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Benchware Discovery 360 Product Overview

Introduction to Benchware Discovery D360^o

Executive Summary

Benchware[®] Discovery 360^o (D360) allows organizations to improve their research efficiency in a cost effective manner by allowing research scientists to readily access, analyze and share their data. The product has demonstrated excellent usability, high performance query capability, comprehensive data analysis functionality and scalability to 1000s of users.

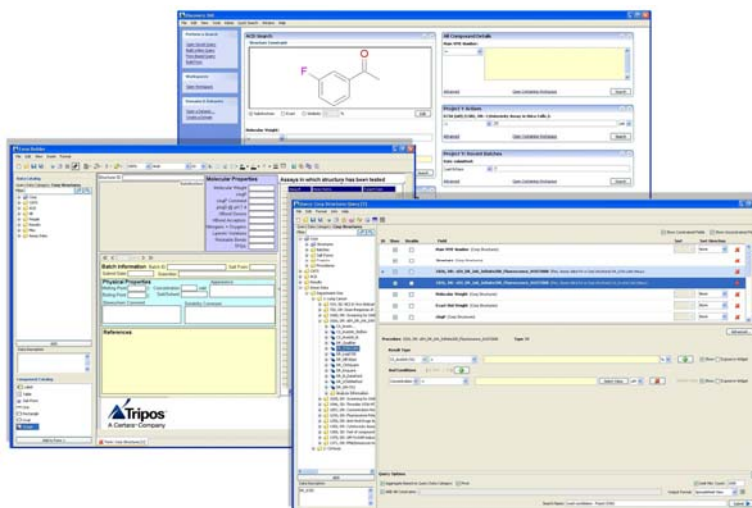
“After working with Tripos, our colleagues internally and with Accenture, we were able to put D360 in play February, 2008. To date, we have deployed to over 700 scientists, including chemists and biologists ranging in specialties. We’ve been very pleased with the feedback from scientists. They have come to us and said they have seen tremendous time savings and can use D360 to ask questions of the Wyeth data that simply weren’t possible before, or would take hours for the query to actually return with information. The scientists have been finding a functionality that they didn’t have access to before and seem to be generally enthusiastic about using it.....”

“Overall, the benefit we’re seeing is how this application is giving scientists time to focus on science and innovate and extend their capabilities.”

-Steve Howes, Senior Director, Bioinformatics, Wyeth Pharmaceuticals
Excerpt from Future Pharmaceuticals podcast April 2009

Data Access

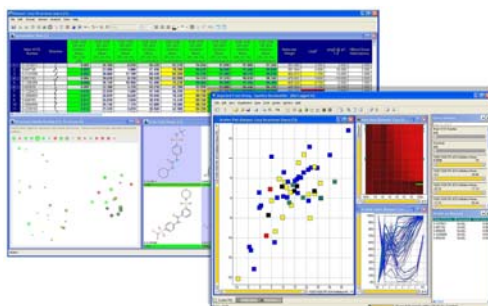
D360 is a multi-tiered application that allows researchers to effectively access, analyze and share vast quantities of research data of a complex nature. D360 allows both simple and complex query construction covering different aspects of research data (chemical, biological, logistical...) through intuitive building interfaces. Queries can be easily stored and shared with project team members and research managers or exposed as simple searches for the most common research workflows.



**Main Application window (top) showing QuickSearch widgets.
Form Builder Interface (left) with partially built Form template and
Query Builder window (right) containing constrained query.**

Data Analysis

Users can readily generate and *explore research data* to gain the understanding that drives projects forward through multiple, interlinked data viewers along with Tripos' established R-Group analysis and structure similarity projections. D360 allows visualization of complex, multidimensional datasets through forms, chemically aware spreadsheets, grids, graphs & charts along with Tripos' innovative structure similarity maps. Advanced analysis capabilities are provided through built-in integration with 3rd party analysis and statistical tools (TIBCO Spotfire, SAS, JMP...) or through integration of proprietary scientific techniques through D360's APIs.



D360 dataset window showing integrated Spotfire viewer.

Sharing

Effective reporting is ensured by the smooth data export functionality to 3rd party applications including MS Excel & PowerPoint.

Project Management and Decision Support is an integral part of D360 and allows effective knowledge sharing through a fully configurable personal and shared workspace system supporting audit trailing and access rights assignments.

Who is using D360?

Benchware[®] Discovery 360[°] has proven to reduce the amount of time scientific teams spend on retrieving, manipulating, analyzing and distributing knowledge and leads quickly to a strong return on investment.

