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MEETING ABSTRACTS

PREDICTION OF DRUGS' SIDE EFFECTS *IN SILICO*

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The goal of this project is to create algorithm and software solution for prediction of drugs' side effects. The algorithm is based on calculations of interactions between active substances and known macromolecules.

Methods of molecular docking and reverse molecular docking are used there. Each exanimated drug substance is docked into binding site of each macromolecule of sc-PDB database while the interaction between them is calculated. A set of decoys is selected from the ZINC database based on chemical properties. Decoys are docked into binding site of each macromolecule as well as exanimated drug substances. The docking results of exanimated substances and decoys are compared to determine the specificity of interactions. These methods are implemented using AutoDock Vina. All of docking interactions are analyzed by R software and the list of resulting macromolecules are released. The active drugs substances can be a substrate, inhibitor, or inducer of resulting macromolecules and they are suitable for *in vitro* testing.

The software solution is designed as a public service accessible by a web browser.

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Keywords: in silico prediction; molecular docking; off-target; side effects

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