Après-Midi Thématique

"Computational methods in chemistry"

College Européen Doctoral, jeudi 15 Février 2024

14:00 - 14:20	***Amiram Goldblum*****,** Hebrew University, Israel, Solving Tough Challenges in Drug Discovery
14:20 - 14:40	***Hanoch Senderowitz*****,** Bar-Ilan University, Israel, Optimization of QSAR Models for Virtual Screening
14:40 - 15:00	***Dragos Horvath,*** University of Strasbourg, France, The Chemical Library Space
15:00 - 15:20	***Barak Akabayov,*** Bar-Ilan University, Israel, Expanding the Chemical Space of a Hit Molecule Obtained by Fragment-Based Screening
15:20 - 15:50	***Coffee break***
15:50 - 16:10	***Didier Rognan,*** University of Strasbourg, France, Organic chemistry-driven structure-based screening of ultra-large chemical spaces
16:10 - 16:30	***Igor Baskin,*** Technion, Israel, The Concept of Electrochemoinformatics
16:30 - 16:50	***Alexandre Varnek,*** University of Strasbourg, France, In silico design of new enantioselective catalysts
16:50 – 17:10	***Jürgen Bajorath*****,** University of Bonn, Germany, Computational analysis of kinase inhibitors with different modes of action