

Supporting Information

New Terphenyl based Ensemble for the Detection of Acetate Ions in Plasma like System

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General Experimental Procedures

UV-Vis and fluorescence Titrations

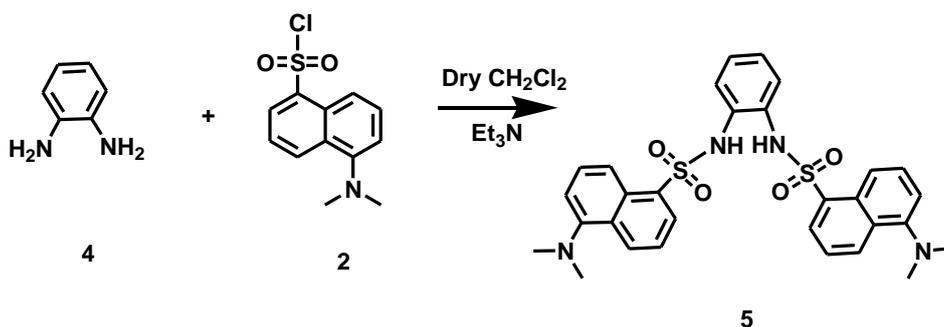
UV-Vis and fluorescence titrations were performed with 1×10^{-5} M solution of receptor **3** in THF. Typically, aliquots of freshly prepared standard solutions (10^{-1} - 10^{-3} M in THF) of metal perchlorates (Pb^{2+} , Hg^{2+} , Ba^{2+} , Cd^{2+} , Ag^+ , Zn^{2+} , Cu^{2+} , Ni^{2+} , Co^{2+} , Fe^{3+} , Fe^{2+} , K^+ , Mg^{2+} , Na^+ and Li^+) were added and the UV-Vis spectra of the samples were recorded. Similarly, aliquots of freshly prepared solutions of anions (F^- , Cl^- , Br^- , I^- , HSO_4^- , H_2PO_4^- , CH_3COO^- , NO_3^- , N_3^- , SO_4^{2-} , SO_3^{2-} , $\text{Cr}_2\text{O}_7^{2-}$) were added to record the absorption behaviour of **3**.

^1H NMR Experiments

The stock solution of compound **3** (10^{-2} M) and perchlorate salts of Hg^{2+} (2×10^{-2} M) were prepared in $\text{CDCl}_3:\text{CD}_3\text{CN}$ (8:2) for ^1H NMR titration experiments. Tetrabutylammonium salts of fluoride and acetate were prepared in CDCl_3 .

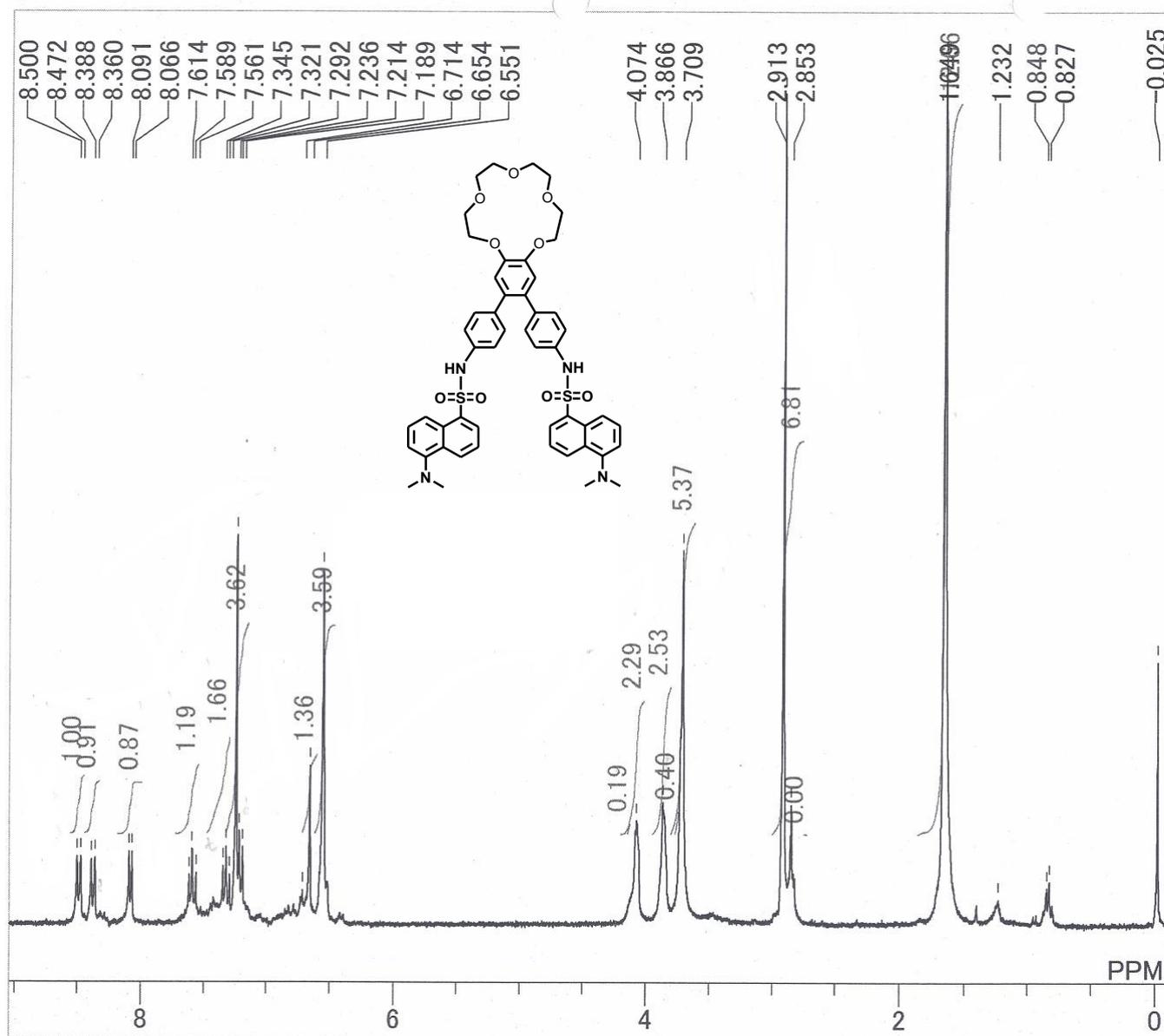
Experimental Procedure for synthesis of **4**¹

A solution of dansyl chloride (0.27 g, 1.02 mmol) in dichloromethane (5 ml) was added to the solution of diamine **1** (0.05 g, 0.22 mmol) in minimum amount of dichloromethane. To the above solution triethylamine (90 μL) was added. The resultant reaction mixture was stirred for overnight at room temperature. The mixture so obtained was treated with dichloromethane and dried over anhydrous Na_2SO_4 . The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography (CH_2Cl_2) to give 70 mg of **4** (yield 70%).

