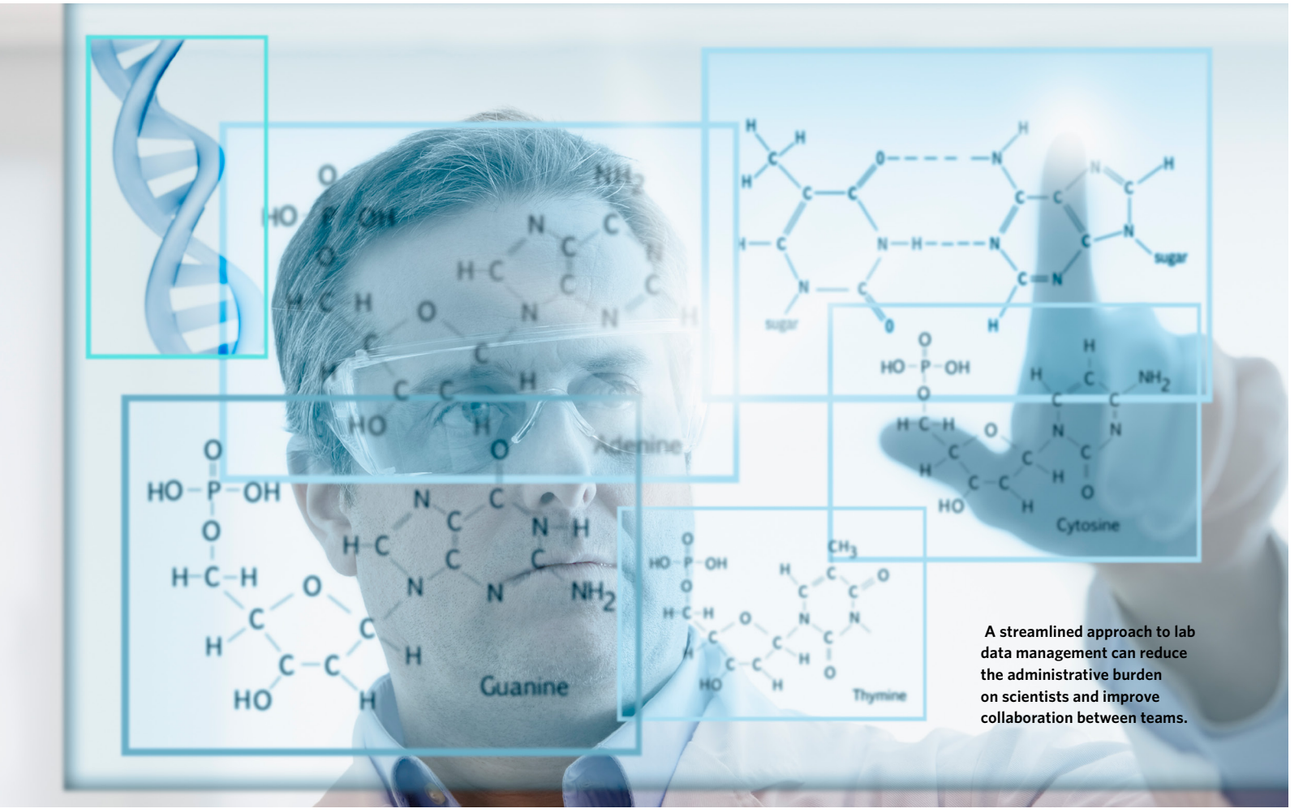


**A streamlined approach to lab data management can reduce the administrative burden on scientists and improve collaboration between teams.**

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# MAKE, TEST, DECIDE: HOW TO SAVE PRECIOUS TIME IN DRUG DISCOVERY

**FOR DRUG DISCOVERY LABS,** finding the right informatics tools is more important than ever as medicinal chemists look to maximize 'scientific quality time'.

**Time is of the essence in drug discovery.** And while the process is inherently complex and labour-intensive, biotech and pharma researchers continue to develop efficient ways to synthesize, screen and test ever-larger libraries of candidate molecules. But labs are always on the lookout for new ways for their researchers to claw back 'scientific quality time': vital breathing room, away from repetitive administrative tasks, to be creative.

"Our oncology work tends to move quickly," says Jennifer Fulton, a medicinal chemist at precision therapy-focused biotech, Cogent Biosciences. Against this backdrop, the choice of laboratory informatics tools is essential; the wrong product could gum up the gears rather than grease the wheels of progress.

Revvity Signals Software's Signals Research Suite is a good fit for the brisk pace of R&D at Cogent Biosciences, providing an array of tools that enables easy management of information from the laboratory bench to boardroom presentations. Signals Research Suite, Fulton says, has given Cogent Biosciences the kind of data analytics capabilities that were once the sole domain of big pharma companies with deep pockets and extensive IT departments.

