



Way2Drug Cheminformatics Platform for Drug Repurposing

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What is drug repurposing (DRP)?

“The process of finding new uses outside the scope of the original medical indication for existing drugs is also known as redirecting, repurposing, repositioning and reprofiling.”

Ashburn, T.T. and Thor, K.B. Drug repositioning: identifying and developing new uses for existing drugs. *Nat. Rev. Drug Discov.* **2004**, 3, 673–683.

THE 6TH ANNUAL

Drug Repositioning, Repurposing and Rescue Conference

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Global Health Focus: Repurposing for Rare
Diseases and Orphan Drug Development

June 27-28, 2017 | Chicago, IL

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Featured Speakers

Ron Alfa, MD, Ph.D., Vice President, Discovery
and Product, Recursion Pharmaceuticals

Bobbie Ann Austin, Ph.D., Program Officer, Drug
Development Partnership Programs, NCATS,
Office of the Director, National Institutes of
Health

Xavier Paoli, CCO and VP of R&D Operations,
PharNext SA

About the Conference

Join us in Chicago, where we will highlight the latest developments in the fields of drug repositioning, repurposing and rescue. This conference continues to serve as a global meeting place for those engaged in efforts to further drug development through new means of collaborations, including patient advocacy efforts and industry/academic/government cooperation.

A central focus at this year's event will be **the use of repurposing to find and develop new therapies for rare diseases**. Many rare diseases and disorders are serious conditions with no approved treatments. There is thus significant unmet needs for patients. The pharmaceutical industry has become engaged in a greater effort to develop drugs for these "orphan" indications. The FDA has supported this effort via various special protocols as well. There is a growing amount of evidence which suggests repurposing or repositioning research can greatly aid in the development of drugs for rare diseases. By using a more systematic approach, existing compounds are being tested for both common and neglected diseases faster and with more success.

Key Themes at This Year's Conference

PATIENT ADVOCACY EFFORTS

Emphasis on and engagement with patient advocacy groups, who are investing in drug repositioning efforts to an unprecedented degree

NEW PARTNERSHIPS

The conference will explore how new partnerships between various groups, including government, industry and academia are teaming up to advance repurposing efforts

<http://www.drugrepositioningconference.com/index/>

Drug Repurposing, Rescue, and Repositioning



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A New Journal for the Drug Repurposing Community

Hermann A.M. Mucke, PhD

European Editor, Drug Repurposing, Rescue, and Repositioning.
H.M. Pharma Consultancy, Wien, Austria.

Dear reader:

What you are holding in your hand—or what you are looking at on your screen—is the premier issue of the first journal that is exclusively dedicated to new medical uses of known pharmaceutically active compounds: *Drug Repurposing, Rescue, and Repositioning*.

So, another peer-reviewed journal for the medical sciences. Why should this be necessary? Hundreds exist already.

INTERDISCIPLINARY BROADNESS DEMANDS HIGH-LEVEL INTEGRATION

To be sure, it is not as if there were no proper opportunities to publish quality articles addressing drug repurposing. Pertinent articles appear in life sciences journals that specialize in medicinal chemistry, systems biology, molecular modeling,

has been missing until now. The product you are looking at is the first coordinated and well-supported attempt to remedy this.

OPTIMAL RESOURCE UTILIZATION IS NOT RECYCLING

Several common myths need to be dispelled before experts from so many diverse fields can collaborate with maximum efficacy. Number one is that drug repurposing, rescue, and repositioning is an inherently defensive concept, promoted by pharmaceutical companies to recoup at least part of their investments in the development of their failed late-stage drug candidates, or in drugs that had to be removed from the market for safety reasons. While such things do happen, this is only the “rescue” part of the story—and probably the least significant one in economic terms.

Nor is the *repositioning* of marketed drugs something as simple as what business developers call a line extension—such as expanding the approval of a cancer drug to include additional tumor types. Rather, drug repositioning implies the use in a different disease class, and while this often exploits

Drug Repurposing, Rescue, and Repositioning

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Current Volume: 1

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DRUG REPURPOSING NEWS

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Astellas continues IT-enabled Drug Repurposing Deal Drive with Excelra hook-up

June 10th 2016, Posted By: [Drug Repurposing Portal](#)



Astellas Pharma has struck its third drug repurposing agreement of the past 6 months. The latest collaboration sees Astellas start working with Excelra, an Indian informatics company that has landed 8 similar deals on the strength of its drug repurposing database and accompanying algorithms. For Excelra, the deal with Astellas marks an advance in its attempts to establish itself as a standalone business.

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GVK^{BIO}
Accelerating Research

Generate extra value from existing assets

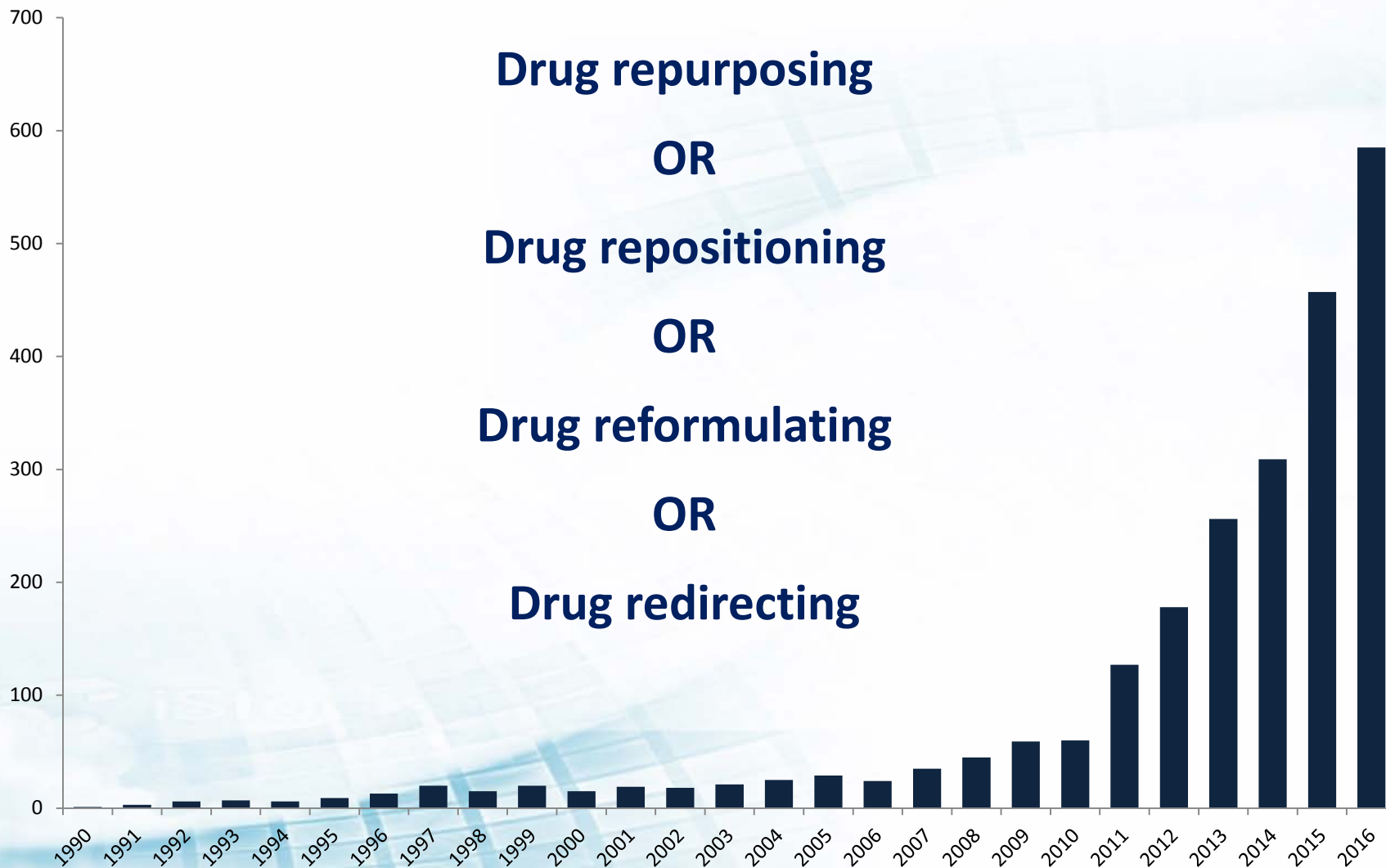
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<http://drugrepurposingportal.com/drug-repurposing-news.php>

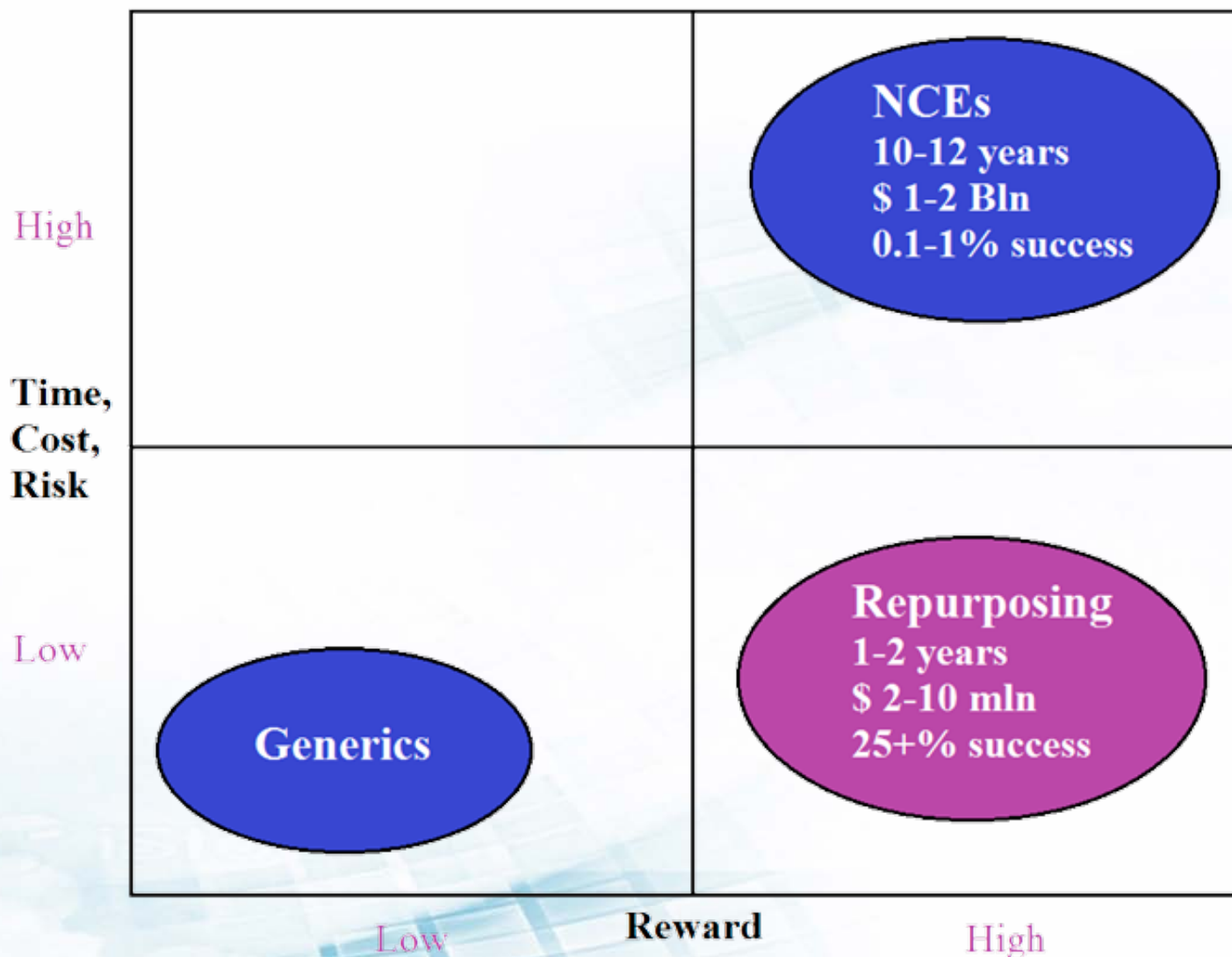


Web of Science statistics on drug repurposing (01.07.2017)





