Summary
This course introduces computational electronic structure methods and their broad applications to organic chemistry. It also discusses physical organic concepts to illustrate the stability and reactivity of organic molecules.

Content

Computational Methods
• Electronic structure approaches for organic chemistry
• Overview of density functional theory and post-Hartree-Fock methods

Fundamentals of physical organic chemistry
• Thermodynamic stabilities
• Stabilizing effects
• Computation of reaction mechanisms
• Radicals, diradicals, carbenes and spin multiplicity
• Kinetic isotope effects
• (Organic reactions dynamics)

Special topic in physical organic chemistry
• Aromaticity
• Carbocation
• Molecular Strain

Selected article for presentation

Keywords
Computational organic chemistry, chemical concepts

Learning Outcomes
By the end of the course, the student must be able to:
• Choose an appropriate computational method to address a given chemistry problem
• Estimate the uncertainties associated with the use of a given computational approach
• Assess / Evaluate the (de)stabilizing effects of a molecule
• Elaborate orbital energy diagrammes
• Interpret the forbidden/allowed nature of a chemical reaction
• Specify the type of kinetic isotope effects
• Identify the main message of an article

Transversal skills
• Communicate effectively, being understood, including across different languages and cultures.

Expected student activities
resolve the weekly mini-quiz and the two maxi-quiz
read, understand and present a scientific article

Assessment methods
1/3 présentation; 2/3 oral exam

Resources
Ressources en bibliothèque
• Modern Physical Organic Chemistry / Anslyn
• Computational Organic Chemistry / Bachrach

Websites
• http://scgc.epfl.ch/telechargement_cours_chimie

Moodle Link
• http://moodle.epfl.ch/course/view.php?id=15018