Supporting Information

A highly selective pyridoxal-based chemosensor for the detection of Zn(II) and application in live cell imaging; X-ray crystallography of pyridoxal-TRIS Schiff-base Zn(II) and Cu(II) complexes.

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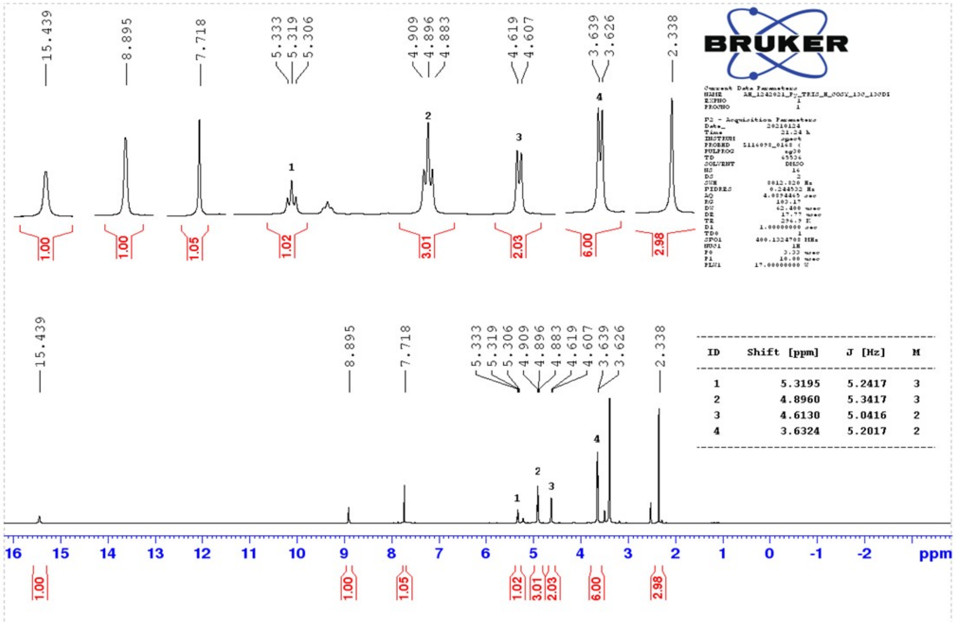

Figure S1: [1]H NMR of compound 1 in DMSO-d6.

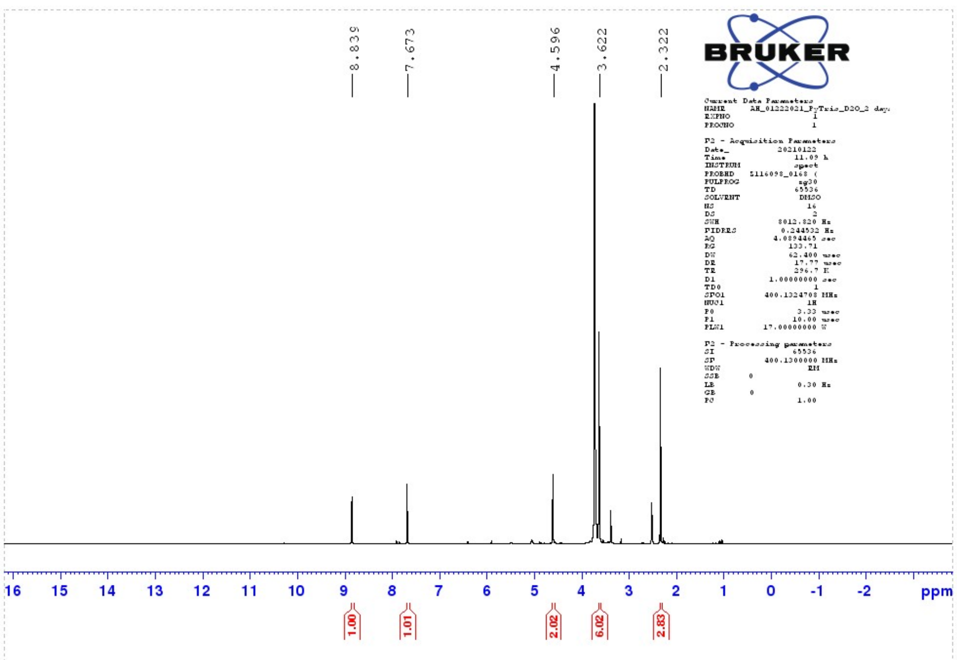

Figure S2: [1]H NMR of compound 1 in DMSO-d6 with added D_2O.