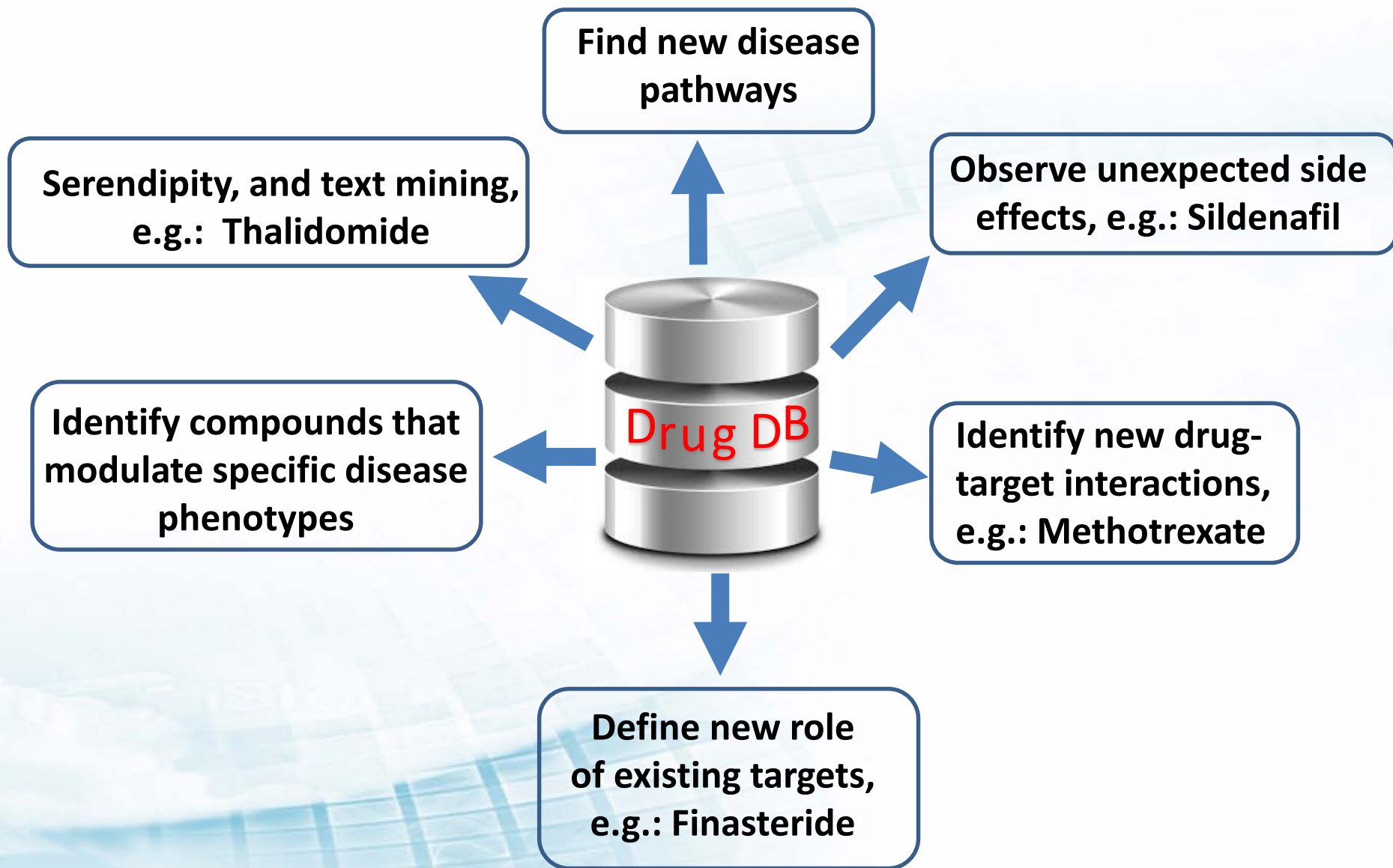
DRP: Time/Cost/Risk values



Ashburn T.T. and Thor K.B., 2004; Cavalla D., 2009.
 Flower D.R., 2013; Naylor S. and Schonfeld J.M., 2014.



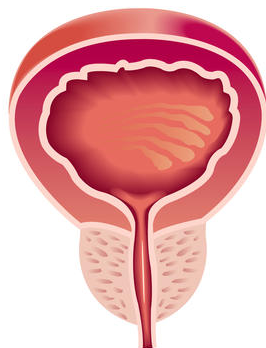
DRP: How it happens?





Define new role of existing targets: Finasteride

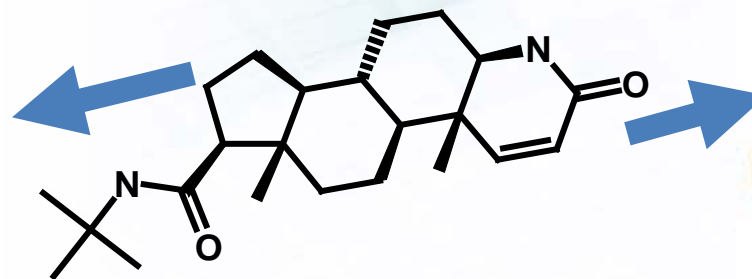
5-alpha-reductase inhibitor, Benign prostatic hyperplasia - 1992 (Proscar; Merck)



Normal prostate



Prostatic hypertrophy



**5-alpha-reductase inhibitor, Hair loss treatment - 1997
 Propecia (with a fivefold lower dose), had worldwide sales
 of US \$239 million in 2003**



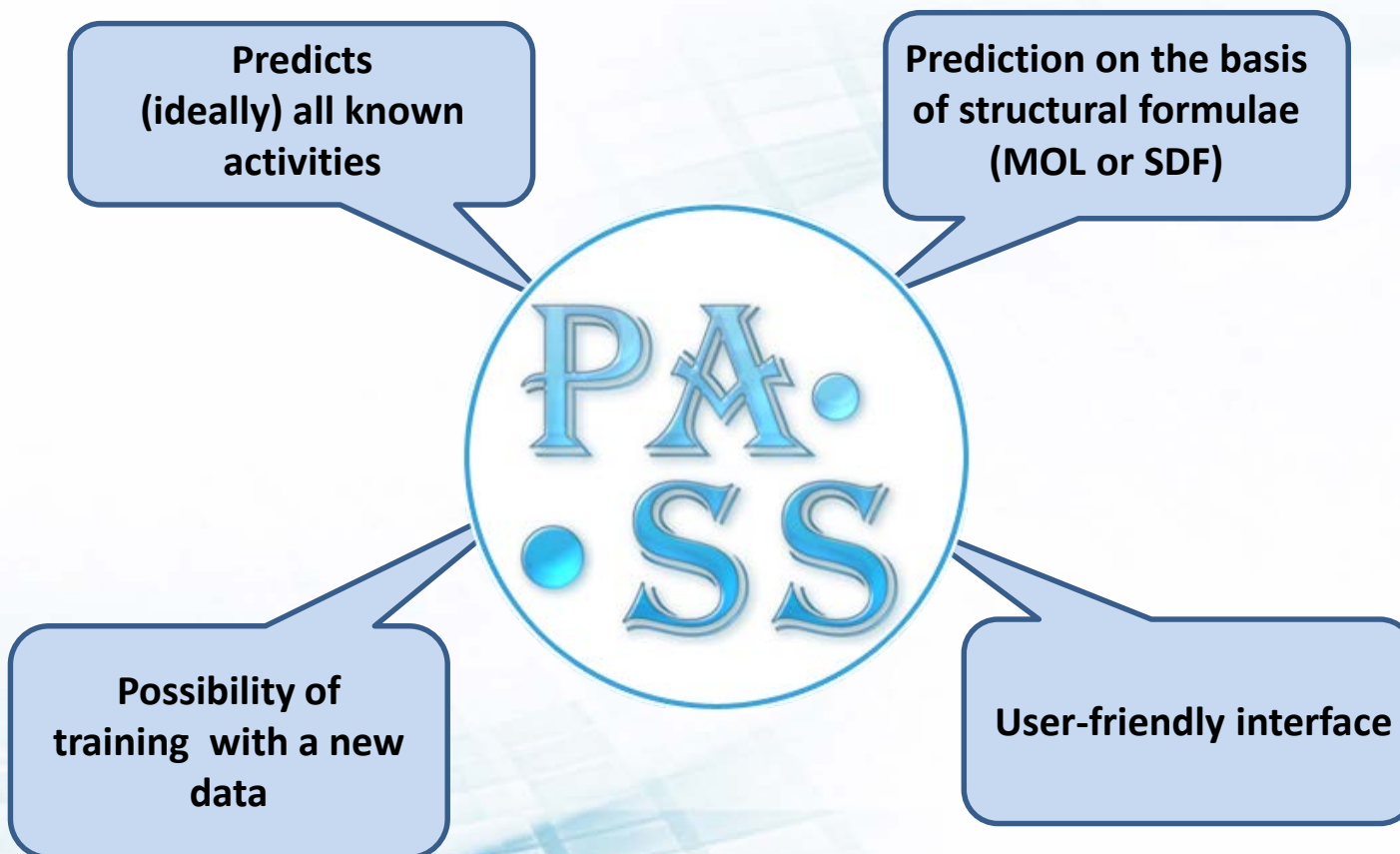
If you can predict the most probable targets
& new effects for the existing drugs by the
current chemoinformatics tools?

Yes, you can!

**Both structure-based and ligand-based methods
may be applied for this purpose: (Q)SAR,
pharmacophore sets, inverse docking, etc.**



Computer program for evaluating biological activity profiles (spectra)



PASS: Prediction of Biological Activity Spectra for Substances



PASS: Development & updating workflow

Full text publications, databases, presentations at conferences, etc.

Reliable data on structure and activity of drug-like molecules





Example of prediction for Clopidogrel

C:\PASS 2012\Drugs_Example.sdf

5x5 4x4 3x3 2x2 Molecular Structure MNA

1

2

3

4

5

6

Antithrombotic

Effects Mechanisms Toxicity Antitargets Metabolism Gene Exp

45 of 464 Possible Pharmacological Effects at Pa > Pi

0.951	0.004	Neuroprotector
0.886	0.005	Acute neurologic disorders treatment
0.723	0.006	Antithrombotic
0.712	0.004	Platelet aggregation inhibitor
0.618	0.019	Antianginal
0.553	0.013	Atherosclerosis treatment
0.463	0.048	Analgesic
0.385	0.009	Platelet antagonist
0.361	0.027	Stroke treatment
0.352	0.026	Angiogenesis stimulant
0.332	0.017	Anticoagulant
0.366	0.083	Diabetic neuropathy treatment
0.292	0.013	Analgesic, opioid
0.324	0.049	Antiinflammatory, ophthalmic
0.341	0.116	Spasmolytic, urinary
0.290	0.102	Cell adhesion molecule inhibitor
0.301	0.135	Neurodegenerative diseases treatment
0.261	0.098	Antipsoriatic
0.167	0.005	Acetylcholine release stimulant
0.199	0.057	Fibromyalgia syndrome treatment
0.236	0.104	Age-related macular degeneration treatment
0.202	0.075	Pancreatic disorders treatment
0.228	0.104	Amyotrophic lateral sclerosis treatment
0.375	0.254	Vasodilator, cerebral
0.176	0.058	Lipoprotein disorders treatment
0.156	0.047	Diabetic retinopathy treatment
0.257	0.150	Psychotropic

42 Substructure Descriptors; 0 new.

246 of 6400 Possible Activities
45 of 464 Possible Pharmacological Effects
79 of 3850 Possible Mechanisms of Action
106 of 321 Possible Toxic and Adverse Effects
5 of 118 Possible Antitargets
12 of 195 Possible Metabolism-Related Actions
17 of 1610 Possible Gene Expression Regulation
4 of 68 Possible Transporters-Related Actions

> <NAME> (0)
Clopidogrel

1/129 0.723 0.006 Antithrombotic

Clopidogrel: predicted vs. known activities

Abdominal pain
 Acute neurologic disorders treatment
 Agranulocytosis
 Allergic reaction
 Anaphylaxis
 Anemia
 Angioedema
 Angiogenesis inhibitor
 Antianginal
 Antiarthritic
 Anticoagulant
 Antineoplastic
 Antipsoriatic
 Antithrombotic
 Anxiety
 Arthralgia
 Atherosclerosis treatment
 Back pain
 Behavioral disturbance
 Blindness
 Bronchoconstrictor
 Cardiotoxic
 Cataract
 CCL4 expression enhancer
 CCL5 expression enhancer
 Chest pain
 Colic
 Colitis

Conjunctivitis
 Consciousness alteration
 Constipation
 Cough
 CYP2 substrate
 CYP2C substrate
 CYP2C19 inhibitor
 CYP2C19 substrate
 CYP2C9 inhibitor
 CYP3A substrate
 CYP3A4 substrate
 Cytochrome P450 inhibitor
 Dermatitis
Dermatologic
 Dizziness
 Drug eruption
 Dyspepsia
 Emetic
 Eosinophilia
 Erythema
 Erythema multiforme
 Exanthema
 Flatulence
GP IIb/IIIa receptor antagonist
 Hallucinogen
 Headache
 Heart failure
 Hematotoxic
 Hemorrhage

Henoch-Schonlein purpura
 Hepatic failure
 Hepatitis
 Hepatotoxic
 Hypertensive
 Hyperthermic
 Hypotension
 Infection
 Insomnia
 Lassitude
 Leukopenia
 Lichen planus
 Lichenoid eruption
 Malaise
 Menstruation disturbance
 Myalgia
 Nausea
 Necrosis
 Nephrotoxic
 Neuroprotect
 Neutropenia
 Ocular toxicity
 Pain
 Pancreatitis
 Pancytopenia
 Platelet aggregation inhibitor
 Platelet antagonist
 Pruritus
 Pulmonary embolism

Purinergic P2 antagonist
 Purinergic P2T antagonist
 Purinergic P2Y antagonist
 Purinergic P2Y12 antagonist
 Purinergic receptor antagonist
 Purpura
 Renal colic
 Reproductive dysfunction
 Rhinitis
 Sensory disturbance
 Serum sickness
 Shock
 Sinusitis
 Sleep disturbance
 Stomatitis
 Syncope
 THBS1 expression enhancer
 Thrombocytopenia
Toxic
 Toxic epidermal necrolysis
 Toxic, gastrointestinal
 TP53 expression enhancer
 Urticaria
 Vasculitis
 Vertigo
 Vision disturbance

Blue – predictions coincided with the experiment.
Black – unpredictable activities.
Red – unpredicted activities.

