Beyond a Drawing Tool:

The Evolution of a Comprehensive, Chemically-Intelligent Solution for Chemistry Communication

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How Innovative Software Can Empower Today's Chemists to Search, Reuse, and Report Their Data Efficiently and Seamlessly

INTRODUCTION

Connected technologies have transformed many different fields of study in the last two decades, and the scientific lab has not remained immune.1 Across the globe, labs big and small have adopted technologies such as electronic lab notebooks cloud platforms, enhanced automation, and dedicated software to accelerate research, increase reproducibility, and improve productivity.

It's clear that technology has vastly improved the way science is being done, and in many cases, new software and robotics have rendered tedious manual processes obsolete.2 The current coronavirus pandemic offers a great example – scientists have begun to run complete experiments through automation and remote monitoring, without physically being present in the lab.3

As the world is definitively moving towards these trends in automation, electronic record-keeping, and cloud connectivity, there is also significant innovation happening in communication tools. Particularly for chemists, these innovations are bringing about a revolutionary change in how they are sharing their research. This article delves into the current communication struggles in chemistry research and how they can be easily overcome with purpose-built, innovative software such as ChemDraw and Signals ChemDraw.

Chemists routinely need to find, collate, and reformat pre-existing chemical structure drawings and associated scientific results into reports, presentations, publications and patent submissions. This is a labor intensive and highly inefficient process, requiring manually opening and browsing through a multitude of files, followed by copying and pasting selected structures into new reports which must be carefully formatted to combine molecules with their properties and assay results. Signals ChemDraw, the latest tool in the ChemDraw arsenal, is a refreshing solution to this problem – it facilitates quick structure searches in all documents where chemical information is stored and allows creating collections of select chemical structure drawings and their associated properties. It also enables users to automatically generate consistently formatted reports. The following discussion presents a more in-depth look at both the challenges and novel solutions.

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Top Challenges in Chemistry Reporting and Communication

Chemists deal with many different challenges when finding, reusing, and organizing chemical information to create publishable reports and presentations. Here, we've grouped these challenges into three main buckets.

Lack Of Efficiency in Conducting Admin Tasks

Any scientist would know too well the struggle of having to balance research with routine admin tasks, such as tracking work, searching through archives, and recording protocols and observations. This type of work is painfully time-consuming, taking away precious hours that could be dedicated to actual science. But they must be done.

There is also the reporting aspect, which includes presentations and posters for lab meetings/conferences, patent applications, journal publications, thesis-writing, etc. Science reporting requires several layers of communication and many hours of preparation. Luckily, with software like ChemDraw, chemistry research has moved far beyond the times when stencils were used to draw and copy chemical structures. But even today, despite a diminishing trend, the majority of chemists still capture their experimental data on paper lab notebooks and conduct manual data searches. Reusing data in this manner is completely inefficient, error-prone, and irreproducible.

"That's why electronic lab notebooks or ELNs are such a valuable tool for chemists – they automate some of these mundane, housekeeping tasks. You can simply search for and duplicate an existing experiment, slightly modify the chemical reaction scheme, and insert pre-defined text templates for experimental procedures.," says Dr. Pierre Morieux, organic chemist, Global Marketing Manager for ChemDraw at Revvity Signals, and all-around ChemDraw Wizard. "This is where software applications play a very important role in getting those inefficient admin tasks out of the way, and giving back valuable time to research scientists."

Dealing with Limited "Chemical-Intelligence" in Applications Every day, chemists access a variety of different applications, websites, and online databases when conducting their research. Unfortunately, not all of them are able to understand the language of chemistry, with all its diverse molecules and intricate chemical structures. For example, one cannot simply use a ChemDraw structure to search and organize data in these applications. This makes it difficult for chemists to quickly perform structure searches and compile lists or transfer information, and there is a real need for more chemically-intelligent software applications. "Chem-ignorant software can be a real challenge," Morieux says. He believes that research software developers and IT organizations will help change that landscape.

ChemDraw JavaScript was developed for this exact purpose. It's a building block easily integrated into modern web technology so that the application becomes chemically smart and able to recognize molecules and reactions. As an example, Revvity Signals's Cloud ELN Signals Notebook integrates this web-enabled version of ChemDraw, which allows chemists to seamlessly draw molecules and reactions in the browser or through the ChemDraw Desktop application.

