PharmaExpert

This is an optional extension of the PASS system, allowing for a systematic data mining and biological interpretation of PASS results.

PharmaExpert analyzes mechanism-effect relationships, identifies the probable drug-drug interactions for pairs of molecules, and searches for molecules acting on multiple targets. The software can also help to identify molecules with desired activities and without toxic or side effects.

The analysis is based on a "mechanism-effect(s)" relationship knowledgebase (MER base) that is collected by experts from literature of more than 12 years and includes over 11,000 relationships at the present time.

PASS

The acronym PASS stands for "Prediction of Activity Spectra for Substances". Upon entering a structural formula of a chemical substance, the program returns the potential biological activities of this compound.

PharmaExpert allows to:

- Select compounds with required therapeutic, but without adverse effects;
- Comparatively analyze compounds with similar structures;
- Select compounds with multiple mechanisms of action;
- Assess drug-drug interactions with regard to their pharmacokinetic, pharmacodynamic, and adverse effects.

Recent PharmaExpert publications

Lagunin A., Filimonov D., Poroikov V. (2010) Multi-targeted natural products evaluation based on biological activity prediction with PASS. *Curr. Pharm. Des.* **16**:1703-1717.

Geronikaki A.A., Lagunin A.A., Hadjipavlou-Litina D.I., Eleftheriou P.T., Filimonov D.A., Poroikov V.V., Alam I., Saxena A.K. (2008) Computer-aided discovery of anti-inflammatory thiazolidinones with dual cyclooxygenase/lipoxygenase inhibition. *J. Med. Chem.* **51**:1601-1609.

Filz O., Lagunin A., Filimonov D., Poroikov V. (2008) Computer-aided prediction of QT-prolongation. *SAR QSAR Environ. Res.* **19**:81-90.

PharmaExpert

About geneXplain

The geneXplain GmbH is a young company with a growing portfolio of useful software for life scientists. Whether you are working on genome, network or compound analysis, we have what you need!

Our **geneXplain platform** is the online toolbox and workflow management system for scientists in the fields of transcriptomics and proteomics. Here, you can store and analyze your experimental data (including raw microarray results), search for master regulator molecules, map to GO terms, and even add your own workflows and scripts.

We distribute software developed by in silico molecular biology, Inc., Japan, for geneticists. **In-Silico Molecular Cloning (IMC)** lets you handle annotated DNA, conduct cloning experiments in silico, map features and sequences, and compare and align genomes. **GenomeTraveler (GT)** takes this to the next level by adding the possibility to visualize and interpret your Next Generation Sequencing (NGS) data.

For scientists working on drug discovery and drug optimization, we distribute a range of tools from the Institute of Biomedical Chemistry (IBMC), Russia. **PASS (Prediction of Activity Spectra for Substances)** predicts whole bioactivity spectra for your compounds qualitatively, based only on 2D structural formulae. **PharmaExpert** is the additional software to help you choose the most suitable substance from a set of PASS predictions. **GUSAR (General Unrestricted Structure-Activity Relationships)** predicts biological activities quantitatively, based on (Q)SAR models, which can also be created with the software.

It is geneXplain's mission to provide the computational methodology required to achieve the goal of "personalized pharmacogenomics". We wish to help academic researchers in their daily work with easy-to-use tools that are compatible with the low-budget requirements of most academic groups. At the same time, we shall provide high-end technology platforms to fulfill bioinformatics requirements to industrial standards. Finally, we intend to offer partnerships for research and training in the area of our expertise.

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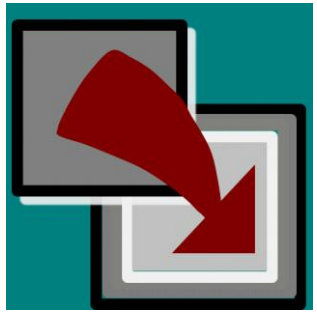
PharmaExpert

