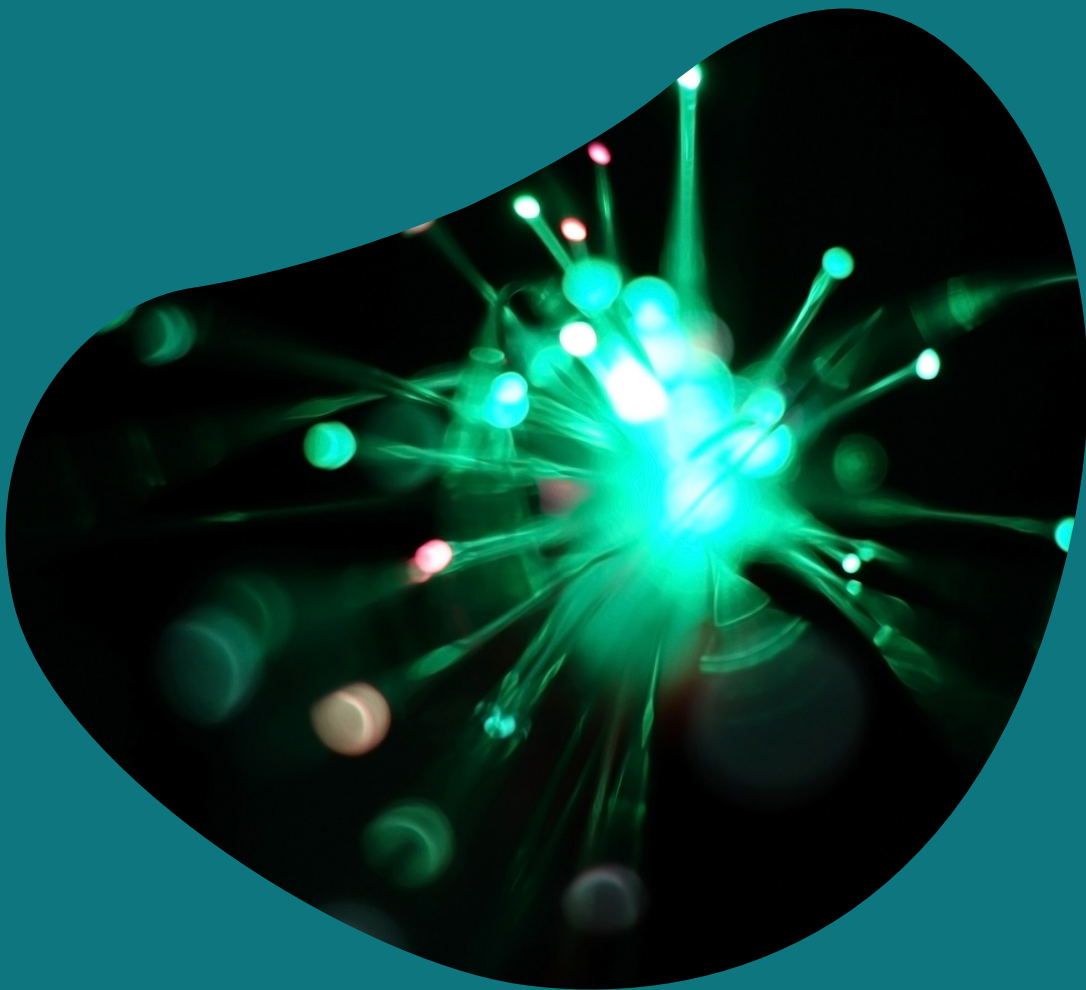




Upgrade to Lead Discovery Premium



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)		✓

Revvity Signals Software, Inc
940 Winter Street | Waltham, MA 02451 USA
P: (800) 762-4000 or (+1) 203-925-4602
revvitysignals.com/company/contact

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