Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

An Imidazo-phenanthroline Scaffold Enables Both Chromogenic Fe(II) and Fluorogenic Zn(II) Detection

Aykut Yoldas[‡], Fatih Algi[†,*]

[‡] Laboratory of Organic Materials (LOM), Canakkale Onsekiz Mart University, TR-17100 Canakkale, Turkey.

[†] Department of Biotechnology and Molecular Biology & ASUBTAM BioNanoTech Lab., Aksaray University, TR-68100 Aksaray, Turkey.

*Corresponding author: E-mail: falgi@aksaray.edu.tr; Tel: +903822882138; Fax: +903822882185

Table of Contents

Copies of ^{1}H NMR and ^{13}C NMR Spectra

Copies of Mass Spectra

Figures of Job plot, LOD and Linear regression curve

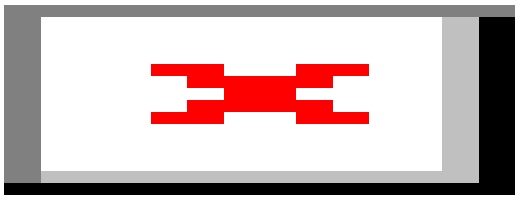

Figure S1. ^{1}H NMR spectrum of **3** ($CDCl_3$).

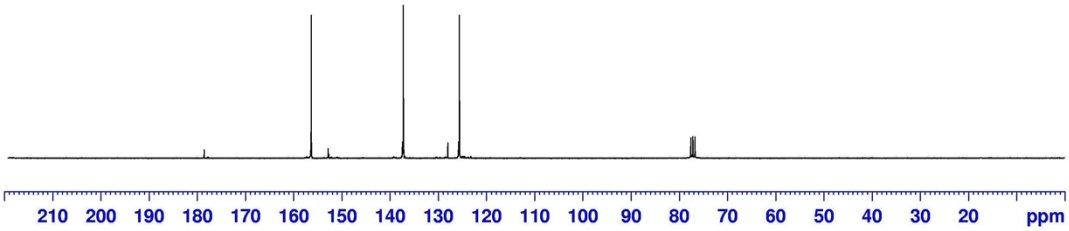

Figure S2. ^{13}C NMR spectrum of **3** ($CDCl_3$).

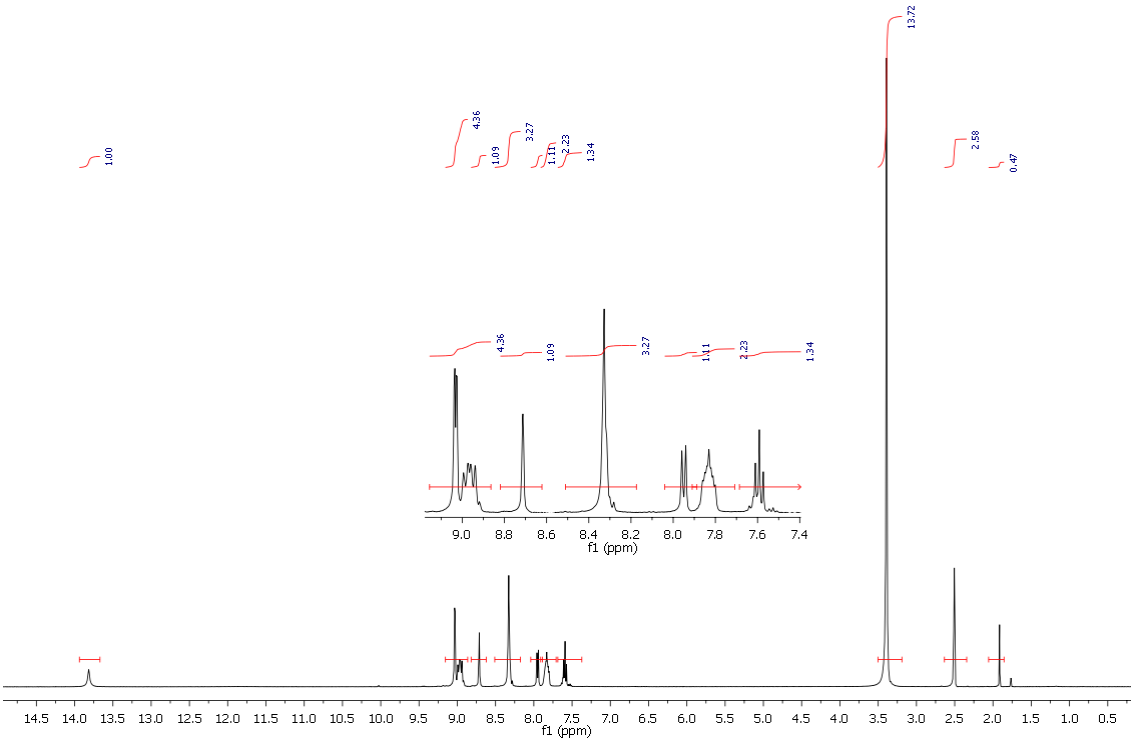

Figure S3. ^{1}H NMR spectrum of **1** (DMSO-d_6).

