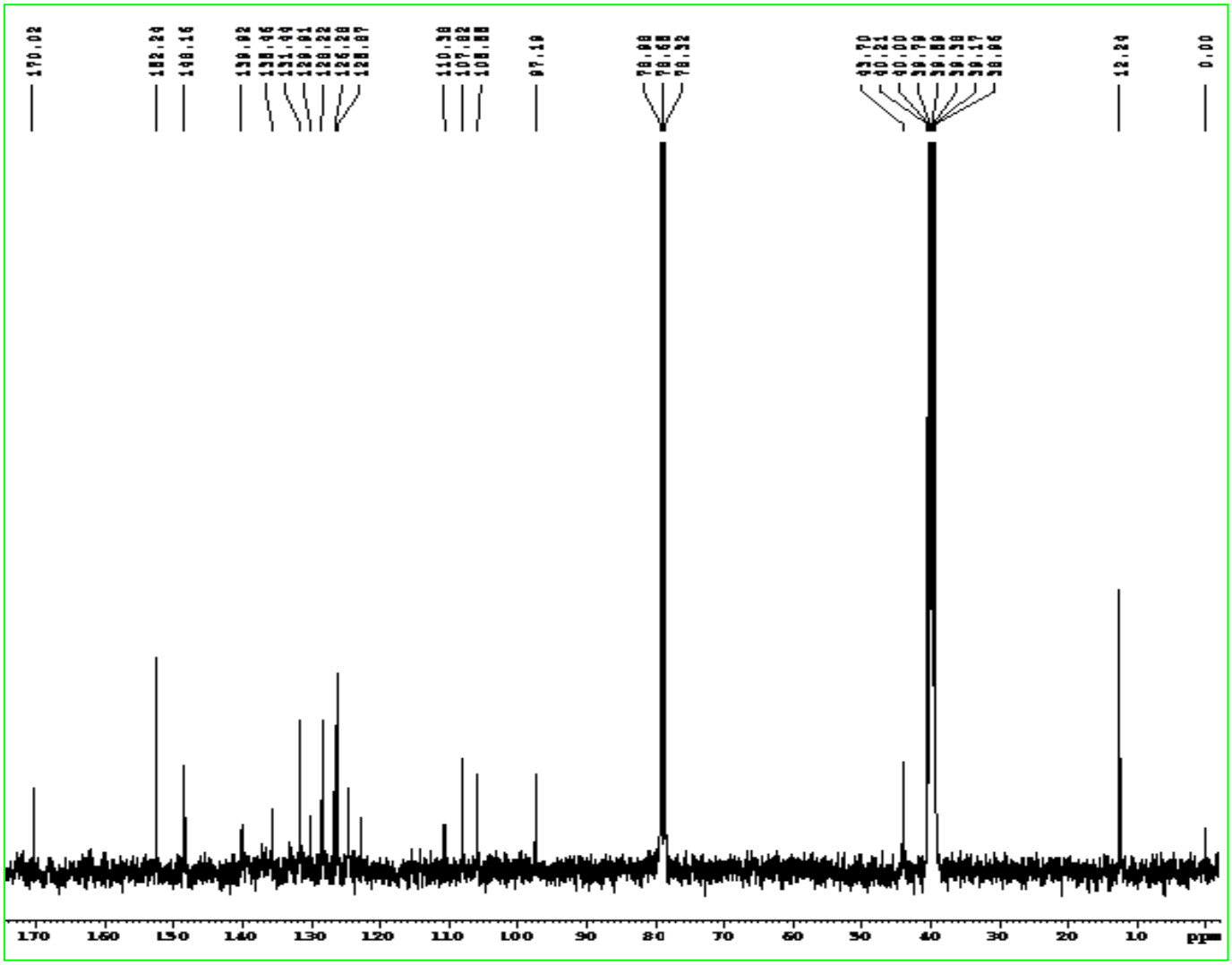
MALDI-TOF of compound 5



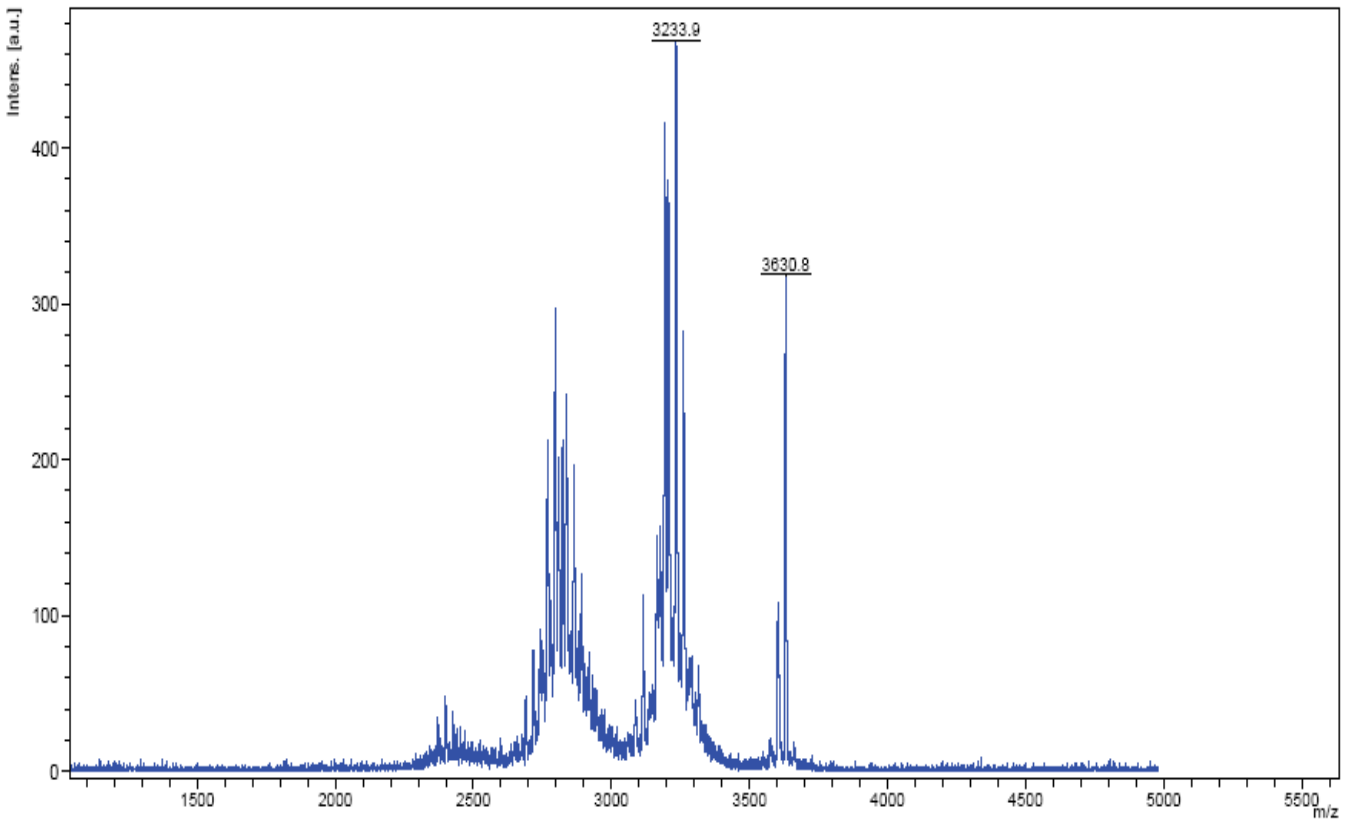
^{1}H NMR spectrum of compound 7 (300 MHz, $CDCl_3$)



