

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

Figure S1. ^1H NMR spectrum of 3 (CDCl_3).....	SI-4
Figure S2. ^{13}C NMR spectrum of 3 (CDCl_3).....	SI-4
Figure S3. ^1H NMR spectrum of 1 (DMSO-d_6).....	SI-5
Figure S4. ^{13}C NMR spectrum of 1 ($\text{DMSO-d}_6 / \text{CDCl}_3$).....	SI-5
Figure S11. ^1H NMR spectrum of 1+Zn(II) complex (DMSO-d_6).....	SI-11
Figure S12. Partial ^1H NMR spectra of 1 (up) and 1+Zn²⁺ complex (down) in (DMSO-d_6).....	SI-11

Copies of Mass Spectra

Figure S5. HRMS spectrum of 1	SI-6
Figure S13. MALDI TOF mass spectrum of 1+Zn²⁺ complex.....	SI-12

Figures of Job plot, LOD and Linear regression curve

Figure S6. Job plot diagram of 1 for Fe^{2+} at a constant total concentration of 2.5×10^{-5} M in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), pH= 7.2, 25°C.....	SI-7
Figure S7. Plot of normalized absorbtion intensity of 1 as a function of $\log[\text{Fe}^{2+}]$ in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v, pH=7.2) at 25°C, ($\log[\text{Fe}^{2+}] = -5.31$).....	SI-8
Figure S8. Linear regression curve for 1	SI-9
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.....	SI-9

Figure S10. Job plot diagram of **1** for Zn²⁺ (ΔI indicates the change of emission intensity at 498 nm) at a constant total concentration of 2.5×10^{-5} M in 0.1 M HEPES buffer containing 0.1% CH₃OH (v/v), pH= 7.2 at 25°C, $\lambda_{\text{exc}}=308$ nm.....SI-10

Figure S11.Job plot diagram of **1** for Zn²⁺ (ΔI indicates the change of emission intensity at 498 nm) at a constant total concentration of 2.5×10^{-5} M)..... SI-11

Figure S14. Fluorescence emission spectra of **1** (5.20×10^{-5} M) in the absence and presence of Zn²⁺ (10 equiv) and/or all other ions (Ag⁺, Al³⁺, Au³⁺, Cd²⁺, Co²⁺, Cu⁺, Cu²⁺, Fe²⁺, Fe³⁺, Hg²⁺, K⁺, Li⁺, Mn²⁺, Mg²⁺, Na⁺, Ni²⁺, Pb²⁺, Pt²⁺ and Pd²⁺) (10 equiv) in 0.1 M HEPES buffer containing 0.1% CH₃OH (v/v), pH = 7.2, 25°C, $\lambda_{\text{exc}}=308$ nm.....SI-13

Figure S15.Plot of normalized fluorescence intensity of **1** as a function of log[Zn²⁺] in 0.1 M HEPES buffer containing 0.1% CH₃OH (v/v, pH=7.2) at 25°C, $\lambda_{\text{exc}}=308$ nm (log[Zn²⁺] = -6.171)..... SI-14

Figure S16.Linear regression curve for **1**..... SI-14

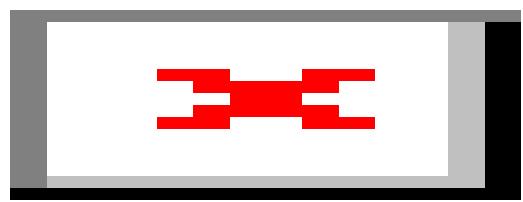


Figure S1. ^1H NMR spectrum of **3** (CDCl_3).

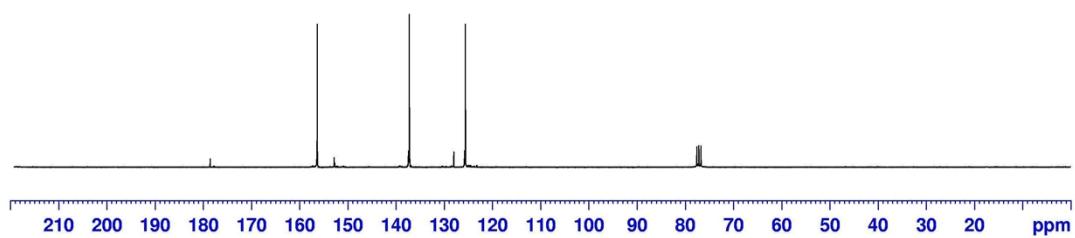


Figure S2. ^{13}C NMR spectrum of **3** (CDCl_3).