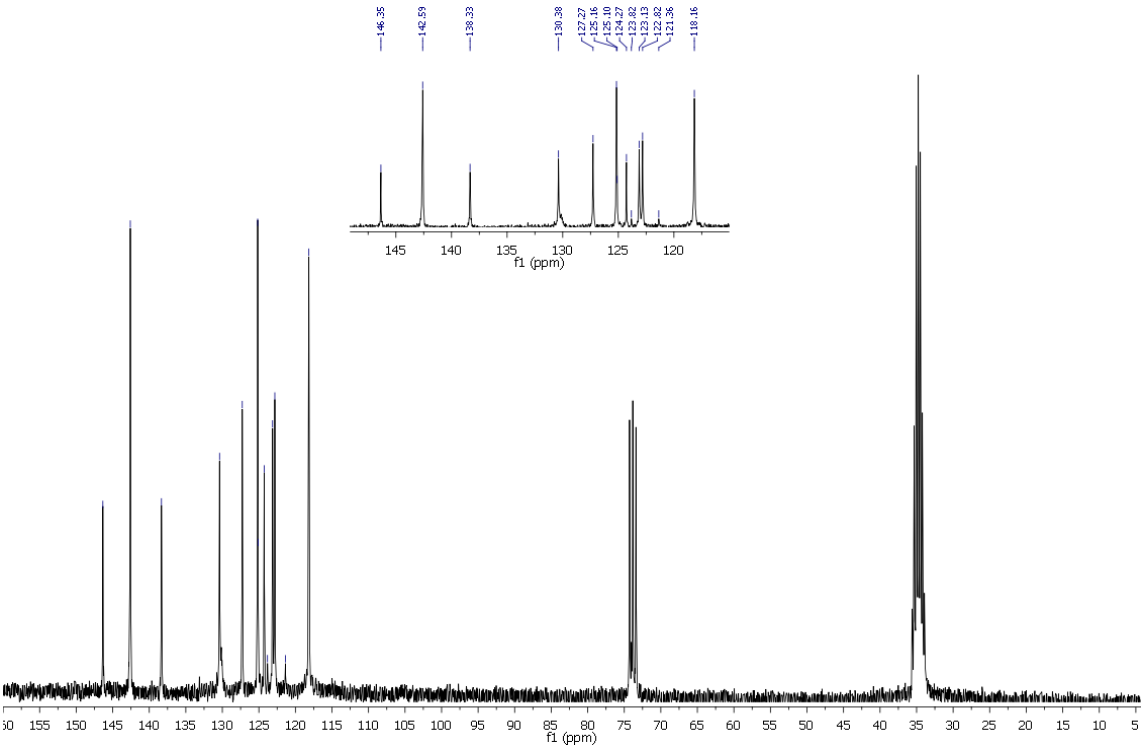

Figure S4. ^{13}C NMR spectrum of **1** (DMSO-d_6 /$CDCl_3$).

