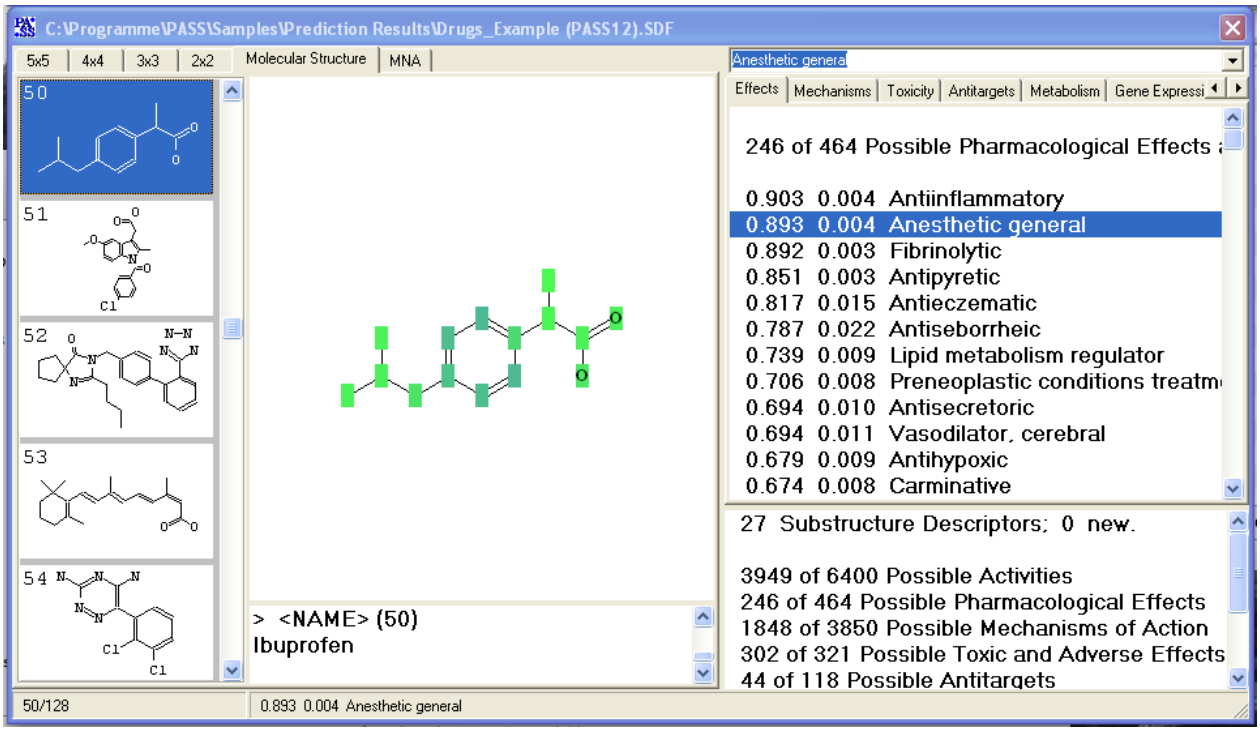
PASS & PharmaExpert 2012 Release Announcement

The geneXplain team is proud to announce the new release of the PASS and PharmaExpert software for qualitative biological activity prediction. These programs have been developed by V. Poroikov, D. Filimonov and Associates, Moscow, Russia.



New features of the 2012 releases:

PASS

- Improved SAR base contains 313345 substances and 75875 descriptors
- Number of predictable activity types has increased by more than 3000 terms, and number of recommended activity types has increased by more than 2000 terms
- Considerable increase of the number of predictable effects on gene expression by more than 1500 terms
- Considerable increase in the number of predictable mechanisms of action, by more than 470 terms

- New functionality enabling direct communication between PASS and structure-drawing programs, e.g. Marvinsketch
    - Copy any individual structure from PASS directly to clipboard, as Bitmap or as MOL file
    - Open a structure in PASS directly from clipboard

Statistics

	PASS 2011	PASS 2012
substances	250,407	313,345
descriptors	69,950	75,875
activity types	4,444	7,527
activity types, recommended	4,366	6,400
pharmacological effects	497	464
mechanisms of action	3,378	3,850
toxic and adverse effects	274	321
antitargets	116	118
metabolism-related	206	195
gene expression	31	1,610
transporter-related	49	68

PharmaExpert

- Number of activity types has increased by over 3000 terms
- Improved MER Base
    - 450 activity-activity relationships have been added
- Enhanced functionality for drug-drug interaction analysis: automatic pair-wise analysis for two sdf files with pass prediction results added

About PASS and PharmaExpert:

With ***PASS***, you can easily make qualitative predictions of the biological activity spectra for your compounds of interest. This process is fast and effective, even for huge libraries of chemical structures. Thus, you can estimate the general biological potential of chemical substances as well as discover new possible activities for known drugs. PASS also assesses the impact of separate atoms on a particular activity, which opens up the possibility to optimize a lead structure for a certain purpose.

PASS uses 2D structural formulas in SDF or MOL format for prediction. This enables the user to perform predictions for new substances for which more information is

not yet available. Predictions can be viewed directly on the PASS interface and can be saved as text, SD or CSV files.

PharmaExpert is a useful tool to mine the data obtained with PASS. The program simplifies the process of selecting compounds with desirable activities, but without side effects. With PharmaExpert, you can also compare compounds, discover drug-drug interactions of two substances, or select compounds acting via multiple mechanisms leading to the same effect.

Both programs are locally installed on a PC and come with a predefined SAR (Structure-Activity Relationships) or MER (Mechanism-Effect Relationships) base, respectively, which can be adjusted to the user's needs, or, in case of PASS' SAR base, can also be created from scratch with the user's own data.

Application areas include: medicinal chemistry, computational chemistry, drug discovery and drug development, drug repositioning, chemical toxicity, safety assessment, pharmacogenomics, chemogenomics, SAR, natural compound effects, translational research and translational medicine.

Links

More information about the software and free demo versions are available on our website: http://www.genexplain.com/pass

Read what experts in cheminformatics think about PASS on LinkedIn: http://www.linkedin.com/company/genexplain/cheminformatics-software-pass-171755/product

The PASS homepage at the Institute of Biomedical Chemistry, Russian Academy of Sciences: http://www.pharmaexpert.ru/PASSOnline/

Other products distributed by geneXplain GmbH:

geneXplain platform, an online toolbox and workflow management system for a broad range of bioinformatic and systems biology applications.

IMC (In silico Molecular Cloning), a software package to analyze and visualize whole genome data.

GT (GenomeTraveler), a software package to analyze whole genomes, including mapping and assembly of next generation sequencing data and all features of IMC.

GUSAR (General Unrestricted Structure-Activity Relationships), software to create models on quantitative structure-activity relationships (QSAR models) for organic drug-like compounds.

QSAR models, a library of pre-calculated QSAR models (LD50 values for acute rat/mouse toxicity; IC50, K_i and K_{act} for interactions with antitargets) that can be used together with GUSAR software is available on request.

About geneXplain GmbH

GeneXplain GmbH has been founded in April 2010 and is based in Wolfenbüttel, Germany. The company aims at providing a comprehensive set of computational tools supporting the complete drug development pipeline from the statistical evaluation of high-throughput data, their biological interpretation, identification of potential targets to the prediction of most promising lead structures. The geneXplain platform is based on BioUML and has been developed together with the Institute of Systems Biology, Novosibirsk, Russia, where this leading-edge technology has been developed.

Your geneXplain team

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