

Lead Discovery powered by TIBCO Spotfire®

At a Glance

Lead Discovery is a highly visual, interactive software tool 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

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.

Lead Discovery combines the power of TIBCO Spotfire® with the scientific intelligence that chemists have come to expect from ChemDraw. These two tools empower both life science chemists and physical science chemists - whether the desired result is a novel small molecule inhibitor of a protein kinase or a unique ligand for catalyzing the mass production of terephthalic acid. Lead Discovery is the optimal interactive visualization tool for the investigation of large data sets of chemical information. Eliminate the hassle of pivot tables and transferring molecules from a database into Excel. With Lead Discovery, the chemical structures and related information are at your fingertips, with the added familiarity of ChemDraw.

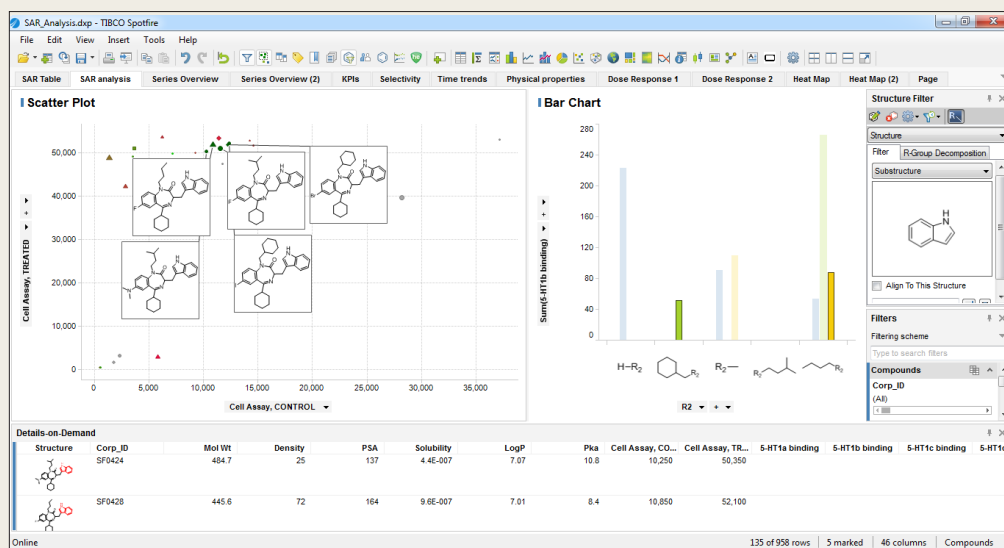


Figure 1. Lead Discovery has the capability to rapidly and accurately filter by chemical structure. The above image shows the ability of Lead Discovery to narrow down a large data set to a specific collection of compounds. Once filtered, chemists can select, label, and highlight the desired data. Chemists can render structures in data tables, directly on visualizations, and directly on graphical axes for easy SAR analysis.

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 SDF files 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.

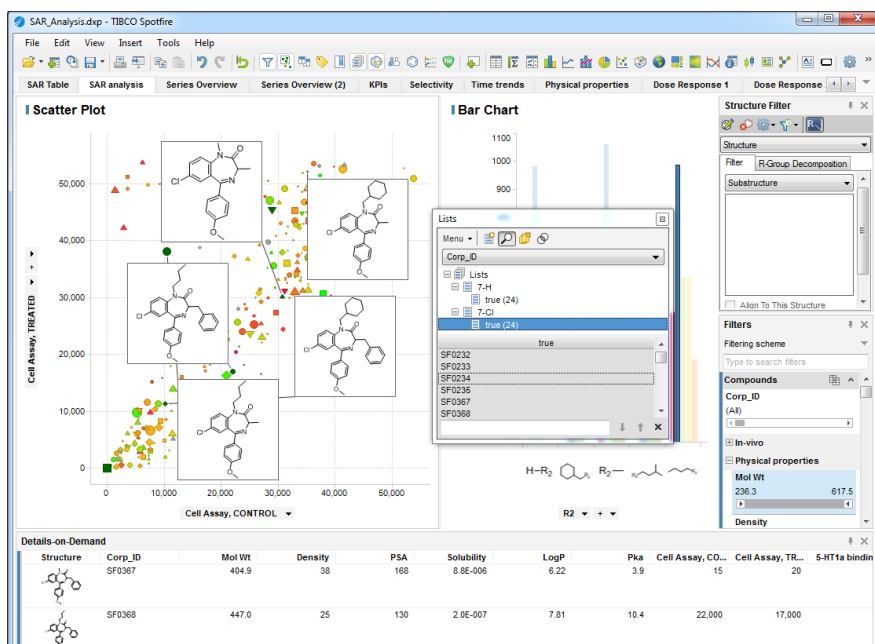


Figure 2. With Lead Discovery, chemists can easily create lists of compounds as highlighted above. Once a list (or series of lists) has been created, chemists can apply grouping techniques to complete Matched Molecular Pair Analyses (MMPA).

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.

Download Free Trial of Lead Discovery at www.perkinelmer.com/spotfire-leaddiscovery

PerkinElmer, Inc.
940 Winter Street
Waltham, MA 02451 USA
P: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com



For a complete listing of our global offices, visit www.perkinelmer.com/ContactUs

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