Supporting Information for

A novel chromo- and fluorogenic dual sensor for Mg^{2+} and Zn^{2+} with cell imaging possibilities and DFT studies†.

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18. Chemical shifts in NMR of **DFC-8-AQ** , Zn^{2+} and Mg^{2+} complex. Table S1

19. LOD determination

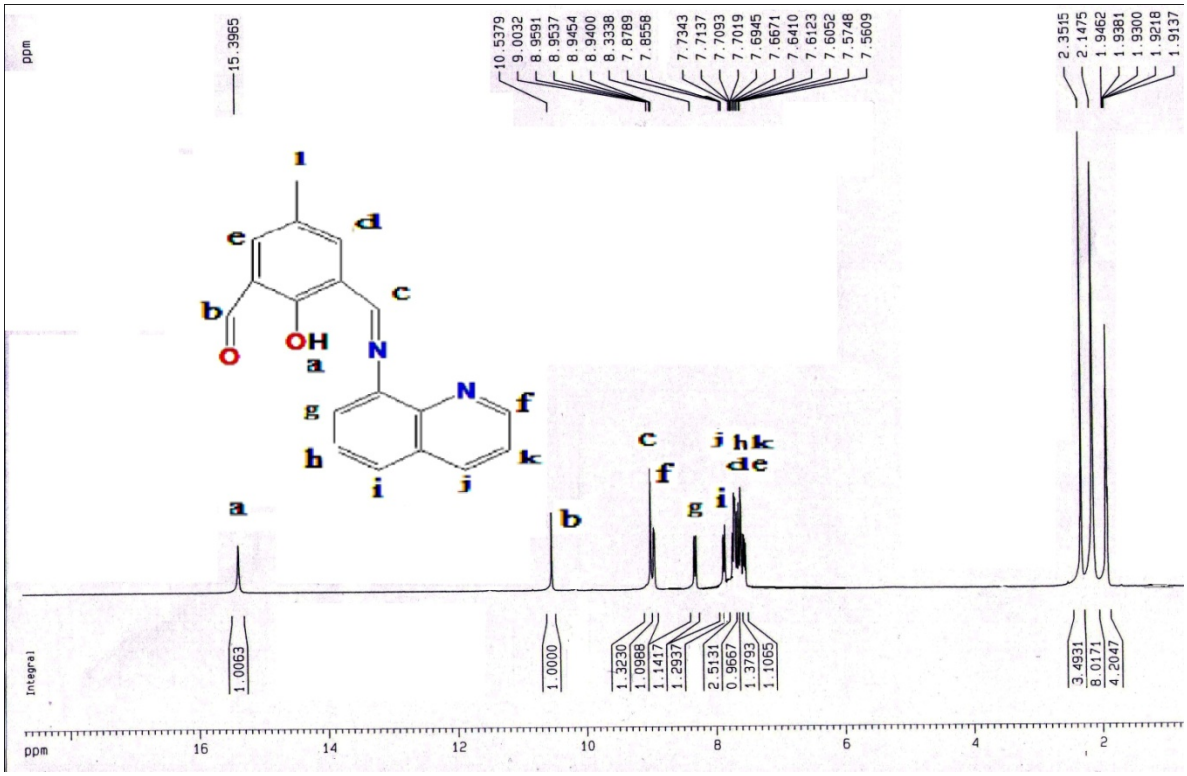
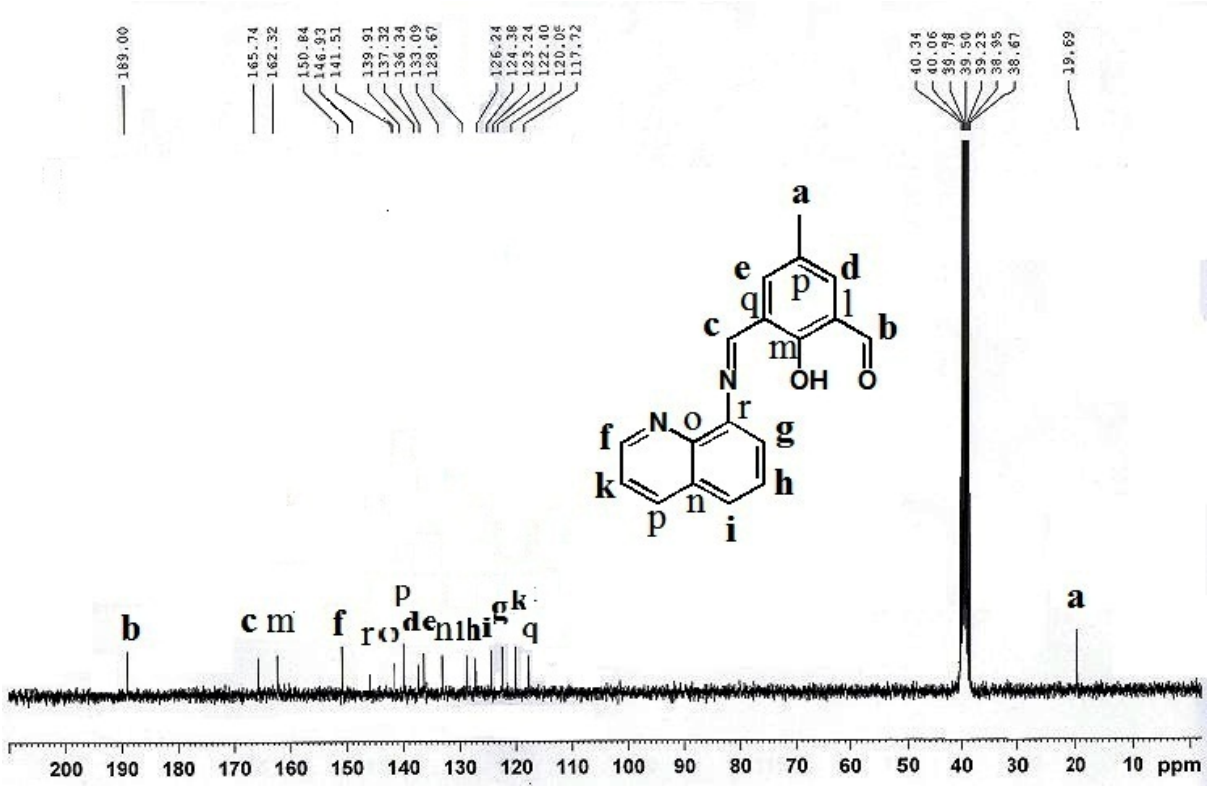


Figure S1. ^{1}H NMR spectrum of **DFC-8-AQ** in CD_3CN, in Bruker 300 MHz instrument.



S1a. ^{13}C NMR of the ligand **DFC-8-AQ** in DMSO-d_6.

