INSTITUTO DE INGENIERÍA
BIOLÓGICA Y MÉDICA
PONTIFICIA UNIVERSIDAD CATÓLICA DE CHILE

IIBM Seminar

"Computational approaches to drug design and their application to anticancer and antifungal targets"

Andreas Schüller, Dr. phil. nat.
Department of Molecular Genetics and Microbiology,
School of Biological Sciences
Institute for Biological and Medical Engineering
Pontificia Universidad Católica de Chile

Wednesday 30th November 2022 - 13:00 Hrs - Lunch included
Hybrid Seminar – Sala C-306 Const. Civil
Zoom link: Contact **secretariaiibm@uc.cl**

INSTITUTO DE INGENIERÍA
BIOLÓGICA Y MÉDICA
PONTIFICIA UNIVERSIDAD CATÓLICA DE CHILE

"Computational approaches to drug design and their application to anticancer and antifungal targets"

Overview:

Computer-aided drug design (CADD) is a multidisciplinary area that employs a broad range of computational methods for the design and discovery of drugs and is an important element of the modern drug discovery process. Here, we present recent advances of CADD applied to anticancer and antifungal targets. Tumor cells have altered metabolism relying on lactate as a major energy source and signaling molecule. Cell-cell transport of lactate is mediated by monocarboxylate transporters (MCT) where subtypes MCT1 and 4 are evaluated as targets for chemotherapy. While MCT1 inhibitors have advanced into clinical trials, no potent and selective inhibitors against MCT4 are available. Here, we provide preliminary evidence for a novel MCT4 inhibitor discovered by an in silico drug design strategy. On the other hand, fungal infections cause millions of deaths per year, especially in the immunosuppressed population. Available
antifungal drugs are structurally conserved, and novel algorithms are needed to discover new chemical scaffolds. We have developed a novel prediction algorithm for drug candidates and targets based on network-based inference. This algorithm is inspired by notions of social network theory for improved scaffold and target hopping. Preliminary results confirm the antifungal activity of several candidates predicted by our method.