PharmaExpert: Interpretation of the predictions

PharmaExpert

Prediction & Interpretation - H:\DATABASES\DRUG-BANK\approved (PASS2014).SDF. 57/1278

Cholecalciferol, Menadione, Adenosine triphosphate, L-Proline, Adenine, L-Asparagine, Pravastatin, Fluvoxamine, Valsartan, Ranipril, Masoprocol

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Pa	Pi	Activity	Predicted value descending
0.791	0.009	Abdominal distension	
0.791	0.011	Toxic, vascular	
0.775	0.003	Diuretic	
0.785	0.014	Excitability	
0.778	0.008	Dry eye	
0.782	0.017	Glucanase 2-dehydrogenase (acceptor) inhibitor	
0.763	0.002	Dermatomyositis	
0.762	0.005	Vasodilator	
0.725	0.016	Inflammation	
0.712	0.007	Gynaecostasia	
0.709	0.005	Scleroderma	
0.714	0.017	Diplopia	
0.707	0.013	Induration	
0.714	0.023	Atrial natriuretic peptide agonist	0.714 0.023
0.710	0.019	Stevens-Johnson syndrome	
0.706	0.016	Dyspnea	
0.702	0.016	Swelling	
0.691	0.007	QT interval prolongation	
0.684	0.006	Immunotoxin	
0.695	0.018	Anemia	
0.701	0.026	Breast pain	
0.688	0.018	Angioedema	
0.671	0.005	Carcinogenic, mouse, female	
0.665	0.006	Vasodilator, coronary	
0.656	0.001	Henoch-Schönlein purpura	
0.681	0.034	TGFB1 expression inhibitor	
0.661	0.015	Stidor	
0.671	0.035	Taste disturbance	
0.631	0.007	Psychostimulant	0.470 0.038
0.620	0.007	Antihypertensive	0.620 0.007

Substance intended to prevent damage to the brain or spinal cord from ischemia, stroke, convulsions, or trauma. Some must be administered before the event, but others may be effective for some time after.

UniProt ID	Gene name(s)	Species

KEGG | NCI Pathways | Reactome | Gene Ontology

- 0.714 0.023 Atrial natriuretic peptide agonist
 - HIF-1 signaling pathway
- 0.401 0.002 Angiotensin-converting enzyme inhibitor
 - Chagas disease (American trypanosomiasis)
 - Hypertrophic cardiomyopathy (HCM)
- 0.390 0.039 Interleukin 2 agonist
 - Renin-angiotensin system
- 0.386 0.005 P-glycoprotein 1 inhibitor
 - ABC transporters
- 0.343 0.152 Insulin like growth factor 1 agonist
 - Adherens junction
 - Bile secretion
 - Endocytosis
 - Focal adhesion
 - Glioma
 - HIF-1 signaling pathway
 - Long-term depression
 - Melanoma
 - Oocyte meiosis
 - Pathways in cancer

Therapeutic effects

- Analgesic
- Anesthetic, non-opioid
- Antianginal
- Antidiabetic
- Antidiabetic symptomatic
- Antidiarrheal
- Antiglaucomatous
- Antihypertensive
- Antinflammatory
- Antischemic, cerebral
- Antimigraine
- Antipneumonia
- Atherosclerosis treatment
- Cardiotonic
- Chronic obstructive pulmonary disease treatment
- Diuretic
- Heart failure treatment
- Hypolipemic
- Myocardial infarction treatment

Side effects

- Alpecia (hair loss)
- Alveolitis
- Anaphylaxis
- Anemia
- Angioedema
- Anuria
- Bone marrow suppression
- Bullous pemphigoid
- Cholestatic jaundice
- Cytotoxic
- Diarrhea
- Dizziness
- Dysethesia
- Edema
- Exanthema

Pa > Pi Antihypertensive

Pa > Pi Angiotensin-converting enzyme inhibitor

Pa = None Mutagenic

Number of selected compounds: 45

Poroikov V. et al. PharmaExpert: diseases, targets and ligands – three in one. In: *QSAR and Molecular Modelling in Rational Design of Bioactive Molecules*. Ankara (Turkey), CADD & D Society, 2005, p.514-515.



PharmaExpert: Search for multitargeted antineoplastic agents

PharmaExpert

File Tools View Help

Pa > 0.100

36 from 23768

Prediction & Interpretation - G:\DATABASES\PRESTWICK\PRESTWICK-4\prestwick_chemical_library_cured (PASS2014)-20.SDF. 1/1074

Az Guanidine-90 Allantoin Acetazolamide Metformin hydrochloride Isotretinoin acetate Amloride hydrochloride dihydrate Hydrochlorothiazide Sulfaguanidine Meticranolol Benzocaine

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Pa Pi Types of Activities Pa-Pi descending

Pa Pi <chemical_name>

Pa	Pi	Types of Activities
0.989	0.000	Pterin deaminase inhibitor
0.931	0.003	Pure red cell aplasia
0.916	0.001	ANCA-positive vasculitis
0.872	0.000	Sepiapterin deaminase inhibitor
0.837	0.004	Peripheral neuropathy
0.837	0.007	ANKRD1 expression enhancer
0.830	0.004	Status epilepticus
0.819	0.001	Queuine tRNA-ribosyltransferase inhibitor
0.814	0.004	Splenomegaly
0.812	0.033	Bone marrow suppression
0.779	0.004	MAPT expression inhibitor
0.804	0.029	Renin release stimulant
0.765	0.024	Neural tube defect
0.730	0.001	Purine biosynthesis inhibitor
0.723	0.004	Mediator release inhibitor
0.717	0.006	Mitochondrial processing peptidase inhibitor
0.727	0.043	Hyperpigmentation
0.680	0.002	Pteridine reductase inhibitor
0.676	0.005	Undecaprenyl-phosphate mannosyltransferase inhibitor
0.683	0.025	Stevens-Johnson syndrome
0.684	0.027	Multiple organ failure
0.654	0.011	ADP-thymidine kinase inhibitor
0.671	0.031	Nail discoloration
0.645	0.005	Thiol oxidase inhibitor
0.666	0.042	Antineoplastic
0.664	0.047	Hallucination, visual
0.646	0.038	CASP10 expression enhancer
0.614	0.010	Antineoplastic (renal cancer)
0.642	0.062	TSC2 expression enhancer
0.587	0.009	Natural killer cell stimulant
0.580	0.002	Folate antagonist
0.596	0.020	Allergic conjunctivitis treatment
0.605	0.037	Hemolysis
0.569	0.011	Thrombocytopenia inhibitor
0.557	0.002	Xanthine dehydrogenase inhibitor
0.606	0.059	SP1 expression enhancer
0.581	0.041	Acute neurologic disorders treatment
0.580	0.041	Alopecia (hair loss)
0.565	0.032	Nephritis
		Substance stimulates expression of ANKRD1.

Multitargeted actions

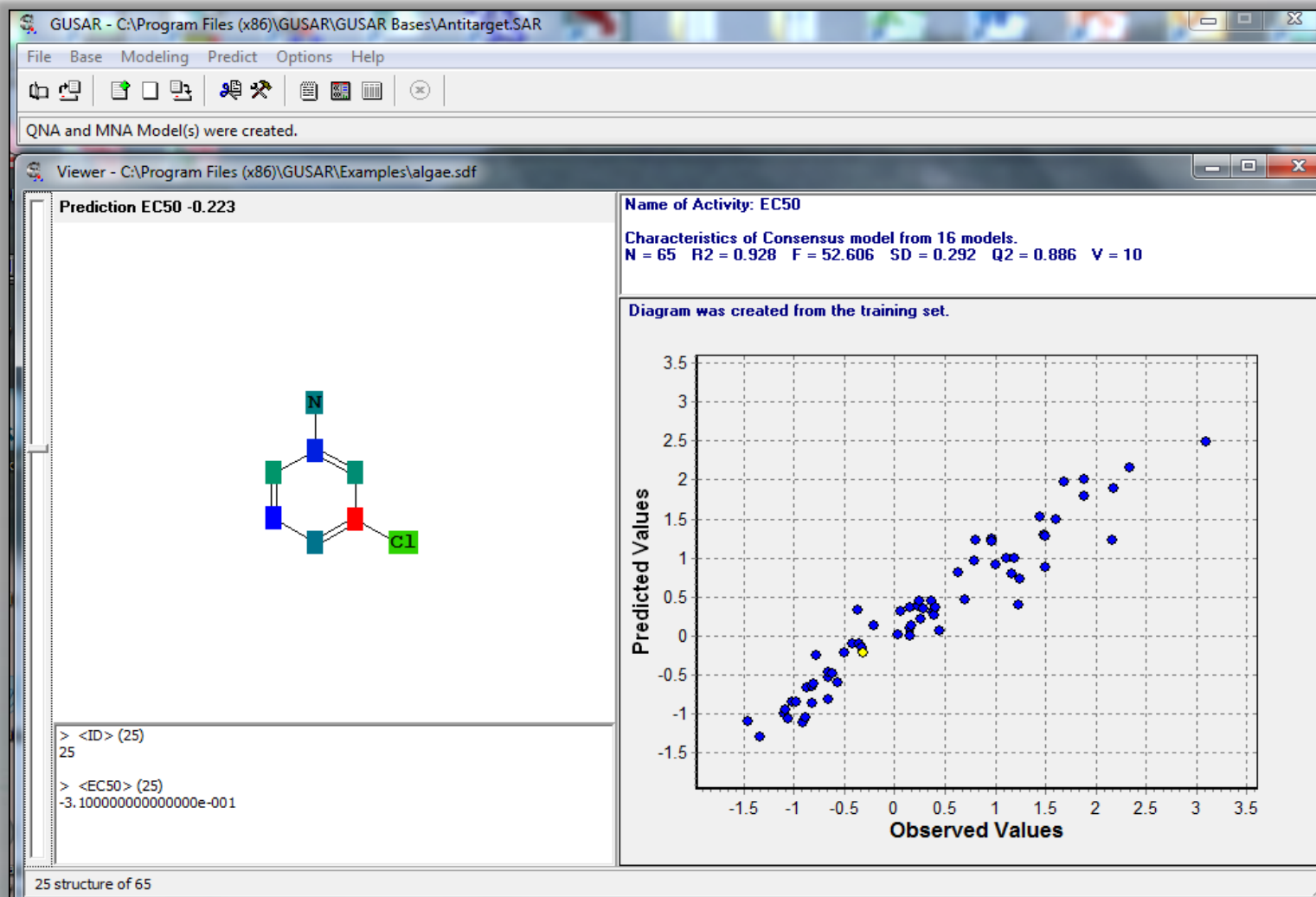
Effects: Antineoplastic (breast cancer) Number of targets: 3

