Electronic Supplementary Information

An Efficient, Schiff-base Derivative for Selective Fluorescent Sensing of Zn^{2+} Ions: Quantum Chemical Calculation Appended by Real Sample Application and Cell imaging Study

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1.

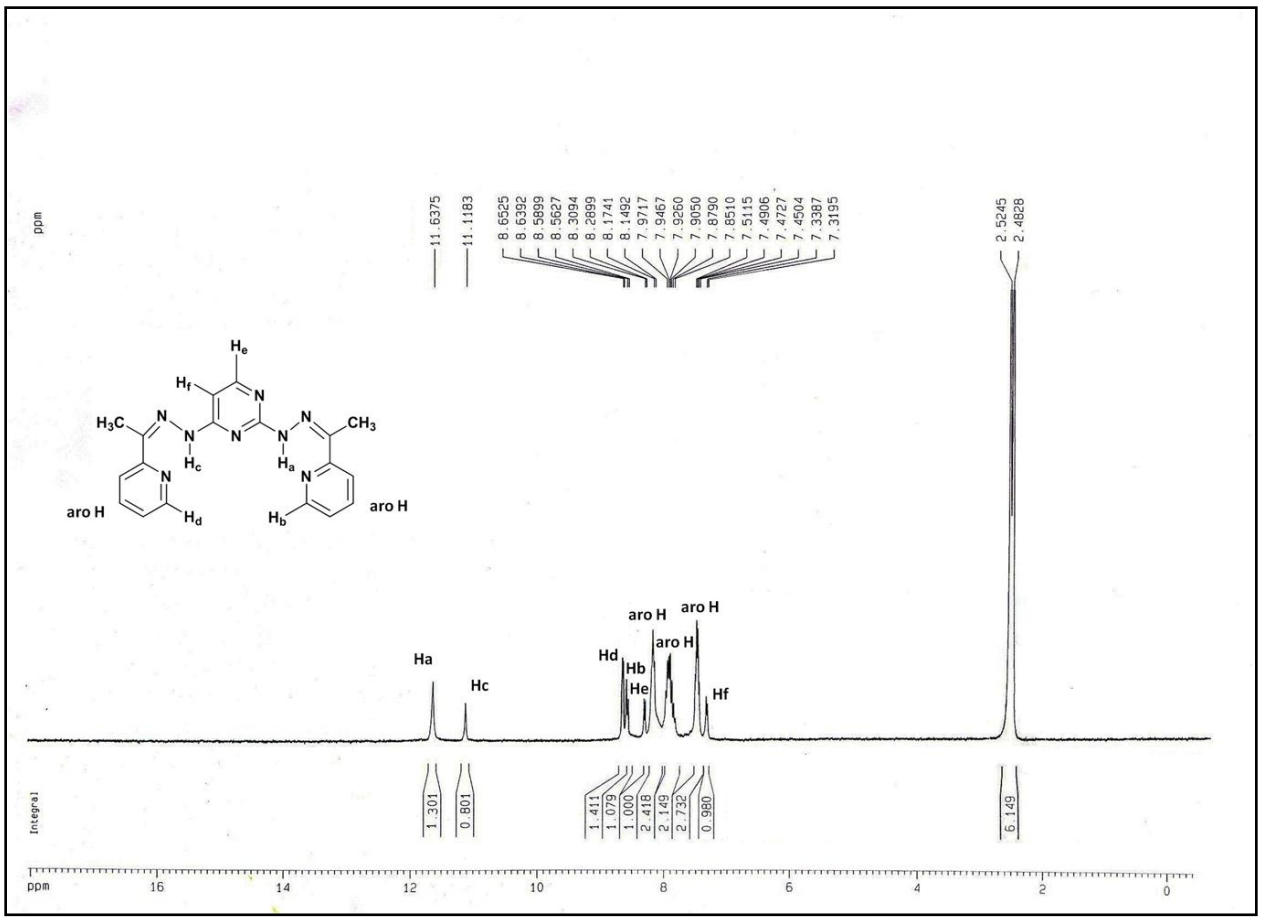

Figure S1a. ^{1}H NMR spectra of ligand PyHP.

