

METADRUG

SYSTEMS PHARMACOLOGY



USE METADRUG TO

- Find known and predict possible targets of small molecules
- Find biological pathways affected by small molecules
- Predict indications your drug may be active for
- Discover biomarkers of drug efficacy
- Predict compound metabolites, ADME properties and side effects

WHO CAN BENEFIT

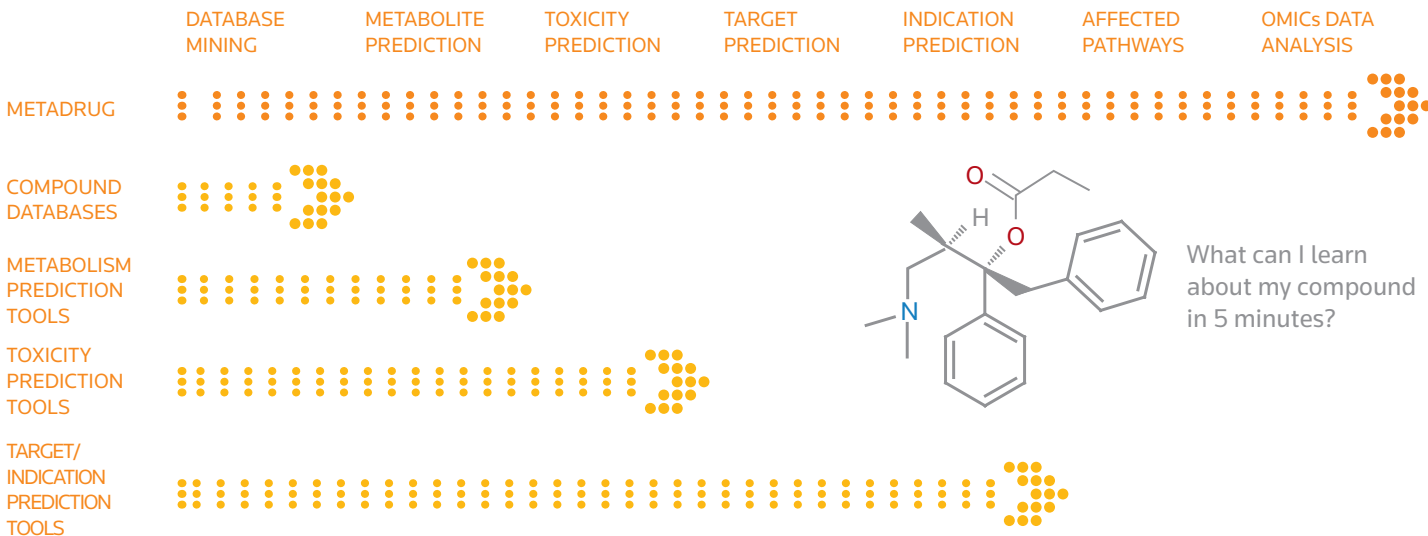
- Drug discovery and development groups
- Lead identification and optimization groups
- Target discovery groups
- Disease area groups
- Compound screening groups
- Chemoinformatics and medicinal chemistry groups
- Pharmacokinetics and metabolism groups
- Toxicity assessment groups

How much do you know about compounds available at your company? What solutions would you use if you would like to know their primary and secondary protein targets, potentially active and toxic metabolites, biological pathways that may be affected by them, and a spectrum of indications they may be useful for?

MetaDrug is a leading systems pharmacology solution that incorporates extensive manually curated information on biological effects of small molecule compounds. Predictive and analytical algorithms look at chemical compounds from different angles in one integrated workflow are available for:

- Individual previously described compounds to look up their known information and predict currently unknown properties
- Individual newly synthesized or isolated compounds to predict their properties from its structures
- Compound libraries to extract known and predict new properties of individual compounds and perform their comparison and prioritization

FIGURE 1: METADRUG PREDICTION TOOLS



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HARDWARE REQUIREMENTS

CLIENT (FOR WEB PORTAL AND IN-HOUSE INSTALLATIONS):

- P4 CPU and 1GB RAM
- Internet Explorer 6.0 or higher
- Adobe 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
- *MetaDrug* supports x86-64bit architecture

MetaDrug predictions rely on manually curated information about compound targets, metabolic fate, ADME properties, and therapeutic and side effects. Nearly 6,000 human proteins are covered by compound information, which is the largest collection of druggable targets available anywhere. Every target in *MetaDrug* comes with protein interactions to explore biological pathways affected by your compounds and network neighborhood of drug targets. OMICs data analysis capabilities provide an additional approach for solving your compound's mechanisms of action, discovering drug efficacy biomarkers, and corroborating your hypotheses generated by classical structure-based methods.

