

# Benchware LibraryDesigner

Library Design on the Desktop



Given the vast universe of potential chemical entities to be synthesized, the design of small parallel libraries and large combinatorial libraries has increasingly becoming a strategic challenge for many Life Science discovery companies. To make these libraries, chemists must decide which reactants to use, usually from a very long list of potential reactants. Benchware® LibraryDesigner is a unique program which was developed to assist the laboratory chemist specifically with this decision-making process.

## Key Benefits

- Empowers laboratory chemists to design compound libraries
- Reduces workload of computational chemists, allowing them to focus time on non-routine tasks best handled by expert users
- Expands the enumeration functionality of Benchware LibraryMaker
- Increases productivity by accelerating decision making ability in the laboratory

## Key Features

- Utilizes easy to use, wizard-based interface to reactant-biased, product-based design algorithm
- Seamlessly integrates with functionality of Benchware LibraryMaker
- Supports design of many types of focused and diverse libraries
- Addresses iterative nature of library design with unique library re-design feature
- Imports virtual product scores such as docking and QSAR scores
- Automatically computes BCUT descriptors for design of various types of libraries

## Decision Support for Library Design

It is actually more important to use library design software to assist with the selection of reactants for small parallel libraries than for large combinatorial libraries. A few poor choices when selecting 80 A-type reactants from a list of 500 potential reactants is far less costly than a few poor choices when selecting just 4 or 8 A-type reactants from the same list of 500. The functionality of Benchware LibraryDesigner supports such decisions, saving time and money in the discovery process.

## Enhance the Functionality of Benchware LibraryMaker

Benchware LibraryDesigner is provided as an optional module within the Benchware LibraryMaker application environment and is seamlessly interfaced with that application's powerful enumeration, reactant-filtering, and product-filtering functionality. Benchware LibraryDesigner consists of a wizard-based interface to Tripos' unique, industry-validated reactant-biased, product-based (RBPB) library design functionality. The RBPB approach was first implemented in Tripos' DiverseSolutions®, an application that addresses many diversity-related tasks which arise in pharmaceutical and agrochemical discovery situations.

## Reactant Biased, Product Based Design

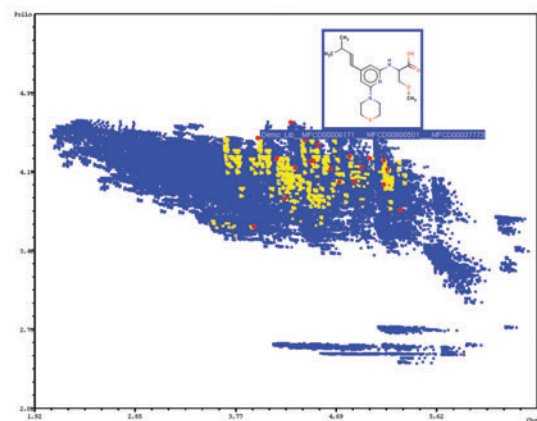
Historically, chemists have had two opposing objectives to satisfy when designing libraries: to satisfy the organization's 'economic' constraints

and to optimize library design criterion.

Achieving a satisfactory balance between these two objectives can be seen as the essence of library design. Therefore it is important that library design software enable a user-specified level of compromise between economic considerations and design criterion. Such compromise requires a reactant-biased, product-based approach to library design (RBPB design). Benchware LibraryDesigner has been built with this approach in mind.

## Supported Platforms

- Windows 98
- Windows NT 4.0
- Windows 2000 Professional
- Windows XP Professional



Above: Benchware LibraryDesigner plots descriptor values for molecular structures. In this view of chemistry space, red dots represent known lead compounds and blue dots represent compounds in a large virtual library. Yellow dots in this plot represent compounds in a new focused library that was designed by selecting a subset of the larger virtual library (blue dots) that cluster near the lead compounds (red dots).