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Research Article

## Coumarin-Oxazolyl-Based Chemosensor for Selective Detection of Fe<sup>2+</sup> Ions: Preparation, Spectral Characterization, Theoretical Studies and Cellular Bioimaging

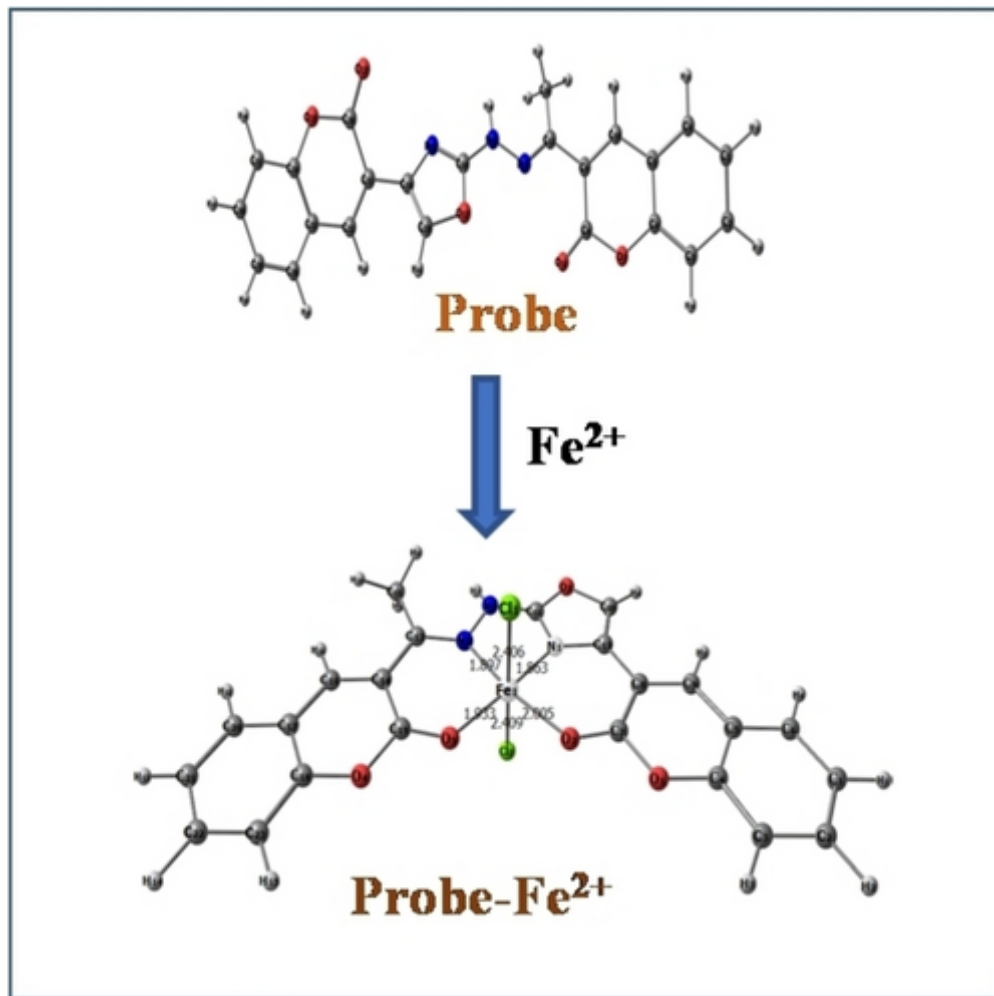
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### Graphical Abstract

AOX has the ability to sense Fe<sup>2+</sup> ions by “naked-eye” detection with an apparent colour change from pale yellow to brown in Water:DMSO (4 : 1 v/v) medium. The true nature of resulted fluorophore-quencher complex (AOX–Fe<sup>2+</sup>) and its 1 : 1 stoichiometry was confirmed using Job's plot and various spectroscopic techniques. Further, the binding constant (K<sub>a</sub>) and the detection limit (LOD) of AOX towards Fe<sup>2+</sup> were found as  $3.97 \pm 0.26 \times 10^7 \text{ l mol}^{-1}$  and  $7.15 \times 10^{-8} \text{ M}$  respectively. Theoretical calculations (density functional theory) were done to confirm the existence of the fluorophore-quencher complex. The in vitro cytotoxic nature of AOX and AOX–Fe<sup>2+</sup> was examined with HeLa cells using MTT assay and their activity was compared with standard doxorubicin. The IC<sub>50</sub> values were found to be  $24.0 \pm 0.6 \text{ } \mu\text{M}$ ,  $17.3 \pm 1.5 \text{ } \mu\text{M}$  and  $15.1 \pm 1.0 \text{ } \mu\text{M}$  for AOX, AOX–Fe<sup>2+</sup> and doxorubicin respectively, the compounds possessed significant cytotoxicity towards HeLa cells. The results of fluorescence cell imaging studies of AOX and AOX–Fe<sup>2+</sup> in HeLa cells revealed the imaging efficacy of AOX in detecting Fe<sup>2+</sup> ion effectively in the living cells.



## Abstract

New coumarin-oxazolyl derived receptor (*E*)-3(2-(2-(1-(2-oxo-2H-chromen-3-yl)ethylidene)hydrazinyl)oxazol-4-yl)-2H-chromen-2-one (**AOX**) was designed, synthesised from the reaction of 3-acetyl-coumarin semicarbazone with 3-bromoacetyl coumarin in chloroform/ethanol and the formation of **AOX** was confirmed by using different spectroscopic methods. The interaction of the **AOX** with different metal ions was investigated using photometric titrations and its selectively detected the Fe<sup>2+</sup> ions.

## Conflict of interest

The authors declare no competing financial interest.

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## Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

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