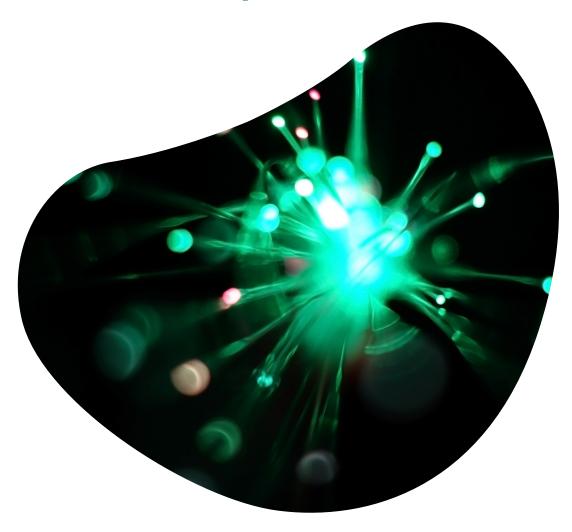
## Upgrade to Lead Discovery Premium





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

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