

The main goal of the project is to understand how one can identify more effectively new chemicals that can possess activity towards biological macromolecules, such as enzymes or receptors. The ability to predict the effect of chemicals on biologically important targets has long been sought by humanity. It would help design new and safer drugs faster, such as finding compounds inhibiting a mutated protein causing a disease. A chemical compound (e.g. a drug) can interact with a biological target in a dynamical manner as both entities are flexible. Unfortunately computationally it is extremely difficult to account for this effect with the currently prevailing methodologies. This project aims to systematically address this problem by proposing a novel way to account for the dynamical nature of ligand-receptor interactions.

In order to achieve this goal we focus on applying a specially designed procedure which includes molecular docking and molecular dynamics simulations to generate a diverse dataset of protein-ligand complexes. Combined with descriptors extraction this type of dynamical target-ligand interactions provide a novel way of training machine learning and deep learning based predictors. The predictive models developed in this project will be tested especially on biologically relevant targets that have been shown to be challenging for computational drug discovery methods.

Results of this project will broaden our understanding of the different binding mechanisms employed by nature to regulate cellular processes. The methodology and tools which will be developed have the potential to become the state-of-the-art for the development of novel compounds or derivatives of known ligands. All datasets and models will be publicly available to test and reuse by the scientific community and interested general public.