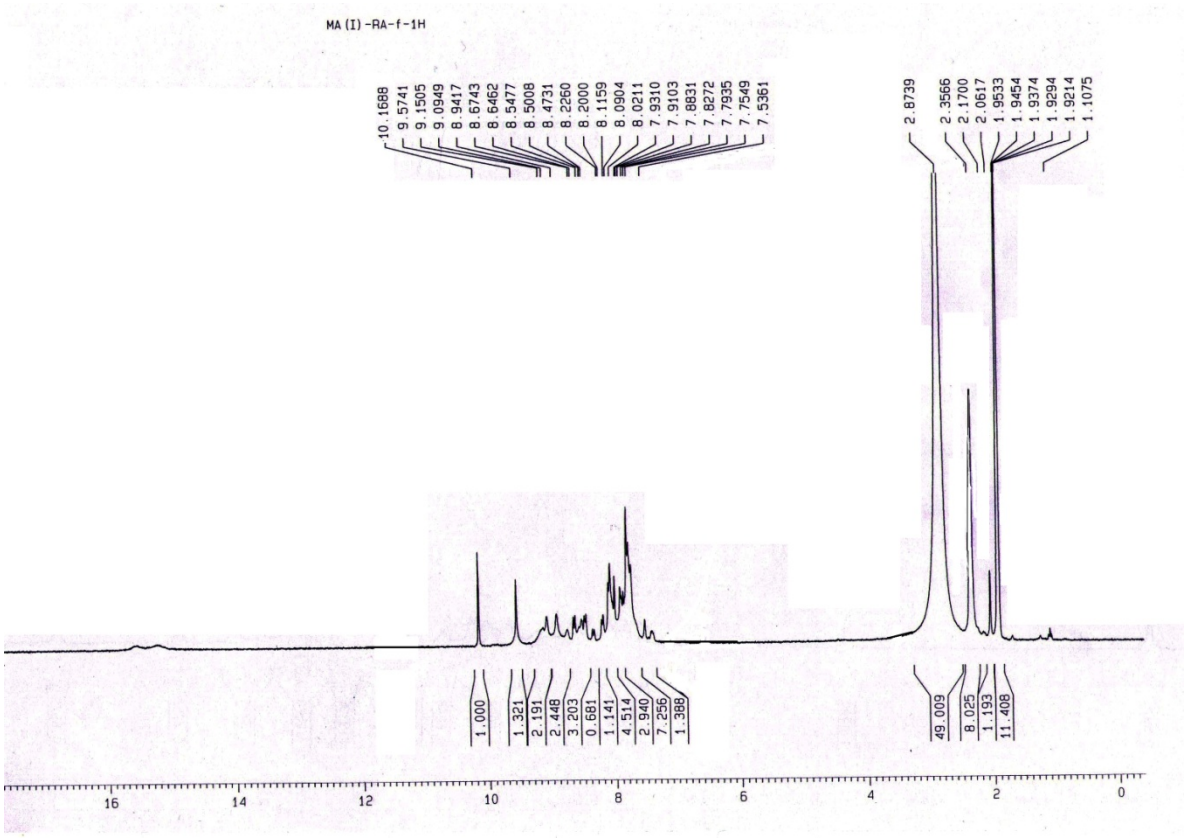


Figure S1b. ^{1}H NMR spectrum of **DFC-8-AQ** +Mg^{2+} in CD_3CN, in Bruker 300 MHz instrument.

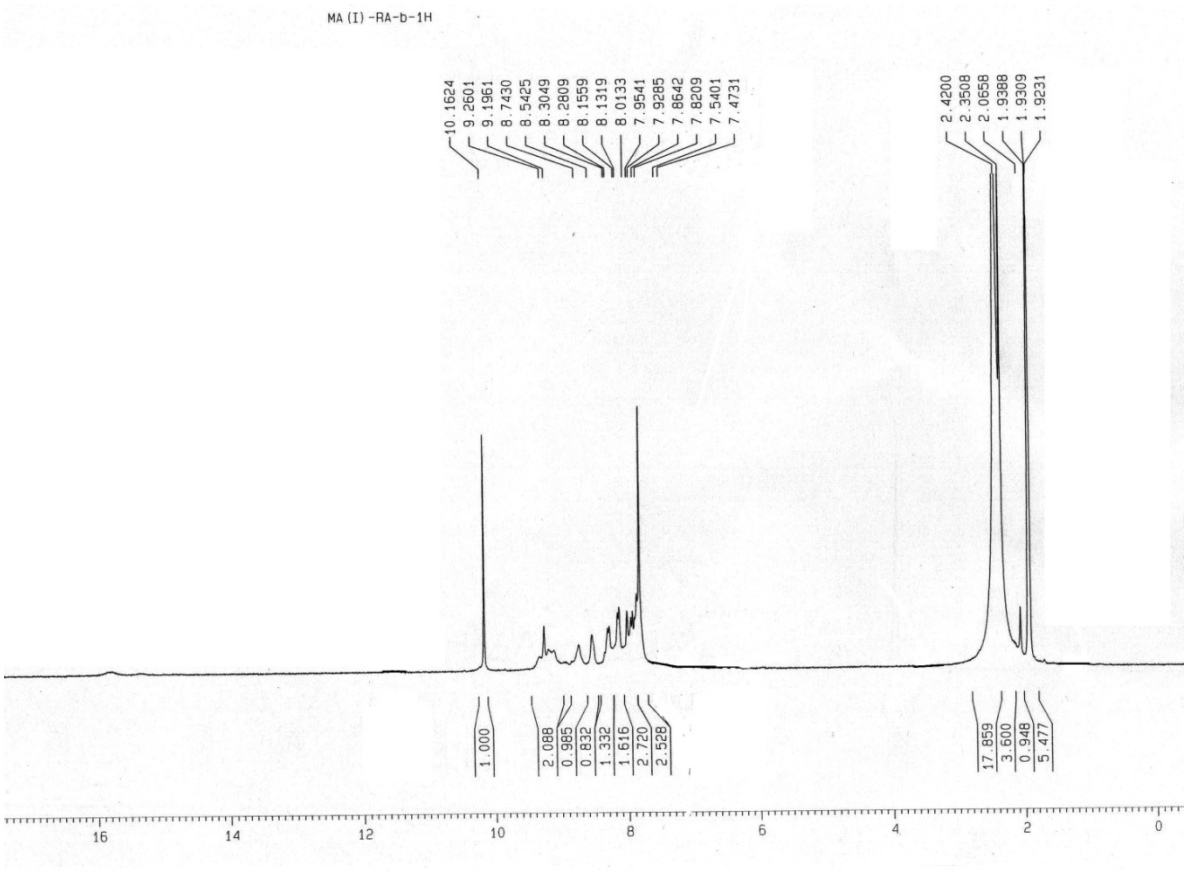


Figure S1c. ^{1}H NMR spectrum of **DFC-8-AQ** $+Zn^{2+}$ in CD_3CN, in Bruker 300 MHz instrument.

