# Signals<sup>™</sup> Research Suite for New Biological and Chemical Modalities Research

A unified, cloud-native SaaS platform that drives scientific collaboration across Drug Discovery





### Complexity in New Drug Modalities Requires Multidisciplinary Collaboration

Emerging classes of therapeutics exacerbate the challenges in drug discovery because they often force the rapid adoption of new assay techniques or require different data representations. Partnerships between biologists and medicinal chemists are driving development in novel drug modalities, including technological advances in protein degraders, peptide therapeutics, antibody development, cell and gene therapies, and RNA-based therapeutics.

Supporting these new scientific endeavors requires efficient collaboration across multidisciplinary, globally distributed teams. These dispersed teams can collaborate efficiently with cloud-based, workflow-focused solutions.

### Challenges and Opportunities in Integrating Informatics for Drug Discovery

Historically, drug discovery information has been captured in self-managed informatics systems, using bespoke software targeting individual subdomains of the overall process. These include medicinal chemistry, lead optimization, in vitro assays, cell line optimization, biologics process optimization, in vitro drug metabolism and pharmacokinetics (DMPK ) assays, animal pharmacokinetic studies, and animal efficacy and safety studies. The fragmented nature of this informatics environment has created several key challenges:

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

## Advanced Workflow Focused Solutions are Critical

To address the increasing complexity of NBE and NCE research while accelerating innovation, scientists need a paradigm change in their current point-solution-based software. Researchers supporting the drug discovery process need a workflow-focused solution that enables them to focus on solving challenging scientific problems in Drug Discovery within one comprehensive platform instead of jumping from one informatics system to the next to get the job done. A common platform is essential today due to the focus on new drug modalities, such as protein degraders, mRNA, and antibody-drug conjugates, which require extensive collaboration between scientific disciplines.

### Introducing the Signals<sup>™</sup> Research Suite for Drug Discovery

Revvity Signals understands these needs and has developed a tailor-made workflow-focused tool for drug discovery. The Signals<sup>™</sup> Research Suite is an ideal solution for scientists working on new drug modalities or those who want to expand the power of Signals Notebook across the entire Make-Test-Decide R&D lifecycle for better data, insights, and outcomes.

It is the only complete, unified SaaS software that collectively addresses the endto-end needs of research scientists in a collaborative and user-friendly platform. Equipped with powerful visual data analytics tools, the Signals Research Suite enables researchers to gain insights that leverage their creative expertise to bring promising new therapeutics to patients in need. A common platform is essential today due to the focus on new drug modalities, such as protein degraders, mRNA, and antibodydrug conjugates, which require extensive collaboration between scientific disciplines.

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#### **Built on Best-in-Class Products**

Powered by industry-leading ChemDraw<sup>®</sup> and Spotfire<sup>™</sup>, the Signals Research Suite includes a trio of scientific and integrated software capacities:

- Signals<sup>™</sup> Notebook, the premier cloud-based electronic lab notebook for biologists and chemists to collaborate, capture, organize, share, and explore data
- The data processing capability leverages Spotfire<sup>™</sup> for data analysis and visualization of all modalities, uniting assay development, low- to ultra-throughput product assays, and in vivo studies
- The Data-driven analytics capability is the next-generation data management system, analyzes scientific results and enables efficient access and analysis of all scientific results collected throughout the R&D life cycle

Together, the platform delivers best-in-class analysis and data visualization for the Make-Test-Decide R&D life cycle, fostering rapid innovation in the development and optimization of candidate therapeutics to expedite their journey to market.





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#### Make

**Signals™ Notebook** is intuitive. It has DNA fluency for biologists, HELM integrations to support the bridge between chemically modified biopolymers , and is natively integrated with ChemDraw to allow chemists to properly document their work. The notebook digitally maintains scientific integrity and encourages creativity and productive thinking, all while fostering collaboration across multidisciplinary teams. Finally, it fundamentally supports intellectual property protection for patents.

- 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



*Figure 2.* Signals Notebook represents the first step the Make-Test-Decide R&D workflow. Signals Notebook can be used to plan, capture data, and collaborate.

**ChemDraw**<sup>®</sup>, the trusted chemistry gold standard for the last 35+ years, has been continuously upgraded to include colorful, interactive features to make highquality chemical drawings and 3D models, including the ability to copy 3D figures into PowerPoint<sup>®</sup> (3MF copy) to enhance communication with collaborators and stakeholders. ChemDraw is the chemical brain that natively powers the Signals Research Suite.