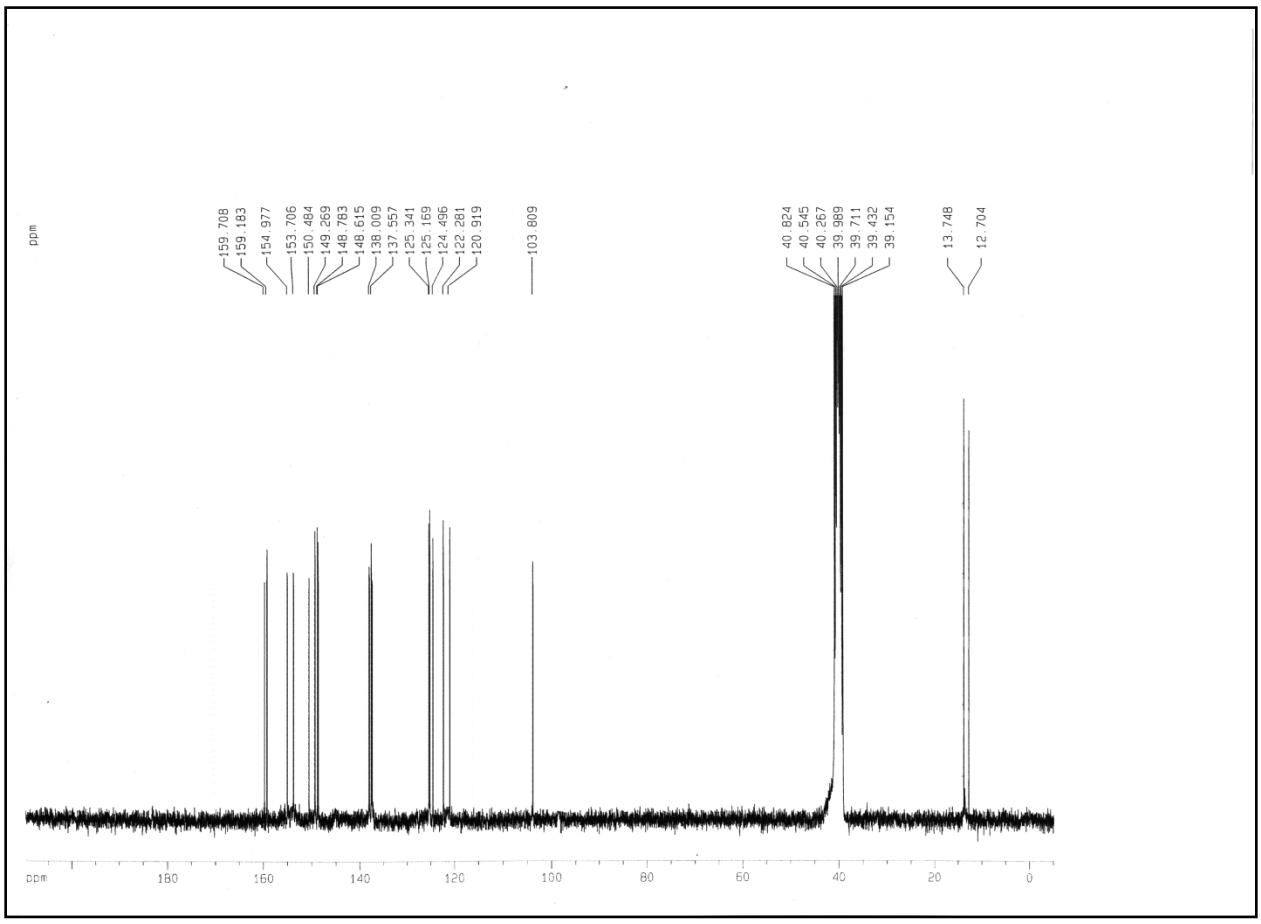

Figure S1b: ^{13}C NMR spectra of ligand PyHP.

2.

