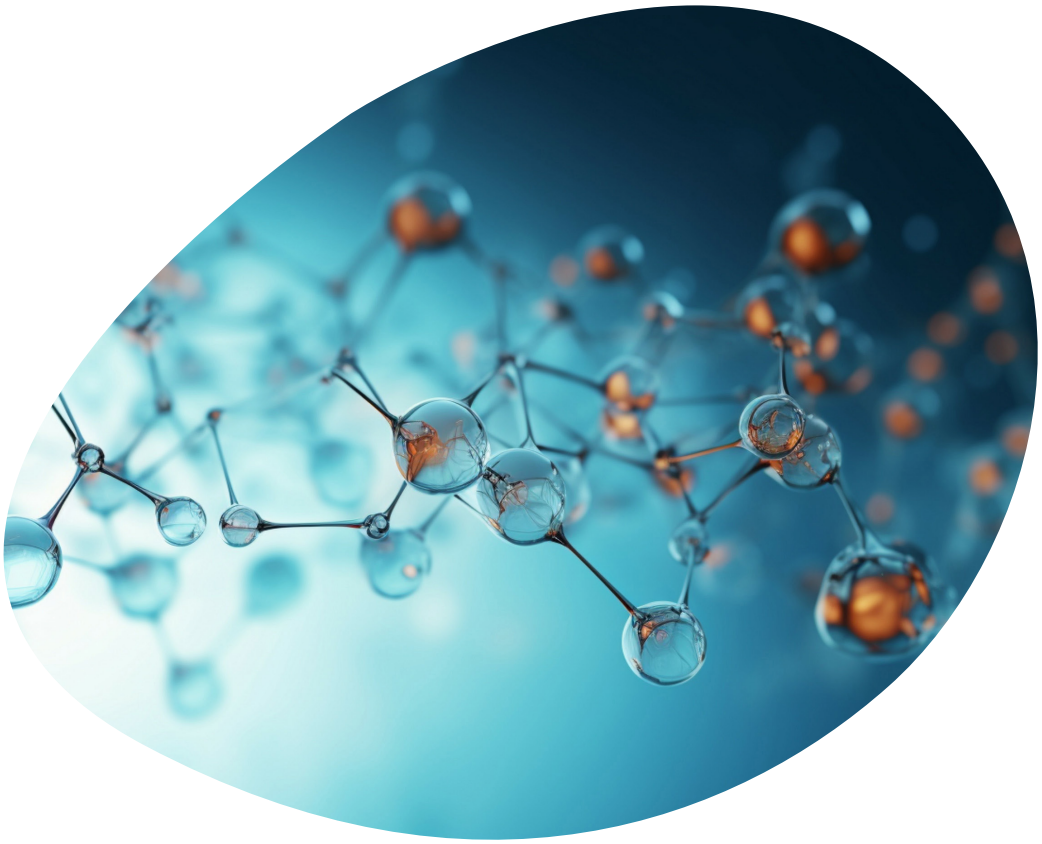
E-BOOK

REACHING THE NEXT FRONTIER

Digital transformation in the specialty chemical industry



revvity signals

TABLE OF CONTENTS

CLICK TO SEE INTERACTIVE DEMO

INTRODUCTION

Digital Transformation To Accelerate Product R&D To Market

Innovation is critical for sustainable long-term growth in any industry. Recent trends are prompting specialty chemical and related companies to reconsider their R&D laboratory operating models. Advances in technology and instrumentation and rapidly evolving consumer and market needs have disrupted the status quo,[1,2] and the age-old approach to product development may no longer be an option.

With the staggering amount of change happening in the industry, the rise of digital technologies can help companies apply data-driven decision-making — derived through ideation, data management, and analysis — that can accelerate the innovative breakthroughs they need to stay competitive.