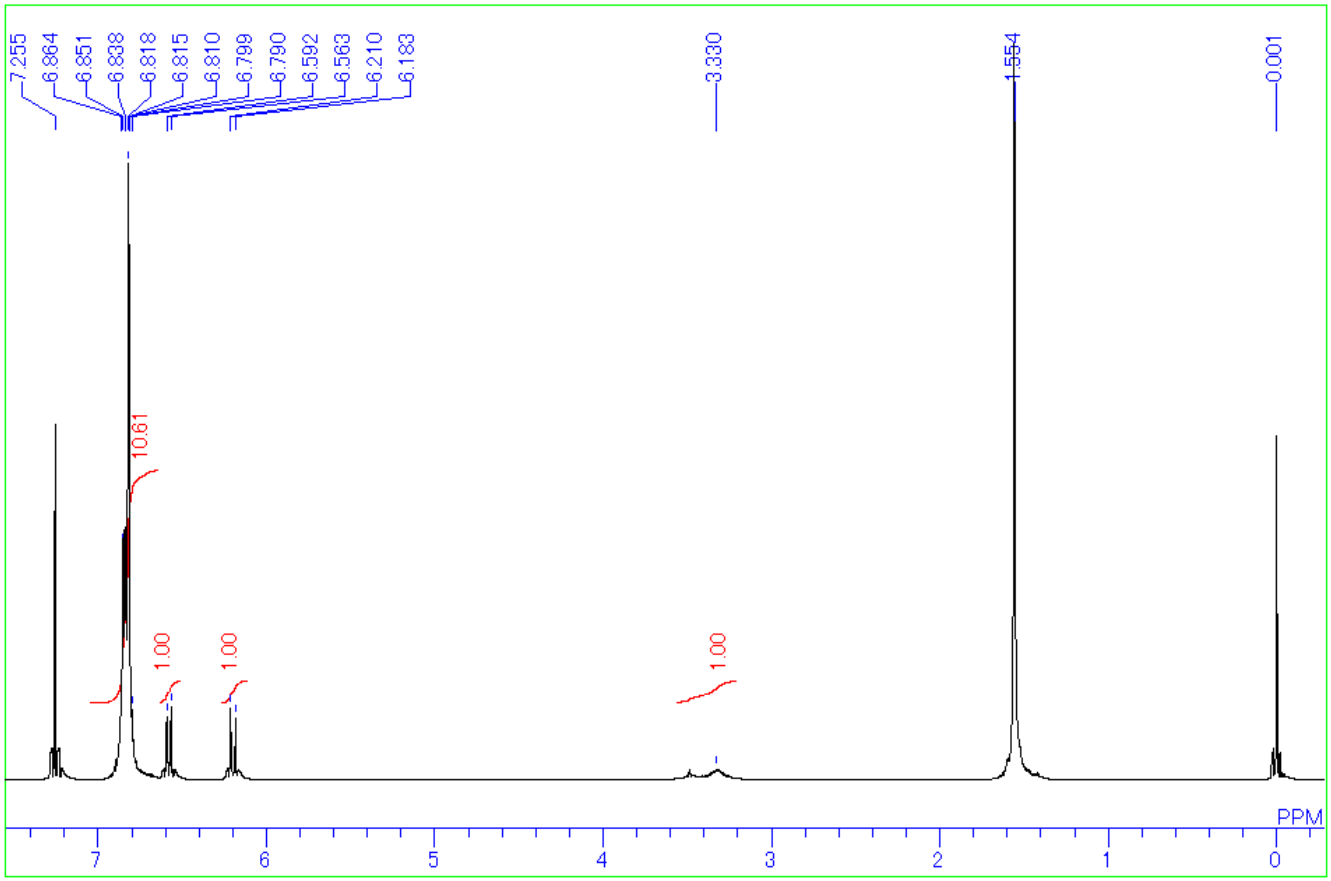
^{13}C NMR spectrum of compound 7 (100 MHz, $CDCl_3$:DMSO; 8:2)



