

Biocatalysts in
organic synthesis

 Selective and novel
transformations
catalysed by enzymes
and analogues

 Developed in
collaboration with
Professor Bryan Jones

 Searchable by
exact structure,
substructure, free text,
keywords

BioCatalysis

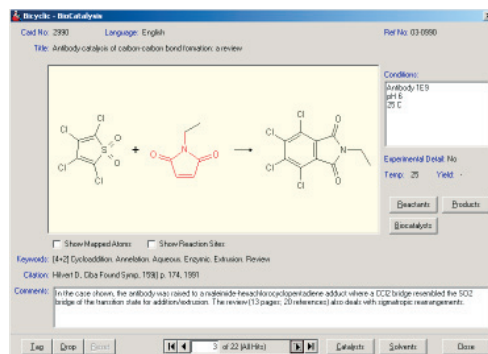
Accelrys' BioCatalysis database has been developed in recognition of the increasing importance of biomolecules as catalysts in organic synthesis.

Users of the database will discover for themselves the wide range of possibilities offered by biocatalysts, both in achieving novel transformations and as versatile replacements for traditional catalysts. The database focuses on the synthetic use of enzymic systems and micro-organisms, techniques which offer advantages of selectivity (chemo-, regio- and enantio-), ease of use and environmental friendliness.

Selection of relevant material for inclusion in the database is the responsibility of Professor Bryan Jones (University of Toronto) – an acknowledged expert in the field. Entries are selected to illustrate the types of reactions catalysed, with an emphasis on preparatively useful transformations. In addition to natural enzymes, the database also includes information on artificial enzymes, enzyme mimics, modified enzymes and catalytic antibodies. About 20% of the database represents patent information.

As well as offering literature references and searchable structures, the database also includes a wide range of important non-structural information – all searchable. So data on, for example, reaction conditions, yield, e.e. & d.e., scale, EC & CAS numbers of the biocatalysts, etc. can all be retrieved. In addition, extensive use of keywords makes it easy to formulate efficient and effective queries based on reaction characteristics.

BioCatalysis is designed to help you apply the rapidly growing body of knowledge coming out of one of the most active research areas in chemistry.



A reference to antibody catalysis in the Accord version of BioCatalysis. Note the query substructure highlighted in red. Buttons on the right lead to further information on the substances involved.

Viewing a record on antibody catalysis in ISIS/Base. In this example, the red highlighting in the structures indicated reacting centers.

Key Features

- Thorough coverage of the scientific literature, including patents, from 1903 to the present.
- Fully structure searchable.
- Keywords offer powerful, fast searches.
- Bi-annual updates, totalling approximately 3,000 reactions per year, ensure you keep up-to-date.
- Developed in collaboration with academic expert Professors Bryan Jones (Toronto)

BioCatalysis System Specifications

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

Supported Platforms

Accord Unix & Windows
 ISIS/Host™ 2.1 or higher VMS, Unix & Windows
 Other systems Please inquire