Run Load Save

No	Pa	Number	Activity type	Activity type	Activity type
462	0.632	2	Cyclic GMP phosphodiesterase inhibitor	Epidermal growth factor receptor kinase inhibitor	Vascular endothelial growth factor 2 antagonist
463	0.632	2	Cyclic GMP phosphodiesterase inhibitor	ErbB-2 antagonist	Vascular endothelial growth factor 2 antagonist
464	0.632	2	Cyclic GMP phosphodiesterase inhibitor	MAP kinase kinase inhibitor	Vascular endothelial growth factor 2 antagonist
465	0.632	2	Cyclic GMP phosphodiesterase inhibitor	Platelet activating factor beta antagonist	Vascular endothelial growth factor 2 antagonist
466	0.632	1	Cyclic GMP phosphodiesterase inhibitor	Transcription factor NF kappa B inhibitor	Vascular endothelial growth factor 2 antagonist
467	0.632	3	Cyclic GMP phosphodiesterase inhibitor	Tyrosine kinase inhibitor	Vascular endothelial growth factor 2 antagonist
468	0.632	1	Cyclic GMP phosphodiesterase inhibitor	Vascular endothelial growth factor 1 antagonist	Vascular endothelial growth factor 2 antagonist
469	0.632	3	Cyclic GMP phosphodiesterase inhibitor	Vascular endothelial growth factor antagonist	Vascular endothelial growth factor 2 antagonist
470	0.322	1	Cyclin-dependent kinase 2 inhibitor	Tyrosine kinase inhibitor	Vascular endothelial growth factor 2 antagonist
471	0.322	1	Cyclin-dependent kinase 2 inhibitor	Vascular endothelial growth factor antagonist	Vascular endothelial growth factor 2 antagonist
472	0.632	2	EphB2 kinase inhibitor	Epidermal growth factor antagonist	Vascular endothelial growth factor 2 antagonist

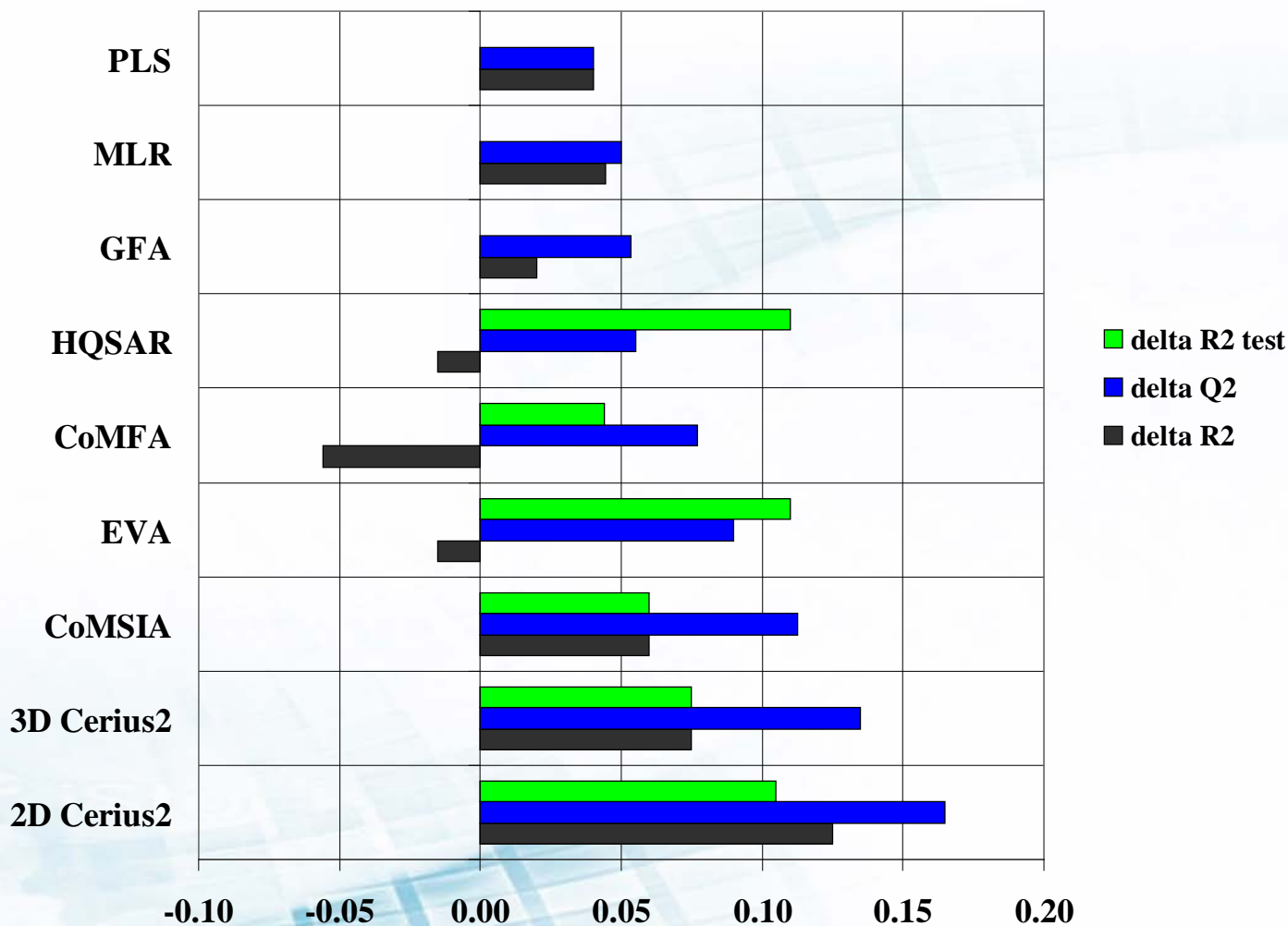


GUSAR: General Unrestricted Structure-Activity Relationships





GUSAR: Superiority in performance in comparison with some other (Q)SAR methods





PASS: Methods and some applications

Filimonov D.A., Lagunin A.A., Gloriozova T.A., Rudik A.V., Druzhilovskiy D.S., Pogodin P.V., Poroikov V.V. (2014). Prediction of the biological activity spectra of organic compounds using the PASS online web resource. *Chemistry of Heterocyclic Compounds*, 50: 444-457.

Filimonov D.A., Poroikov V.V. (2008). Probabilistic Approach in Virtual Screening. In: *Chemoinformatics Approaches to Virtual Screening*. Alexander Varnek and Alexander Tropsha, Eds. RSC Publishing, 182-216.

Filimonov D.A., Poroikov V.V. (2006). Prediction of biological activity spectra for organic compounds. *Russian Journal of General Chemistry*, 50: 66-75.

Chemical Similarity Assessment through Multiset Neighborhood of Atoms: Definition and Comparison with the Other Descriptors

Denis Filimonov, Vladimir Poroikov, Yulia Bronina, and Terence Greenaway

Journal of Chemical Information and Modeling, 2009, 9, 1233-1240

Received September 10, 2008

A new method for assessment of molecular similarity based on original definitions of chemical similarity is described. The novelty of molecular similarity method with the method is compared with that of the methods of other approaches. The same evaluation set is used to predict the binding power of 120 molecules and the comparison of 2 descriptors. The results show that proposed method performs better than the other approaches.

INTRODUCTION

Assessment of chemical similarity is widely used in computer-aided drug design (CADD) to find new molecules or to select the most promising ones. The most common methods for similarity assessment are based on the comparison of molecular fingerprints. The most popular methods are the Tanimoto coefficient, the Dice coefficient, and the Jaccard coefficient. The most common methods for similarity assessment are based on the comparison of molecular fingerprints. The most popular methods are the Tanimoto coefficient, the Dice coefficient, and the Jaccard coefficient.

RESULTS

The results of the comparison of the proposed method with the other methods are presented in Table 1. The proposed method shows the best results in terms of the number of correct predictions and the number of false predictions.

Robustness of Biological Activity Spectra Predicting by Computer Program PASS for Nontoxic Set of Chemical Compounds

V. V. Poroikov, V. D. A. Filimonov, T. A. Gloriozova, A. A. Lagunin, and A. V. Rudik

Journal of Chemical Information and Modeling, 2008, 8, 1233-1240

Received March 15, 2008

The computer program PASS provides simultaneous prediction of several kinds of biological activity spectra for organic compounds. The PASS prediction of activity spectra for nontoxic set of chemical compounds is investigated. The results show that the proposed method performs better than the other methods.

INTRODUCTION

The PASS program is a software tool for the prediction of biological activity spectra for organic compounds. The program is based on the probabilistic approach to the prediction of biological activity spectra.

RESULTS

The results of the prediction of biological activity spectra for nontoxic set of chemical compounds are presented in Table 1. The proposed method shows the best results in terms of the number of correct predictions and the number of false predictions.

BIOINFORMATICS APPLICATIONS NOTE

PASS: prediction of activity spectra for biologically active substances

Alsey Lagunin, Alisa Stepanovichna, Dmitri Filimonov and Vladimir Poroikov

Journal of Chemical Information and Modeling, 2000, 4, 1233-1240

Received November 18, 1999; revised December 11, 1999; accepted on March 21, 2000

ABSTRACT

The PASS program is a software tool for the prediction of biological activity spectra for organic compounds. The program is based on the probabilistic approach to the prediction of biological activity spectra.

INTRODUCTION

The PASS program is a software tool for the prediction of biological activity spectra for organic compounds. The program is based on the probabilistic approach to the prediction of biological activity spectra.

Discriminating between Drugs and Nondrugs by Prediction of Activity Spectra for Substances (PASS)

Denis Filimonov, Vladimir Poroikov, Yulia Bronina, and Terence Greenaway

Journal of Chemical Information and Modeling, 2009, 9, 1233-1240

Received September 10, 2008

A new method for assessment of molecular similarity based on original definitions of chemical similarity is described. The novelty of molecular similarity method with the method is compared with that of the methods of other approaches. The same evaluation set is used to predict the binding power of 120 molecules and the comparison of 2 descriptors. The results show that proposed method performs better than the other approaches.

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PASS Biological Activity Spectrum Prediction in the Enhanced Open NCI Database Browser

Denis Filimonov, Vladimir Poroikov, Yulia Bronina, and Terence Greenaway

Journal of Chemical Information and Modeling, 2009, 9, 1233-1240

Received September 10, 2008

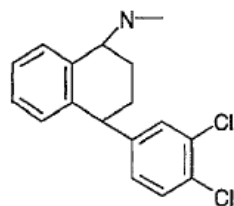
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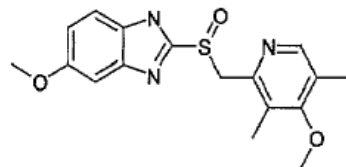


Our experience in DRP: Prediction for Top200 drugs



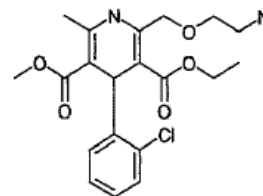
Sertraline

Adrenergic transmitter uptake inhibitor (0.770)
Antiparkinsonian (0.609)
Leukopoiesis inhibitor (0.582)
Cocain dependency treatment (0.560)
Acute neurologic disorders treatment (0.541)



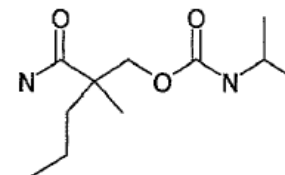
Omeprazole

TNF-alpha release inhibitor (0.658)
Atherosclerosis treatment (0.541)



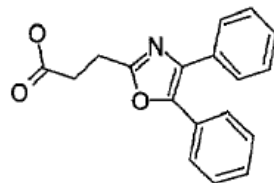
Amlodipine

Antineoplastic enhancer (0.608)
Multiple sclerosis treatment (0.508)



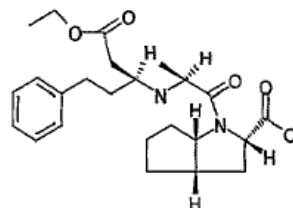
Carisoprodol

Angiogenesis inhibitor (0.569)
Multiple sclerosis treatment (0.549)



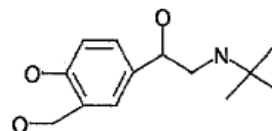
Oxaprozin

Bone formation stimulant (0.785)
Interleukin 1 antagonist (0.640)



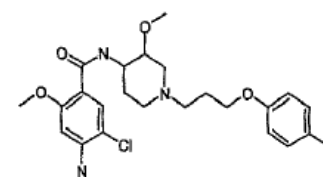
Ramipril

Multiple sclerosis treatment (0.589)
Cognition disorders treatment (0.562)
Antiarthritic (0.454)



Albuterol

Antiobesity (0.784)



Cisapride

Irritable Bowel syndrome therapy (0.720)
Rhinitis treatment (0.524)

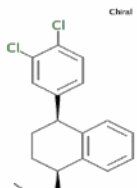
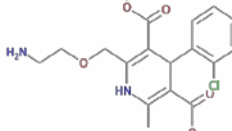
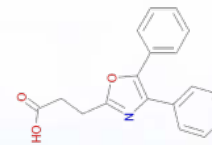
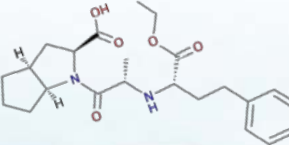
FIGURE 3 Examples of biological activities predicted de novo for some pharmaceuticals from the Top 200 list, which may become a reason for a new application. Pa values are given in brackets.



Four new indications confirmed by further studies

In 2001 we published predictions of new effects for 8 medicines from the list of Top200 Drugs [1].