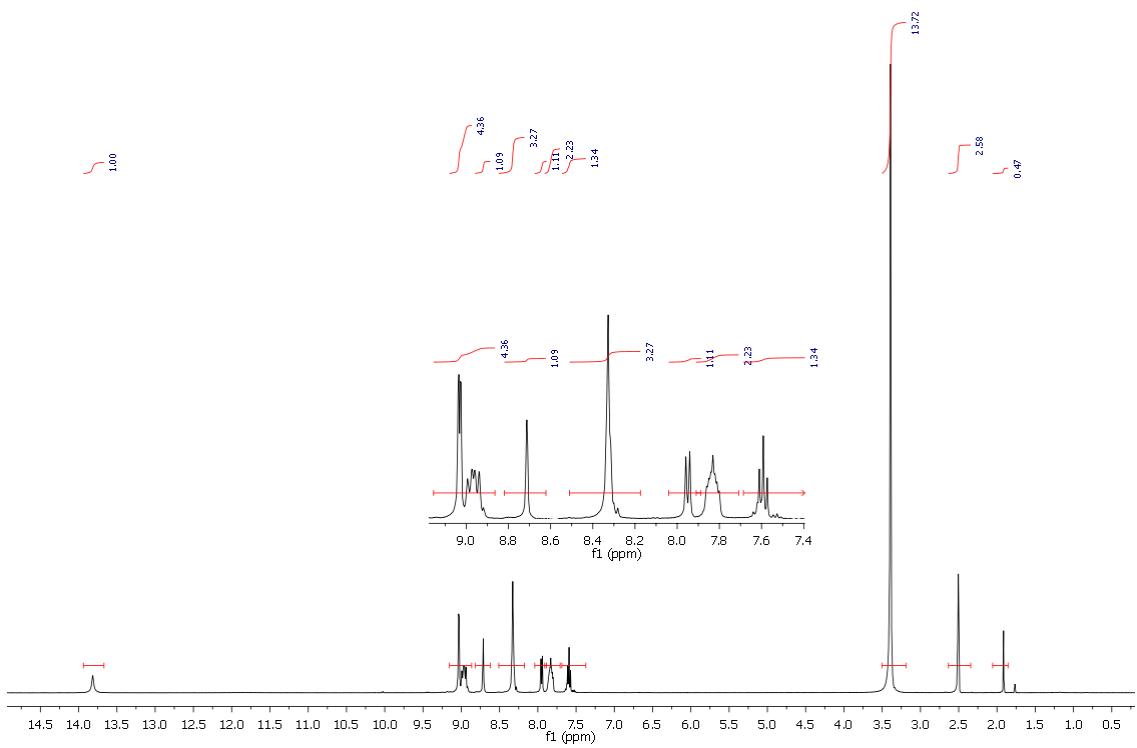


Figure S3. ^1H NMR spectrum of **1** (DMSO-d₆).