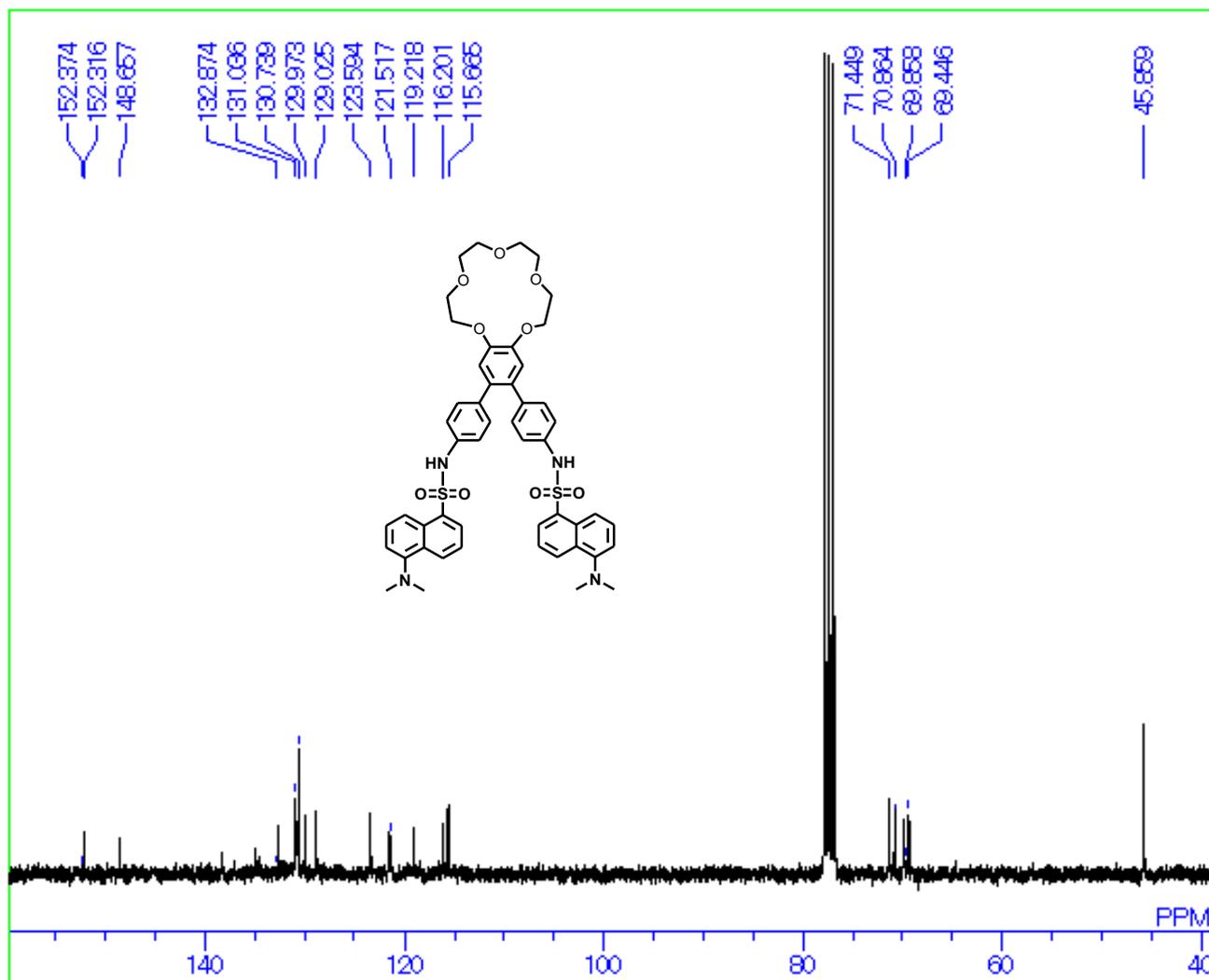


¹ Kavallieratos, K.; Rosenberg, J. M.; Chen, W.-Z.; Ren, T. J. Am. Chem. Soc. 2005, 127, 6514.