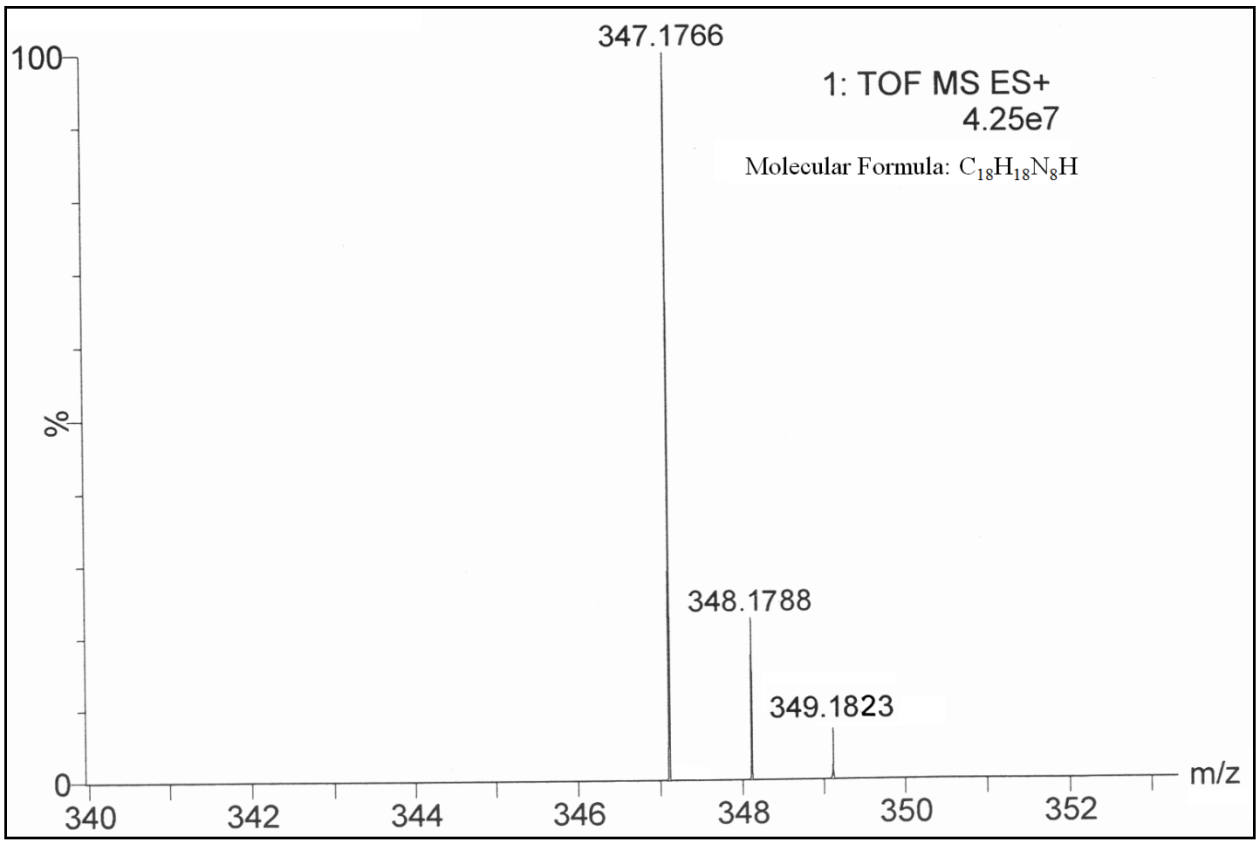

Figure S2: HRMS spectra of PyHP ligand.

3.

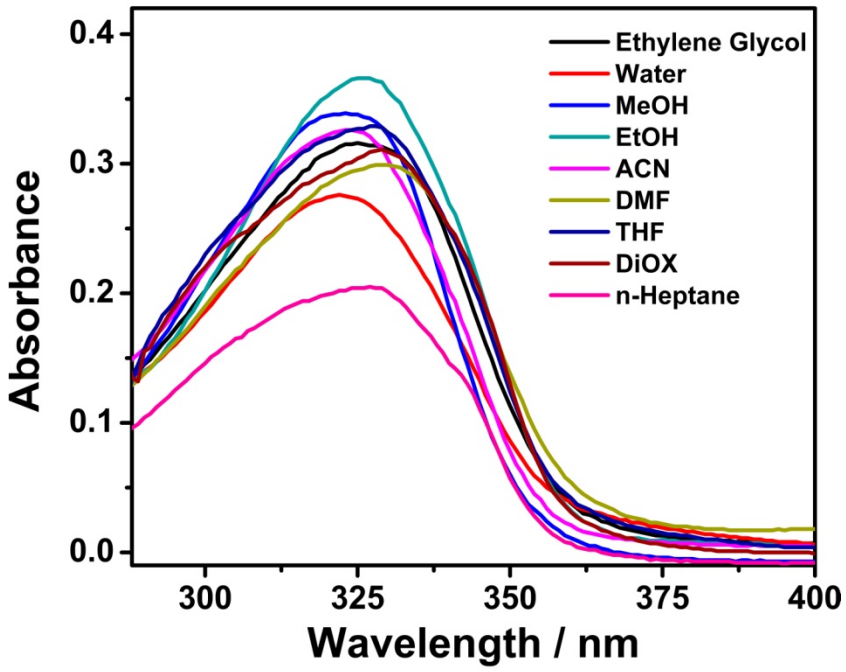

Figure S3: Absorption spectra of PyHP in different solvents.

