



CHIMIE MOLÉCULAIRE ET SUPRAMOLÉCULAIRE

MOLECULAR AND SUPRAMOLECULAR CHEMISTRY

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| Lecturers : 12.0 | TC : 18.0 | PW : 0.0 | Autonomy : 18.0 | Study : 0.0 | Project : 0.0 | Language : FR

Objectives

Metabolites are low molecular weight species, present in blood, among an abundant background of high molecular weight species. Metabolites are the biomarkers of a large range of pathologies. However their detection, for clinical use, is still a global challenge. Chemical functionalization of porous silicon surfaces, by using specific molecules, could allow the selective trapping of metabolites. Such a trapping could allow to improve the sensitivity of the detection tools, classically used in hospitals (mass spectrometry).

Objectives of this course is to study the effects of the physico-chemical properties of molecules (structure, hydrophile-lipophile balance, charges) on the intermolecular interactions. A large part of the course will be

Keywords : Intermolecular interactions, Molecular Dynamics simulations, innovative clinical diagnostic tools

Programme

This course will be presented in the form of a case study.

First, the physicochemical properties of single molecules will be presented (structure, hydrophilic hydrophobic balance, charges).

Secondly, the physicochemical properties of supramolecular structures will be analyzed from the properties of the single molecules that constitute them by molecular modeling (energy of interactions...).

The results of this analysis will be used to design a biomedical analysis tool.

Learning outcomes

- C2N1: Define a system and its boundaries, identify the phenomena involved and propose a simple model. Formulate the hypotheses.
- C2N3: Characterize the complexity of a system, identify interactions and sources of uncertainty.
- C1I1: Carry out a state of the art and implement creative methods, on a problem open to technical-scientific-economic questions, and formalize the result.

Independent study

Objectifs : Molecular modeling on computer

Méthodes :

Core texts

Franck, *CHIMIE PHARMACEUTIQUE*, De Boeck, 2005

J.-M. Lehn *LA CHIMIE SUPRAMOLÉCULAIRE, CONCEPTS ET PERSPECTIVES*, De Boeck, 1997

Trong Anh *INTRODUCTION À LA CHIMIE MOLÉCULAIRE*, Ellipses, 1994

Assessment

Score = 50% knowledge + 50% know-how

Knowledge score = 50% final exam + 50% continuous assessment

Know-how score = 50% final exam + 50% continuous assessment