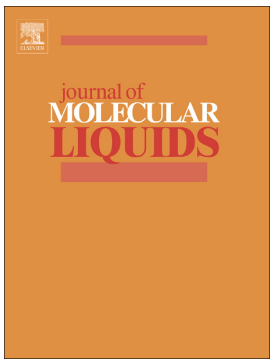


# Selective fluorescence sensing of Cu(II) ions using calix[4]pyrrole fabricated Ag nanoparticles: A spectroscopic and computational approach

Anita Kongor, Manthan Panchal, Mohd Athar, P.C. Jha, Devendrasinh Jhala, Gaurang Sindhav, Naumita Shah, Vinod Jain

PII: S0167-7322(18)32820-4
DOI: doi:10.1016/j.molliq.2018.08.014
Reference: MOLLIQ 9459

To appear in: *Journal of Molecular Liquids*

Received date: 31 May 2018
Revised date: 31 July 2018
Accepted date: 3 August 2018

Please cite this article as: Anita Kongor, Manthan Panchal, Mohd Athar, P.C. Jha, Devendrasinh Jhala, Gaurang Sindhav, Naumita Shah, Vinod Jain , Selective fluorescence sensing of Cu(II) ions using calix[4]pyrrole fabricated Ag nanoparticles: A spectroscopic and computational approach. Molliq (2018), doi:10.1016/j.molliq.2018.08.014

# Selective fluorescence sensing of Cu(II) ions using calix[4]pyrrole fabricated Ag nanoparticles: a spectroscopic and computational approach

Anita Kongor[a], Manthan Panchal[a], Mohd Athar[b], P.C. Jha[c], Devendrasinh Jhala[d], Gaurang Sindhav[d], Naumita Shah[d], Vinod Jain[a*]

[a]Department of Chemistry, School of Sciences, Gujarat University, Ahmedabad – 380009, Gujarat, India
[b]CCG@CUG, School of Chemical Sciences, Central University of Gujarat Gandhinagar Gujarat- 382030.
[c]CCG@CUG, Centre for Applied Chemistry, Central University of Gujarat Gandhinagar Gujarat- 382030
[d]Department of Zoology, School of Sciences, Gujarat University, Ahmedabad – 380009, Gujarat, India
*Corresponding author: Tel.:+91-9327013263; Fax: +91-079-26303263; E-mail:drvkjain@hotmail.com

## Abstract

The presence of Cu(II) at excessive levels can cause several undesirable issues to human health and to the environment as well. Hence, a simple, fast and selective method is needed to be developed to monitor the occurrence of Cu(II). In the present study, we report a novel fluorescent sensor for the selective and sensitive detection of Cu(II) using calix[4]pyrrole fabricated nano-Ag particles (CPTH-AgNPs). The selectivity of the method has been evaluated under optimal conditions of pH and temperature. A theoretical molecular dynamics method has been implemented to understand the coating of calix[4]pyrrole tetrahydrazide around nano-Ag particles. The computational approach predicts the grafting of CPTH on the surface of AgNPsand unveils the role of non-covalent pi-pi intermolecular and H-bonding interactions. The conjugated features of calix[4]pyrrole and nanoparticles provide deep insights into the ion sensing phenomenon. The non-covalent interaction of Cu(II) with CPTH-AgNPs disturbs the intramolecular hydrogen bonding networks and causes aggregation of the nanoparticles which has been demonstrated using FT-IR, DLS and TEM analysis. The present work has also been extended for some bio-analytical applications such as antibacterial, and DNA (CT-DNA) binding studies, which indicate the importance of CPTH-AgNPs for designing an efficient drug-target carrier system. Moreover, the *in vitro* HeLa cell imaging based on fluorescence microscopy predicts the potential application of CPTH-AgNPs for targeted cancer treatment in living systems.

**Keywords:** Calix[4]pyrrole; Silver nanoparticles; Computational approach; Cu(II); fluorescence sensor; HeLa cell imaging

## 1. Introduction