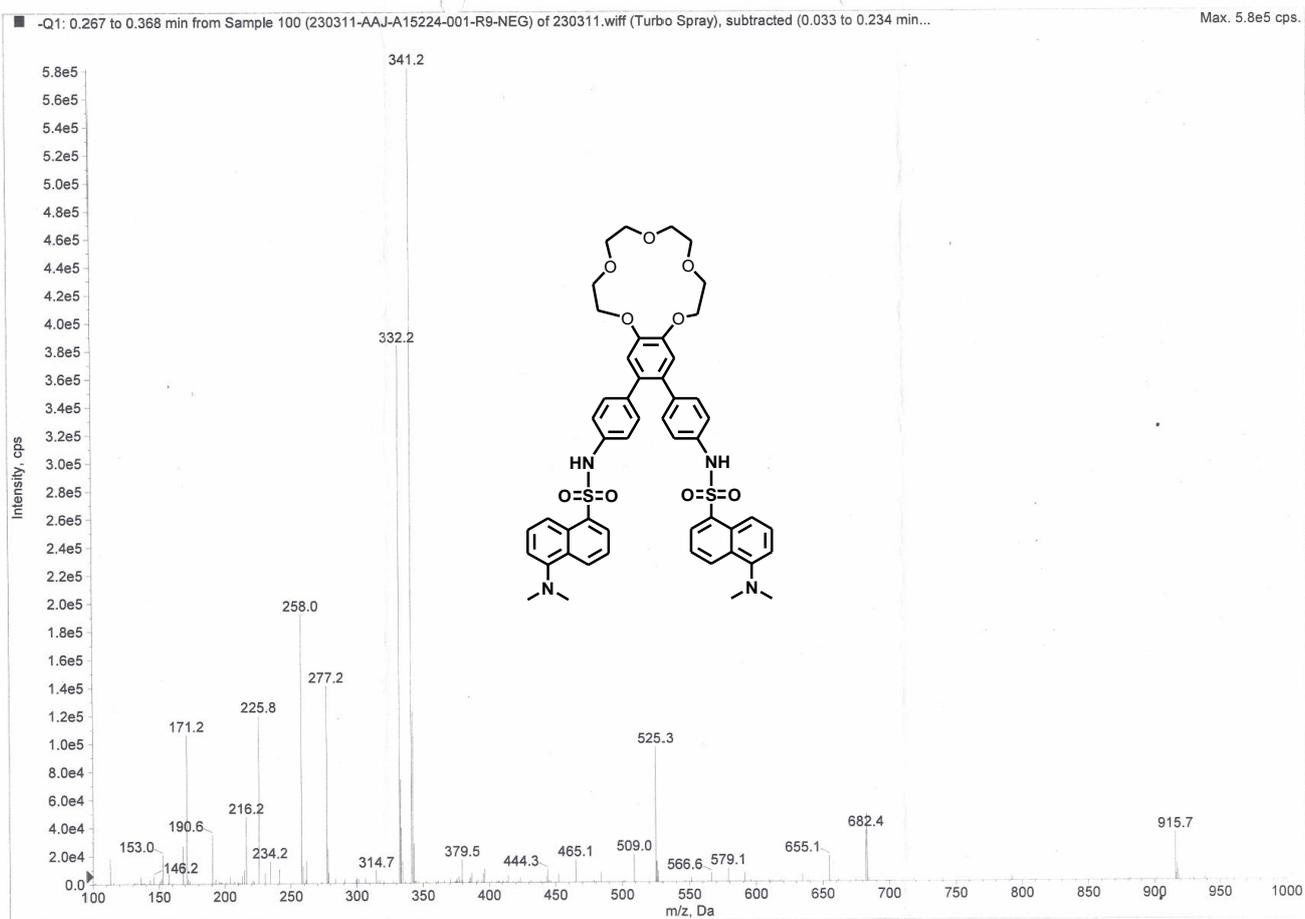
¹H NMR of Compound 3



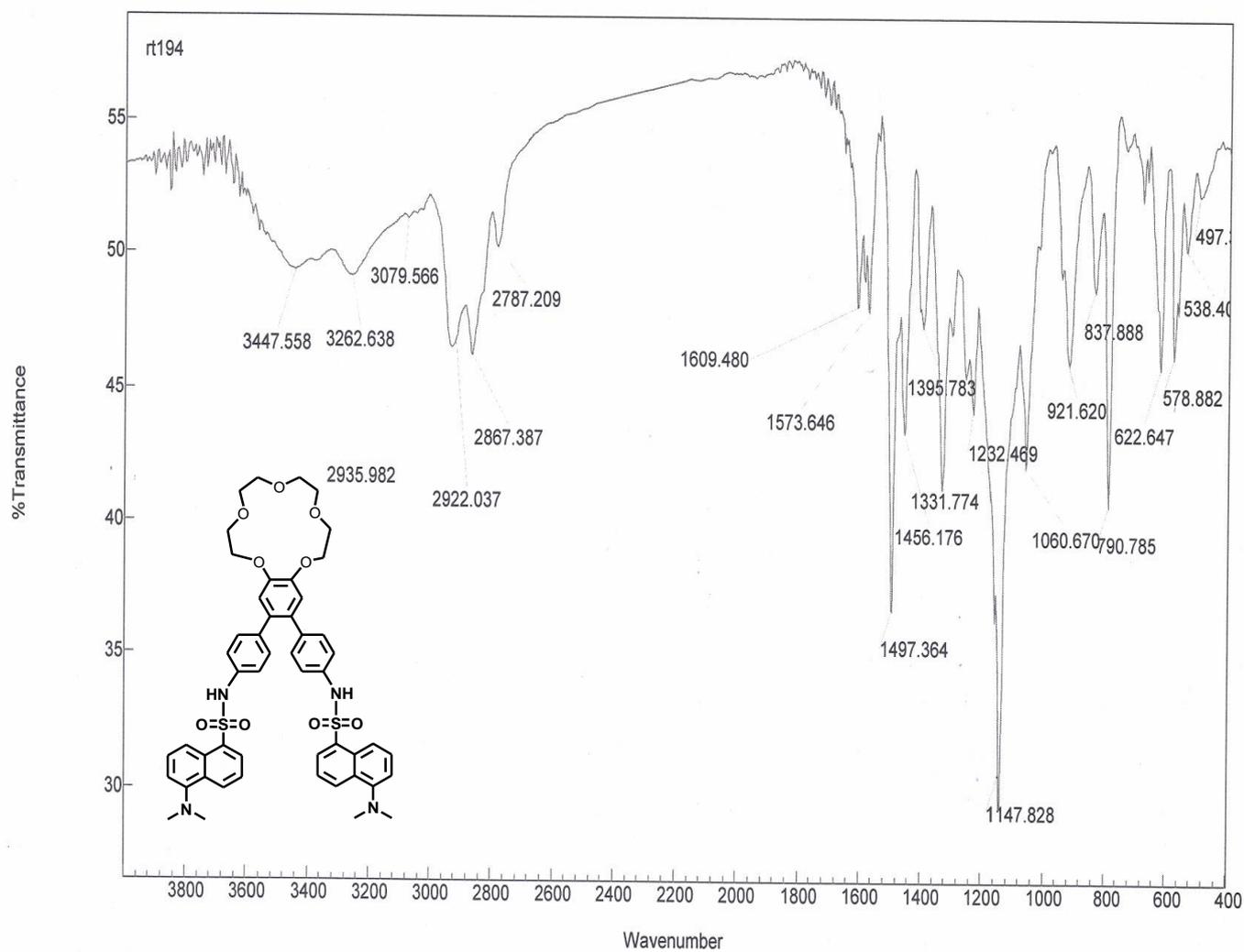
^{13}C NMR of Compound 3



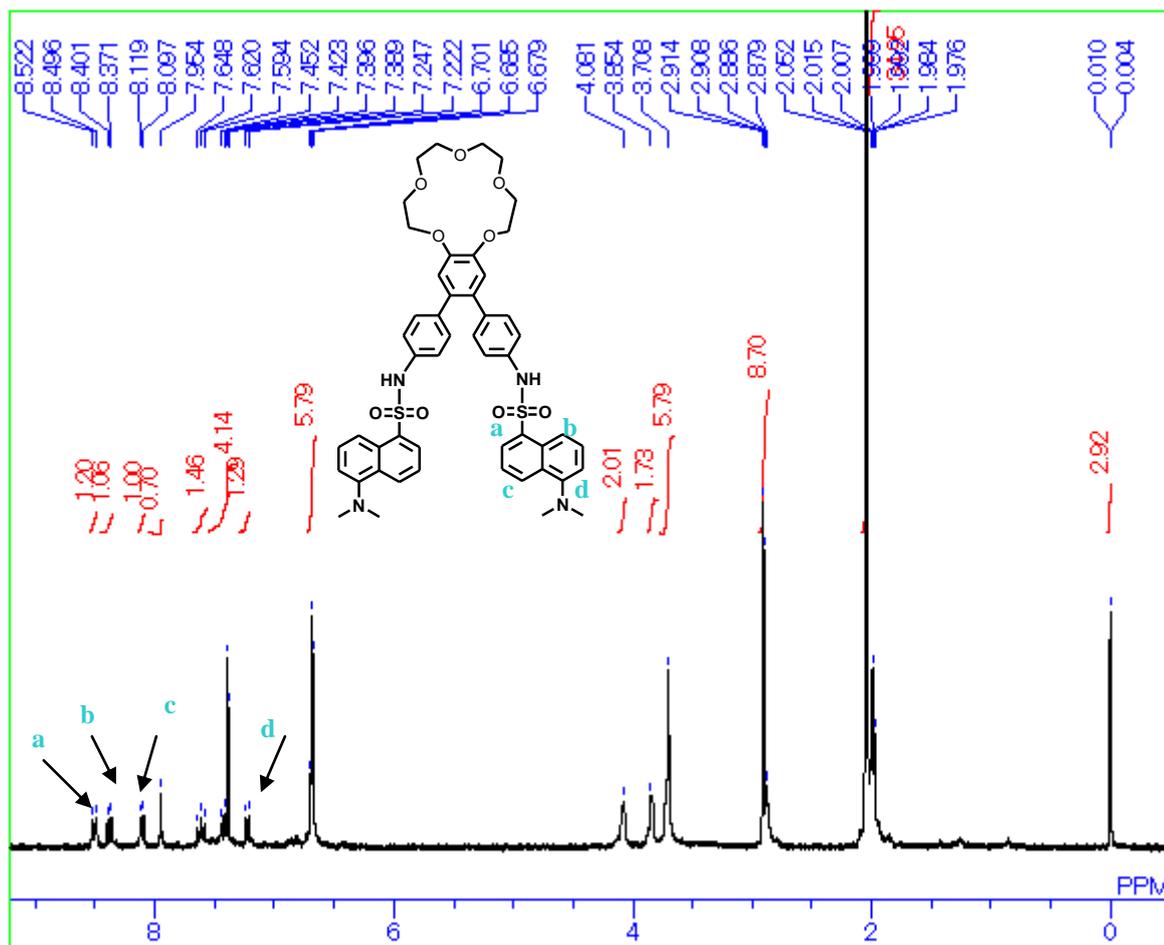