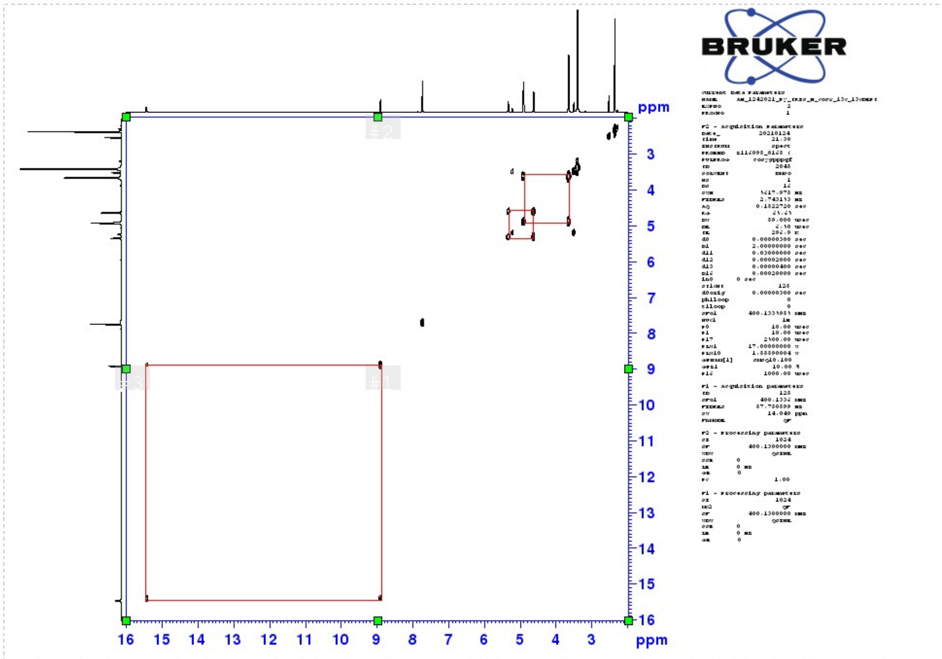

Figure S3: ^{1}H-^{1}H Correlation Spectroscopy (COSY) NMR of 1 shows the correlation between hydrogens coupled to each other in the ^{1}H NMR spectrum in DMSO-d6.

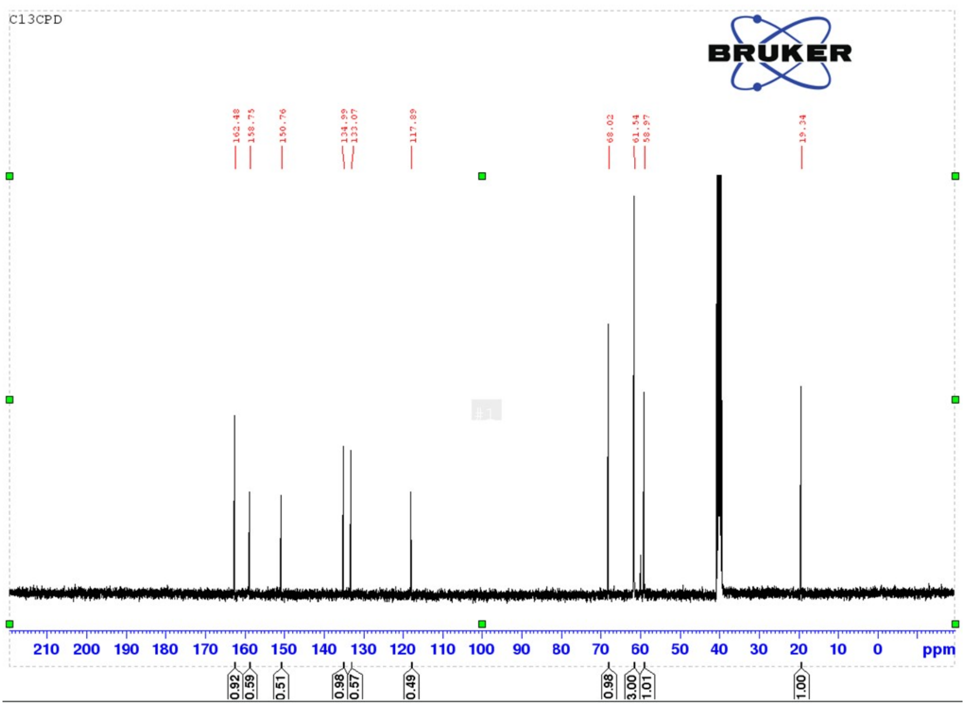

Figure S4: ^{13}C-CPD NMR of compound 1 in DMSO-d6.

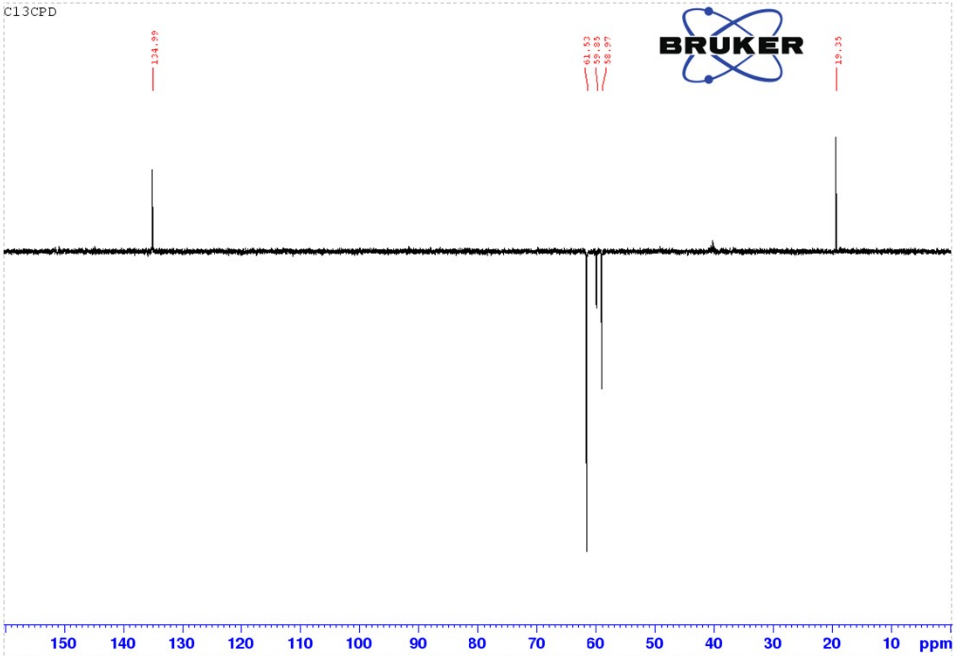

Figure S5: ^{13}C-DEPT135 NMR of 1 in DMSO-d6.