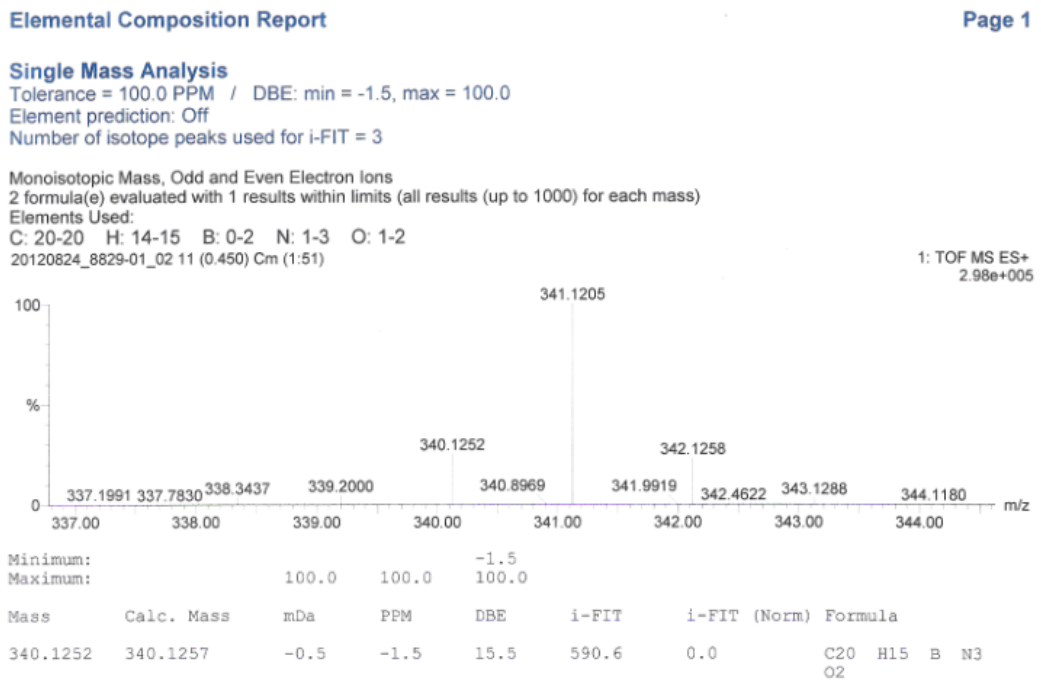

Figure S5. HRMS spectrum of **1**.

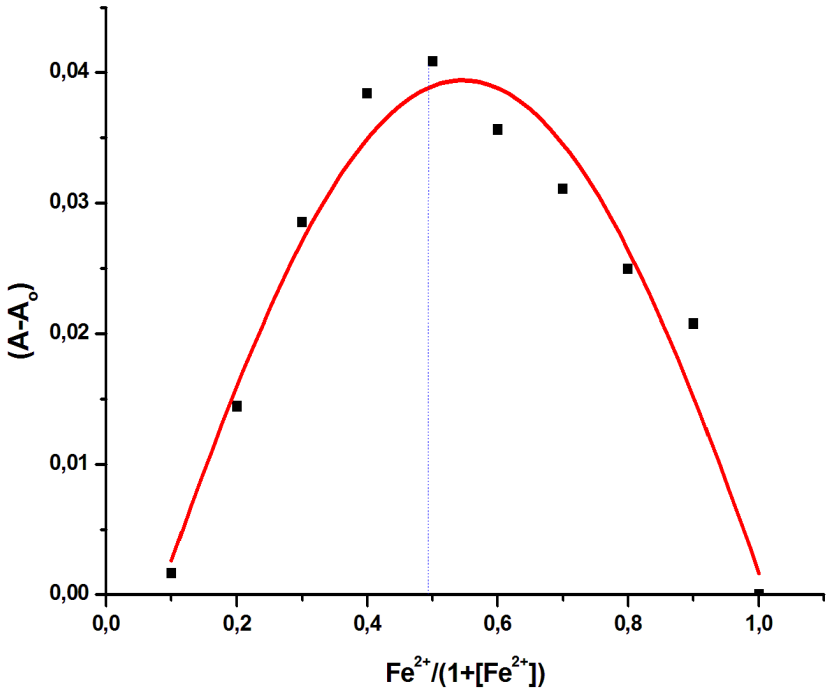

Figure S6. Job plot diagram of **1** for Fe^{2+} at a constant total concentration of $2.5x10^{-5}$ M in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), pH= 7.2, 25°C.

