User-friendly Database Querying for Decision Making in Drug Discovery

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Introduction

A key challenge in drug discovery is ensuring that project leaders and decision makers have access to the latest and most relevant data for their projects. In this poster we present the results of a collaborative effort to develop a user-friendly graphical tool for creating, sharing and executing structured database queries and presenting the results in a format that enables the user to visualise and analyse the data without further processing to guide the optimisation of compounds in drug discovery.

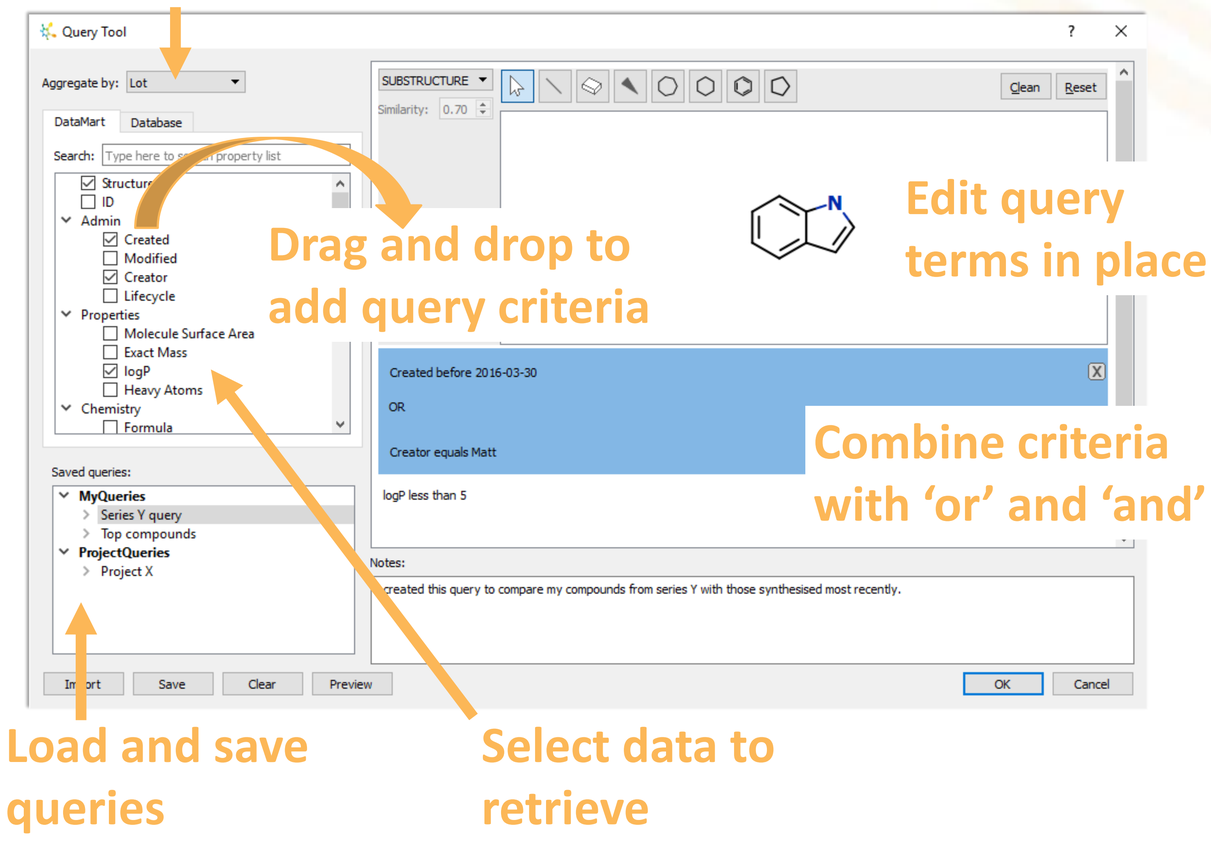
Query Tool

Requirements

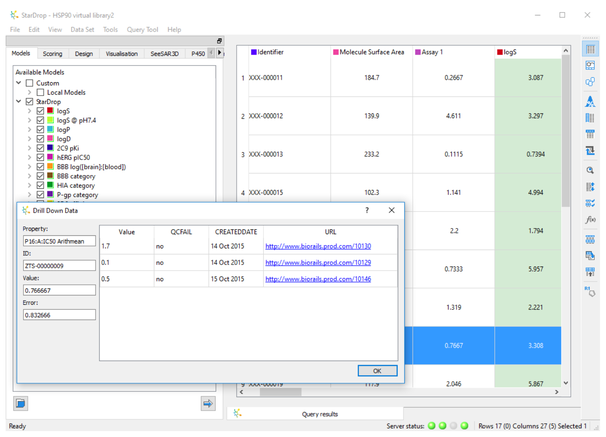
- User-friendly definition of search criteria and fields
- Save, share, edit and execute pre-defined queries
- Support for criteria based on chemical structure, numerical, date, textual and categorical fields
- Support for multiple data aggregation levels
- On demand drill down to data underlying aggregated values
- Refresh query to update results and analyses with new data
- Provide access to multiple data sources

Solution

A query tool was developed within the StarDrop™ software platform.