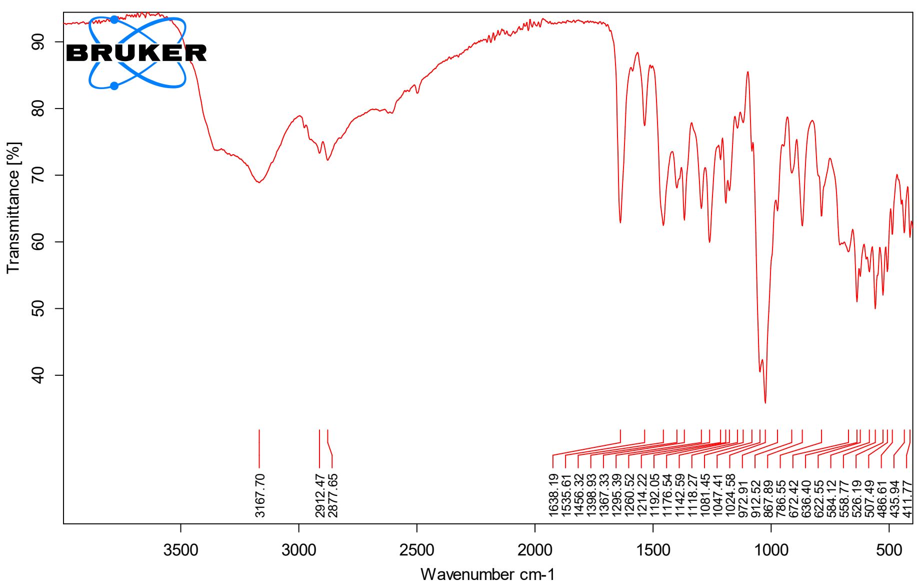

Figure S6: IR spectrum of compound 1.

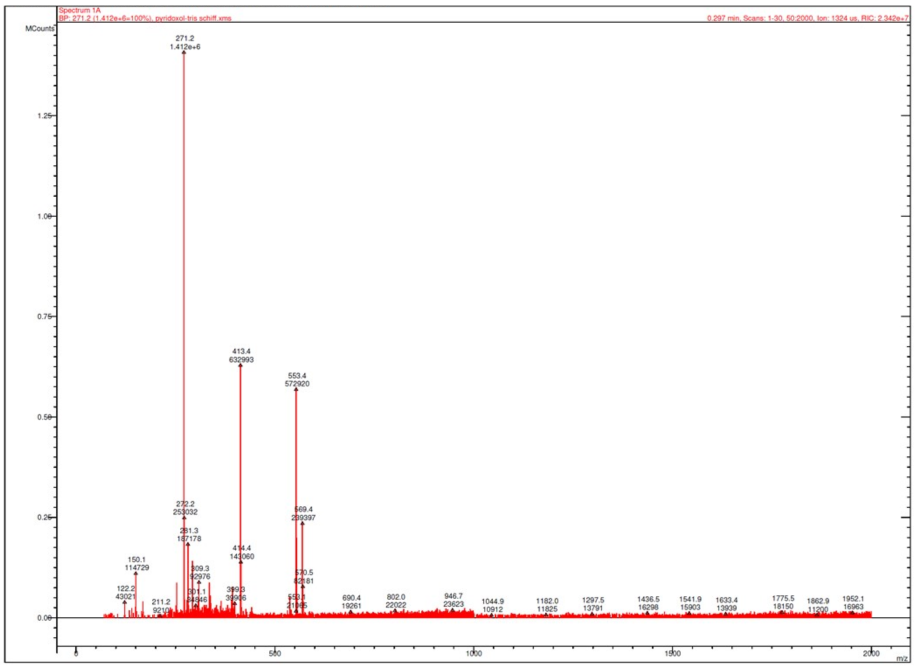

*Figure S7: ESI-MS Spectra of **1** showing a molecular ion peak at 271.2 $[M+H]^+$ referring to the molar mass of compound **1** (270.28 g/mol).*