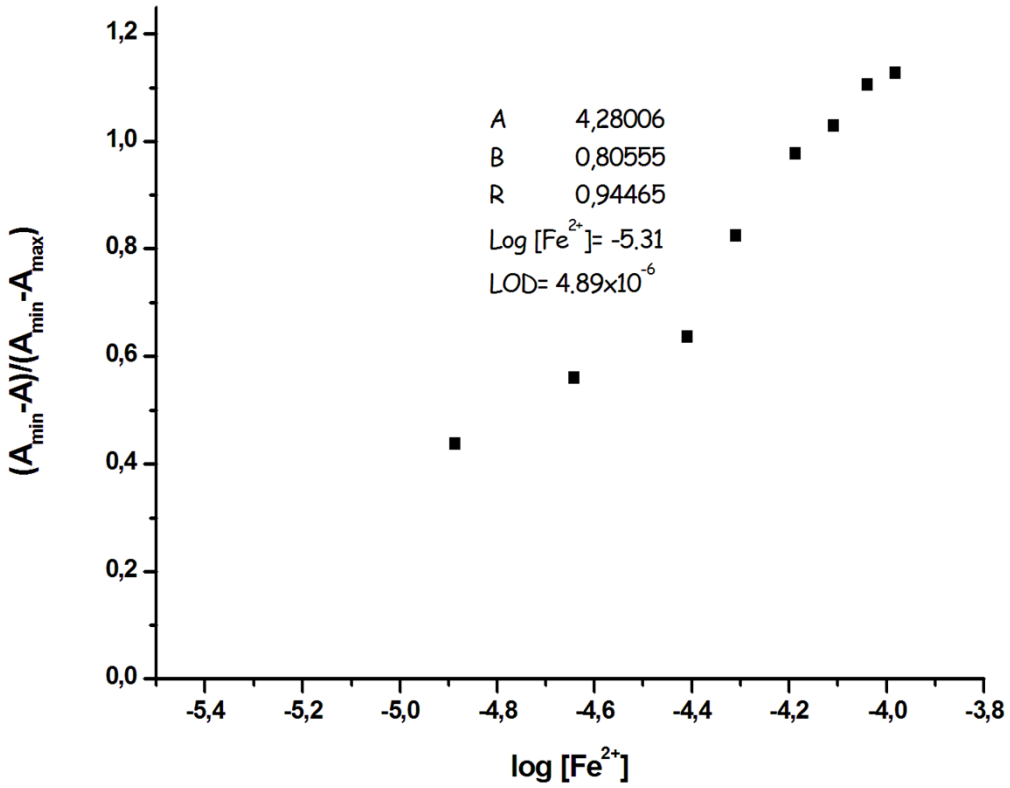

Figure S7. Plot of normalized absorbtion intensity of **1** as a function of log[Fe^{2+}] in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v, pH=7.2) at 25°C, (log[Fe^{2+}] = -5.31).

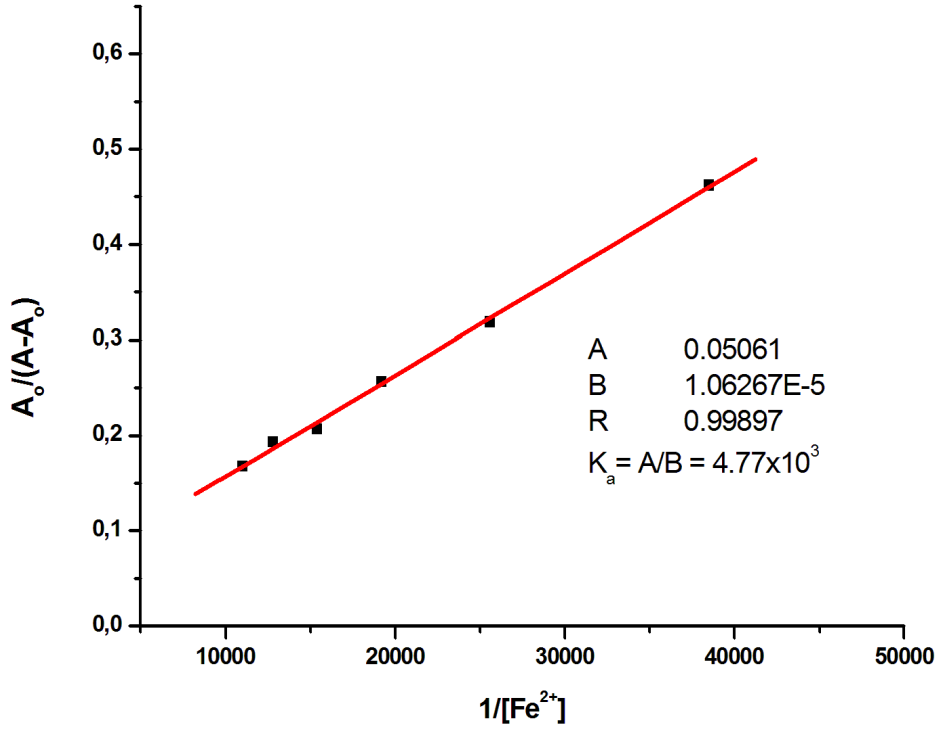

Figure S8. Linear regression curve for **1**.

Figure S9. Chromogenic (left) and fluorogenic (right) responses of **1** to metal ions in aqueous 0.1 M HEPES containing 0.1% CH_3OH (v/v) solution (pH= 7.2, 25°C) under room light and UV illumination (365 nm), respectively.

