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WAY2DRUG CHEMINFORMATICS PLATFORM FOR DRUG REPURPOSING

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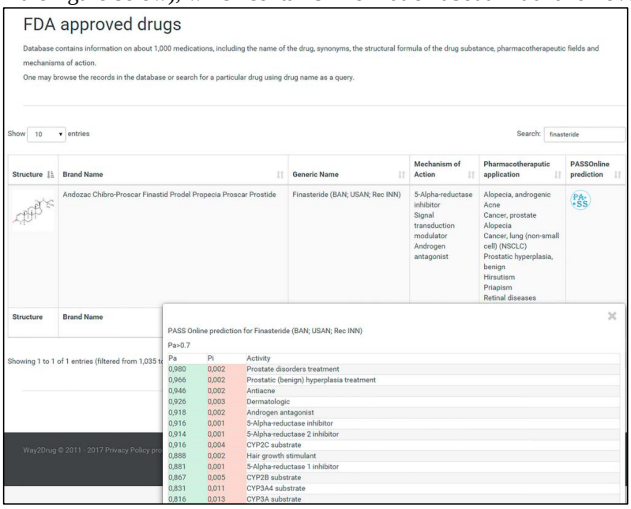
The Way2Drug platform [1] provides access to information about drugs launched in U.S. and Russian Federation, and the opportunities of computer-aided prediction of biological activity for drug-like compounds. Current computational components of the platform provide the prediction of interaction with molecular targets, influence on gene expression, pharmacotherapeutic and side effects, metabolism, acute toxicity in rats with four modes of administration, cytotoxicity, etc., by the structural formula of the drug-like compound.

Clicking on the "**PASS**" button in the right column of the table with the drug information, one obtains the predicted biological activity spectra (PBAS) for the particular drug (see prediction for Finasteride in the figure below), which contains information about initial and novel indications.



Besides, one may find drug substances similar to the structural formula of the compound used as a query by application MNA-, QNA- or PBAS-based similarity assessment. It is also possible to create the exclusive training set with the SAR Creator tool and obtain a (Q)SAR model using PASS or GUSAR software. This model could be applied for prediction of novel bioactivites of FDA approved drugs. Finally, some physicochemical and ADMET characteristics may be estimated for the compound under study using the computational tools of our Indian collaborators [2].

1. Way2Drug. – URL: http://www.way2drug.com/dr.
2. MPDS – URL: http://mpds.osdd.net/.

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