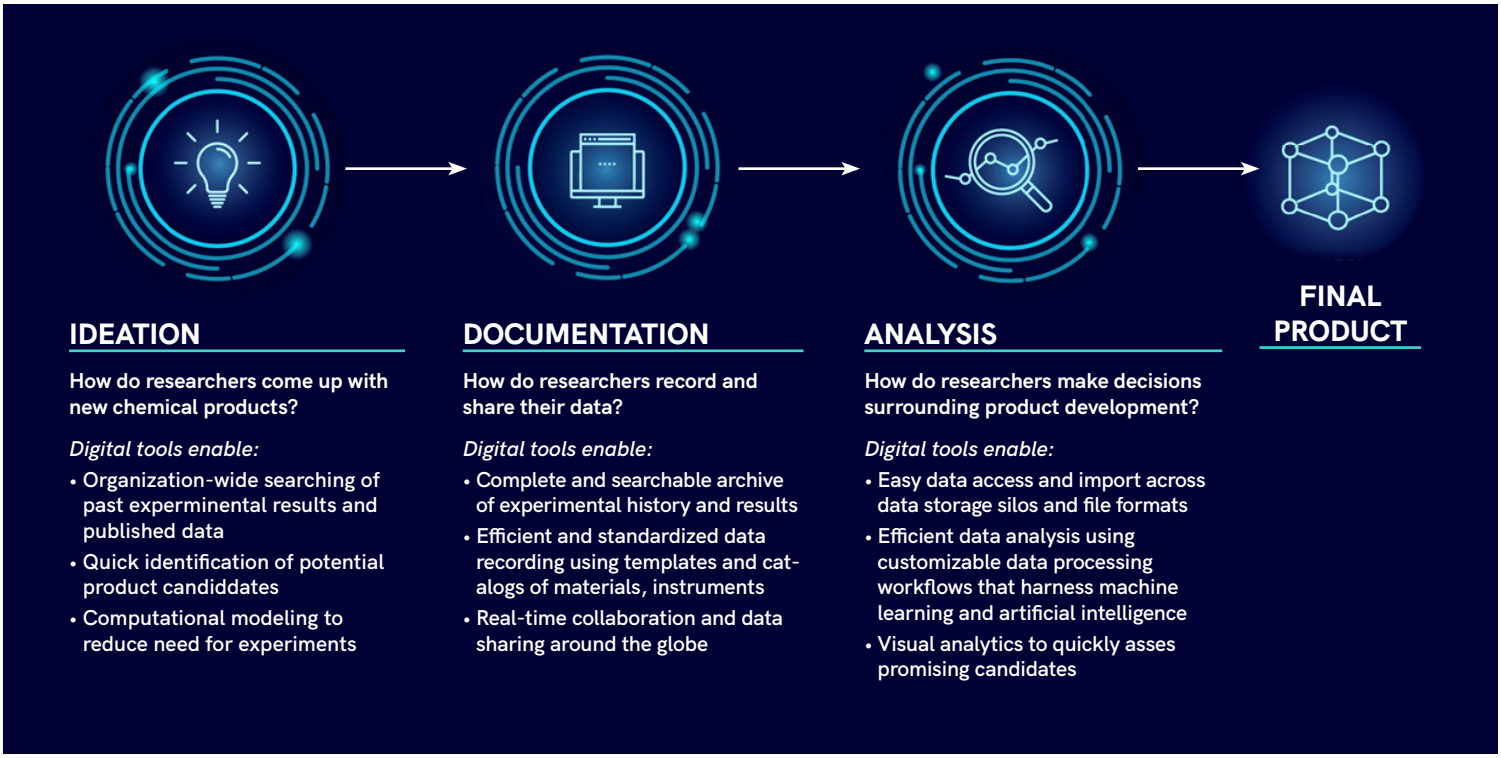
All chemical companies use some digital technologies, but most do so in a siloed and limited fashion, to address narrow or specific needs.[3] Leading chemical companies, however, are moving toward what is known as *digital transformation* — the adoption and integration of digital tools across an organization's entire operation. Such transformation equips organizations to meet the world's needs with better products now and in the future.

A pivotal aspect of digital transformation involves harnessing the latest cloud-based technologies in research and development (R&D). Without digital transformation, the process of developing new products is fragmented, with researchers working in isolation, wasting time searching for data, and often repeating experiments because past results are not readily accessible. They also face enormous challenges to analyze vast amounts of experimental data to make good decisions.

In contrast, with the latest digital tools, chemical companies can accelerate product innovation through three main phases of research: ideation, data management, and analysis, as described below and in Figure 1.

Ideation: Advanced technology and software enable industrial chemists to effectively harness existing data from internal and external research, and then to process that data to formulate hypotheses and experimental plans for developing new products.

Data management: As researchers conduct experiments, advanced digital tools provide access to all data and software tools in a single interface and allow them to use the data effectively with features like templating and tagging. They also collaborate easily with colleagues, across teams and organizations, in real time.