The tool for estimation of safety and efficacy of new pharmaceutical agents

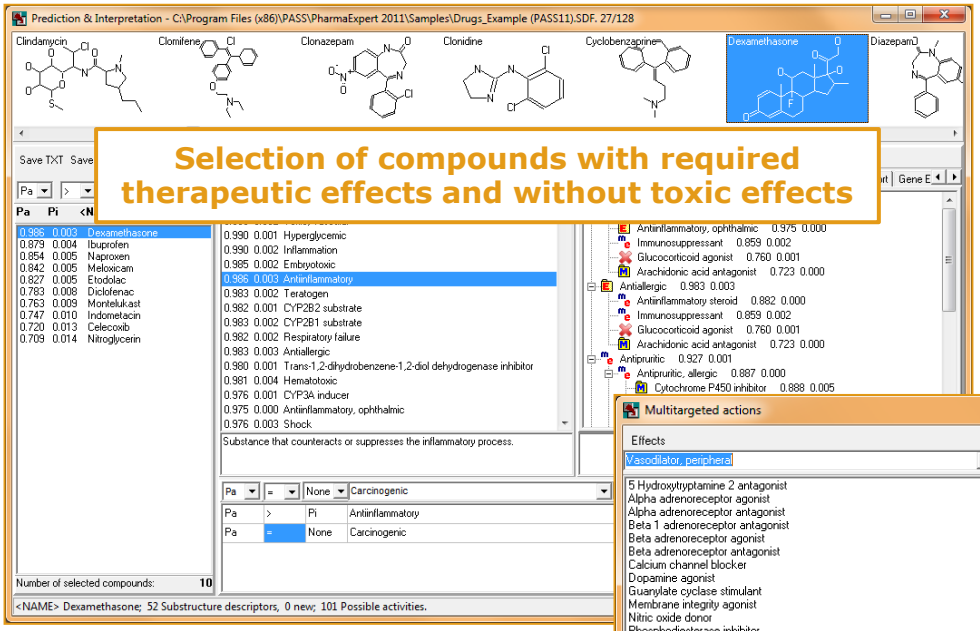


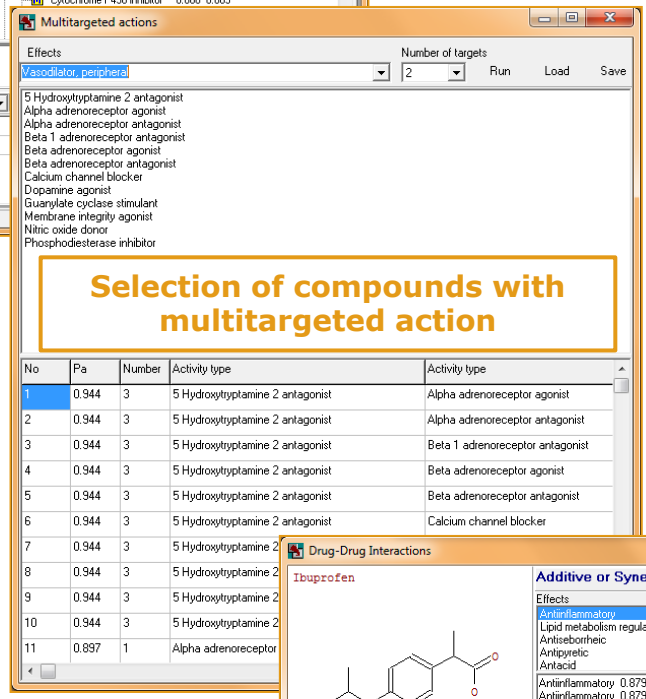
geneXplain

PharmaExpert - a tool for the estimation of safety and efficacy of new pharmaceutical agents

How to select the most promising compounds among those predicted to interact with the selected target(s) and to cause the required pharmacotherapeutic effect(s)?

PharmaExpert, as a pharmacological knowledge-based tool, provides *in silico* screening of compounds using the PASS prediction of their biological activities.





PASS and PharmaExpert: The optimal combination

In a first step, PASS has predicted biological activities for chemical compounds based on a library containing more than 250,000 structures (known drugs and drug-like compounds).

As the next step, PharmaExpert selects those chemical compounds that exhibit the required biological activity spectra with low probability of adverse or toxic effects.

Out of the thousands of biological activities predicted by PASS, PharmaExpert identifies rational combinations of multi-targeted action and finds the suitable pharmaceutical agents among commercially available chemical compounds.

