Signals One for New Biological and Chemical Modalities Research

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

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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 Signals One™ for Drug Discovery

Revvity Signals understands these needs and has developed a tailor-made workflow-focused tool for drug discovery. AI-enhanced Signals One 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 Design-Make-Test-Decide R&D lifecycle for better data, insights, and outcomes.

It is the only complete, unified SaaS software that collectively addresses the end-to-end needs of research scientists in a collaborative and user-friendly platform. Equipped with powerful visual data analytics tools, Signals One enables researchers to gain insights that leverage their creative expertise to bring promising new therapeutics to patients in need.

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One solution for Design-Make-Test-Decide

Powered by Revvity Signals technology platform, Signals One addresses the end- to-end needs of research scientists throughout the Design-Make-Test-Decide R&D Lifecycle.

Design:
- Signals One is integrated with ChemDraw®, the gold-standard chemical drawing and communication software.
- Leverage structured, high-quality data and open APIs to integrate AI algorithms for predictive modeling, hypothesis generation, and design optimization.

Make:
- Facilitates collaboration and data management to capture, organize, share, and explore data.
- Plan, perform, and document experiments to avoid duplication of work and to maximize insights into your wet-lab workflows.

Test:
- Simply handle common visualization and analytics uses cases including in vitro curve fitting, in vivo data visualization, and group-comparison with Signals Native Analytics
- For more advanced analysis needs, leverage natively integrated Spotfire® for data analysis and visualization of all modalities, this capability unites assay development, low- to ultrahigh-throughput production assays, high content screening, and in vivo studies, enabling users to search across all assay and screening data in a single solution.
- As a central data processing platform for all types of experiment workflows, Signals Data Processing lets you parse instrument files, process data using automatable calculation templates, and capture results.

Decide:
- This next-generation data management system analyzes scientific results. Data-driven Analytics capabilities enables efficient access and analysis of all scientific results collected throughout the R&D life cycle.
- With all the chemical and biological analytic functionality of Revvity Signal's Lead Discovery Premium, plus advanced query and data management capabilities, it helps users find and retrieve any test or assay result plus associated compound or biologic sequence information across experiments, projects, and departments.
- The Data-driven Analytics capabilities provide sub-second query responses across even the largest of databases. Scientists can easily transfer the relevant subsets of data into analytic dashboards without any programming, manual data-wrangling, or reformatting.

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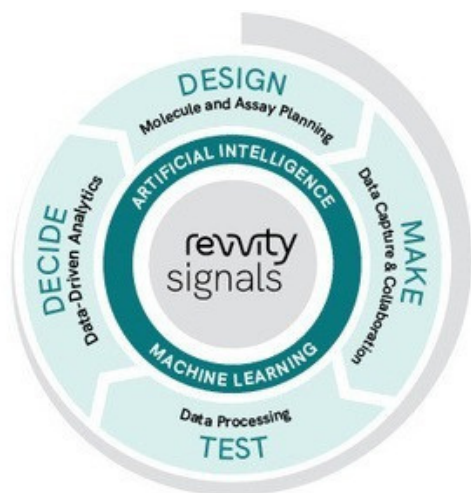

Figure 1. Signals One unites all scientific program work into one platform, spanning early research to in vitro testing and safety to early development.