4.

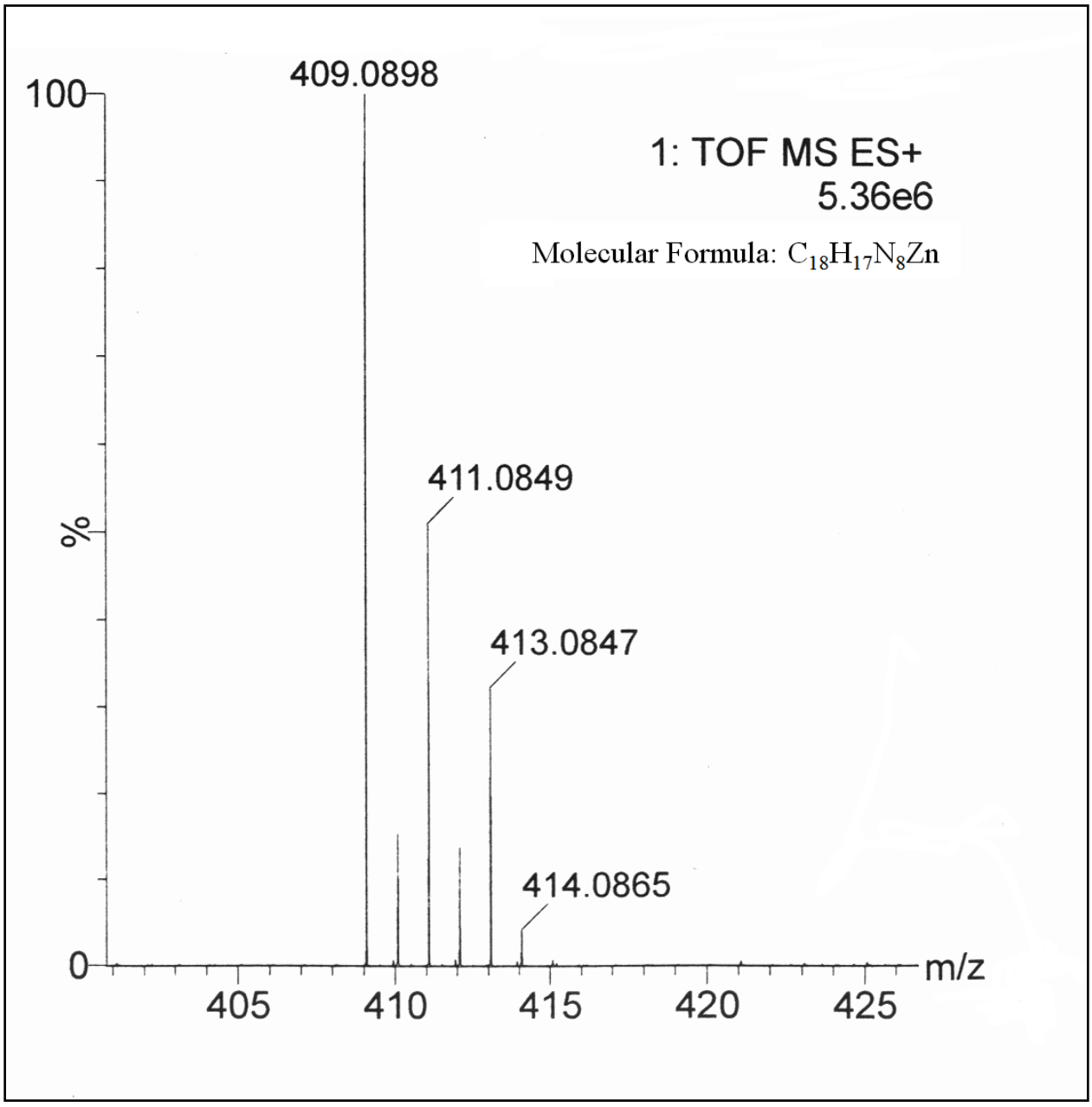

Figure S4: HRMS spectra of PyHP-Zn^{2+} complex.

5.

