

Imine-Linked Chemosensors for the Estimation of Zn²⁺ in Biological Samples

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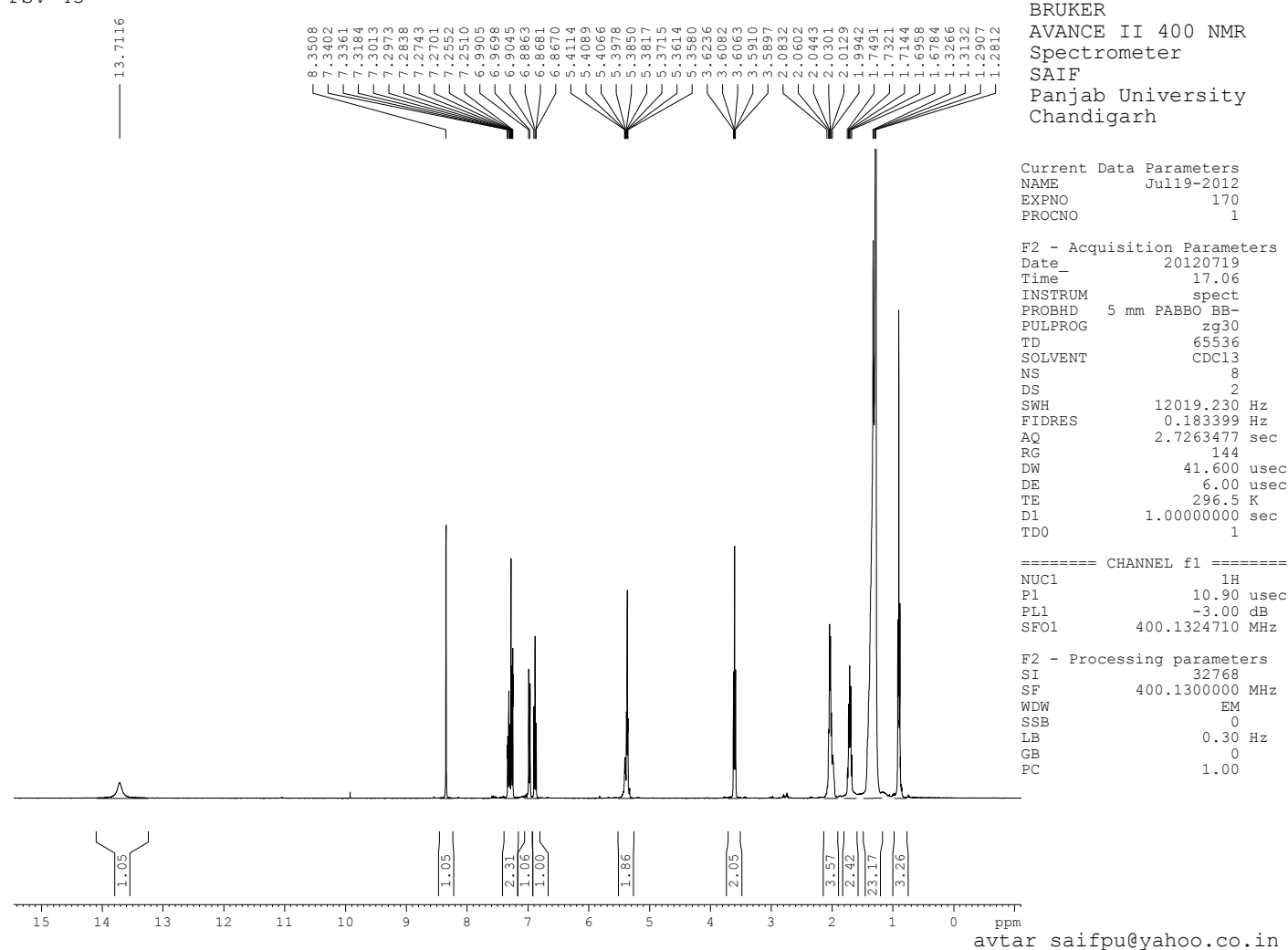


Figure S1: ¹H NMR spectrum of sensor **1** in CDCl₃

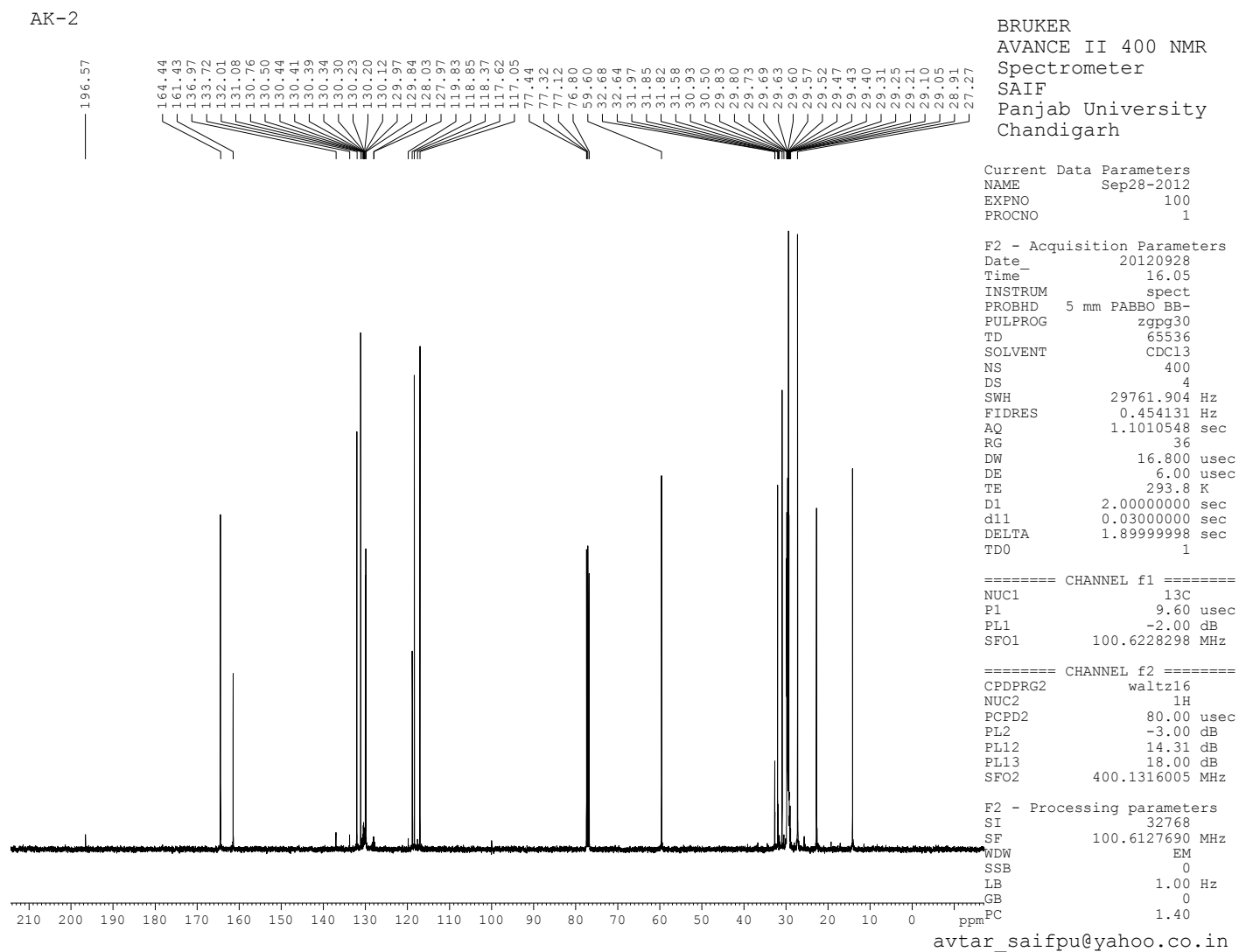


Figure S2: ^{13}C NMR spectrum of sensor **1** in CDCl_3 .

