



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student : MAHHMUDA KHANNAM

Roll Number : 136122016

Programme of Study : Ph.D.

Thesis Title: Synthesis, Characterization and Investigation on Water-Soluble, Aquated Gd(III) and Mn(II) complexes as MRI Contrast Agents.

Name of Thesis Supervisor(s) : Dr. CHANDAN MUKHERJEE

Thesis Submitted to the Department/ Center : CHEMISTRY

Date of completion of Thesis Viva-Voce Exam : 14/03/2019

Key words for description of Thesis Work : MRI contrast agents, longitudinal relaxivity, T1-weighted images, and stability.

SHORT ABSTRACT

MRI is an effective diagnostic imaging modality. The low sensitivity of the technique can be overcome by injection of a class of substances prior imaging, termed as contrast agents. These contrast agents can enhance the image contrast by catalytically shortening the relaxation times of in vivo water protons. Metal complexes containing paramagnetic Gd(III) and Mn(II) ions are usually used as T1-contrast agents. The main objective of this thesis has been the development of new thermodynamically stable, water-soluble, Gd(III) and Mn(II) complexes with better relaxivity value compared to current commercially available Gd(III)-based MRI contrast agents.

In this context, we have synthesized two hexadentate picolinate-based ligands Li₃cbda and H₂hbda to prepare their corresponding Gd(III) and Mn(II) complexes. The respective Gd(III) complexes (3A and 3B) possess more than one coordinated-water molecules, thus offered relaxivity values greater than clinically approved mono(aquated) Gd(III) complexes. Both of the complexes showed sufficient thermodynamic stability and impressive contrast efficiency to behave as T1-weighted contrast agents.

The respective Mn(II) complexes of these two ligand frameworks (5A and 6A) also showed impressive thermodynamic stability. With one coordinated-water molecule they offered longitudinal relaxivity value comparable to some of clinically approved mono(aquated) Gd(III) complexes. Their behavior under physiologically abundant anions and T1-weighted phantom images under clinical scanner were also studied.

The lipophilic piperidine-based pentadentate ligand H₃cpmda used to synthesize Mn(II) complex (4B) with one-coordinated water molecule. The complex offered impressive thermodynamic stability due to presence of rigid ligand framework. With one coordinated-water molecule it showed relaxivity value comparable to already reported mono(aquated) Gd(III) complexes and impressive contrast efficiency.

Herein, we have synthesized two Gd(III) complexes and three Mn(II) complexes and studied their thermodynamic stability, relaxivity and contrast efficiency as T1-weighted contrast agents.