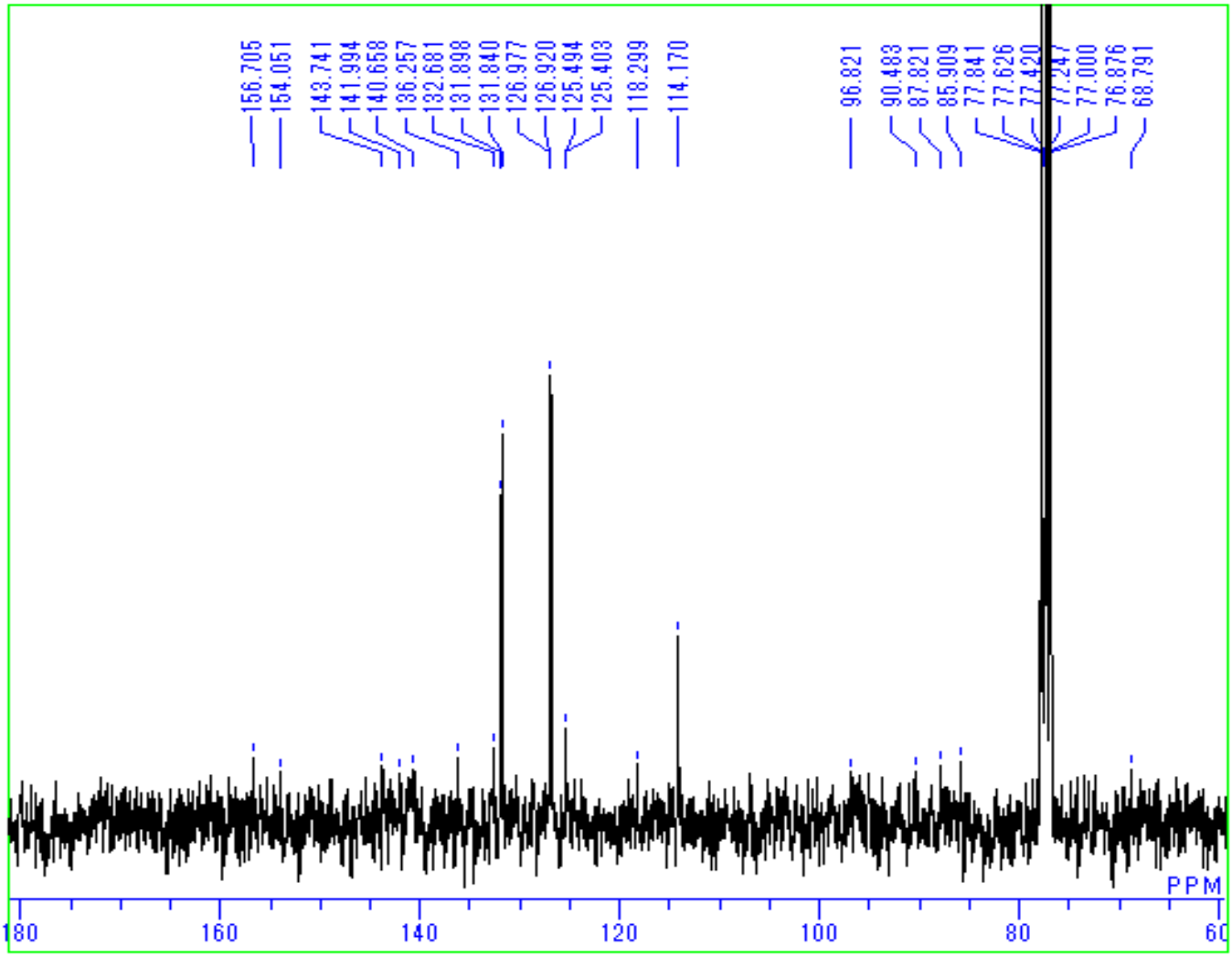
MALDI-TOF of compound 7



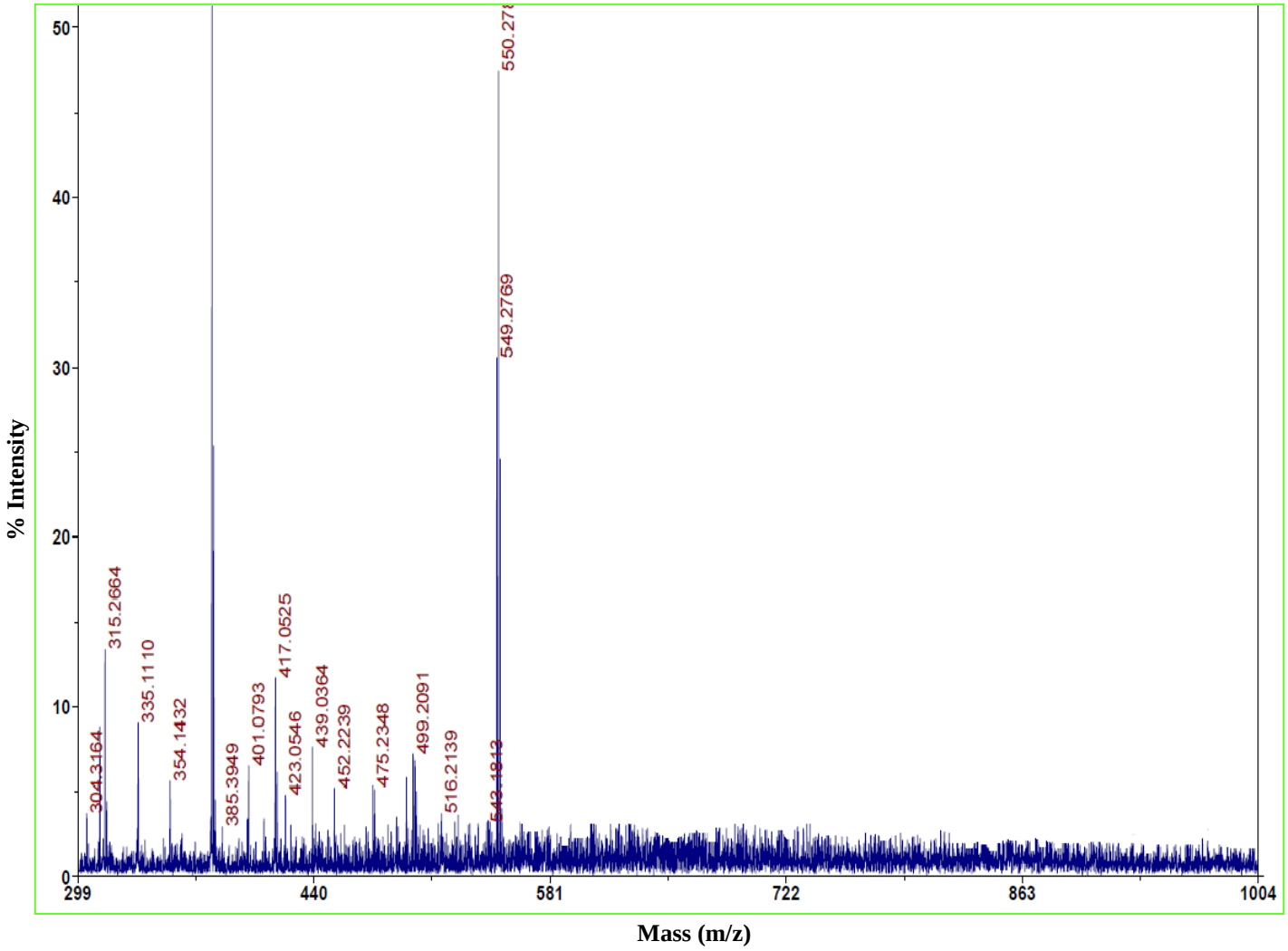
^{1}H NMR spectrum of compound 10 (300 MHz, $CDCl_3$)



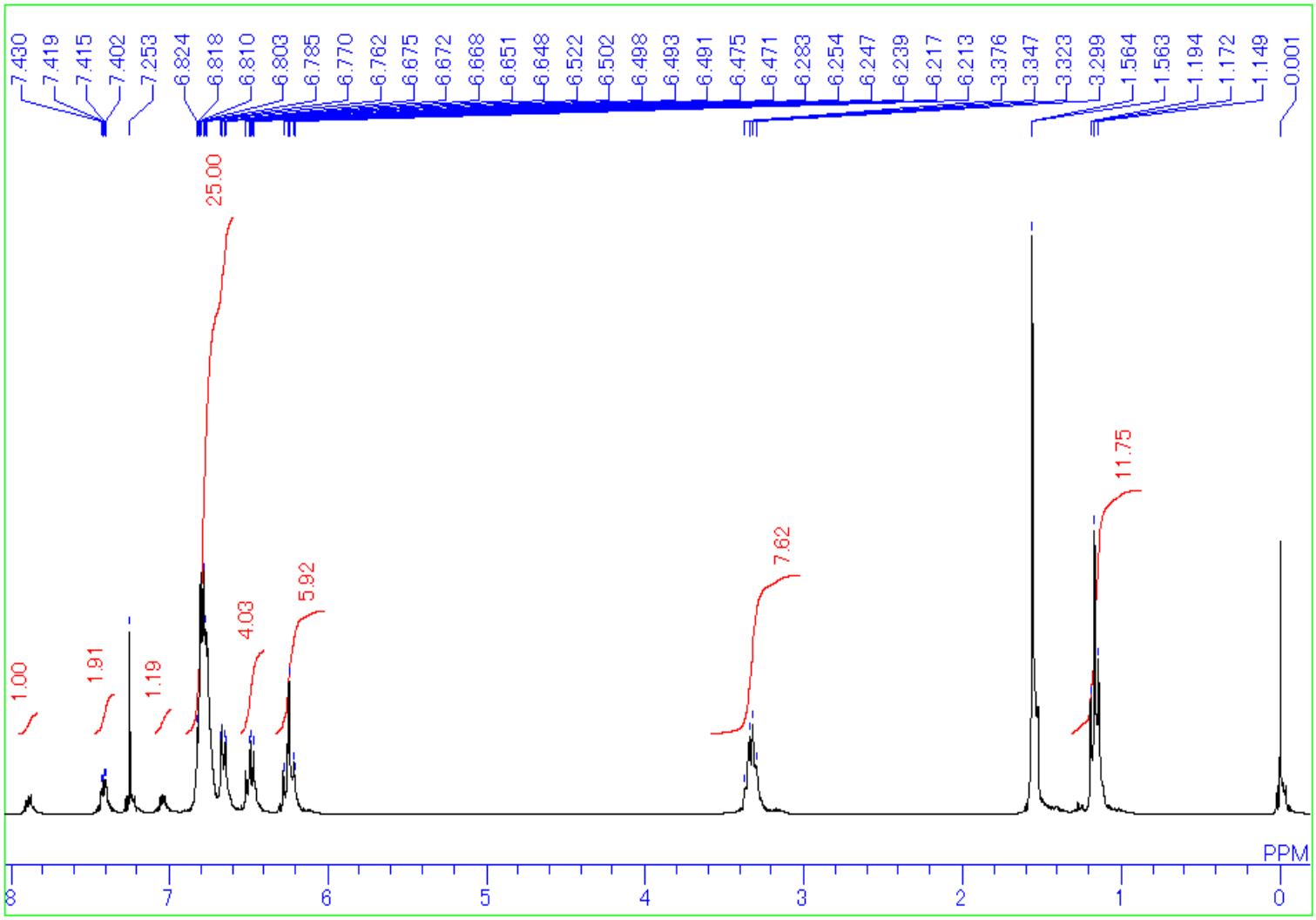
^{13}C NMR spectrum of compound 10 (75 MHz, $CDCl_3$)



