



Enterprise Solutions for Discovery Chemistry

Increase Your Chances of Bringing a New Drug
to Market with Signals One

revvity
signals



Medicinal chemistry is rapidly evolving

Medicinal chemistry is a critical component of the drug discovery and design process, ensuring the efficacy of candidate pharmaceuticals in preclinical tests. Technological advances in peptide therapeutics, antibody development, cell and gene therapies, and even RNA-based therapeutics have presented medicinal chemists with an entirely new challenge. Already struggling to achieve the speed and accuracy required during small molecule target identification, hit identification, hit-to-lead optimization, lead optimization, and preclinical testing, medicinal chemists are now faced with more demands regarding speed and accuracy to deliver these novel modalities from bench to clinic as well. Meeting these demands requires not only close and efficient collaboration across multidisciplinary teams, but also streamlined data management that facilitates rapid, efficient, reproducible workflows, and a return of scientific quality time to medicinal and synthetic chemists.

Lead Discovery ChemCharts

Lead Discovery ChemCharts

Structure	Code	SaR	Parent_MW	MW	Salt_MW	cLogP	HBA	HBD	Rot_Bonds
	MBX033906	H	451.11	609.02	127.91	5.57	6	2	5
	MBX00573	CF3COOH	174.21	285.23	114.02	0.10	3	2	1
	MBX027792	HBr	427.48	508.38	80.91	0.88	6	1	6
	MBX027815	HBr	404.52	485.43	80.91	2.84	7	1	6
	MBX028116	HBr	350.47	431.38	80.91	1.61	4	0	4
	MBX020135	HBr	420.53	501.44	80.91	3.63	3	0	6
	MBX043057	HBr	369.47	458.38	80.91	1.28	6	1	6
	MBX043191	HBr	424.51	505.42	80.91	-0.35	7	1	6
	MBX044017	HBr	412.54	493.45	80.91	1.50	5	0	6
	MBX044036	HBr	446.60	527.51	80.91	3.44	6	0	6
	MBX044435	HBr	407.52	488.43	80.91	1.25	5	1	5
	MBX044439	HBr	395.51	476.42	80.91	1.12	5	1	7

Lead Discovery ChemCharts

Code: MBX001023
 Name: N-methyl-6-(piperidin-4-yl)pyridine-2-carboxamide
 Salt: HCl
 Parent_MW: 219.29
 MW: 255.75
 Salt_MW: 36.46
 TPSA: 54.02
 Rot_Bonds: 2
 Heavy_Atoms: 16
 cLogP: 0.45
 HBA: 3
 HBD: 2
 N+O: 4
 Substructure Filter (Temp): True
 StereoComment: None
 Structure search: False
 Tag Column:

5,783 of 10,674 rows 3 marked 18 columns table



Evolving technologies have introduced new challenges

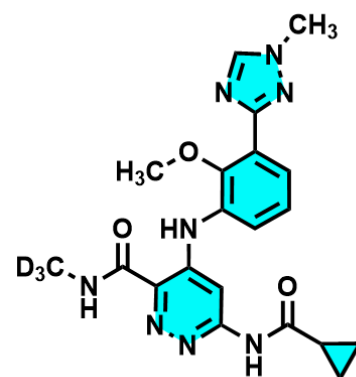
The success of every medicinal chemistry project from conception to clinical trials is predicated on the ability to manage vast quantities of computerized data. The quantity and nature of these data have created several important challenges:

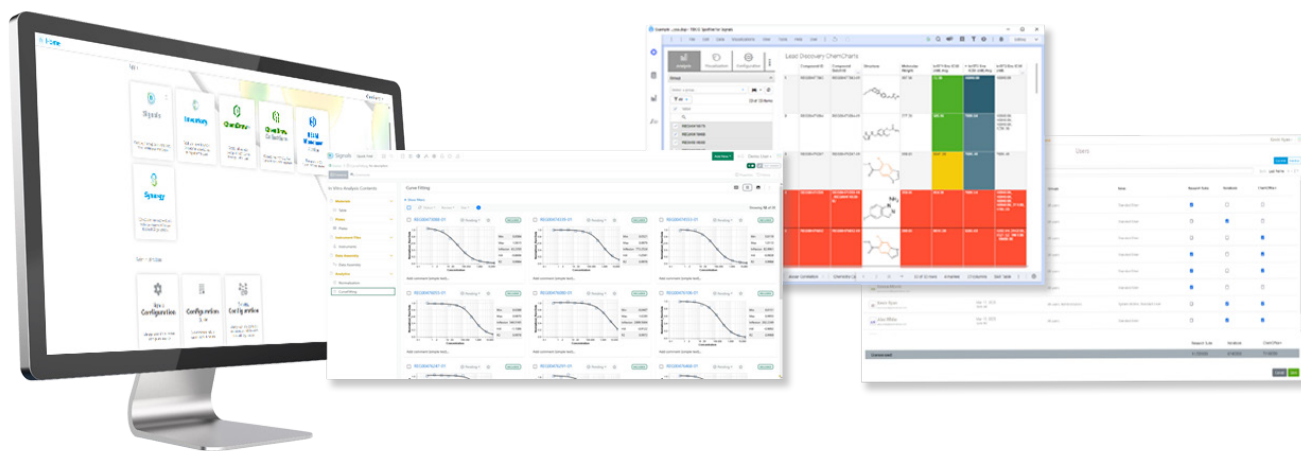
- **Data integration.** Medicinal chemistry generates vast amounts of data from various sources, including experiments, literature, and databases. Integrating and analyzing these data is a challenging task, requiring the development of new data management and analysis tools.
- **Data quality.** Quality data are necessary for making accurate and reliable predictions. Intra-source variability in data quality can make it challenging to integrate and analyze data effectively.
- **Machine learning.** Machine learning (ML) has become an essential tool in medicinal chemistry, aiding chemists in predicting properties of new molecules and identifying targets. Developing accurate and reliable ML models requires high-quality data and sophisticated algorithms.
- **Visualization.** Medicinal chemistry generates complex data that can be difficult to interpret and analyze. Effective data visualization tools are necessary for chemists to identify patterns and trends in the data and make more informed decisions.
- **Legal considerations.** The use of informatics in medicinal chemistry raises several legal considerations, including data privacy, intellectual property, and regulatory compliance. Informatics research must be conducted in compliance with relevant laws and regulations.
- **Collaboration.** Medicinal chemistry research is often a multidisciplinary collaborative effort. Effective collaboration tools and platforms are necessary to facilitate research and accelerate drug discovery.

Advanced software solutions are needed

To increase research efficiency, and give back scientific quality time to researchers, better solutions are needed. Historically, medicinal chemists relied on incomplete software solutions that siloed data and forced manual efforts to find, aggregate, and analyze those data. Struggling to trace molecules from discovery to manufacture, or to disseminate information to up- and downstream teams, these chemists found it challenging to produce reproducible, quality data, increasing the risk of failure.

To adapt and thrive in a competitive market facing ever-increasing quality requirements from regulatory agencies, pharmaceutical companies can support their discovery chemists with streamlined, globally accessible software solutions that enable early, critical insights to increase the success rate of drug discovery projects.





Introducing the Signals One Solution for Discovery Chemistry

Revvity Signals Software understands these needs and has developed a solution tailor-made for medicinal chemistry. The Signals One solution includes unified software applications that collectively address the end-to-end needs of research scientists. It is the only complete, unified SaaS software for scientific research that gives discovery chemists a collaborative platform with complete control over their data workflows across every step of the discovery process in a user-friendly, intuitive, and streamlined manner. Equipped with powerful visual data analytics tools, the Signals One enables chemists to gain the insights that leverage their creative expertise to bring promising new therapeutics to patients in need.

Built on trusted standards

Powered by ChemDraw® and Spotfire®, Signals One includes Signals™ Notebook, the premier electronic lab notebook for chemists and biologists to collaborate; a data processing capability for in vitro and in vivo analysis; and a data-driven analytics capability for no-code query building – even for complex queries – and visual analytics for both chemical and biological preclinical research data, no matter the data source.

Together, the platform delivers best-in-class analysis and data visualization for the Design-Make-Test-Decide cycle, increasing the efficiency with which candidate therapeutics can be iterated, optimized, and brought to market.

Design.