You will be interested in D360 if:

- Your researchers spend significant amounts of time and effort getting to and understanding their data.
- Your researchers need to use multiple applications to generate the data views they need.
- You find inter-project comparisons difficult due to data package inconsistencies.
- You are considering building a data access and analysis system in house.
- You are replacing or enhancing an existing in-house developed system.

Summary

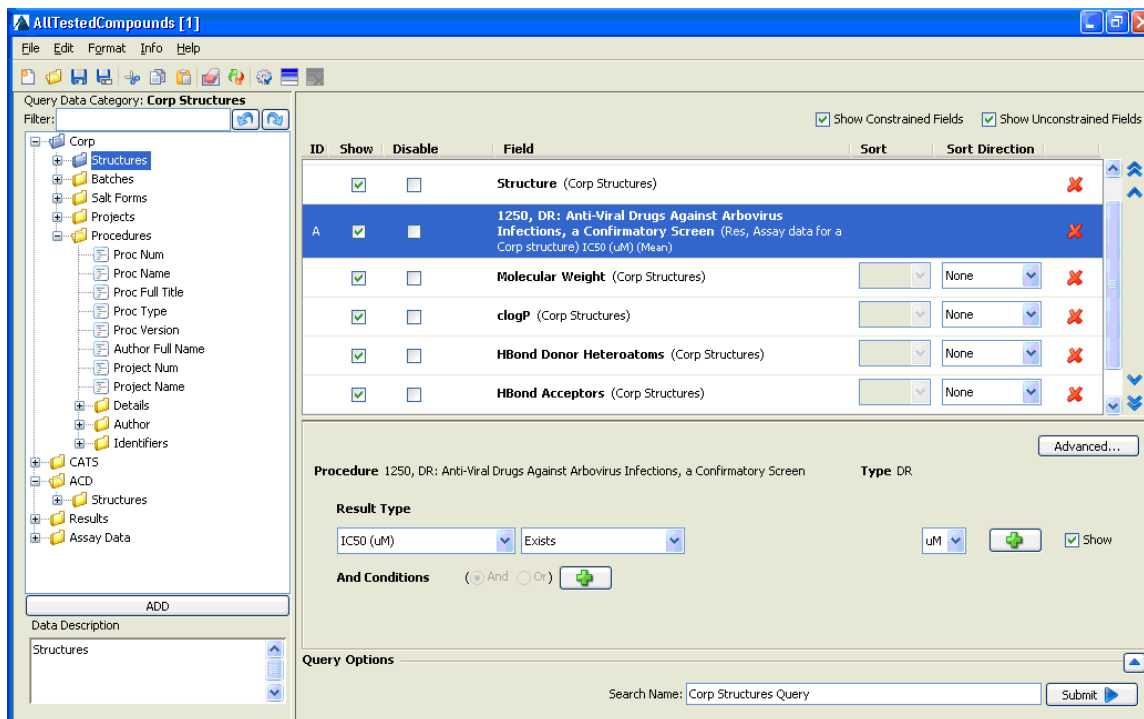
Benchware[®] Discovery 360[°] (D360) is the first comprehensive product solution that provides life science researchers a *single point of access* to retrieve, analyze, and share scientific data. It eliminates time-consuming, error prone, non-productive hours that scientists spend merging and manipulating data from multiple, disparate sources. Using D360, assembly of a project SAR dataset is reduced from hours to minutes allowing researchers to spend more time at the bench.

D360 is the only enterprise application for pharmaceutical data access, analysis, and sharing that is both easily configured to the requirements of a particular research organization *and* can provide the scalability and performance necessary for even the largest life sciences organizations. D360 is a product solution rather than a one-off custom development and has been deployed to thousands of scientists to increase the speed, accuracy, and effectiveness of research.

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.