Analysis: Using customizable data-processing workflows that harness statistical analysis, data mining, machine learning, and artificial intelligence, chemists can make sense of multiparametric data and adopt mathematically rigorous approaches to product decisions, as well as to identify potential future areas of growth .

Digital transformation throughout the product development process reinforces a company's competitive edge by allowing it to efficiently develop new products. Enhanced data management and analysis, including data capture from consumers about product use and performance, can further improve the cycle, creating the lasting growth and innovation needed to meet changing market needs and consumer demands.[3]

This e-book explores how digital transformation across the product development process can lead to faster product development via better use of data, collaboration, and computation power. By addressing how advanced digital tools can specifically aid each step of product development—ideation, data management, and analysis—chemists can begin to understand the potential benefits of full digital transformation to their organizations and the industry.

CLICK TO SEE INTERACTIVE DEMO

SOURCES

1. Knut Alicke et al., "End-to-End Digital Transformations for Chemical Companies," McKinsey & Company, Aug. 25, 2020, https://www.mckinsey.com/industries/chemicals/our-insights/end-to-end-digital-transformations-for-chemical-companies.
2. Florian Budde et al., "The State of the Chemical Industry—It Is Getting More Complex," McKinsey & Company, Nov. 10, 2020, https://www.mckinsey.com/industries/chemicals/our-insights/the-state-of-the-chemical-industry-it-is-getting-more-complex.
3. 2023 Chemical Industry Outlook," Deloitte, n.d., https://www2.deloitte.com/us/en/pages/energy-and-resources/articles/chemical-industry-outlook.html

CHAPTER 1

ACCELERATING THE MOVE FROM BRAINSTORM TO BENCH

The universe of chemical products is vast and varied. In the United States alone, the chemical industry produces tens of thousands of products. Yet regardless of what's being made, whether it be a water-resistant paint or biodegradable plastic, every new or improved product starts with an idea.

During the ideation phase, researchers assess existing data to identify potential products with a particular end use. They also develop a testable hypothesis and design experiments to analyze specific metrics that help identify the best candidate. For greater market share and higher profits, this work must be done quickly.

The iterative process of deciding which parameters to test, how to test them, and in what order is the first half of what is referred to as *design of experiments* (DOE); the second half consists of carrying out the tests. The test conditions are often multiparametric and may involve permutations of pressure, temperature, time, or other metrics. These carefully selected readouts will give scientists an idea of how the set of potential products will perform under diverse conditions relevant to the end use.

DOE has historically been described as more of an art than a science. During DOE, experts use their knowledge of the product and available testing techniques to thoughtfully determine which set of metrics and variations to test and in what order.[1]

Yet chemical products, materials, formulations, and markets have become increasingly complex, and relying solely on human processing power is no longer an adequate approach.[2]

An Expanded Digital Tool Kit

The digital tool kit available to chemists has expanded along with the volume and diversity of chemical products. Today's chemist can leverage these advanced tools to accelerate the ideation phase of development. Access to centrally stored data, enabled by cloud storage, and software that integrates literature search capabilities help chemists understand what already exists in their chemical space.

> **"Companies could be much more productive in their research if they increase their digital technology resoures."**
>
> *-Tom Runge, process chemist and founder of Runge Consulting*

By having existing data at their fingertips, chemists can more efficiently formulate hypotheses and experimental plans. This lets them spend less time planning and more time focusing on experiments and identifying candidates.

Leverage Past Data for Better DOE

Tom Runge, a process chemist who founded Runge Consulting, says integrating the latest digital tools into experimental ideation and planning is key to accelerating research. He's found that when researchers are able to stay focused on conducting experiments, an organization increases the chances that its product will beat the competition to market.

Runge, who worked in the chemical and pharmaceutical industries before starting his consulting business, observed that researchers who don't use advanced digital tools spend more time sifting through data to conduct DOE for new products.

"You might as well try to glean as much wisdom from all of your experiments done beforehand than try to set up new ones," he says. "Companies could be much more productive in their research if they increase their digital technology resources."