Which predictions are confirmed? (informational search, September 2014)

				Ref.
	Sertraline	Cocain dependency treatment	+	[2]
	Amlodipine	Antineoplastic enhancer (moderate BCRP/ABCG2 inhibitor)	+	[3]
	Oxaprozin	Interleukin 1 antagonist (Inhibitor of production of Interleukin 1β)	+	[4]
	Ramipril	Antiarthritic	+	[5]

1. Poroikov V. et al. *SAR and QSAR Environ. Res.*, **2001**, 12: 327-344.
2. Mancino M.J. et al. *J. Clin. Psychopharmacol.*, **2014**, 34: 234–239.
3. Takara K. et al. *Mol. Med. Rep.*, **2012**, 5: 603-609.
4. Rainsford K.D. et al. *Inflammopharmacology*, **2002**, 10: 85–239.
5. Shi Q. et al. *Arthritis Res. Ther.*, **2012**, 14: R223.

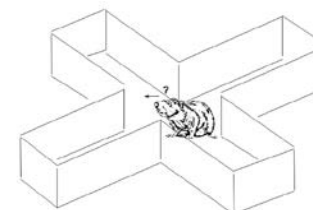


Nootropic effect in some antihypertensive drugs?

1



3



4

Perindopril in dose of 1 mg/kg, and quinapril and monopril in doses of 10 mg/kg improved the patrolling behavior in the maze, like piracetam and meclofenoxate (in doses of 300 and 120 mg/kg, respectively).

2

Name	Pa (Nootropic effect), %
Captopril	44,6
Enalapril	65,5
Lisinopril	61,8
Perindopril	60,9
Quinapril	65,1
Ramipril	63,3
Monopril	30,9
Piracetam	81,7
Amlodipin	-
Hydrochlorothiazide	-

5

BMJ Open 2013;3:e002881 doi:10.1136/bmjopen-2013-002881

Geriatric medicine

Effects of centrally acting ACE inhibitors on the rate of cognitive decline in dementia

Yang Gao^{1,2}, Rónán O’Caoimh¹, Liam Healy¹, David M Kerins^{3,4}, Joseph Eustace⁵, Gordon Guyatt⁶, David Sammon², D William Molloy^{1,7}

+ Author Affiliations

Correspondence to
 Professor D William Molloy; w.molloy@ucc.ie

Published 22 July 2013



PASS Online: The first publication & Some comments

BIOINFORMATICS APPLICATIONS NOTE

Vol. 16 no. 8 2000
Pages 747-748

PASS: prediction of activity spectra for biologically active substances

Alexey Lagunin, Alla Stepanchikova, Dmitrii Filimonov and Vladimir Poroikov

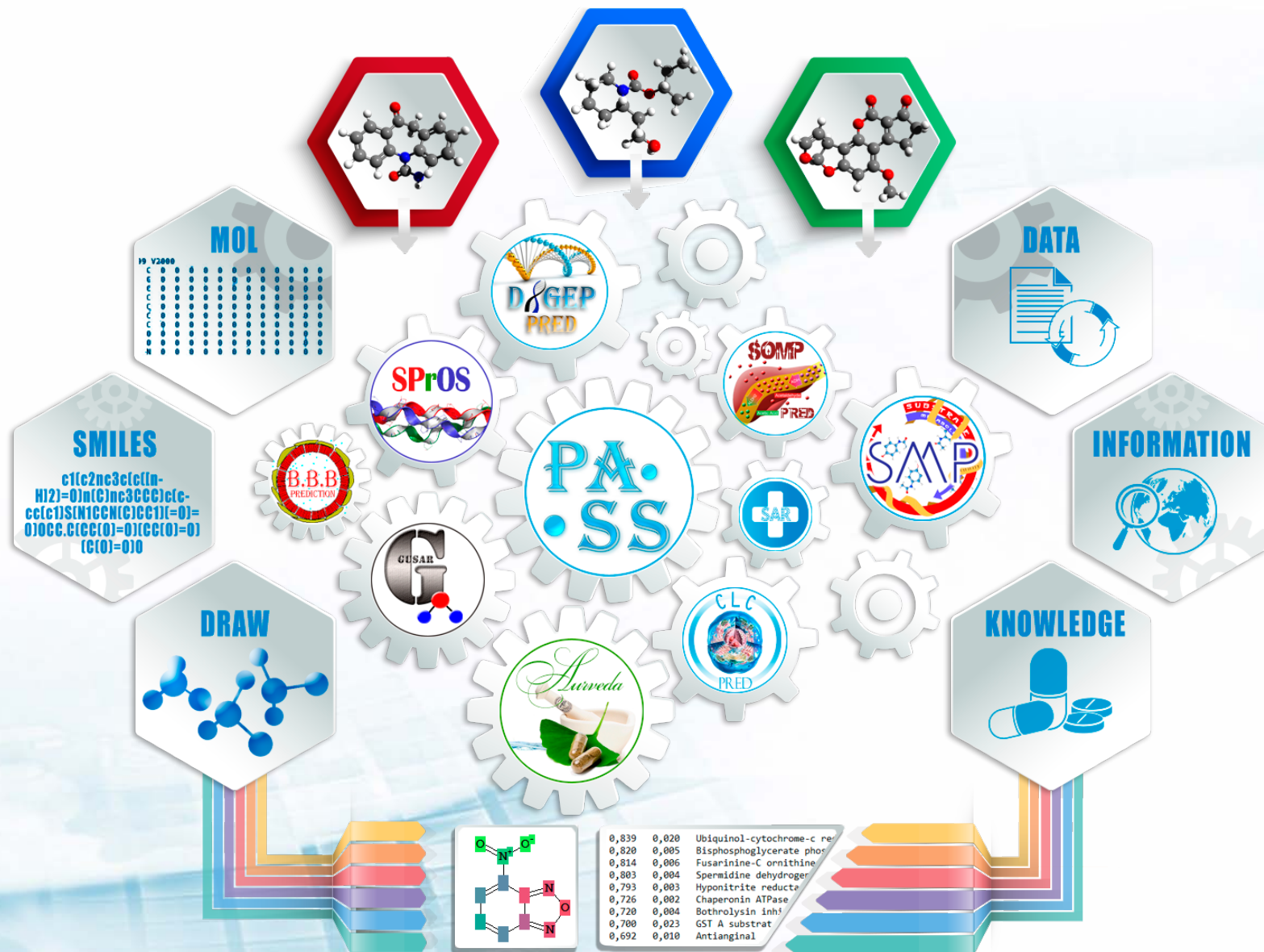
Laboratory of Structure-Function Based Drug Design, Institute of Biomedical Chemistry RAMS, Moscow, Pogodinskaya str., 10, 119832, Russia

Received on November 26, 1999; revised on December 11, 1999; accepted on March 21, 2000

“One of the earliest and most widely used examples of data-mining target elucidation is the continuously curated and expanded Prediction of Activity Spectra for Substances (PASS) software, which was assimilated from the bioactivities of more than 270,000 compound-ligand pairs.”

Mervin L.H., ... , Bender A. J. Cheminform., 2015, 7: 51.

Way2Drug web platform





Way2Drug available online

India

Russia

Ukraine

Mexico

China

United States

Egypt

Kazakhstan

Brazil

Other

Cross-browser and cross-platform support

630 818 molecules

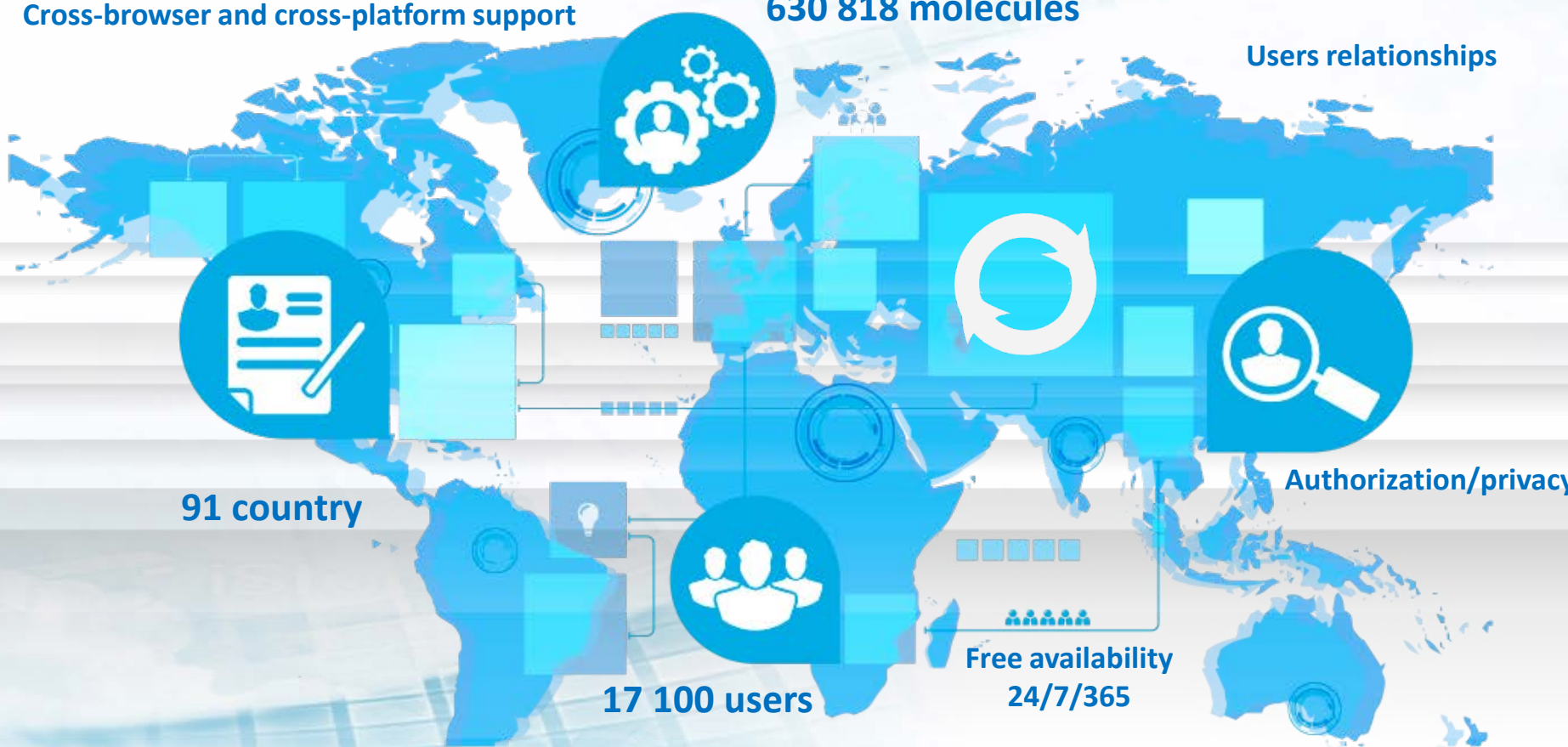
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European Journal of Medicinal Chemistry 43 (2008) 1015–1024

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Original article

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Bioorganic & Medicinal Chemistry Letters 15 (2005) 2145–2148

Bioorganic & Medicinal Chemistry Letters

ANTIMICROBIAL AGENTS AND CHEMOTHERAPY, Jan. 2003, p. 174–180
0066-4804/03/S08.00+0 DOI: 10.1128/AAC.47.1.174-180.2003
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Vol. 47, No. 1

In Vitro Activities of 7-Substituted 9-Chloro and 9-Amino-2-Methoxyacridines and Their Bis- and Tetra-Acridine Complexes against *Leishmania infantum*

Carole Di Giorgio,^{1*} Florence Delmas,¹ Nathalie Filloux,² Maxime Robin,² Lactitia Seferian,²

azolines revisited: search for novel anxiolytic

rganic Chemistry, 2013, Vol. 39, No. 2, pp. 202–210. © Pleiades Publishing, Ltd., 2013.
E. Smirnova, H. Do Tkhi Tkhu, Tkhanh Tra Nguen, G.N. Apryshko, O.S. Zhukova, N.I. Medvedeva, T.I. Nazyrov, E.V. Tret'yakova, D.V. Kazakov, F.E. Safarov, G.A. Tolstikov, 2013, published in Bioorganicheskaya Khimiya, 2013, Vol. 39, No. 2, pp. 230–237.

Chemistry of Heterocyclic Compounds, Vol. 49, No. 1, April, 2013 (Russian Original Vol. 49, No. 1, January, 2013)

A DRUG MYSTERY OF HETEROCYCLES: VARIOUS MOLECULES FOR ONE TARGET OR ONE COMPOUND FOR MULTIPLE TARGETS?

