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A new multifunctional benzimidazole tagged coumarin as ratiometric fluorophore for the detection of Cd²⁺/F⁻ ions and imaging in live cells

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ABSTRACT

A novel multifunctional ratiometric fluorescent probe has been designed and synthesized for the selective recognition of Cd²⁺/F ions. The probe (3)-((2)-(1H-benzoimidazole-2-yl)-phenylimino) methyl-4-chloromethyl-2H-chromen-2-ene (**BIMC**) displays excellent ratiometric responses towards Cd²⁺/F ions over the tested cations/anions. The lowest detection limits observed for Cd²⁺ and F are 1.5×10⁻¹⁰ mol/L and 1.2×10⁻¹⁰ mol/L respectively. Job's plot and Electro spray Ionization mass spectral (ESI-MS) studies confirms 1:1 binding stoichiometry of **BIMC** with Cd²⁺/F ions, which is further evidenced by ¹H-NMR titration studies. The reversibility studies of **BIMC** with Cd²⁺ have been investigated using ethylenediaminetetraacetic acid (EDTA). Upon binding to Cd²⁺/F ions, the probe features strong ratiometric response in both UV-Visible and fluorescence spectra due to the inhibition of intramolecular charge transfer (ICT). Furthermore, the mechanism of ICT has been rationalized via solvatochromism and DFT calculations.

1. Introduction

The widespread occurrence of heavy metals and anions in both industry and agriculture wastes causes harmful effects on human health and are recognized as eco-pollutants [1]. Chemosensors have the potential to detect various ion and neutral species due to their high sensitivity, selectivity, versatility and relatively simple handling. Hence nurturing multifunctional receptors have become more attractive and also gained much more importance in recent era of research due to their ecological potentials [2–4]. However, only few receptors are available in the literature for simultaneous detection of multianalytes with different optical responses [5–7].

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