Mass spectrum of 3



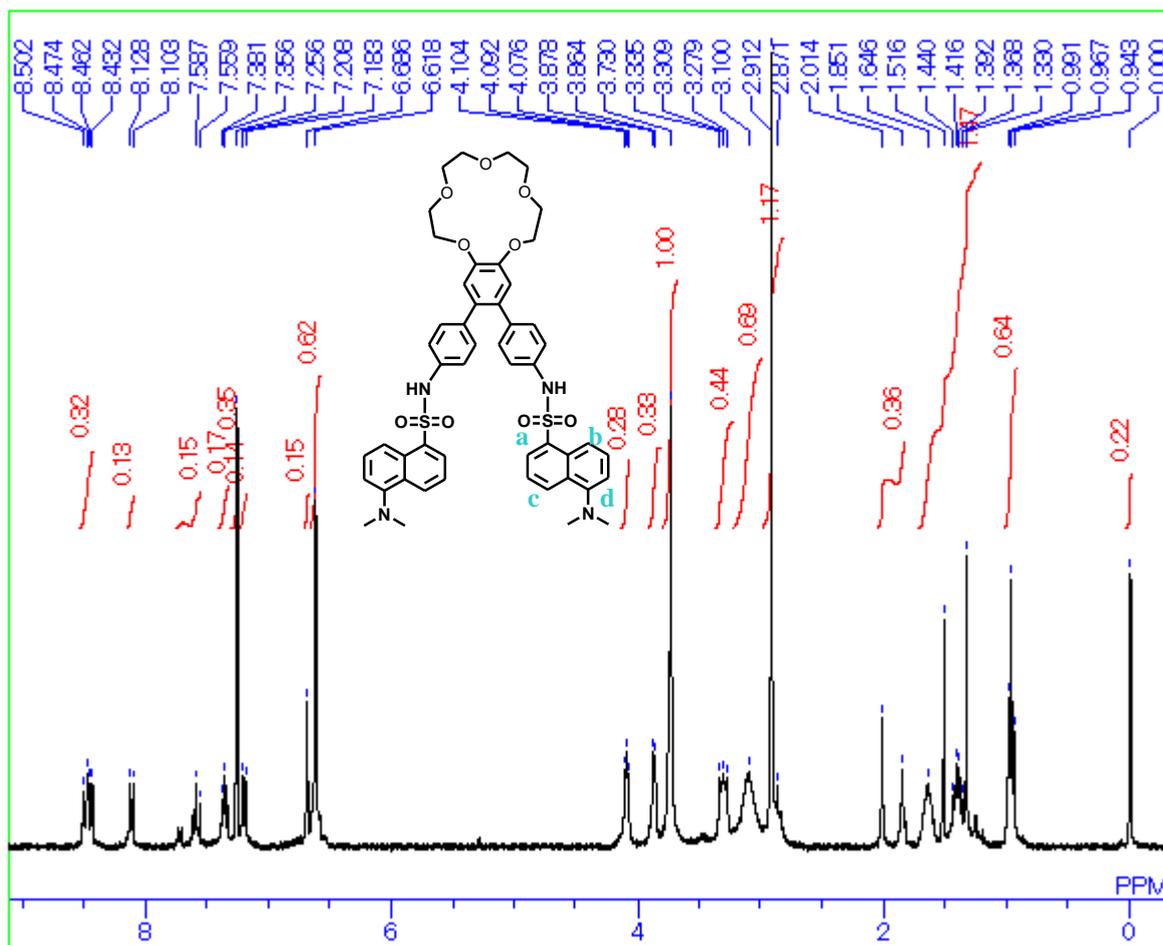
IR spectrum of 3



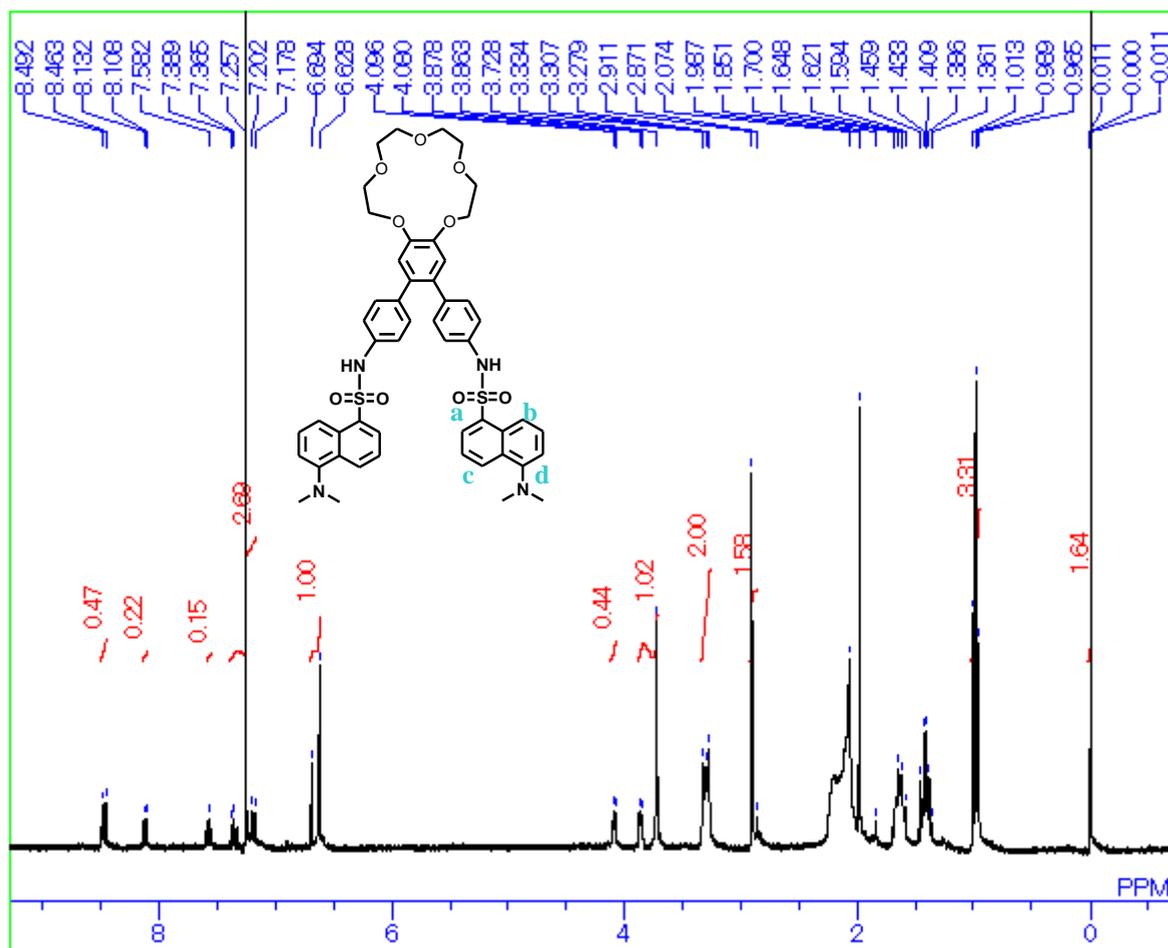
^1H NMR of Compound 3 in CDCl_3



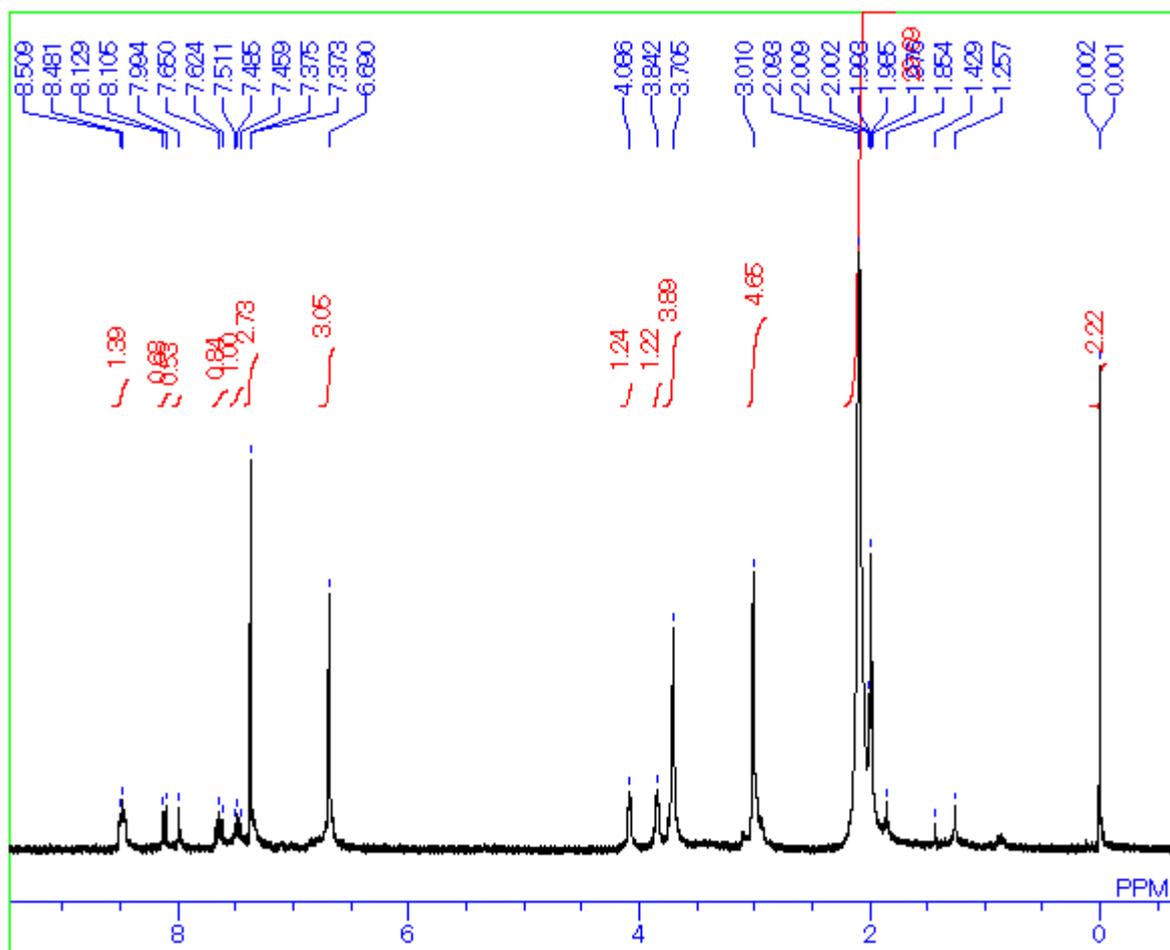
