

# TIBCO Spotfire® Lead Discovery

Chemists 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 drug discovery and development process.

TIBCO Spotfire® Lead Discovery software provides chemists with the capability to access 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 to design effective drugs. 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 flexibility to evaluate the chemical space in a number of different ways provides high value to teams of both medicinal and computational chemists.

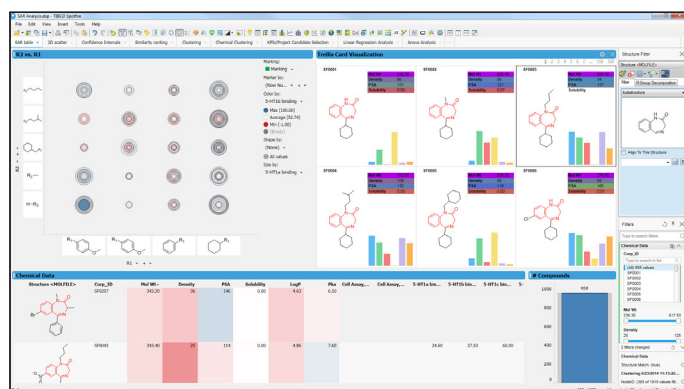


Figure 1. TIBCO Spotfire® Lead Discovery software provides powerful visualization of structure analysis chemical structures linked with properties, additional experimental data and analytics for medicinal and computational chemists.

## At a Glance

TIBCO Spotfire® 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 for further analysis
- Interactive tools for structure searching, activity profiling, clustering on properties/structural descriptors 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

## Attributes and Capabilities

TIBCO Spotfire® Lead Discovery software 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 and analysis performed on subsets or the entire data set to reveal trends in a compound series or particular structural motifs, thus improving the efficiency and quality of decisions. Capabilities of TIBCO Spotfire® 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.

Interactive filters – Data filtering via range sliders, check boxes, radio buttons, list box or text search.

One-click data access – Access relational databases, flat files via simple links that are configurable within a TIBCO Spotfire® analysis file. Load multiple data tables into a single TIBCO Spotfire® analysis file.

Chemical structure viewing and searching – View structures from Mol files, SMILES, or chemistry databases and perform similarity and substructure searches. Import and export SDF files.

Tagging – Attach tags or annotations to records in your data set, helping you track records of interest and makes for easy filtering.

Bookmarks – Capture snapshots of your analysis, which can be applied at any time, allowing you to return to a previously created view of the data.

**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® Enterprise Player** – Enables organizations to easily deploy rich interactive analysis applications and workflows to a wide audience of analysis consumers. Analyses created and saved by TIBCO Spotfire® Lead Discovery users are available to TIBCO Spotfire® 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.

TIBCO Spotfire® Lead Discovery software helps chemists 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.

For more information visit [www.perkinelmer.com/product/spotfire-leaddiscovery](http://www.perkinelmer.com/product/spotfire-leaddiscovery)

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