

# Accelrys Bioactivity Databases

Authoritative Bioactivity, Metabolism, and Toxicity  
Information for Lead Selection and Design

# Accelrys Bioactivity Databases: Authoritative Collection of Bioactivity Information for Lead Selection and Design



- Access related therapeutic activity, metabolism, toxicity, literature, and patent information for investigational drugs in a unified electronic environment
- Compare new compounds to those tested in humans for greater biological relevance
- Monitor competitive intelligence on investigational drugs
- Identify training sets and validation compounds for SAR studies
- Uncover metabolic liabilities related to investigational compounds



# MDDR (Drug Data Report) Database

## What is it?

A trusted, structure-searchable library of 197,500+ biologically active molecules and related information (monthly updates). Contains 3D models, biological activities, activity classifications.

## What questions can I answer?

- What patented compounds like my compound are reported in existing drug discovery pipelines?
- What companies are working on these compounds?
- What phase of development have these compounds reached?
- What compounds are best suited for SAR training sets?

## How can it help me?

- Correlate chemical structure to known therapeutic activity
- Readily retrieve compounds with related therapeutic activities
- Readily obtain transportable chemical structures (SDFfile)



## What is it?

Structure-searchable database of 9,000+ launched drugs and compounds studied as medicinal agents in humans from 1900 to present. Includes 3D models and biochemical properties such as drug class, logP, and pKa, and links to primary literature and patents

## What questions can I answer?

- What are reported activities of known drugs?
- To what activity classes are these compounds assigned
- What are source companies, physical properties and leading references for these compounds?

## How can it help me?

- Identify pharmacophores for compounds with well established activities
- Create transportable chemical structures of know drugs (SDFFile)
- Identify compounds suitable for use in SAR training sets



## What is it?

World's most comprehensive collection of xenobiotic compounds and biotransformations with 13,400+ parent compounds and >95,000 known biotransformations.

## What questions can I answer?

- What are the likely metabolic liabilities for compounds based on comparison to reported metabolism of similar structures?
- Should lead compounds be failed early based on expected metabolic liabilities?
- Are metabolic derivatives of a compound under investigation associated with adverse toxic effects?

## How can it help me?

- Anticipate metabolic activities of novel compounds based on comparisons with known structures
- Locate full metabolic schemes for known compounds
- Correlate known metabolites with adverse effects and other activities



## What is it?

Largest structure-searchable compendium of in vivo and in vitro public toxicity study data (185,000+ compounds) including acute toxicity, mutagenicity, skin and eye irritation, tumorigenicity and carcinogenicity, reproductive effects, and multiple dose effects

## What questions can I answer?

- Does a novel compound fall into a class of structures with known toxic properties?
- Do materials used exhibit safety hazards?
- Are structures of interest with known adverse effects recognized as metabolites of other compounds

## How can it help me?

- A single, definitive source saves time searching for toxicity data
- Direct links go to related information in Symyx Metabolite Database
- Links to primary literature save time finding source information



# Please Contact Us

To learn more about the Accelrys Bioactivity Databases, please contact Lydia Pollitt at Accelrys.



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