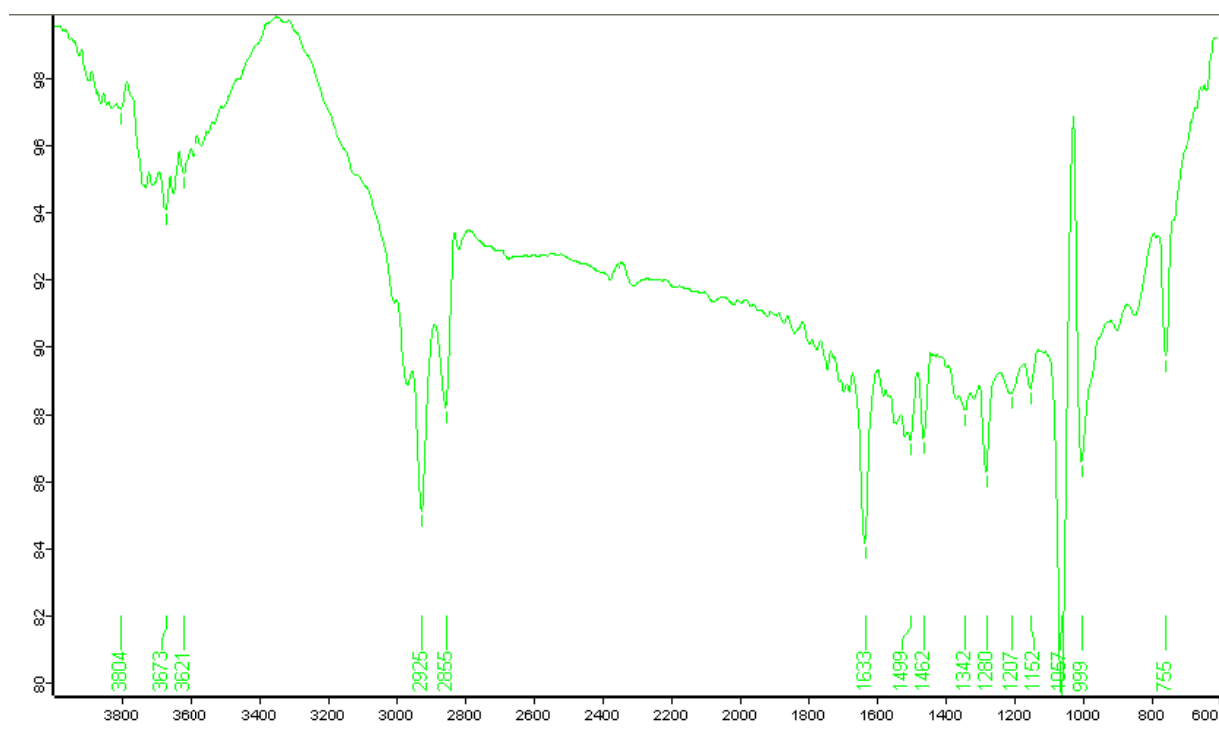


Figure S3: IR spectrum of sensor 1.

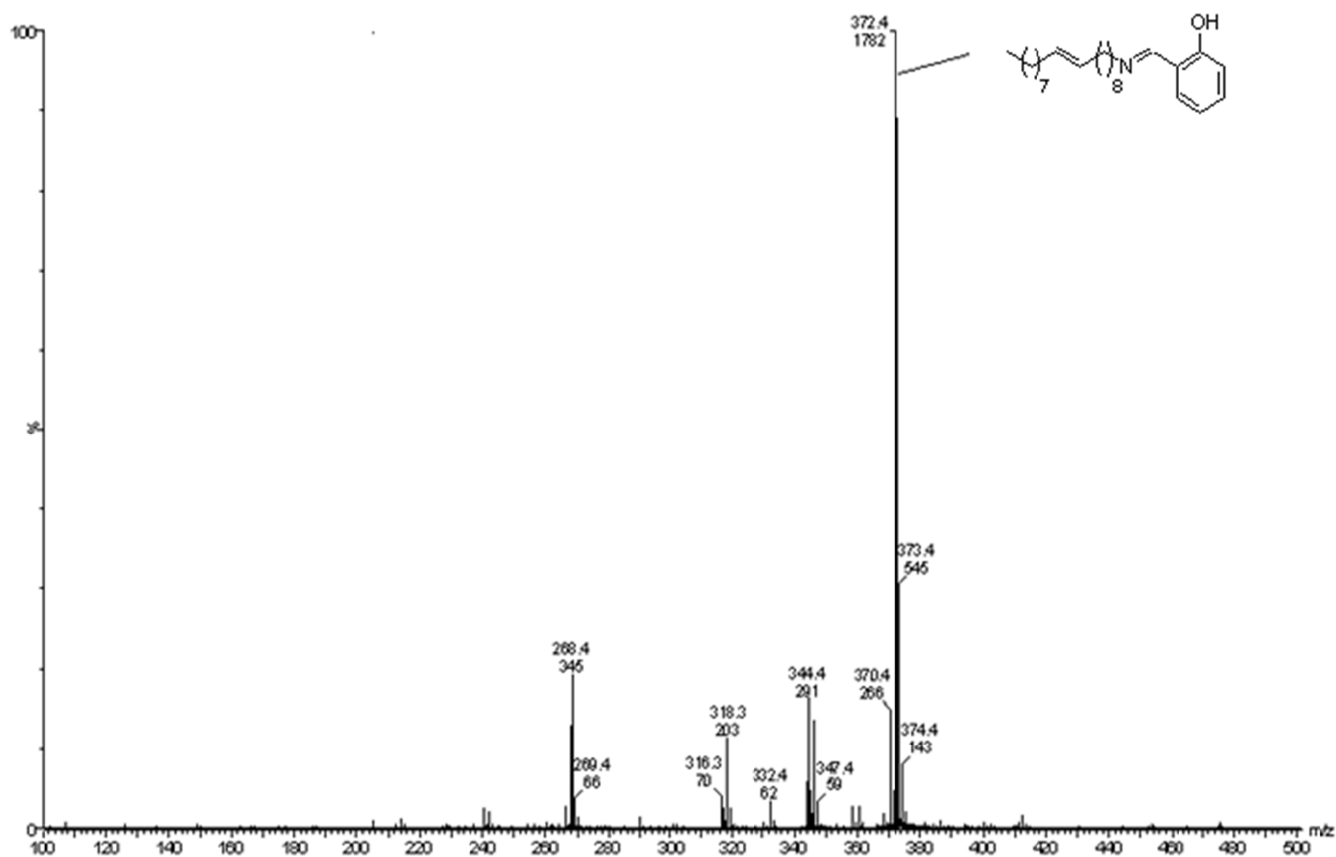


Figure S4: Mass spectrum of sensor 1 with peak at 372.4 corresponds to $[M+1]^+$ peak.