OUR PUBLICATIONS

- Kleemann R, et al A systems biology strategy for predicting similarities and differences of drug effects: evidence for drug-specific modulation of inflammation in atherosclerosis. *BMC Syst Biol.* 2011 Aug 12:5:125.
- Myshkin E, et al. Prediction of Organ Toxicity Endpoints by QSAR Modeling Based on Precise Chemical-Histopathology Annotations. *Chem Biol Drug Des.* 2012 Sep 80:3:406

CONTENT HIGHLIGHTS

- More than 70 QSAR models to predict compound toxicity, ADME properties and therapeutic activity
- More than 160 metabolic rules for metabolite predictions
- More than 1,400 interactive canonical pathway maps capturing nearly 200,000 human, mouse, and rat fine metabolic and signaling canonical pathways depicted based on consensus literature findings
- More than one million interactions of proteins with other proteins, DNA, RNA, metabolites, and xenobiotics
- Thousands of disease biomarkers
- Nearly 700,000 compounds with targets and bioactivity information
- More than 9,000 metabolic reactions
- More than 7,200 drugs
- 5,000 endogenous metabolites
- Millions of synonyms resolved for genes, proteins, and compounds
- Protein complexes and protein families in human, mouse, and rat

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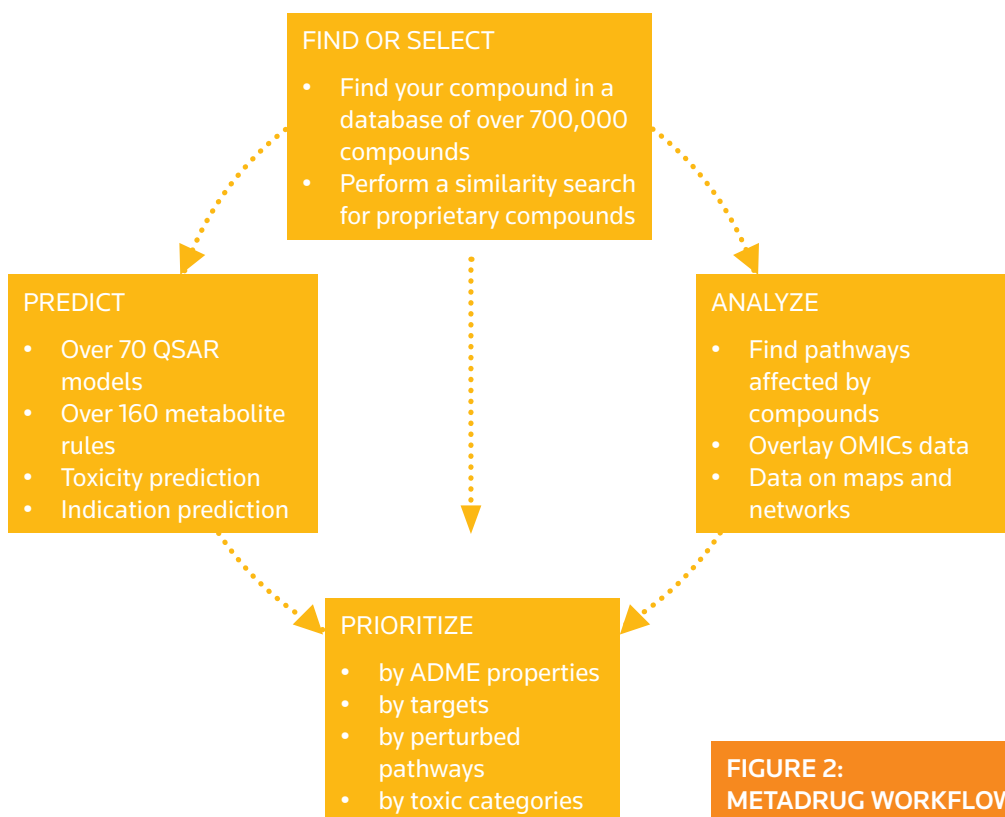


FIGURE 2: METADRUG WORKFLOW

For a complete office list visit:
ip-science.thomsonreuters.com/contact

Contact us to find out more about *MetaBase* or visit
thomsonreuters.com/diseaseinsight

