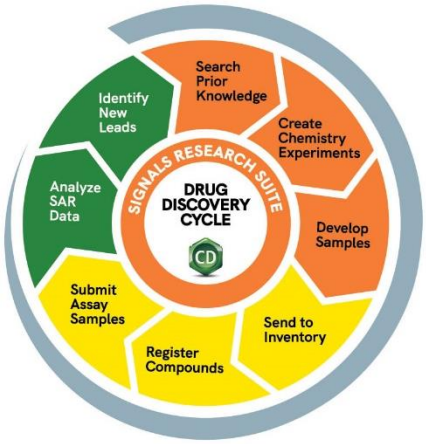
Signals Notebook for Discovery Chemistry

Give back more scientific quality time to chemists, and increase chances of drug discovery success

Revvity Signals Notebook, integrated with the industry-standard ChemDraw, provides chemists involved in drug discovery with an intuitive, cloud electronic lab notebook (ELN) that streamlines data management, promotes collaboration, and enables rapid insights to accelerate innovation and discovery.

Chemists involved in drug discovery are challenged by an abundance of data, a lack of integrated tools, and ever-shrinking time for creative scientific exploration. More than a productivity tool, Signals Notebook speeds users to insight, fosters insightful collaborations, improves decision-making, and accelerates discovery.



Signals Notebook- The Starting Point for Drug Design in the Signals Research Suite

Signals Notebook is part of the Signals Research Suite that is powered by ChemDraw, the chemical communication solution and TIBCO® Spotfire®, the leading visual data analytics software. By combining all the software applications needed for the Make-Test-Decide drug discovery cycle in one integrated platform, Signals Research Suite helps discovery chemists improve research efficiency and uncover unforeseen insights. This ultimately improves the

success rate of drug discovery projects and hence the likelihood of bringing novel drugs to market.

The only ELN with Native ChemDraw Integration

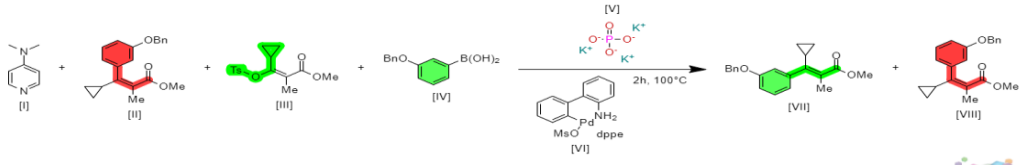
Experience the unmatched benefits of integrating the industry's gold standard chemical drawing and communication solution, ChemDraw, directly within the Signals Notebook. This native ChemDraw integration transforms Signals Notebook into a chemistry-intelligent platform, offering a wide range of advanced features such as:

- Automated Stoichiometry Calculations and Auto Text: Signals Notebook automatically populates stoichiometry tables, adjusts calculations based on reaction stoichiometry and number of equivalents, providing appropriate units of measure, and ensuring accuracy in experimental data. Updated amounts from the stoichiometry table are automatically updated in the written experimental procedure.

- Comprehensive Search Functionality: Users can search for chemicals using their CAS Number, structure, or name. Additionally, Signals Notebook offers full access to PubChem material safety data sheets, and a wealth of other valuable resources, simplifying the process of finding and referencing essential information.

- Multiple structural formats: Create drawings of structures and reactions by simply pasting SMILES strings or drag and drop ChemDraw or .mol files directly into the canvas. Researchers get greater flexibility in visualizing and handling chemical structures.

- ChemACX Explorer enables searching for chemical supplier information and chemical property exploration for compounds that are commercially available as well as CAS Registry number search to find chemical structures. Those chemicals can then directly be added to an experiment reaction scheme.



