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Synthesis, characterization, and biological potential of new Zn(II) complexes with naphto[1,2-d]oxazol-type ligands

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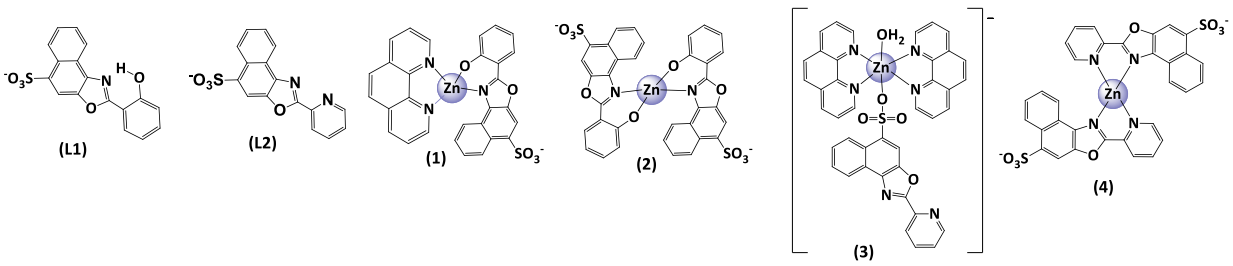
Naphtoxazoles are known for their diverse biological properties, such as anticancer, anti-inflammatory, and antimicrobial activities[1]. In our aim to develop potent biological agents, we synthesized two new naphto[1,2-d]oxazol-type ligands, **L1** and **L2**, and their zinc(II) complexes, **1** – **4** (Fig. 1). These compounds were fully characterized using elemental and conductimetric analysis; FTIR, UV-vis, ^{1}H- and ^{13}C-NMR spectroscopies; mass-spectrometry; and the structures of some of these compounds were determined by single crystal X-ray diffraction (**L1**, **L2**, and **3**). The coordination mode of the Zn^{2+} to the ligands depends on the structure of the ligand: **L1**, which possesses the phenolic derivative, allows the bidentate zinc(II) coordination to N-oxazolic and O-phenolic moieties, while **L2**, which holds a pyridine derivative, coordinates to metal ions by the sulphonate group. The zinc(II) complexes have enhanced fluorescence emission compared to the free ligands and antioxidant potential analyzed by DPPH assay, which indicates their potential as biological fluorescent probes and antioxidant agents. In addition, the mode of interaction with the DNA of the ligands and the complexes were analyzed by spectroscopic titration and viscosity experiments. The viscosity measurements and the intrinsic DNA-binding constants $(K_b)^2$ obtained by electronic absorption titration indicate that the complexes interact with the DNA by groove binding mode. The higher K_b value found for **2** ($1{,}1 \times 10^5$) may be due to the enhanced planarity extension of **L1** after bidentate coordination to zinc(II), which permitted improved interaction between **2** and the DNA helix. The results revealed that the complexes demonstrated significantly enhanced biological properties compared to the free ligands, paving the way for promising future research and development.

Figure 1. Proposed structures for ligands (**1**, **2**) and their complexes (**3**, **4**, **5**, **6)**



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