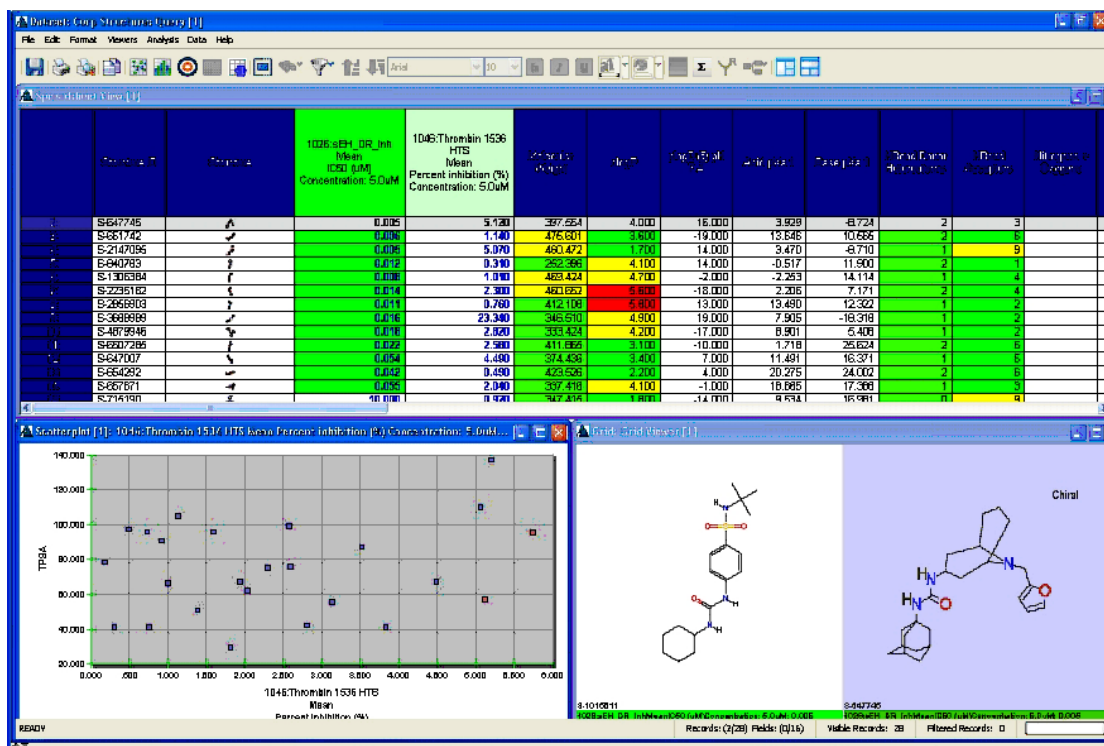
Query Construction



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.

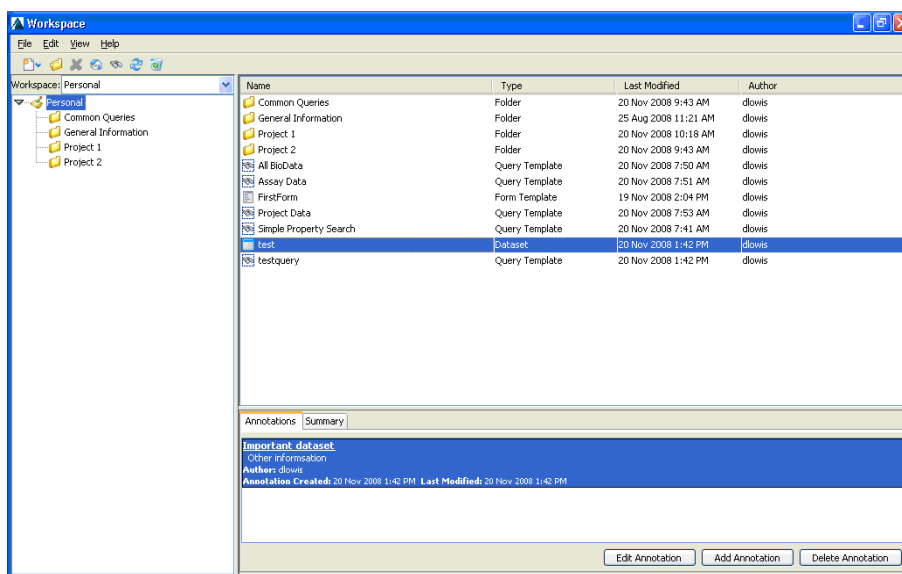
When a user has multiple views within a dataset, the system provides several options for linking viewers together. Selections made within one viewer are propagated to all other viewers, and a "primary viewer" mode can be used to show detail in a viewer based on selection in another.