Bioorganic & Medicinal Chemistry 20 (2012) 2930–2939

Structure, and Pharmacological Activity of 1-(13R,17R)-Epoxy-(13R,17R)-trioxolane Abietic Acid

UDC 547.67

V.I. Zvarych, R.Ya. Musyanovych, V.G. Chervetsov, O.Z. Komarovska-Porokhnyavets, M.V. Stasevych, V.P. Novikova, Department of Technology of Biologically Active Substances, Pharmacy and Biotechnology

Contents lists available at SciVerse ScienceDirect

Bioorganic & Medicinal Chemistry

journal homepage: www.elsevier.com/locate/bmc

SYNTHESIS OF NEW DERIVATIVES OF 2-ACYLISOTHIOCYANATE OF 1-NITRO-9,10-ANTHRAQUINONE WITH

УДК 378.147:547

Identification of novel isocytosine derivatives as xanthine oxidase inhibitors from a set of virtual screening hits

European Journal of Medicinal Chemistry 45 (2010) 2606–2612

Contents lists available at ScienceDirect

European Journal of Medicinal Chemistry

Комбинаторная химия в высшей школе: десятилетний опыт научных учебных и организационных проектов

Е.В. Бабаев



Way2Drug Drug Repurposing Platform

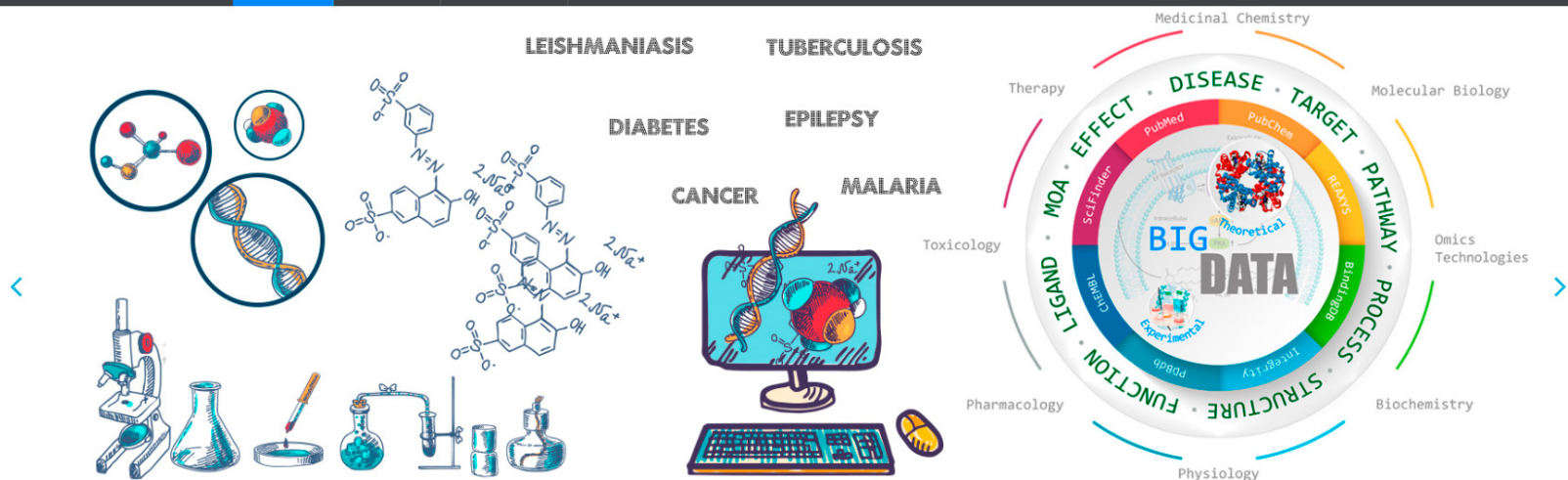
Way2Drug PREDICTIVE SERVICES
Understanding Chemical-Biological Interactions

Molecular Property Diagnostic Suite (MPDS™)
An Open Source Chemoinformatics Portal

A Knowledge Based Approach to Drug Repurposing for Socially Important and Rare Diseases.

RSF - DST Project # 16-45-02012 - INT/RUS/RSF/12

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<p>Global research</p> <p>Discovery of new safe and potent medicines based on cutting-edge knowledge of a certain pathology at the molecular, cellular, tissue and organism levels, and the most</p>	<p>Referential ideas</p> <p>Integration of the currently available biomedical and chemical data, extraction of the useful information and generation of new knowledge in the field of chemical-biological</p>	<p>New services</p> <p>Computational predictions based on perpetually updated information, which overcome the limits of the current knowledge and allow to expand predictive functionalities of</p>	<p>Collaboration</p> <p>Providing framework for effective interaction of researchers working in the multidisciplinary field of drug design & discovery, to combine their complementary background.</p>
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<http://www.way2drug.com/dr>

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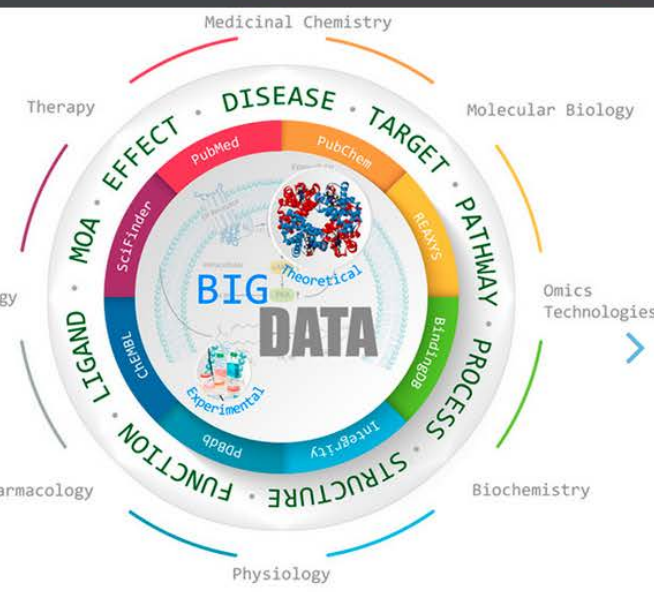
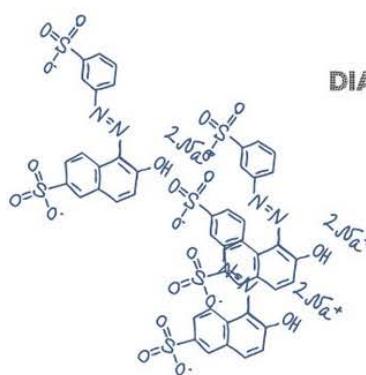
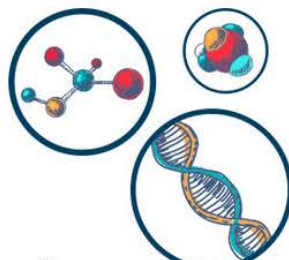
TUBERCULOSIS

DIABETES

EPILEPSY

CANCER

MALARIA



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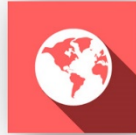


Way2Drug DRP: Pharmacotherapeutic Areas

Orphan diseases

A disease is considered rare* when no more than **1 out of 2000** people suffer from it

Estimates indicate **>300 million** people living with a rare disease worldwide



Tests for **3500** rare diseases are now available...



...but only about **400 rare diseases** have therapies



80% of rare diseases have a genetic component

50% of those affected by rare diseases are children

Reported rates of medication adherence range from **58-65%**



There are **6,000 to 7,000** rare diseases



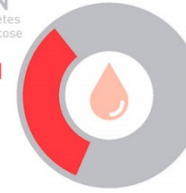
DIABETES

DIABETES IS ON THE RISE

422 MILLION adults have diabetes

3.7 MILLION deaths due to diabetes and high blood glucose

1.5 MILLION deaths caused by diabetes



Epilepsy

Epilepsy is a condition that affects the brain and causes repeated seizures



65 MILLION people worldwide currently live with epilepsy.

200,000 people per year are diagnosed with epilepsy

TUBERCULOSIS (TB) FACTS

TB is a serious disease. It can infect many body parts, but is most common in the lungs.



9,000,000 people fell ill with TB

TB is a leading cause of death in patients with HIV.



1,500,000 died from the disease*

MALARIA FACTS

Malaria is a serious disease that is **PREVENTABLE** and **TREATABLE**.

97 countries and territories had ongoing malaria transmission in 2015.



a child dies from malaria in Sub-Saharan Africa.



Cancer Facts

approximately 14 million new cases



The disease accounts for **7.4 million deaths worldwide**. It's the leading cause of death worldwide, causing around 13% of all deaths worldwide



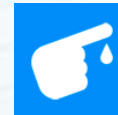
Tuberculosis



Leishmaniasis



Malaria



Diabetes



Cancer



Epilepsy

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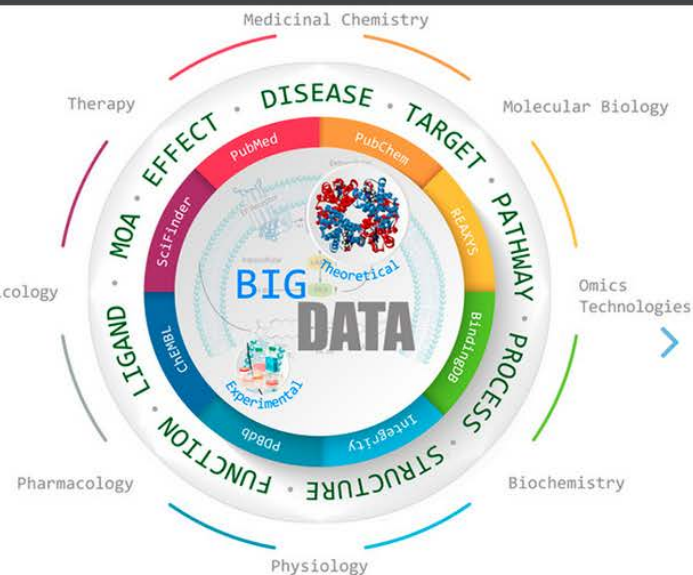
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- SAR Creator
- PASS Online Total
- PASS Online Selector
- MNA/QNA Similarity

LEISHMANIASIS TUBERCULOSIS
DIABETES EPILEPSY
CANCER MALARIA



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SAR Creator

PASS Online Total

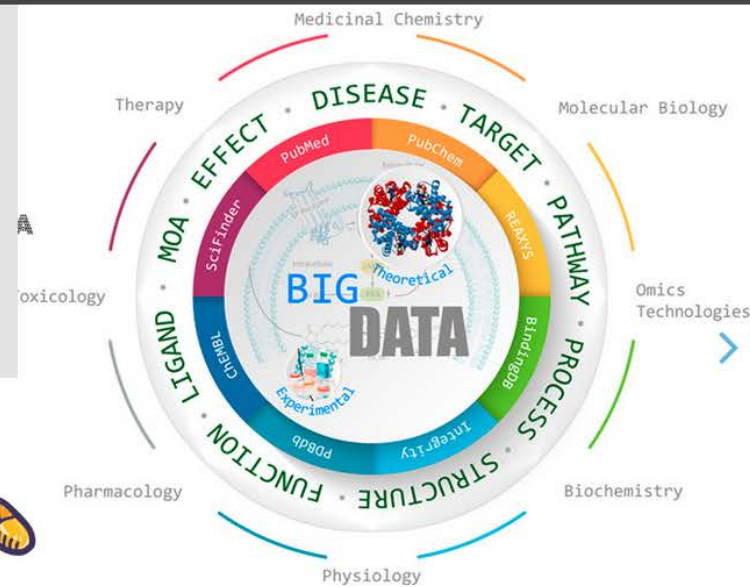
PASS Online Selector

MNA/QNA Similarity

Pharmacological Targets

FDA Approved Drugs

Pharmaceutical Substances Registered in Russia



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Way2Drug DRP: Molecular targets

Pharmacological Targets

Show entries

Search:

Target's name	UniProt	PDB	Kegg	Pharmacotherapeutic application		
				PreClinical	Clinical	Launched
1-deoxy-D-xylulose 5-phosphate reductoisomerase	Q8IKG4				Tuberculosis	Malaria
1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-1	P19174				Cancer	
11beta-Hydroxysteroid Dehydrogenase (nonspecified subtype)	P24385					Diabetes Cancer
14-3-3 protein epsilon	P62258			Cancer		
15-hydroxyprostaglandin dehydrogenase (NAD+) (isoform 1)	P15428				Cancer	
17beta-Hydroxysteroid dehydrogenase (nonspecified subtype)	P24864				Cancer Diabetes	
2-amino-3-carboxymuconate-6-semialdehyde	Q8TDX5				Diabetes	
3-oxoacyl-(acyl-carrier protein) reductase	Q8I2S7				Cancer Leishmaniasis Malaria	
3-phosphoinositide-dependent protein kinase 1 (isoform 1)	O15530				Diabetes	Cancer
4F2 cell-surface antigen heavy chain	P08195			Cancer		
Target's name	UniProt	PDB	Kegg	Pharmacotherapeutic application		
				PreClinical	Clinical	Launched