Search function

The search mask of PharmaExpert allows to find any number of desired activities with specified thresholds of the probability to be active (Pa). At the same time, it is possible to exclude unwanted activities by simply setting their Pa to equal zero.

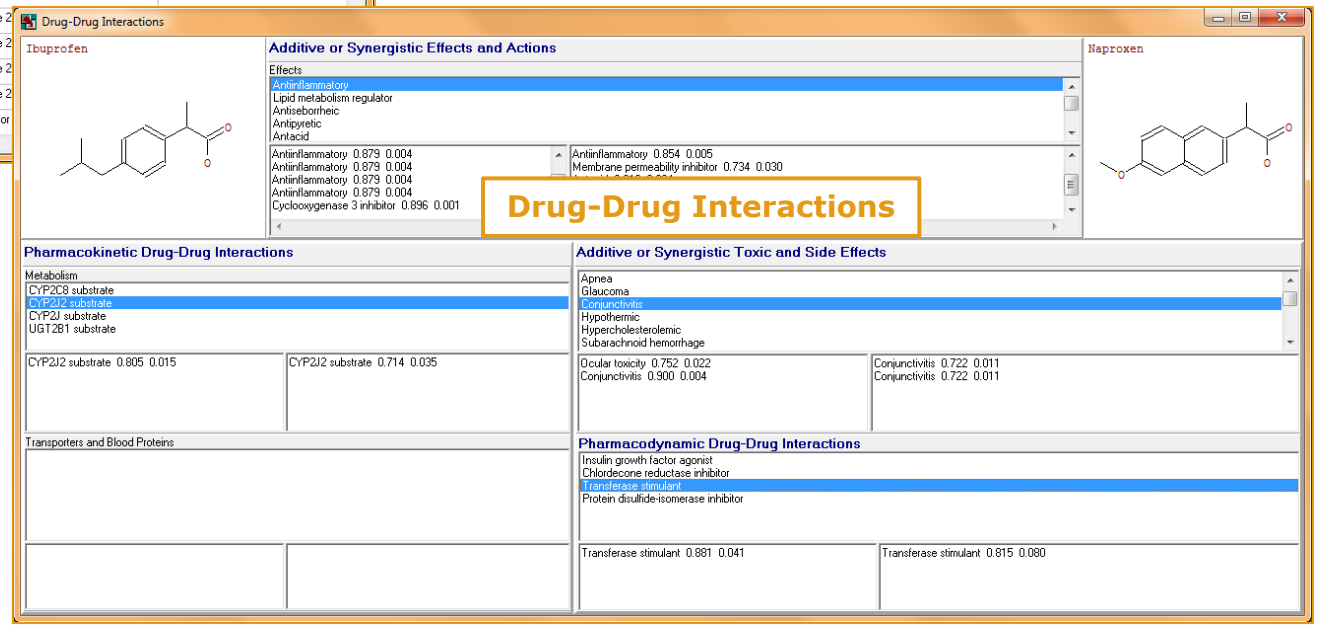
Mechanism-effect relationships

PharmaExpert comes with a database, manually curated by experts, containing 11,049 mechanism-effect relationships (MER), which is used to analyze the PASS prediction data.

In this MER base, biological activities are described as mechanisms of action and/or pharmacological effects, and their records contain lists of relationships with other types of biological activity, including references to publications.

Multitarget selection

With PharmaExpert it is possible to identify substances with multitargeted actions. Simply choose a desired effect and a number of mechanisms that should lead to it will be displayed automatically. The software will then return a list of substances displaying more than one mechanism leading to the effect.



Drug-drug interactions

PharmaExpert provides a comfortable interface to reveal the most important types of drug-drug interactions for pairs of pharmaceutical agents.

A dedicated option allows to classify interactions of the compounds with metabolic enzymes and protein transporters, thus facilitating the estimation of *pharmacokinetic drug-drug interactions*.

Pharmacodynamic interactions are estimated with respect to molecular targets and pharmacotherapeutic effects.

Synergistic or additive effects of two compounds are provided for *adverse and toxic effects* as well.

A slide show with screenshots can be found on our homepage (www.genexplain.com) and also on our Facebook account (www.facebook.com/genexplain), and recommendations from experts for the PASS software can be found on our LinkedIn profile (http://www.linkedin.com/company/genexplain/products).