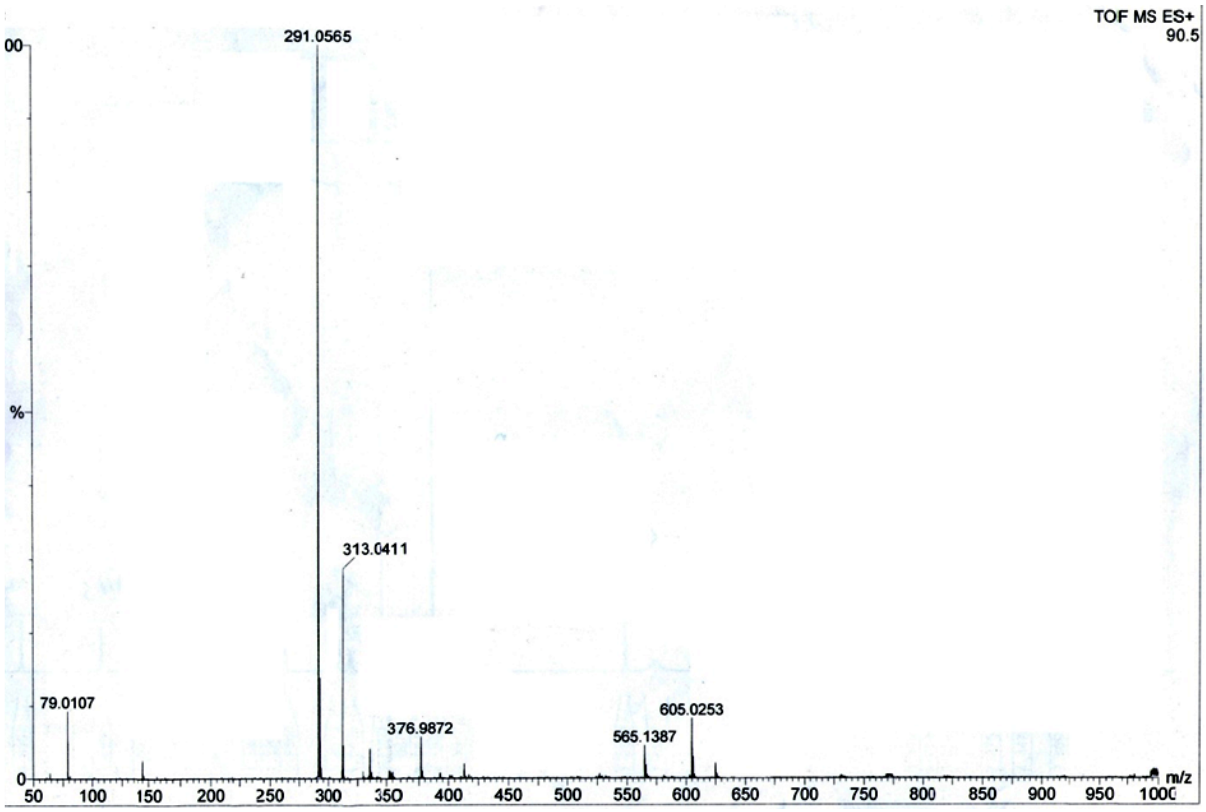


Figure S2. Mass spectrum of **DFC-8-AQ** in MeCN .

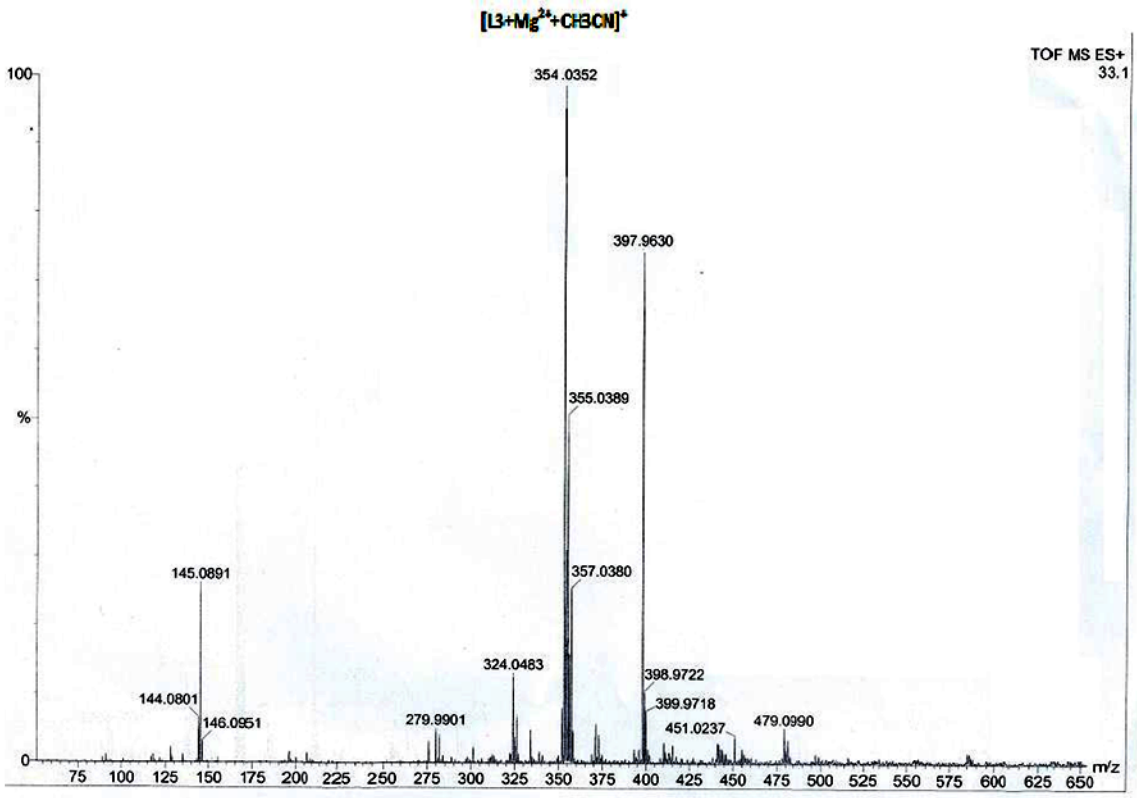


Figure S2a. Mass spectrum of **DFC-8-AQ** +Mg^{2+} in MeCN.

