## Machine learning estimated docking scores

Docking programs, used for virtual screening of molecular docking, are rather difficult to operate and time and hardware demanding. In our project, we sought to develop methods for predicting docking scores using machine learning (ML) and deep learning (DL) and thus address mentioned problems and the need to use specialized docking software. The necessary data were obtained using the MOE docking software; the dataset was used for designing, implementation and testing machine learning methods. We compared the regression models of ML methods and new approach in natural language processing - Transformers architecture trained on a body of chemical data presented as SMILES strings.