

ENERGYPOLIS SEMINAR

15. 3. 2017, 11:00 - 12:00, ENERGYPOLIS Sion, 4th floor, Zeuzier

Storing and processing chemical information in the web browser

Luc PATINY (Head of Chemical Information Service EPFL)

EPFL SB ISIC-GE, BCH 4104 (Batochime UNIL), Av. F.-A. Forel 2, CH-1015 Lausanne

Luc Patiny will present the web browser based storing and processing of chemical information. The chemical information service is collaborating with the research groups in ISIC and develop a web based analysis software for the storage of NMR, HPLC and MS spectra and directly retrieve the data from any web-browser.

The development of a worldwide shared database allowing to store any kind of information about chemicals is a priority goal. Many innovative tools allowing to visualize and to analyse the data are being developed in this goal. The automatic analysis of spectra as well as the prediction of physical characteristics are one of our major research topic.

The Chemical Information Service of EPFL funded the webpages like www.nmrdb.org or www.chemcalc.org that receive several thousand visitors per day and e.g. contain one of the most complete database for MS spectra.

Publications:

- [1] Sharing Product Physical Characteristics over the Internet. Patiny, L. Internet Journal of Chemistry 2000; 3, 2.
- [2] Molbank: First fully web-based publication of chemical reaction data of individual molecules with structure search and submission. Lin, S.-K.; Patiny, L. Internet Journal of Chemistry 2000; 3, 1.
- [3] Krompiec, M.; Patiny, L. Easy Calculation of Molecular Formula, Molecular Weight and Isotopic Distribution of Peptides in "Proceedings of ECSOC-5, The Fifth International Electronic Conference on Synthetic Organic Chemistry, <http://www.mdpi.org/ecsoc-5.htm>, September 1-30, 2001", Editors: Oliver Kappe, Pedro Merino, Andreas Marzinzik, Helma Wennemers, Thomas Wirth, Jean-Jacques Vanden Eynde and Shu-Kun Lin, CD-ROM edition, ISBN 3-906980-06-5, 2001, c0016.
- [4] Easy Calculation of Molecular Formula, Molecular Weight and Isotopic Distribution of Peptides. Krompiec, M.; Patiny, L. *Acros Organics Acta* 10, 2003.



CV: Dr. Luc Patiny

Dr. Luc Patiny is the Director of Chemical Information Service at EPFL. He holds a PhD in organic chemistry and did postdoctoral research in the field of NMR spectroscopy. Since the past 13 years he is in charge of the chemical information service of ISIC at EPFL.

Tel. : +41 21 693 94 69

Luc.patiny@epfl.ch

<https://people.epfl.ch/148588>

<http://cheminformatics.epfl.ch>