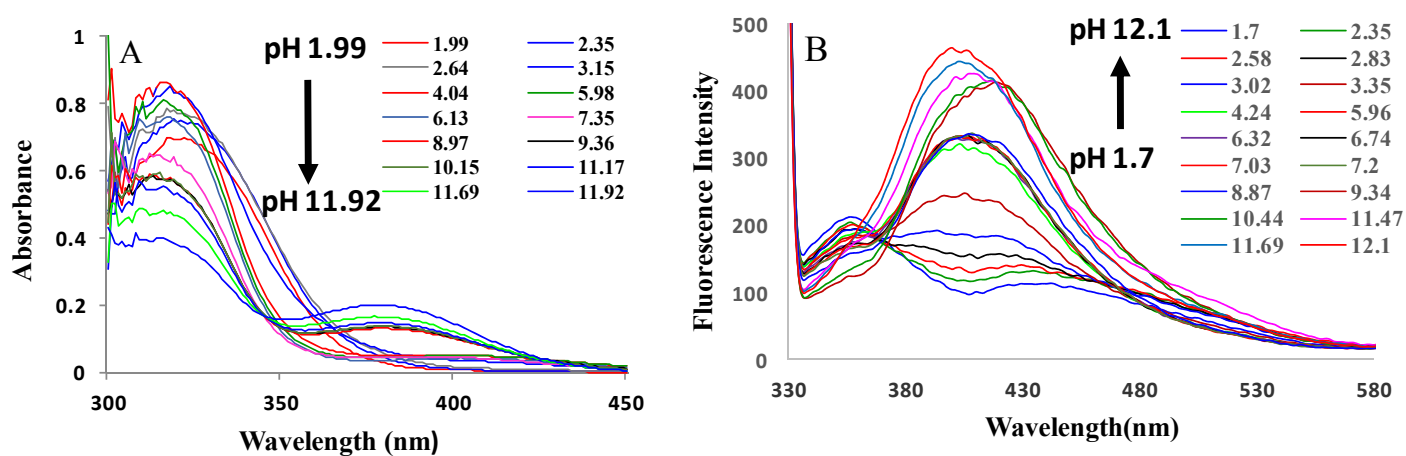


Figure S5: (A) UV-Vis absorption spectrum of sensor **1** (5 μM) and (B) Fluorescent response of sensor **3** (5 μM); with variation of pH in aqueous 1% triton-X-100 solution (inset showing the pH values).

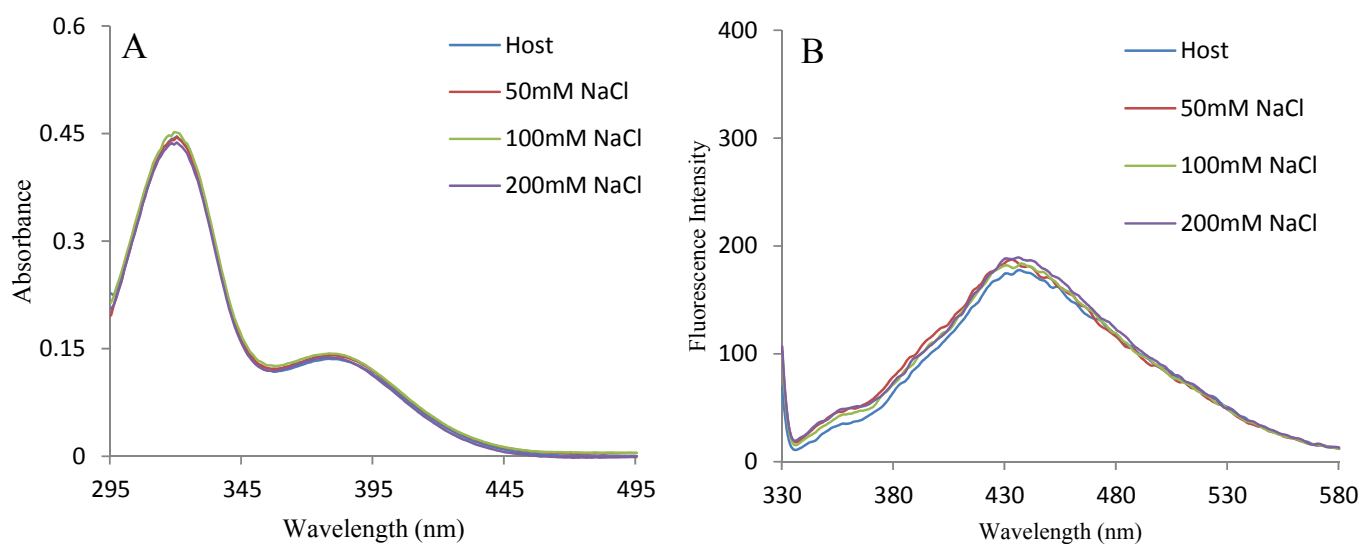


Figure S6: Effect of increasing ionic strength on (A) UV-Vis absorption profile; (B) Fluorescence emission profile of sensor **1** (5 μM) in aqueous 1% triton-X-100 solution.

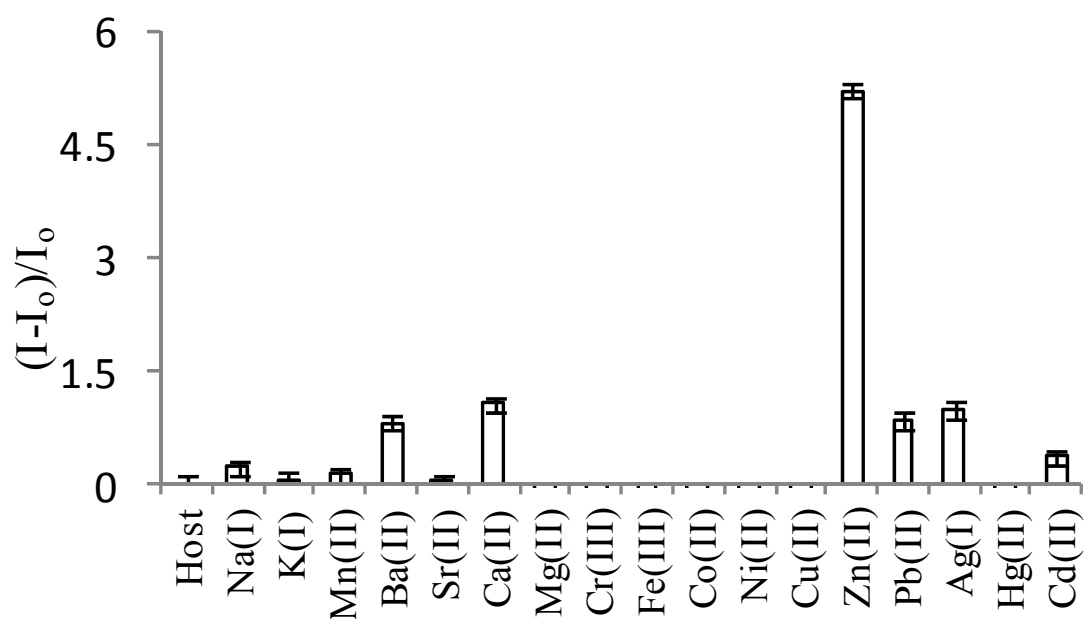


Figure S7: Fluorescence ratio $(I-I_0)/I_0$ of sensor **3** (5 μ M) at 440 nm upon addition of 50 μ M of different metal ions in aqueous 1% triton-X-100 solution; excitation wavelength was 320 nm