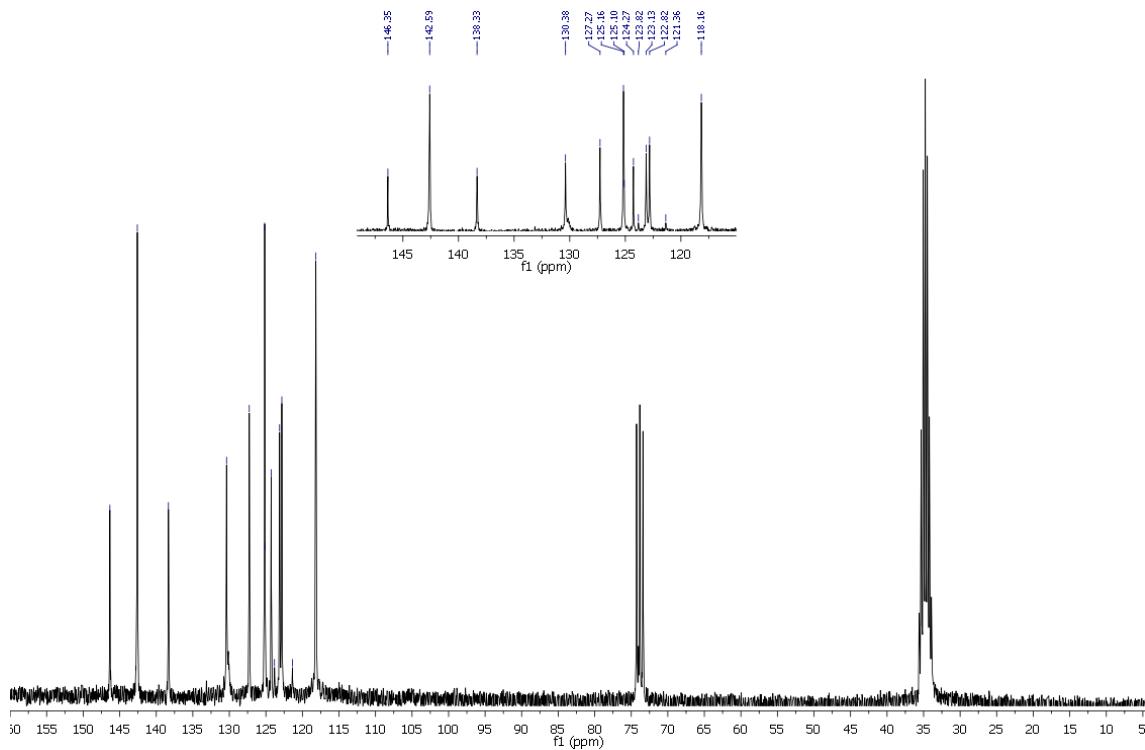


Figure S4. ^{13}C NMR spectrum of **1** (DMSO-d₆ / CDCl₃).

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

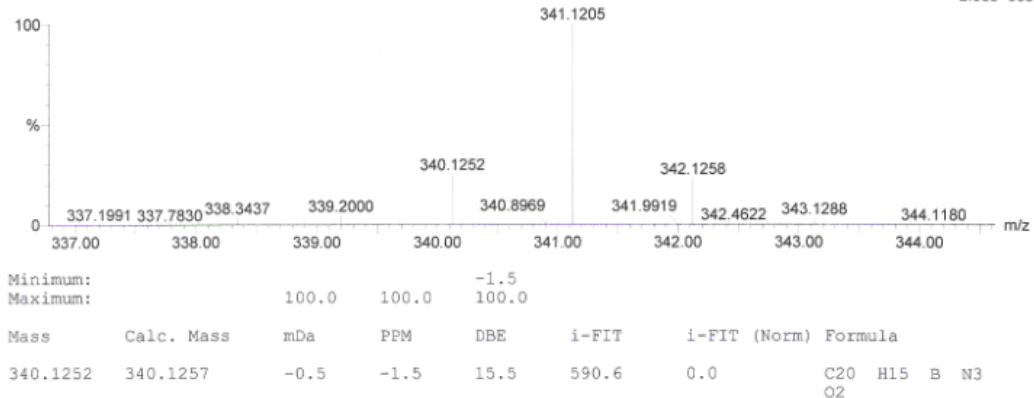
Monoisotopic Mass, Odd and Even Electron Ions

2 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-20 H: 14-15 B: 0-2 N: 1-3 O: 1-2

20120824_8829-01_02 11 (0.450) Cm (1:51)

1: TOF MS ES+
2.98e+005**Figure S5.** HRMS spectrum of **1**.

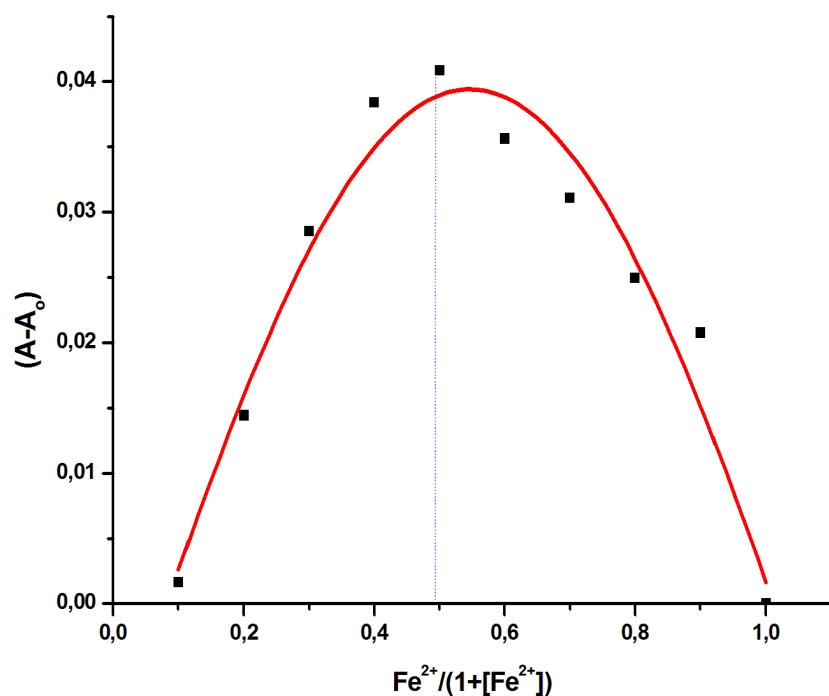


Figure S6. Job plot diagram of **1** for Fe^{2+} at a constant total concentration of 2.5×10^{-5} M in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), $\text{pH}=7.2$, 25°C .

