Supporting Information

Crystal structure, spectroscopic, DNA binding studies and DFT calculations of a Zn(II) complex containing pyridoxal appended Schiff base and its application in Bioimaging of Zn(II)

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Figure S1: Mass spectrum of Complex 1.

Figure S2: $^1$H NMR spectrum of Complex 1.
Figure S3: $^{13}$C NMR spectrum of Complex 1.

Table S2: Analysis of Hydrogen Bonds
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<td>O2-H2A---N3&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.82</td>
<td>2.01</td>
<td>2.787(7)</td>
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<td>0.82(5)</td>
<td>1.90(5)</td>
<td>2.719(5)</td>
<td>176(6)</td>
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<td>C8-H8---O3</td>
<td>0.93</td>
<td>2.54</td>
<td>3.151(5)</td>
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Symmetry operations: a= 1/2+x,1/2-y,-1/2+z; b= 3/2-x,1/2+y,3/2-z; c= 1-x,-y,1-z

Figure S4: IR Spectra of ligand and the complex 1.
**Figure S5:** Job’s plot of complex formation between ligand (host) and the Zn(II). X_h is the ligand mole fraction.

**Figure S6:** Emission spectra of complex 1 in 9:1 methanol:water buffer (pH 7.4, λ_ex 390 nm).
Figure S7: Red bars: Fluorescence Changes of HL (1 × 10⁻⁵ M) in the presence of 1 equiv of Zn(II) solution. Green bars: Enhanced emission upon the addition of different cations (3 equiv). All samples are prepared in 10 mMTris-HCl buffer at pH 7.4 and excited at 385 nm.

Calculation of Binding constant and detection limit for Ligand with Zn(II)complex:

The binding constant value of Zn(II) with ligand has been determined from the emission intensity data following the modified Benesi–Hildebrand equation, 1/ΔI = 1/ΔI_{max} + (1/K[C])(1/ΔI_{max}). Here ΔI = I−I_{min} and ΔI_{max} = I_{max}−I_{min}, where I_{min}, I, and I_{max} are the emission intensities of ligand considered in the absence of Zn(II), at an intermediate Zn(II) concentration, and at a concentration of complete saturation where K is the binding constant and [C] is the Zn(II) concentration respectively. From the plot of [1 / (I_{min}−I)] against [C]⁻¹ for ligand, the value of K has been determined from the slope. As the plot of 1/ (I−I_{min}) vs 1/[C] gives a straight line, indicates the 1:1 complexation of the sensor with Zn(II). The association constant (K_a) as determined by fluorescence titration method for the ligand with Zn(II) is found to be 1.8 × 10⁵ M⁻¹.

Calculation of the detection limit:

The detection limit DL of Ligand for Zn(II) was determined from the following equation:
DL = K* Sb1/S Where K = 2 or 3 (we take 2 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve.

For Ligand with Zn(II):

From the Intensity vs. Zn(II) graph, we get slope = 4.25327E11, and Sb1 value is 62770.41679.

Thus using the formula, we get the Detection Limit = \(2.95 \times 10^{-7}\) M

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<td>B</td>
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**Figure S8:** Association constant and Detection limit calculation Ligand with Zn\(^{2+}\).
**Figure S9:** Fluorescence Microscopic photographs of (a) *Candida albicans* cells treated with ligand, (b) *Candida albicans* cells treated with Zn(II) + followed by the ligand.

**Table S2:** DFT results of Complex 1.

Complex 1 (optimized in Gas phase)

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<th>LUMO+1</th>
<th>LUMO+2</th>
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<td>0.41</td>
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<td>2.03</td>
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<td>0.44</td>
<td>0.52</td>
<td>60.67</td>
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<td>1Zn 10O</td>
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<td>1Zn 12O</td>
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<td>1Zn 15N</td>
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Complex I (optimized in MeOH):

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<th>Atom name and number</th>
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<th>Mayer bond order</th>
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Table S3: TD-DFT calculations of Ligand and Complex 1.

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Optimized Geometries

Complex in gas:

Zn    4.42419100  3.36639100  6.39485700
C     4.48753000  3.35745700  3.42044500
H     3.40876400  3.17836600  3.32268000
H     4.95690900  3.08734600  2.46395900
C     6.52257600  0.84470000  5.34617500
N     5.00286700  2.57390300  4.53261200
C     6.54501500  1.24457000  6.72039500
O     6.05588100  -1.05062300  2.94947300
H     5.57547600  -1.64983500  3.54315900
O     5.91667700  2.27401700  7.20691000
N     8.02209600  -0.61780100  7.23738500
O     4.81057100  4.43667600  8.31636700
H     5.42511600  3.72971500  8.59806800
C     7.27914600  -0.30623900  4.96198000
N     2.59929200  3.09996200  7.20511400
C     4.76271300  4.83887700  3.72831500
H     5.84766700  4.98338500  3.75483600
H     4.35718200  5.48325100  2.93315800
C     7.34795600  0.45063800  7.62247300
C     7.33651400  -0.80835100  3.53479500
H     7.81022000  -0.07246500  2.87367000
H     7.96218900  -1.71216100  3.50205100
C     5.83187000  1.60105200  4.32410700
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Complex in MeOH:

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