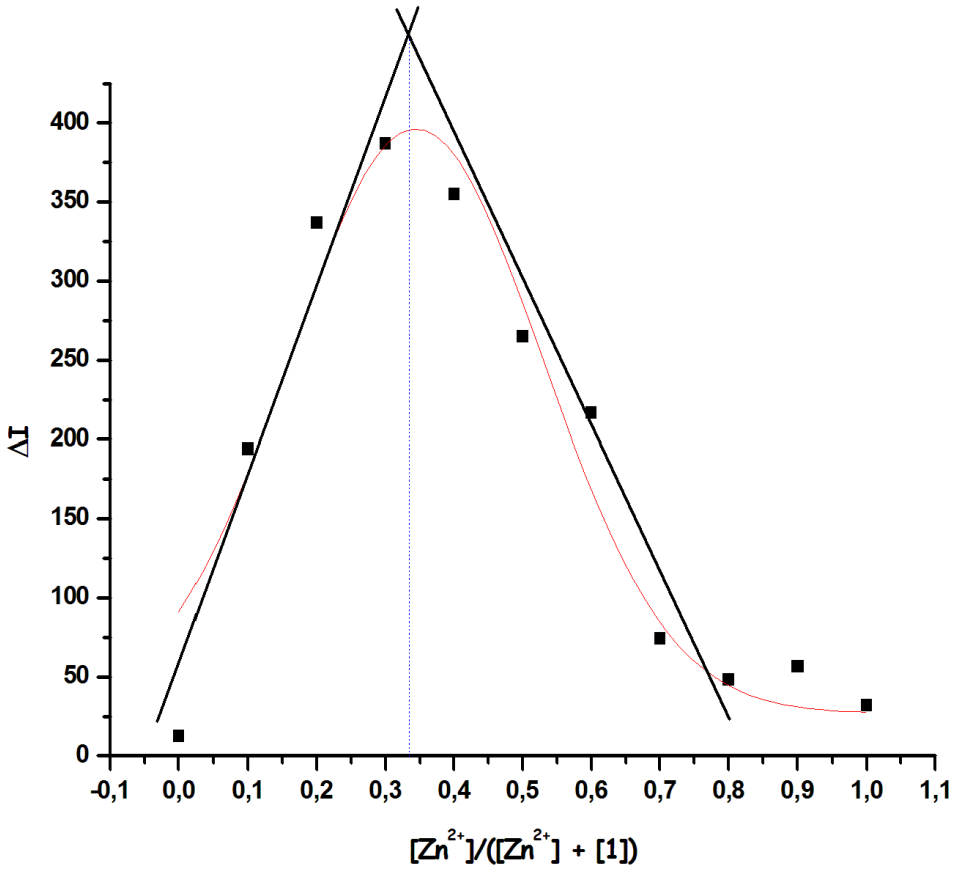

Figure S10. Job plot diagram of **1** for Zn^{2+} (ΔI indicates the change of emission intensity at 498 nm) at a constant total concentration of $2.5x10^{-5}$ M in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), pH= 7.2 at 25°C, λ_{exc}=308 nm.

