

Dual mode chemosensor for fluorescence detection of zinc and hypochlorite on fluorescein backbone and cell imaging application

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1. General procedure for drawing Job plot by Fluorescence method:

Stock solution of same concentration of **FAD** and Zn^{2+} were prepared in the order of $\approx 1.0 \times 10^{-5}$ M in acetonitrile/aqueous HEPES buffered solution (1:1, pH 7.2) solution. The emission in each case with different *host-guest* ratio but equal in volume was recorded. Job plots were drawn by plotting $\Delta I \cdot X_{\text{host}}$ vs X_{host} (ΔI = change of intensity of the fluorescence spectrum at 426 nm during titration and X_{host} is the mole fraction of the host in each case, respectively).

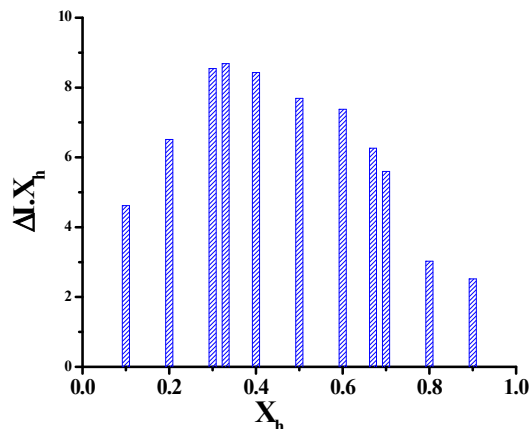


Figure S₁: Jobs plot diagram of **FAD** for Zn^{2+} (where X_h is the mole fraction of host and ΔI indicates the change of the emission intensity).

2. Binding constant

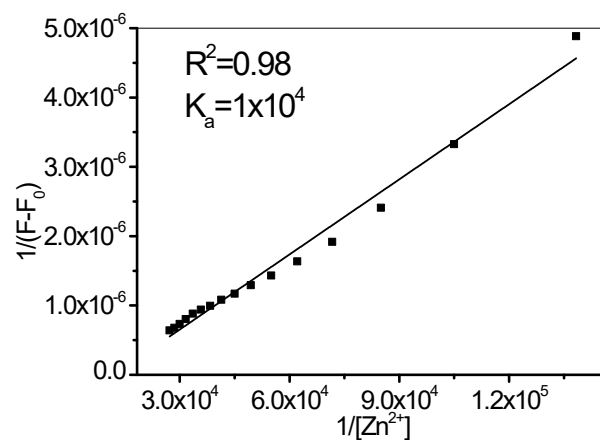


Figure S₂: Changes of Fluorescence Intensity of **FAD** ($c=1 \times 10^{-5}$ M) as a function of $[\text{Zn}^{2+}]$ ($c = 2 \times 10^{-4}$ M) at 426 nm.

3. Calculation of the detection limit:

For Zn²⁺

The detection limit (DL) of **FAD** in emission spectra for Zn²⁺ was determined from the following equation:

$$DL = K * Sb1/S$$

Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve.

From the graph Figure we get slope = 51476, and Sb1 value is 30638.11

Thus using the formula we get the Detection Limit for Zn²⁺ = 1.79 μM in Fluorescence spectra.

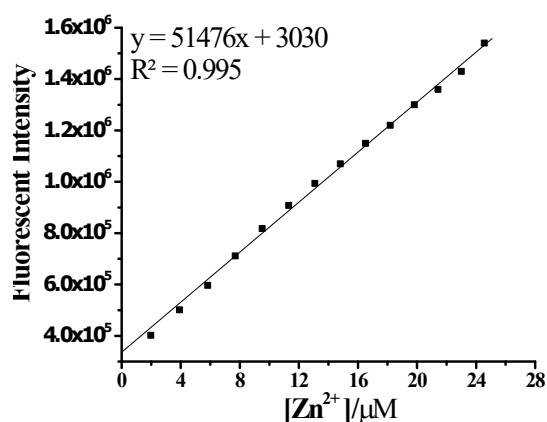


Figure S₃: Changes of Fluorescence Intensity of **FAD** ($c = 1 \times 10^{-5} \text{M}$) as a function of $[\text{Zn}^{2+}]$ ($c = 2 \times 10^{-4} \text{M}$) at 426 nm.

