StarDrop™

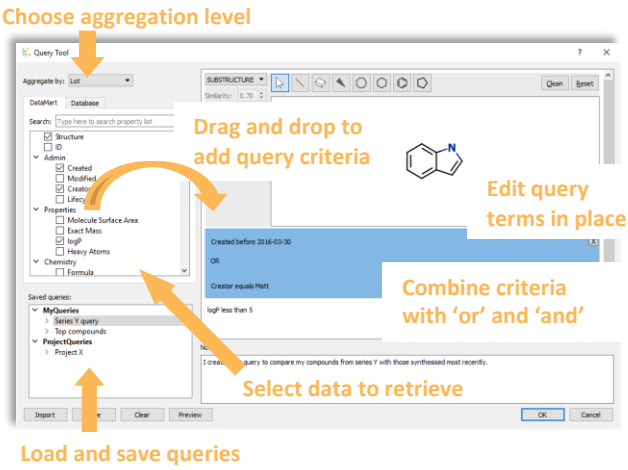
Customisation and Integration:

Overview

As an enterprise platform, StarDrop's comprehensive data analysis, visualisation and compound design environment has been built to work seamlessly with your informatics infrastructure. Here are a just few examples…

Database Query Interface

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. StarDrop provides a user-friendly graphical tool for creating, sharing and executing structured database queries, returning the results ready for visualisation and analysis. Features include:



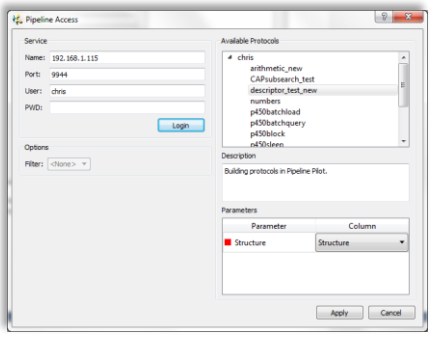
- User-friendly definition of search criteria
- Saving, sharing and running predefined queries
- Easy editing of criteria based on chemical structure, numerical, date, textual and categorical fields
- Access to multiple data sources
- Support for multiple data aggregation levels with on demand drill down to underlying data
- Refresh capability to update results and analyses with new data

Certara D360™ Integration

D360 provides scientific data integration, access, analysis, and visualisation capabilities for early discovery through to the preclinical and clinical phases of drug development. D360 solves both intra and inter-domain research challenges by integrating data from multiple source systems. From within StarDrop, users can link directly to D360, accessing their workspaces to pull data directly into StarDrop and guide their compound selection and design decisions. D360 users can also push data straight into StarDrop and so whichever end you start from, the combined capabilities of D360 and StarDrop can easily be applied to every research decision.

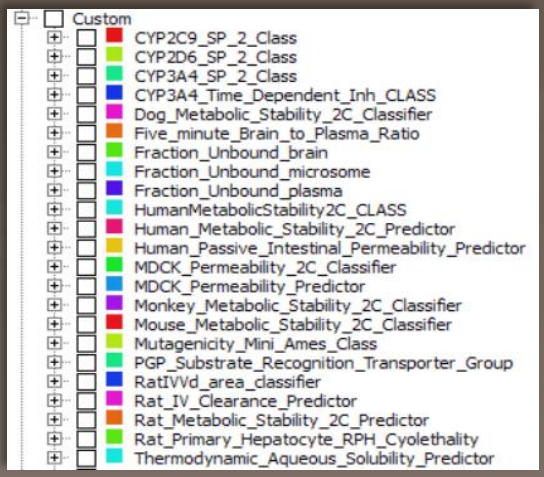
Pipeline Pilot® and KNIME® Integration

If your informatics environment uses pipelining platforms such as Pipeline Pilot or KNIME, StarDrop can be linked directly to this infrastructure. A dedicated Pipeline Pilot interface enables StarDrop users to log in, select and run protocols, providing instant access to your own informatics methods. StarDrop's Python scripting environment means that KNIME users can also connect to any protocols available as part of your infrastructure. Furthermore, StarDrop's ADME QSAR models, quantum mechanical P450 models and Probabilistic Scoring approach to multi-parameter optimisation are also available as web services enabling them to be part of your own pipelines, without need to use the StarDrop user interface.



In-house and 3rd Party Predictive Models

Whether you have built custom, in-house models or are using predictive technologies from 3rd parties, StarDrop's flexible model interface provides a front-end to work with all of your models in one place. Using a simple API to connect each model StarDrop can work with any models that take a structure as input and return numerical, categorical or text results. Created to provide easy customisation, you can quickly add predictive models that you have built or to which you have access via a command-line or web service interface.



Models can be accessed directly through the StarDrop desktop application or via a model server. On the server, you can control the way that model calculations are batched together and configure the number of molecules passed into the calculations in each batch. The StarDrop application can connect with one or more model servers, enabling you to organise your models to run most efficiently, and each model server can be configured to use multiple machines, CPUs or cores, so that you can add computational power where it is needed most.

Python Scripting

Much of StarDrop's customisation environment has been facilitated using Python. The StarDrop client scripting interface provides Python modules that give you direct control of the user interface and manipulation of data sets. You can use the Python modules from StarDrop's built-in console (interactively) and through items selected from a customisable menu. To take advantage of StarDrop's Card View™ for visualising relationships between compounds, the scripting interface also enables you to create and specify your own layouts. If desired, StarDrop can be configured to run a script when launched from the command line.

Web Services Interfaces

StarDrop's *in silico* predictive ADME QSAR models, quantum mechanical predictions of P450 metabolism and Probabilistic Scoring approach to multi-parameter optimisation (MPO) can all be accessed via web services. These enable your in-house or 3rd party tools to access StarDrop's prediction and MPO algorithms directly without needing to use the StarDrop client interface.

About Optibrium

Optibrium provides elegant software solutions for small molecule design, optimisation and data analysis. Optibrium's primary product, StarDrop™, brings confidence to the selection and design of high quality candidate compounds.

Founded in 2009, Optibrium continues to develop new products and research novel technologies to improve the efficiency and productivity of the drug discovery process. Optibrium works closely with its broad range of customers and collaborators that include leading global pharma, agrochemical and flavouring companies, biotech and academic groups.

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