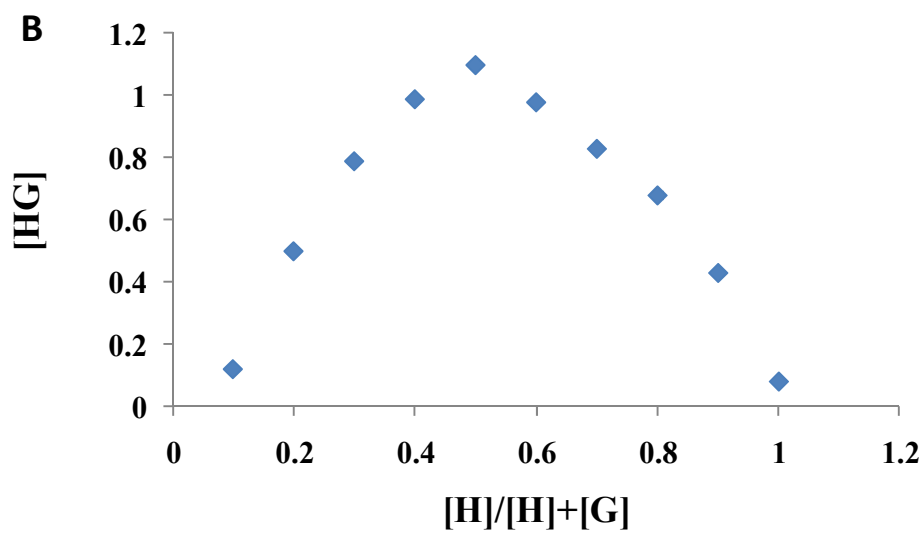
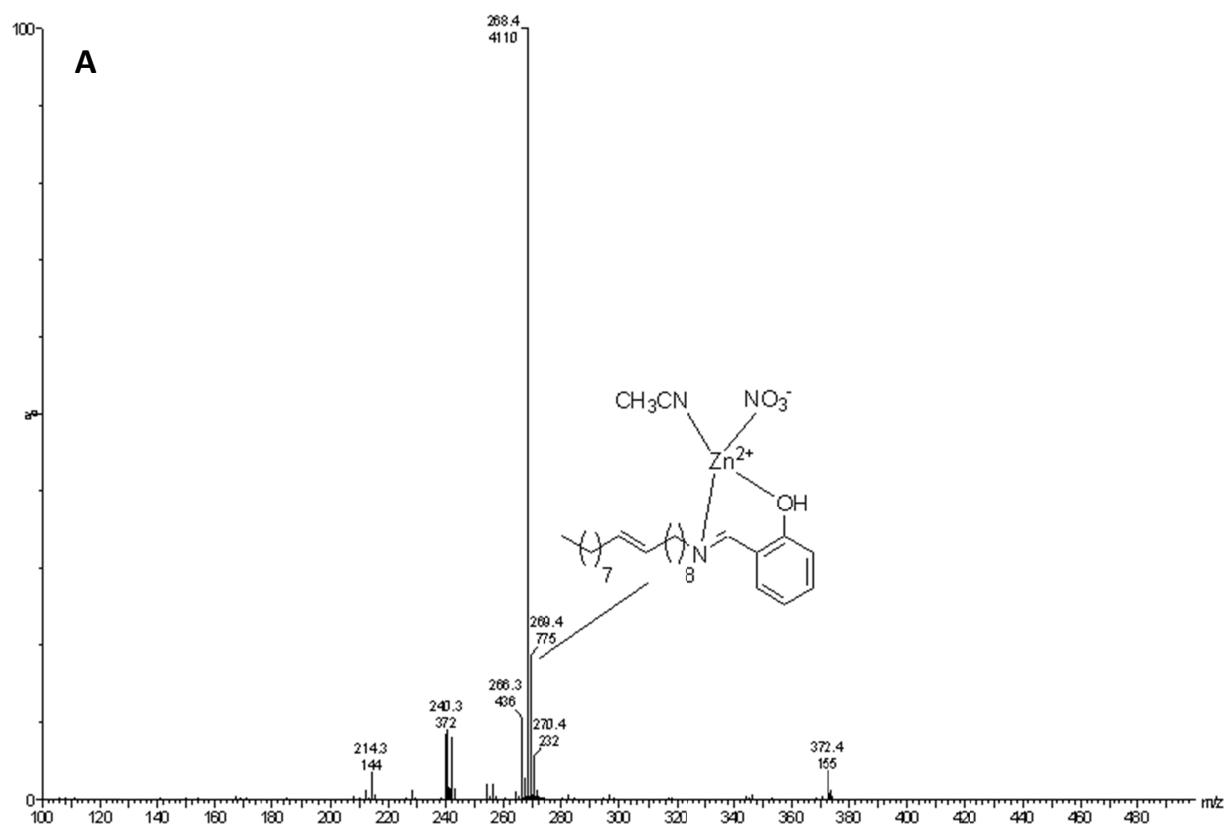


Figure S8: (A) Mass spectra of complex **1**.Zn²⁺ with peak at m/z value 269.4 corresponds to [M+1]²⁺, where M is [**1**+Zn²⁺+NO₃⁻+CH₃CN] (B) Job's plot for complex formed between receptor **1** and Zn²⁺. The fluorescence intensity at 440 nm was used for calculations. The concentration of [HG] was calculated by the equation [HG] = $\Delta I/I_0 \times [H]$.

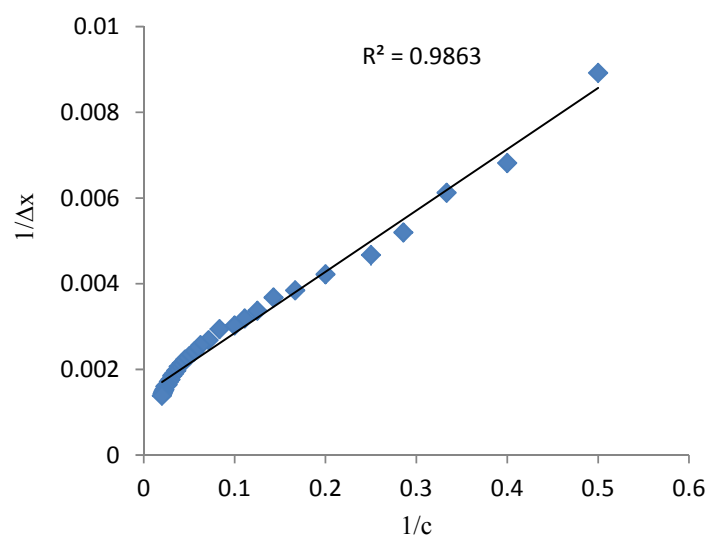


Figure S9: Calculation of binding constant using Benesi-Hildebrand plot with fluorescence titration data.