For hypochlorite,

The detection limit (DL) of **FAD** in fluorescence spectra for OCl^- was determined from the following equation:

$$DL = K * Sb1/S$$

Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve.

Thus, using the formula, we get the Detection Limit for $\text{OCl}^- = 2.24 \mu\text{M}$ in Fluorescence spectra.

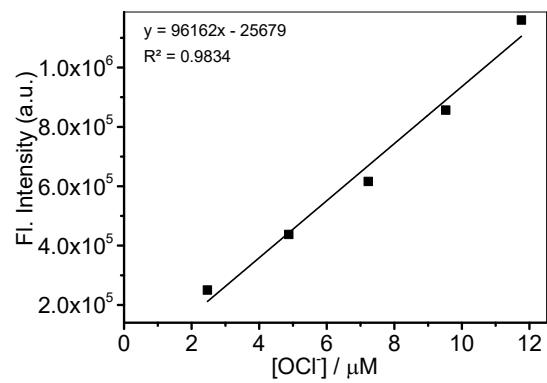
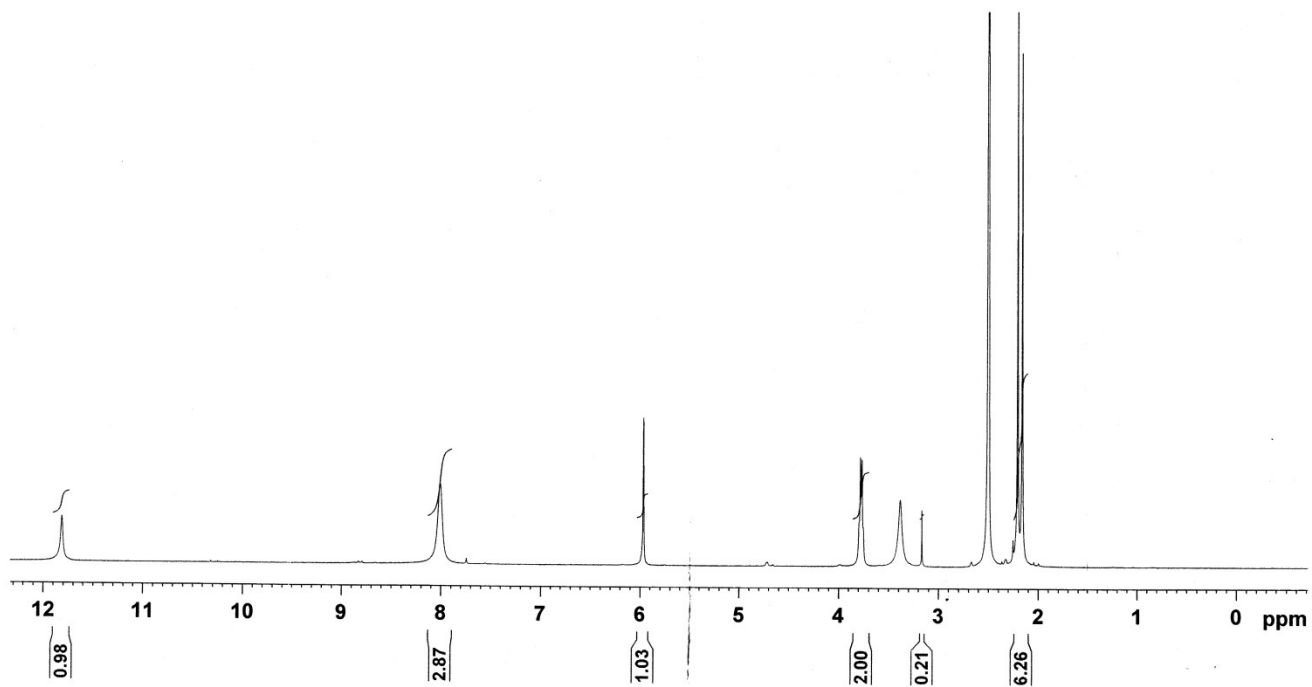
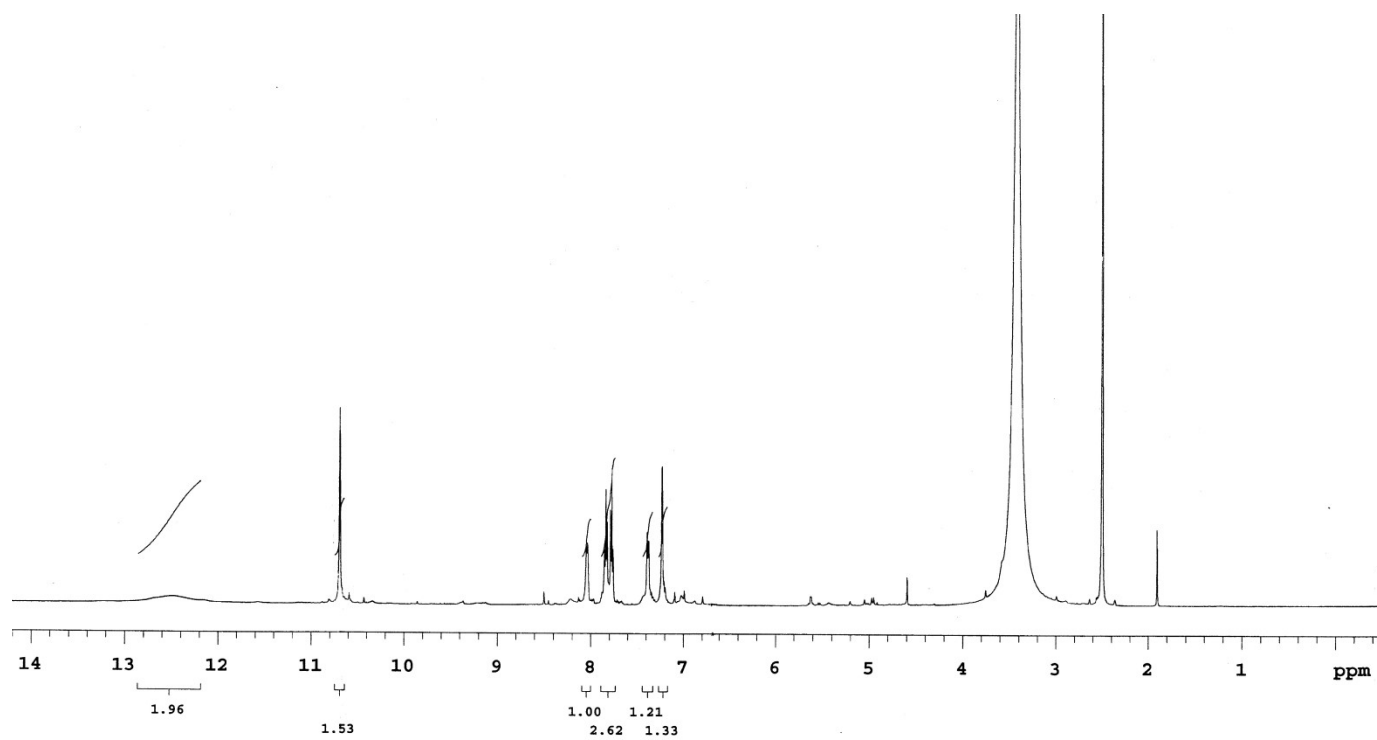


Figure S₄: Changes of Fluorescence Intensity of **FAD** ($c = 1 \times 10^{-5} \text{M}$) as a function of $[\text{OCI}^-]$ ($c = 2 \times 10^{-4} \text{M}$) at 520 nm.

