

Benchware Discovery 360° for the End User

D360's end user interface comprises a single application (one stop shopping for discovery data) that provides access to the key capabilities of the system for Query Construction, Query Execution, Dataset Analysis, and Workspaces for saving and sharing information.

Query Construction

The screenshot displays the 'AllTestedCompounds [1]' application window. The interface is divided into several sections:

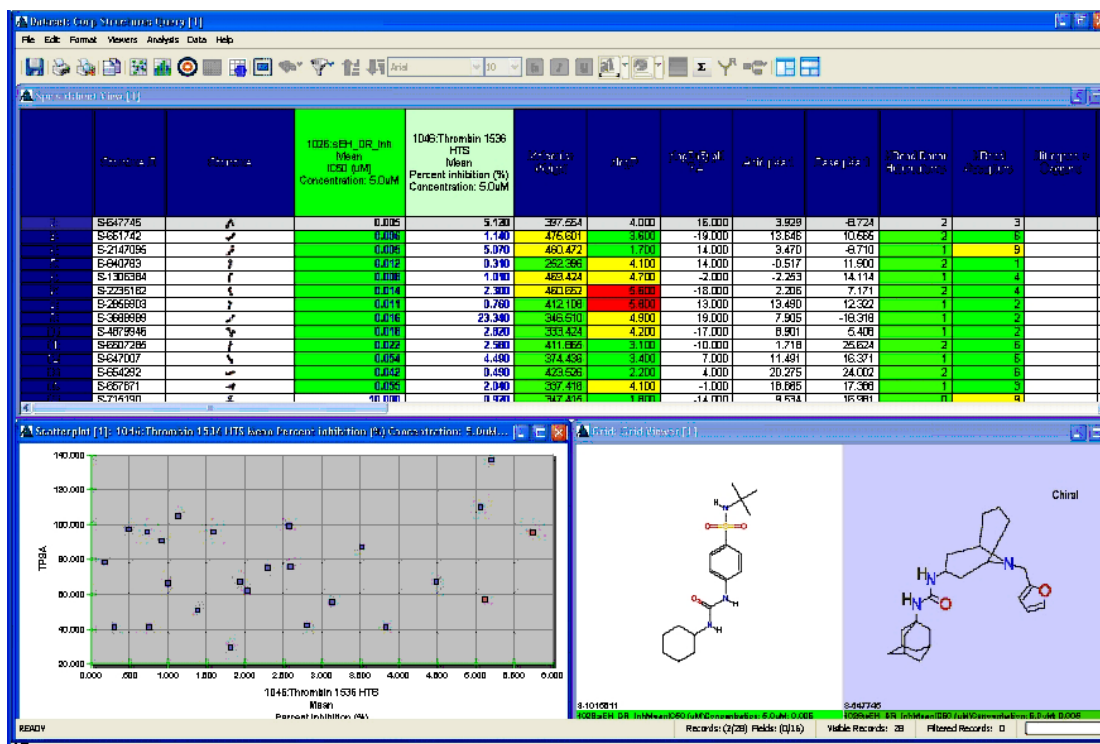
- Left Panel:** A tree view showing a hierarchy of data categories. The 'Corp Structures' category is selected, and its sub-items (Proc Num, Proc Name, Proc Full Title, Proc Type, Proc Version, Author Full Name, Project Num, Project Name, Details, Author, Identifiers, CATS, ACD, Structures, Results, Assay Data) are visible.
- Top Panel:** 'Query Data Category: Corp Structures' and a 'Filter:' field. Checkboxes for 'Show Constrained Fields' and 'Show Unconstrained Fields' are present.
- Table:** A table with columns 'ID', 'Show', 'Disable', 'Field', 'Sort', and 'Sort Direction'. It lists several fields for selection:

ID	Show	Disable	Field	Sort	Sort Direction
	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Structure (Corp Structures)		
A	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1250, DR: Anti-Viral Drugs Against Arbovirus Infections, a Confirmatory Screen (Res, Assay data for a Corp structure) IC50 (uM) (Mean)		
	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Molecular Weight (Corp Structures)		None
	<input checked="" type="checkbox"/>	<input type="checkbox"/>	clogP (Corp Structures)		None
	<input checked="" type="checkbox"/>	<input type="checkbox"/>	HBond Donor Heteroatoms (Corp Structures)		None
	<input checked="" type="checkbox"/>	<input type="checkbox"/>	HBond Acceptors (Corp Structures)		None
- Bottom Panel:** 'Procedure' and 'Type' fields. A 'Result Type' section with dropdowns for 'IC50 (uM)', 'Exists', and 'uM'. 'And Conditions' section with radio buttons for 'And' and 'Or'. 'Query Options' section with a 'Search Name' field containing 'Corp Structures Query' and a 'Submit' button.

