# QSPRpred, Spock and DrugEx: Developing an Open Source Ecosystem for Cheminformatics

**Šícho Martin**1,2, van den Maagdenberg Helle W.2, Bernatavicius Andrius2,3, Svozil Daniel1,van Westen Gerard2,

1 CZ-OPENSCREEN: National Infrastructure for Chemical Biology, Department of Informatics and Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology Prague, Technická 5, 166 28, Prague, Czech Republic

2 Leiden Academic Centre for Drug Research, Leiden University, 55 Einsteinweg, 2333 CC, Leiden, The Netherlands

3 Leiden Institute of Advanced Computer Science, Leiden University, Niels Bohrweg 1, 2333CA Leiden, The Netherlands.

This talk presents **QSPRpred**, **Spock**, and **DrugEx**, an open-source cheminformatics ecosystem designed to accelerate drug discovery by integrating predictive modeling, molecular docking, and generative chemistry. QSPRpred is a modular Python framework for building robust QSPR/QSAR models with automated preprocessing and hyperparameter optimization. Spock serves as an automated molecular docking framework that generates and stores ligand-protein complexes, enabling structure-based virtual screening to identify promising ligands. Complementing these, DrugEx leverages both Spock pipelines and QSPRpred models to guide *de novo* molecular generation. Together, these tools facilitate streamlined workflows from property prediction and docking to compound design, improving reproducibility and reducing complexity through interoperable, version-controlled components. Case studies demonstrate how this ecosystem enhances virtual screening campaigns by combining data-driven modeling with structure-based docking, supported by open-source development and community collaboration.