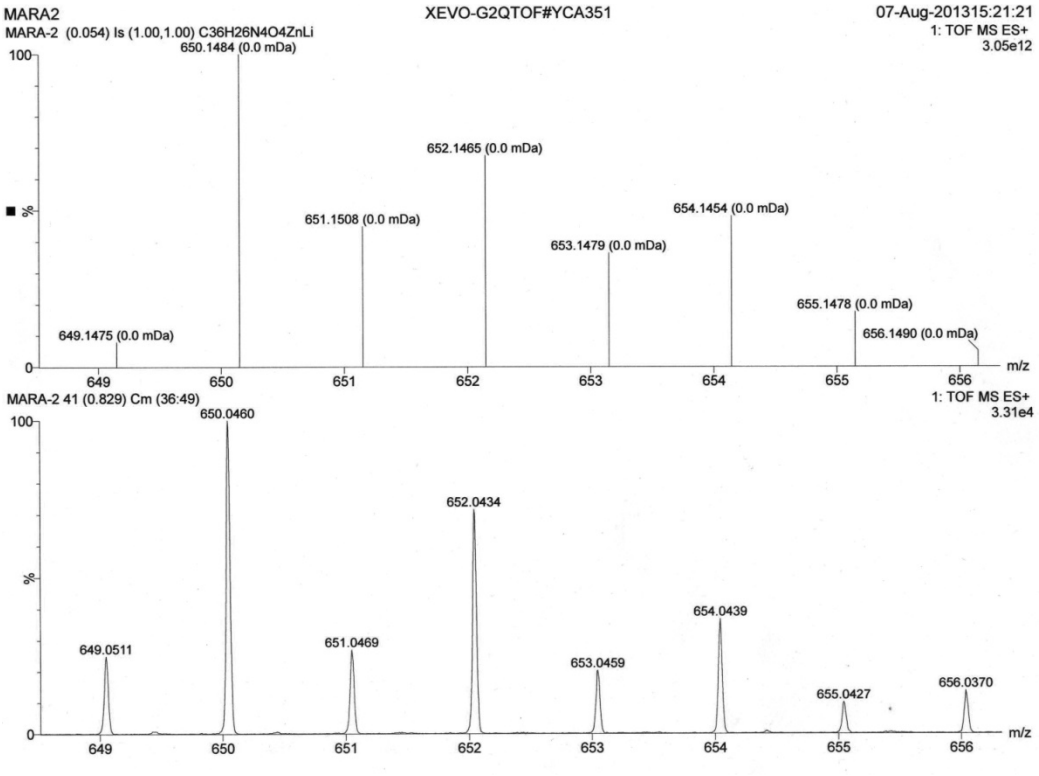


Figure S2b. Mass spectrum of **DFC-8-AQ** +Zn^{2+} in MeCN.

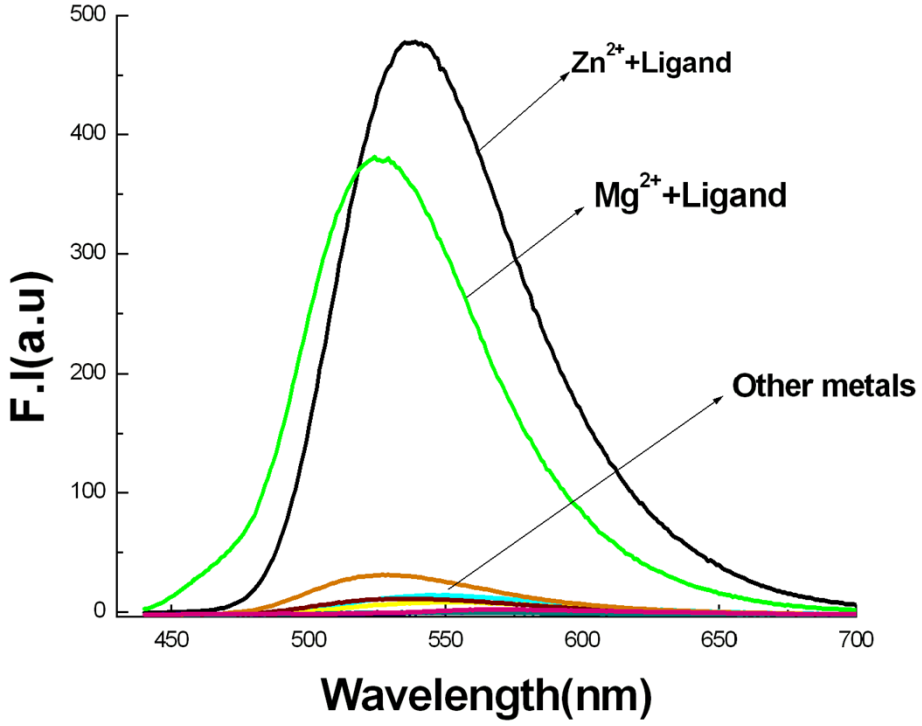


Figure S3. Selectivity of **DFC-8-AQ** towards Mg^{2+} and Zn^{2+} over other biologically relevant metal ions.

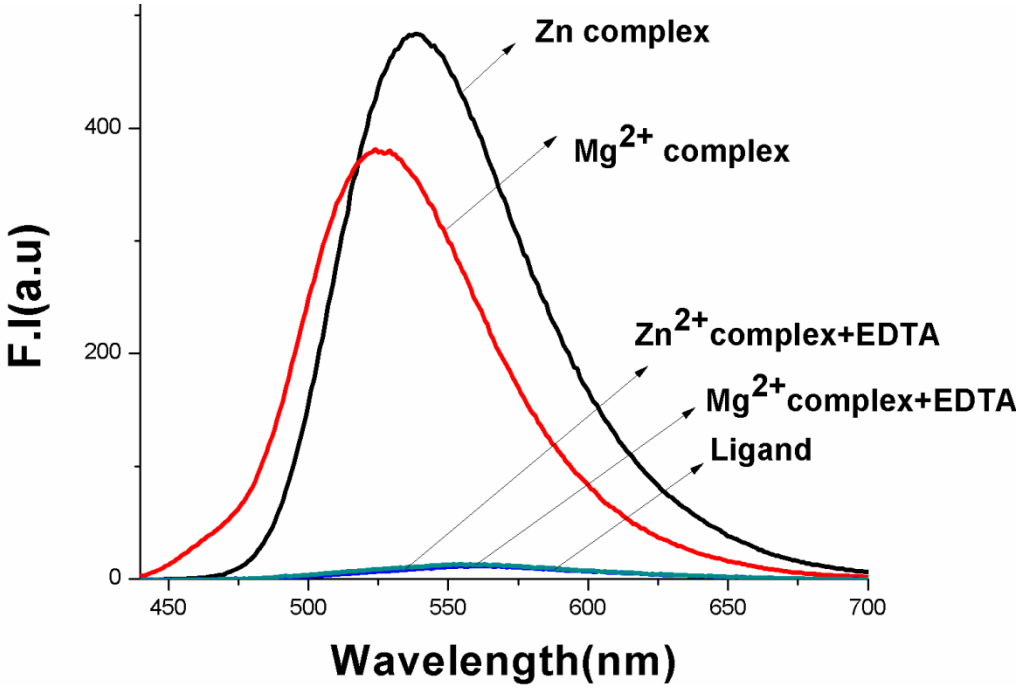


Figure S4. Reversibility plot of Zn complex and Mg complex With excess EDTA.