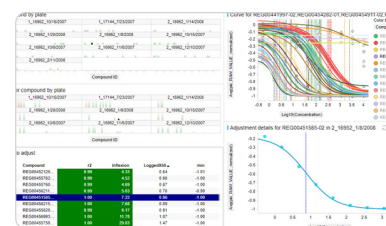
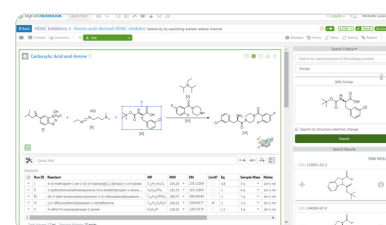
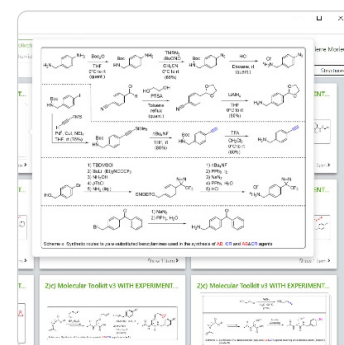
- **ChemDraw® & Signals™ ChemDraw** – Rapidly sketch, enumerate, and analyze molecular structures while seamlessly integrating intelligence from SciFinder, Reaxys, and Google Scholar/Patents.
- **Chemical Property Calculation within ChemDraw**– Instantly assess key molecular properties to refine design decisions early in the process.
- **AI-Ready Data & Signals™ API** – Leverage structured, high-quality data and open APIs to integrate AI algorithms for predictive modeling, hypothesis generation, and design optimization.

Signals One delivers best-in-class analysis and data visualization for the Design-Make-Test-Decide cycle so that you never miss an insight, increasing the efficiency with which candidate therapeutics can be iterated, optimized, and brought to market.



Make.

- ChemDraw®, the trusted chemistry gold standard for the last 40 years, has been continuously upgraded to include colorful, interactive features to make high-quality chemical drawings and 3D models, including the ability to copy 3D figures into PowerPoint® (3MF copy) to enhance communication with collaborators and stakeholders. ChemDraw is the chemical brain that natively powers Signals One.
- Hierarchical Editing Language for Macromolecules (HELM), another new ChemDraw feature, facilitates accurate visual representation of new drug modalities by allowing investigators to include amino acids, peptides, and nucleic acids in core molecular structures and to manage those biomolecules through shared libraries in Signals Notebook.
- Additionally, teams can cut time spent on back-and-forth emails and meeting preparation with the easy reporting capabilities of Signals ChemDraw.
- Signals™ Notebook is intuitive, chemically intelligent, and natively integrated with ChemDraw to allow chemists to properly document their work digitally, maintaining scientific integrity, encouraging creativity and productive thinking, and fostering collaboration across multidiscipline teams.



Test.

- Powered by Spotfire, analyses data and converts complex results into intuitive graphics. This facilitates unified assay data management, rapid assessment of hit compounds, and graphing of IC curves, kinetics, and other results from critical assays to evaluate efficacy and determine whether modifications are needed.

Decide.

- Providing next-generation data management, guided search and advanced Structure Activity Relationship (SAR) analysis, features an easy-to-use point-and-click query builder to access, parse, and analyze large datasets without the need for writing code. Chemists can visualize every experiment and project holistically, gaining unique, unforeseen insights critical to the discovery process in hours instead of months and facilitating the advancement of molecules to clinical trials, ultimately increasing the chances of bringing a new drug to market.



Key capabilities address data analysis scalability, collaboration, and data management challenges

Signals One is an end-to-end solution that helps medicinal chemists transition drug candidates to preclinical and clinical trials faster than ever, enabling companies to be first to market and first to patient. This is achieved through three key capabilities.

#1 | Data analysis scalability and collaboration

- *Infuse chemical and biological intelligence into visual analytics*
- *Leverage intuitive visualization tools to make complex chemistry easy to understand by all stakeholders and provide visibility into the research process*
- *Communicate more effectively and accelerate the rate of advancing*

Combining new features simplifies data analysis in Signals One and facilitates cross-team collaboration and decision-making. Chemists can make elegant, high-quality, engaging, and interactive chemical models with ease. Even macromolecules are simple to model with the addition of new HELM capabilities to ChemDraw, expanding the medicinal chemist's ability to evaluate and share information about not just small molecules, but also the next generation of biologics. Through advanced coloring options, easy-to-export 3D models (3MF format) make it easy for therapeutics developers to share their work with key stakeholders and clients.