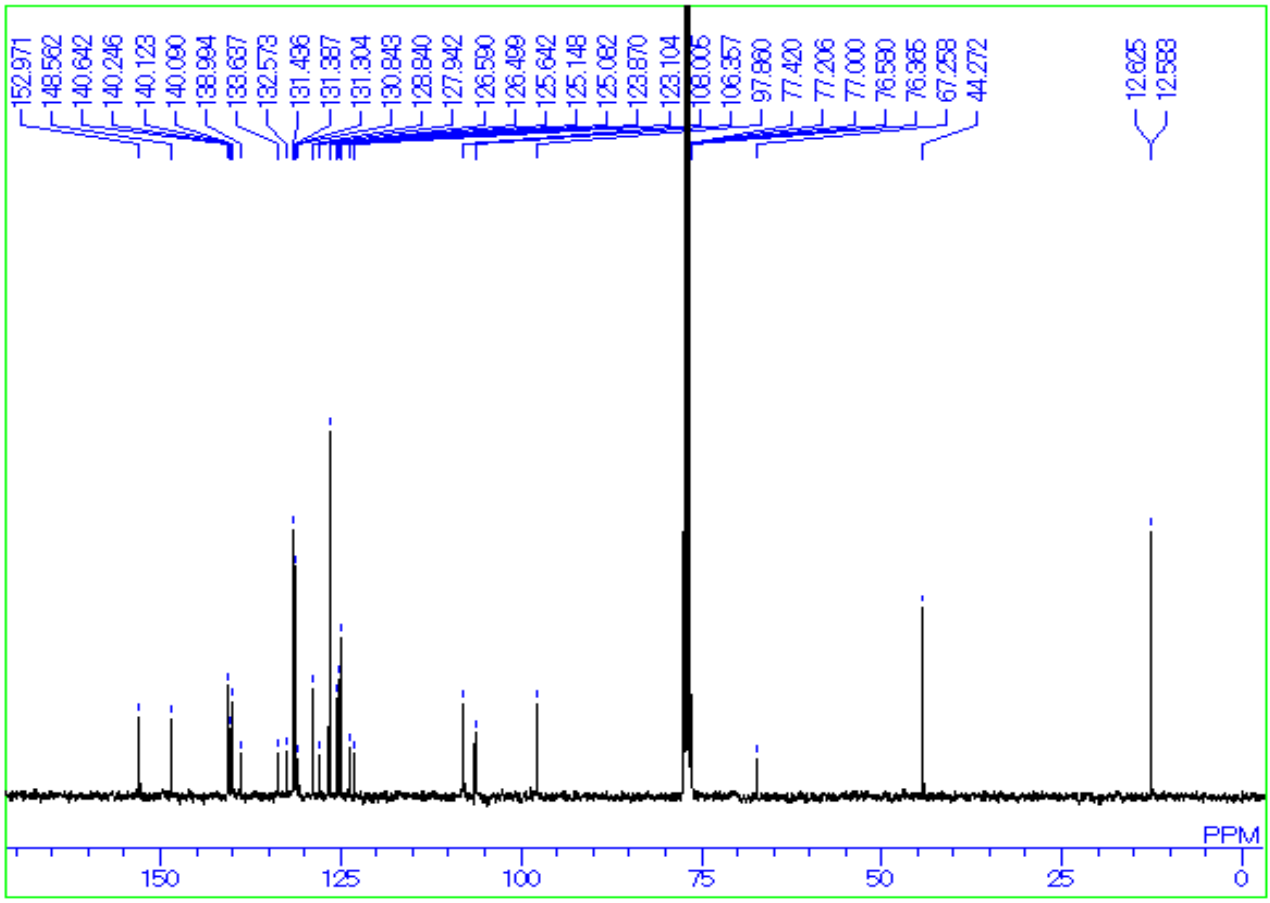
MALDI-TOF of compound 10



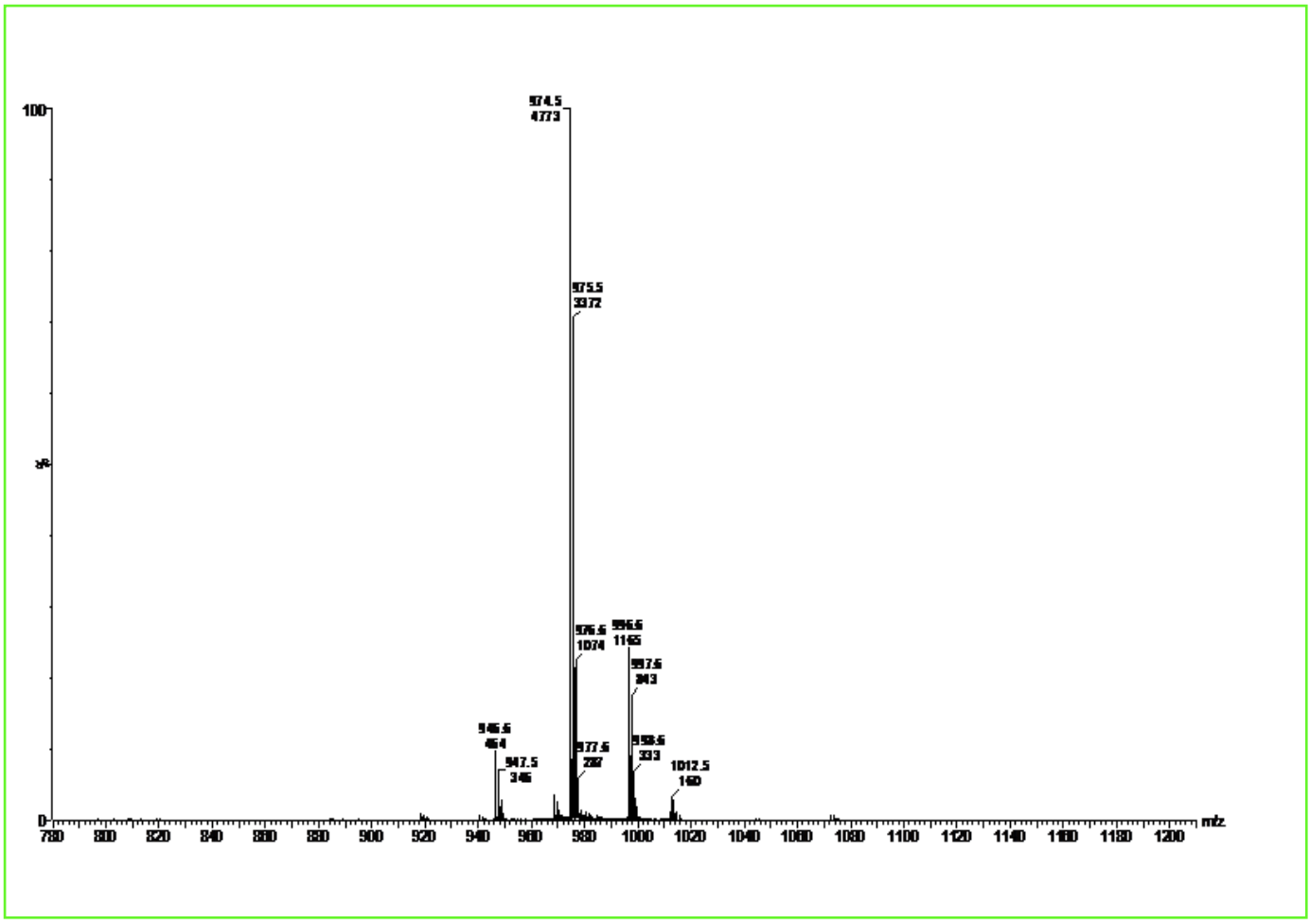
^{1}H NMR spectrum of compound 11 (300 MHz, $CDCl_3$)



^{13}C NMR spectrum of compound 11 (75 MHz, $CDCl_3$)



Mass spectrum of compound 11



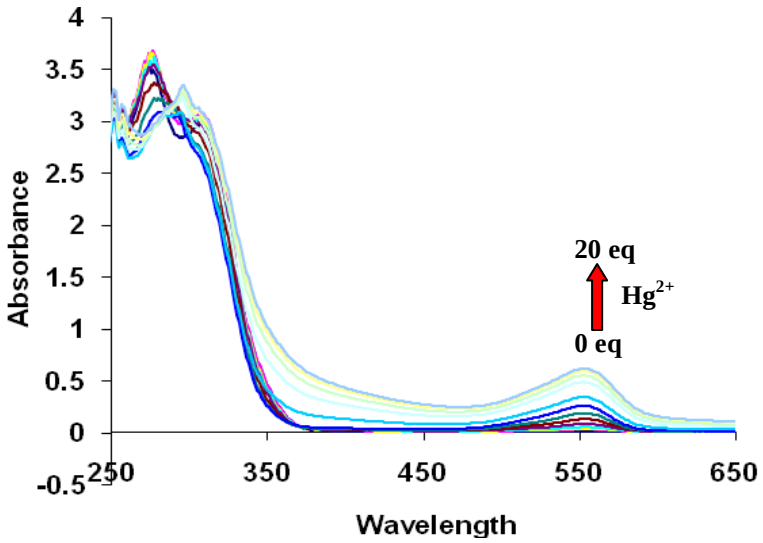


Figure S1. UV-vis spectra of receptor **7** (5 μM) in the presence of Hg^{2+} ions (0- 20 eq) in THF.

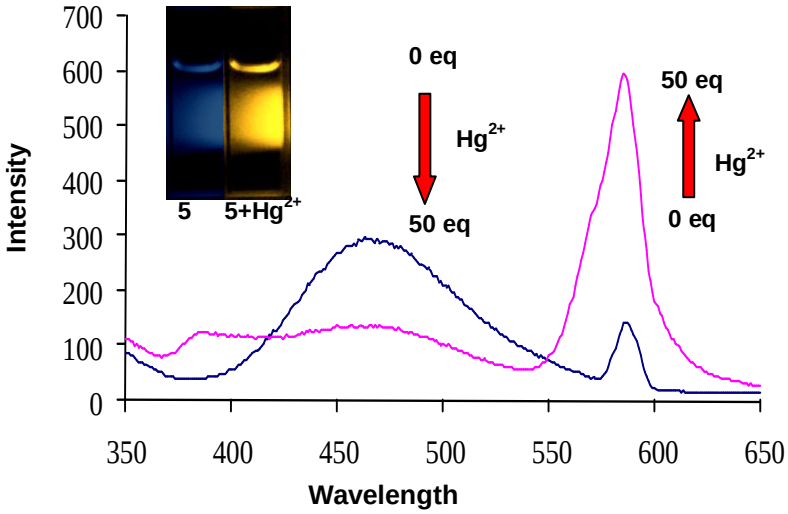


Figure S2. Fluorescence response of receptor **5** (1 μM) on addition of Hg^{2+} (50 eq) in THF, λ_{ex} = 290 nm. Inset shows the change in the fluorescence of compound **5** on addition of Hg^{2+} ions.

