

Metabolic transformations of drugs and chemicals

Includes drugs, agrochemicals, food additives, and industrial and environmental chemicals

Developed in association with expert collaborators, including Dr. David Hawkins. Includes information from all volumes of 'Biotransformations'

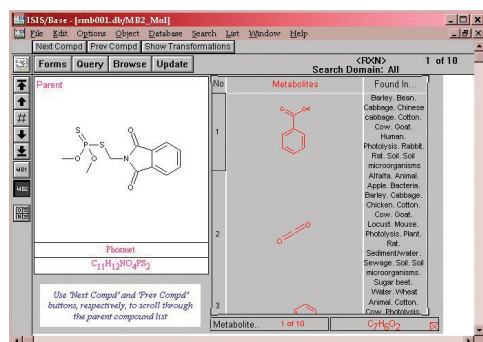
Convenient and flexible retrieval of pathways and related compounds

Searchable by exact structure, substructure, free text, keywords

You are welcome to evaluate the database on-site for 30 days with no obligation.

# Metabolism

Accelrys' Metabolism database focuses on the metabolic fate of chemicals (including pharmaceuticals, agrochemicals, food additives, and environmental and industrial chemicals) in vertebrates, invertebrates, and plants.



View showing the metabolites of a parent compound

The first release of the Metabolism database was derived from the Royal Society of Chemistry (RSC) publication, Biotransformations. The database is expanding rapidly and now includes data from the primary literature as well as information from another RSC publication, Metabolic Pathways of AgroChemicals, giving enhanced coverage of pesticides and plant systems.

Metabolism has been developed under the expert guidance of Dr. David Hawkins at Huntingdon Life Sciences in the UK.

Each record in Metabolism represents one transformation and shows the use or occurrence of the parent compound along with the biological system in which the transformation was observed. At the click of a button, you can see all the metabolites arising from a parent molecule. Another click shows you all the compounds that give rise to a particular metabolite. Actual or hypothetical metabolic pathways are indexed alpha-numerically.

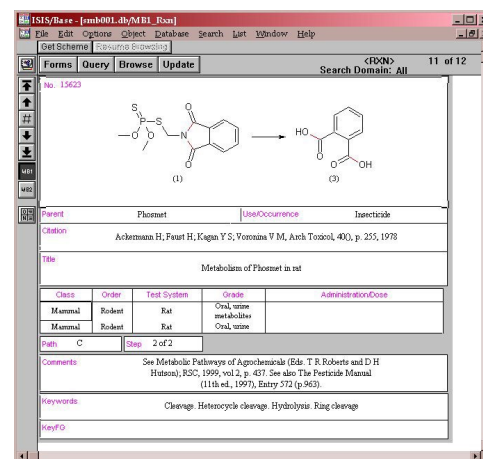
The database may be searched graphically using exact, similar, or substructure search options,

including changed bond information where appropriate. More generic searches may be performed using a variety of keyword options.

Chemists, biochemists and toxicologists in industry, regulatory authorities and government bodies around the world are already using Metabolism daily.

## Metabolism System Specifications

Accelrys' Metabolism database was designed for use with the popular ISIS reaction-retrieval systems on both desktop and client/server platforms. Metabolism is compatible with reaction databases supplied by Accelrys and other reputable database vendors, as well as with in-house databases built using the same systems.



The results of a search in Metabolism under ISIS/Base

## Supported Platforms

ISIS/Host	2.1 or higher	VMS, Unix and Windows
ISIS/Base	2.1 or higher	Windows
Other systems		Please inquire