But to glean wisdom from past experiments, scientists must be able to access and assess experimental history. An estimated 55% of data stored by organizations is dark data — data that is difficult to access and left unused.[3] It can be labor- and time-intensive if scientists have to manually curate the data to find relevant chemical information.[4]

Researchers may be required to search the literature with SciFindern or Google Scholar in one browser, access past experimental data from their digital notebooks on a local server, and email with collaborators to exchange data and ideas.

Adopting advanced digital tools means researchers need not spend time finding and piecing together existing data. Instead, the software does the work for them.

Smart software helps researchers find existing data and unify it, providing recommendations and visualizations before they even start doing an experiment. This can help accelerate speed to market, which is always one of the most important goals of product development.

Chemical Queries Made Easy

"Where is my data?"

That may be one of the first questions researchers ask themselves at the start of the ideation process. During past experiments, researchers may have recorded chemical structures or reactions using software such as ChemDraw® from Revvity Signals and then copied the structure into another application, such as Microsoft Word or PowerPoint, where the data is stored long term.

"Once inside a Microsoft Office document, the data is essentially dead and buried," says Pierre Morieux, Global Product Marketing Manager for Revvity Signals. "It requires a lot of effort or a really good memory for researchers to reuse it or do something meaningful with it."

Researchers would need to track down the file and page with the relevant information and then extract it for their new use. Chemistry-focused tools like ChemDraw, integrated into Signals Notebook, help accelerate the process of finding chemical data.

"ChemDraw can take those scattered chemical drawings and help transform them into an easily accessible database of chemical knowledge," Morieux says.

The program extracts chemical structures and related information from a document, perhaps a Word file or PowerPoint presentation, and brings them to the ChemOffice+ Cloud environment without having to find or open the original document. Chemical drawings can be selected, copied, and pasted into a new document or into ChemDraw for further editing (Figure 1).

Researchers can also create and manage custom lists of molecules based on user-defined properties. For example, those developing new synthetic dyes can add compounds with certain properties, such as pigmentation, to specific lists. They can then quickly review the collection of compounds when looking to design a dye with specific pigmentation properties. The chemical

record and lists can be maintained and updated in real time, so researchers have the most current database to work with.

"This allows researchers to recycle, reuse, and repurpose already-existing chemical data without having to guess which document it's stored in," Morieux says.

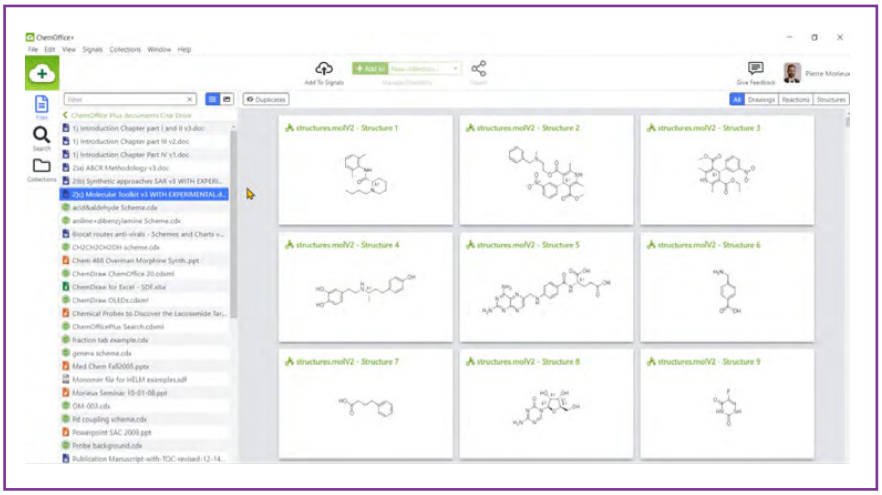


Figure 1. *Cloud-based ChemOffice+ Cloud offers a database of chemical knowledge in real time. On the left, discrete files including those from ChemDraw and Microsoft Office are uploaded to the ChemOffice+ Cloud suite. On the right, the extracted chemical drawings are shown. Users can select specific drawings and copy them for further editing or use, or they can create custom lists of selected chemical structures.*

Easy access to data can jump-start the ideation process. Once scientists understand what's been done, they can start identifying what existing chemicals, formulations, or materials have features that may meet the requirements for the new product.

Vivek Kalihari, Senior Market Development Manager at Grace, says efficient identification of a narrow list of possible product candidates is a key benefit of digital transformation.

