Centre for Research in Molecular Modeling
CERMM
Centre de recherche en modélisation moléculaire

UNIVERSITÉ Concordia UNIVERSITY

Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING
and the DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY

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Jean-François Truchon
Vertex Pharmaceuticals (Canada) Inc. and Université de Montréal

Computer Aided Drug Design: When Water Swamps the SAR?

The optimization of biologically active molecules requires an iterative process of chemical matter modifications and biological assay measurements. It is beyond the realm of possibility to synthesize all molecule variations in order to reach the optimal molecule properties. Computer aided methods and protein X-ray crystallography are a proven combination to speed-up the optimization process and progress faster toward a good quality drug candidate. In this talk, attention will be turned to a single molecule: water. Its role in protein-ligand association will be discussed together with ways that modern techniques can be used and improved to better take advantage of its peculiar behavior.

Jean-François Truchon is currently working as a molecular modeler at the Laval site of Vertex Pharmaceuticals. Prior to joining Vertex in 2013, he created the water analysis application in MOE while at Chemical Computing Group. He previously worked at Merck Frosst from 2002 to 2010 as an application scientist in molecular modeling where he contributed to basic research projects aimed at treating diseases such as osteoporosis, COPD, HIV and chronic pain. His first professional experience was however at Lockheed Martin Canada where he spent two years developing artificial intelligence algorithms and programs devoted to military defense.