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

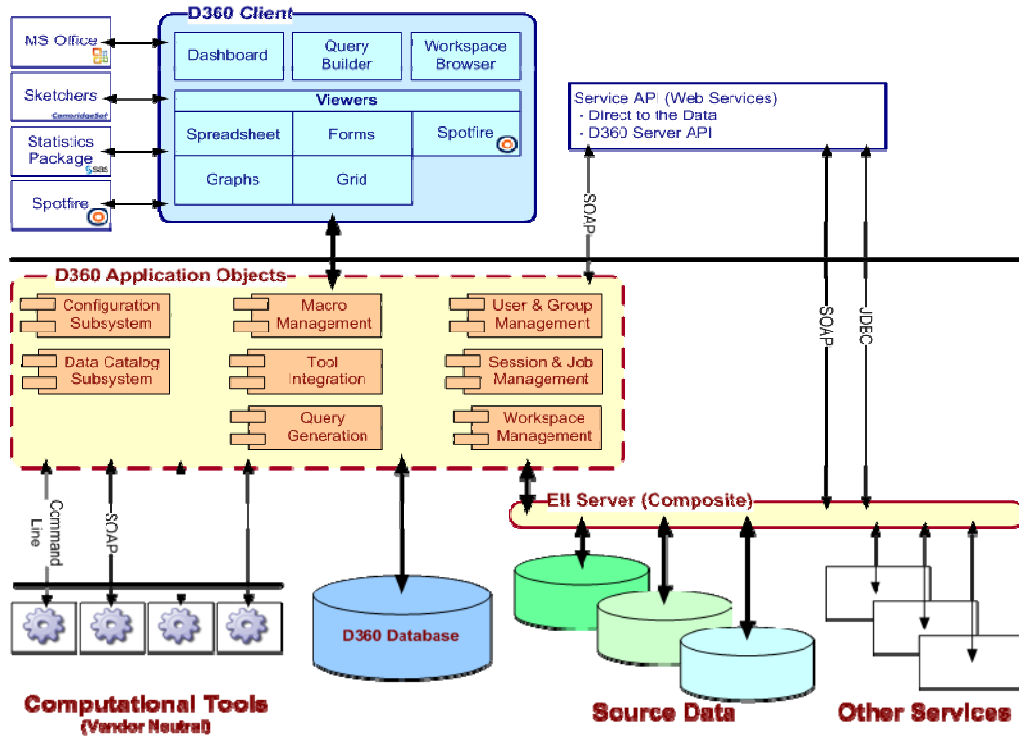
The final area of D360 is the workspace system, which is designed to facilitate capturing information generated in the application (queries, datasets, results of analysis), and sharing and reuse of that data between users. All users of the system have access to a personal workspace, in which they can 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.

Benchmark Discovery 360° for the Technical User

Architecture

D360 is a multi-tiered application built from a dynamic collection of interchangeable components and services, as shown in the diagram below.



The system has several major architecture components:

- **D360 Client:** A rich tool through which users interact with the functionality of the system. This is a Java application, which can be deployed as standard desktop-installed software, or through a web-based deployment mechanism (Java WebStart).
- **D360 Application Server:** The server is a collection of services that store configuration, generate queries, manage sessions and user jobs, execute data transformation logic, manage user workspaces, and interact with computational tools and other services. These are typically deployed within a Java/J2EE environment on a variety of supported platforms (Windows, Linux, Solaris).
- **EII Server:** A key component of the solution is an Enterprise Information Integration server. D360 uses an embedded solution from Composite Software. The Composite engine is a proven system, used in large organizations in a variety of industries to access diverse types of data. The EII server supports access to “federated” data, from a variety of data sources. These data sources may be underlying databases, external services and tools, files, etc. Combined with the scientific knowledge provided through D360, the solution is optimized for dealing with the typical source database systems used throughout discovery organizations.
- **D360 Database:** An Oracle database is used to store information about jobs being run, store virtual data sets while users are interacting with them, and provide storage for the workspace subsystem.
- **Tools, Source Systems and Services, and Computation Engines:** As described below, D360 is often integrated with a variety of end-user tools, source systems, customer and third-party services, and computation engines. D360 includes “out of the box” integration with the most common tools and services in each of these areas, and simple mechanisms (through configuration and pluggable components) to add integration with new services and tools.