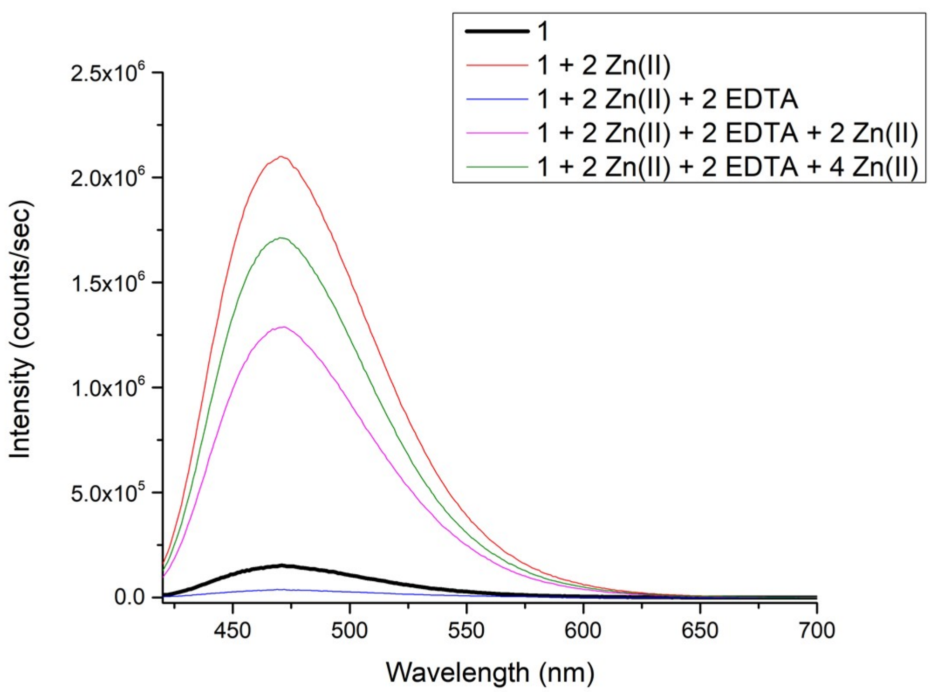

Figure S8: Fluorescence emission spectra of compound 1 in the presence of Zn(II) followed by addition of Na_2EDTA and followed by the addition of Zn(II) (λex=413 nm).

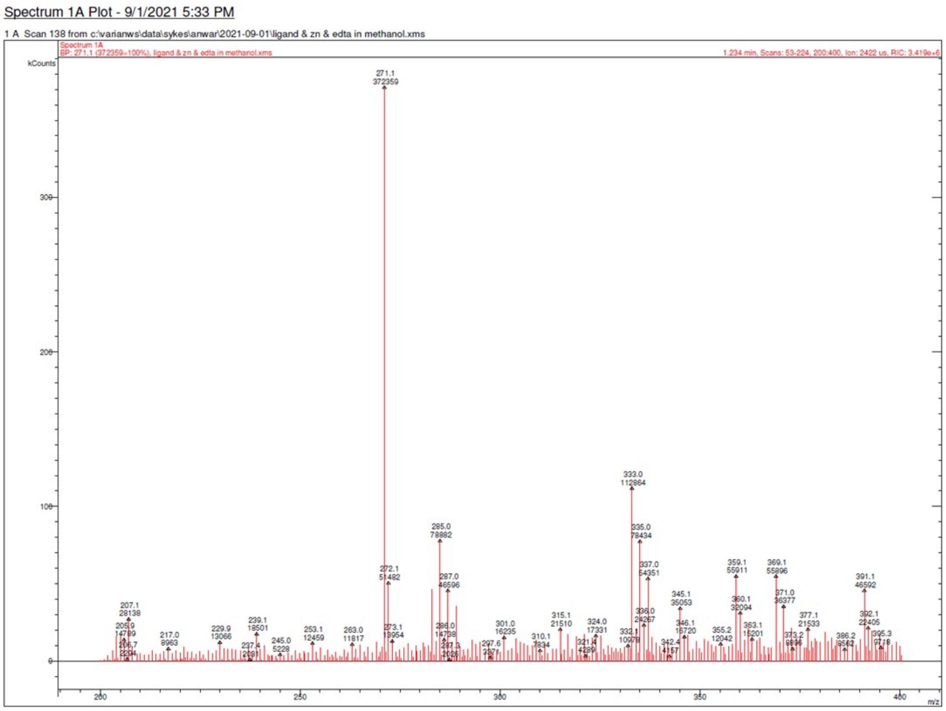

*Figure S9: ESI-MS Spectra of recovered **1** after addition of EDTA showing a molecular ion peak at 271.1 [M+H]+ referring to the molar mass of compound **1** (270.28 g/mol).*

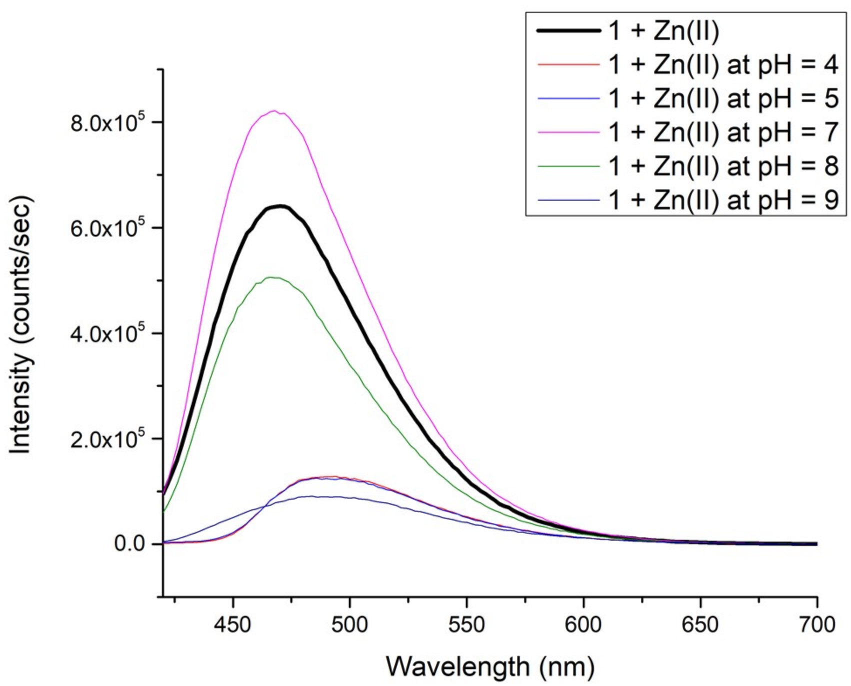

Figure S10: Effect of the pH on the fluorescence intensity of compound 1 in the presence of 2 equivalent of Zn(II) ions (λex=413 nm).