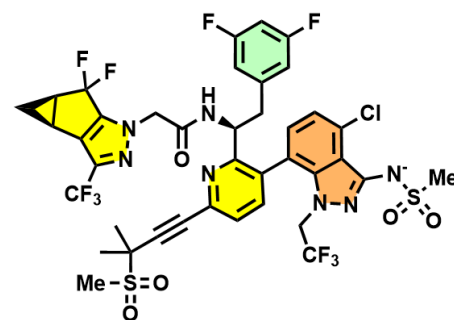
Signals ChemDraw makes the graphics created in Signals One easy to share, and Signals Notebook tracks all reagents, solvents, products, and properties utilized from start to finish, eliminating confusion about what was done, when, and by whom.

Collaboration and decision-making are further supported by tools that enable biologists to graph data from multiple pharmacokinetic (PK) assays performed on hit compounds. Results are then immediately accessible by the medicinal chemists making critical decisions about whether to advance a therapeutic candidate, enabling them to work on refinements as soon as possible and propelling new discoveries to market with accuracy and efficiency.

Easily repurpose already-existing organic chemistry experiments

- The only cloud Electronic Lab Notebook (ELN) with native ChemDraw integration
- Lightning-fast structure search for small molecules
- HELM capabilities empowering new drug modality research
- Easy to share analyses with key stakeholders and external collaborators
- Faster insights to make critical go/no-go decisions

The ability to collect, find, and analyze data across multidisciplinary teams is critical for determining the efficacy and safety of novel therapeutic candidates.



#2 | A collaborative ELN built for modern drug discovery

- *Facilitate cross-team collaboration with integrated, multidisciplinary platform*
- *Create more time for scientific creativity by reducing administrative work and number of point solutions used by researchers*

Effective and efficient collaboration between chemists, biologists, and computer scientists rely on an integrated platform. Complex and time-consuming workflows must be streamlined, and researchers require a way to easily capture, store, make improvements to, and share information on experiments.

Signals Notebook increases efficiency at every step in the drug discovery process, reducing the time and resources spent on administrative tasks and providing a space for scientists to create. This creates more time to brainstorm ideas focused on scientific research and to increase productivity. Ultimately, more important discoveries are brought to the market to help patients live better lives, and there is company-wide success and growth. As the only ELN integrated with ChemDraw, Signals Notebook seamlessly records complex chemical drawings and reaction mechanisms in visually pleasing, publication-ready formats.

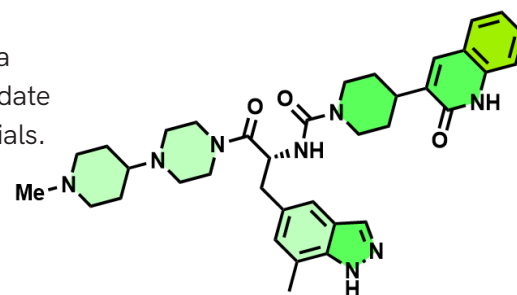
- Data are easily accessible from one location
- Automated stoichiometric calculations
- Search for prior knowledge
- Material inventory management and safety information
- Access controls enable group-specific data access
- Support for patent applications

#3 | Democratized digital visualizations for chemists

- *Self-serve data management delivers results in minutes, not months, giving back scientific quality time to researchers*
- *Surpass Excel's limitations by capturing data relationships and resulting activity*
- *Provides holistic view of all preclinical research data necessary to quickly identify the best candidates for success*

Democratize your data analysis and visualization with a fit for purpose Spotfire powered application developed to do what Excel can't: capture the relationship between the chemical structure of a candidate therapeutic and its resulting activity on the target biology. Signals One gives the power to analyze and visualize data directly to the chemist, without the need to code. They gain answers in minutes, versus months of development.

Controlled, self-serve access to data enables chemists to extract actionable insights from millions of rows of data all without the need for expensive and time-consuming IT support. Full integration permits seamless, real-time data sharing between chemists and biologists, facilitating rapid iteration on candidate therapeutics and ensuring only the best advance to preclinical and clinical trials.