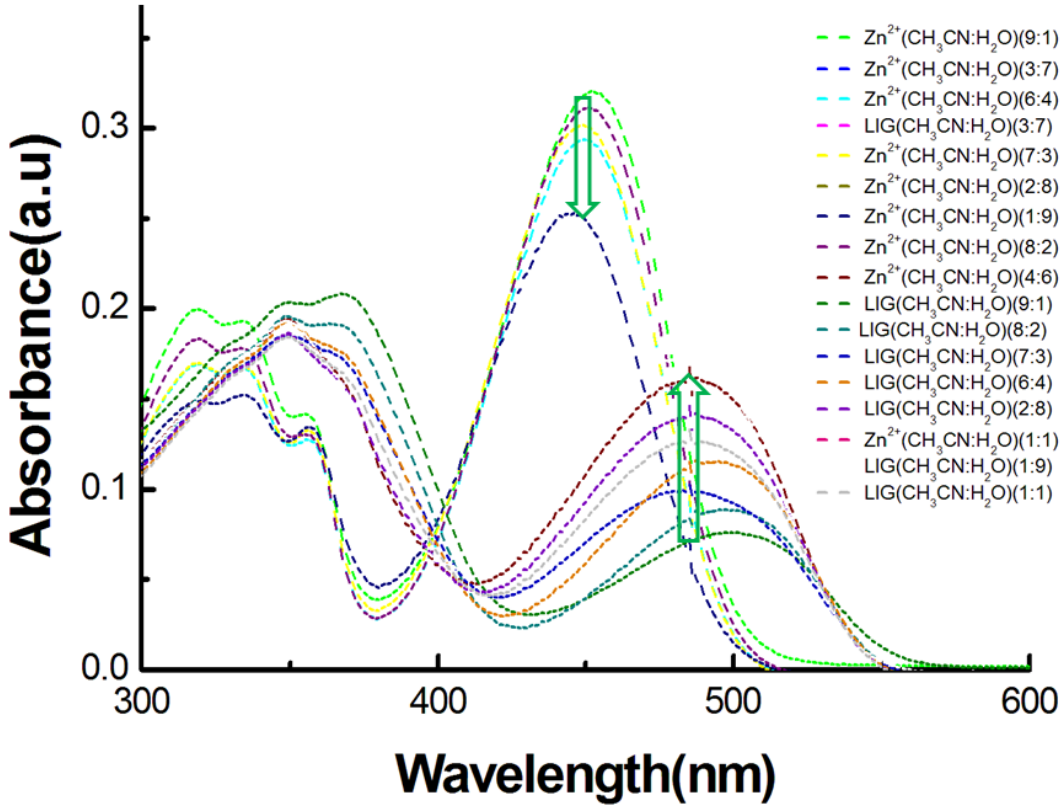


Figure S5(a). UV-vis spectra of the ligand and Zn^{2+} complex in various ratio of CH_3CN-H_20 mixture

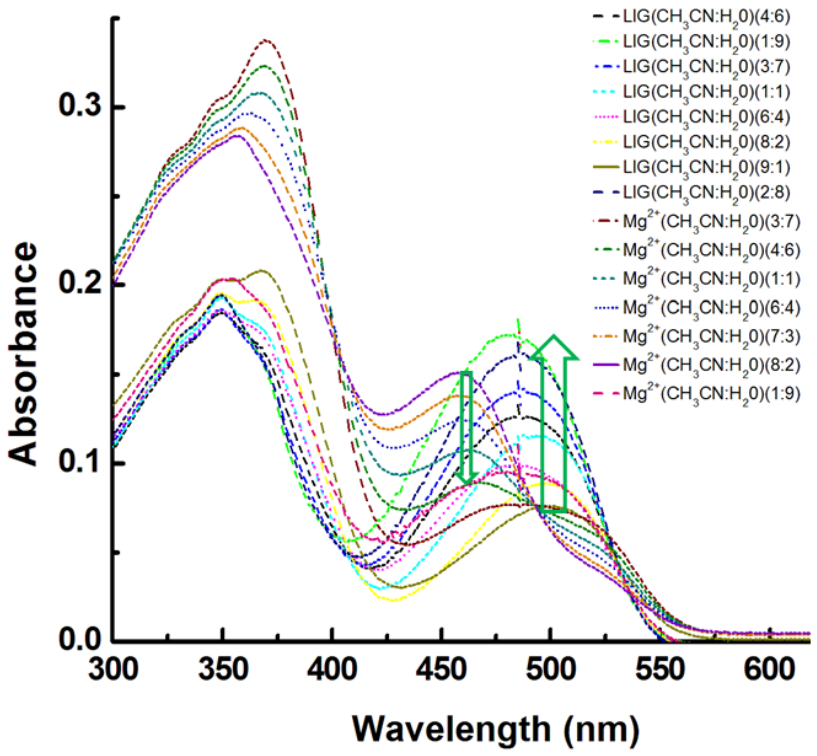


Figure S5(b). UV-vis spectra of the ligand and Mg^{2+} complex in various ratio of CH_3CN-H_20 mixture

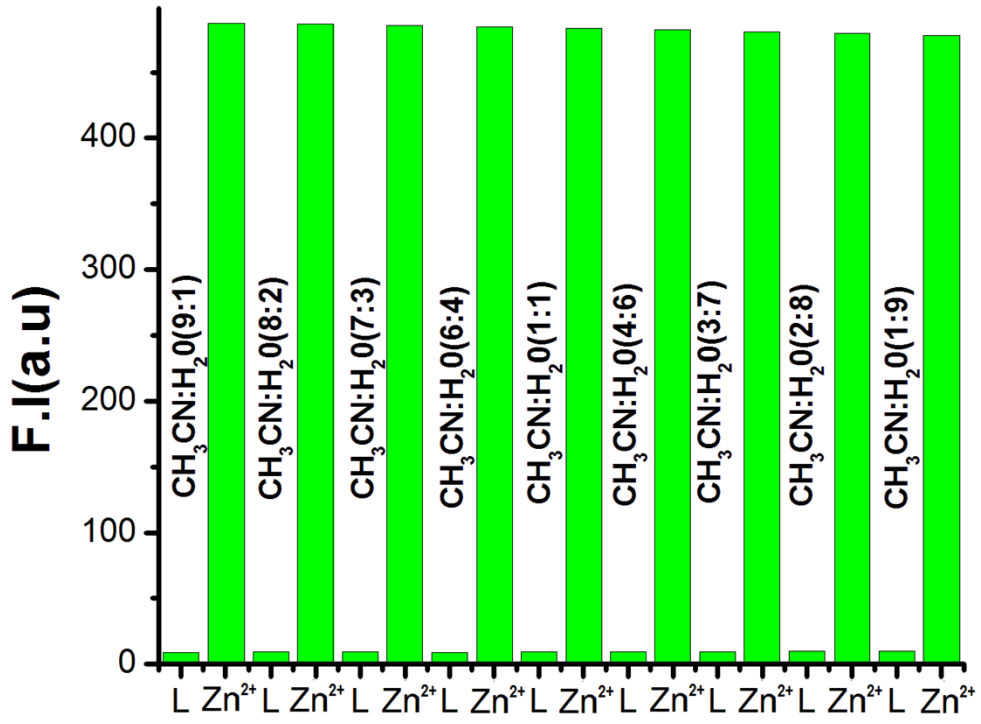


Figure S5(c). Flurescence spectra of the ligand and Zn^{2+} complex in various ratio of CH_3CN-H_20 (HEPES buffer) mixture.

