



# Upgrade to Lead Discovery Premium



# Visualize and Analyze Small Molecules and Biologics in One Solution

If you need more powerful visualization and analysis, it's time to upgrade from Lead Discovery to Lead Discovery Premium:

- Guided Workflows empower scientists with the ability to find and assemble any data they want to answer any scientific question in seconds or minutes rather than days, independent of IT
- Lead Discovery Premium transforms Spotfire® from the best general data visualization and analysis tool to the best scientific discovery tool
- Lead Discovery Premium really changes the game from what Spotfire® has historically been capable of and now enables Structure / Sequence to be coordinately visualized with \*all\* results
- Update your project tracking data instantly and use our analysis tools to surface your best candidates automatically

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 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)		✓

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