The architecture of D360 has been designed to fulfill several high-level design goals:

- **Proven performance and scalability:** In order to support the needs of users throughout large discovery organizations, a solution such as D360 must perform well, and scale from small numbers of users up to large deployments with thousands of users. D360 has been optimized to ensure response time and query performance are as fast as possible, allowing users to focus on analyzing their data and making decisions rather than waiting for query results. In addition, real-world deployments of D360 have had utilization of greater than 10,000 queries per month, and scalability testing has been performed to significantly higher levels.
- **Modular collection of components and services:** Although D360 is a comprehensive solution that can be used “out of the box”, an important consideration was to ensure that customers could extend, replace, remove, or add modules as necessary. This includes components within the user interfaces as well as services and data sources on the back end.
- **Configuration-driven:** All aspects of the application make use of the D360 configuration system, allowing their behavior to be determined dynamically, and to be changed without the need to develop or modify any code. In most cases, configuration can be applied globally, on an individual user basis, or to groups of users.
- **Open integration options:** Users of D360 typically have a variety of tools they interact with, ranging from Microsoft Office to Spotfire to highly specialized applications. In addition, customer organizations typically have a variety of services, data sources, and computational tools they need to tie together into a comprehensive solution. D360 has been designed to provide open integration options for hooking these tools and services together as necessary.
- **Easy to setup, use and maintain:** Finally, Tripos has focused on ensuring that the power added through D360 to satisfy the design goals above is achieved while also maintaining ease of use and maintenance. Though a number of extension and configuration points are available, the system is usable after deployment simply by configuring at least one data source. Tripos has also worked to ensure ongoing maintenance and support activities are minimized, to ensure the overall cost of ownership is as low as possible.

Configuration and Customization

Data Sources

The most obvious and immediate need for configuration arises with access to data sources, as access to data is required to make use of functionality in the system. Data sources are connected to the EII server through a graphical configuration mechanism, which mostly involves simply providing connection information and then using “auto-discovery” capabilities to find and interpret the available data. Query generation and data display within the D360 application are controlled by the Data Catalog. The Data Catalog controls how fields are presented to users, manages important relationships between data, and provides metadata which will be used in visualization or analysis. Tripos provides administrative tools for building the data catalog.

Data Transformation and Business Rules

Once D360 has been connected to data sources, customers frequently chose to implement business rules for transforming data as it is retrieved. This often involves operations such as pivoting result data into distinct columns, aggregating values at various levels, or automatically converting data from storage units to an alternate display format. Most of these operations can be controlled by an end user through the query user interfaces, but defaults or corporate business rules can be implemented through configuration. When more advanced transformation or specialized aggregation rules are desired, new services can be deployed into the system as pluggable components available to the user.

Service and Tool Integration

A variety of mechanisms are commonly utilized to integrate external services and tools. First, customers frequently have compute engines and predictive models (in-house or third party) that they desire to connect to datasets. These tools may generate additional data to be included in datasets, or calculate data based on other information or structures in those datasets. D360 includes a framework for integration of these tools, which can invoke engines locally on the server machine (as executables) or defer to remote services. Remote services are typically deployed as SOAP web services, which are then hooked up to D360 through simple configuration. This configuration involves providing a definition for the service API, typically in a Web Services Definition Language (WSDL) file, and providing metadata about how dataset information should be passed to the service and how results should be displayed in the UI. Current customers use this to connect not only to standalone compute tools, but also to workflow tools and integrated models, including those utilizing Pipeline Pilot.

In addition to services invoked from the system, customers frequently desire to connect desktop tools within the D360 client. D360 contains standard integration with the most common desktop tools, including Microsoft Excel, PowerPoint, Spotfire, and various statistical packages. This tool integration can appear in a variety of ways. In the most common scenario, data is exported to the external tool from D360. When the external tool accepts standard data formats, this export can simply be defined through new configuration entries, including invoking the tool through command line or direct APIs. For more complex data needs, or for deeper integration of the tool within the client application, components can be implemented to D360 APIs and then “plugged in” to the client. In the most advanced cases, complex components and tools are tied deeply into menus, datasets, and functionality throughout the system, building a powerful integrated application utilizing D360 as a platform.

Visualization

A number of visualizations (spreadsheets, graphs and charts, grids, forms, similarity maps, etc) are available in D360 datasets out of the box. However, customers occasionally desire to extend these visualizations, and add new ways to visualize data.

Many types of data presentation can be created through configuration of existing components. In fact, the available viewers are determined dynamically based on configuration data. In some cases, a customer may choose to add a new viewer by going beyond configuration, and creating new visualization code. This code is implemented to standard product APIs, and “plugged in” to the D360 client dynamically. In other cases, a customer may desire to integrate an existing tool as a visualization mechanism. This can be done through configuration and connections of the external tool to standard interfaces. These interfaces provide several levels of integration – ranging from simply pushing data out, to deep, two-way communication.