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Reactants

Rxn ID	Reactant	MF	MW	EM	Limit?	Eq	d	Sample Mass	Moles
I	N,N-dimethylpyridin-4-amine	$C_7H_{10}N_2$	122.17	122.084398		2		0.51 g	4.2 mmol
II	methyl (Z)-3-(3-(benzyloxy)phenyl)-3-cyclopropyl-2-methylacrylate	$C_{21}H_{22}O_3$	322.40	322.15689		1		0.67 g	2.1 mmol
III	methyl (E)-3-cyclopropyl-2-methyl-3-(tosyloxy)acrylate, 4 water, 4...	$C_{15}H_{18}O_5S{\cdot}4H_2O$	310.36	310.08749	✓	1	1.12 g/mL	0.80 g	2.1 mmol
IV	(3-(benzyloxy)phenyl)boronic acid	$C_{13}H_{13}BO_3$	228.05	228.09577		1		0.48 g	2.1 mmol
V	potassium phosphate	K_3O_4P	212.26	211.84454		3		1.3 g	6.3 mmol
VI	precatalyst	$C_{39}H_{37}NO_5P_2PdS$	768.16	767.10042		1.5		2.4 g	3.1 mmol

Figure 1. An example of a coupling reaction drawn with ChemDraw in Signals Notebook and its corresponding, automatically populated stoichiometry table.

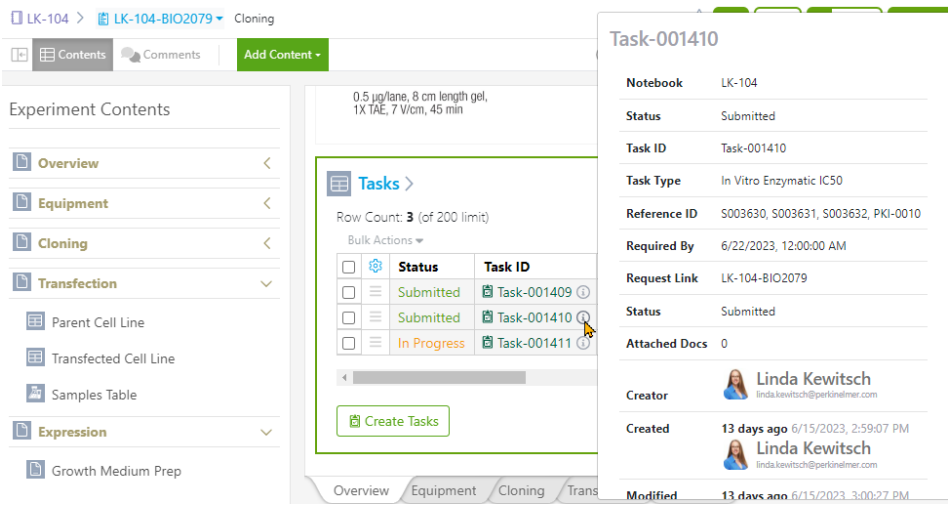


Figure 2. An example of a biological task request within a Signals Notebook experiment, allowing for seamless cross-disciplinary collaboration. A simple hover over tasks immediately gives a glance of important sample information.

Support Chemistry/Biology Collaboration

Signals Notebook encourages real-time multidisciplinary collaboration with on-demand experiment-sharing within and outside organizations. As analytical methods progress through the drug development process, Signals Notebook supports workflows including and beyond pharmaceutical R&D. Synthetic, analytical, (bio)formulation, and (bio)process scientists and biologists working in areas from screening to preclinical and clinical development can now share the same ELN.

Their research and experimental needs are supported in Signals Notebook so they can share and exchange data in the same environment. This integration becomes more critical as more drug discovery methods and new modalities call for the input, analysis, and sharing of chemical data and structures, as well as biological peptides, proteins, viral vectors, sequence, and expression data.

As a productivity solution, Signals Notebook automates data capture and experiment note-taking, is user-friendly for data management, and natively integrates with Microsoft Word, Excel, PowerPoint, PDFs. Scientific papers, spectral scans, and more can be directly included in experimental procedures in the notebook.

Parallel Chemistry Experiments: Library Creation (Combinatorial Chemistry)

Added at customers' request, this ability to create sub-experiments within an experiment helps enumerate compound libraries and keep track of syntheses. Parallel experiments streamline the process and allow for efficient organization and management of complex synthesis projects. This

feature is particularly useful in combinatorial chemistry, where numerous compounds are synthesized simultaneously to expedite the drug discovery process.

By facilitating the management of multiple reactions and conditions, Signals Notebook enables researchers to optimize their experimental design, compare results, and identify the most promising candidates for further investigation. The parallel experiments functionality empowers chemists to maximize productivity and accelerate the discovery of novel compounds, contributing to the development of new therapeutics.