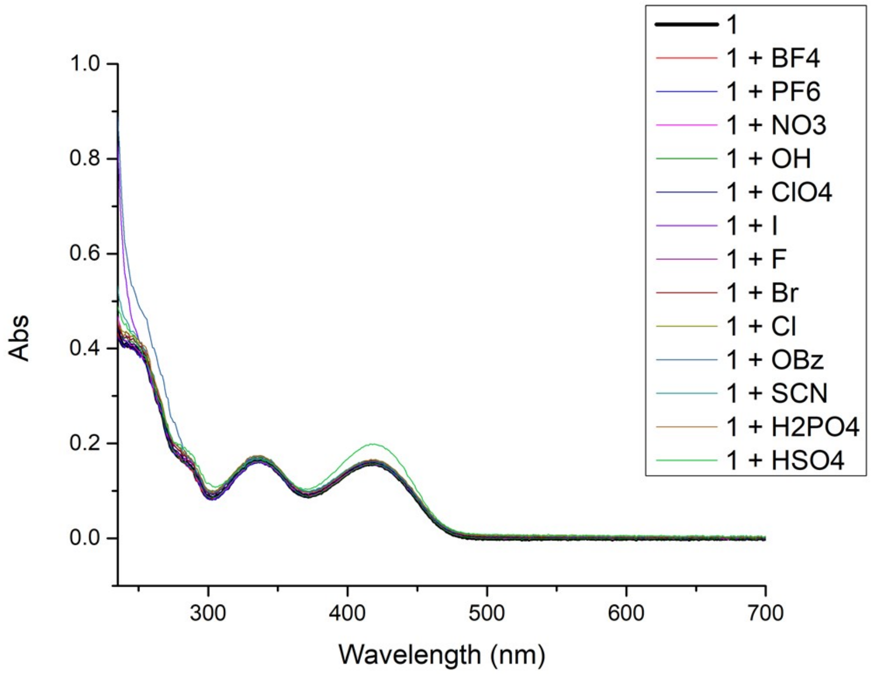

*Figure S11: UV-Vis spectra of compound **1** (5.0 x10^{-5} M) in CH_3OH before (black) and after the addition of 2.0 equivalents of anions as tetrabutylammonium salts.*

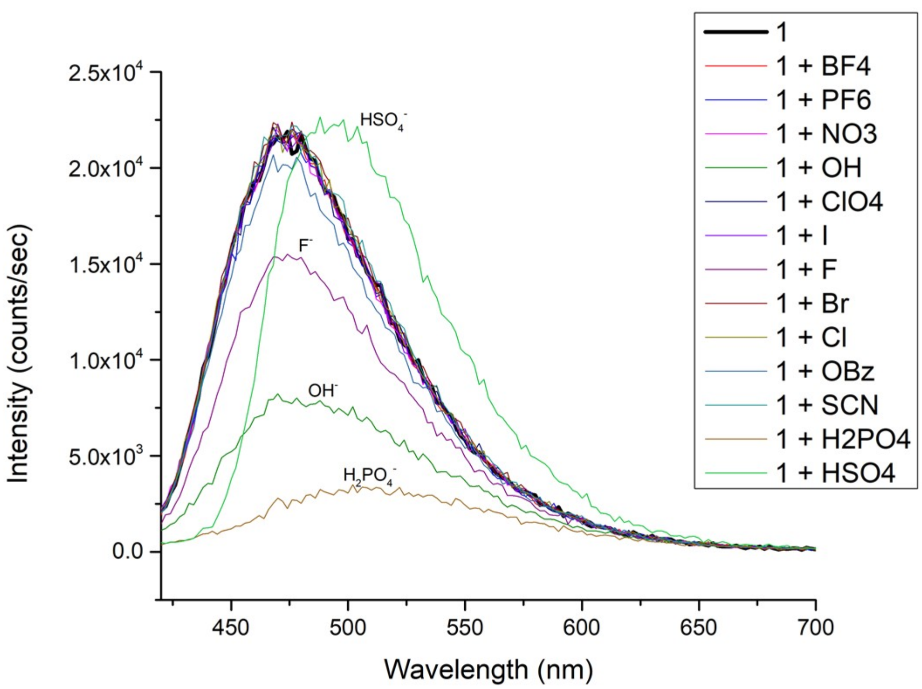

*Figure S12: Emission spectra of compound **1** (5.0 x10^{-5} M, λ_{ext} = 413 nm) in CH_3OH before (black) and after the addition of 2.0 equivalents of anions as tetrabutylammonium salts.*