Navigating Siloed Reporting Applications and Databases
There are numerous different applications and web resources that chemists turn to, for their communications activities (e.g. Microsoft Word, PowerPoint, Excel, Outlook, Teams, etc.), but there is no cross-talk between them. The fact remains that searching for chemical structures across these different applications is no easy task – it's a tiresome manual process, which, in turn, leads to information being buried and forgotten in various documents, spreadsheets, and decks.
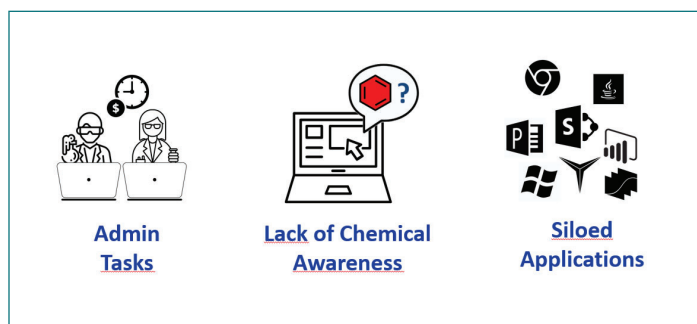

Figure 1. The top challenges faced by chemists in communicating their work.

More often than not, there are vast amounts of data stored disparately in a chemist's personal or lab computer. This renders the data almost unusable and hard to locate. Such siloed applications become graveyards of chemical information; researchers are stuck wasting hours trying to find already existing drawings and schemes, perhaps created months or years ago.

"Ideally, a chemist should be able to easily find, reuse, and repurpose these existing chemical drawings and share them in a streamlined way. That's the goal Revvity Signals, as a developer of technology solutions, is working towards – the ability to give users tools that can break down these silos."

Developing Solutions Through a Suite of Innovative Software Tools

To address the above challenges and help chemists overcome horrible inefficiencies in reporting and sharing their work, Revvity Signals has been developing an "ecosystem of applications" that together provide a comprehensive solution. These applications are integrated to work seamlessly to cover each step in the so-called "Make/Test/Decide" workflow.

"As a chemist you make compounds or materials, you test them, and then you decide which ones you should make next. ChemDraw comes into play for ideation at the "Make" stage, when you plan out what you're going to synthesize," Morieux explains. "Then for testing and analysis, we have the Signals Lead Discovery platform that offers analytics and visualization software to help you manage large quantities of test samples and analyze results."

Signals Lead Discovery, powered by TIBCO Spotfire®, provides guided search and analysis workflows (with feedback on availability of assay data) and intuitive visualizations to identify patterns, trends, and outliers within the data. Morieux says this platform was designed to assist chemists in making faster, yet more insightful, decisions about their research. When it comes to recording experiments and data, the Signals Notebook allows chemists to keep track of their work in a cloud-native platform, that also functions as a handy data management tool.
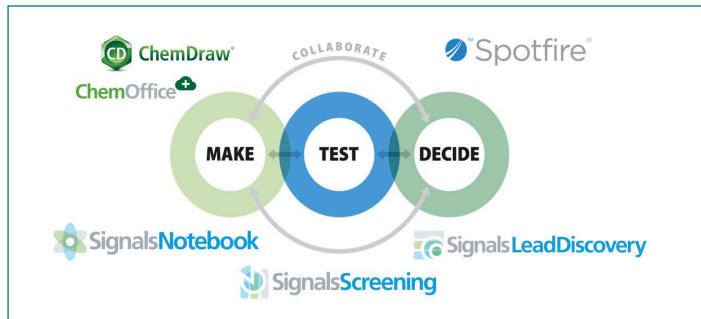

Figure 2. Revvity Signals's Suite of applications that address each step of the Make/Test/Decide workflow.

The latest addition to Revvity Signals's suite of applications, that focuses specifically on accelerating chemical communication, is Signals ChemDraw (Version 20). To understand what Signals ChemDraw makes possible for chemists, it's important to revisit its core component – ChemDraw.

ChemDraw, as a drawing tool, offers many features that not only enable chemists to draw and represent their chemical research in an artful and efficient way, but also facilitate processing and structuring experimental data. ChemDraw's capabilities support chemists of all levels, from aspiring to experienced, allowing them to sketch out reactions and conceptualize experiments, without having to be a master at drawing structures. The software includes hotkeys, color options, 3D displays, and NMR

predictions. It has several, extremely useful integrations with databases to enable searching for different types of information through chemical structures.