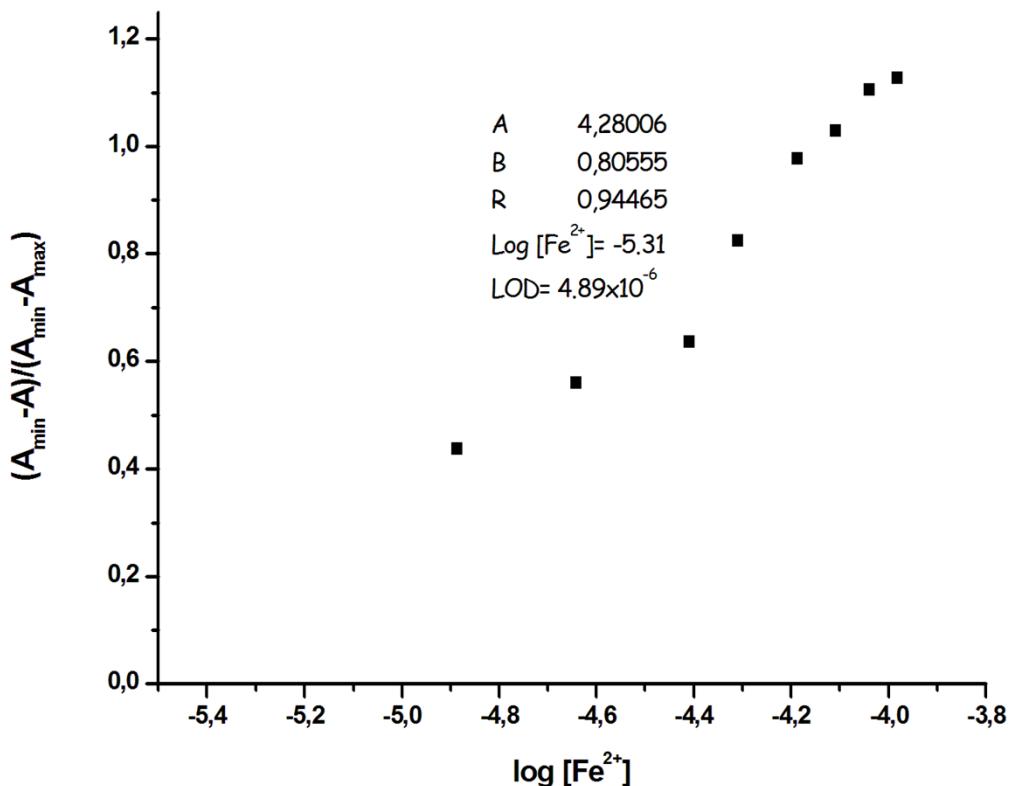


Figure S7. Plot of normalized absorbtion intensity of **1** as a function of $\log[Fe^{2+}]$ in 0.1 M HEPES buffer containing 0.1% CH₃OH (v/v, pH=7.2) at 25°C, ($\log[Fe^{2+}] = -5.31$).

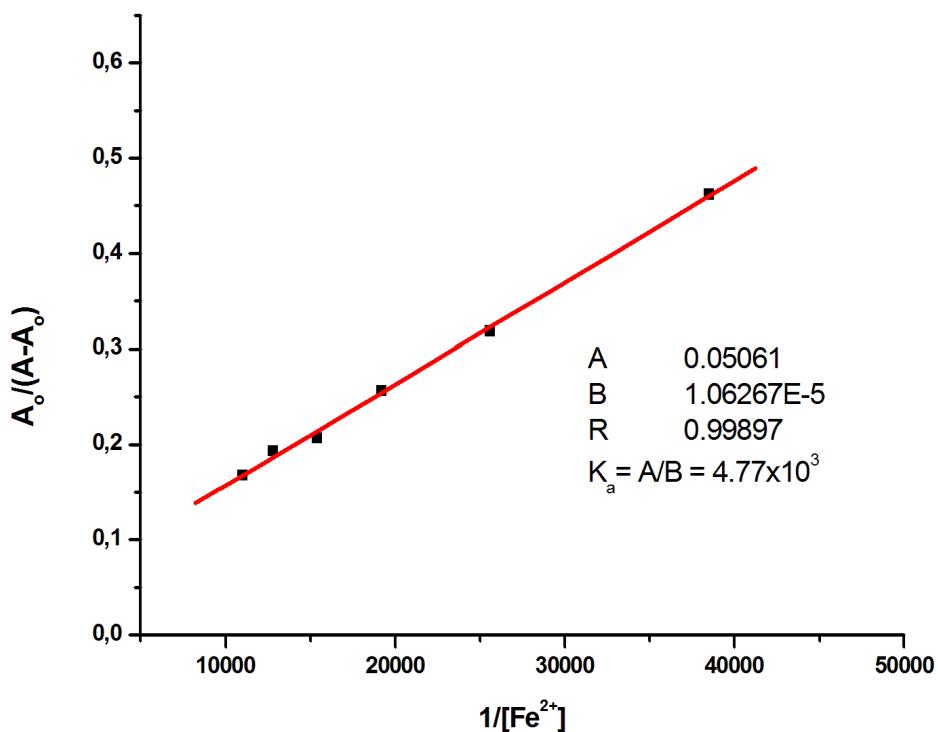


Figure S8. Linear regression curve for **1**.



