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Chemical Space: Make it, See it, Use it

Prof. Dr. Jean-Louis Reymond Department of Chemistry, Biochemistry and Pharmaceutical Sciences University of Bern

19.12.2023, 4:15 pm Lecture hall EG16, DCBP

Apéro in front of EG16 at the end of the seminar

Abstract:

Since the advent of organic chemistry as a basis for drug development, millions of molecules of various sizes and shapes have been discovered or synthesized and tested for various properties, and thousands of them have become clinical drugs. Can we understand this data and use it to discover new drugs addressing unmet medical needs? To contribute to this endeavor, we develop computational tools to enumerate, visualize and search the vast chemical space of drug-like molecules and use our tools in applied projects involving organic as well as peptide synthesis and bioassays. Illustrative application examples include small molecule ion channels, transporter and kinase inhibitors as well as peptides as antibacterials, anticancer, and immunomodulatory agents, and as transfection reagents.

About the speaker: **Prof. Dr. Jean-Louis Reymond**

Jean-Louis Reymond (https://orcid.org/0000-0003-2724-2942) is a Professor of Chemistry at the University of Bern, Switzerland. He studied Chemistry and Biochemistry at the ETH Zürich and obtained his Ph.D. at the University of Lausanne on natural products synthesis (1989). After a Post-Doc and Assistant Professorship at the Scripps Research Institute, he joined the University of Bern (1997). His current research focuses on chemical space exploration methods combining data science, artificial intelligence, organic synthesis and bioassays to discover new bioactive small molecules and peptides (https://gdb.unibe.ch).