Signals Notebook Inventory Management

No solution is better equipped to manage your lab inventory than Signals Notebook. Not only does it track inventory ordering, stock, and location, it also monitors consumption for a complete understanding of what you have and when you'll need more, without leading to excess. Combining Signals Notebook with inventory management best practices among scientists helps calibrate appropriate stock levels and enhancement management of the ebbs and flows of the supply chain.

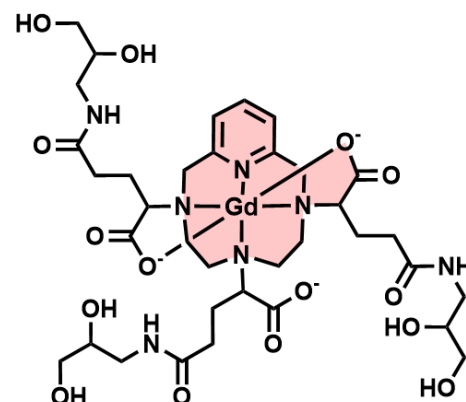
Data processing capability

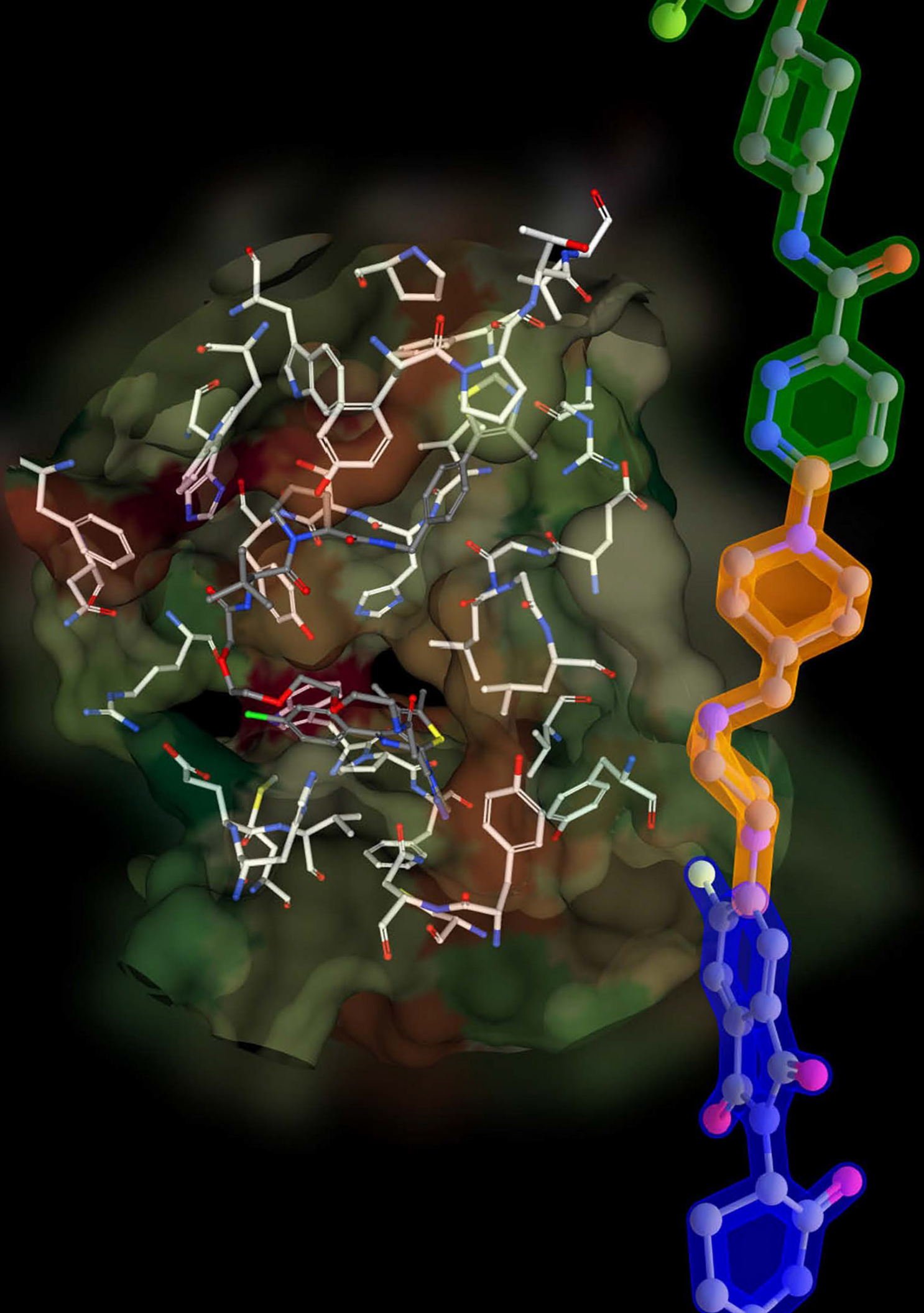
- One software application for unified assay data management covering multiple instruments and assay types saving time and increasing data accuracy
- Workflow templates are set up once, used multiple times
- Graphics driven by Spotfire enable meaningful visualization of data
- Standardized Statistical Analysis providing cluster analysis and unsupervised machine learning
- Manage vast amounts of data
- Simplified reporting that pushes directly into Signals Notebook and export into Microsoft Office and PDF format
- Automatic round trip of experimental results from Signals VitroVivo into Signals Notebook

