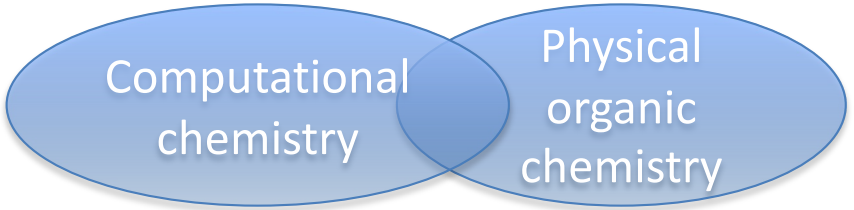
Physical and Computational Organic Chemistry

Connection with other lectures



Bachelor

1st year: AIMF and General Overview
2nd year: Fonctions et réactions chimiques I et II
2nd year: Chimie quantique
3rd year: *An asset*: Introduction to Electronic Structure methods

Master

Fifth semester: Structure and Reactivity
Fifth semester: Computational methods in molecular quantum mechanics

The aim of this lecture series is to become familiar with diverse standard and modern computational and physical organic chemistry approaches, appreciate their applications in the field of organic chemistry and realize their strengths and limitations.

Physical and Computational Organic Chemistry

Structure of the lecture

Lecture notes and ex-cathedra lecture on the blackboard.

Mini Quiz: A set of quick questions at the end of a chapter. The answers will be provided directly during the course.

Quiz of the month: Typical questions relevant to the course. The corrections will be provided to those answering the quiz.

Presentation of special topic of physical/computational organic chemistry: In groups of two, you will select one research article relevant to the course. A list will be provided around Easter, but you are welcome to pick article with my approval. The last two weeks of the semester will be devoted to the presentations of the articles by each group of two students (~Max. 12 minutes per group).

Exam: Oral exam, 20 minutes long (5 minutes of preparation, 15 minutes of exam)

Grade: 1/3 presentation + 2/3 oral exam

Literature

Physical Organic Chemistry

- Steven M. Bachrach, ***Computational Organic Chemistry***, First Edition, 2007, Wiley-Interscience.
  Application of computations to some of the most relevant problem of organic chemistry. Include conversations with six computational physical organic chemists. Also read the blog: **http://comporgchem.com/blog/**

- Eric V. Anslyn and Dennis A. Dougherty, ***Modern Physical Organic Chemistry***, First edition, 2006, University Science Books 2006.
  Here is a modern textbook written by two distinguished researchers in this field. The book makes explicit the many connections between physical organic chemistry and critical fields such as organometallic chemistry, materials chemistry. It covers the core areas of physical organic chemistry as well.

- Ian Fleming, ***Frontier Orbitals and Organic Chemical Reactions***, 6th edition, 2006, John Wiley & Son.
  A simplified account of frontier orbital theory and an overview of its applications in organic chemistry.

Literature

Computational and theoretical Chemistry

- Willam B. Smith*, **Introduction to Theoretical Organic Chemistry and Molecular Modeling***, X Edition, 1996, Wiley-VCH.
  A book on theoretical chemistry written by an organic chemist for organic chemists.

- Eric V. Anslyn and Dennis A. Dougherty, ***Modern Physical Organic Chemistry***, First edition, 2006, University Science Books 2006.
  The foundations and applications of modern computational methods are also developed in this book.

- Attila Szabo and Neil S. Ostlund, ***Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory***, First Edition, 1996, Dover.
  The bible of quantum chemistry.

- Christopher J. Cramer, ***Essentials of Computational Chemistry, Theories and Models***, Second Edition, 2004, Wiley.
  For those specifically interested in Computational Chemistry.

Course Schedule

I. Electronic Structure Theory for Organic Chemistry

17.02.25 « *Why is computational chemistry useful and how did it evolve*? »
24.02.25 Introduction / 1. Computational Methods: 1.1. Ab initio
03.03.25 Computational Methods: 1.1. (suite et fin) 1.2. DFT
10.03.25 Computational Methods: 1.2. DFT (suite et fin)

II. Fundamentals of Physical Organic Chemistry

17.03.25 Thermodynamic Stability and Additivity Rules
24.03.25 Stabilizing Effects in Hydrocarbon Chemistry
31.03.25 Aromaticity
07.04.25 Reaction mechanisms
14.04.25 Pericyclic Reactions and Isotope Effects/Special topic in catalysis
21.04.25 Easter Holidays

III. Special Topics

28.05.25 Special Machine learning in chemistry
05.05.25 Machine learning applications in chemistry

IV. Presentations

12.05.25 Presentation of the articles
19.05.25 Presentation of the articles
26.05.23 Pentecôte
xxxxx.25 Exam