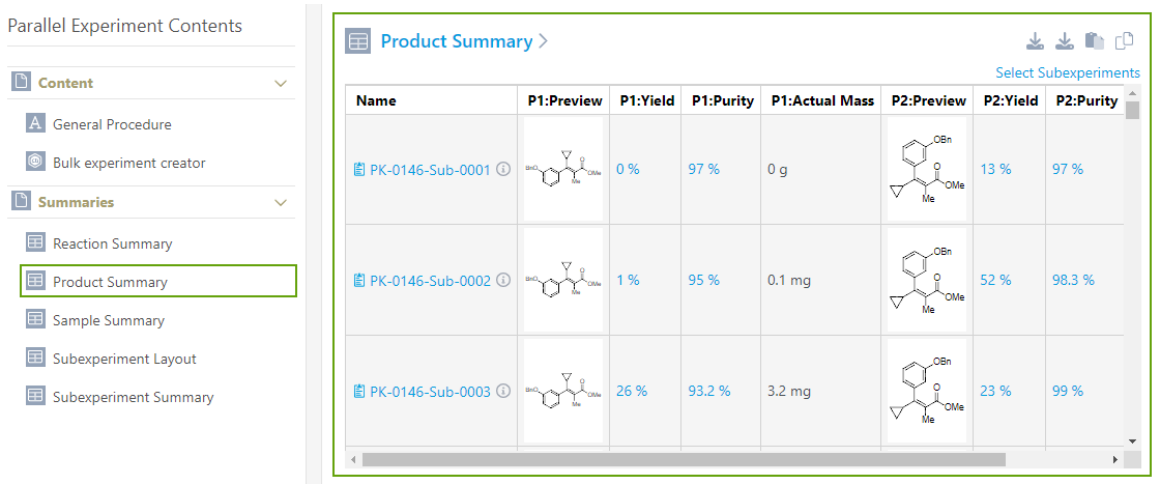
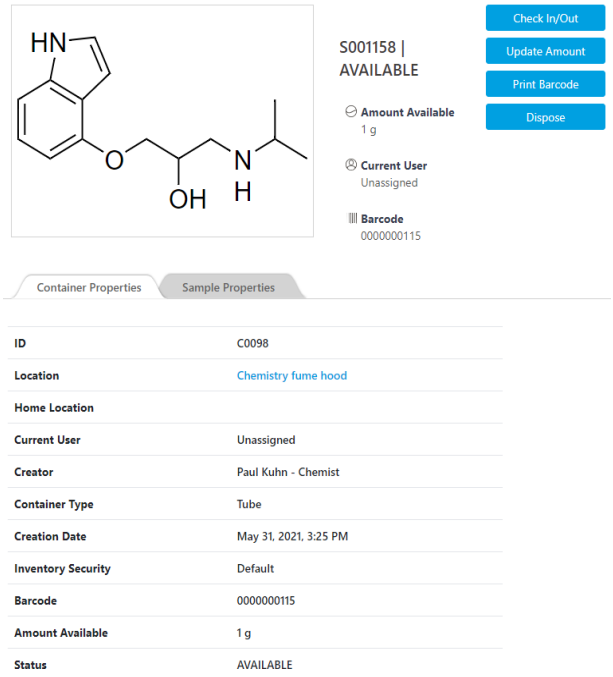


Figure 3. A screenshot of a parallel (combinatorial) chemistry experiment in Signals Notebook. Reactants and various conditions can be loaded as a .csv file to generate all the necessary conditions and variations. A summary view of the enumerated reactions, products



Materials Inventory

Search for chemicals and compounds in your materials inventory with ease and obtain their precise storage location, streamlining the process of locating and retrieving necessary resources. Easily track chemicals via barcode, enabling accurate and efficient inventory management. The system provides real-time information on what is available in-house for use and generates alerts for when to order or reorder chemicals, ensuring that essential supplies are always on hand.

Figure 1. An example of an Inventory item in Signals Inventory. The chemical can be readily inserted into a chemistry experiment stoichiometry table, and the amount used in the experiment will be decremented from the Inventory container.