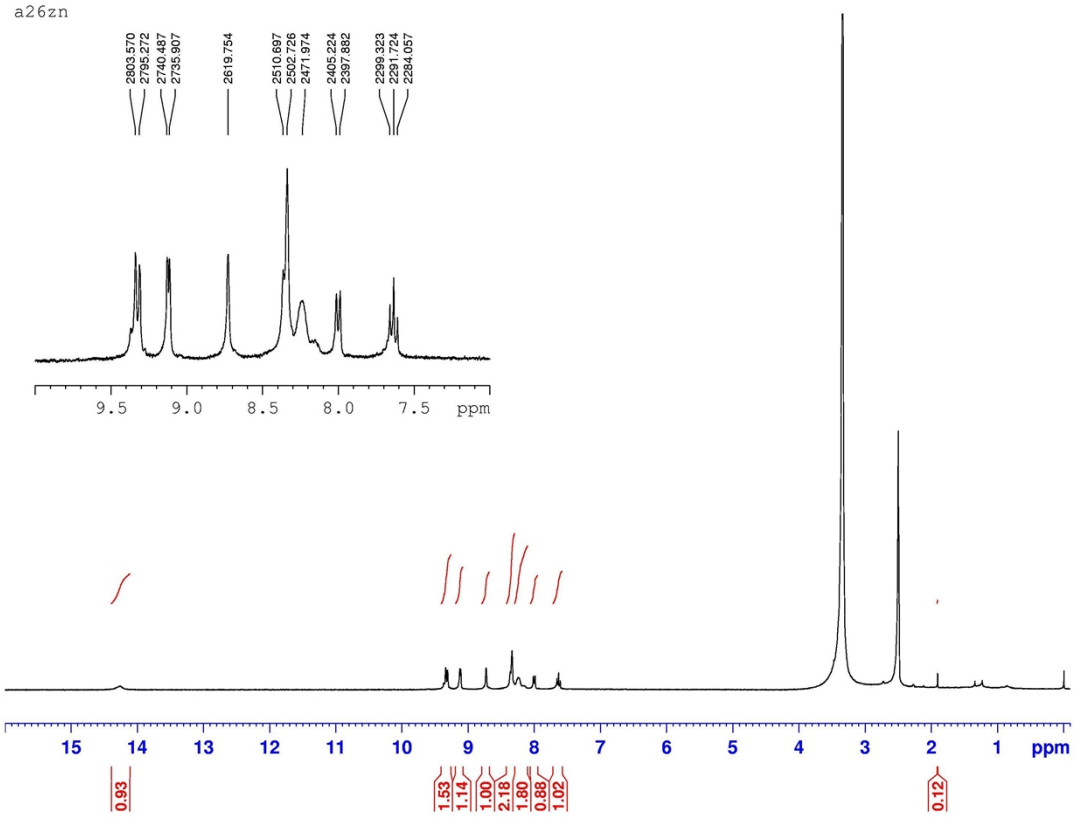

Figure S11. ^{1}H NMR spectrum of **1**+Zn(II) complex (DMSO-d_6).

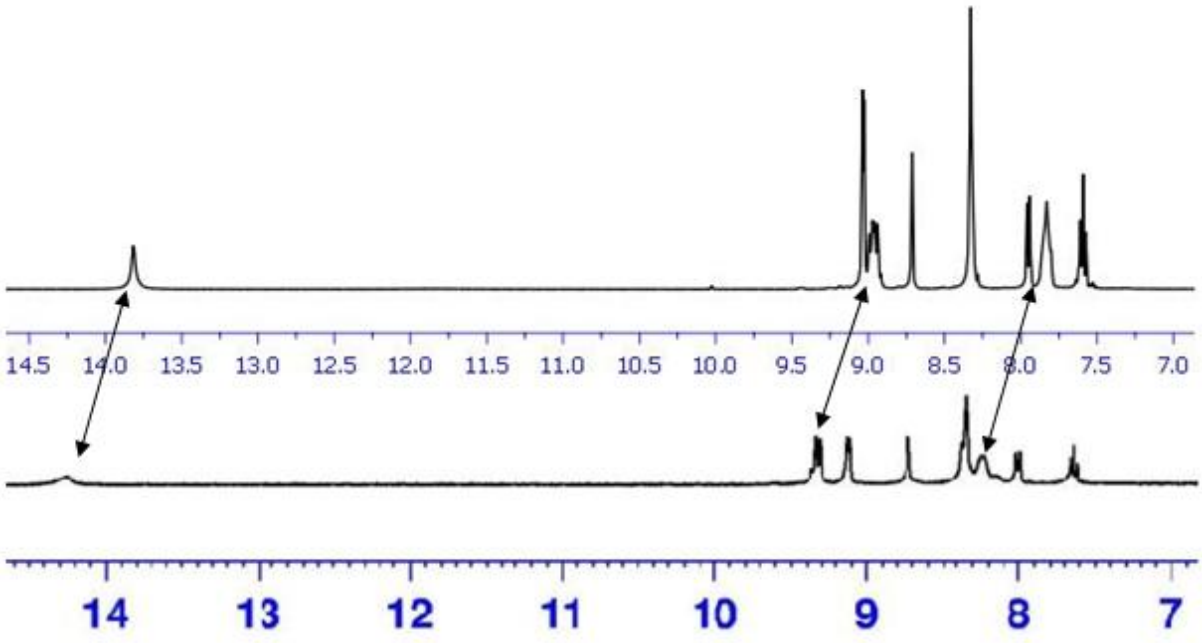

Figure S12. Partial ^{1}H NMR spectra of **1** (up) and **1**+Zn^{2+} complex (down) in (DMSO-d_6).