Showing 1 to 10 of 2,322 entries



Molecular targets: Links to the external resources

UniProt
UniProtKB ▾

BLAST | Align | Retrieve/ID mapping | Peptide search
Help | Contact

UniProtKB - O00763 (ACACB_HUMAN)

Basket ▾

RCSB PDB | Deposit ▾ | Search ▾ | Visualize ▾ | Analyze ▾ | Download ▾ | Learn ▾ | More ▾
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Display

- Entry
- Publications
- Feature viewer
- Feature table

An Information Portal to
126809 Biological
Macromolecular Structures

Advanced Search | Browse by Annotations

Amyotrophic lateral sclerosis (ALS)

[Pathway menu | Organism menu | Pathway entry | Download KGMML | Show description | User data mapping]

Reference pathway (KO) 100%

Similarity

Structure Similarity

Experiment

of RSGI RUH-053, an Apo-Biotin Carboxy Carrier Protein from Human

Released: 2006-10-25

[Ruhul Momen, A.Z.M., Hirota, H., Hayashi, F., Yokoyama, S., RIKEN Structural Initiative](#)

well free synthesis

Knowledgebase: 2DN8 (3 models >19 annotations) [SBKB.org](#)

Snapshot

wwPDB Validation

Metric	Percentile Ranks	Value
Clashscore	<div style="width: 100%; height: 10px; background: linear-gradient(to right, red, white, blue);"></div>	14
Ramachandran outliers	<div style="width: 100%; height: 10px; background: linear-gradient(to right, red, white, blue);"></div>	1.7%
Sidechain outliers	<div style="width: 100%; height: 10px; background: linear-gradient(to right, red, white, blue);"></div>	25.0%

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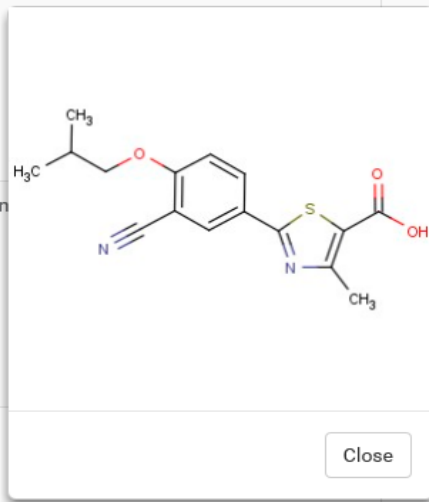
Way2Drug DRP: FDA Approved Drug Substances

Show 10 entries

FDA approved drugs

Search:

Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application
	Adenuric Febric Feburic Uloric	Febuxostat (USAN; Rec INN)	Xanthine Oxidase Inhibitors	Gout Hyperuricemia Cancer therapy associated disorders Angina pectoris, stable Hematologic-blood cancer
	Edecrin Hydromedin	Acetazolamide (Rec INN; JAN) Acetazolamide (BAN; USAN)	Wnt Signaling Inhibitors	Hypertension
	Potiga Trobalt	Retigabine (USAN) Retigabine (Prop USAN)	Voltage-Gated K(V) 7.2/7.3 (KCNQ2/3) Channel Activators Voltage-Gated K(V) 7.2 (KCNQ2) Channel Activators Voltage-Gated K(V) 7.3 (KCNQ3) Channel Activators P-Glycoprotein (MDR-1; ABCB1) Inhibitors GABA Aminotransferase Inhibitors	Epilepsy Lennox-Gastaut syndrome Neuralgia, postherpetic (PHN) Amyotrophic lateral sclerosis Epilepsy, partial seizures



Neoplastic disorders
(234 drugs)

Malaria
(12 drugs)

Tuberculosis
(20 drugs)

Epilepsy
(41 drugs)

Diabetes
(84 drugs)

Way2Drug DRP: Search for Clopidogrel

A Knowledge Based Approach to Drug Repurposing for Socially Important and Rare Diseases

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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.

Show 10 entries

Search: Clopido

Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application	PASSOnline prediction
	Iscover Plavix	Clopidogrel bisulfate (USAN) Clopidogrel hydrogensulfate	Purinergic P2T antagonist Signal transduction modulator	Arrhythmia Stroke Disorders of hemostasis Fibrillation, atrial	



Way2Drug DRP: PASS Prediction for Clopidogrel Bisulfate

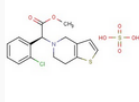

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One may browse the records in the database or search for a particular drug using drug name as a query.

 Show entries

 Search:

Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application	PASSOnline prediction
	Iscover Plavix	Clopidogrel bisulfate (USAN) Clopidogrel hydrogensulfate	Purinergic P2T antagonist	Arrhythmia Stroke	
				Atherosclerosis Thrombosis Systemic lupus erythematosus Angina pectoris, stable Acute coronary syndrome	
Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application	PASSOnline prediction

Components: 2

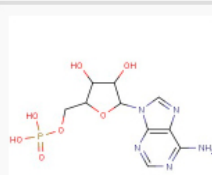
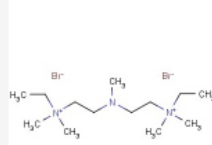
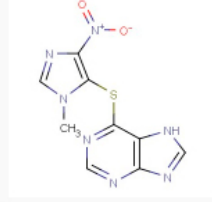
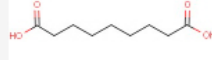
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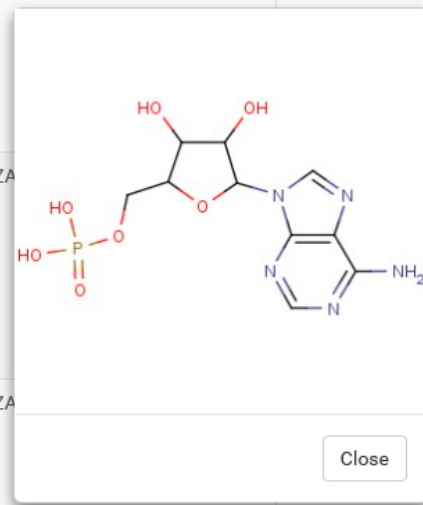
Way2Drug DRP: Drug Substances Registered in Russia

Show entries

Pharmaceutical Substances Registered in Russia

Search:

Structure	Trade name	Substance name	Comments
	Фосфаден	ADENOSINE PHOSPHATE	Торговое название: Фосфаден Международное название: Аденозина фосфат Страна: Россия . дата актуализации - 17.05.1999 (РЛС)
	Пентамин	AZA	Торговое название: Пентамин Международное название: Азаметония бромид Страна: Россия . В нескольких препаратах, несколько дат регистрации.
	Азатиоприн	AZA	Торговое название: Азатиоприн Международное название: Азатиоприн Страна: Россия
	СКИНОРЕН	AZELAIC ACID	мазь . Торговое название Скинорен (Skinoren) Страна-производитель Германия Фирма-производитель Schering AG - 10.11.1998 . . .



Close



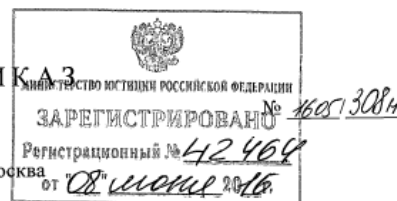
New opportunities for drug repurposing?

**МИНИСТЕРСТВО
ПРОМЫШЛЕННОСТИ И
ТОРГОВЛИ РОССИЙСКОЙ
ФЕДЕРАЦИИ
(Минпромторг России)**

**МИНИСТЕРСТВО
ЗДРАВООХРАНЕНИЯ
РОССИЙСКОЙ ФЕДЕРАЦИИ
(Минздрав России)**

19 мая 2016 г.

П Р И К А З



Об утверждении перечня биомиметов для разработки схожих по фармакотерапевтическому действию и улучшенных аналогов инновационных лекарственных препаратов

В соответствии с пунктом 3 Правил предоставления субсидий из федерального бюджета российским организациям на возмещение части затрат на реализацию проектов по разработке схожих по фармакотерапевтическому действию и улучшенных аналогов инновационных лекарственных препаратов, утвержденных постановлением Правительства Российской Федерации от 30 декабря 2015 г. № 1503 (Собрание законодательства Российской Федерации 11.01.2016, № 2 ст. 377), **п р и к а з ы в а е м :**

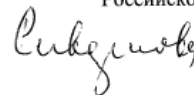
Утвердить прилагаемый перечень биомиметов для разработки схожих по фармакотерапевтическому действию и улучшенных аналогов инновационных лекарственных препаратов.

Врио Министра промышленности и торговли Российской Федерации



Г.С. Никитин

Министр здравоохранения Российской Федерации



В.И. Скворцова



Partial statistics of PASS predictions

Pa>50%	Pa>70%	Types of Activity
227	73	Proteasome ATPase inhibitor
89	31	Meprin B inhibitor
63	52	Androgen antagonist
55	37	Estrogen antagonist
45	23	Phenylalanine 4-hydroxylase inhibitor
40	22	Progesterone agonist
32	10	Fibroblast growth factor 1 agonist
30	5	Fibroblast growth factor 4 antagonist
26	10	Potassium channel (Voltage-sensitive) blocker
24	17	Interleukin 6 antagonist
20	8	5 Hydroxytryptamine 2A antagonist
18	10	Dopamine D2 antagonist
18	11	Interleukin 5 antagonist
14	4	Meprin A inhibitor
13	5	Tumour necrosis factor alpha release inhibitor
11	1	AMP-activated protein kinase, alpha-1 subunit inhibitor
10	6	Opioid kappa receptor agonist
10	9	Dopamine D2 agonist
9	2	Histone deacetylase SIRT1 inhibitor

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• • •

PharmaExpert Search: 5 HT 2A antagonists

PharmaExpert

Prediction & Interpretation - H:\DOCUMENTS\DRUG-SUBSTANCES-REGISTERED-IN-RU

ZIPRASIDONE ZOLEDRONIC ACID ZOLMITRIPTAN

Pa	Pi	<substance_name>
0,892	0,003	ZIPRASIDONE
0,882	0,003	Ergotamine
0,876	0,003	MIANSERIN
0,827	0,003	Dihydroergocristine
0,791	0,004	Serindole
0,765	0,004	Paliperidone
0,740	0,004	RISPERIDONE
0,711	0,004	MIRTAZAPINE
0,669	0,004	DROPERIDOL
0,659	0,004	OLANZAPINE
0,632	0,004	DIHYDROERGOCRISTINE
0,607	0,004	AMITRIPTYLINE

Save TXT Save SD Clipboard Exclude

Pa Pi Activity

Pa	Pi	Activity
0,954	0,003	Dopamine D2 antagonist
0,892	0,003	5 Hydroxytryptamine 2A antagonist
0,767	0,003	HERG 1 channel blocker
0,604	0,001	5 Hydroxytryptamine 2A agonist
0,590	0,006	Potassium channel (Voltage-sensitive)
0,550	0,002	Dopamine D2S antagonist

0,892 0,003 ZIPRASIDONE

0,882 0,003 Ergotamine

0,876 0,003 MIANSERIN

0,827 0,003 Dihydroergocristine

0,791 0,004 Serindole

0,765 0,004 Paliperidone

0,740 0,004 RISPERIDONE

0,711 0,004 MIRTAZAPINE

0,669 0,004 DROPERIDOL

0,659 0,004 OLANZAPINE

0,632 0,004 DIHYDROERGOCRISTINE

0,607 0,004 AMITRIPTYLINE

Species: Homo sapiens

Number of selected compounds: 20

<substance_name> ZIPRASIDONE; 48 Substructure descriptors, 0 new; 6 Possible activities.