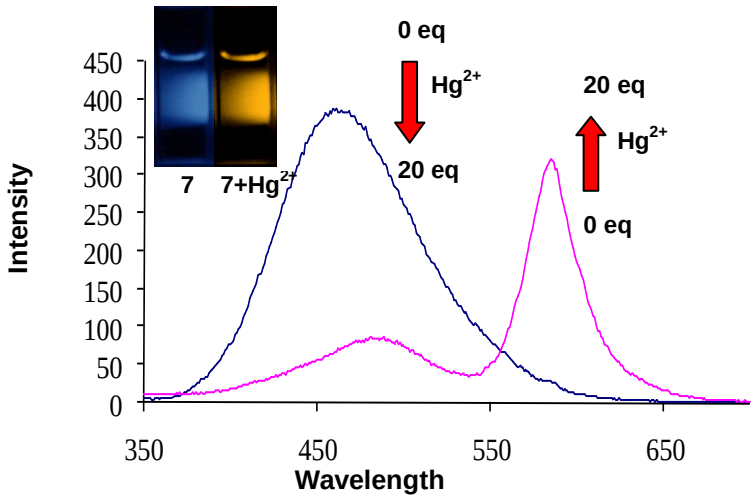


Figure S3. Fluorescence response of receptor **7** (1 μM) on addition of Hg^{2+} (0-20 eq) in THF, λ_{ex} = 290 nm. Inset shows the change in the fluorescence of compound **7** on addition of Hg^{2+} ions.

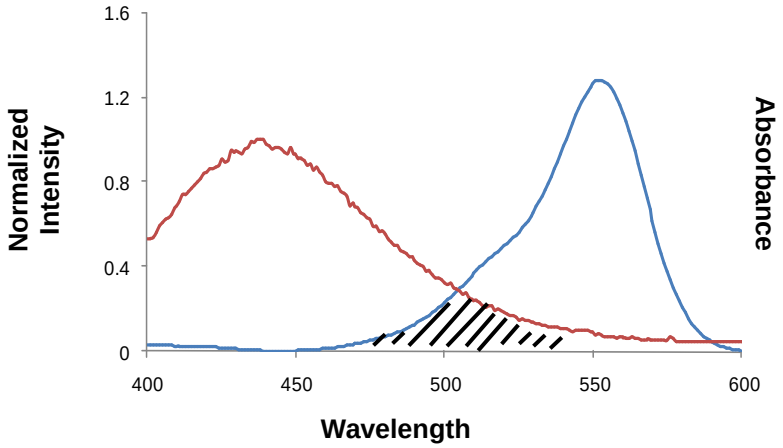


Figure S4 Spectral overlap of the absorption spectrum of rhodamine B (2.0 μM in THF) and emission spectrum of diamine **3** (2.0 μM in THF)

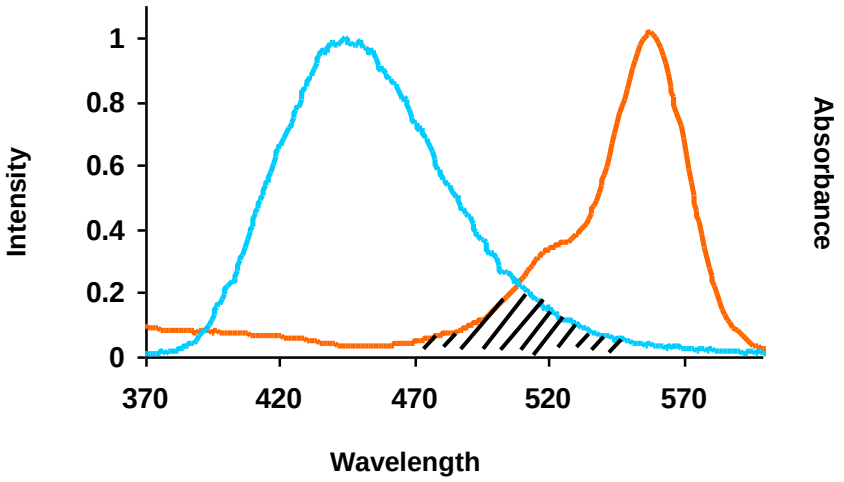


Figure S5 The spectral overlay of the absorption spectrum of rhodamine B, (2.0 μM in acetonitrile) and fluorescence spectrum of compound **6** (2.0 μM in acetonitrile).

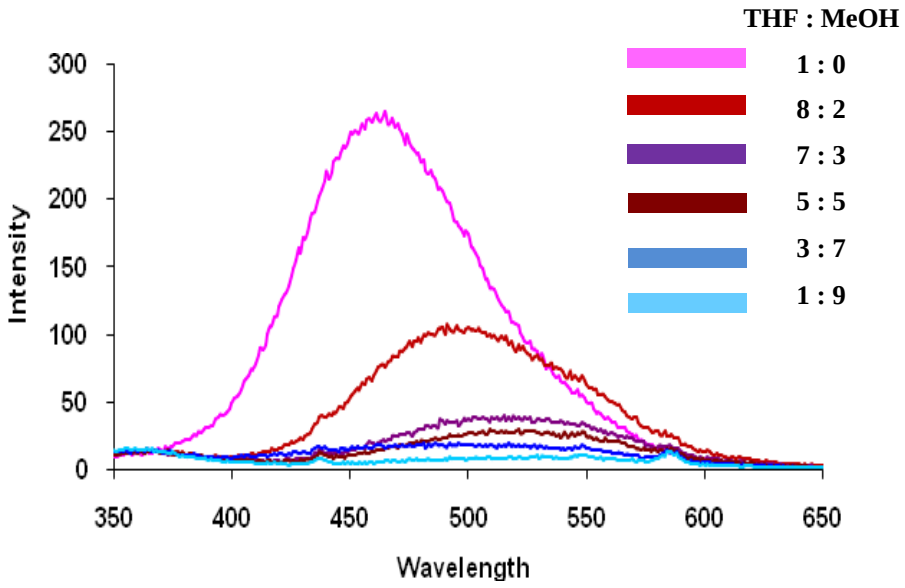


Figure S6 The fluorescence spectrum of compound **5** (1 μM) in different ratios of THF and methanol

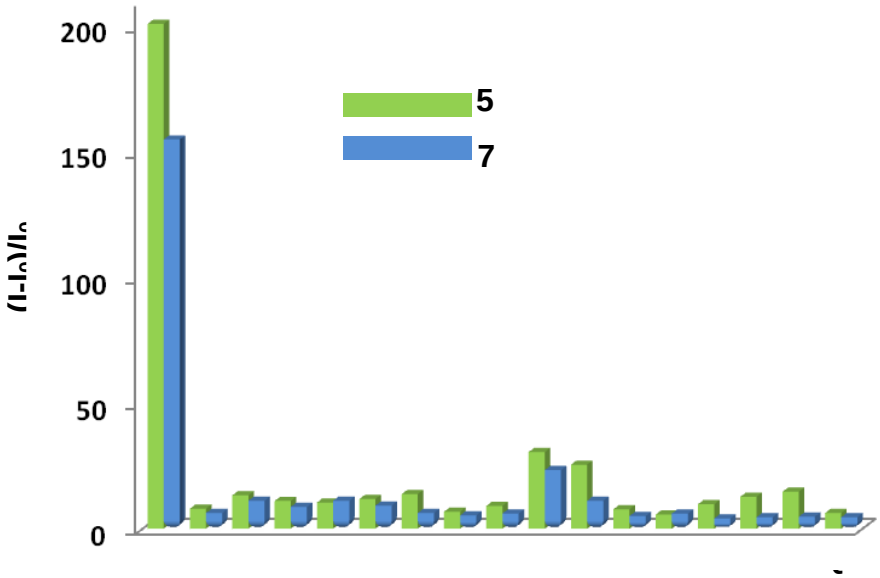


Figure S7. The selectivity graph of derivative **5** (1 µM) and **7** (1 µM) towards Hg^{2+} ions at 585 nm; A = Hg^{2+}, B = Pb^{2+}, C = Ba^{2+}, D = Ag^{+}, E = Cd^{2+}, F = Zn^{2+}, G = Cu^{2+}, H = Ni^{2+}, I = Co^{2+}, J = Fe^{2+}, K = Fe^{3+}, L = Mn^{2+}, M = Ca^{2+}, N = K^{+}, O = Mg^{2+}, P = Na^{+}, Q = Li^{+} in THF.