D360 includes an example of this with the standard integration to Spotfire. A user can choose to invoke Spotfire as a D360 viewer, which launches the external tool and provides access to data from the user’s dataset automatically. Events are then propagated in both directions between D360 and Spotfire, allowing a user to make selections and changes in either application and see the results in the other. Finally, when the user saves the D360 data set, the entire Spotfire session, including all setup, visualization, selections, and data, are persisted, and restored in the original format if the dataset is opened at a later point.

External Access and Sharing

Finally, in many D360 deployments it is desirable to access data in D360 (including visualizations, queries, etc) in external tools such as SharePoint. These systems can be connected together by hooking into standard APIs within the D360 application server.

Other Areas

The areas listed above provide several examples of the typical configuration and customization that customers may choose. Many other aspects of D360 are configurable and extensible, allowing customers to utilize D360 as a platform on which broader solutions are built, and to integrate D360 into other applications used throughout Discovery workflows.

Frequently Asked Questions about Benchware Discovery 360°

Data Access

- **What types of data can D360 work with?**
 - D360 provides an integrated view of all discovery data. Data can be presented from compound or batch/lot perspective or from the point of view of a project. D360 allows users to ask any question of the data rather than being limited to a particular data “view” and can provide for standard SAR table generation through investigation of batch level variation of biodata to project management.
 - D360 allows users to search for, constrain, present and analyze numerical, modified numerical, text, date, chemical structure and image data from a variety of sources such as chemical registration systems, compound & reagent inventory systems, biological data repositories and electronic lab notebooks.
- **Does D360 require a data warehouse?**
 - D360 employs a commercial Enterprise Information Integration (EII) component that allows the application to be deployed either on top of an existing data warehouse or to federate disparate data systems which may be a variety of storage formats from relational data systems to Excel files to text files.
- **How can I integrate new data sources as new technologies become available?**
 - D360’s configuration system allows new data sources to be made available to end users with no need for additional coding. Once configured the new data source will be automatically available to users at their next login.
 - In the case that D360 is operating in a data warehouse environment, new sources of data can be rapidly federated into the system making the data available to users while the process of loading the data into the warehouse proceeds.
- **Can user’s query data at both the compound and the batch/lot level?**
 - D360 allows presentation of data at both the compound and batch/lot level but goes significantly further and allows users to generate datasets where returned records represent Projects, Assays or Procedures, People etc. Alternate views of data allow D360 to be used as a research and project management tool in addition to understanding how chemical structure affects biological activity profiles.
- **How does D360 deal with data aggregation and pivoting?**
 - Data aggregation and pivoting is done automatically in D360 so that users do not have to manually aggregate and pivot using Excel tools or their equivalent. Because business rules are employed to determine default pivot conditions and aggregation functions datasets produced through D360 are more consistent and error free than those created by users performing aggregation and pivot tasks manually.
 - Power users can readily access multiple different aggregation functions and alter pivot conditions in order to understand more detail in the data that is retrieved. Custom aggregation functions are readily implemented through the configuration system.
- **What is the learning curve for a new user of D360?**
 - D360 is a single point of access for fundamental day-to-day activities like reagent searches, project tracking and SAR generation. Building simple queries is a straightforward process through the intuitive interface that also allows users to quickly select the data that they want to see and provide constraints to limit the retrieved data.
 - Users who are uninterested in building their own queries can utilize those built by others and published in the workspace system. In D360 version 5.0 (available in Feb '09) queries will be savable as quick search widgets which provide Google like access to common workflows from the main application window.
 - Data analysis functionality has been designed to mimic tools that users tend to be familiar with such as Excel for spreadsheet manipulations., iGoogle or Yahoo web pages for QuickSearch widgets, Windows Explorer for workspace exploration.