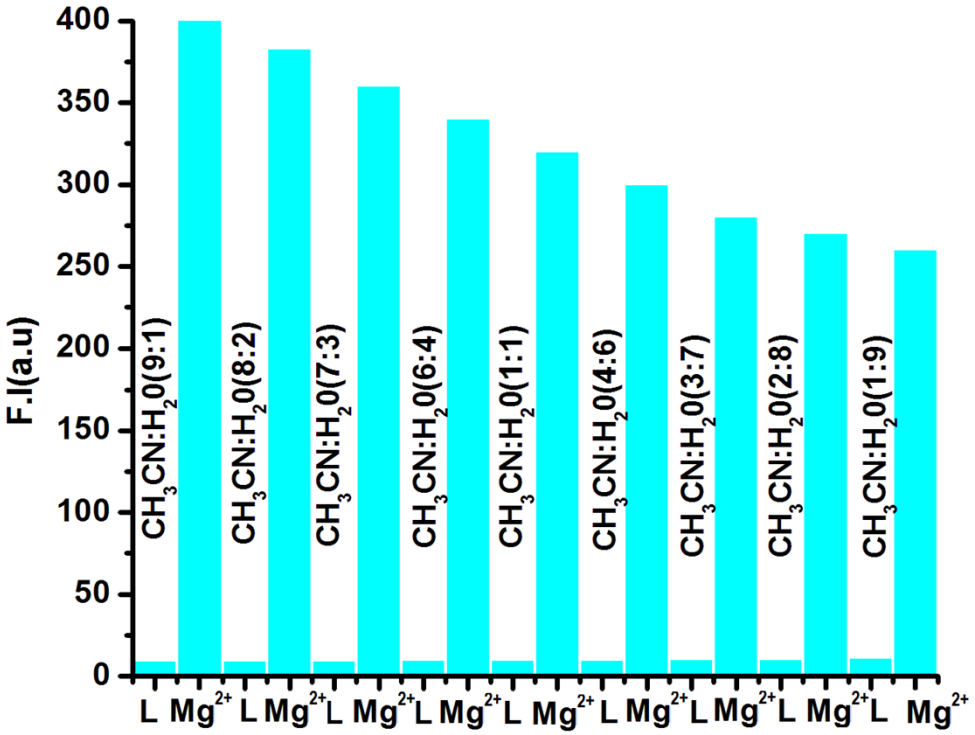


Figure S5(d). Flurescence spectra of the ligand and Mg^{2+} complex in various ratio of CH_3CN-H_20 (HEPES buffer) mixture