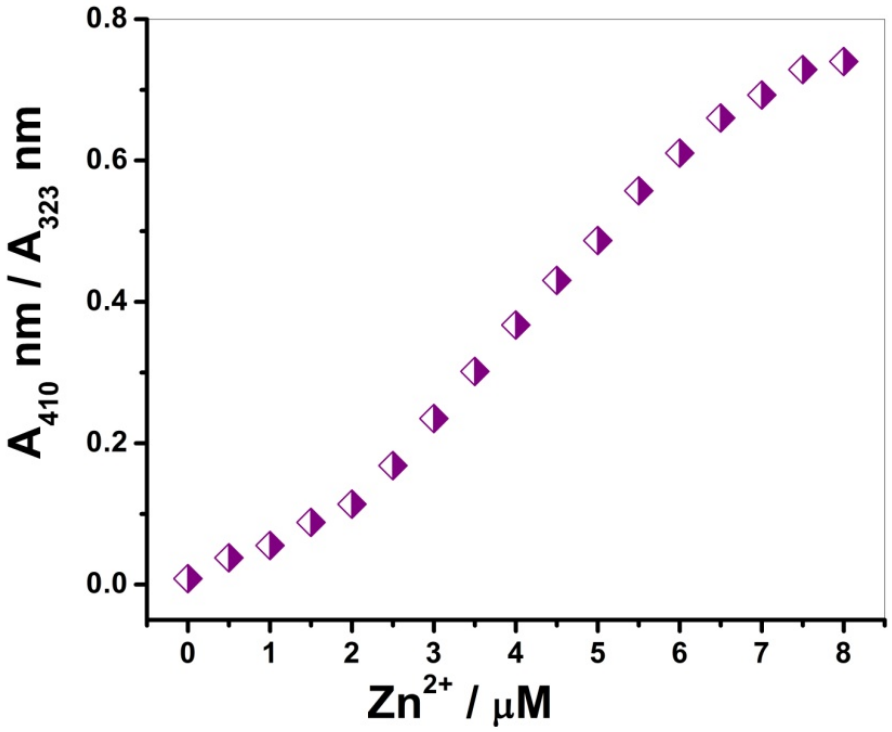

Figure S5: Plot of A_{410} / A_{323} vs. $[Zn^{2+}]$ (μM)

6.

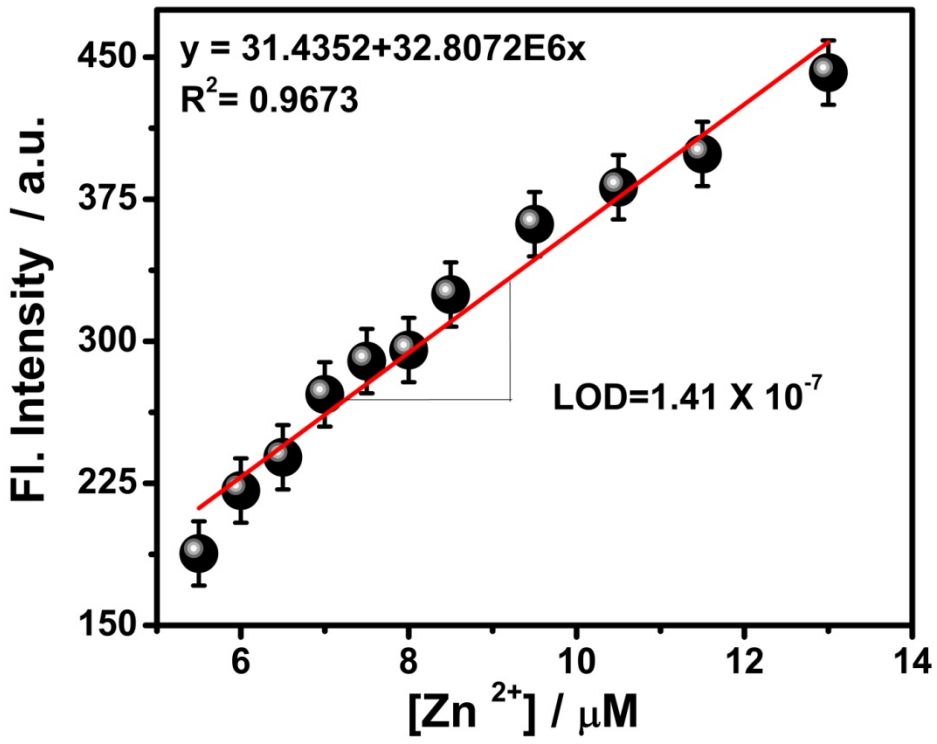

Figure S6: Fluorescence intensity at 489 nm of PyHP as a function of concentration of Zn^{2+}.

7.