"It's a long process to start with lab-scale experiments and analysis and then move up to success at a commercial scale, but if improved analytics help me analyze the 100 formulations I've tried before and quickly decide which five look promising for a new use, that's huge," Kalihari says. "Then when you start to do experiments or increase production to commercial scale, you're only dealing with five candidates instead of 100, which is a big savings in terms of time, money, and energy."

All the Data in One Place

An application programming interface (API), the software that allows sharing and integration of data, can be used to create a database of what is already known about a particular chemical product, formulation, or material. APIs can then be leveraged to create a single interface for the user to explore all that data. Think of the process of searching for flights online using a travel website. You enter your departure and destination locations and travel dates, and results from several airlines that meet your criteria are produced. This is a real-life example of an API—instead of the user going to each individual airline's website to type in the same information and compare across browser windows, the software does the work for you and returns the results in one screen.

With digital tools such as Signals Research Suite, a cloud-native collaboration platform for R&D from Revvity Signals, chemists can use the same process to find past experimental data as well as published data from the scientific literature (Figure 2). But in this case, the flights are chemical product candidates, and the filtering options are characteristics known from existing data.

Figure 2. Advanced digital tools allow all relevant data to be displayed on one screen. Researchers can use this single interface to search through published data as well as past in-house experimental data of their own and across their organization.

CASE STUDY:
Accelerating Target Identification with Advanced Digital Tools

Adoption of the latest digital tools can help transform the R&D process for a new chemical or chemical product. Consider the experience of a global agriscience company working to develop herbicides, insecticides, and fungicides for use in crop protection.

Crop protection discovery focuses on developing small organic molecules that modulate targeted biological processes, and the analysis tools used may rely on structure–activity relationships, physical property analysis, and binding properties.

Agricultural chemistry has the added complexity that most applications are outdoors, bringing additional requirements for formulation stability. Cost also needs to be considered carefully, as growers may not have big budgets.

With digital tools that aren't custom built for the chemist, like Microsoft Excel, researchers may be left to identify and assess candidate pools for new fungicides or other crop protectants one by one, which may limit how many options they can explore. Depending on the actual product and application, the number of potential compounds could well exceed the number a human could assess and process in a reasonable time.

The agriscience company identified additional challenges for crop chemists:

- Data was fragmented and difficult to query, making data review a time-intensive process during candidate identification.
- Throughout R&D, from compound selection to reporting, various discrete software and digital tools were used, making the process discontinuous.
- Charts that effectively visualized and communicated chemical data were needed to identify promising candidates.

To address these challenges, the company decided to incorporate the Signals Inventa data analytics solution, part of the Signals Research Suite, into its R&D pipeline. Cloud-based data access facilitated by Signals Data Factory, an add-on storage component, allowed for rapid data accessing and querying from both internal and external data storage locations. This enabled researchers to quickly access past experimental data, chemical structures, and reaction chemistry in one interface.

To better identify promising product candidates from past experimental data, researchers used Signals Inventa, which incorporates data analysis and visualization enabled by Spotfire®, a powerful scientific data analytics engine licensed exclusively by Revvity Signals. The R&D leader guiding the project described that platform as "easy test-driven data querying" with the ability to filter for specific tests, data, or projects; to search by chemical structures or activity criteria; and to analyze results in real time.

Chemical data visualizations helped researchers further narrow the selection of the test panel by identifying trends in past data. For example, they used the analysis technique known as R-group decomposition (Figure 3) to better understand structure–function relationships in the context of their chemistry. In this analysis, a central core structure—a scaffold—is used as the search query to identify all chemical molecules that contain that scaffold structure. The attached chemical arms that extend from the scaffold at distinct attachment sites, the R-groups, can then be identified, analyzed, and correlated to chemical and physical properties determined from previous experiments. In this way, chemists can break down a panel of chemical structures to understand which R-groups and attachment patterns may yield the desired traits for a new product.