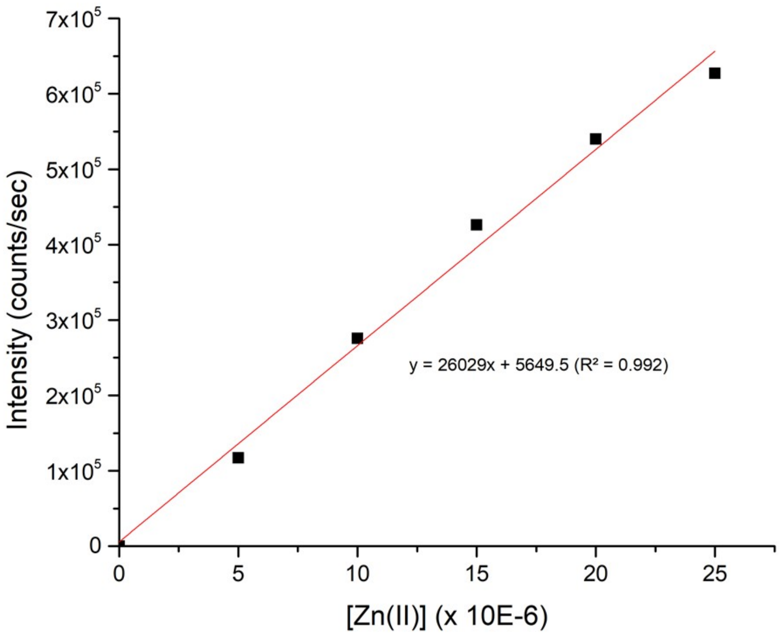

Figure S13: Normalized response of fluorescence signal of 1 (5.0×10^{-5} M, CH_3OH) in the presence of the increasing amount of Zn(II) ($5 - 25 \times10^{-6}$ M, ACN) (λ_{ex} = 413nm; λ_{em} = 470nm)

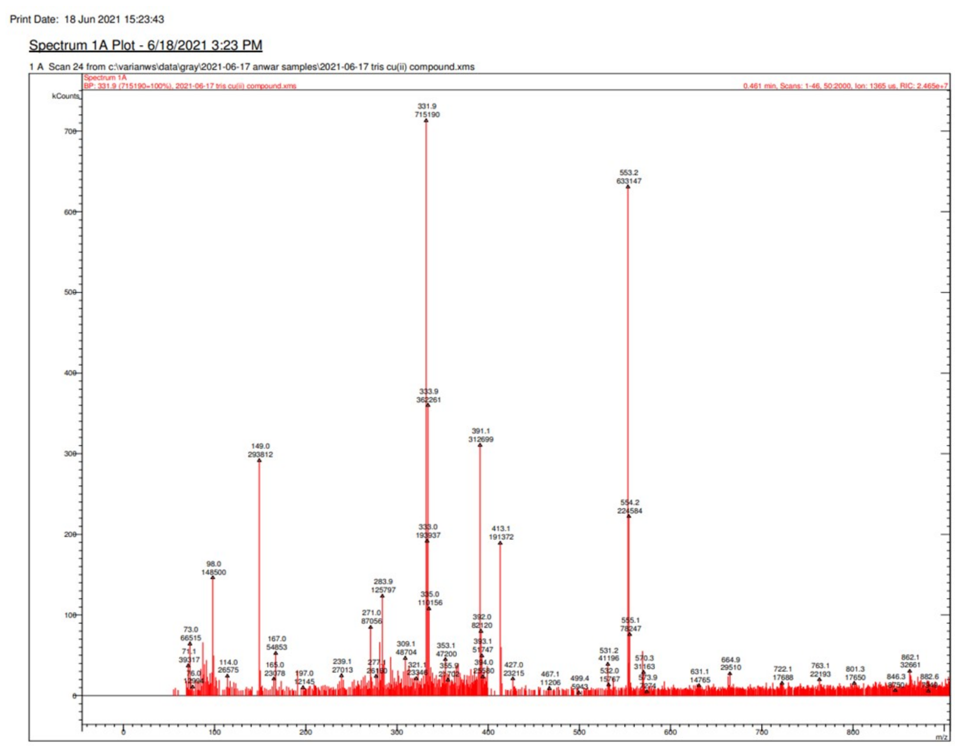

*Figure S 14: Electrospray mass spectrum (ESI-MS positive) of Cu(II) complex of compound **1**.*