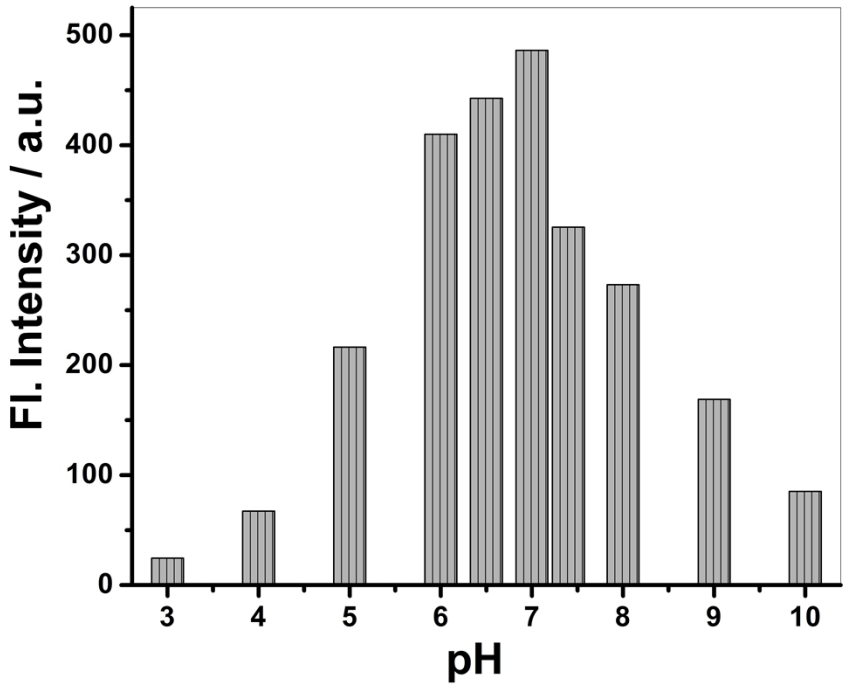

Figure S7: Bar diagram of Fluorescence Intensity vs. pH (of MeOH-HEPES buffer solvent mixture) indicate that sensing selectivity of Zn^{2+} bound PyHP state is maximum at pH=7.0.

8.

