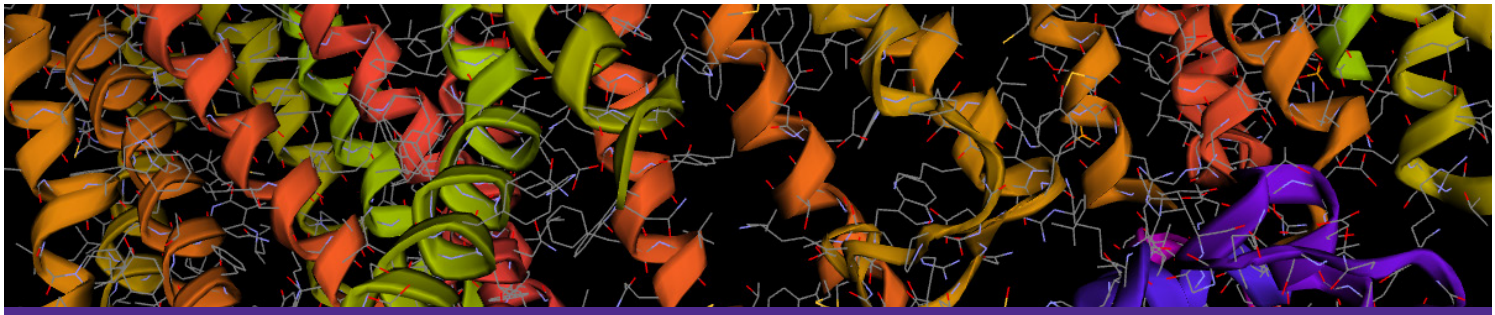

Lead Discovery Premium

At a Glance

Lead Discovery Premium combines the power of TIBCO Spotfire® with the chemistry smarts of Lead Discovery and adds advanced chemical structural and biological sequence intelligence to create the premier platform for powerful and incisive chemical and biological analytics.

Benefits

- All the core chemistry capabilities of Lead Discovery (See page 2) augmented with powerful advanced chemical and biological analysis and display tools
- Powerful tools that enable scientists to fully explore the complex data sets that are now common in the search for novel small molecule and biologic therapeutic agents
- A rich palette of intuitive data display options to uncover and highlight key relationships, including one-click SAR table transposition, form views, radar charts, violin plots and SAR maps of R-group decompositions
- Robust multi-parameter optimization visualization and scoring to home in on promising structural motifs and sequence modifications
- 3D View of structures for large and small molecules and tools to visualize and explore biological sequences and relate structural features and modifications to changes in activity and other properties
- Full set of biosequence analysis tools, including sequence search (BLAST) and alignment (Clustal Omega), highlight differences relative to a reference sequence, relate bioactivity to monomer substitutions, and relate sequence regions and monomer positions to 3D structure

Lead Discovery Premium combines the power of TIBCO Spotfire® with the chemistry smarts of Lead Discovery and adds advanced chemical and biological intelligence to create the premier platform for powerful and incisive chemical and biological analytics.

Today's drug discovery scientists working on small molecule or, increasingly, on biologic therapeutic agents are faced with an ever-increasing array of parameters. Some data is generated in-house, other results may come from external collaborators, and some may be available on the internet. Volumes, storage locations and formats may vary, and researchers need all the help they can get to locate and navigate the available relevant data and assemble it into meaningful and accessible sets for further analysis.

With Lead Discovery Premium, scientists can easily import, sift through and interpret chemical structures and biological sequences combined with other relevant data in a highly visual, intuitive and interactive environment. Building on the core set of chemical capabilities (handle common chemistry file formats, editors and renderers; substructure, tautomer and similarity search; R-group analysis; calculate physical properties), Lead Discovery Premium equips chemists with the following powerful SAR tools and capabilities for deeper and more precise exploration of their structures and related data: fast chemical search; one-click transposable SAR table; form views of data; SAR map of R-group decomposition, including combining multiple R-group analyses for a set of structures, R-group decomposition on R-groups themselves, and property calculations on R-group fragments; extended palette of data visualizations (radar chart, violin plots, etc.); multi-parameter optimization visualization and scoring; and 3D View of structures. This rich set of capabilities will enable chemists to rapidly detect trends and identify the most promising structural motifs for further elaboration.

PerkinElmer®
For the Better

For scientists working with biologic entities, Lead Discovery Premium now includes tools to import, align, and analyze sequences and to correlate the sequence differences to activity data to help speed biologics discovery. Sequence search using BLAST on internal and external databases can be used to combine all available sequences for analysis, and sequences can be aligned using CLUSTAL Omega. Sequence analysis and visualization tools include the ability to highlight sequence differences relative to a reference sequence, to relate monomer substitutions to bioactivity, and to relate sequence regions and monomer positions to 3D structure. This combined analysis of sequence and activity data lets scientists focus on sequence differences that are related to efficacy, safety, and production measures, and will enable the discovery and nomination of the optimal drug candidate faster.

Lead Discovery Premium is a powerful way to explore and probe complex chemical and biological data so that key relationships can be better understood and decisions can be made more quickly and with increased confidence.

Feature	Lead Discovery	Lead Discovery Premium
Visualize small molecule structures	✓	✓
Find structures in external data sources	✓	✓
Define compound series via structure filters	✓	✓
Analyze R-groups contribution to activity	✓	✓
Utilize all major chemistry renderers and editors	✓	✓
Autodetect chemical columns within loaded data	✓	✓
Calculate physical properties	✓	✓
Auto-update compound series as new compounds are added	✓	✓
Auto-update R-group analyses as new compounds are add	✓	✓
Publish to TIBCO Spotfire® Consumer with full chemistry analysis capabilities	✓	✓
Global set the preferred chemistry renderer	✓	✓
One-click switching of chemistry format (ChemDraw, SMILES, etc)	✓	✓
Tautomeric substructure searching	✓	✓
One-click transposable SAR table		✓
Form views data		✓
SAR map of R-group decomposition		✓
Broadened palette of data visualizations (radar chart, violin plots, etc.)		✓
Multi-parameter optimization visualization and scoring		✓
3D view of structures for large and small molecules		✓
Visualize and analyze biological sequences		✓
Highlight sequence differences relative to a reference sequence		✓
Align sequences through CLUSTAL Omega		✓
BLAST searching over internal or external sequence databases		✓
Sequence Analysis of biological molecules, relate therapeutic agent activity to monomer substitutions		✓
3D biomolecule analysis relate sequence regions and monomer positions to 3D structure		✓
Incorporate your own analysis pipelines through extensible web services framework		✓
Matched Molecular Pair analysis		✓
Core Decomposition analysis		✓
Property and activity compound neighborhood analysis		✓
Numerical sorting and coloring of textual columns (e.g. ">50nM" sorted and colored by the number 50)		✓

For more information, please visit www.perkinelmerinformatics.com/products/research/lead-discovery-premium/

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