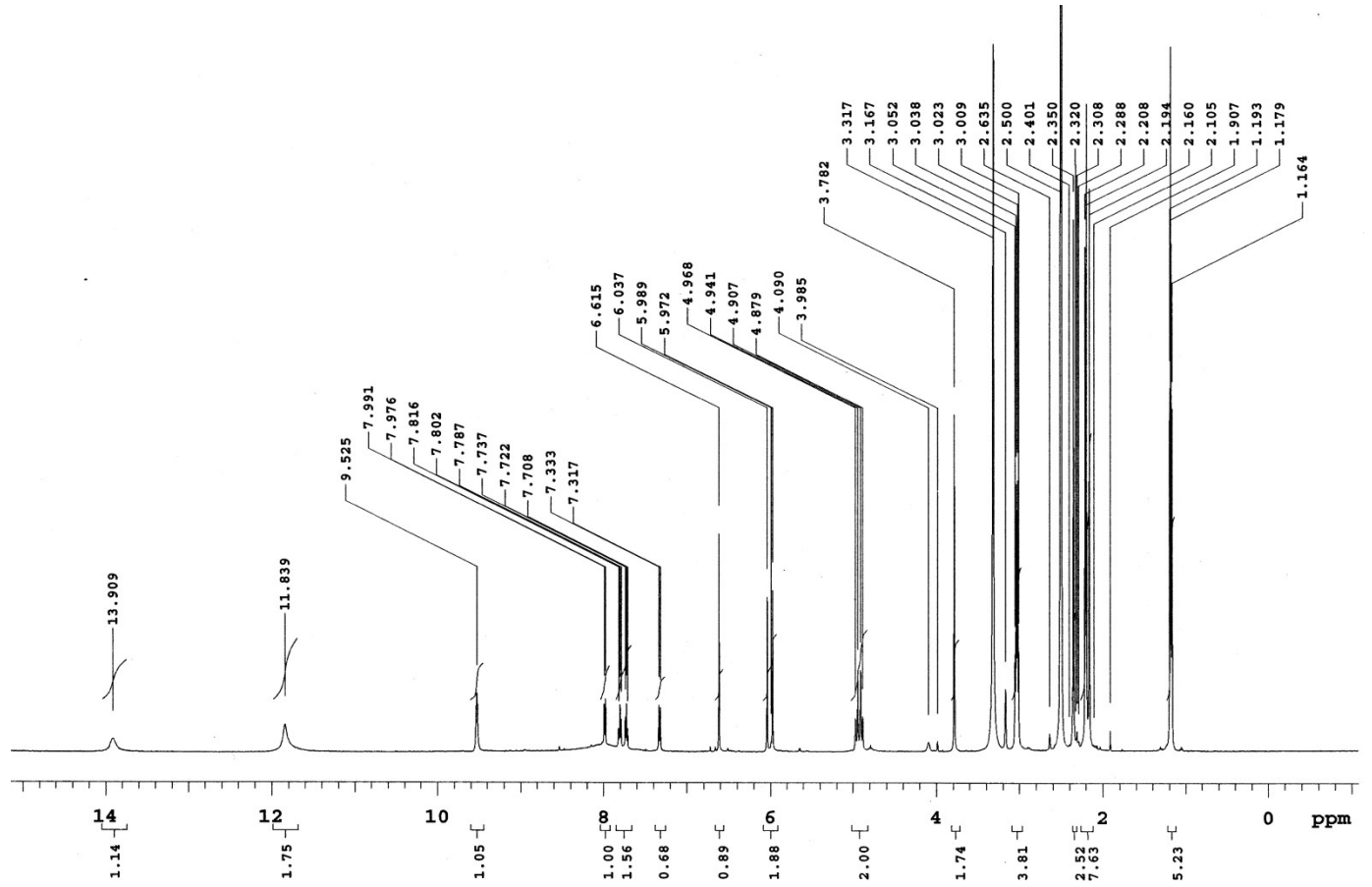
4. ^1H NMR spectrum of Compound 1 in $\text{d}_6\text{-DMSO}$ (500 MHz):