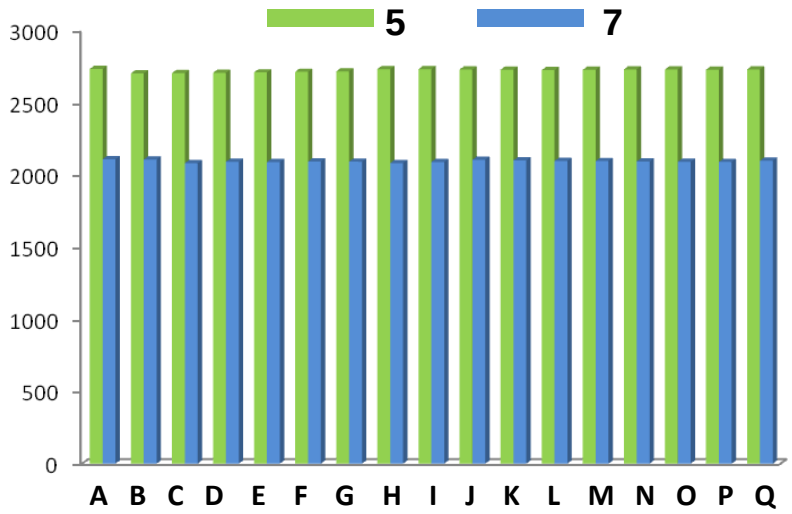


Figure S8. Competitive selectivity of receptor **5** (1.0 µM) and **7** towards Hg^{2+} ions (20 eq and 60 eq , respectively) in the presence of other metal ions (100 eq) A = none, B = Pb^{+}, C = Ba^{+}, D = Ag^{+}, E = Cd^{2+}, F = Zn^{2+}, G = Cu^{2+}, H = Ni^{2+}, I = Co^{2+}, J = Fe^{2+}, K = Fe^{3+}, L = Mn^{2+}, M = Ca^{2+}, N = K^{+}, O = Mg^{2+}, P = Na^{+}, Q = Li^{+} in methanol.

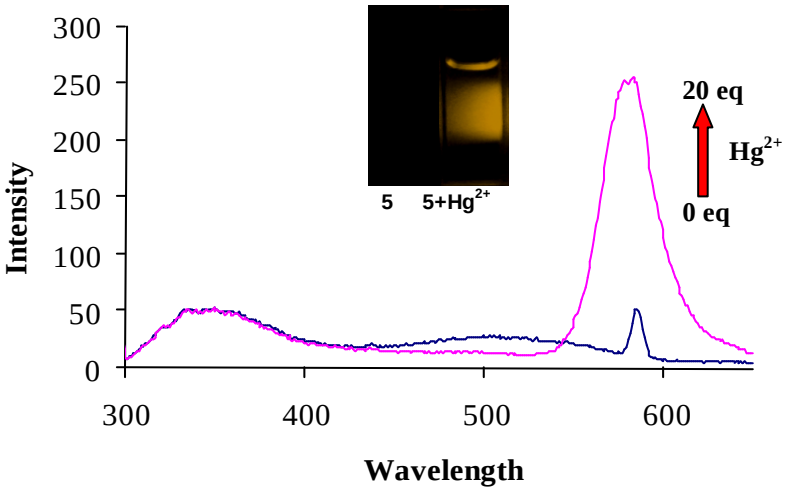


Figure S9. Fluorescence response of receptor **5** (1 μM) on addition of Hg^{2+} (0-20 eq) in n-butanol, λ_{ex} = 290 nm.

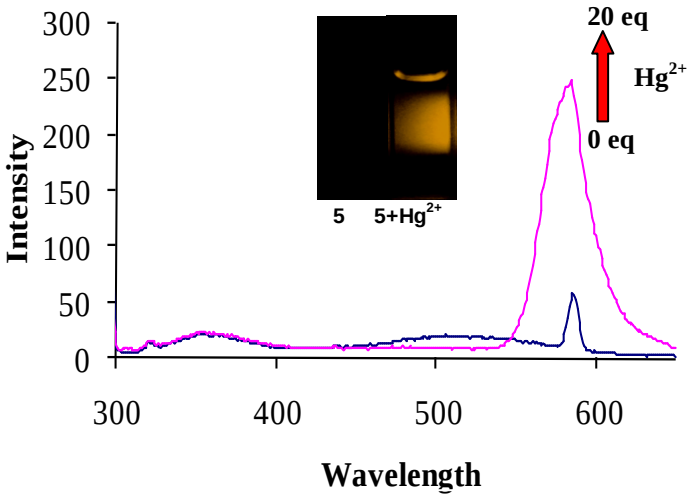


Figure S10. Fluorescence response of receptor **5** (1 μM) on addition of Hg^{2+} (0-20 eq) in n-propanol, λ_{ex} = 290 nm.

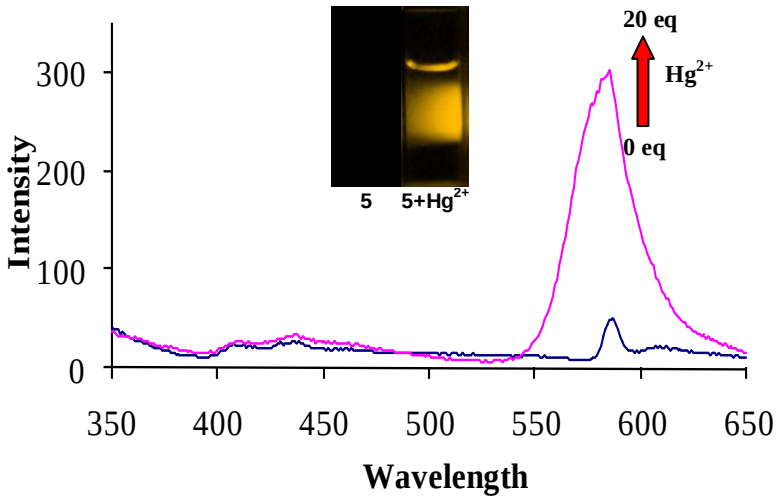


Figure S11. Fluorescence response of receptor **5** (1 μM) on addition of Hg^{2+} (0-20 eq) in ethanol, λ_{ex} = 290 nm.

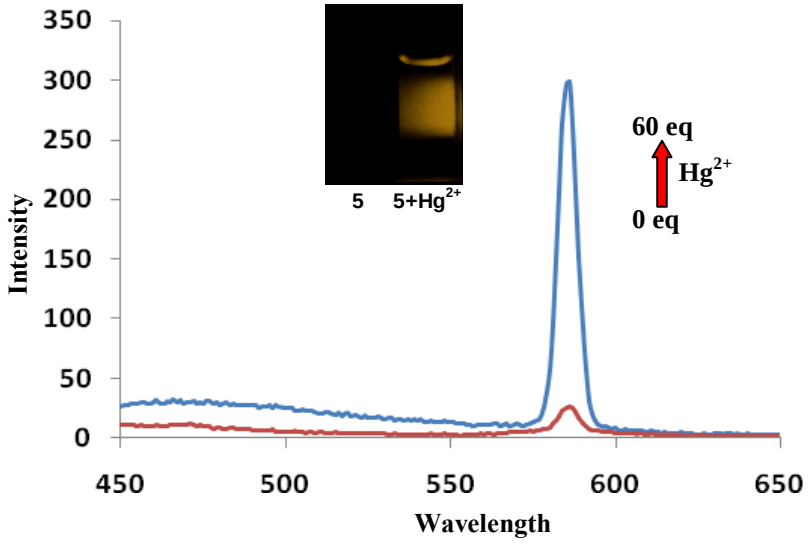


Figure S12. Fluorescence response of receptor **7** (1 μM) on addition of Hg^{2+} (0-60 eq) in n-butanol, λ_{ex} = 290 nm.

