Research project for Master degree

Field:
Coordination Chemistry

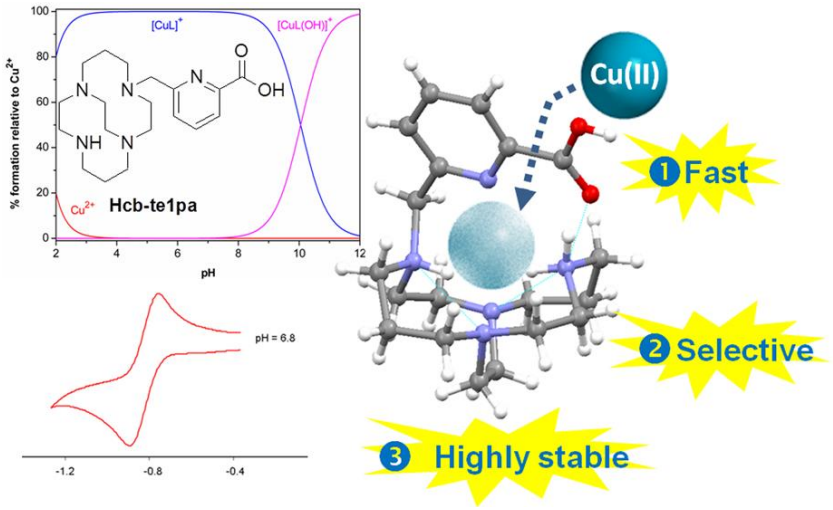
Title:
Design and study of metal complexes interesting for nuclear imaging applications

Workplace:
Coordination and Supramolecular Chemistry Laboratory, ITQB NOVA, Oeiras, Portugal.

Duration of the work:
As required by the student's Master degree plan.

Supervisors:
Dr. Luís M. P. Lima (llima@itqb.unl.pt); Prof. Rita Delgado (delgado@itqb.unl.pt)

Background:
The field of medical imaging using radiopharmaceuticals is experiencing a great development mainly due to the growing availability of a variety of suitable metal radionuclides. Among the most pursued nuclides are those dedicated to positron emission tomography (PET) such as ^{64}Cu and ^{68}Ga. Radiopharmaceuticals usually employ bifunctional chelating agents (BCA's) containing a chelator moiety linked to a conjugation function, where the former is responsible to form strong complexes with the metal cation while the latter allows for the conjugation with biomolecules for targeted applications.[1]



We are interested in developing new chelators for the efficient complexation of copper(II) and gallium(III) cations, and the most important properties required are the stability, the formation rate, and the kinetic inertness of the complexes. The chelators will be based on small polyamines selectively functionalized with appropriate donors groups for metal coordination such as carboxyl, pyridyl and pycolinate ones, following our recent research in the field (see example in the Figure).[2]

1. E.W. Price and C. Orvig, *Chem. Soc. Rev.* **2014**, *43*, 260–290.
2. L. M. P. Lima, Z. Halime, R. Marion, N. Camus, R. Delgado, C. Platas-Iglesias, and R. Tripier, *Inorg. Chem.* **2014**, *53*, 5269–5279.

Objectives:

- Synthesis of a new organic ligand for the efficient complexation of relevant metal cations such as copper(II) and gallium(III).
- Study of the metal complexes of the synthesized ligand regarding structural, thermodynamic stability and kinetic properties.

Work plan:

An organic ligand (chelator) suitable for strong complexation of copper(II) and/or gallium(III) cations will be rationally designed. Synthesis and isolation of the ligand will be performed by suitable organic chemistry reactions and techniques, and its structure will be characterized by NMR spectroscopy. Potentiometric titrations will be used to determine the protonation constants of the ligand. The metal complexation properties of the ligand will be studied mainly by potentiometric and/or UV-vis spectrophotometric titrations, to determine the thermodynamic stability constants for the complexes and also to calculate their formation rate and kinetic inertness. Additional characterization of the complexes may be performed by EPR spectroscopy and electrochemistry in case of copper(II) or by NMR spectroscopy in case of gallium(III). The obtained compounds will also be subjected to crystallization attempts to allow for determining their solid state structure by X-ray diffraction.