D360 Query Builder with a query involving compound and biological data

D360 includes a powerful system for constructing queries. This system allows a range of queries, from simple queries on compound related data fields, to complex queries involving advanced constraints, biological data, a variety of data categories, and query logic. Users can browse through the Data Catalog, which presents all available data in an organized manner, and choose data that they wish to constrain and data that will be included in their datasets. Based on the available data and related business rules configured in the system, complex options are supported, allowing users to dynamically pivot and aggregate data, constrain based on relationships between fields, and define their output formats. Queries can be built dynamically as they are needed, or can be saved and shared within D360 or as objects on a file system. Release 5.0 of D360 (early 2009), will provide Form based querying and data presentation as well as QuickSearch widgets providing instant access to commonly used searches for all D360 users.

Dataset Analysis



D360 client application with a simple project dataset with multiple views and formatting
Data from PubChem

Once a query has been submitted, a dataset is generated and presented to the users. Datasets provide one or more methods of visualizing data, and access to all of the analysis tools and related capabilities in the system. Many queries will begin with a spreadsheet view of data, and then use additional viewers within the dataset to visualize data in a variety of ways. Standard viewer types include:

- Spreadsheets – standard table-based views of data, with basic functionality similar to standard desktop spreadsheet tools, and advanced capabilities based on knowledge of scientific data and integration to all of the D360 capabilities.
- Grids – a tile-based presentation of structures and selected fields, allowing a more compact representation of data when users are focused on structures
- Graphs and Charts – Graphs such as scatter plots and histograms for displaying and exploring data graphically
- Similarity Maps – A tool for visual analysis of data (commonly used for structure similarity) which allows user's to easily understand the make-up of a dataset with the ability to plot data across multiple dimensions.
- Forms - Beginning with D360 5.0 in early 2009, forms-based views will be supported
- Other views, including both those included with D360, and those added by customer configuration and extensions.

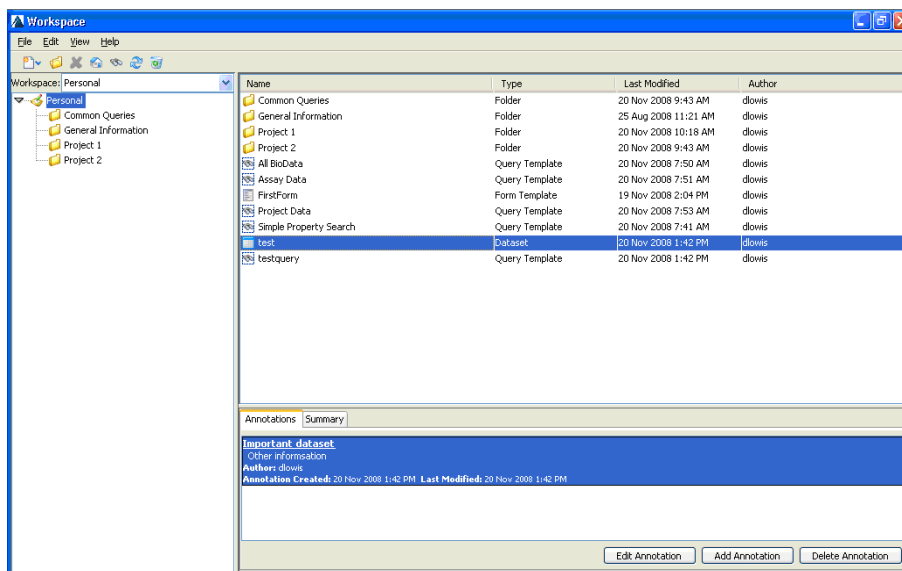
When a user has multiple views within a dataset, the system provides several options for linking viewers together. Selections made within one viewer are propagated to all other viewers, and a "primary viewer" mode can be used to show detail in a viewer based on selection in another.

Datasets also include standard tools for refining data, including filter, find and selection tools that can be used in simple cases as well as for more advanced logic. Formatting can be applied in viewers based on manual selection, or based on "color by value" and similar rules. Viewers can be printed and exported in a variety of formats, as can their underlying data.

Integrated tools and services provide the ability to perform advanced analysis and calculations based on the data in the dataset. These may generate additional views, or add data to the set. Users can add custom data to the dataset, utilizing manual input, import, or equation capabilities. A variety of built in analysis mechanism, including R-Group analysis, can also be accessed.

Finally, datasets provide access to simple mechanisms for following workflows or drilling down into aggregated data. Configurable follow-on queries allow users to browse through related views with a single click – following a path through the data available to the system as they work through their analysis and experiment planning.

Workspaces



D360 Workspace Browser

The final area of D360 is the workspace system, which is designed to facilitate capturing information generated in the application (queries, datasets, results of analysis), and sharing and reuse of that data between users. All users of the system have access to a personal workspace, in which they can store queries and datasets. In addition, an unlimited number of group workspaces can be established, and users can publish data into these groups. Security can be configured within these groups, allowing some shared workspaces to be available globally, while others can be further restricted. Distinction of read and write permissions can be set on individual groups for each user.

The workspace tool provides a familiar, “Windows Explorer” style user interface for browsing this data. In addition, users can directly browse all workspaces when retrieving or saving data through other portions of D360. An annotation facility is provided for capturing relevant information about items stored in workspaces.