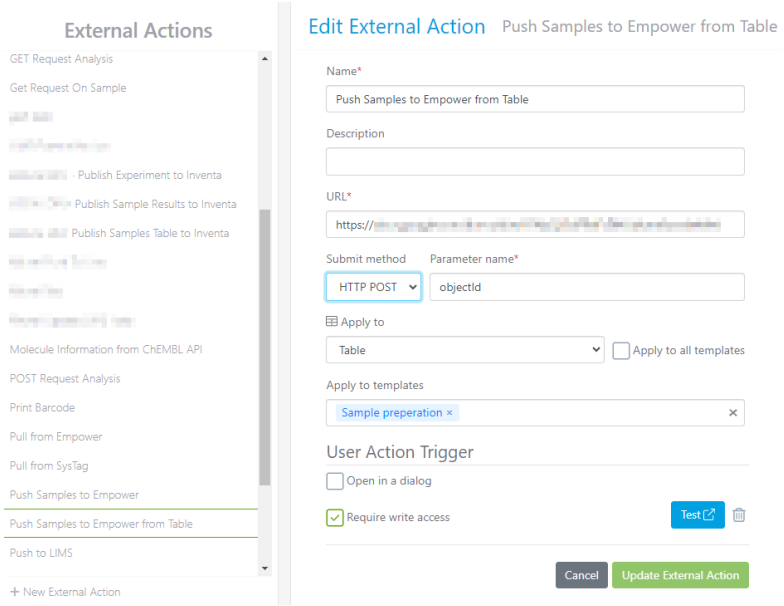
Signals Notebook keeps track of amounts used in each experiment through automatic decrements, providing an accurate record of material consumption. This feature not only helps researchers monitor their usage but also assists in maintaining up-to-date inventory levels, reducing the risk of running out of crucial chemicals during an experiment.

Security

The security features in Signals Notebook ensure that organizations maintain the highest level of data protection and integrity. Controlled permissions and data access safeguard sensitive information, allowing only the necessary and approved data to be shared with specific individuals or groups. This robust security extends not only to internal teams but also to external contract research organizations, ensuring that collaboration remains secure and confidential.

Signals Notebook allows for the creation of locked fields and entries in worksheets, preventing unauthorized alterations and maintaining data integrity. By restricting the ability to modify these fields, organizations can ensure that critical information remains accurate and unaltered while still being compliant with established procedures.

Moreover, the security measures in Signals Notebook include regular data backups, advanced encryption, and the user authentication protocols one can expect from a modern software solution. These features work in tandem to protect your organization's valuable intellectual property and minimize the risk of data breaches or unauthorized access.



Seamless Integration through APIs (Application Programming Interfaces)

In today's rapidly evolving digital landscape, Application Programming Interfaces (APIs) play a crucial role in connecting various software applications and services. For cheminformaticians, APIs enable seamless integration and data exchange between Signals Notebook and common chemistry sources, services, and third-party applications.

Figure 2. An admin view of the integrations dashboard in Signals Notebook, showing various possible interactions with 3rd party applications that are enabled by the Signals Notebook Application Programming Interface (API).

APIs provide the flexibility to integrate Signals Notebook with other essential tools, such as data analysis platforms, laboratory information management systems (LIMS), and enterprise resource planning (ERP) systems. These integrations facilitate more efficient data management, collaboration, and reporting, driving productivity and innovation within research teams.

Reclaim Lost Scientific Quality Time

Signals Notebook, integrated with ChemDraw, gives time back to discovery chemists. It enables them to quickly enter procedures, experimental findings, data, and analyses that are shareable with others. Access to previous experimental results and history makes it easy to build upon previous work, while capturing methods and procedures within Signals Notebook facilitates the retention of intellectual property information.

With procedures clearly outlined in Signals Notebook worksheets, there is less room for error, leading to increased consistency and control over protocols and standard operating procedures (SOPs). This clarity helps streamline the research process and minimize mistakes, saving valuable time and resources.

Better, cloud-based data management in the collaborative, integrated Signals Notebook equips discovery chemists with the necessary tools to work more efficiently and effectively. By providing a user-friendly platform for managing and sharing data, Signals Notebook increases the chances of success in bringing new therapies to market, driving innovation, and improving patient outcomes.

FREE TRIAL

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