dotmatics
knowledge solutions

Datasheet

DOTMATICS CHEMSELECTOR

Dotmatics Chemselector manages very large chemistry datasets with fast search and trivially simple update. It has a streamlined user interface focused on browsing and filtering for molecule, reagent and sample selection. The available eMolecules+ for Chemselector dataset provides access to highly curated eMolecules sourcing data.

SUPPORTING CHEMISTRY DESIGN WORKFLOWS

Chemselector provides high performance chemical searching, filtering and selection designed to support critical medicinal and synthetic chemistry tasks including

- building block selection
- fragment set design
- screening molecule selection for scaffold hopping
- chemical series validation for hit to lead campaigns ("SAR by catalog")

Chemselector's modern web user interface is designed to facilitate the selection of interesting molecules, samples or packages that are collected into carts to send to purchasing or for further processing

Chemselector uses Dotmatics provided datasets such as the eMolecules+ for Chemselector sourcing data and ChEMBL for Chemselector, or datasets built in-house from corporate or public databases (details overleaf)

It provides fast exact, substructure, similarity and match molecular pair searching and filtering by properties, substructures and packages on massive chemistry datasets

EASE OF UPDATE

Chemselector uses a novel search technology that allows datasets to be stored as files on the application server. With no database to build, updates are as simple as replacing a file, ensuring critical information is always up to date

INTEGRATION

Chemselector is fully integrated with the Dotmatics suite allowing Carts to be sent to Vortex for refinement or Reaction Workflows for use in library design

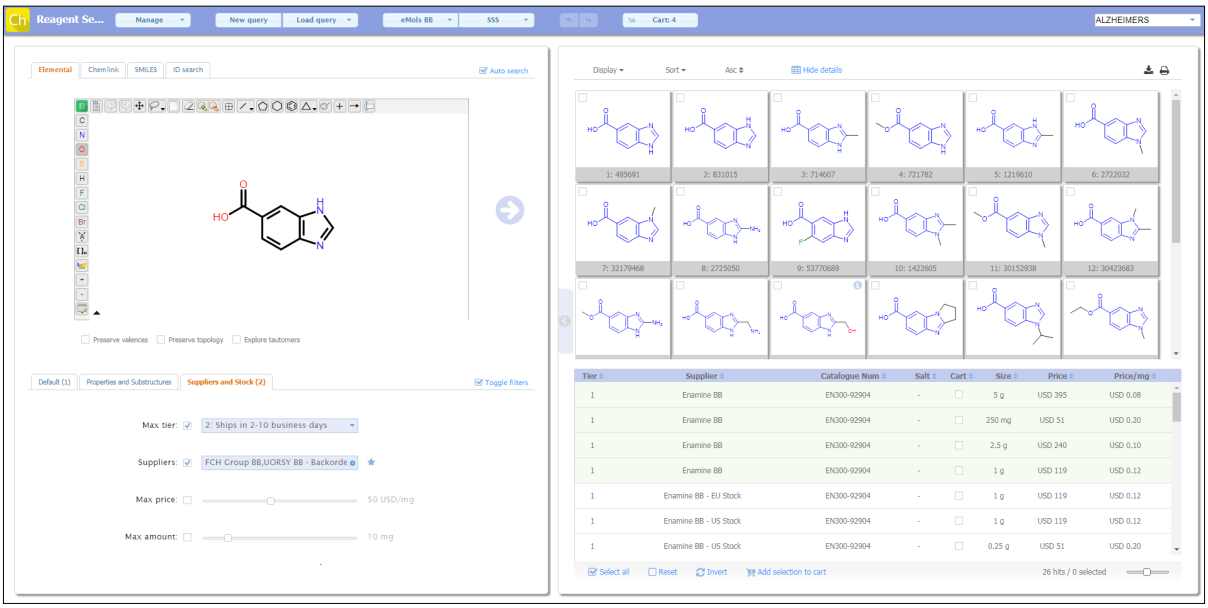

Figure 1: Reagent search and package selection using the eMolecules Building Blocks dataset

