**INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI**
**SHORT ABSTRACT OF THESIS**

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Programme of Study : **Ph.D.**

Thesis Title: **Recognition of Some Metal Ions Using N,N-, N,O- or N,S-Donor Ligands and Cytotoxicity, Cell Imaging Studies**

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Thesis Submitted to the Department/ Center : **Chemistry**

Date of completion of Thesis Viva-Voce Exam : **27-04-2022**

Key words for description of Thesis : Heterocyclic, Isoquinoline, Colorimetric, Fluorescence, DFT/TDDFT calculation, Cell imaging, Trivalent ions, Coumarin, Pyrene, Hydrazinecarbothioamide, 1,8-naphthalimide

## SHORT ABSTRACT

My Thesis contains five chapters. Chapter 1 is about Introduction, Materials and Methods. In this chapter introduction about Fluorescence and various sensing mechanisms are explained. Some recent literature reports based on metal ion detection using different fluorescent probes have been discussed. Along with this, materials, methods and instrumentation related to this thesis are described in details. In Chapter 2 the heterocyclic probe 3-(1-isoquinolinyl)imidazo[5, 1-*a*]isoquinoline (**L1**) in $CH_3OH$/HEPES buffer system (5 mM, pH = 7.4, 6:4, *v/v*), exhibits blue fluorescence ($\lambda_{em}$ = 454 nm) upon excitation with 359 nm light. Upon adding $Pd^{2+}$ ion solution, **L1** shows "*turn-off*" response. Job's plot and ESI mass spectrometric analysis reveal a 1:1 ratio for binding of **L1** with Pd(II) ion. DFT/TDDFT calculations performed on $[Pd(\mathbf{L1})Cl(CH_3CN)]^+$ ion support the experimental findings. Fluorescence imaging in the absence and presence of $Pd^{2+}$ revealed that **L1** can be successfully applied on living cells with outstanding sensitivity. In Chapter 3 the heterocyclic probe 3-(2-hydroxyphenyl)imidazo[5, 1-*a*]isoquinoline (**L2H**) has exhibited specific recognition of $Cu^{2+}$ ion by forming a complex of formula $[Cu(\mathbf{L2})_2]$, which in

turn showed recognition for $CN^-$ ions with in $CH_3CN$/aqueous HEPES-buffer solution (5 mM, pH = 7.4, 6:4, *v/v*). Based on the cytotoxic analysis, 5 μM of **L2H** was selected for determining its fluorescence attributes in cellular imaging in MDA-MB-231 and HDF cells. In Chapter 4 Schiff base probe (**L3**) containing coumarin and pyrene moieties is synthesized and characterized which can detect trivalent M(III) ions (M = Al, Cr and Fe) through "OFF-ON" fluorescence process. Fluorescence intensity of these M(III) bound **L3** complexes is quenched by fluoride ions. From cytotoxicity analysis, 7.5 μM of probe **L3** was selected to analyze its fluorescence attributes in cellular imaging. In Chapter 5 the probe (**L4**) having hydrazinecarbothioamide and 1,8-naphthalimide moieties has been synthesized and evaluated for its metal ion sensing ability. It exhibits a selective and sensitive colorimetric as well as fluorescent recognition of $Hg^{2+}$ and $Ag^+$ ions in $CH_3OH$ - HEPES buffer solution (5 mM, 7:3, *v/v*, pH = 7.4). The DFT/TDDFT calculation has revealed a decrease in energy of the HOMO-LUMO gap in mercury and silver complex thereby supporting the experimentally observed red shift in absorption bands. Based on the cytotoxic assay, 5 μM concentration of probe **L4** was considered for intracellular detection of $Hg^{2+}$ and $Ag^+$ ions in MDA-MB-231 and HDF cells through "*turn-on*" fluorescence response.