Séminaire du département N2EV
Avec le soutien LUE

Computer- Assisted Asymmetric Synthesis with VIRTUAL CHEMIST

Vendredi 30 juin 2023 à 11h15
Salle de séminaire Patrick ALNOT (N° 4-A014), IJL, Campus Artem

Nicolas Moitessier *MC Gill University*

A received his undergraduate training and his Ph.D (1998) from Université Henri Poincaré-Nancy I (France) under the guidance of Dr. Yves Chapleur (carbohydrate chemistry) working in close collaboration with a theoretical chemistry group (Dr. Maigret). His PhD was followed by post-doctoral studies with Prof. Shephen Hanessian (1998-2000, medicinal chemistry, asymmetric synthesis). In 2001, he moved back to Nancy to start an academic career (Chargé de Recherche, CNRS) then back to Montréal in 2003 (Assistant Professor, McGill University), where he is now Full Professor.

His research spans from software development and artificial intelligence to medicinal chemistry and drug synthesis. For this work, Moitessier received a number of awards including the first Reginald Fessenden Professorship in innovation for the development of the Forecaster platform in drug discovery, the AstraZeneca Award in Chemistry and recently the Canadian Society of Chemistry Medicinal and Biological Chemistry Lectureship award.

In 2010, he co-founded Molecular Forecaster, a company distributing the developed software and providing service and consulting to local and international pharmaceutical and biotechnology companies. In 2016 he was appointed as Associate Editor of the European Journal of Medicinal Chemistry

Abstract: Most catalysts are currently optimized through trials-and-errors, a very tedious and inefficient approach. Alternatively, some process chemistry groups are using robotics to screen several catalysts experimentally. However, this approach can hardly be used to discover new ones or optimize existing ones as it is restricted to commercially available chemicals (or chemicals available in house) and does not explore a significant portion of the vast chemical space. In general, efficient design and discovery of novel organic synthetic methodologies (including catalytic processes) calls for the large organic chemistry toolbox including nuclear magnetic resonance, mass spectrometry, and crystallography. These complex scientific technologies are largely accessible without expert knowledge of their inner workings with synthetic chemists running standard 1D and 2D NMR experiments without necessarily understanding and/or manipulating the magnetic pulse sequences. With the rise of Quantum Mechanics methods – Hartree-Fock and density functional theory (DFT) – Molecular Mechanics and Machine Learning methods, organic chemists have caught a glimpse of the power and utility of such computations. However, this array of methods remain largely inaccessible to the experimental chemistry community. We propose to deliver computational chemistry methods to the hands of organic chemists. For this purpose, we have been developing VIRTUAL CHEMIST, a computational platform aiming at assisting chemists in the design of novel reactions. We have demonstrated that this platform was able to simulate research programs of multiple human years within a week or so. The data could now be used to streamline the discovery and/or improve the discovery rate. We will present this platform, its developments, applications, strengths and weaknesses and how it can assist chemists in the day-to-day research.