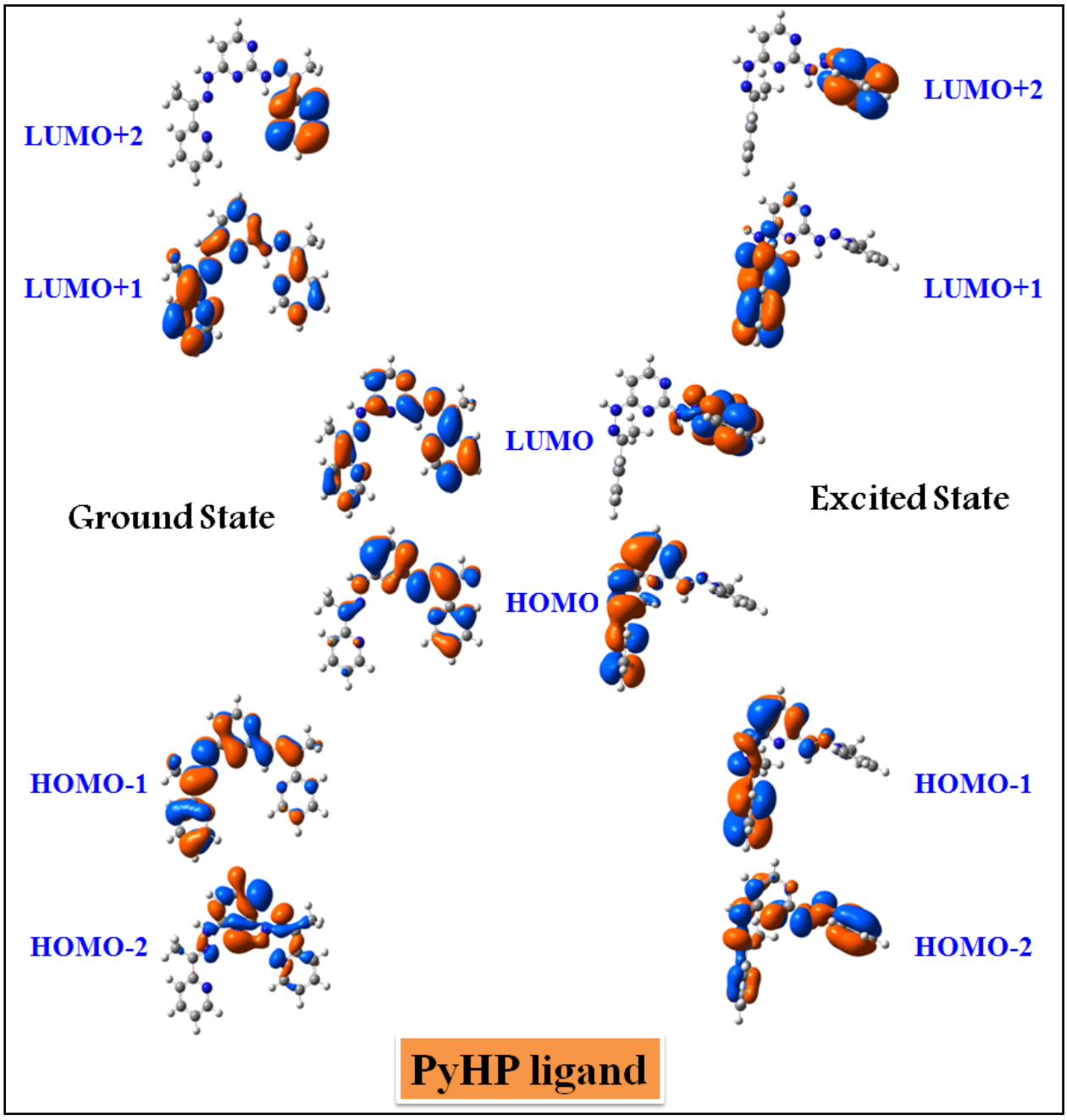

Figure S8: Frontier Molecular Orbital (FMO) diagram of PyHP ligand in ground (DFT/6-31G(d,p)) and excited state (CIS/6-31G(d,p).

9.