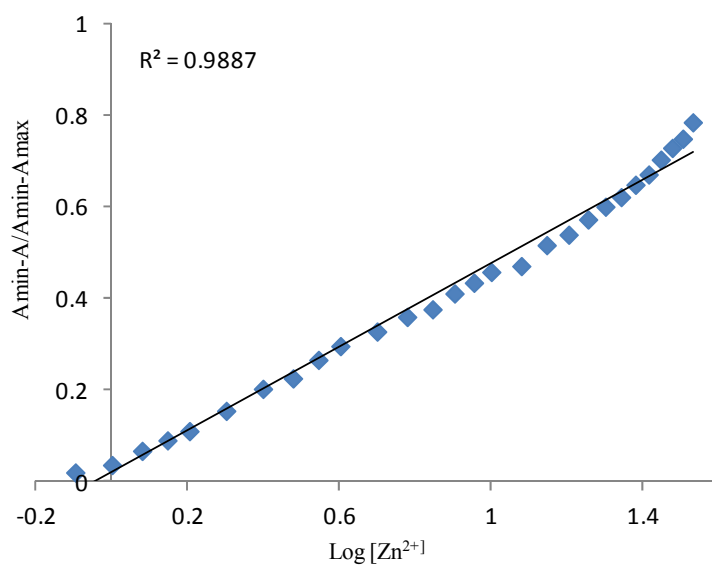


Figure S10: Calculation of detection limit for estimation of Zn^{2+} by sensor **1**.

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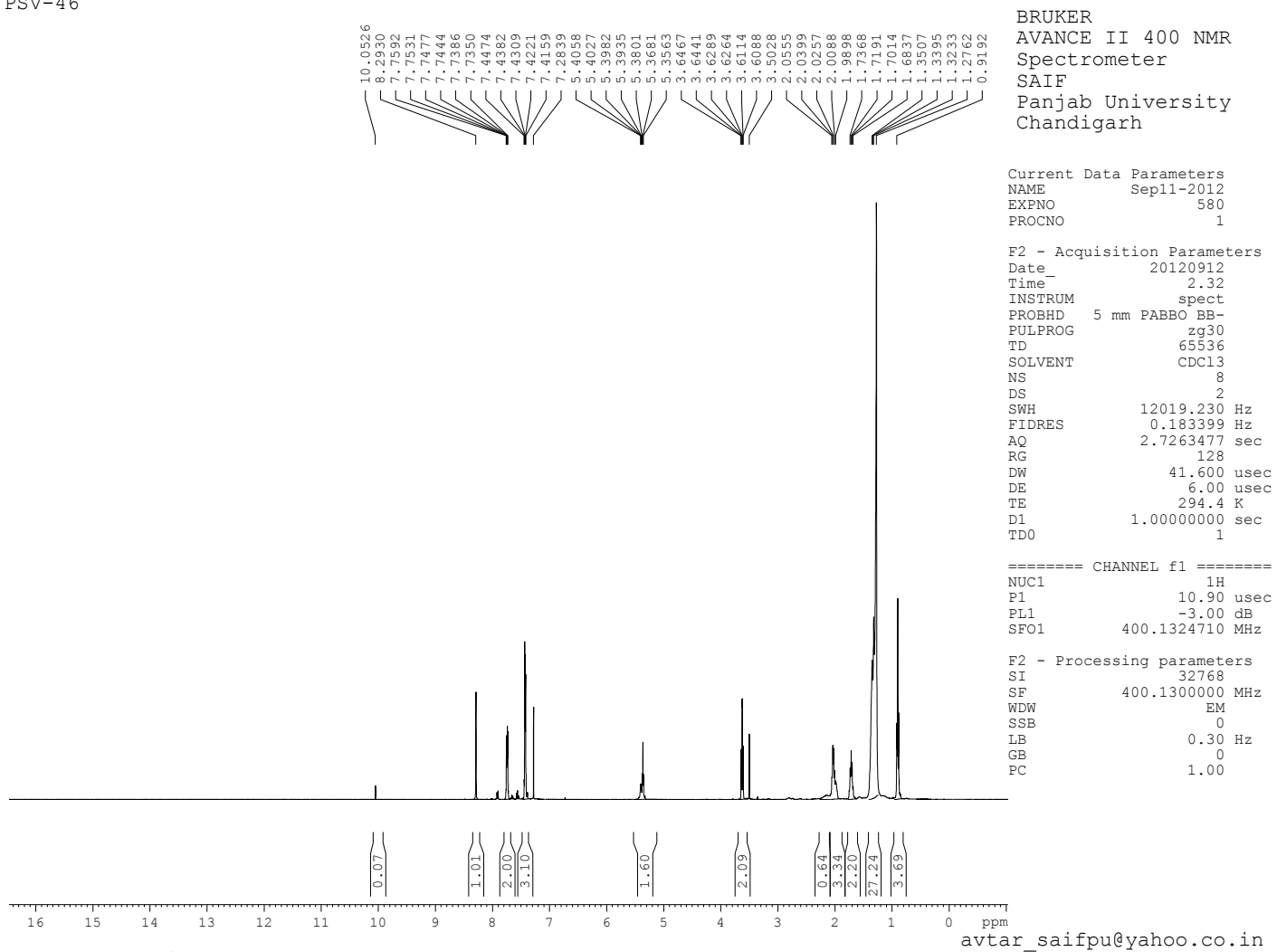


