Data Visualization with Chemical Intelligence

Scientists are continually asked to evaluate an ever-increasing number of parameters that include chemical properties, biological assays and ADME results in order to make better decisions about which compounds to synthesize next to optimize the product.

Lead Discovery software provides scientists with the capability to access scientific data easily and transparently. One-click access to both chemistry and biology data for visualization, analysis and association with other information, helps to drive structural recommendations and improve the choice of synthesis paths. Medicinal chemists can investigate structure activity relationships (SAR) and explore the available compound library, searching by structures chosen from visualizations of available data or structure searches. Computational chemists can visualize and explore chemical scaffolds and compound library motifs in order to improve the design of compound libraries. The chemical intelligence built into Lead Discovery renders it invaluable to research chemists.

At a glance

Lead Discovery software provides an easy-to-use, highly visual and interactive environment for exploring chemical structures and any associated data such as biological assay results.

Benefits

- Access and display a wide range of multivariate chemistry data including chemical structures
- Load multiple linked chemical and biological data tables in a single TIBCO Spotfire analysis file
- Highly interactive visualization and filtering facilitates the rapid isolation of compounds based on key criteria and chemical structure for further analysis
- Interactive tools for structure searching, activity profiling, R-group decomposition, clustering and list management
- Quickly build hierarchies and aggregations allowing navigation through different levels in your data, plate to compound level, project to compound series to individual compound level
- Capture and collaborate around analysis workflows
- Shared environment for making structural recommendations to project teams
- Build best-practice applications for chemical structure analysis

Figure 1. Lead Discovery powered by TIBCO Spotfire software provides powerful visualization of chemical structures linked with properties, additional experimental data and analytics for medicinal and computational chemists.
Attributes and capabilities

Lead Discovery provides a wealth of visualization options for exploration and analysis of chemical properties, assay results and chemical structures. The data can be combined, visualized and filtered for analysis to be performed either on subsets or the entire data set to reveal trends in a compound series or particular structural motifs. With better visualization, the speed, efficiency and quality of decisions can be significantly improved.

Capabilities of Lead Discovery software include:

Visualizations — 3-D scatter plots, line charts, pie charts, summary statistics table, bar charts and histograms. Drag-and-drop visualization and analysis creation and modification on-the-fly.

Chemical structure viewing and filtering — View structures from molfiles, SMILES, CDX (ChemDraw), or chemistry databases and filter using trusted similarity and substructure algorithms. Import and export SDfiles and ChemDraw for Excel documents. Align all structures in a dataset to a chosen scaffold. Tag data based on chemical attributes for further classification and analysis.

Interactive filters — Data filtering via chemical structure (full, substructure, or similarity) range sliders, check boxes, radio buttons, list box or text search.

R-Group Decomposition — Define a common scaffold in a series of related structures and Lead Discovery will analyze and display all the attached R-groups so that scientists can discern favorable substitution patterns and preferred substituents to aid in lead optimization.

Clustering by chemical structure — Clustering based on any column including chemical structure (fingerprint) similarity.

Chemical property calculators — Dynamically calculate chemical structure properties based on built in prediction algorithms.

Substructure searching and hit highlighting — When importing structures from a database.

TIBCO Spotfire Platform Components

TIBCO Spotfire Asset Management Analytics Library — Share analysis files and interactive discussions that include visualization and filtering capabilities from a secure centralized repository accessible across the organization.

TIBCO Spotfire Analytics Server — Provides centralized administration of end user access rights and client configurations, making it easy to deploy analytics across the enterprise. Role-based access to data and functionality maps to existing security infrastructures. Desktop clients remotely updated from server, including deployment of custom extensions.

TIBCO Spotfire Web Player — Enables organizations to easily deploy rich interactive analysis applications and workflows to a wide audience of analysis consumers. Analyses created and saved by users of TIBCO Spotfire Pro with Lead Discovery are available to TIBCO Spotfire Pro with Web Player users.

TIBCO Spotfire Developer — A complete set of application programming interfaces (APIs) that allow developers to integrate and automate the platform, as well as extend it with entirely new custom tools, visualizations and more.

Lead Discovery software helps scientists focus on making decisions — such as which particular path of compound synthesis to follow — by providing a way to ask questions of all of the data that is available within a single environment. The ability to associate data points in multiple visualizations with structures in the structure viewer is a powerful way in which to represent complex data so that key relationships can be better understood and the decisions that follow can be made with increased confidence.