

**V. Poroikov<sup>1</sup>**  
**D. Druzhilovskiy<sup>1</sup>**  
**A. Rudik<sup>1</sup>**  
**P. Pogodin<sup>1</sup>**  
**D. Filimonov<sup>1</sup>**  
**A. Lagunin<sup>1,2</sup>**  
**N. Sastry<sup>3</sup>**

## WAY2DRUG CHEMINFORMATICS PLATFORM FOR DRUG REPURPOSING

<sup>1</sup> Institute of Biomedical Chemistry, 10 Bldg. 8, Pogodinskaya Str., Moscow, 119121, Russia;

<sup>2</sup> Medico-biological Faculty, Pirogov Russian National Research Medical University, Ostrovitianov str. 1, Moscow, 117997, Russia;

<sup>3</sup> Centre for Molecular Modeling, CSIR-Indian Institute of Chemical Technology, Hyderabad - 500007, India

*vladimir.poroikov@ibmc.msk.ru*


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.

**FDA approved drugs**

Database contains information on about 1,000 medications, including the name of the drug, synonyms, the structural formula of the drug substance, pharmacotherapeutic fields and mechanisms of action.  
One may browse the records in the database or search for a particular drug using drug name as a query.

Search:

Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application	PASSOnline prediction
	Andozac Chibro-Proscar Finastid Prodel Propecia Proscar Prostate	Finasteride (BAN; USAN; Rec INN)	5-Alpha-reductase inhibitor	Alopecia, androgenic Acne Cancer, prostate Signal transduction modulator Cancer, lung (non-small cell) (NSCLC) Prostatic hyperplasia, benign Hirsutism Priglamin Retinal diseases	<b>PASS</b>

PASS Online prediction for Finasteride (BAN; USAN; Rec INN)

Pa=0.7

Ps	Pi	Activity
0.990	0.002	Prostate disorders treatment
0.986	0.002	Prostate (benign) hyperplasia treatment
0.946	0.002	Anticancer
0.926	0.003	Dermatologic
0.918	0.002	Androgen antagonist
0.916	0.001	5-Alpha-reductase inhibitor
0.914	0.001	5-Alpha-reductase 2 inhibitor
0.916	0.004	CYP2C substrate
0.898	0.002	Hair growth stimulant
0.891	0.001	5-Alpha-reductase 1 inhibitor
0.857	0.003	CYP2B substrate
0.831	0.011	CYP3A4 substrate
0.816	0.013	CYP3A substrate

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 bioactivities 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/>.

*The work is supported by RSF-DST grant (project No. 16-45-02012 - INT/RUS/RSF/12).*