Figure S9. Chromogenic (left) and fluorogenic (right) responses of **1** to metal ions in aqueous 0.1 M HEPES containing 0.1% CH₃OH (v/v) solution (pH= 7.2, 25°C) under room light and UV illumination (365 nm), respectively.

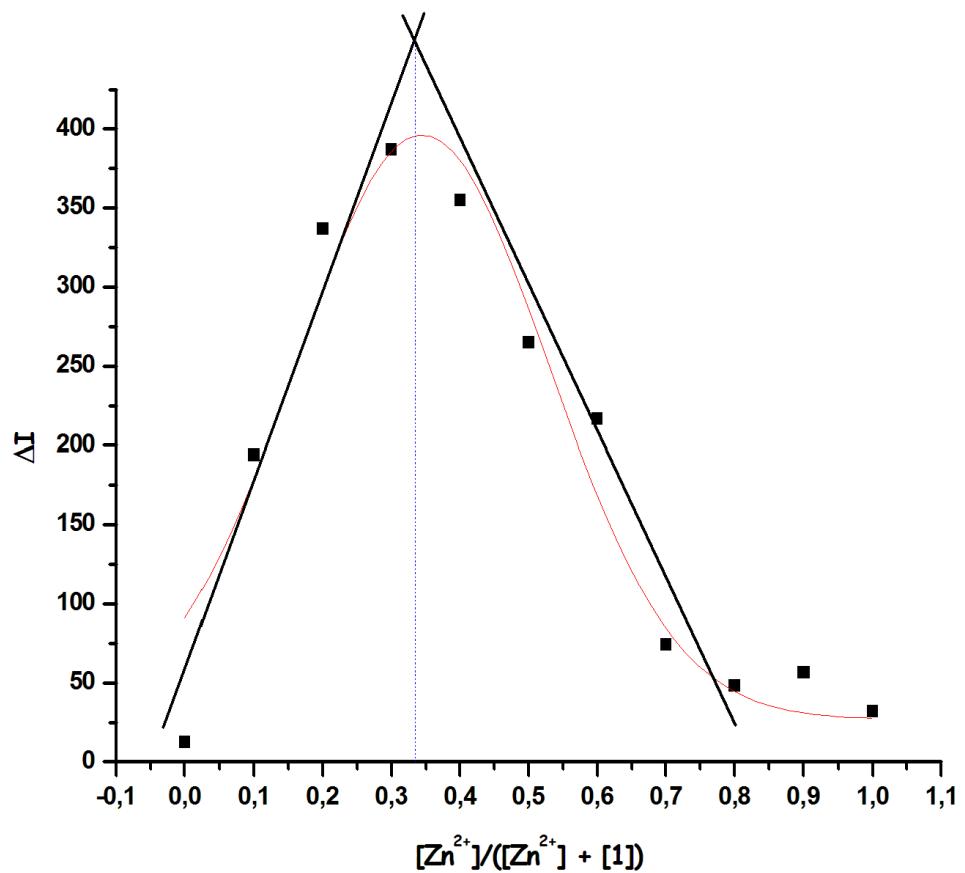


Figure S10. Job plot diagram of **1** for Zn^{2+} (ΔI indicates the change of emission intensity at 498 nm) at a constant total concentration of 2.5×10^{-5} M in 0.1 M HEPES buffer containing 0.1% CH_3OH (v/v), $\text{pH} = 7.2$ at 25°C , $\lambda_{\text{exc}} = 308$ nm.