5. ^1H NMR spectrum of Compound 2 in $\text{d}_6\text{-DMSO}$ (500 MHz):



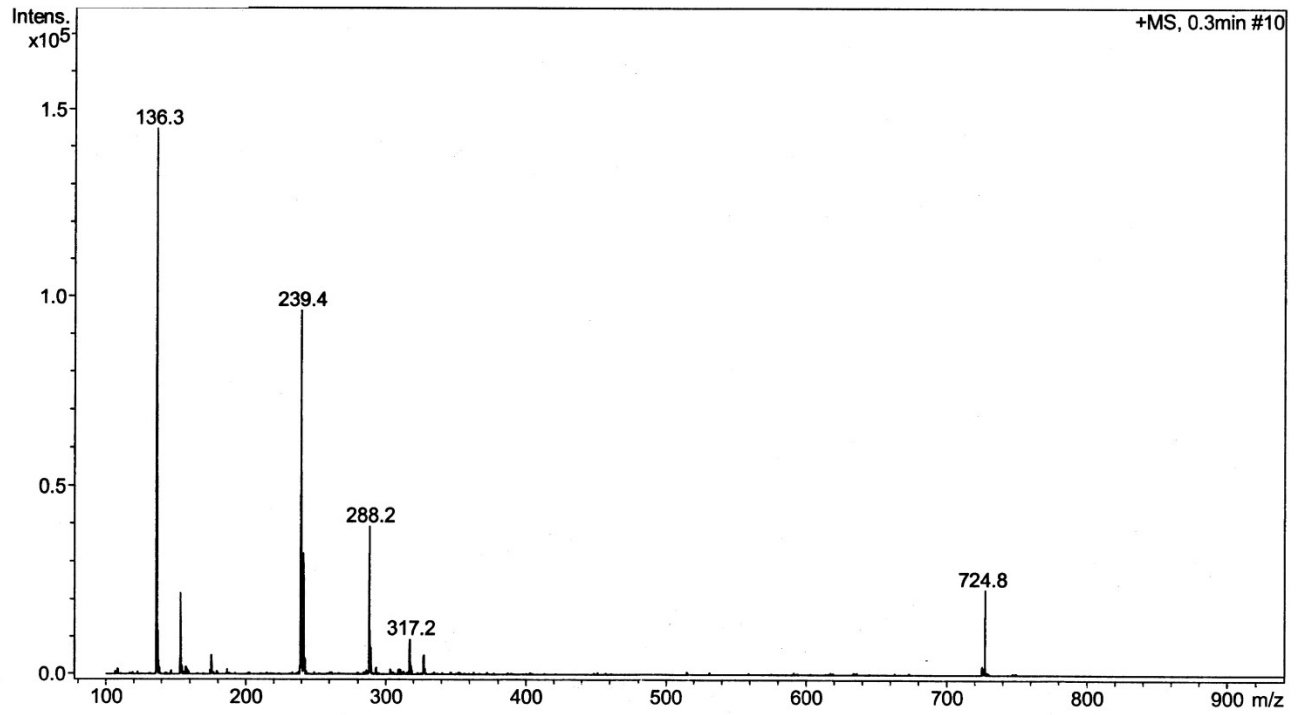
6. ¹H NMR spectrum of FAD in d₆-DMSO (500 MHz):



7. Mass spectrum of FAD

Instrument: Agilent 6310 Ion Trap

Operator: Suhi



Analysed By