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

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

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

https://github.com/DrrDom

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

De novo design:

crem – Python module for structure generation

https://github.com/DrrDom/crem

3D pharmacophore modeling:

pmapper – 3D pharmacophore processing, signatures and fingerprints

https://github.com/DrrDom/pmapper

psearch – automated 3D ligand-based modeling and screening

https://github.com/meddwl/psearch

pharmd – retrieve 3D pharmacophores from MD trajectories and screening

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

MD modeling:

md-scripts – automated pipeline for high-throughput MD simulations

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

Molecular docking:

docking-scripts – Python module to run automatic molecular docking using vina, smina and gnina

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

Machine learning:

sirms – 2D descriptors for single compounds, “quasi”-mixtures, mixtures and reactions

https://github.com/DrrDom/sirms

spci – automatic QSAR model building and interpretation

https://github.com/DrrDom/spci

rspci – R package to analyze fragment contributions from spci output

https://github.com/DrrDom/rspci

ibenchmark – benchmark interpretability of machine learning models

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

Auxiliary RDKit repositories:

Various RDKit scripts

https://github.com/DrrDom/rdkit-scripts

Scripts to create local databases for similarity and substructure search with RDKit

https://github.com/DrrDom/chemicalite-scripts