Virtual high-throughput screening of novel pharmacological agents based on PASS predictions

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Among the numerous tools currently used for virtual screening, PASS (http://pharmaexpert.ru/passonline) occupies a special place. PASS predicts 6400 biological activities of drug-like compounds with a mean accuracy of about 95%. Its training set consists of 330,000 biologically active compounds. Since PASS calculations for 50,000 structures take a few minutes on an ordinary PC, PASS is applicable to chemical libraries containing millions of compounds. Based on PASS predictions, novel pharmaceutical agents have been discovered with anxiolytic, anti-inflammatory, antihypertensive, anticancer and other actions. To find new anticancer agents, we have analyzed dozens of millions of structures from ChemNavigator and selected a few dozens for biological testing. Two out of eleven tested compounds were found to be potent anticancer NCEs, which are under preclinical studies now. We also present recent results of virtual screening for HIV-1 microbicides.

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