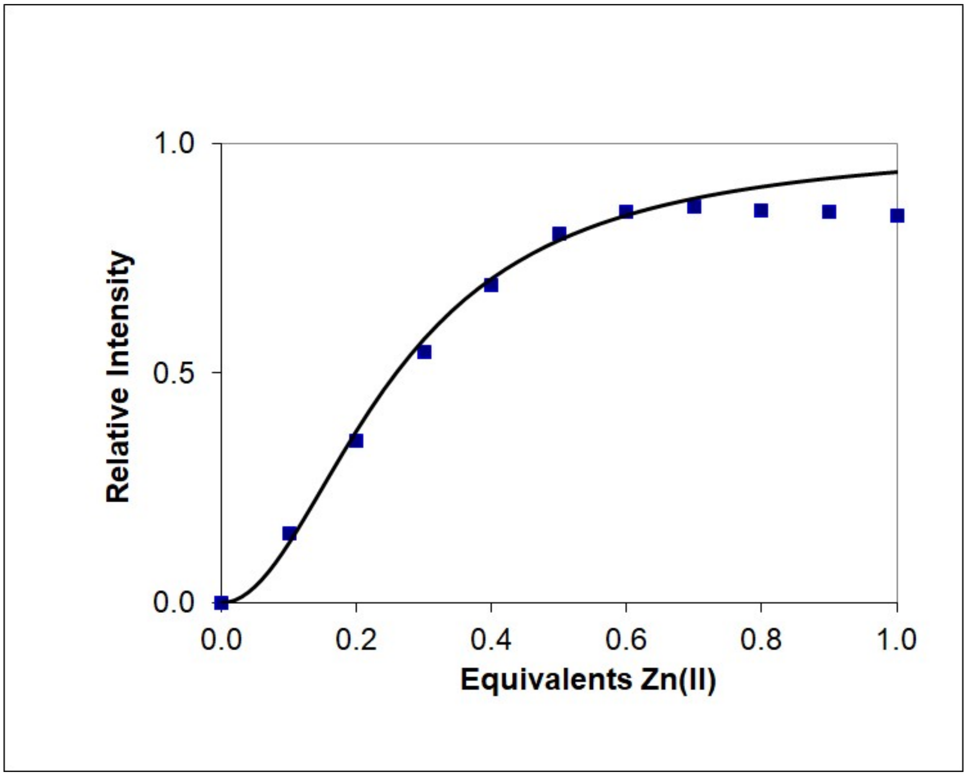

Figure S15: Relative fluorescence intensity at 470 nm on the added equivalent of Zn(II); best fit for 2:1 compound 1:Zn(II) association. Association constant for 2:1 best fit equal 6.0 x 10^9 M^{-2} (±10%).

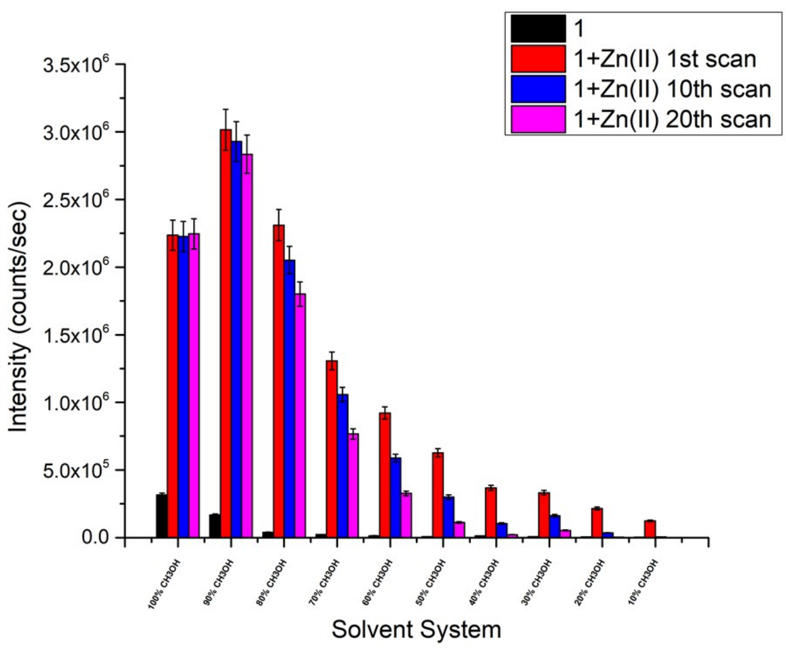

Figure S16: Relative fluorescence intensity of compound 1 at 470 nm on addition of 2.0 equivalents Zn(II) as perchlorate salts in different fraction of CH_3OH and H_2O (0.1 M HEPES buffer, pH = 7.3) showing the loss of emission at higher content of water. 20 scans with interval of 1 min, 10^{th} scan: approx. 15 mins, and 20^{th} scan: approx. 30 mins.

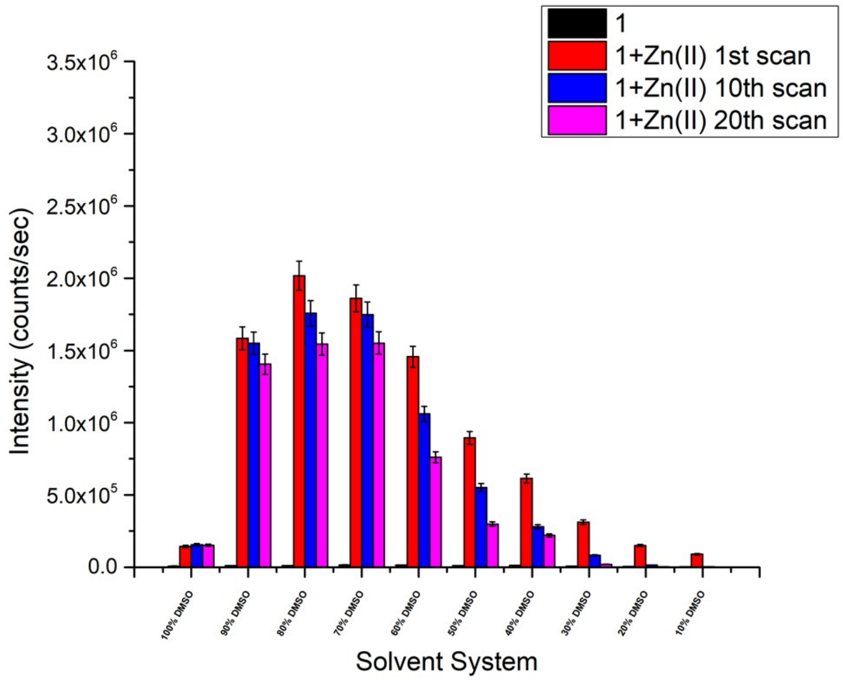

Figure S17: Relative fluorescence intensity of compound 1 at 470 nm on addition of 2.0 equivalents Zn(II) as perchlorate salts in different fraction of DMSO and H_2O (0.1 M HEPES buffer, pH = 7.3) showing the loss of emission at higher content of water. 20 scans with interval of 1 min, 10th scan: approx. 15 mins, and 20th scan: approx. 30 mins.