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*Figure 3.* Native ChemDraw integration in Signals Notebook. Chemical synthesis reactions can be easily drawn using ChemDraw and stoichiometry tables automatically update.

**Hierarchical Editing Language for Macromolecules (HELM)**, another new Signals Suite feature, facilitates accurate visual representation of new drug modalities by allowing investigators to include amino acids, peptides, and nucleic acids in core molecular structures. Researchers can communicate and manage biomolecules through shared libraries in Signals Notebook. This enables biologists and chemists to accurately, and easily represent modified small- to medium-sized biomolecules and all their associated scientific testing in one easy-to-use place.



*Figure 4.* Using the HELM Editor in ChemDraw to draw Terlipressin in amino acid notation (top) and conversation of the amino acids into a chemical structure (bottom).

#### Test

**The data processing capability,** powered by Spotfire<sup>¬</sup>, 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. The data processing capability facilitates templatizations for faster analysis and the standardization of analysis practices across researchers and research teams contributing to data consistency.

- 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 and used multiple times.
- Graphics driven by Spotfire<sup>™</sup> enable meaningful visualization of data.
- Standardized Statistical Analysis provides cluster analysis and unsupervised ML.
- Manage vast amounts of data.
- Simplified reporting pushes directly into Signals Notebook and exports into Microsoft Office and PDF format.
- Automatic round trip of experimental results from the data processing capability into Signals Notebook



*Figure 5.* The Data processing capability represents the Test phase of the Make-Test-Decide R&D workflow. The capability provides provides guided workflows for data import and analysis so that visualization and analytics are consistent and reliable.

#### Decide

**The data-driven analytics capability provides** provides next-generation data management, guided search, and advanced Structure Activity Relationship (SAR) analysis. It features an intuitive point-and-click query builder to access, parse, and analyze large datasets without the need for writing code. Biologists and chemists can visualize every experiment and project holistically, gaining unique, unforeseen insights critical to the discovery process in hours instead of months. This facilitates the advancement of molecules to clinical trials, ultimately increasing the chances of bringing a new drug to market.

## The Only 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.



*Figure 6.* The Data-driven analytics capability represents the Decide phase of the Make-Test-Decide R&D workflow. Researchers can compare many assay results at once in SAR Analysis tables, perform R-group decomposition, and make decisions about next steps.

#### Secure Data that Supports Regulatory Compliance

Developed in line with best practices for data security and integrity, the Signals Research Suite implements 24/7 global security monitoring, alerting and escalation by the Revvity Signals Software Security Operations Center. The platform can be deployed in either a multi-tenant or private-cloud environment and is designed to meet standard IT requirements for automatic updates and cloud security controls. Also, by automating routine tasks and workflows, data within the Suite is findable, accessible, interoperable and reproducible (FAIR), aiding in data integrity and regulatory compliance.

#### Save with 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, but 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 helps calibrate appropriate stock levels and manage the ebbs and flows of the supply chain.

#### 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:

- Business & Scientific Use Case Consulting
- Technology & Architecture Consulting
- Implementation & Deployment
- Systems Integration & Data Migration
- Data Science & Advanced Analytics
- Organizational Change Management
- Validation Services & Compliance Support
- Education and Enablement

The Revvity Signals team leverages science and technology expertise to deliver solutions that meet and exceed customer expectations.



With secure single-sign-on access to all applications, as well as centrally located data tutorials, training videos and software release information, Signals Research Suite lets users spend more time on their experiments, collaborate with peers, and speed innovation. switching between independent solutions.

#### Better Data, Insights, and Outcomes

The Signals<sup>™</sup> Research Suite is the first fully integrated SaaS platform for new biological and chemical modalities research, ideally suited for research use cases involving early and late-stage in vitro assays, cell line optimization, biologics process optimization, in vitro DMPK assays, animal pharmacokinetic studies, stage animal efficacy and safety studies. The Signals Research Suite is an ideal solution for scientists working on new drug modalities or who want to expand the power of Signals Notebook across the entire Make-Test-Decide R&D lifecycle for better data, insights, and outcomes.

revvity signals To learn more about the Revvity Signals Research Suite for new biological and chemical modalities research and to increase your chance for market success, visit: <u>https://revvitysignals.com/products/research/signals-research-suite</u>

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