

A structural database for analogue design

Substructure or keyword searches. Find compounds or replaceable fragments

Thousands of active compounds and bioanalogue pairs, abstracted from the chemical and biological literature

Includes drugs, agrochemicals, enzyme inhibitors, pro-drugs, etc

BIOSTER

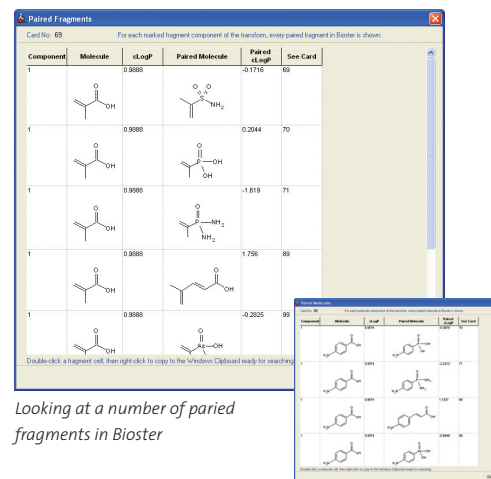
Developed by Dr István Ujváry at the Hungarian Academy of Sciences, the BIOSTER database is a compilation of many thousands of critically selected pairs of molecules having similar biological activities.

Selection of database entries is based on the well-known principle of bioisosterism - a proven technique used in the design of bioactive compounds. However, in order to provide the widest possible choice of fragments for use in lead generation and optimisation, other structurally and biologically related molecule pairs are also indexed. These include transition state analogue enzyme inhibitors, pro-drugs, propesticides and peptidomimetics.

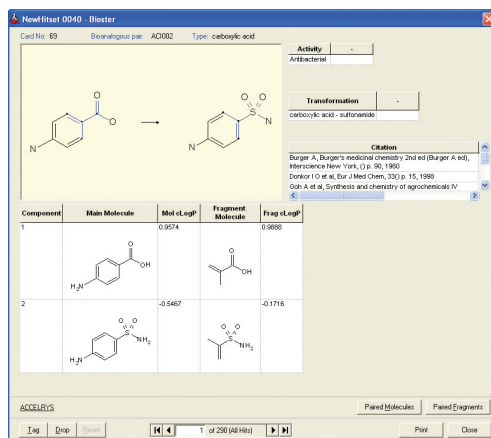
BIOSTER is useful for the design of novel, biologically active analogues of natural products, synthetic drugs, and agrochemicals. As such, it can be applied to the design of combinatorial libraries, helping to identify the most appropriate candidates from a cluster of potentially active compounds. You can also use BIOSTER's rich toolbox of proven examples of structural modifications to stimulate and explore ideas around your own lead progression and optimization studies to assist in the generation of potent, active molecules.

BIOSTER System Specifications

BIOSTER is available in a variety of formats including ISIS/Host and Accord Database Explorer (ADE) local and server. The ADE local version is ideal for providing individual desktop access to users. The ADE server version utilizes the power of the Accord Chemistry Cartridge and Oracle to give you fast network access to BIOSTER data. Both ADE format versions provide easy access to BIOSTER data via a simple easy to use interface that runs on Windows XP and Windows Vista.



Looking at a number of paired fragments in Bioster



Viewing a typical Bioster record in the Accord Database Explorer

Supported Platforms:

Accord format..... Unix and Windows
 ISIS/Host™ 2.1 or higher Unix and Windows
 ISIS 6 and other platforms . . . Please enquire
 You are welcome to evaluate the database on-site for 30 days with no obligation.