^1H NMR of Compound 3 in the presence of F^- ions in CDCl_3



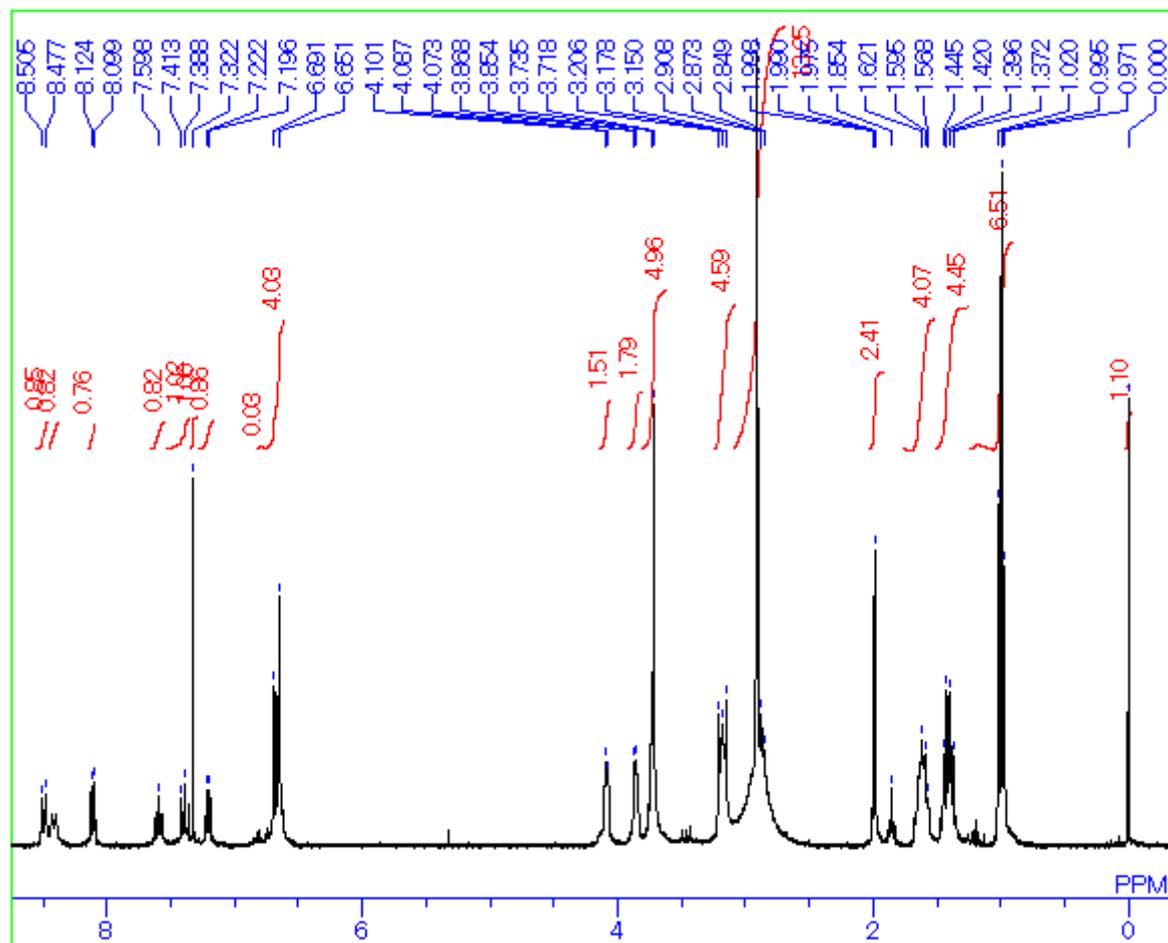
^1H NMR of Compound 3 in the presence of CH_3COO^- ions in CDCl_3