Data-driven analytics capability

- The only Structure Activity Relationship (SAR) software application with native ChemDraw integration
- Holistic view of all preclinical research data (chemical and biological) with the target engagement profiling app increases your chances of identifying the right drug candidate
- Dedicated, specialized visualizations for advanced structure-activity relationships, e.g., R-group decomposition, matched molecular-pair analysis, activity cliff, etc.
- Connections to multiple data sources without hard coding
- Guided analysis workflows eliminating the need to learn yet another new application
- Horizontally scalable search platform provides the search experience needed, regardless of data volume and complexity
- Uses the FAIR (findable, accessible, interoperable, and reusable) data standard

The only cloud ELN and SAR application software with native ChemDraw integration



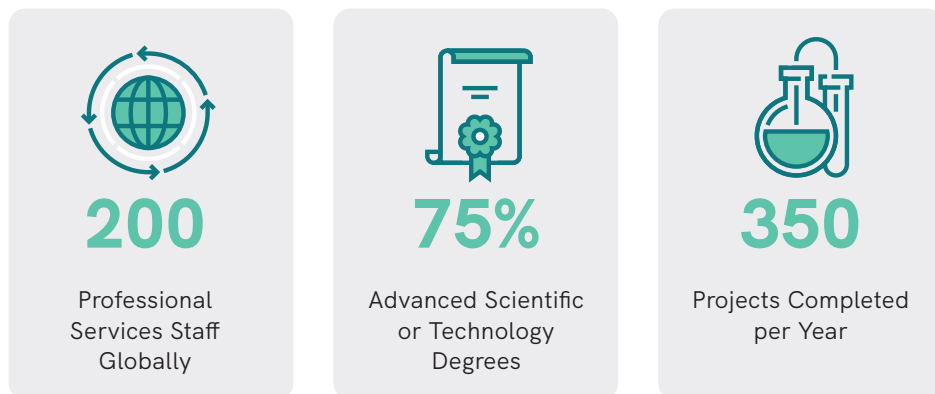


One Team, One Goal – Harmonized Alignment for Scientific Excellence

The Enterprise Customer Experience team delivers a wide range of services for designing, deploying, and managing an informatics solution that aligns with your organization's R&D Informatics needs. Service offerings include:

- Implementation Services
- Validation Services
- Consulting & Design Services
- Configuration & Integration Services
- Education Services

We understand technology and the science of our customers. We apply that expertise to delivering solutions that meet and exceed customer expectations.



Increase the success rate for your drug discovery

Signals One gives more scientific quality time to medicinal and synthetic chemists, improving their chances of successfully bringing new therapeutics to market. The only chemistry software platform powered by ChemDraw and Spotfire, Signals One is a feature-rich, flexible solution supporting all scientific workflows and all types of chemistry experiments. With a modern user interface and integrations to multiple data sources without coding, it encourages multidisciplinary collaboration around FAIR datasets.

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To learn more about Revvity Signals One for discovery chemistry, and increase your chances for market success, visit:
<https://revvitysignals.com/solutions/drug-discovery>



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