Design & Make

Signals One 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
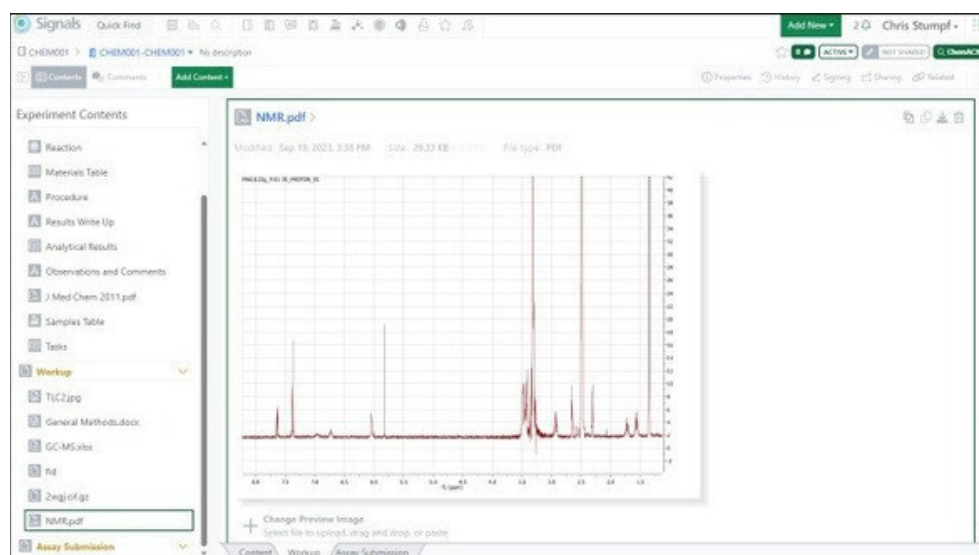- Support for patent applications

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

ChemDraw®, the trusted chemistry gold standard for the last 35+ 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 the Signals One.
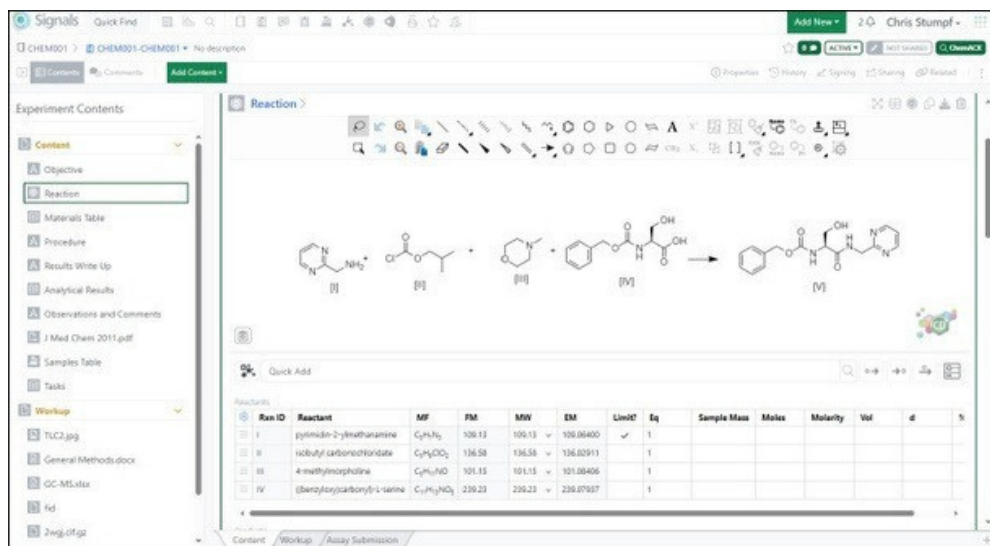
Figure 3. Native ChemDraw integration in Signals One. Chemical synthesis reactions can be easily drawn using ChemDraw and stoichiometry tables automatically update.

Hierarchical Editing Language for Macromolecules (HELM), another new Signals One 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 One. 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.
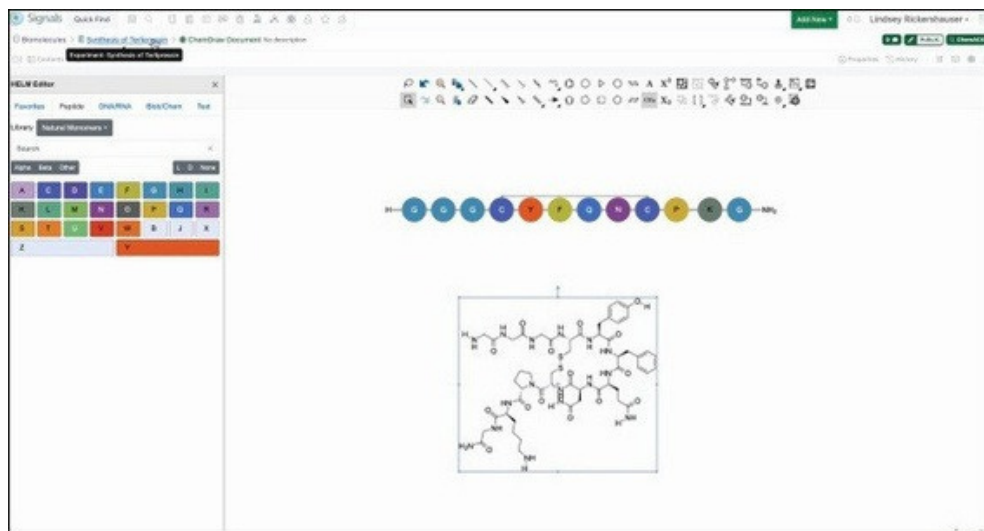