- Training for a standard D360 user generally takes about 4 hours to cover basic query building, dataset browsing and analysis and sharing through the workspace system. Advanced training for power users is usually conducted over 1 to 2 days depending on the functionality to be covered. Generally it has been found that users quickly become familiar with D360 after training and that they find D360 significantly easier to use than the multiple applications they employed prior to D360 deployment.
- **How does a user construct a new query?**
 - Construction of a D360 query comprises 3 steps:
 - i) Decide what type of entity you are searching for (Compound, Batch/Lot, Project...) – this is similar to selecting whether you are performing a Google search for web pages, News, Images...
 - ii) Select the data you wish to see in the final dataset. Data fields are picked from an organized, filterable list that can be customized through the D360 configuration system.
 - iii) Enter constraints – constraint operators are selected from a pulldown menu and constraints entered by either typing in values or selection from a list of options. After one or more constraints have been provided the user can submit the search.
 - For more advanced users a variety of additional capabilities are easily accessible from the search interface: Changing aggregation functions, changing pivot conditions, specification of logic between constraints, specification of output format, specification of result sort order and color by value criteria. All advanced options are saved with the query so that any user can run the most advanced query with ease once it has been constructed and shared.
- **How does a user execute a query and get a dataset?**
 - The query would be opened from the workspace system (similar to opening a file from Windows Explorer), optionally add or edit constraints and execute the query with a single click.
 - QuickSearch widgets (available in version 5.0 – Feb '09) provide up-front access to commonly used queries from the main application window which alleviates the need for the user to find and open a workspace query.
- **How can queries be shared?**
 - D360 queries saved to a user's personal workspace can be published to group workspaces where they can be accessed by all members of the group. Group members can open and execute the query or save it to their personal workspace for modification.
 - In version 5.0 (Feb '09) users will be able to present D360 queries as QuickSearch widgets. When the user saves a query they can select which constraint fields to expose and save the query as a QuickSearch widget. When this "widgetised" query is published to a group workspace it places a new search panel on the main application window of all users who are members of the group workspace.

Data Analysis

- **What analysis tools does D360 offer?**
 - D360 provides discovery scientists with a rich set of data analysis tools to help them make sense of discovery data. Highlights are as follows:
 - i) Data viewers: Spreadsheet, Grid, Form (in version 5.0), scatter plots, histograms, similarity maps, Spotfire integrated as a data viewer.
 - ii) Data Analysis: Sorting, Data statistics, Equation columns, Color data by value, Graph point options (color, size, shape), Data correlation matrix, R-Group analysis, Structure similarity maps, Clustering ect.
 - iii) Data manipulation: Find, Filter, User defined columns, Data Record selection by criteria, Export ect.
 - iv) Additional data: Ability to add additional data to a current dataset, Follow-on queries, creation of identifier lists ect.
- **Can users find underlying data values (drilldown) used to obtain aggregated data?**
 - D360 allows users to drill down on aggregated data values to view the underlying values. Drilldown tables display not only the constituent data that was aggregated but also additional, related information e.g. when drilling down on a mean IC50 the user will see the individual IC50 values along with additional data on the experiments used to determine those values such as Run Date, Analysis comments ect.
- **Does D360 handle modified numerical data (e.g. <5)?**
 - D360 is designed to deal with data columns which are nominally of numeric type but also contain modified numeric values (e.g. >10) and also text comments (e.g. "Limit of Detection"). Modified data values are sorted and filtered in numeric fashion; taking account of the modifier and text values in nominally numeric columns do not cause error conditions.
 - Modified numeric values and text values for data fields that are nominally numeric in type are subject to specific, configurable business rules during data aggregation.
- **When users are employing multiple data viewers is the selection status maintained between those viewers?**
 - D360 datasets maintain full selection propagation between all data viewers. If data is selected in one viewer then it is selected in all viewers including Spotfire if the user is employing Spotfire as a D360 data viewer.
 - D360 datasets have a primary viewer mode that allows users to navigate the dataset using a particular data viewer. This "primary viewer" displays all dataset data while the remainder of the viewers display only the data selected in the primary viewer.
- **Is it straightforward to integrate additional data analysis tools with D360?**
 - A frequently cited concern regarding data analysis products is that they do not offer a proprietary advantage. D360 aims to provide a rich set of base functionality that is common to pharmaceutical research and then to allow customization and modification by individual organizations. Using D360s APIs much new data analysis functionality can be added to the application either in the form of new functionality in the client application, integration with other desktop applications or integration with server side algorithms through web services.
 - Out of the Box D360 is integrated with the following data analysis tools: Spotfire (tight integration as a data viewer), Excel, JMP, SAS for Excel, SIMCA-P.
- **Given a D360 dataset how easy is it to find related information?**
 - D360 employs 3 mechanisms to obtain information related to data displayed in a dataset:
 - i) **Drilldown:** As previously mentioned, double clicking on an aggregated data field will display a drilldown table that shows the underlying data that was aggregated to produce the summarized value and additionally data related that is closely related to the underlying values.
 - ii) **Get Additional Data:** Additional data related to records in a dataset can be added to a dataset without the need for the user to re-execute the whole query.
 - iii) **Follow-on Queries:** Follow-on queries allow the user to follow a train of thought through the data available through D360. Follow-on queries are defined and configured at a system

level and are accessible to users through the right click menu on an appropriate data field. An example of follow on queries might be “Batches of this compound” or “Inventory information for this batch”. A user examining a dataset could right click on selected compound IDs and select the “Batches of this compound” follow-on query which would result in a new dataset that displayed all batches of the selected compound IDs. The user could then select specific batch IDs, right click and select the “Inventory information for this batch” follow-on query which would result in inventory information (location, quantity, container etc.) for the selected batch IDs.