But larger companies, too, are recognizing the advantages of leaving software implementation to the experts. Joost Brakkee, an IT director at Janssen, notes that after years of working with an internally developed electronic lab notebook, his company finally decided to begin transitioning its R&D teams to Signals Research Suite. "You don't have to reinvent the wheel," he says. "It allows us to integrate with other systems, and above all, it helps us collaborate with all the different scientific communities that we need to support."

## ACCELERATING THE CYCLE

The Signals Research platform is the foundation of the Signals Research Suite, a software platform designed to facilitate the research efforts of chemists, biologists and clinical experts, and to enable knowledge-sharing and coordination between these specialized teams. Pharmaceutical chemist Pierre Morieux, chemistry product marketing manager at Revvity Signals Software, says the platform encompasses the entire 'make-test-decide' cycle that forms the backbone of scientific research. It's the iterative process that starts with basic discovery and informs researchers' decision-making as they work towards their goals. "We want our software to cover the workflow end-to-end," says Morieux, who is affectionately known as ChemDraw Wizard on the Internet.

The entry point for this process is Signals Notebook, which records critical experimental information, including the chemical structures of compounds and the synthetic procedures used to generate them. This is supported by Notebook's integration of ChemDraw, a widely used chemical structure and reaction drawing tool. Although initially developed for small-molecule compounds, ChemDraw's capabilities now extend to the complex world biopolymers such as nucleic acid- and protein-based drugs — a critical need amid the industry's surging interest in biologics, and new complex chemical modalities. ChemDraw now supports the Hierarchical Editing Language for Macromolecules (HELM) standard for the visual representation of such complex biomolecules, and the company is working on making these as straightforward to manipulate as their small-molecule counterparts.

**"WE WANT OUR SOFTWARE TO COVER THE WORKFLOW END-TO-END."**

Signals Notebook can bring other efficiencies. For example, Fulton's team at Cogent Biosciences also uses Signals Notebook for compound registration, where a molecule is compared against others in a database to determine how distinctive it is, relative to existing compounds. It also eliminates excess manual work in terms of the recording, modification and sharing of experimental procedures associated with the 'make' and 'test' components of the cycle.

For the 'decide' component, medicinal chemists and their colleagues can turn to the Signals Inventa software. This decision-support tool incorporates the popular TIBCO Spotfire platform, coupling its visual data analytics capabilities with a toolbox tailored to dealing with chemical (and biological) entities and their associated assay data. Developmental biologist Daniel Weaver, Revvity Signals Software's product manager for lead discovery and screening, says Inventa is particularly useful in evaluating structure-activity relationship data — a critical resource for optimizing the performance of promising lead candidates.

"We've extended that to being able to do the same kind of assessments on large molecules as you do on small molecules," says Weaver, noting that the software has even proven suitable for evaluating new drug categories such as antibody-drug conjugates (ADCs), in which a monoclonal antibody targeting a tumour-specific antigen is coupled to a potent chemotherapeutic. "It allows you to pull in the annotative context that describes how was the antibody made, what plasmids were used to make it, or what linkers were used in ADCs."

## DATA IN HARMONY

The benefits of this kind of digitalization are also clear at the organizational scale. The Signals platform was conceived from the beginning as a cloud-native platform, which gives it an edge, Morieux believes, in terms of data-sharing relative to locally hosted platforms. "Scalability was one of the key things we looked at, because we know from experience that on-site systems can be slow, and that their performance is also dependent on where the servers are," he says. This means that data and other experimental assets generated by any part of a company can readily be relayed to colleagues and collaborators in other departments. "Before, there were really siloed organizations," says Brakkee. "This has led to better harmonization."

Fulton has seen firsthand the difference these capabilities can make. Prior to working with Spotfire and Inventa, her team was struggling to get by with spreadsheets, which meant a lot of frantic scrolling to uncover relevant experimental data when her team leads would stop by to discuss promising leads for an ongoing drug programme. "We learned very clearly that Excel is not built for this," she says. "Now I can click a button and say, 'these are the compounds I'm thinking of.'"

But it isn't simply a matter of accessing and sharing data. The Signals platform also allows users to tailor how that data is presented for different user groups. "Having various ways to visualize data helps communication, because everybody sees data a little bit differently," says Fulton. This can be helpful when researchers performing biological assays need to discuss their findings with the chemists who generated the compounds being tested, or when the research team needs to present finely polished findings to company leadership in the run-up to a decision about a programme's future in the clinical pipeline.

The road to drug discovery will always be littered with failures and disappointments, but a software platform that streamlines the process can help scientists to cut back on administrative chores and focus on what matters most. "We want to help create new medicines, and everything we develop is geared towards that," Morieux says. "We know the problems, we know the pains, and we know how gruelling research can be, and we're just trying to make the lives of researchers easier." ■

**REFERENCE**

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