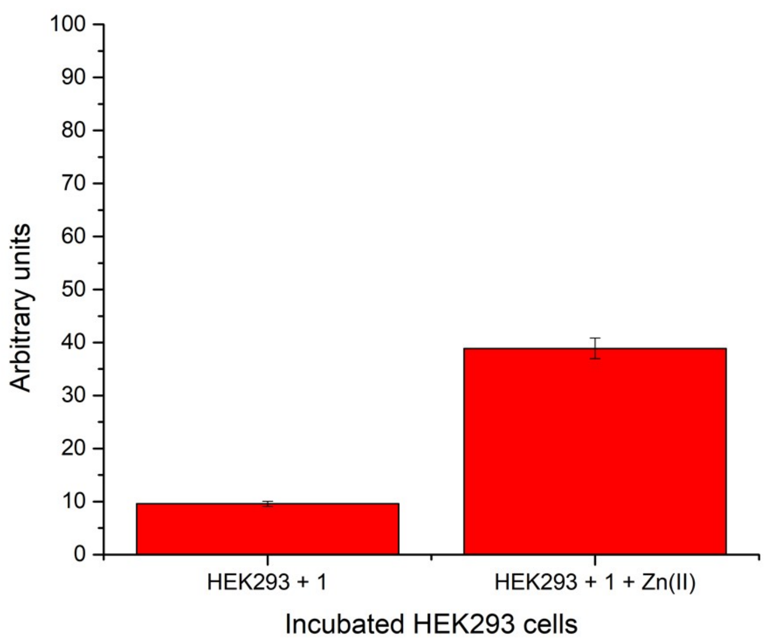

Figure S18: Mean fluorescence intensity(MFI) of compound 1 in HEK293 cells calculated using Fiji software.

Job's Plot

5 x 10^{-5} M of the compound **1** in methanol and 5 x 10^{-5} M Zn(II) as acetate salt in acetonitrile solution were prepared from concentrated stock solutions and 0.25 – 3 mL of **3** and 0 – 2.75 mL of Zn(II) solution were taken in a cuvettes to make total volume of 3 mL and fluorescence spectra were recorded.

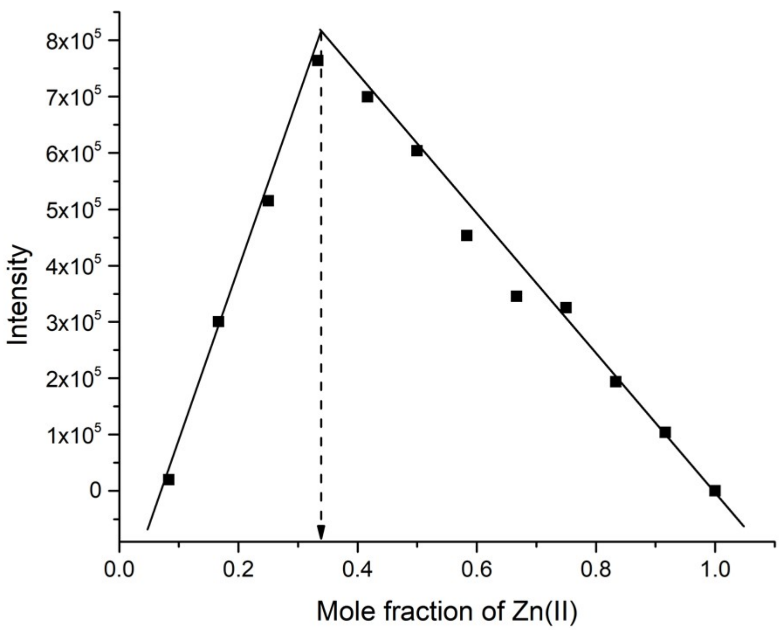

*Figure S19: Job's plot of **1** with Zn(II) with a maxima near to 0.33 confirms the formation of L_2Zn(II) complex. Fluorescence intensity monitored at 470 nm vs. a function of the molar ratio of [**Zn(II)**]/([**1**] + [**Zn(II)**]), λ_{ex} = 413nm.*

Calculation of Quantum Yield

$$\phi_{sample} = \phi_{reference}\, X\, \frac{A_{sample}}{A_{reference}}\, X\, \frac{Abs_{reference}}{Abs_{sample}}\, X\, \frac{{\eta_{sample}}^2}{{\eta_{reference}}^2} \qquad (1)$$

Quantum Yield of Compound 1:

$$\phi_1 = 0.27\, X\, \frac{1.74\ x\ 10^6}{6.93\ x\ 10^7}\, X\, \frac{0.247}{0.042}\, X\, \frac{1.36^2}{1.36^2}$$

$$or,\ \phi_1 = 0.27\, X\, 2.51\ x\ 10^{-2}\, X\, 5.88\, X\, 1 = 0.0398 \cong 0.04$$

Quantum Yield of Zinc complex:

$$\phi_1 = 0.27\, X\, \frac{7.86\ x\ 10^7}{6.93\ x\ 10^7}\, X\, \frac{0.247}{0.157}\, X\, \frac{1.36^2}{1.36^2}$$

$$or,\ \phi_1 = 0.27\, X\, 1.13\, X\, 1.57\, X\, 1 = 0.479 \cong 0.48$$

Calculation of Detection Limit

$$Detection\ Limit = \frac{3\,\sigma}{K} \qquad (2)$$

$$or,\ Detection\ Limit = \frac{3\ x\ 240.145}{26029}\ X\ 10^{-6} = \ 2.77\ x\ 10^{-8}\ M$$