- **How does a user get their data out of D360?**

- D360 allows you to get data out of D360 by 2 main mechanisms:
 - i) **Export:** D360 can export to a variety of file formats: csv, tsv, Excel (xls), SD, mol2, SLN, XML, JPG. Export functionality direct to applications (Excel, JMP, SAS for Excel, Spotfire, PowerPoint) has also been implemented so that users do not have to be concerned about intermediate files or finding the application to which they are exporting. When exporting to Excel and Powerpoint data formatting is maintained.
 - ii) **Copy/Paste:** D360 allows data to be copied and pasted into other applications. Where appropriate data formatting is maintained in this procedure.

- **How can datasets be shared?**

- D360 datasets saved to a user’s personal workspace can be published to group workspaces where they can be accessed by all members of the group. Group members can open and browse the dataset or modify and save it to their personal workspaces.
- Dataset viewers can be printed for hardcopy handouts.

- **How does D360 facilitate communication?**

- In addition to allowing sharing of datasets through the workspace system and queries D360 can also be used as a data presentation tool to allow interactive data analysis sessions in a team environment. For status type presentations data can be transformed into PowerPoint slides in a couple of mouse clicks.

Data Sharing

- **How can users share what they create in D360?**
 - D360 provides a centralized workspace system that acts as a repository for all items created in D360. Each user has their own personal workspace, there is a global workspace that all users can access and additional shared workspaces can be set up for groups (e.g. therapeutic areas, project teams, specific disciplines).
- **Do D360 workspaces have security?**
 - D360 workspaces have role based security. Personal workspaces can be accessed only by the owning user and system administrators. The global workspace can be accessed by all users and administrators. Group workspaces are set up and administered by group administrators who are responsible for group membership and read/write privileges of group members.
- **Are D360 workspaces straightforward to use?**
 - The D360 workspace interface is designed to look and behave like Windows Explorer so all workspace functionality will be highly familiar to D360 users.

Identifier Lists

- **Can users generate lists of identifiers?**
 - D360 allows users to create lists of identifiers in a variety of ways:
 - i) Paste of text
 - ii) From identifier data in a dataset
 - iii) Through editing of existing lists. D360 allows fine (individual item) editing and also gross boolean logic between identifier lists
- **Is building lists easy?**
 - D360 provides a straightforward Wizard interface for the construction of identifier lists.
- **How does D360 use lists of identifiers?**
 - Lists can be employed to constrain D360 searches.
- **How can identifier lists be shared?**
 - D360 lists saved to a user's personal workspace can be published to group workspaces where they can be accessed by all members of the group. Group members can use the list as a constraint in a search or save it to their personal workspace for modification.

System Flexibility (Configuration & Customization)

- **How will D360 provide a competitive advantage for my organization?**
 - It is common to believe that purchasing a product to address a research need does not bestow competitive advantage since competitive organizations are using the same product. D360 is designed to offer a rich set of base functionality for data access, analysis and sharing that is common to all the bespoke data access and analysis systems that have been developed at the larger pharmaceutical organizations with some additional Tripos developed analysis capabilities. Deploying D360 saves on the development risks and maintenance costs of these necessary capabilities while the extensive D360 configuration system and available APIs allow the application to be set up to a particular organization's requirements and provide the infrastructure for an organization to deploy its own proprietary algorithms, visualizations and models to a wide base of end users. Utilizing D360 frees valuable scientific and technical resources from supporting generic functionality such as spreadsheet operations so that they can develop and implement scientific and analysis capabilities that provide a higher level of value to the research process.
- **How is D360 adapted to the needs of my organization?**
 - D360 is an application built from modular system of cohesive components. Each component derives its behavior from the D360 configuration system which allows the behavior and

- computations of the system to be tailored to the requirements of the organization through the editing of text configuration files rather than changing or adding additional code.
- Since D360 is built from components these components can be readily replaced, modified or removed and additional components added through the available APIs. New capabilities such as additional aggregation functions, novel data visualizations and alternative analysis algorithms can be added to the system as new components.
 - D360 interfaces to web services and can be simply configured to communicate with web services for data extraction, property calculations, model predictions and other analysis capabilities.