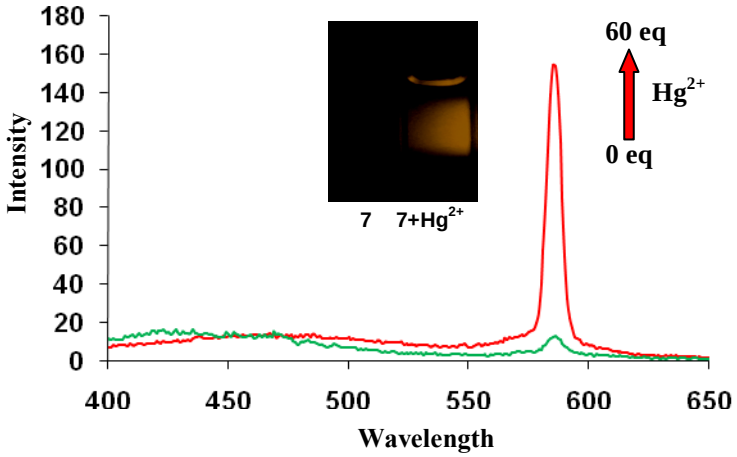


Figure S13. Fluorescence response of receptor **7** (1 μM) on addition of Hg^{2+} (0-60 eq) in n-propanol, λ_{ex} = 290 nm.

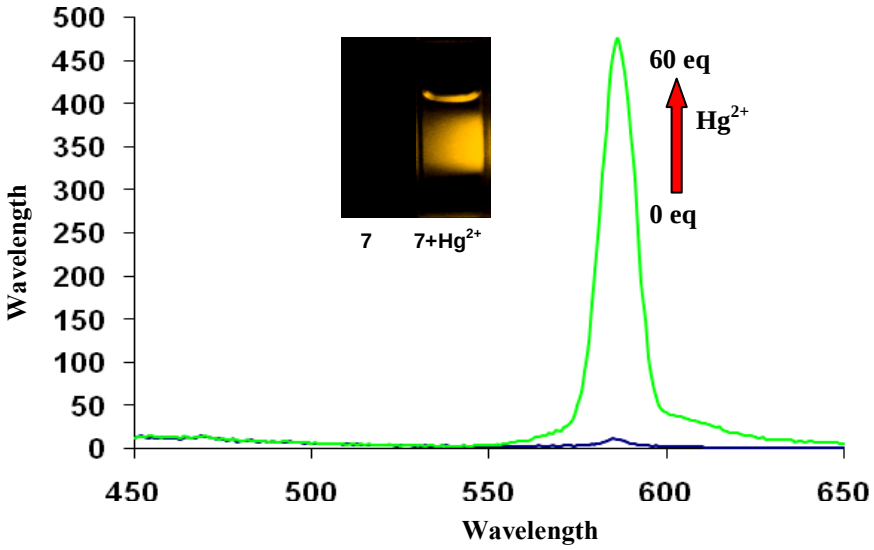


Figure S14. Fluorescence response of receptor **7** (1 μM) on addition of Hg^{2+} (0-60 eq) in ethanol, λ_{ex} = 290 nm.

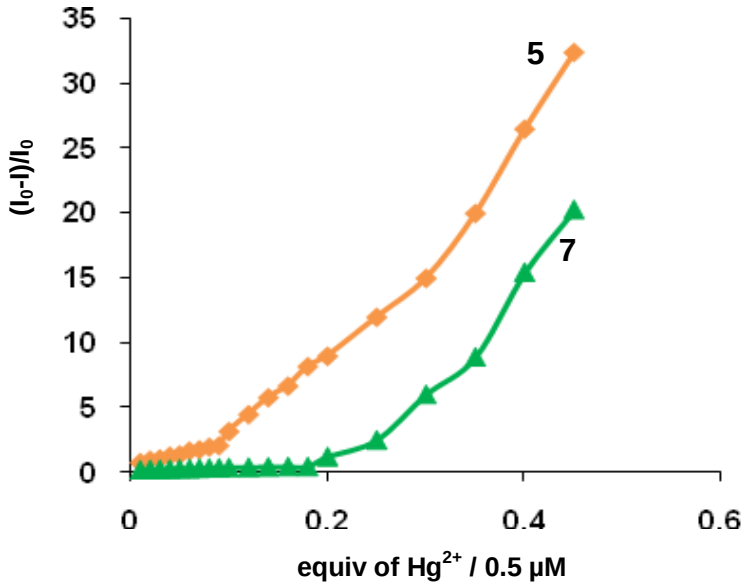


Figure S15. The change in relative intensity on subsequent addition of Hg^{2+} ions in compound **5** (0.5 μM in THF) and **7** (0.5 μM in THF).

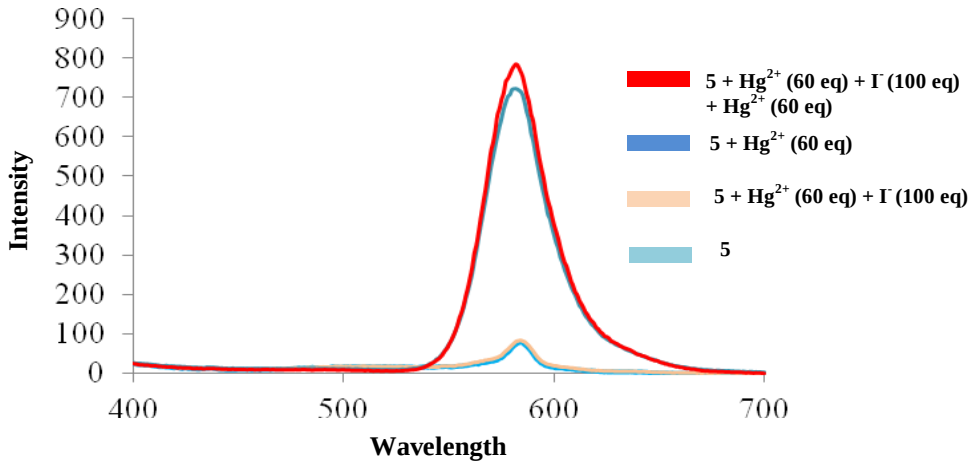


Figure S16. Fluorescence spectra showing reversibility of Hg^{2+} coordination to receptor **5** (1 μM in methanol) by TBAI (100 eq)

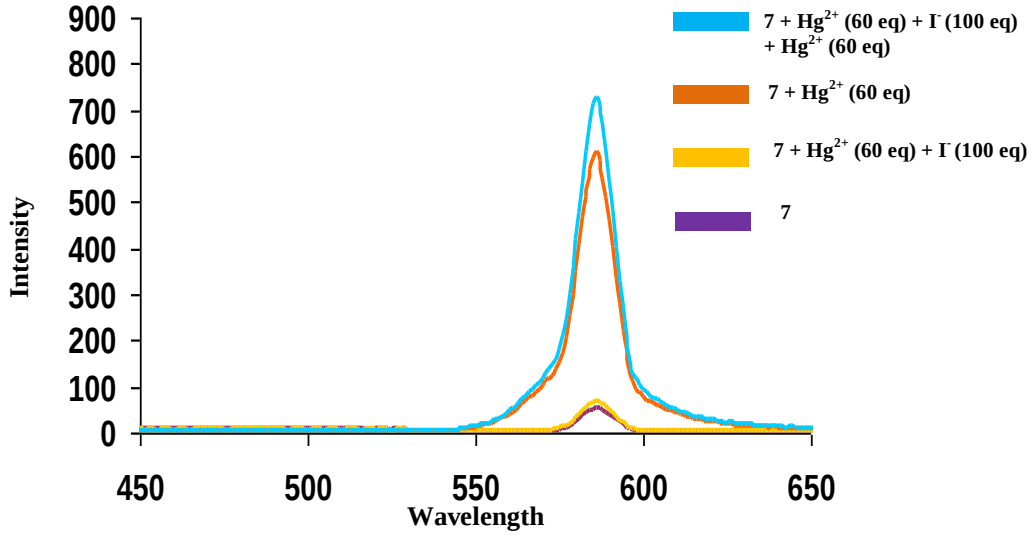


Figure S17 Fluorescence spectra showing reversibility of Hg^{2+} coordination to receptor **7** (1 µM in methanol) by TBAI (100 eq).