For example, with SciFinder, SciFinder-n, and Reaxys integrations, chemists can search large databases of chemical literature with the click of a button. Recently, access to PubChem Chemical Safety information and ChemACX supplier/pricing information were introduced as new capabilities. With the newest version of ChemDraw in Signals ChemDraw, users can now structure search through vast amounts of chemistry and patent literature on Google Scholar and Google Patents, directly from within ChemDraw.
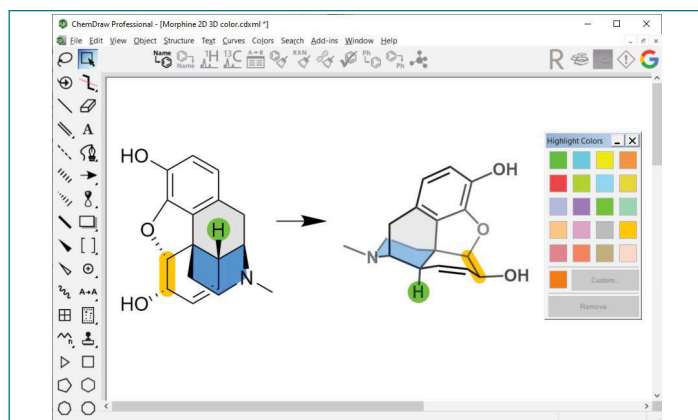

Figure 3. ChemDraw provides powerful drawing, integration, and reporting features to help create and communicate beautiful drawings in seconds.

He notes that drawing a reaction scheme or a molecule is just the beginning of a workflow. While the ChemDraw component of the solution is designed to help chemists more efficiently draw reaction schemes and make them look professional, Signals ChemDraw is designed to meet the overarching goal of facilitating the communication of chemistry ideas. In other words, it helps researchers take their drawing and communicate it with the rest of the world through various mediums, in a simple, straightforward, and hassle-free manner. All the ChemDraw Collections features are designed to boost research and communication productivity by breaking down silos between applications and making admin tasks quick and manageable.

So How is This Done?

In short, the Signals ChemDraw application allows users to perform structure searches on their data directly within documents and disparate locations, organize data into collections, and communicate data through easily created

"With all these capabilities, if ChemDraw can be seen as a well-optimized tool taking chemical drawing to the next level, then Signals ChemDraw is the solution that takes the whole chemical communication workflow to the next level, efficiently turning chemical drawings into chemical knowledge."

Enabling "Chem-munication": Search, Select, Communicate

According to Morieux, Signals ChemDraw introduces a new levelof efficiency and capabilities that have never before been madeavailable to chemists for locating, reusing, organizing, and sharingtheir work. The application enables three main functions that arecritical to chemical reporting.

SEARCH: With Signals ChemDraw's search function, one can quickly search for structures across different locations where chemical information is stored. Most chemists still rely on Microsoft Office applications such as Word, PowerPoint, and Excel to create and store chemistry data – essentially, massive collections of data that have been accumulating over years and years.

"Chemists typically do not store their data as a ChemDraw file, but rather as a file embedded within a document or slide," explains Morieux. "These files accumulate lots of chemical information, but it becomes too difficult to reuse the data. You would need to scroll through hundreds of pages sometimes to manually locate a particular drawing, open it in ChemDraw to tweak or repurpose, and copypaste on to a new report."

Although this process is horribly inefficient, it is currently the standard in industry and academia. Signals ChemDraw is purpose-built to circumvent this inefficiency by allowing a rapid search function across multiple applications and file types (e.g: .cdx files, .cdxml files, .sdf files, and .mol files). Users can now parse and extract drawings, reactions, and structures without even opening the file.

> "With Signals ChemDraw, you can browse what you have locally on your desktop to pick what you would like to upload or reuse. This application looks only for chemistry content,"
> "You can select a 500-page Word document and view only its chemical drawings."
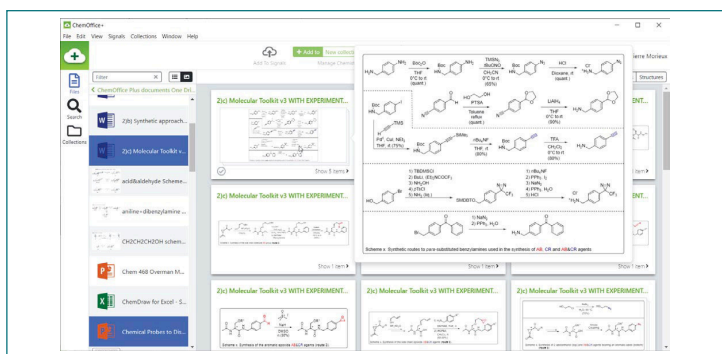

Figure 4. Signals ChemDraw allows users to search and re-use chemical drawings inside MS Office without opening them.

SELECT: Signals ChemDraw has added the ability to select multiple structures and/or reactions and organize them into lists of chemical objects called a collection. A collection is used for a given reporting purpose, for example, reactions prepared in the past week or compounds synthesized in the past 3 months.

