

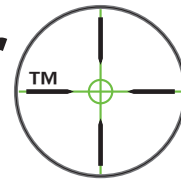


Applications

- Assessment of target safety liabilities
- Evaluation of compounds for in-licensing
- Competitive comparison of in-house development vs competitor compounds
- Mechanistic evaluation of preclinical toxicity findings, and assessment of clinical relevance
- Differentiation of on and off-target effects
- Identification of biomarkers of clinical adverse effects
- Develop screening strategy for follow-up compounds

ToxHunter

Systems toxicology analysis for
MetaCore™ and MetaDrug™

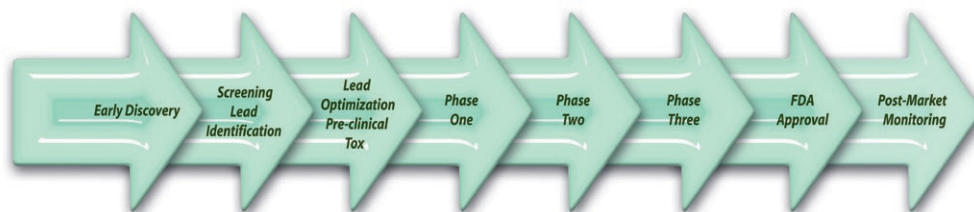


About GeneGo

GeneGo is a leading provider of data analysis solutions in systems biology and systems toxicology. Our tools and manually curated databases help to capture and define the underlying biology behind different types of high-throughput experimental data as well as to understand the effects of small molecule drug compounds in human tissues and other species. We provide solutions for a full range of applications in life science research and drug development, from pre-clinical discovery and NCE applications to clinical trials, covering all aspects of biology and chemistry. GeneGo also provides services for analysis and curation.

ToxHunter™ Overview

ToxHunter is a systems toxicology knowledgebase and data analysis package designed for the assessment of safety liabilities of drugs, environmental contaminants and other xenobiotics at all stages of discovery and development. ToxHunter is available as an add-on feature for GeneGo MetaCore and MetaDrug systems biology and systems pharmacology solutions, and integrates seamlessly with these products.



- Comprehensive target safety assessment
- *In silico* toxicity evaluation of scaffolds/lead compounds
- Comparative analysis of competitor safety profiles
- Analysis of *in vitro* and early *in vivo* systems toxicology experiments
- Toxicity pathways exploration
- Identification and validation of translational biomarkers
- Correlation of target relationship to observed toxicity
- Ranking of candidates by safety profiles
- Understanding of unexpected safety issues and identification of clinical safety biomarkers

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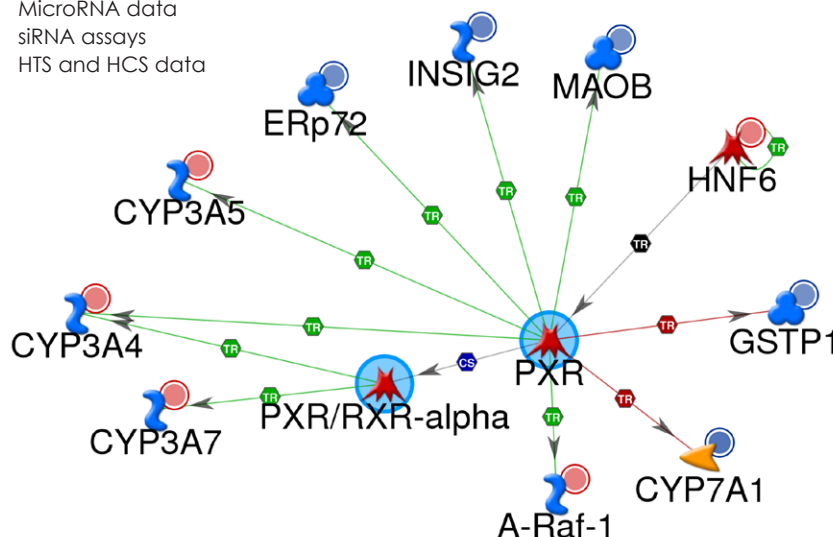
ToxHunter adds to the information mining and data analysis power of the GeneGo platform with a comprehensive, searchable database of gene, protein and metabolite associations to chemical toxicity, new toxicity-related pathway maps, and tools for visualization and filtering of toxicity information on pathway maps and biological interaction networks. Experiments can easily be designed to model specific pathologies, to investigate mechanisms and pathways of toxicity, or to identify safety biomarkers. Molecular safety data can be analyzed in the context of previously reported effects and known signaling and metabolic networks. Automated data analysis and reporting workflows enable rapid interpretation and reporting of experimental results.

ToxHunter was developed under GeneGo's MetaTox™ industry-FDA partnership program. A steering committee of expert representatives from partner organizations discuss the issues being faced in drug safety today, the molecular data types being generated as part of the safety assessment process, and the tools and supporting information necessary to make the best use of these data.

Experimental Data

ToxHunter, as part of the MetaDiscovery platform, allows users to import molecular structures (requires MetaDrug) and experimental data such as genomic, proteomic, metabolomic data, and screening data. A unique feature of the system is concurrent visualization of multiple types of chemical and biological data on pathways and networks. Addressable data types include:

- MOL, SD & CDX structure files
- NMR or MS metabolite data, via CAS numbers, SMILES or brutto formulas
- Gene expression data: whole genome arrays, focused arrays, QPCR and SAGE
- Proteomic data
- MicroRNA data
- siRNA assays
- HTS and HCS data



Key Capabilities

- Browsable toxicity ontology of highly-detailed terms covering multiple target organs, with organ substructures and pathology subtypes differentiated
- High quality manual literature curation of gene, protein and small molecule associations to toxicity terms
- Simple key-word and Boolean searching across toxicity categories for pathology terms, gene, protein or metabolite biomarkers of toxicity
- Ability to flag toxicity associations on maps alongside data, and visualize and filter networks for specific pathologies
- Automated analysis and reporting of experimental data with unique enrichment calculations for specific pathologies and toxicity processes
- QSAR-based prediction of pathological outcomes from chemical structures (with MetaDrug)

Content

ToxHunter adds to the existing content of MetaCore and MetaDrug with:

- 29 new pathway maps representing toxicologically-relevant processes
- > 7000 highly-detailed pathology terms covering 7 target organs (liver, kidney, heart, lung, nose, trachea, forestomach), organized into a browsable ontology with organ substructures and pathology subtypes differentiated
- > 3200 compound-toxicity associations
- > 1500 gene/protein-toxicity annotations
- > 360 small molecule metabolite-toxicity annotations
- 7 additional MetaDrug QSAR models for structure-based prediction of pathological outcomes

Hardware Requirements

Client (for web portal and in-house installations):

P4 CPU and 1GB RAM
 Internet Explorer 6.0 or higher
 Macromedia Flash Player 8 or higher
 Java Runtime Environment (JRE) 1.5.0
 ChemDraw ActiveX / Plugin Net 9.0
 Download Edition

Server (for in-house installations):

2 or more P4/XEON CPU's with
 4GB of RAM recommended
 3.2 GHz CPU and higher recommended
 SCSI HDD with minimum of 250GB of storage
 is recommended
 RAID recommended
 RedHat Enterprise Linux 3, 4 or 5.1; SuSE 9.2;
 CentOS 4.4
 X development package installed
 Oracle 10.2 DBMS and client tools
 MetaCore and MetaDrug support x86-64bit
 architecture

ToxHunter™ Flexible Business Models

- Web portal access or in-house installation
- Annual or multi-year licenses are available
- Named or concurrent users