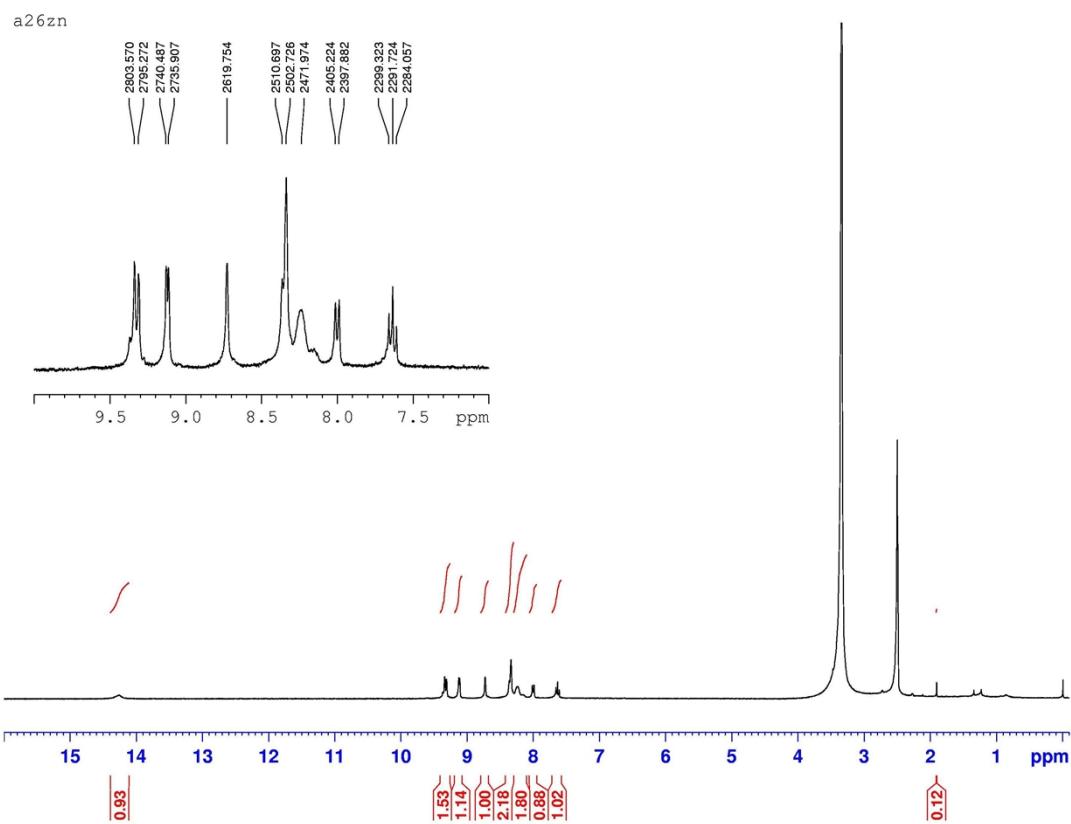


Figure S11. ^1H NMR spectrum of **1**+Zn(II) complex (DMSO- d_6).

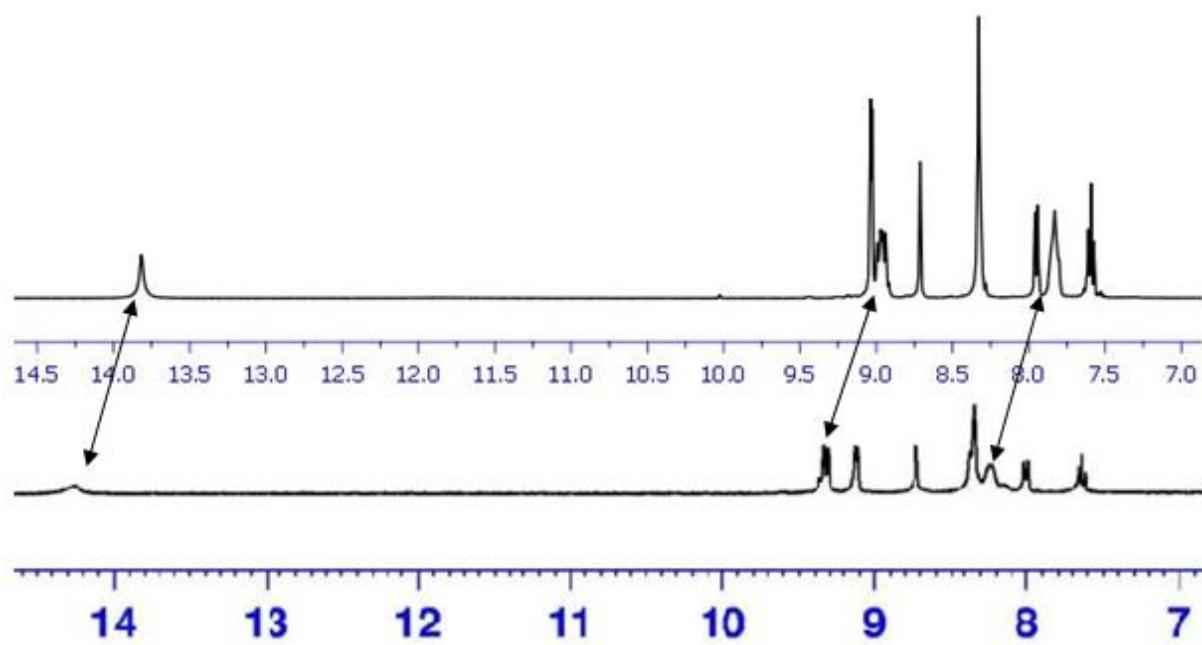


Figure S12. Partial ^1H NMR spectra of **1** (up) and **1**+Zn $^{2+}$ complex (down) in (DMSO- d_6).