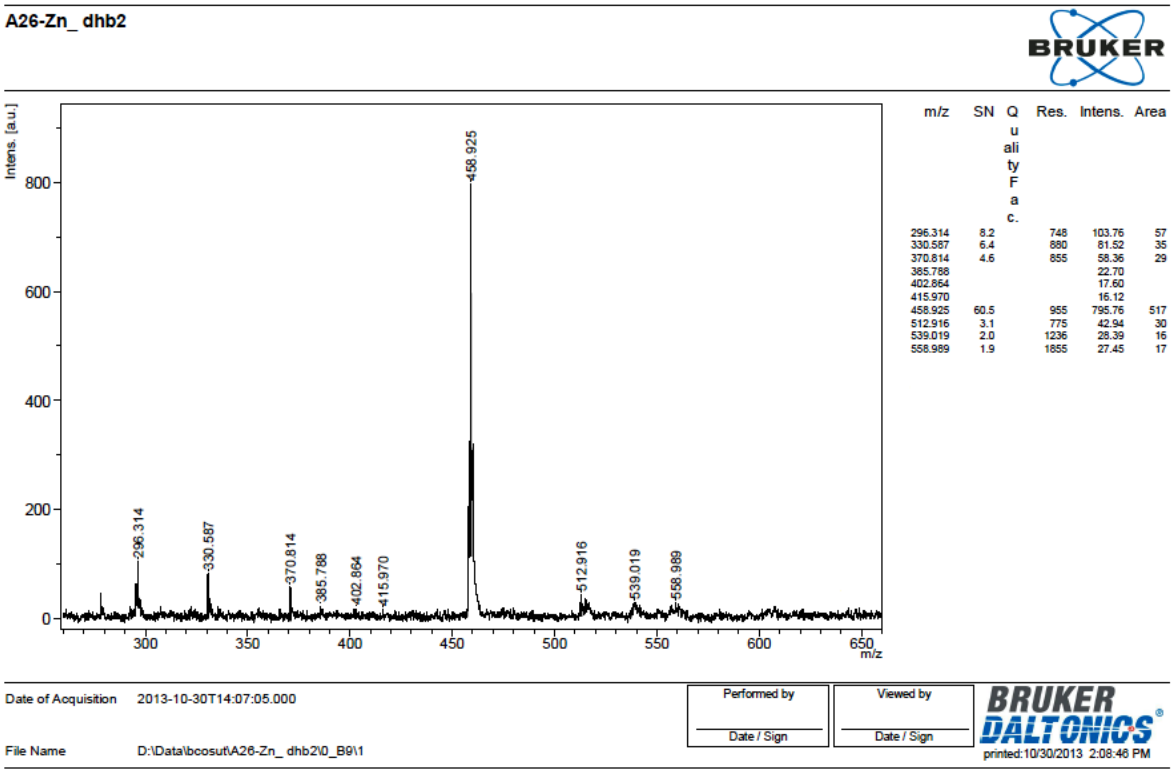

Figure S13. MALDI TOF mass spectrum of **1**+Zn^{2+} complex.