Figure 4. Using the HELM Editor in ChemDraw to draw Terlipressin in amino acid notation (top) and conversation of the amino acids into a chemical structure (bottom).

Test

Signals One includes two-levels of data processing capabilities to provide a flexible environment that caters to a wide range of analytics needs:

For routine use cases including in vitro curve fitting, in vivo data analysis, or group comparisons, Signals One keeps simple analytics simple with native analytics that is designed to be intuitive.

For advanced use cases, where research applications are more complex, researchers can use the data processing powered by Spotfire to analyze data and convert 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™ 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 One and exports into Microsoft Office and PDF format.
- Automatic round trip of experimental results from the data processing capability into Signals One
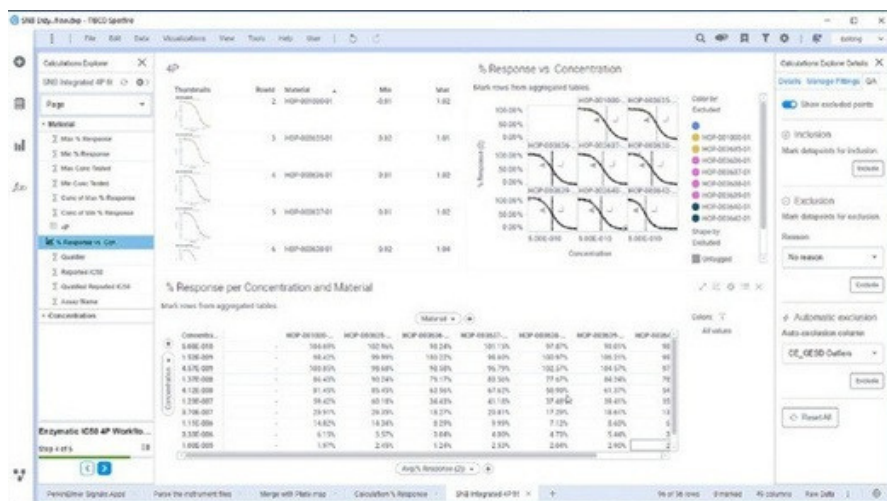

Figure 5. The Data processing capability represents the Test phase of the Design-Make-Test-Decide R&D workflow. The capability provides provides guided workflows for data import and analysis so that visualization and analytics are consistent and reliable.

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.

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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 Design-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 One 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 One Inventory Management
No solution is better equipped to manage your lab inventory than Signals One. 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 One with inventory-management best practices helps calibrate appropriate stock levels and manage the ebbs and flows of the supply chain.

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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 One lets users spend more time on their experiments, collaborate with peers, and speed innovation. switching between independent solutions.

200
Professional Services Staff Globally

75%
Advanced Scientific or Technology Degrees

350
Projects Completed per Year

Better Data, Insights, and Outcomes

Signals One 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. Signals One is an ideal solution for scientists working on new drug modalities or who want to expand the power of Signals Notebook across the entire Design-Make-Test-Decide R&D lifecycle for better data, insights, and outcomes.

To learn more about the Signals One by Revvity Signals for new biological and chemical modalities research and to increase your chance for market success, visit:
https://revvitysignals.com/products/research/signals-one

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