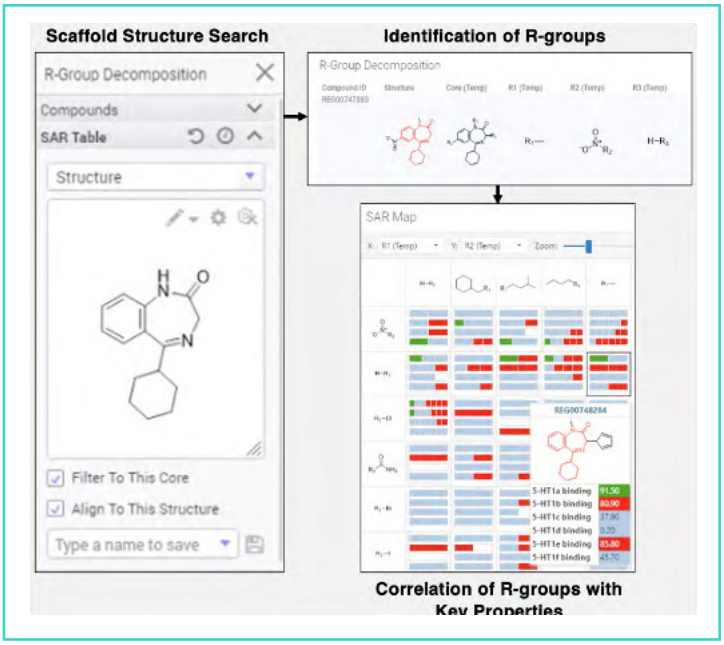


Figure 3. *Analytical approaches such as R-group decomposition can help researchers identify candidates for new chemical products. A chemical scaffold is used as the search query and all molecules with that core structure are returned. The R-groups and their attachment sites of each molecule are identified and can then be correlated with chemical and physical properties. Images sourced from 5.*

This can allow crop scientists to start with a vast panel of potential protection agents and narrow it down to a specific subtype—fungicides, say—and then further focus on the specific chemical features needed for the new application. In this way, researchers can use their past data to better understand what potential candidate molecules may be successful (Figure 4).

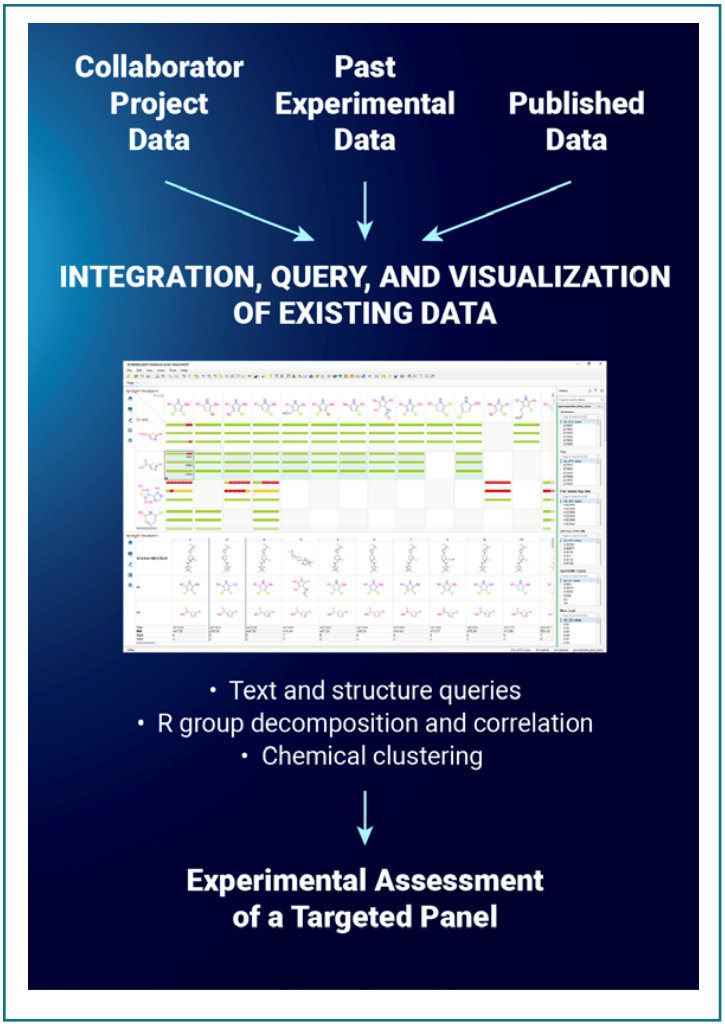


Figure 4. *Overview of how advanced digital tools can help accelerate product development. Integrating the entire data landscape into a single user-friendly interface allows chemists to quickly search through existing experimental data and chemical structures. Statistical analysis and data mining can be applied to better understand how specific chemical structure properties correlate with desired metrics, narrowing a pool of potential candidates to those most likely to succeed.*