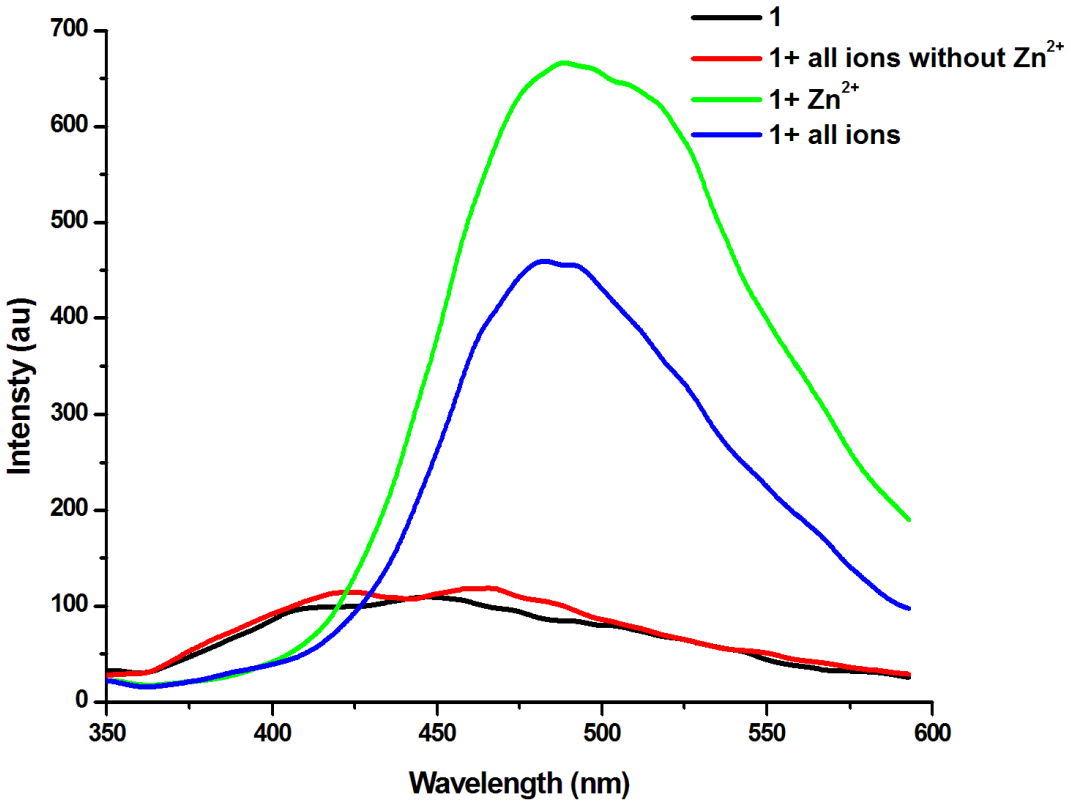

Figure S14. Fluorescence emission spectra of **1** (5.20 x 10^{-5} M) in the absence and presence of Zn^{2+} (10 equiv) and/or all other ions (Ag^{+}, Al^{3+}, Au^{3+}, Cd^{2+}, Co^{2+}, Cu^{+}, Cu^{2+}, Fe^{2+}, Fe^{3+}, Hg^{2+}, K^{+}, Li^{+}, Mn^{2+}, Mg^{2+}, Na^{+}, Ni^{2+}, Pb^{2+}, Pt^{2+} and Pd^{2+}) (10 equiv) in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), pH = 7.2, 25°C, λ_{exc}=308 nm.

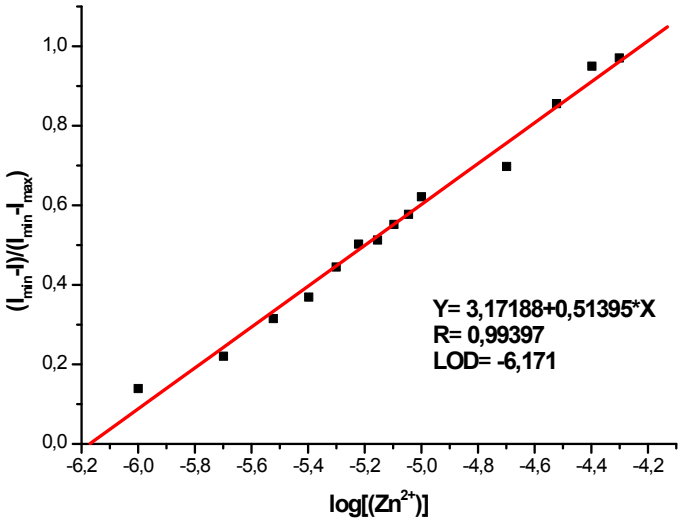

Figure S15. Plot of normalized fluorescence intensity of **1** as a function of log[Zn^{2+}] in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v, pH=7.2) at 25°C, λ_{exc}=308 nm (log[Zn^{2+}] = -6.171).

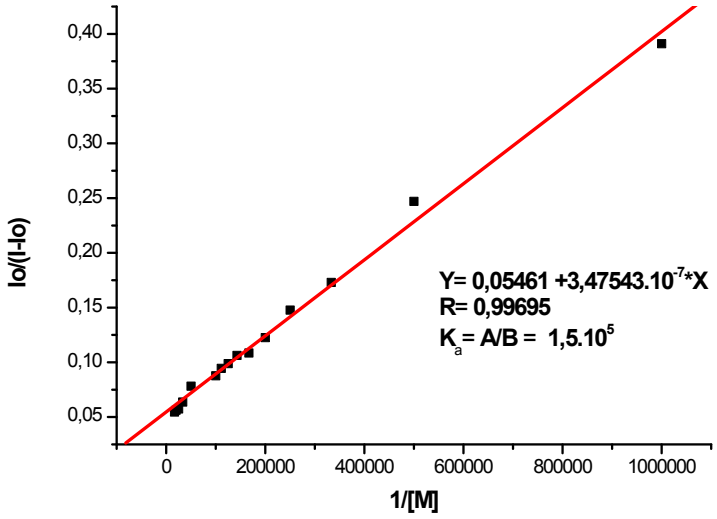

Figure S16. Linear regression curve for **1**.