A26-Zn_dhb2

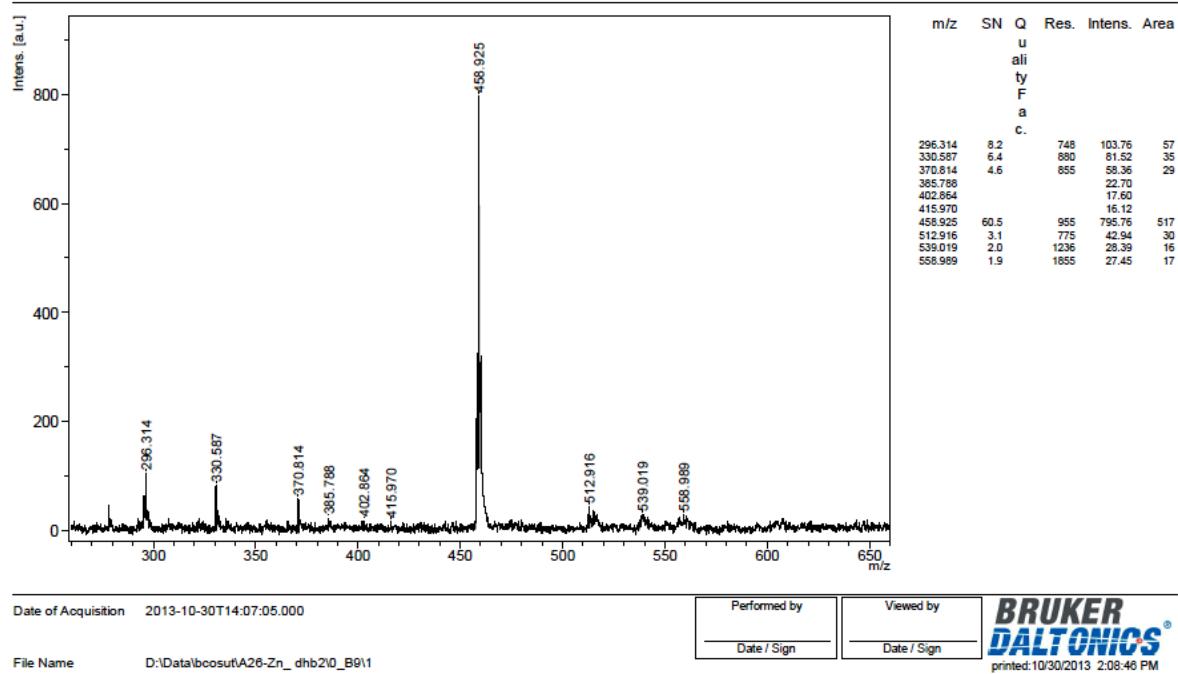


Figure S13. MALDI TOF mass spectrum of **1**+Zn²⁺ complex.