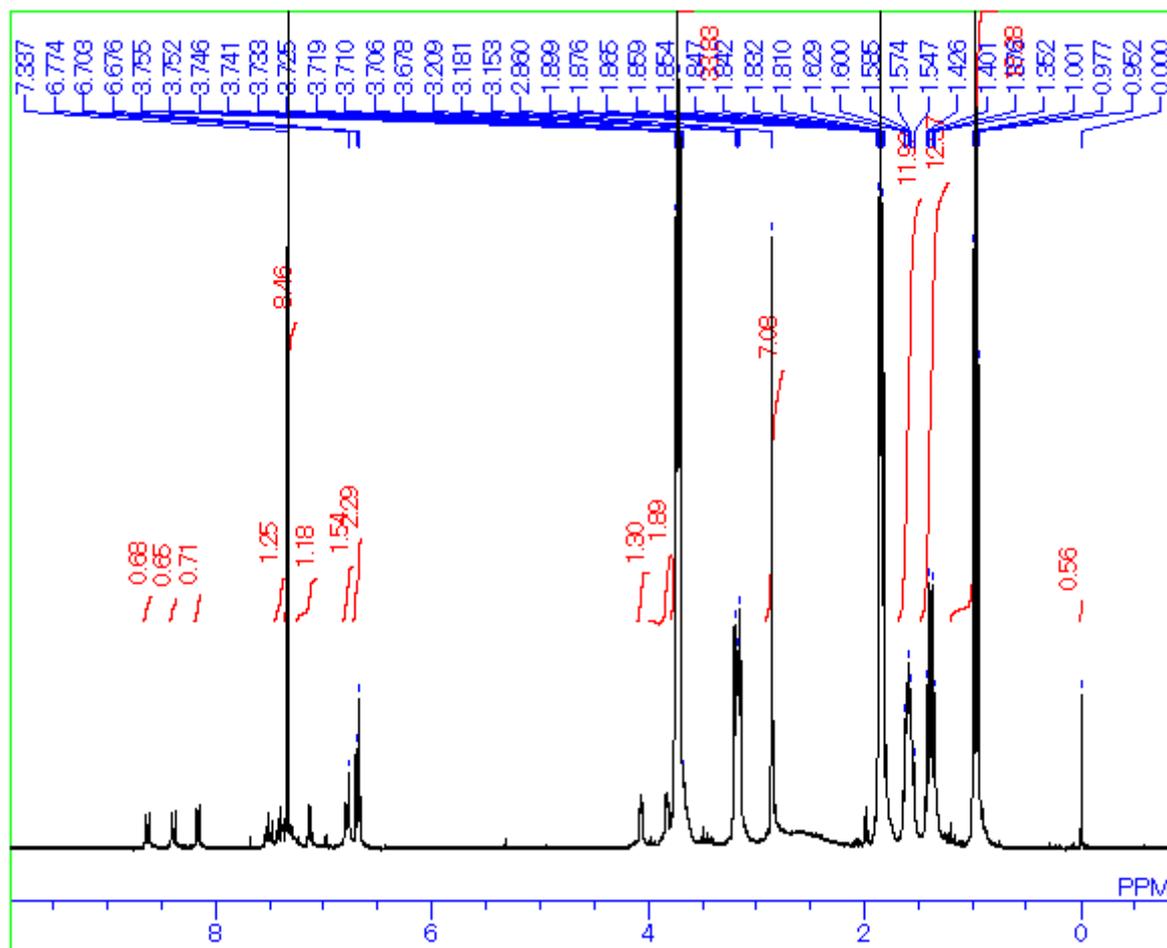
^1H NMR of ensemble 3 + Hg in $\text{CDCl}_3:\text{CD}_3\text{CN}$ (8:2)



^1H NMR of Ensemble 3-Hg in the presence of CH_3COO^- ions in CDCl_3



^1H NMR of Ensemble 3-Hg in the presence of F^- ions in CDCl_3



Compiled UV Titration data of receptor 3 with F^- , CH_3COO^-

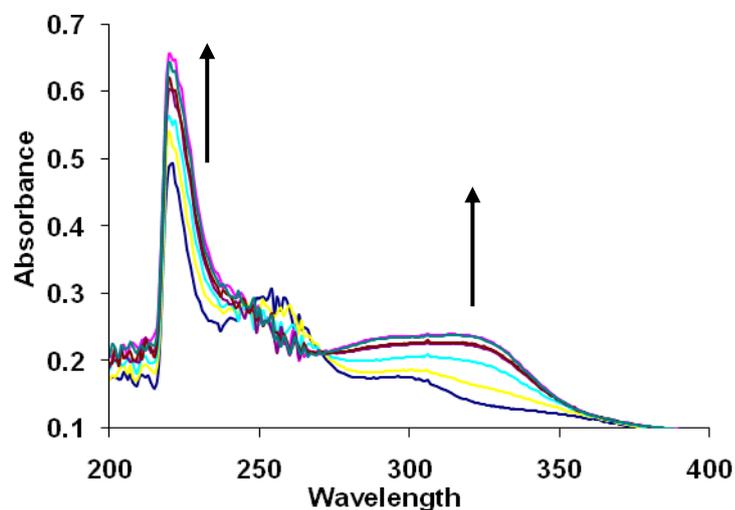


Fig. 1. UV-Vis spectra of receptor 3 (5 μ M) upon addition of CH_3COO^- ions (0.1 – 10.0 equiv) in THF

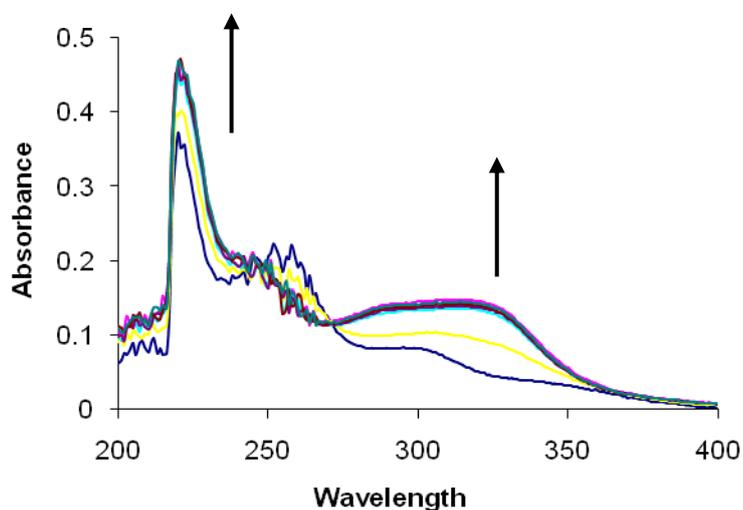


Figure 2. UV-Vis spectra of receptor 3 (5 μ M) upon addition of F^- ions (0.1 – 10.0 equiv) in THF

Compiled UV Titration data of receptor 3 with OH⁻

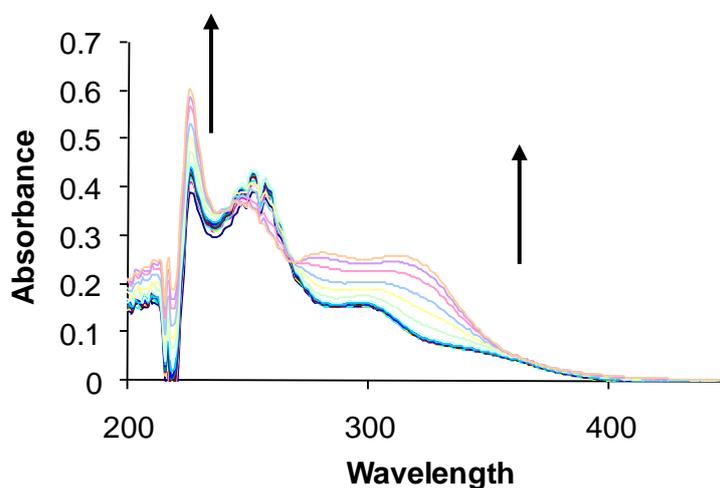


Figure 2. UV-Vis spectra of receptor 3 (5 μM) upon addition of OH⁻ ions (0.1 – 200.0 equiv) in THF