Figure S11A: ^1H NMR spectrum of sensor **2** in CDCl_3

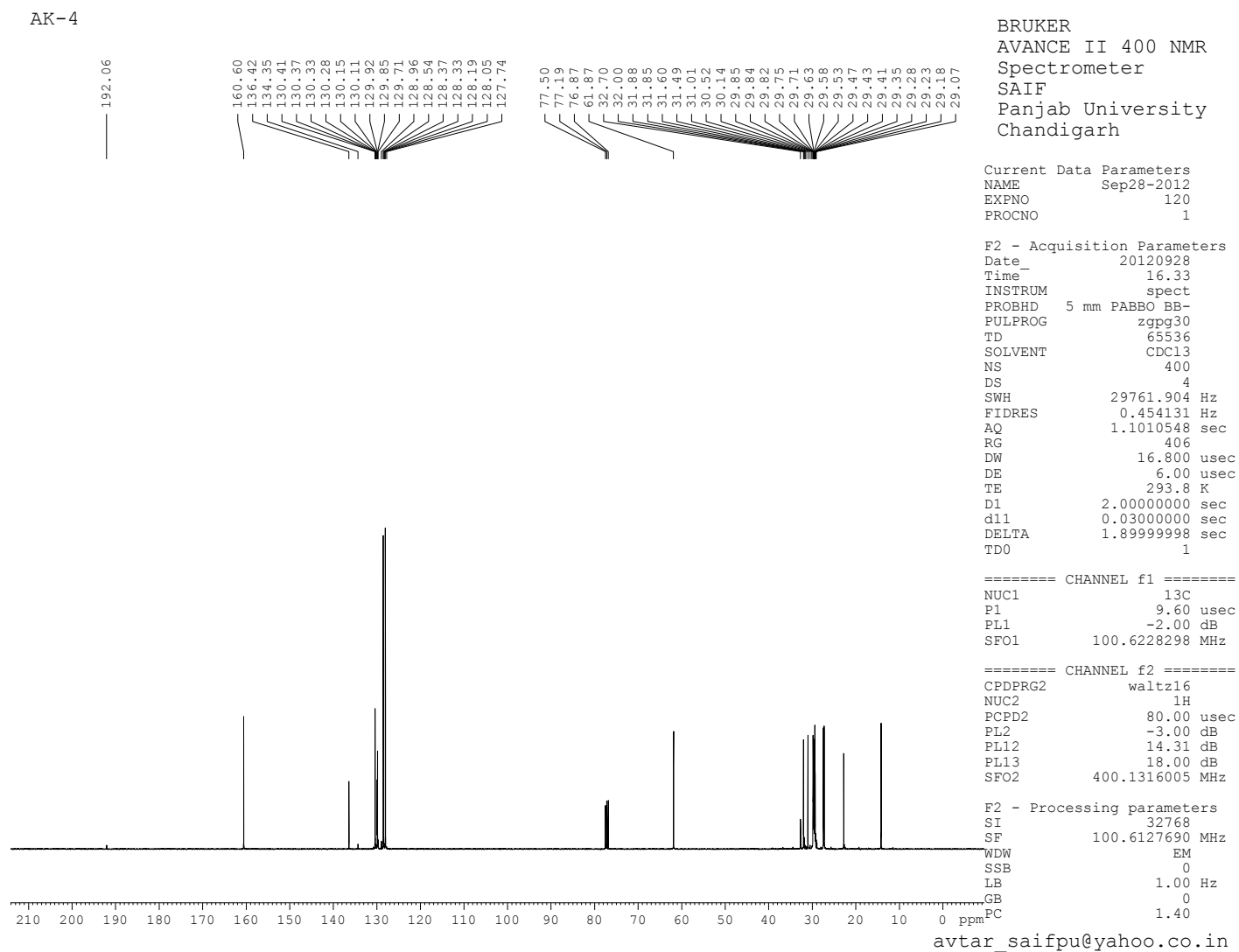


Figure S11B: ^{13}C NMR spectrum of sensor **2** in CDCl_3 .

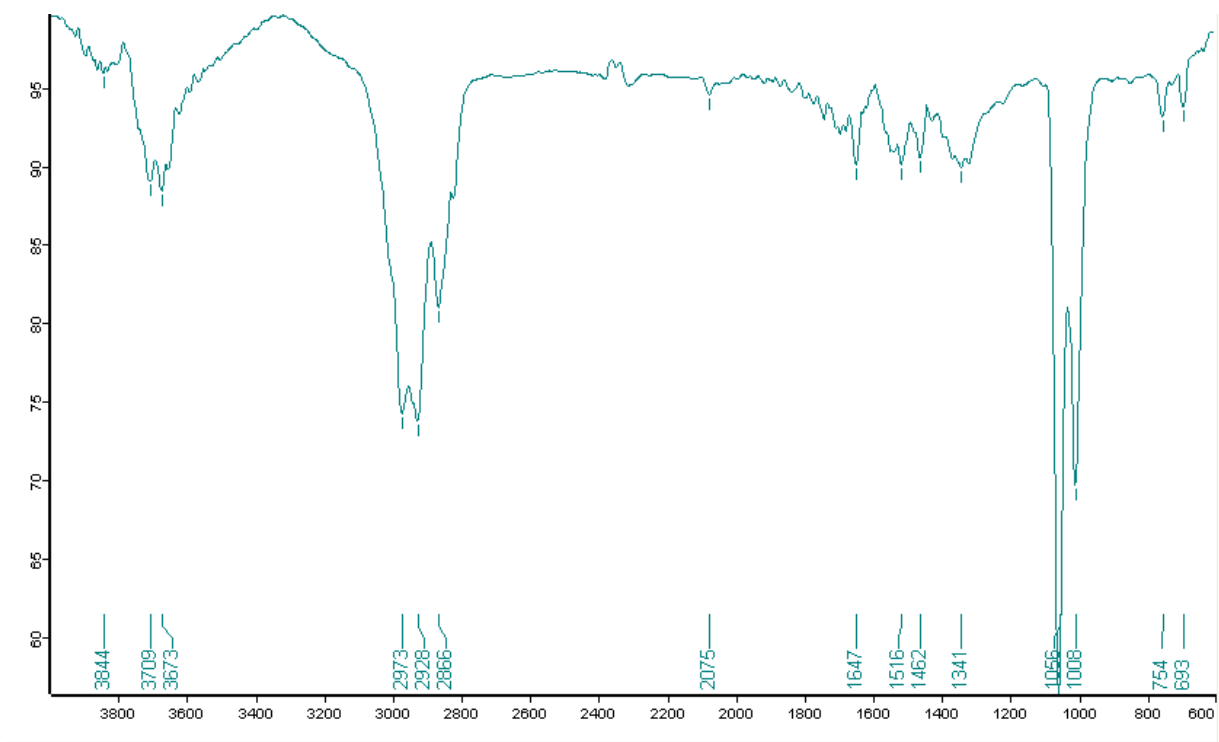


Figure S11C: IR spectrum of sensor 2.

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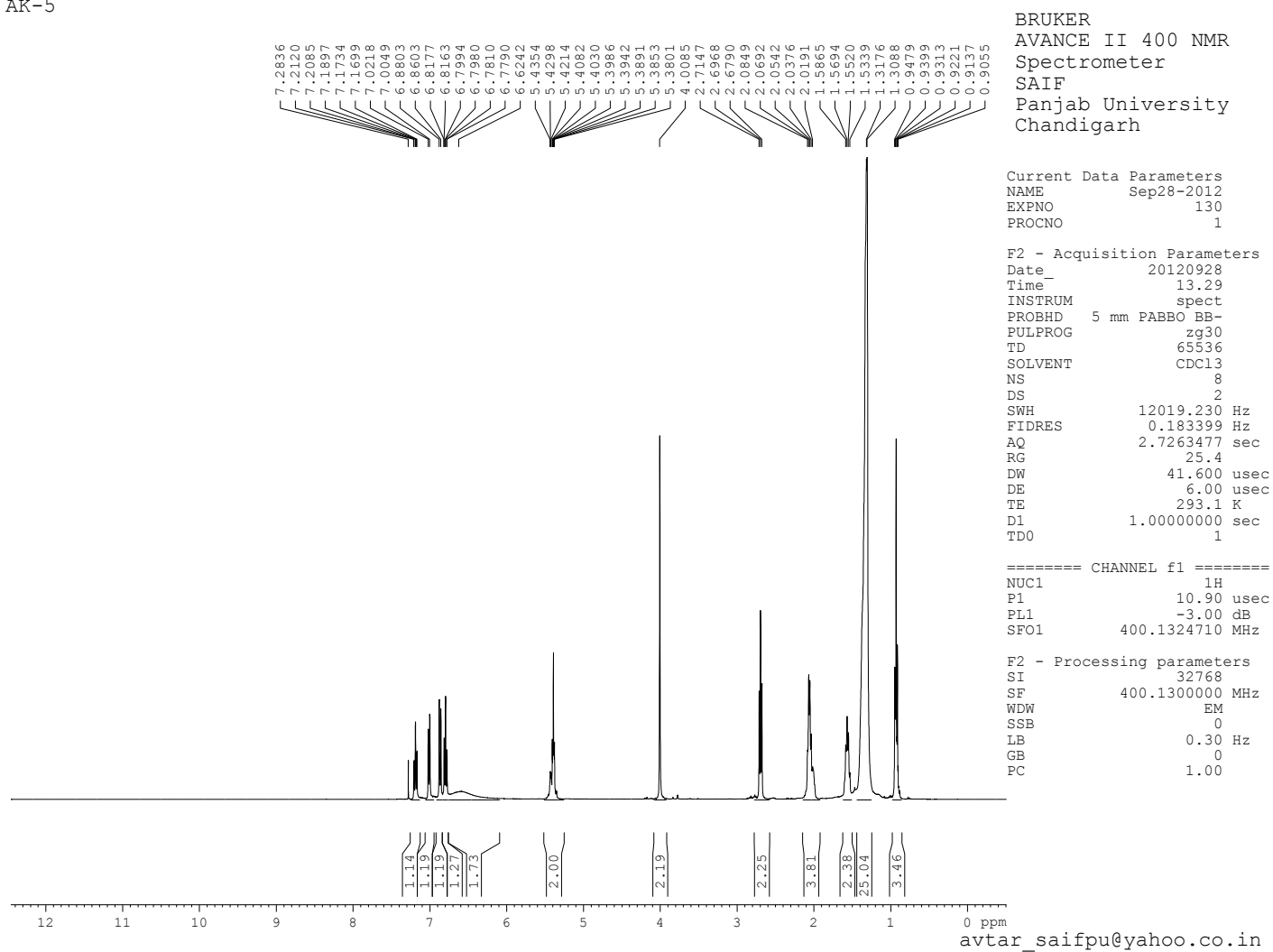