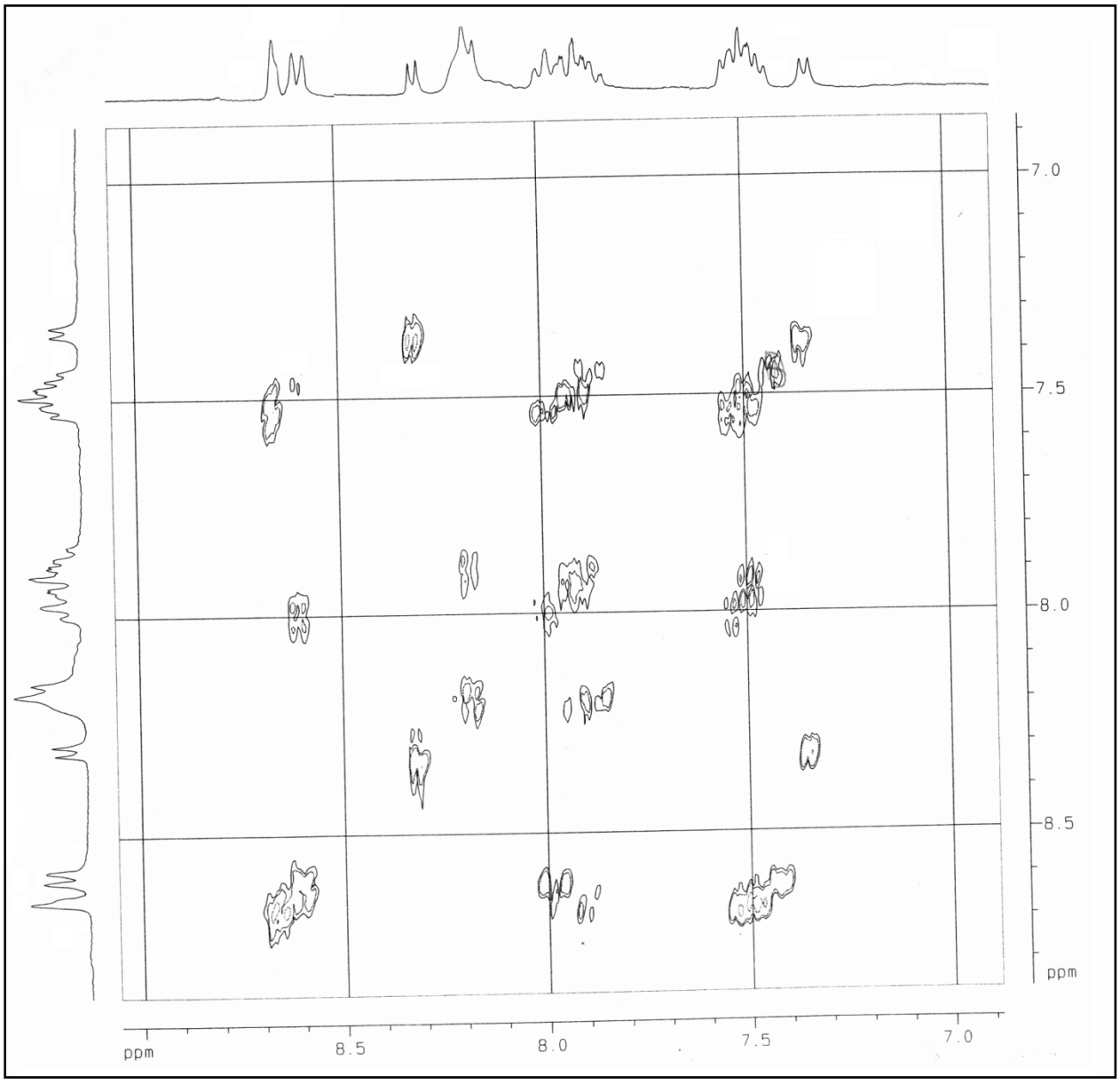

Figure S9: COSY NMR spectra of PyHP.

10.

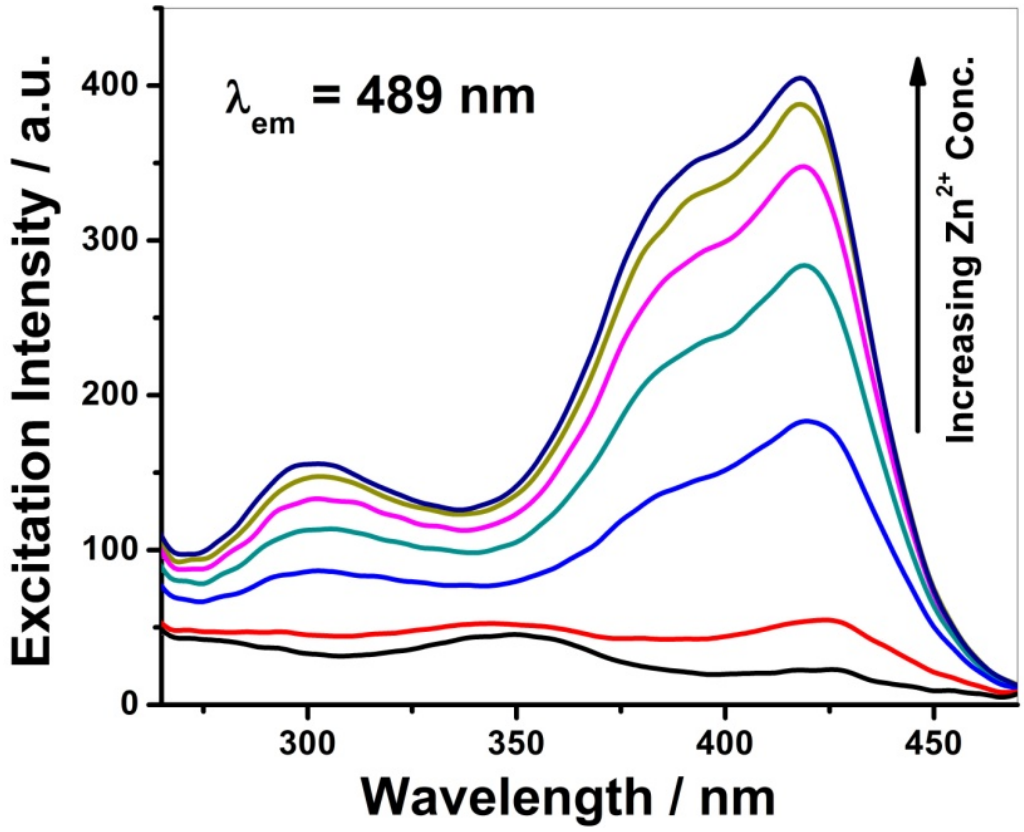

Figure S10: Excitation spectra of PyHP after addition of Zn^{2+} (0-15μM)

Note S1. Zinc Estimation from real samples:

The graph related with emission intensity and Zn concentration (Figure S6) plays the key role in this calculation. Final emission intensity was noted after the complete addition of real sample aliquot in PyHP solution. Final intensity corresponding to Zn concentration was found out from Figure S6 as other parameters (probe conc. slit etc) are same. Now in reverse procedure we can quantitatively estimate the amount of zinc in simple volumetric calculation.