# Lead Discovery powered by TIBCO Spotfire®

## At a Glance

**Lead Discovery** solves the data analysis problems that chemists face every day. With Lead Discovery, chemists can now create SAR/SPR tables in minutes, perform clustering analysis to find the most common scaffold in a data set and calculate/list chemical properties all in the same visualization.

## 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. With Lead Discovery, chemists of all kinds can eliminate the hassle of Excel spreadsheets and bring the familiarity of ChemDraw to their data analysis workflows.

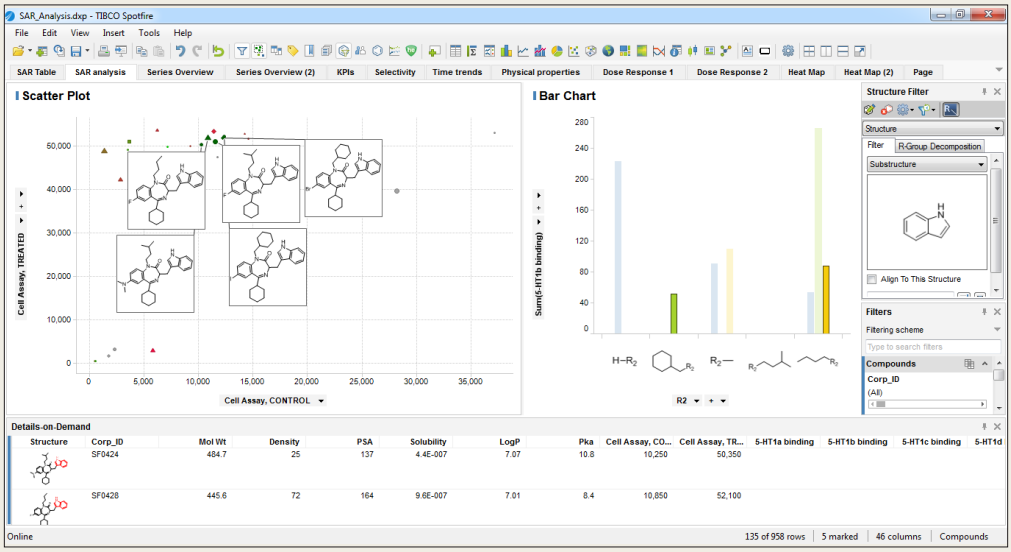


*Figure 1.* Lead Discovery has the capability to rapidly and accurately filter by chemical structure. The above image shows the ability of Lead Discovery to narrow down a large data set to a specific collection of compounds. Once filtered, chemists can select, label, and highlight the desired data. Chemists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

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## 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.

## Lead Discovery within the TIBCO Spotfire® Platform

Users of Lead Discovery for Business Author or Consumer can now perform highly valued chemical structure filtering workflows within the web. Users of Business Author can create visualizations by leveraging the chemical structure filter to fine tune the data to be presented in the visualization. Additionally, consumer users can filter off un-desired chemical structures through the chemical structure filter. The filter is powered by ChemDraw Direct, our HTML5 chemical sketcher, so there is no need to download or install any plugins to leverage the chemical structure filter. Lastly, users can copy and paste directly from ChemDraw desktop (v14 or newer) any chemical structure needed to be used as a filter in their visualization.

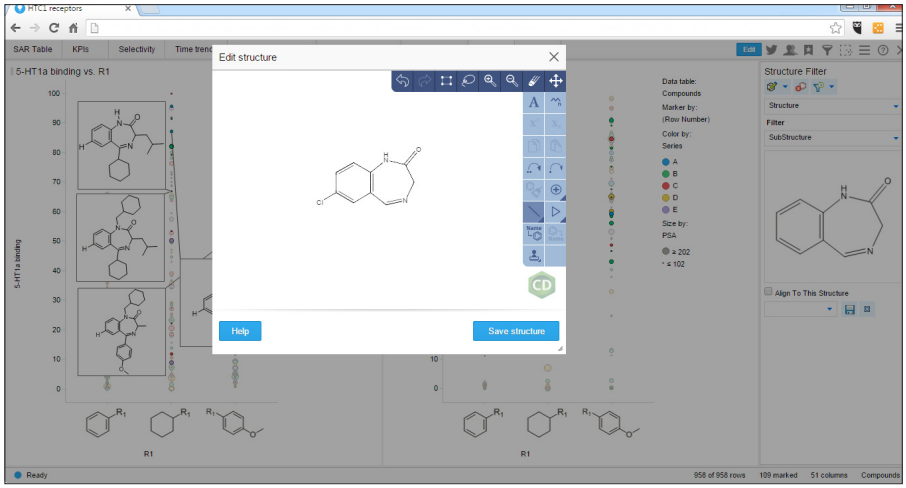


*Figure 2.* ChemDraw Direct is now leveraged for chemical structure filtering in Lead Discovery Business Author and Consumer.

**For more information, please visit www.cambridgesoft.com/ensemble/spotfire/LeadDiscoverypoweredbyTIBCOSpotfire**

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