Way2Drug DRP: Selection of the desirable properties

Draw a structure:

To receive results, please, enter:

Choose activities/properties which you want to predict:

- Select/unselect all
- PASS Online(all activities)
- PASS Online (Effects)
- PASS Online(Mechanism)
- PASS Online(Metabolism)
- PASS Online(Transport)
- PASS Online (Adverse_Effects&Toxicity)
- SOMP (Site of metabolism prediction)
- GUSAR (Antitarget)
- GUSAR (Acute Rat Toxicity)
- GUSAR (Enviromental Toxicity)
- DIGEP-Pred (mRNA Level)
- DIGEP-Pred (Protein Level)
- BBB

And finally:

Click here to predict



Way2Drug DRP: Total predictions for Clopidogrel

To receive results, please, enter:
vvp1951@yandex.ru

Draw a structure:

Chemical structure of Clopidogrel: COC(=O)[C@H](c1ccc(Cl)cc1)N2CCCCC2c3sccc3

Choose activities/properties which you want to predict:

- Select/unselect all
- PASS Online(all activities)
- PASS Online (Effects)
- PASS Online(Mechanism)
- PASS Online(Metabolism)
- PASS Online(Transport)
- PASS Online (Adverse_Effects&Toxicity)
- SOMP (Site of metabolism prediction)
- GUSAR (Antitarget)
- GUSAR (Acute Rat Toxicity)
- GUSAR (Environmental Toxicity)
- DIGEP-Pred (mRNA Level)
- DIGEP-Pred (Protein Level)
- BBB

And finally:

[Click here to predict](#)

<http://www.way2drug.com/dr>



Way2Drug DRP: Prediction results for Clopidogrel

WAY2DRUG results



pass@ibmc.msk.ru pass@ibmc.msk.ru

Вам: vvp1951@yandex.ru

5 июл в 7:07

Язык письма — английский. Перевести на русский?



PASS_Online-
All_Activities.pdf

PDF

PASS_Online-
Effects.pdf

PDF

PASS_Online-
Mechanism.pdf

PDF

PASS_Online-
Metabolism.pdf

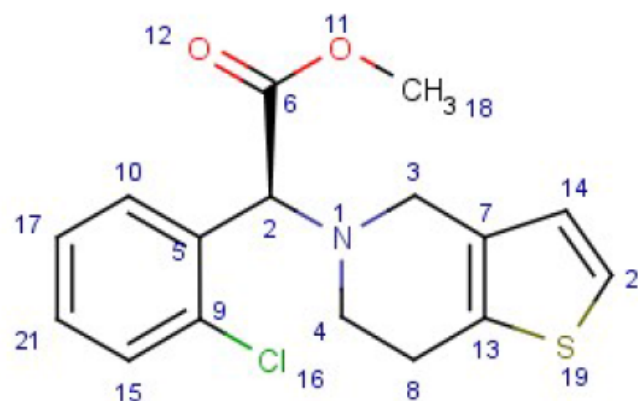
PASS_Online-
Transport.pdf

PASS_Online-
Adverse_Effects

14

This is a file(s) with results from <http://way2d>

PASS_Online-Mechanism Web Server prediction results



Pa	Pi	Activity
0,784	0,008	Muramoyltetrapeptide carboxypeptidase inhibitor
0,768	0,015	Anaphylatoxin receptor antagonist
0,712	0,004	Platelet aggregation inhibitor



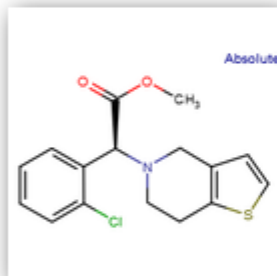
Way2Drug DRP: Similarity search

HOME

ABOUT

SERVICES

Similarity



Cut-off value

0.4



Find structures



Way2Drug DRP: Similarity search

HOME








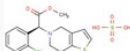
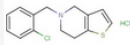
ABOUT

SERVICES

Similarity

Show 10 entries

Search:

Structure 	Brand Name 	Generic Name 	Mechanism of Action 	Pharmacotherapeutic application 	Similarity MNA 	Similarity QNA 
	Iscover Plavix	Clopidogrel bisulfate (USAN) Clopidogrel hydrogensulfate	Purinergic P2T antagonist Signal transduction modulator	Arrhythmia Stroke Disorders of hemostasis Fibrillation, atrial Peripheral arterial disease (PAD) Angina pectoris, unstable Myocardial infarction Thrombotic Disorders Atherosclerosis Thrombosis Systemic lupus erythematosus	1.000	1.000
	Aplaket Ipaton Panaldine Ticlid Ticlofix Ticlodone Tiklid Tiklyd	Ticlopidine hydrochloride (DCF; Rec INN; BAN; USAN)	Purinergic P2T antagonist Signal transduction modulator	Stroke Coronary artery disease Thrombosis	0.609	0.518
Structure	Brand Name	Generic Name	Mechanism of Action	Pharmacotherapeutic application	Similarity MNA	Similarity QNA



Way2Drug DRP: PASS Selector

- PAS
- Antidiabetic
 - Antidiabetic (type 1)
 - Antidiabetic (type 2)
 - Antidiabetic symptomatic
 - Antituberculosic
 - Kegg link**
 - all activity

●Pa>Pi ○Pa>0,3 ○Pa>0,7

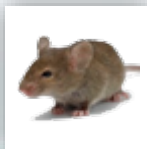
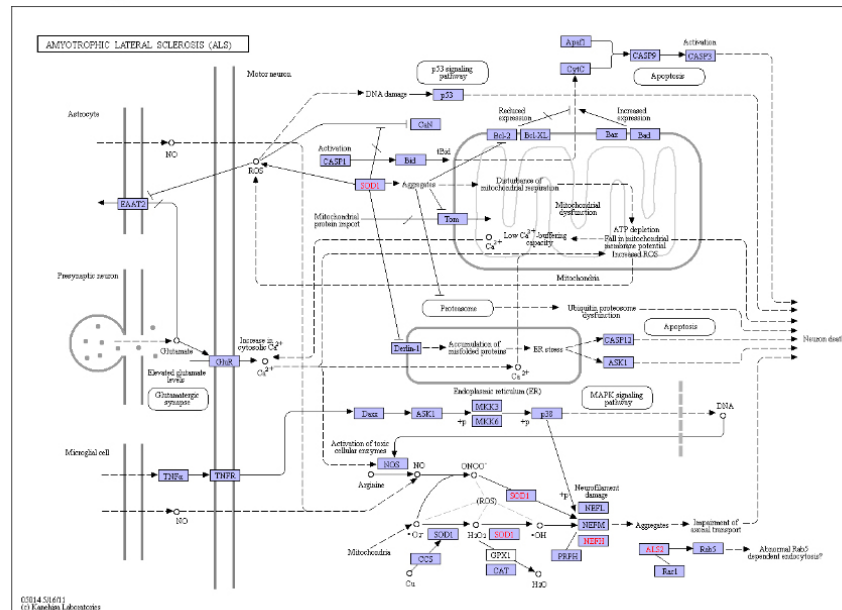
0,847	0,005	Superoxide dismutase inhibitor
0,783	0,004	Transketolase inhibitor
0,646	0,008	Erythropoiesis stimulant
0,575	0,014	APOA1 expression enhancer
0,576	0,033	Calcium channel (voltage-sensitive) activator
0,519	0,014	Caspase 8 stimulant
0,496	0,006	TRPA1 agonist
0,486	0,007	Monophenol monooxygenase inhibitor
0,453	0,036	Caspase 3 stimulant
0,412	0,006	Alcohol dehydrogenase inhibitor
0,361	0,019	Dihydroorotase inhibitor
0,337	0,007	Glutamine-tRNA ligase inhibitor
0,395	0,066	Fibroblast growth factor agonist
0,368	0,047	CF transmembrane conductance regulator

Homo sapiens(P00441)

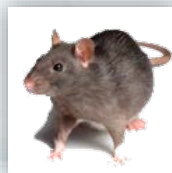
Click to Unirpot

- Peroxisome
- Amyotrophic lateral sclerosis (ALS)
- Huntington's disease
- Prion diseases

Click to view kegg db



Mus musculus



Rattus norvegicus



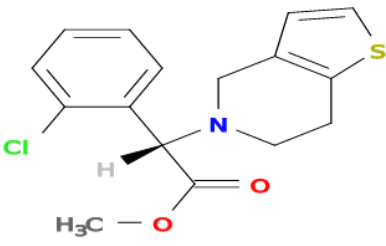
Homo sapiens

Antidiabetic
Antidiabetic (type I)
Antidiabetic (type II)
Antidiabetic symptomatic
Antituberculosic

Molecule Properties Prediction from Molecular Property Diagnostic Suite

Clopidogrel

MPDS Unique ID Card

Molecular Property Diagnostic Suite			
MPDS ID: 25-12-047870			
		Molecular Formula: C ₁₆ H ₁₆ ClNO ₂ S	
		IUPAC Name: 1-[2-(5-bromo-8-hydroxyquinolin-2-yl)ethyl]pyrrolidin-1-ium	
Remarks: Remarks here...			
Name/Synonyms: Name/Synonyms here...			
Molecular Properties:			
Mol. Wt.	321.06	LogP	0.94
HBD	0	LogS	-4.27
HBA	3	pKa	pKa1: ; pKa2: ; pKa3: 4.77; pKa4: -7.74
Molar refractivity	43.95	Polar surface area	57.78
Heavy atoms count	21	Rings count	3.00
Rotatable bonds	6.00	Polarizability	1.78

Molecular Descriptors

Descriptor mol1	Mol.Wt.	AlogP	XlogP	Mol. Refractivity	Pol. Surf. Area	H-Bond Donors	H-Bond Acceptors
	321.059	1.542	2.732	90.777	54.84	0	3
	No. of Atoms	Rot. Bond Count	Acid Group Count	No. of Rigid Bonds	No. of Rings	Struct. Alerts	No. of Aromatic Rings
	37	4	0	19	3	1	2

Biopharmaceutics Classification System (BCS Classification)

Molecule/Descriptor mol1	logS	XlogP	BCS Class	Solubility	Permeability
	-3.675	2.732	I	High	High
	BCS class	Solubility	Permeability		
	I	High	High		
	II	Low	High		
	III	High	Low		
	IV	Low	Low		

Drug-likeness Prediction (DruLiTo)

Filters mol1	Lipinski Rule	Ghose Filter	CMC Filter	Veber Filter	MDDR Like Rule	BBB-Likeness	Unweighed QED	Weighted QED
	+	+	+	+	-	+	+	+

Toxicophoric Groups

```
#####
# Summary of Toxicity Filter results: #
# Date: Wed Jul 05 10:20:39 IST 2017 #
#####

Molecule 1
Structural Alert found: >_2_ester_groups (C(=O)O[C,H1].C(=O)O[C,H1].C(=O)O[C,H1])
Occurrence count: 1
```

MPDS website Hosted at Centre for Molecular Modeling, CSIR-IICT, Hyderabad, India
<http://mpds.osdd.net/>



Way2Drug DRP: SAR Creator

SAR Creator

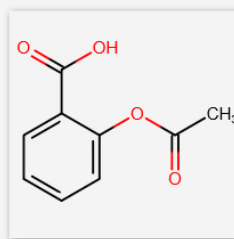
ADD STRUCTURE

VIEW STRUCTURES

VIEW/CREATE SDF FILES

I NEED HELP

Structure



SMILES

CC(=O)Oc1ccccc1C(=O)O

CHEMBL ID

CHEMBL25

INCHI Key

BSYNRYMUTXBXSQ-UHFFFAOYSA-N

Structure

Compound's name

Activity

Group

Save

<http://www.way2drug.com/dr>



Summary

- ✓ Drug repurposing is a promising way for finding new medicines.
- ✓ Chemoinformatics methods help to identify the most prospective directions of research.
- ✓ Based on the long-term projects in chemoinformatics, we are developing Way2Drug Drug Repurposing Platform.
- ✓ Further development of the DRP Platform requires integration, curation of the information, improvement of functionality, etc.
- ✓ Active cooperation between the researchers working in the field of computer-aided drug discovery will be beneficial for all parties.

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Sandeep Kumar, Student

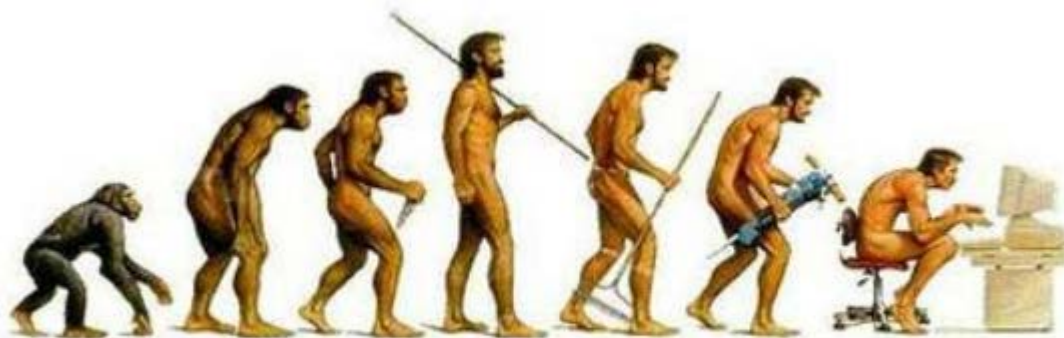
Osmania Medical College & Osmania General Hospital

Rakesh Sahay, M.D

Manisha Sahay, M.D.



Thank you for your kind attention!



We are open for collaboration.

Questions and suggestions:
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vvp1951@yandex.ru