Summary

By leveraging advanced technology and software, industrial chemists can accelerate the ideation phase of their product development. Solutions from Revvity Signals make it fast and easy to search what exists—in an individual scientist's past work, in colleagues' past work, and in the published literature. Data analysis and visualization tools then help the researchers to better identify the most promising product candidates from past experimental data, and then formulate hypotheses and experimental plans to further focus on the specific chemical features needed for the new application. In this way, researchers can spend less time planning and more time running and analyzing experiments. Real-time access to more data, to pursue better leads, helps R&D chemists bring more and better products to market, faster.

SOURCES

1. "Digital Transformation Journeys for Materials Science," Revvity Signals white paper, 2020, https://revvitysignals.com/sites/default/files/2023-12/rs-white-paper-unlocking-lab-efficiency-12.20.23.pdf
2. Florian Budde et al., "The State of the Chemical Industry—It Is Getting More Complex," McKinsey & Company website, Nov. 10, 2020, https://www.mckinsey.com/industries/chemicals/our-insights/the-state-of-the-chemical-industry-it-is-getting-more-complex.
3. Jennifer Sexton, Dark data in R&D: How knowledge management can uncover hidden value, CAS Insights, October 25, 2022. https://www.cas.org/resources/cas-insights/digital/dark-data-knowledge-management
4. Accenture, "Six building blocks for digital R&D in chemicals," June 24, 2021, https://www.accenture.com/us-en/insights/chemicals/digital-research-development-chemicals.
5. Revvity Signals Enterprise Scientific Research Solutions: Signals Research Suite," Revvity Signals, video posted to YouTube on Dec. 7, 2020, https://vimeo.com/886495906.
6. "Signals Lead Discovery—Wide Range of Multivariate Chemistry Data," Revvity Signals website, n.d., https://revvitysignals.com/products/research/signals-inventa

CHAPTER 2

ADVANCED, CLOUD-BASED DATA MANAGEMENT DRIVES PRODUCTIVITY AND COLLABORATION

Documentation of scientific thought, study, and experimental analysis is a cornerstone of research and is key to progress. With the most advanced, cloud-based digital tools, research becomes more efficient and more collaborative, facilitating product development and spurring innovation.

Increasing Workflow Speed and Efficiency

The latest generation of cloud-based electronic laboratory notebooks (ELN) can save researchers time and effort. One feature that increases efficiency is the ability to create custom templates for common experiments, streamlining the process and standardizing how data is captured. Templates can be shared among team members, increasing reproducibility and consistency.

Sharon Feng, Director of Science and Technology and Global Analytical Sciences at PPG Industries, can attest to how using templates helps scientists save time. PPG researchers often need to formulate new paints and coatings, each of which comprises many components.

"Formulations are like a recipe — you start with 10 or more different ingredients and combine them in a specific way," Feng says. "If you create a template for a typical coating formulation, you can reuse it instead of recording each ingredient and recipe every time."

Scientists can then make modifications to achieve specific goals, like changing color. "This enhances efficiency and speed and also standardizes the way scientists record and capture their data," Feng says.

Data Reprocessing Leads to Productivity

Research efficiency is also driven by effectively harnessing past data. Experimental redundancy can cost companies time, money, and other resources. Scientists need to be able to leverage existing data to improve future experiments or drive decisions.

"An ELN that lets you find the data and put it into context will help drive the science forward and have the biggest impact," says David Gosalvez, Executive Director of Science and Technology at Revvity Signals.

The latest, cloud-based ELNs connect experiments from different researchers across time and space to link all relevant data for a particular project — even if researchers were not previously aware of all the past experiments. These tools help scientists harness all the data.

"Without ready access to experimental data, we may run into a scenario where someone doesn't know that a project already exists in a different region or was already done in the past," says Feng. "If we don't have access to this information, we risk double work."

One way researchers can improve the ease and efficiency of searching past data is by embedding tags. This process associates searchable keywords with the tagged information in the ELN, such as a specific experiment or result. Researchers can develop an internal vocabulary of custom tags to help them search quickly and to select related data.

For example, researchers at a company that produces a variety of specialty chemicals can tag their data to associate it with a specific product. This could be as broad as tagging with "adhesives" to encompass all research within that area or as granular as "polyvinyl acetate" to identify experiments related to that one type of adhesive. Tagging can help researchers find relevant experiments during data analysis or ideation of future products.