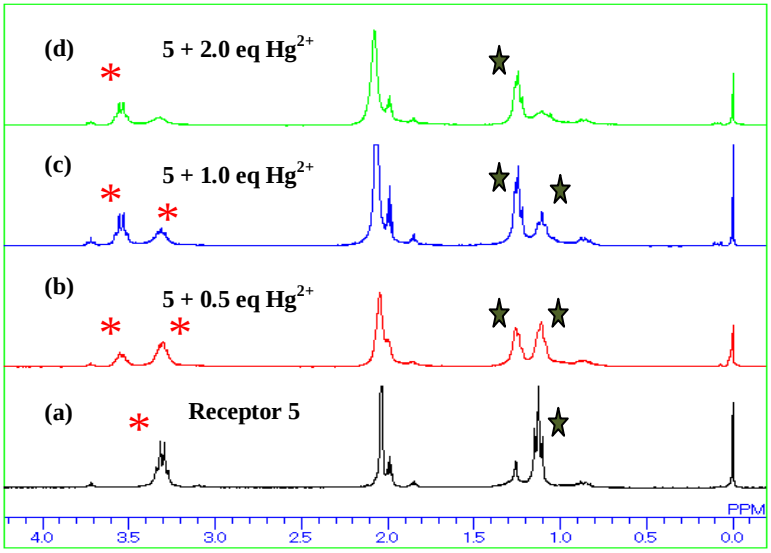


Figure S18. Partial ^1H NMR spectrum of receptor **5** before (a), after addition of 0.5 equiv. (**b**), 1.0 equiv. (**c**) and 2 equiv. (**d**) of Hg^{2+} ions in $CDCl_3$:CD_3CN (8:2)

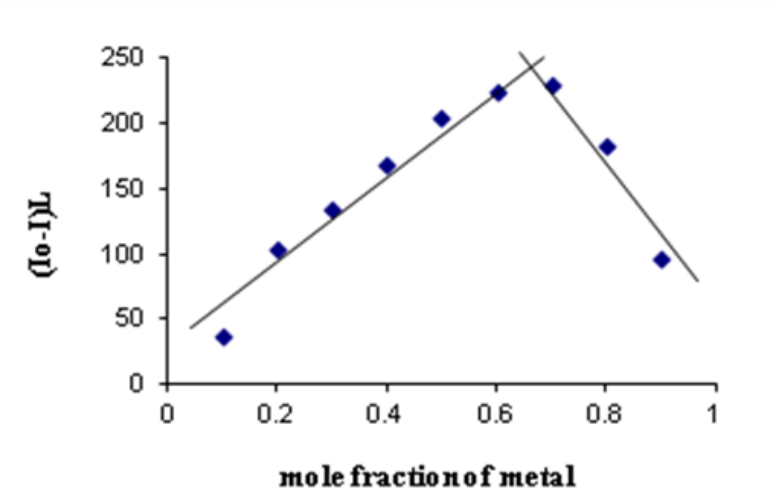


Figure S19. Job's plot for determining the stoichiometry of receptor **5** and Hg^{2+} ion in THF

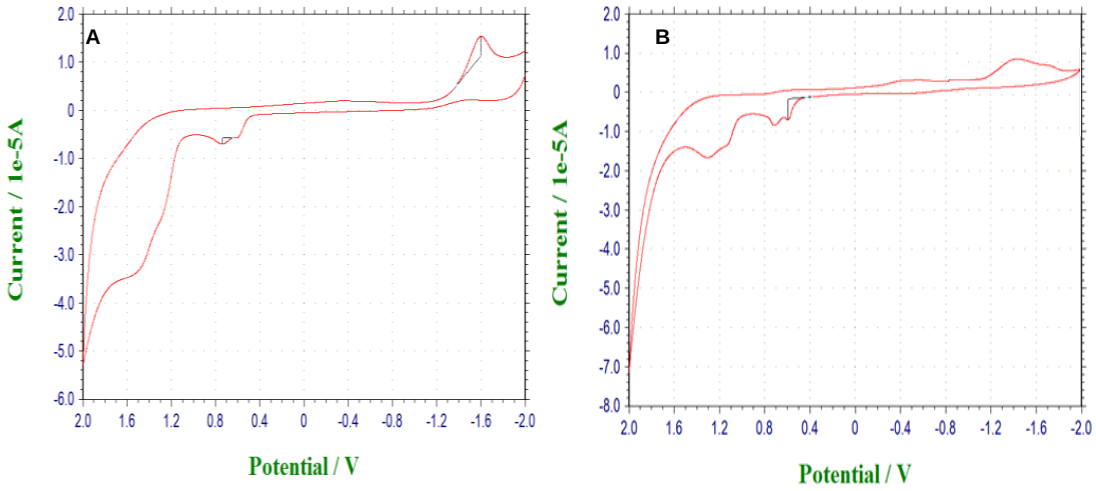


Figure S20 The cyclic voltammograms for derivative **5** before (A) and after (B) addition of Hg^{2+} ions in 1,2dichloromethane (10^{-3} M solution) using ferrocene as internal standard.

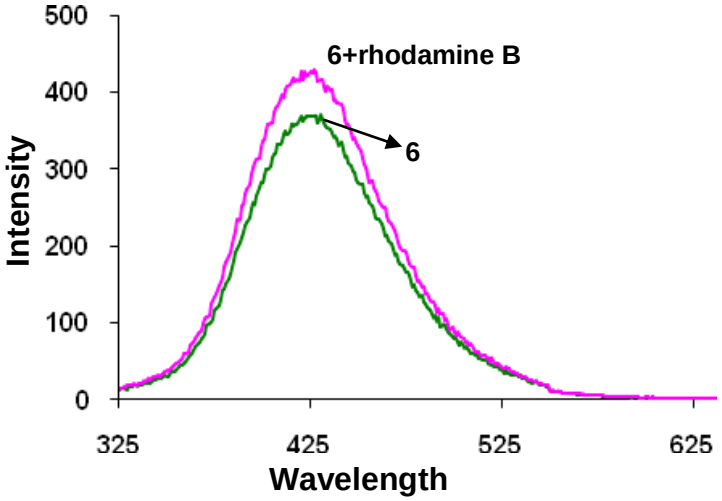


Figure S21. The fluorescence spectrum of compound **6** and equimolar (1 μM) solution of compound **6** + rhodamine B in methanol at excitation wavelength of λ_{eq} = 290 nm.

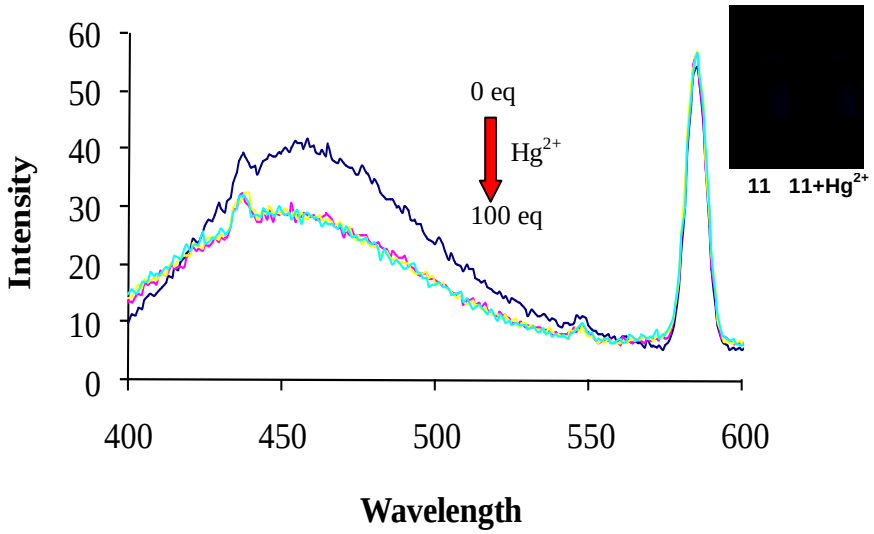


Figure S22 Fluorescence response of receptor **11** (1 μM) on addition of Hg^{2+} (0-50 eq) in THF, λ_{ex} = 290 nm.

Resonance energy transfer efficiency $E = [1 - F_D'/F_D]$

F_D = Fluorescence intensity of free ligand;

F_D' = Fluorescence intensity of corresponding amine

Equation 1

$$\phi_{fs} = \phi_{fr} \times \frac{1-10^{-ArLr}}{1-10^{-AsLs}} \times \frac{N_s^2}{N_r^2} \times \frac{D_s}{D_r}$$

ϕ_{fs} = quantum yield of sample; ϕ_{fr} = quantum yield of reference; A_r = Absorbance of reference; A_s = Absorbance of sample; N_R = refractive index of reference; N_S = refractive index of sample; D_s = area under the curve of fluorescence graph of sample; D_R = area under the curve of fluorescence graph of reference. L_s = length of cell of sample; L_R = length of reference

Equation 2