Intitulé du Sujet de Thèse :

A computational strategy to predict properties of chiral molecular cages

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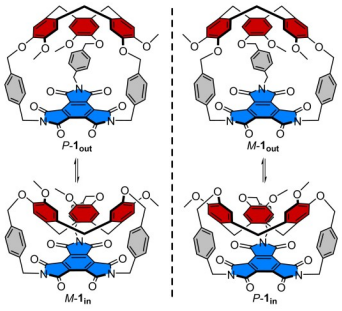
Descriptif du projet

Molecular cages provide well-defined confined environments that can be leveraged to develop selectivity in host-guest chemistry and chemical transformations. Selectivity arises from the precise control of cavity shape and the strategic functionalization of the cage's residues to promote favorable interactions with a target guest. Of particular interest is the ability to engineer chiral environments within these cages, opening the prospect of enantioselective control over chemical processes.

This project aims to develop a computational framework for predicting the properties of chiral, confined molecular environments. Chiral molecules exist as two enantiomers whose configuration can be probed by spectroscopic techniques such as electronic circular dichroism (ECD). However, experimental spectra alone are often insufficient to unambiguously assign absolute configuration, making computational support essential.



The goal is to establish a low-cost yet accurate strategy to rationalize and predict the ECD spectra of new chiral molecules. Calculations using several methods will be performed on molecules of increasing size and complexity, building a reference database serving as a benchmark for spectroscopic assignments.

Special attention will be directed towards chiral molecular cages, which may adopt multiple conformations in solution and can switch their chiral properties in response to an external stimulus, such as solvent change — as exemplified by systems recently characterized in our institute. Depending on progress, the reactivity of these cages will also be investigated, and cage effects, whether geometric or electronic, will be decomposed using established theoretical approaches.

Références Bibliographiques

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