Figure S12A: ^1H NMR spectrum of sensor **3** in CDCl_3 .

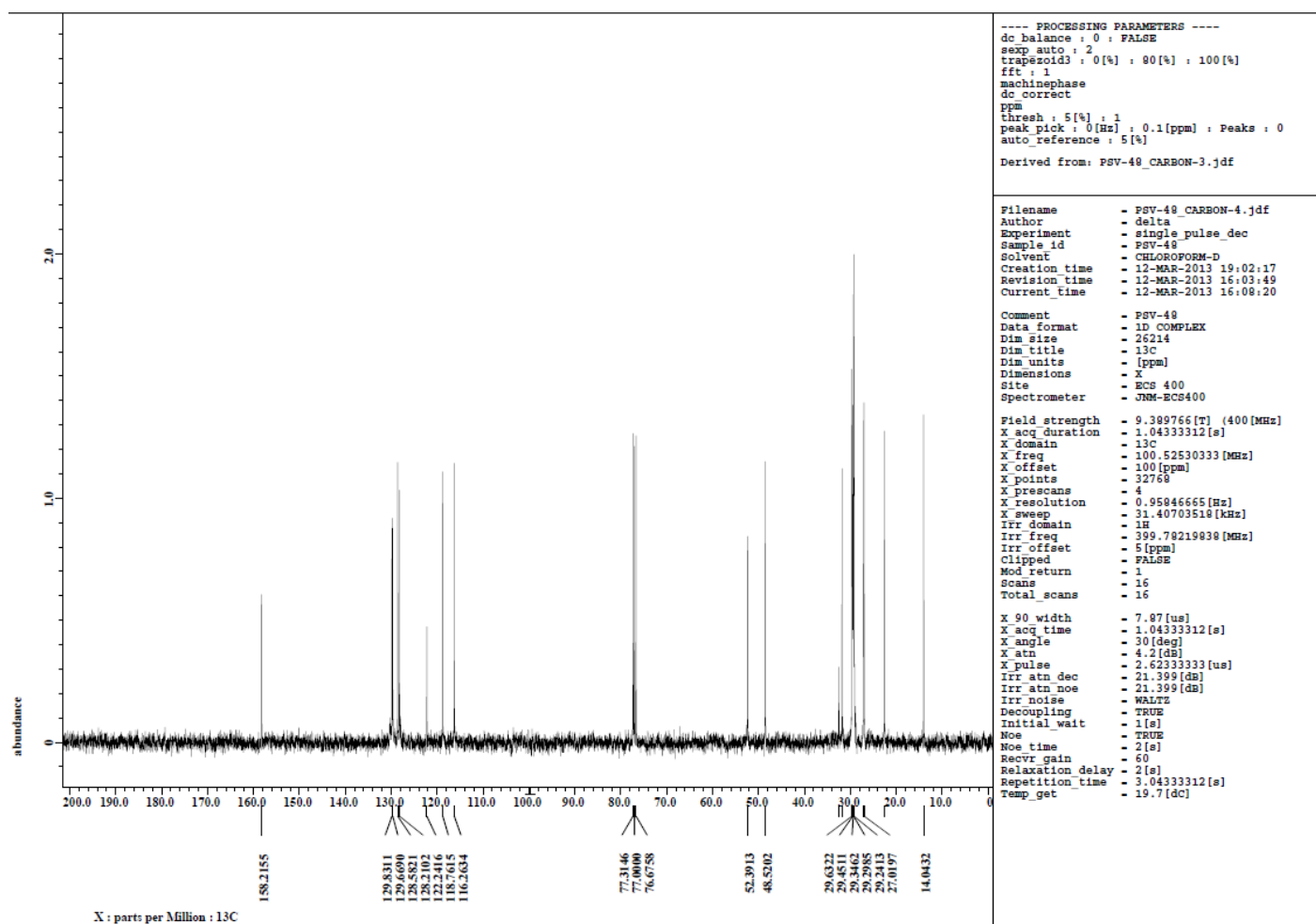


Figure S12B: ^{13}C NMR spectrum of sensor **3** in CDCl_3 .

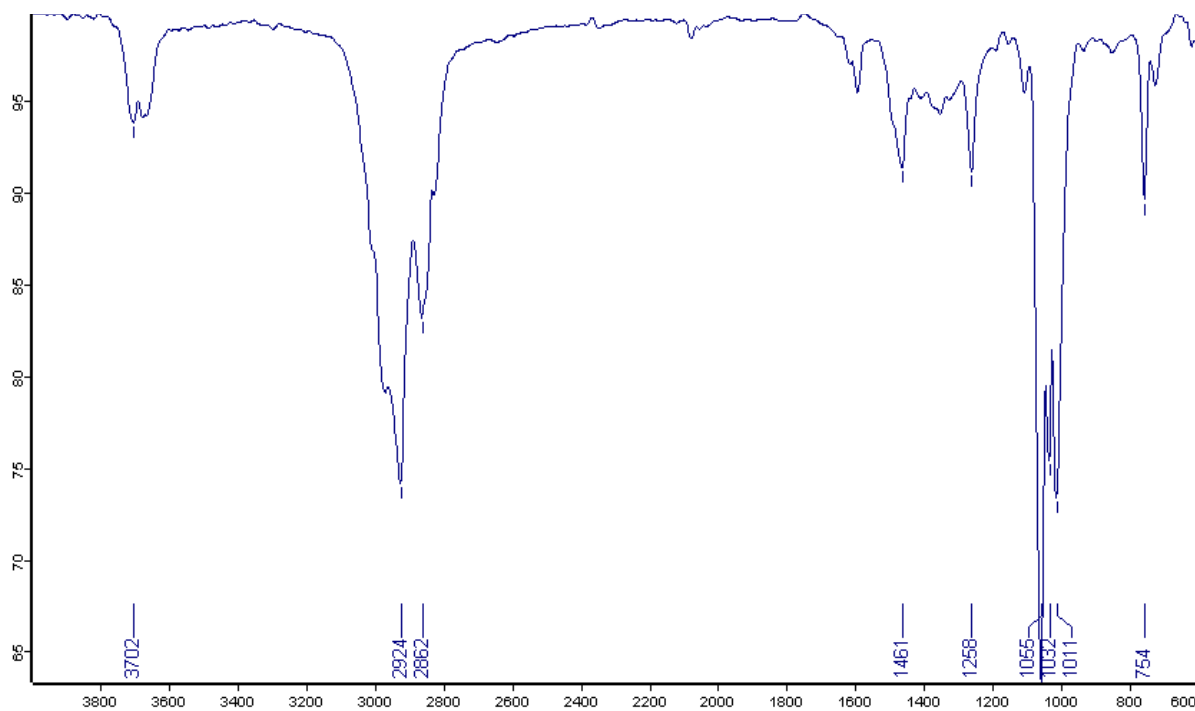


Figure S12C: IR spectrum of sensor **3**.

