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# Synthesis of quinoline functionalized fluorescent chemosensor for Cu (II), DFT studies and its application in imaging in living HEK 293 cells

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ABSTRACT

New fluorescent probes having quinoline moiety have been successfully synthesized for the selective $Cu^{2+}$ ions detection. These sensors show a favorable selectivity towards $Cu^{2+}$ ion over a broad range of other common metal ions in DMSO/$H_2O$ (2:8, v/v) HEPES buffer solution (pH = 7.4), leading to remarkable fluorescence on-off response with very low Limit of Detection (LOD) value. The robust nature of the probes was shown by the detection of $Cu^{2+}$ even after repeated rounds of the experiment. Moreover, the probe can be used to detect $Cu^{2+}$ in real water samples with a high precision and good accuracy. The recognition mechanism of one representative probe towards $Cu^{2+}$ has been properly inspected in details by High Resolution Mass Spectrometry (HRMS) and density functional theory (DFT) calculations. Besides, fluorescence imaging studies in HEK 293 cells of that probe is also indicating that the probe is low cytotoxic and offers good photophysical properties, suggesting that this fluorescent chemosensor can be easily used to track $Cu^{2+}$ ion in cells.

## 1. Introduction

The improvement of chemosensors via optical signal transduction has been of a great interest for the selective recognition of metal ions which can have incredible consequences on the environment as well as health of human [1]. Some essential metal ions, such as $Na^+$, $Ca^{2+}$, $K^+$, $Mg^{2+}$, $Fe^{3+}$, $Cu^{2+}$ and $Zn^{2+}$ may affect biological processes like the conduction of impulses, nerve impulses, muscle contraction, ion-dependent establishment of electrochemical gradients across all the cell plasma membrane, muscle relaxation, cell function etc [2]. Among them, in human body copper is third (in abundance after iron and zinc) most essential metal trace element and plays an significant role in many lifecycle processes such as red blood cell formation, prosthetic group formation, bone formation, respiration etc [3,2,4]. Several research groups have attached the cellular toxicity of $Cu^{2+}$ to serious diseases like Alzheimer's disease [5], familial amyotrophic lateral sclerosis [6], Indian childhood cirrhosis [7], prion disease [8], Wilson and Meknes diseases [9] which are all pathogenically connected with an intracellular deficiency and overload of copper. Monitoring of copper existing in biological resources is an important task all over the world because uptake of excessive copper ions may lead to damage of living organs such as kidney and liver [10]. In our modern society $Cu^{2+}$ is extensively used and it results copper a significant metal pollutant. According to the U.S. Environmental Protection Agency (EPA), the permissible level of copper in drinking water is 20 μM [11]. So the progress of a non-toxic small molecule-based signaling system which is reliable and Compatible for the recognition of $Cu^{2+}$ in living species is a supreme important to us.

In recent years, designing of fluorescent sensors has emerged to be the most popular and significant approach for the detection of metal ions [12]. Even at very low concentration, Fluorescent based sensors can detect common metal ions and can serve up as agents for imaging. The added superiorities over other methods are operational simplicity, high sensitivity, easy operation, remarkable selectivity, rapid response and low cost which makes fluorescent detection a hopeful strategy for the recognition of metal ions [13,14]. Consequently, there has been an enhancing ambition for the synthesis of novel and low cost chemical sensors for $Cu^{2+}$ towards the selective and accurate determination, which consist of rhodamine [15–18], coumarin [19–21], quinoline [22,23] pyrene [24,25] and other fluorophores [26–37]. In recent years, quinoline-based compounds are frequently used as fluorescence sensing system as the quinoline unit has large-conjugated molecular structure which shows excellent spectroscopic properties [38–40]. The nitrogen atom of the heterocyclic quinoline unit has the ability to act as

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