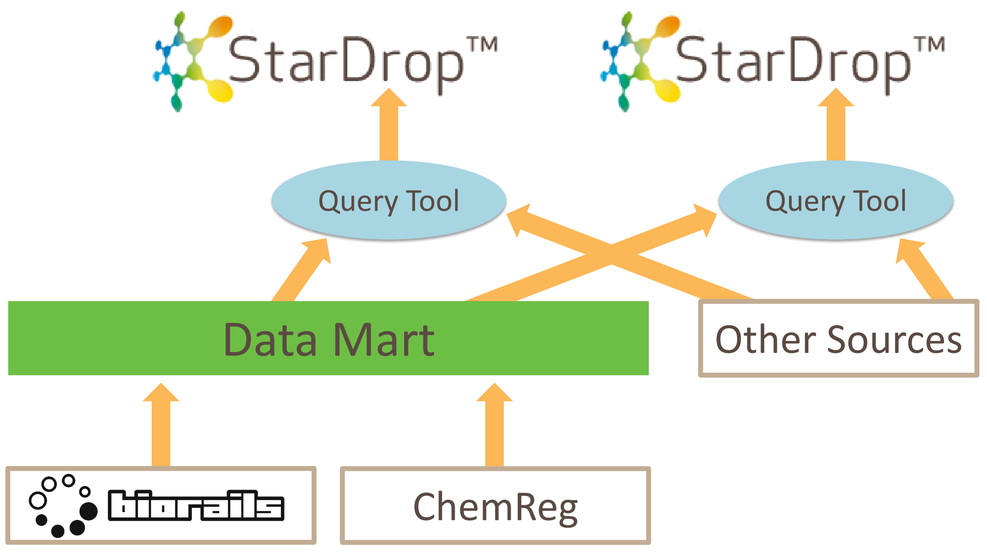


The query tool translates the user input into an SQL query that is run against a data mart via an ODBC connection. Additional data sources may be easily configured and the tool may be adapted to other database APIs.



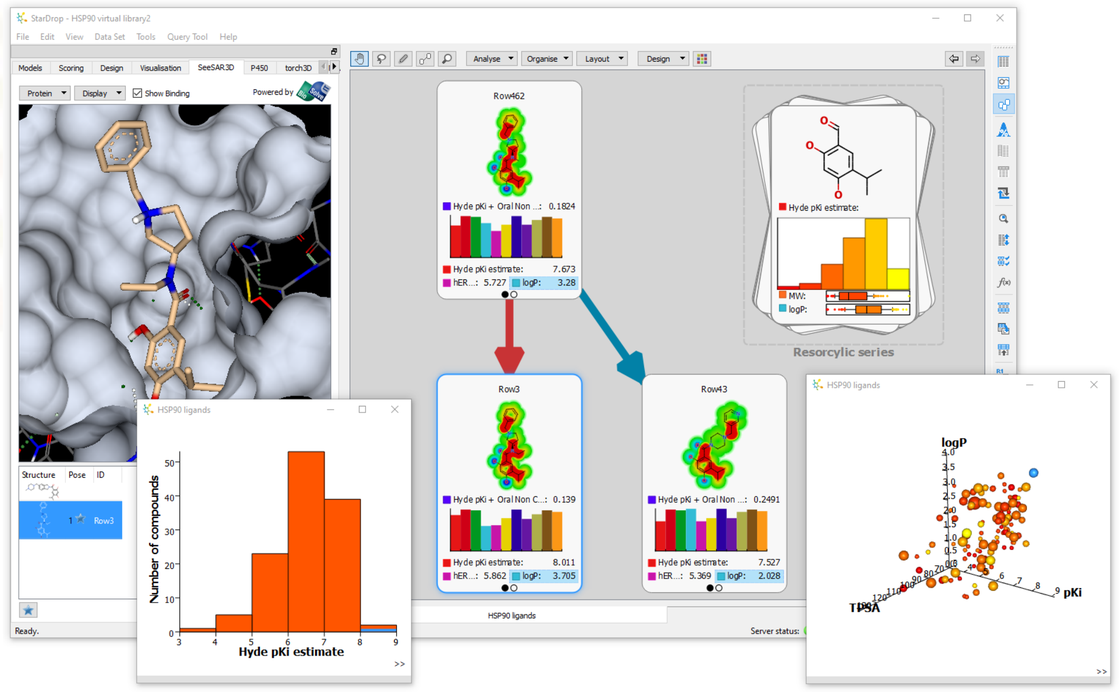
The results displayed may represent aggregated values from multiple measurements. The individual, underlying data points may be easily accessed via a drill-down feature.

Architecture



- Biological data stored in the BioRails™ database is extracted and aggregated by compound, salt and lot nightly
- Results are stored in a data warehouse with associated data from the compound registration database
- These data are pivoted and stored in a data mart which facilitates easy access to results and associated metadata
- StarDrop users can use the query tool to design and run queries against the data mart
- The data returned are displayed in StarDrop

Data Visualisation and Analysis



Value comes from data through the selection and design of high quality compounds, using capabilities such as:

- Data visualisation, including StarDrop’s Card View™
- Analysis of structure-activity relationships
- Multi-parameter optimisation
- *In silico* modelling and d*e novo* design

Conclusion

Seamless connectivity between design and decision making tools and the data management system ensures that project teams have access to the latest information without needing to compile the data manually from many sources. This leads to better decisions and shorter project timelines.

StarDrop: www.optibrium.com/stardrop

BioRails: www.edge-ka.com/products/biorails