DATASETS FOR CHEMSELECTOR

Dotmatics produces sourcing and literature datasets formatted for use with Chemselector. Using these datasets within Chemselector rather than online ensures that commercially sensitive queries are never sent to public webservers. Corporate or other public databases can also be converted for use with Chemselector using provided administrator tools.

eMolecules+ for Chemselector

eMolecules+ provides a screening compound and building block sourcing database of 20 million compounds and 8 million unique chemical structures

- Highly curated sourcing data from eMolecules ensures only in-stock or synthesized compounds from credible vendors are listed
- Accurate and up-to-date availability, supplier, price and packaging information with updated data provided monthly
- eMolecules data is augmented with compound class, physiochemical properties and matched molecular-pairs data for advanced search and filtering
- Chemists use Chemselector workflow to assemble carts to be sent for procurement through existing corporate systems or using eMolecules fulfilment services
- Building block sets can be sent directly to Reaction Workflows for library enumeration

Literature and Patent Datasets

The following are available from Dotmatics formatted for Chemselector

- SureChEMBL for Chemselector - a publicly available large-scale resource containing more than 17 million compounds extracted from the full text, images and attachments of patent documents
- ChEMBL for Chemselector - 1.7 million structures abstracted from the primary published literature
- ChEMBL Drugs for Chemselector - ~9000 structure subset of ChEMBL of known drugs
- PubChem - database of literature chemical molecules and their activities against biological assays

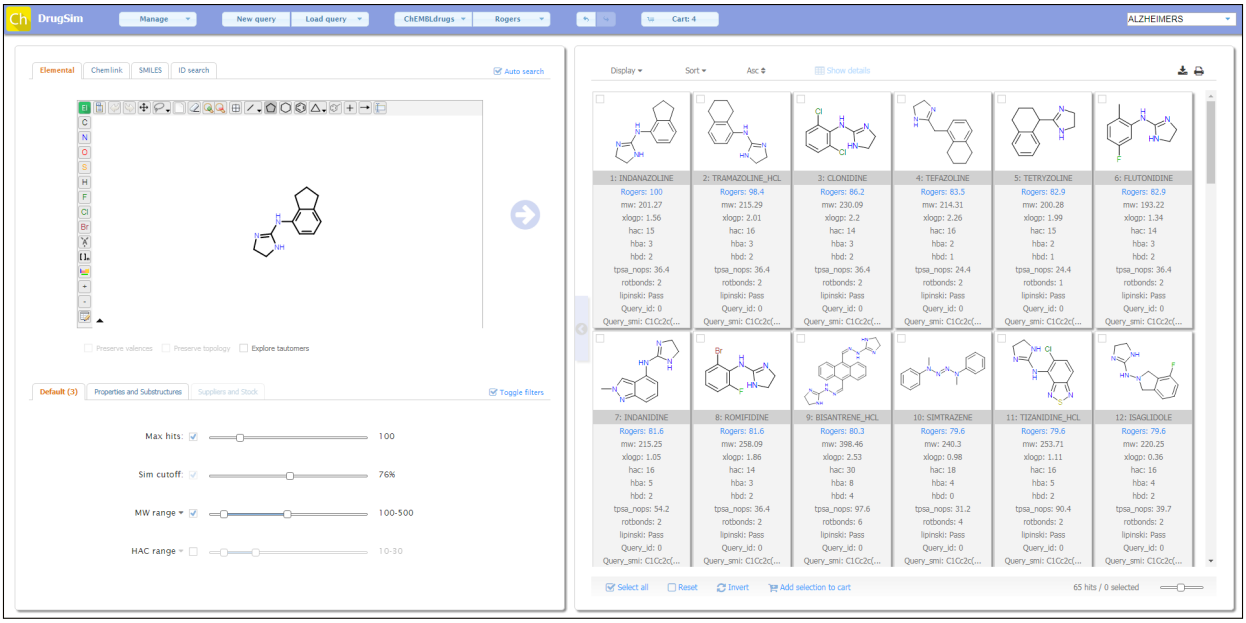

Figure 2: Similarity Search in ChEMBL Drugs for Chemselector

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