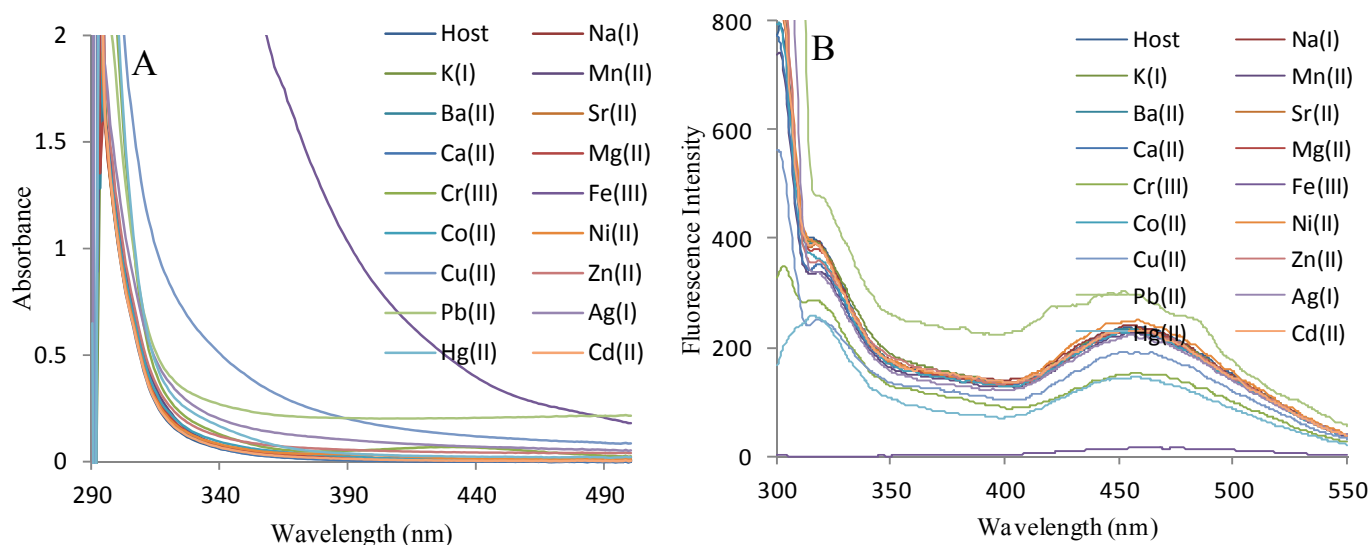


Figure S13:(A)UV-Vis absorption spectra of **2** (10 μM); (B) Fluorescence emission spectra of **2**(10 μM) in presence of different metal ions (50 μM) in aqueous 1% triton-X-100 solution; excitation wavelength was 310 nm.

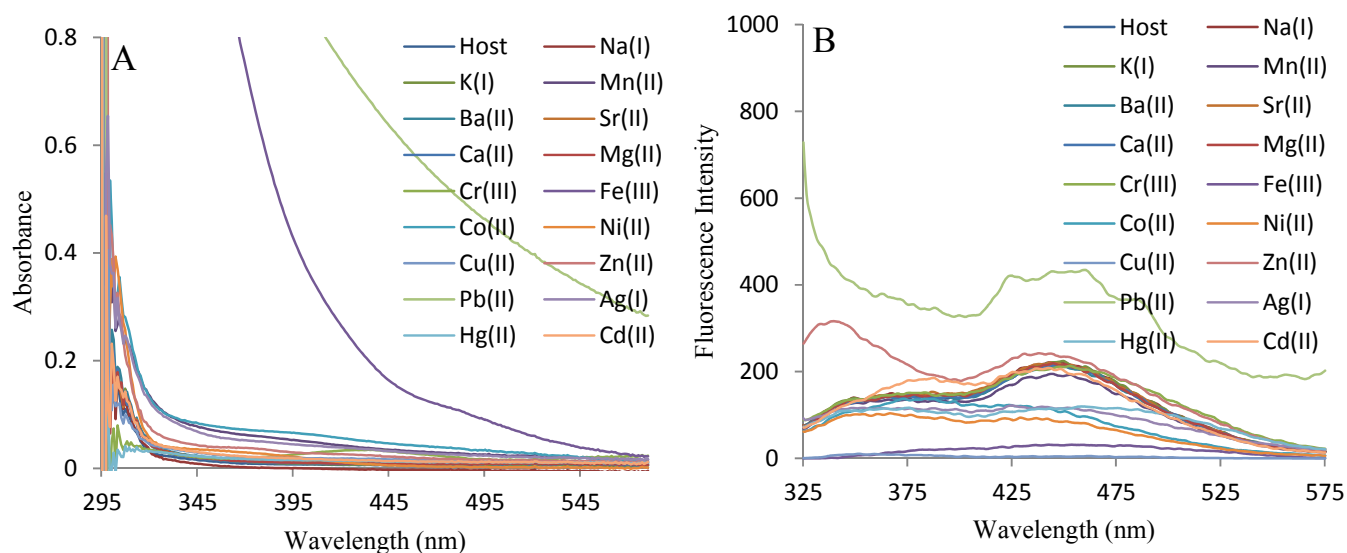


Figure S14:(A)UV-Vis absorption spectra of **3** (10 μM); (B) Fluorescence emission spectra of **3**(10 μM) in presence of different metal ions (50 μM) in aqueous 1% triton-X-100 solution; excitation wavelength was 320 nm

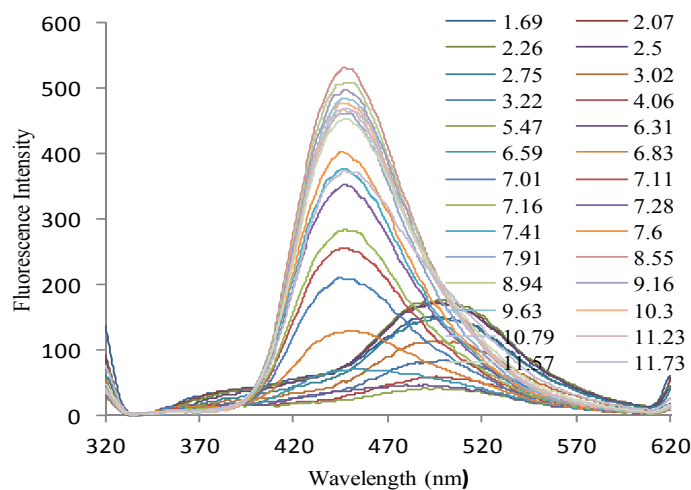


Figure S15: Fluorescence behaviour of **1**.Zn²⁺ complex with variation of pH in aqueous 1% triton-X-100 solution.

Table S1. Total energy values of the keto and enol forms of **3**.

Molecule	Total Energy (a.u.)
Enol form of 3	-1107.0415
Keto form of 3	-1107.0422