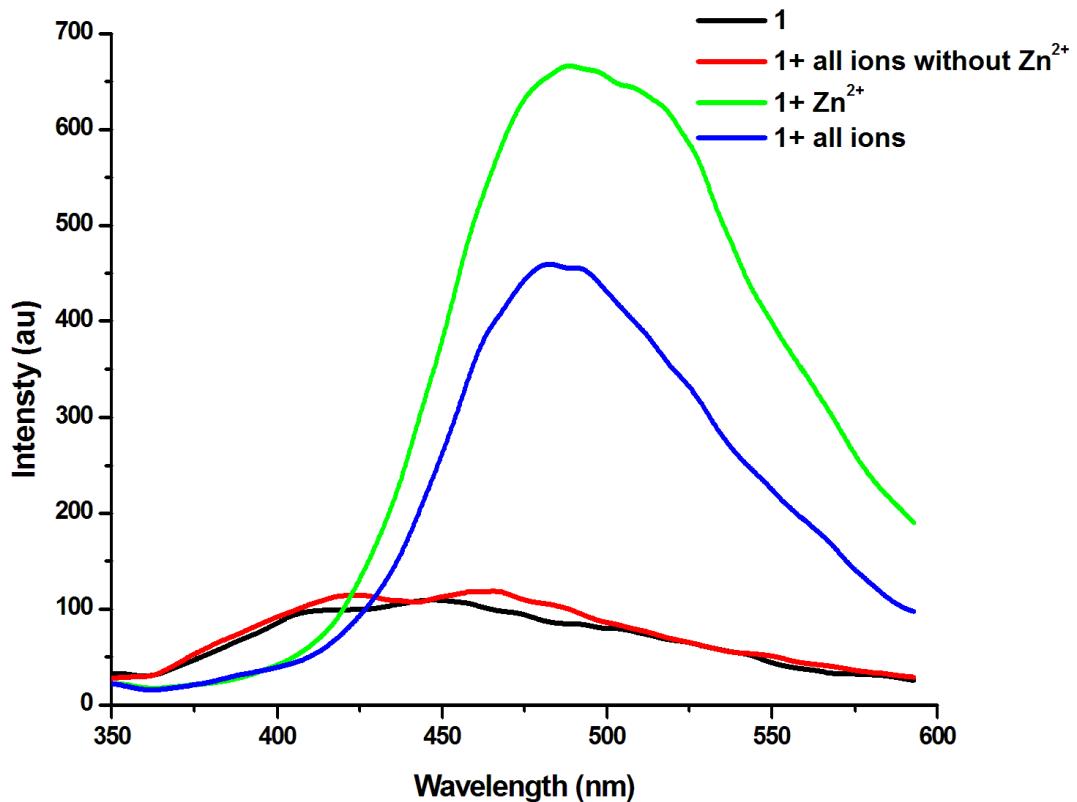


Figure S14. Fluorescence emission spectra of **1** (5.20×10^{-5} M) in the absence and presence of Zn^{2+} (10 equiv) and/or all other ions (Ag^+ , Al^{3+} , Au^{3+} , Cd^{2+} , Co^{2+} , Cu^+ , Cu^{2+} , Fe^{2+} , Fe^{3+} , Hg^{2+} , K^+ , Li^+ , Mn^{2+} , Mg^{2+} , Na^+ , Ni^{2+} , Pb^{2+} , Pt^{2+}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

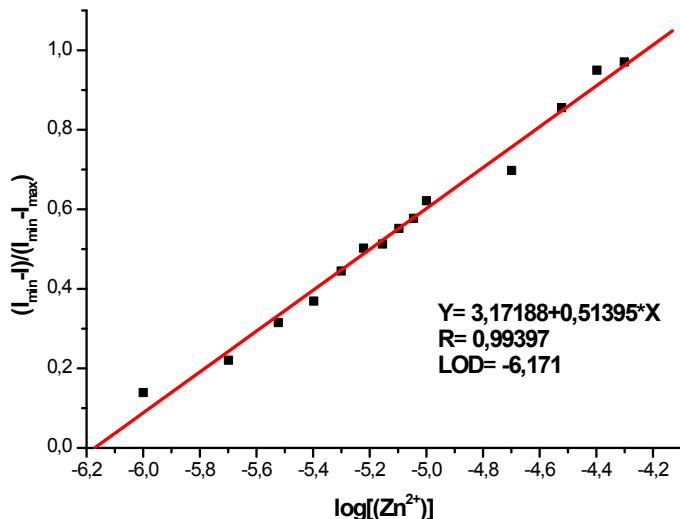


Figure S15. Plot of normalized fluorescence intensity of **1** as a function of $\log[Zn^{2+}]$ in 0.1 M HEPES buffer containing 0.1% CH₃OH (v/v, pH=7.2) at 25°C, $\lambda_{exc}=308$ nm ($\log[Zn^{2+}] = -6.171$).

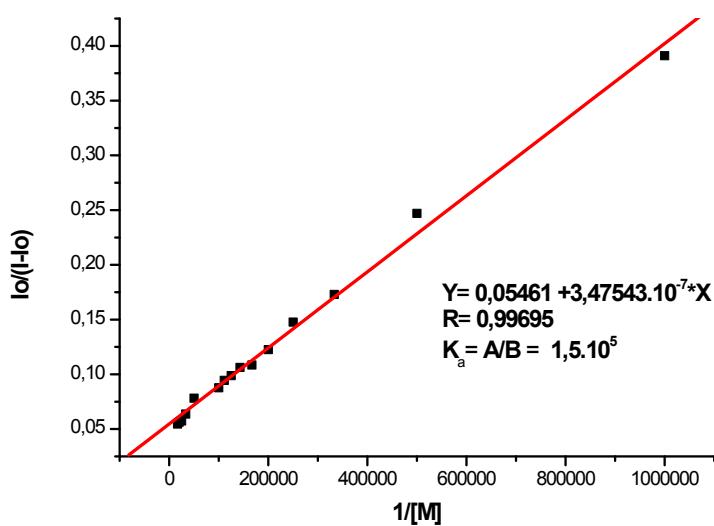


Figure S16. Linear regression curve for **1**.