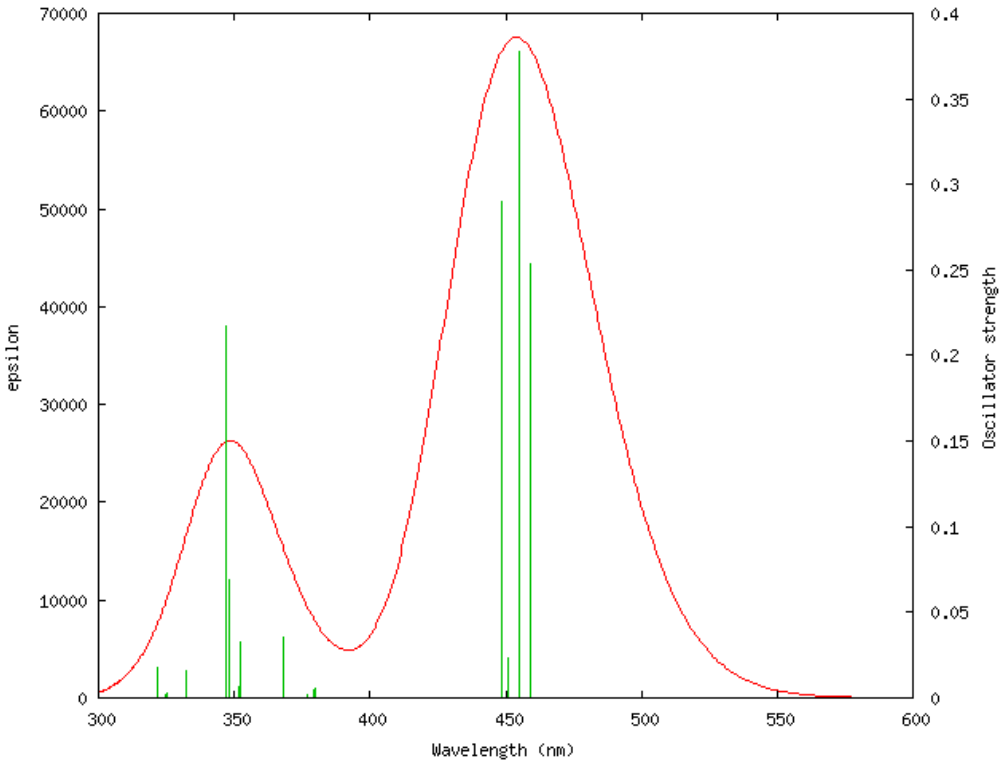


Figure S6. TD-DFT UV-Vis spectrum of [Zn(DFC-8-AQ)$_2$] in MeCN

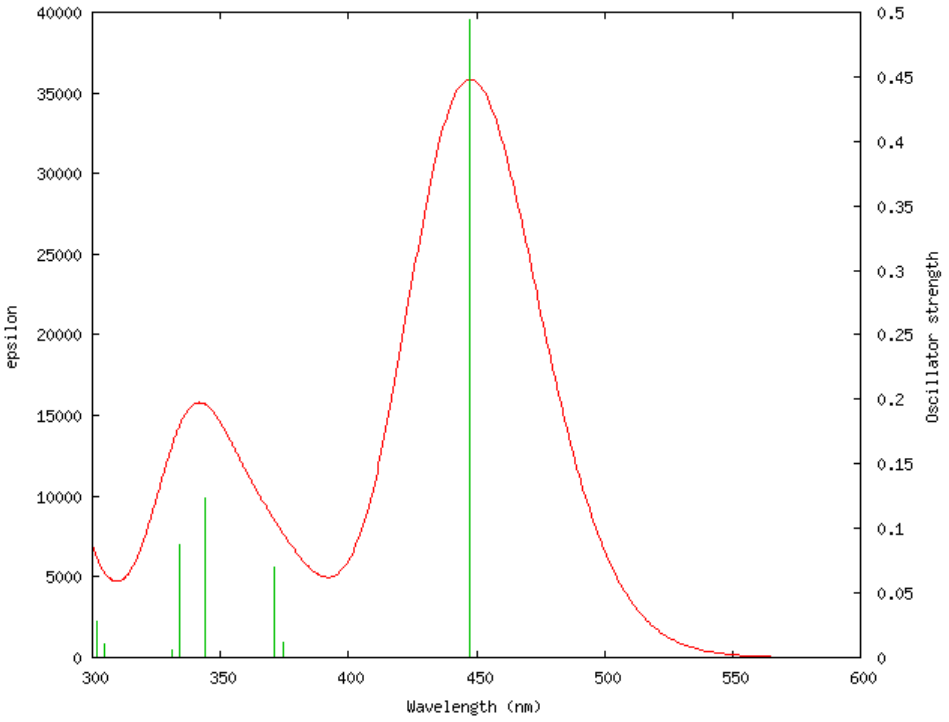


Figure S7. TD-DFT UV-Vis spectrum of [Mg(DFC-8-AQ)(H_2O)$_3$] in MeCN

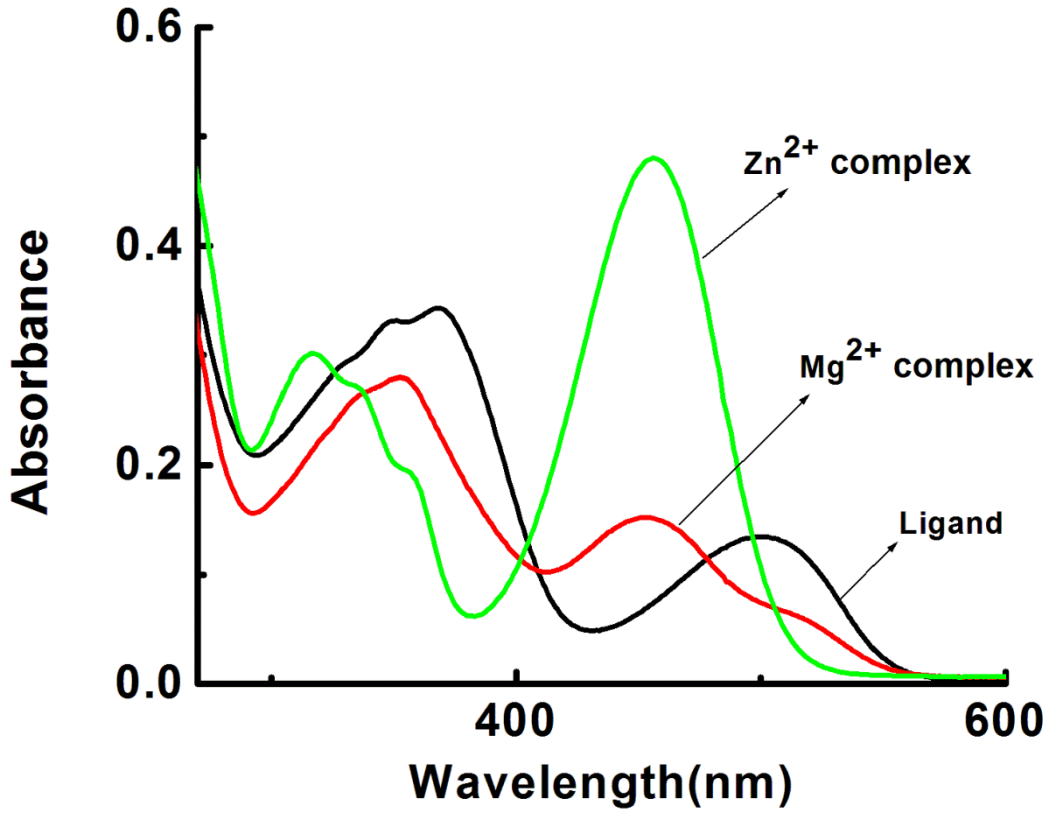


Figure S8. UV-Vis spectra of **DFC-8-AQ** , [Zn(**DFC-8-AQ**)$_2$] and [Mg(**DFC-8-AQ**)(H_2O)$_3$] in MeCN-H_2O 9:1 v/v, 1 mM HEPES buffer, pH 7.2.

Table S1. ^{1}H-NMR chemical shifts in ppm of selected H-atoms in CD_3CN.

Compound	CH=O(b)	CH=N(c)	f	g	OH
DFC-8-AQ	10.53	9.003	8.95	8.33	15.39(b)
DFC-8-AQ -Zn^{2+} (1)	10.16	9.26	9.15	8.94	•••••••••
DFC-8-AQ -Mg^{2+} (2)	10.17	9.57	9.19	8.74	•••••••••

19. Calculation of the detection limit(LOD):

The detection limit DL of **DFC-8-AQ** for M^{2+} (M = Mg and Zn) was determined from 3σ method by following equation: **$DL = K^* Sb_1/S$**

Where K = 2 or 3 (we take 3 in this case); Sb_1 is the standard deviation of the blank solution; S is the slope of the calibration curve obtained from Linear dynamic plot of FI vs. [**M^{2+}**].

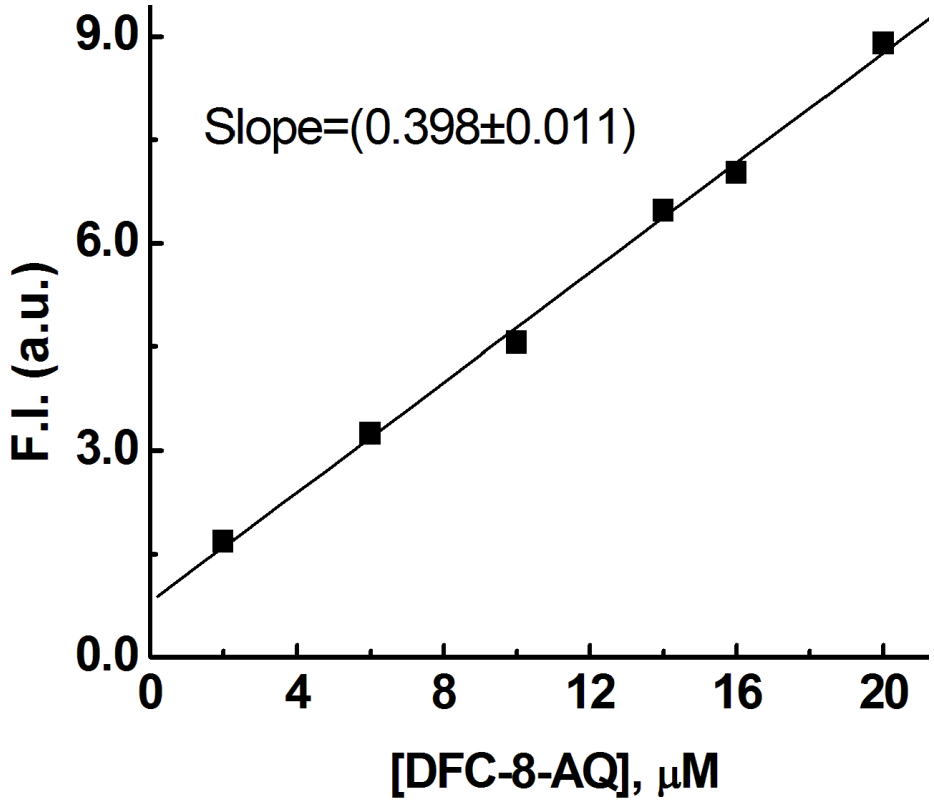


Figure S9a. Determination of Sb_1 or the blank, DFC-8-AQ solution.