Presenting and sharing work is a very regular part of a chemist's job. This may comprise daily reporting, weekly lab meetings, and annual conferences. For such presentations, chemists usually have a large amount of information already drawn in ChemDraw, but organizing and reusing this data is difficult due to the aforementioned inefficiencies with current "chem-ignorant" software.

Enter Signals ChemDraw: This new software can assist in triaging and quickly picking relevant information from the wealth of chemical drawings available. It does this by allowing the user to create a list of molecules or reactions with a purpose. "For example, you can search multiple documents, handpick things that you want to present, and put them in a collection where you can add properties or attributes to a given molecule," Morieux elaborates. "From that collection, you're able to select molecules and accompanying text and drop into a PowerPoint slide – all properly formatted, aligned, and consistent – without having to painstakingly adjust everything manually."

COMMUNICATE: The goal of Signals ChemDraw is to make the mundane task of creating reports to communicate chemical research, much more efficient. With the above capabilities in searching, reusing, selecting, and organizing chemical structures and data, chemists can use Signals ChemDraw to create presentation-ready PowerPoint slides and publication-ready manuscript figures with only a few clicks.
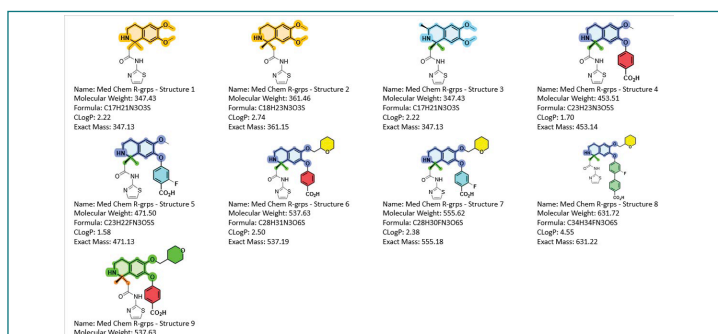

Figure 5. Example of a PowerPoint report slide generated in a few clicks from a ChemDraw Collection.

> "Customer feedback has shown us as that chemists in biotech or pharmaceutical companies often spend up to 2 hours per week drawing, re-drawing, and preparing slides for their meetings."

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This time loss translates to a significant productivity loss for the organization, when work hours of all its chemists are factored in. As a chemically-intelligent solution, Signals ChemDraw was designed to accelerate all the steps in reporting and make the communication process seamless, painless, and efficient. Additionally, being a cloud application, ChemDraw Collections is always running on the latest version available, and updates can be delivered at a much more frequent pace than traditional Desktop applications.

Reaping The Benefits of a Simplified Communication Workflow

According to Morieux, Signals ChemDraw introduces a new "Drawing a molecule structure or reaction scheme is the beginning of a journey for an idea," says Morieux. "The researcher needs to take this idea, share it and convince people of the science, so that it can make its way to a publication, a conference or a patent." In that sense 'perception is reality', he adds. "Without proper communication, a breakthrough discovery will only ever remain an idea buried in a file".

ChemDraw is the technology that parallels and powers the evolution of this journey. It was born as a drawing tool, and over the years, evolved into a highly efficient chemistry application that enables the rapid creation of high-quality, publication-worthy drawings of molecules with ever-increasing complexity.
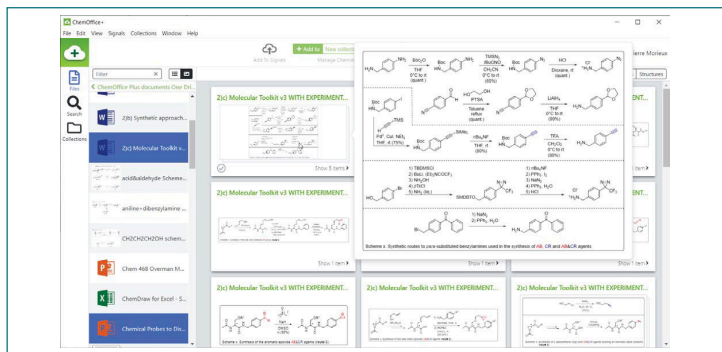

Figure 4. Signals ChemDraw allows users to search and re-use chemical drawings inside MS Office without opening them.

Now, its capabilities extend far beyond a simple drawing tool. With the introduction of Signals ChemDraw, the application has become a robust, comprehensive solution, purpose-built to simplify, facilitate, and accelerate chemistry communication and the transformation of chemical drawings into shareable chemical knowledge.

> "The ability to create a chemical drawing via ChemDraw is not the endgame. The endgame is globally communicating your research to your peers"

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To learn more about Signals ChemDraw and ChemDraw collections, please visit:
www.revvitysignals.com/product/research/chemdraw

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