Software developed at the Group of chemoinformatics and drug design at IMTM

https://imtm.cz/chemoinformatics-and-drug-design

Repositories are located at the personal account and the group account:

https://github.com/DrrDom

https://github.com/ci-lab-cz

De novo design:

CReM	https://github.com/DrrDom/crem https://crem.imtm.cz/
Generic fragment-based structure generation framework allowing growing, mutating and linking molecules	

CReM-dock	https://github.com/ci-lab-cz/crem-dock
Fully automated fragment-based structure generation pipeline guided by molecular docking	

3D pharmacophores

pmapper	https://github.com/DrrDom/pmapper
3D pharmacophore signatures, fingerprints and descriptors	

psearch	https://github.com/meddwl/psearch
Automated pipeline for 3D ligand-based pharmacophore modeling and virtual screening	

pharmd	https://github.com/ci-lab-cz/pharmd
Retrieval of 3D pharmacophores from MD trajectories and virtual screening	

Virtual screening

EasyDock	https://github.com/ci-lab-cz/easydock
Fully automated pipeline for scalable molecular docking. Includes preparation steps (structure checking, stereoisomers enumeration, protonation, etc)	

StreaMD	https://github.com/ci-lab-cz/streamd
Fully automated pipeline for high-throughput MD simulations, including analysis of output trajectories (pose stability, MM-GBSA, ProLIF)	

Machine learning (QSAR)

SiRMS	https://github.com/DrrDom/sirms
2D fragment descriptors to encode single compounds, “quasi”-mixtures, mixtures and reactions	

SPCI	https://github.com/ci-lab-cz/easydock
Fully automatic QSAR model building and structural interpretation with GUI	

rspci	https://github.com/DrrDom/rspci
R package to analyze fragment contributions from SPCI output	

ibenchamrk	https://github.com/ci-lab-cz/ibenchmark
Datasets and metrics to benchmark interpretability of machine learning models	

Auxiliary RDKit repositories:

rdkit-scripts	https://github.com/DrrDom/rdkit-scripts
Python scripts which automates some processing steps (processing SDF files, file format conversion, generation of conformers and isomers, filtering compounds, RMSD calculation, etc)	

chemicalite-scripts	https://github.com/DrrDom/chemicalite-scripts
Scripts to create SQLite databases for similarity and substructure search with RDKit	