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Title: Rhodamine based "turn-on" molecular switch FRET-sensor for cadmium and sulfide ions and live cell imaging study

Author: M. Maniyazagan R. Mariadasse J. Jeyakanthan N.K.

Lokanath S. Naveen K. Premkumar P. Muthuraja P.

Manisankar T. Stalin

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ACCEPTED MANUSCRIPT

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- <AU>M. Maniyazagan a , R. Mariadasse b , J. Jeyakanthan b , N. K. Lokanath d , S. Naveen d , K. Premkumar c , P. Muthuraja † , P. Manisankar † , T. Stalin a *

##Email##drstalin76@gmail.com##/Email##

- <AFF>^aDepartment of Industrial Chemistry, School of Chemical Sciences, Alagappa University, Karaikudi-⁰³, Tamil Nadu, India.
- <AFF>^bStructural Biology and Bio-computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi-04, Tamil Nadu, India
- <AFF>^cCancer Genetics and Nanomedicine Laboratory, Department of Biomedical Science, Bharathidasan University, Tiruchirappalli, Tamil Nadu, India
- <AFF>dDept. of Studies in Physics, University of Mysore, Mansagangotri, Mysore-06, India Physics, Corresponding author. Tel.: +91 9944266475.

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- <ABS-Head><ABS-HEAD>Graphical abstract
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- <ABS-P><xps:span class="xps_Image">fx1</xps:span>
- <ABS-HEAD>Highlights ► A rhodamine-based turn-on fluorescence probe (RBD4) was synthesized and characterized by ¹H NMR, ¹³C NMR and ESI-MS. ► The X-ray crystal structure analyses exhibit the spirolactone of fluorescent sensor RBD4. ► Highly selective towards Cd²+ ion over other metal ions conformed by XRD, SEM, EDAX and FT–IR studies. ► The 1:1 stoichiometric structure between RBD4 and Cd²+ were supported by Job's plot, Benesi-Hildebrand plot and DET theoretical calculations. ► RBD4 fluorescent sensor was
- Benesi-Hildebrand plot and DFT theoretical calculations. ► RBD4 fluorescent sensor was used in imaging Cd²⁺ in cultured HeLa cells.

<ABS-HEAD>Abstract

A">A novel fluorescent chemosensor based on a rhodamine derivative">ABS-P>A novel fluorescent chemosensor based on a rhodamine derivative (RBD4) was designed, synthesized, and used as a selective Cd^{2+} ion sensor. The structure of the fluorescence sensor (RBD4) is confirmed through single crystal X-ray study. On the basis of the Förster resonance energy transfer mechanism between rhodamine and pyridine conjugated dyad, a new colorimetric as well as fluorescence probe was synthesized for the selective detection of Cd^{2+} . This sensor shows high selectivity towards Cd^{2+} ions in the presence of other competing metal ions. On the basis of thorough experimental and theoretical findings, the additions of Cd^{2+} ions to the solution of RBD4 helps to generate a new fluorescence peak at 590 nm due to the selective binding of Cd^{2+} ions with RBD4 in a 1: 1 ratio with a binding constant (K) of $4.2524 \times 10^4 \, \text{M}^{-1}$. The detection limit of RBD4 for Cd^{2+} was $1.025 \times 10^{-8} \, \text{M}$, which presented a pronounced sensitivity towards Cd^{2+} . The *in situ*

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