Compiled UV Titration data of receptor 3 with Hg²⁺

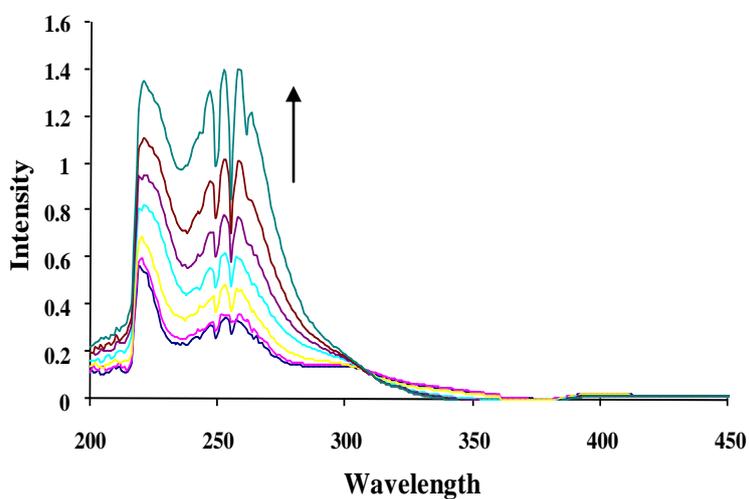


Figure 3. UV-Vis spectra of receptor 3 (5 μM) upon addition of Hg²⁺ ions (0.1 – 20.0 equiv) in THF

Compiled UV Titration data of ensemble 3-Hg with F⁻ and CH₃COO⁻

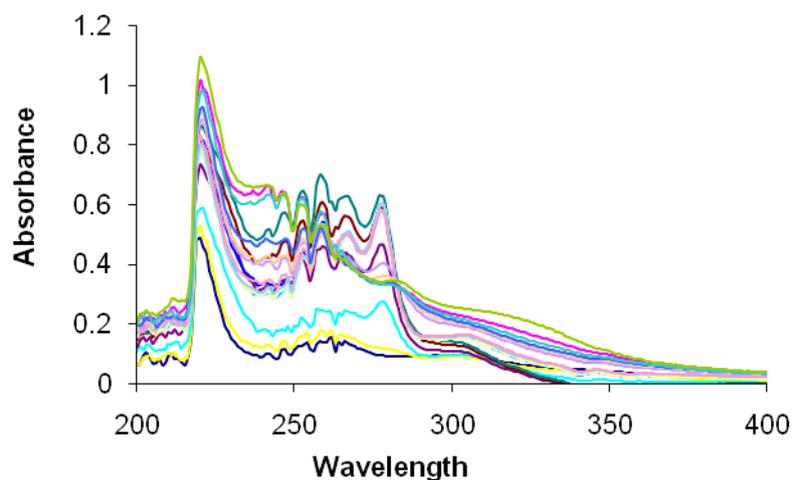


Figure 4. UV-Vis spectra of receptor **1** (5 μM) upon addition of OAc⁻ ions (0.1 – 30.0 equiv) in the presence of PLAS- BSA (10 μl)

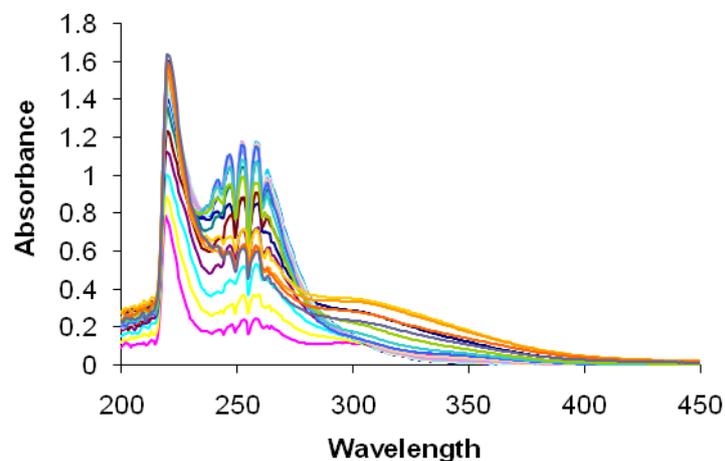


Figure 5. UV-Vis spectra of receptor **1** (5 μM) upon addition of OAc⁻ ions (0.1 – 30.0 equiv) in the absence of PLAS- BSA (10 μl)