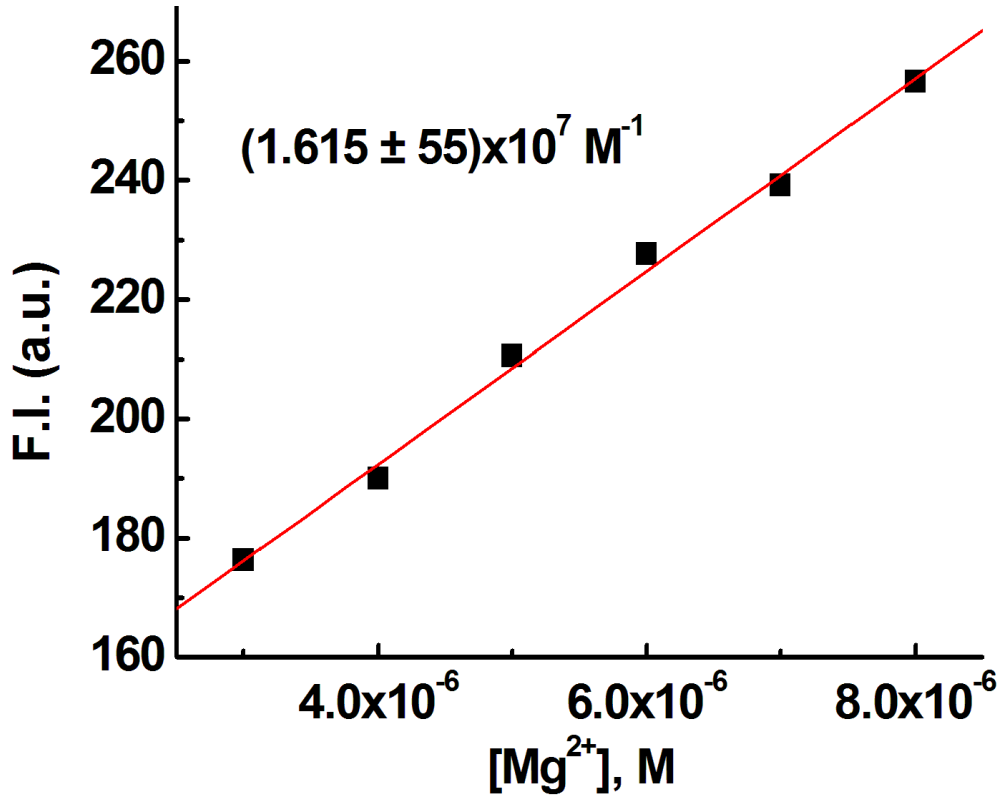


Figure S9b. Linear dynamic plot of FI at 526 nm vs. [Mg^{2+}] for the determination of S (slope); [DFC-8-AQ] =20 µM

LOD (Mg^{2+}) = (3 x 0.011)/1.615 x 10^7 = 2.04 nM

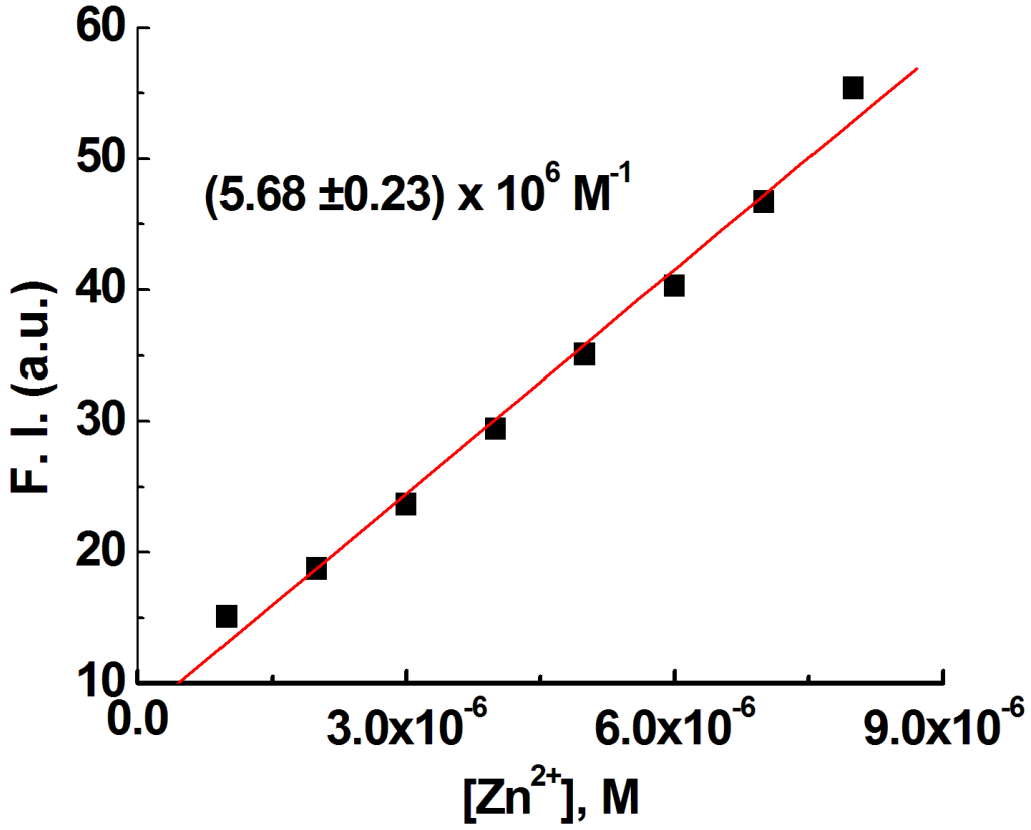


Figure S9c. Linear dynamic plot of FI at 539 nm vs. [Zn^{2+}] for the determination of S (slope); [DFC-8-AQ] =20 µM

LOD (Zn^{2+}) = (3 x 0.011)/5.68x 10^6 = 5.81 nM