

Improving & accelerating library design & profiling



Save time and resources to produce desirable drug-like libraries

OriBase Pharma / Product / EZ Design



Reagent Searching

Include and/or exclude fragment(s) (import or draw)
Import from commercial or in-house databases
Filter by minimum and/or maximum molecular weight



Reagent Filtering

Chemical cleaning / Toxicophore
Unwanted fragment / Properties filtering
(cLogP, HBA, HBD, Rule of five, ...)
Manual picking / Supplier filtering



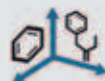
ADME-Tox

In silico prediction and prioritization for Caco-2, BBB, hERG, Cytotoxicity, Cytochromes P450, mutagenicity and carcinogenicity



Library Enumeration & Reverse Enumeration

Enumerate products from reagents following a reaction scheme
Obtain reagents from a set of products using an inverse reaction scheme



Library Profiling

Unwanted fragment / Toxicophore
Manual picking / Checking for duplicates
Properties filtering (cLogP, HBA, HBD, Rule of five,...)
Diversity analysis / Chemical space



EZ Design® is an integrated enterprise solution for reagent selection and filtering, and library enumeration and profiling.

EZ Design®, which bridges computational chemistry & medicinal chemistry, will provide the results you expect intuitively.

Library Design & Profiling

EZ Design® is a reagent selection and filtering, and library design and profiling tool. It has been developed to fit the workflow of both bench and medicinal chemists. It is designed to be portable and features a comprehensive graphical user interface, integrated and fast functionalities needed for reagent retrieval and filtering, product enumeration and library profiling.

EZ Design® uses component-based grouping of four modules: reagent searching, reagent filtering, library enumeration, and library profiling. Each module allows the chemist to access specific functionalities as well as diverse filtering and profiling mechanisms. By delivering the whole picture of reagent selection, and library design and profiling, in which all the relevant functionalities are integrated, EZ Design® drastically reduces the time spent on these processes, from a few days to a few hours.

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