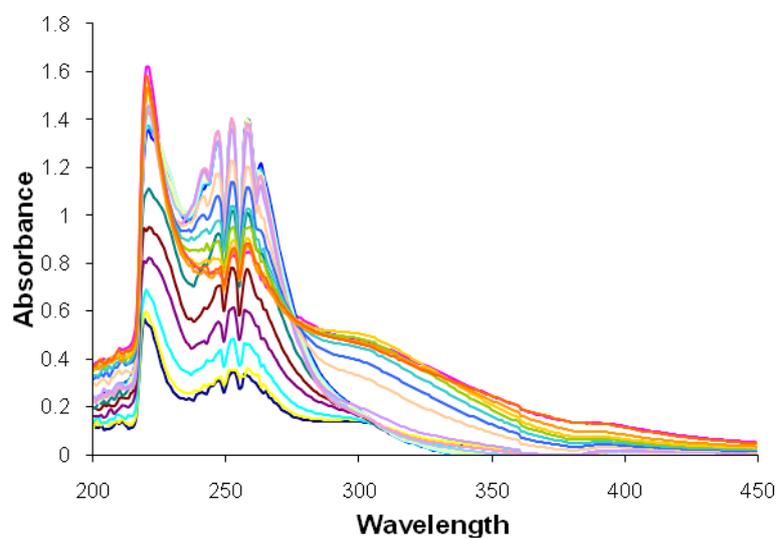
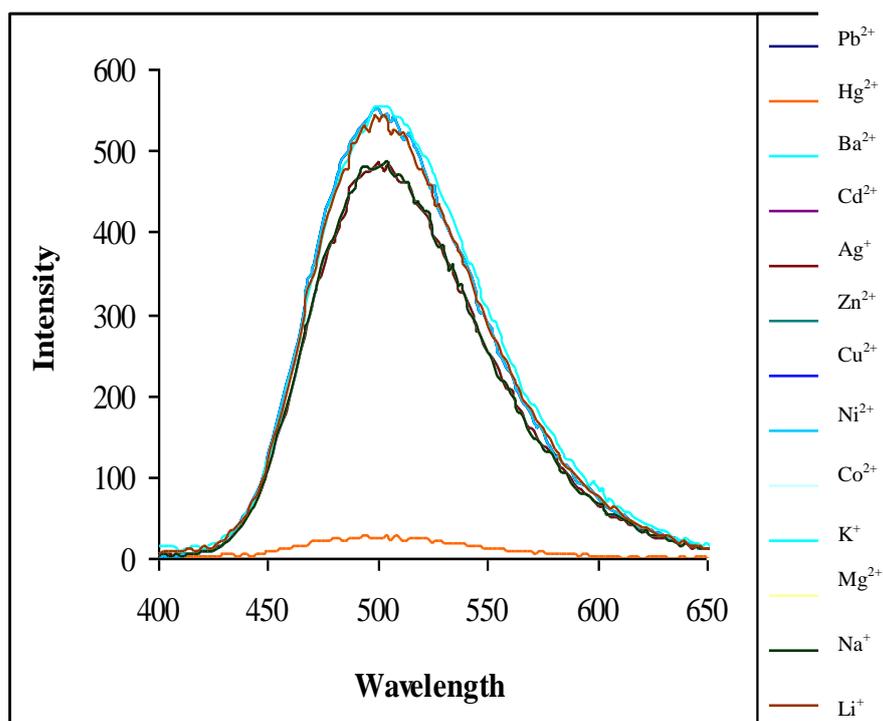
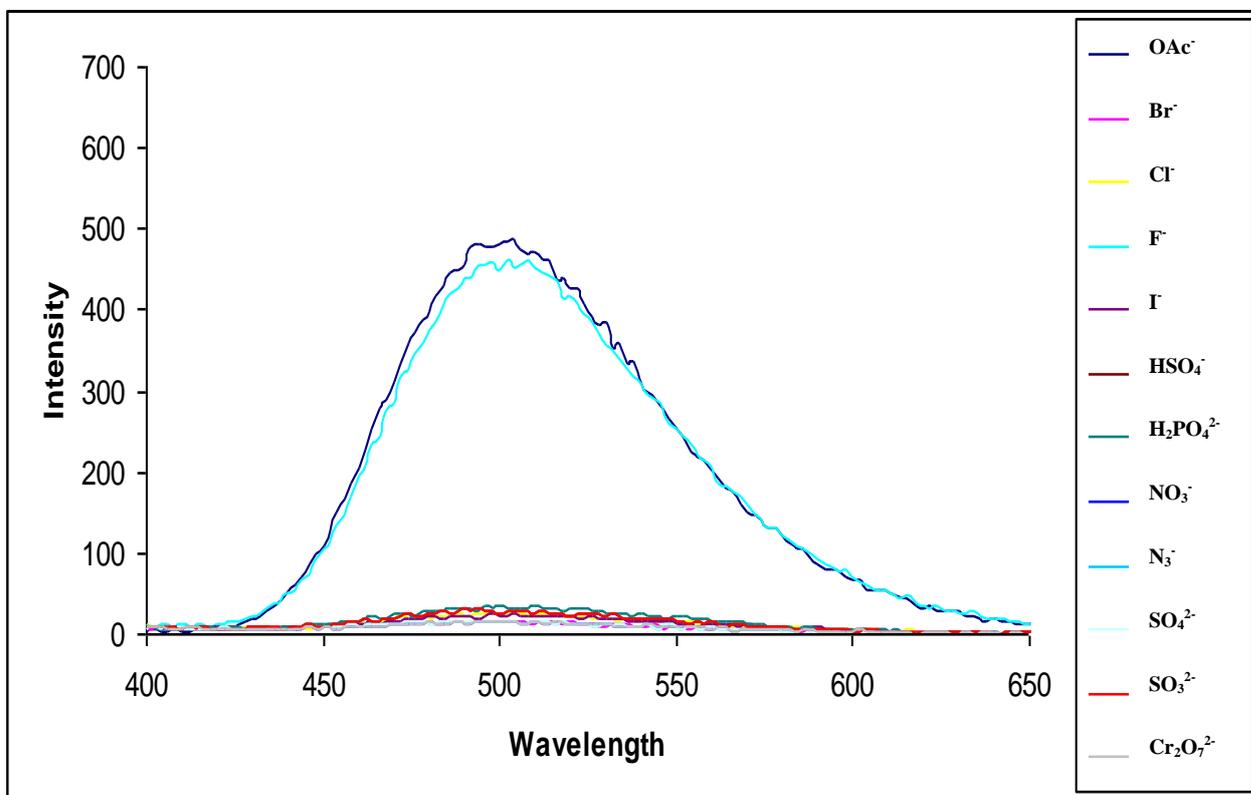


Figure 6. UV-Vis spectra of receptor **1** (5 μM) upon addition of F⁻ ions (0.1 – 30.0 equiv) in THF

Compiled fluorescence behavior of receptor 3 in the presence of various metal ions



Compiled fluorescence behavior of ensemble 3-Hg in the presence of various anions



Fluorescence behavior of ensemble 3-Hg in the presence of CH₃COOK

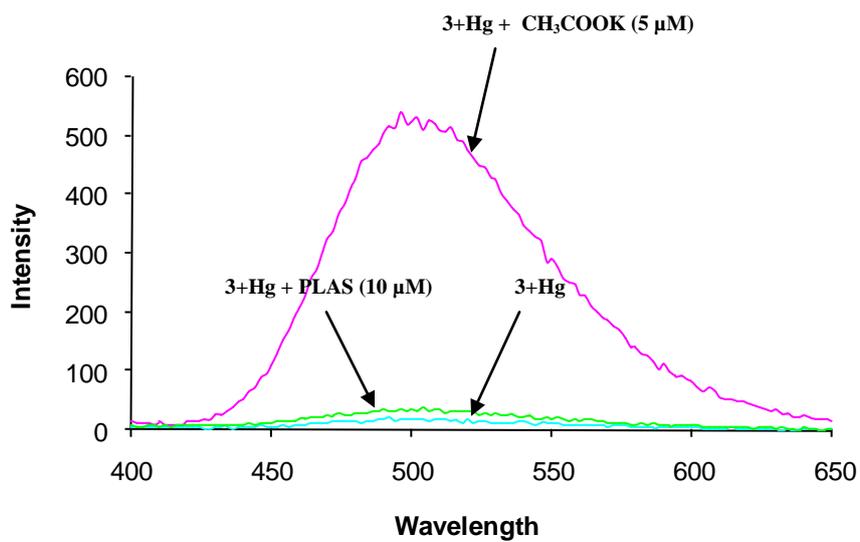


Figure 7. Fluorescence spectra of 3+Hg (10 μM) upon addition of aqueous solution of CH₃COOK (5 equiv)

Fluorescence behavior of reference compound **4** in the presence of Hg

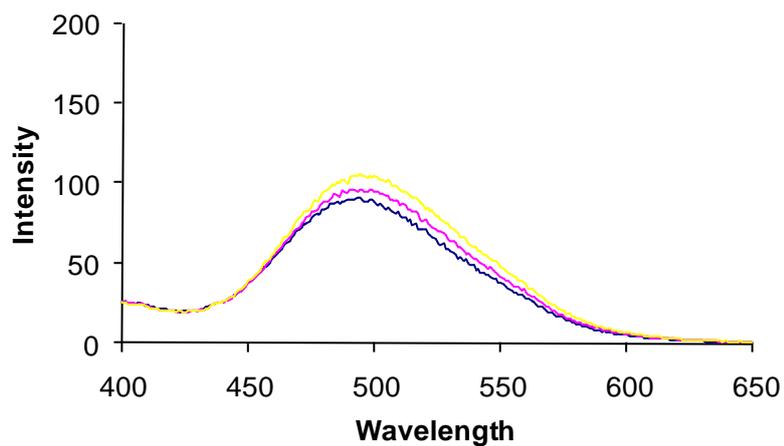


Figure 8. Fluorescence spectra of **4** (2 μM) upon addition of Hg²⁺ ions in THF (50 equiv)