Digital Integration Facilitiates Chemical Innovation

Cloud-based ELNs offer more than a digital store of experimental notes and data, however. The latest ELNs interface seamlessly with other programs, to increase workflow efficiency and allow greater focus on product innovation.

An example of this software integration is the way researchers can access the chemical structure drawing program ChemDraw® directly from Signals Notebook, both from Revvity Signals. This ability to handle chemical structures right in the ELN can provide valuable advantages to the chemical industry.

Recent updates to chemical drawing software can also reduce the time scientists spend drawing structures and recording their data. "Hot keys and keyboard shortcuts make chemical drawing more efficient," says Pierre Morieux, Global Product Marketing Manager. "Chemical drawing can be 5-10 times faster than with simple point-and-click tools."

Expanded capabilities to address complex chemical products like polymers can also improve how scientists visually record their data (Figure 1).

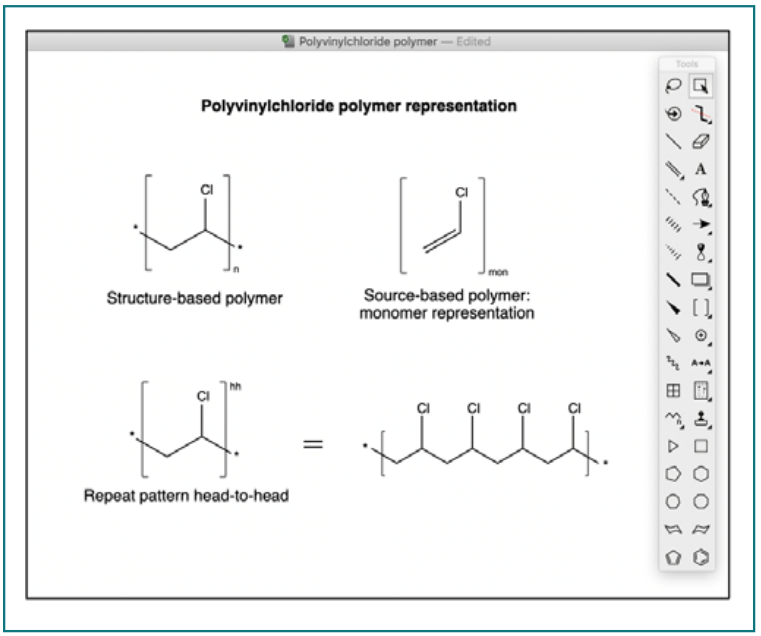


Figure 1. *ChemDraw enables researchers to draw and represent polymers, such as polyvinylchlorides used in plastics, directly in their Signals Notebook interface. Monomeric units can be defined, and polymer repeat numbers can be left general (as "n" number of repeats) or defined. The monomer linking pattern can also be defined. With Signals Notebook, ChemDraw structure drawing can take place within the notebook interface.*

In addition to drawing and recording chemical structures in their Signals Notebook interface, researchers can use structures instead of text as a search feature, which is a big advantage for chemical product development.

"There are plenty of programs that can easily search text information, but we as chemists also have to deal with the communication of chemical structures," says Tom Runge, a chemical industry consultant and the founder of Runge Consulting. "This has always been a major limitation of digital software, including ELNs, and it would be much more efficient to be able to search for a chemical structure."

With the latest ELNs, researchers can do just that. They can enter chemical fragments or whole structures as the search query to identify specific compounds, products, and data quickly

and without text cues. Specifically, ChemDraw, embedded as part of Signals Research Suite from Revvity Signals, can be used to find chemical structures, and then harness them for product development.

"Using ChemOffice+ Cloud to search through existing chemical data, researchers can select specific reactions and create a new experiment within Signals Notebook," Morieux says. "They can then input reaction conditions to populate the new experiment."

The recorded chemical information from the new experiment will likewise be searchable. Spending less time backtracking through a paper notebook to find a particular experiment means researchers can spend more time on activities like ideation and analysis, so that they can generate new concepts to develop more successful products.

Limitless Integration

Integration extends well beyond chemical drawing tools. Through an intuitive user interface or the advanced programming interface (API) technology used to embed ChemDraw, other applications, like Microsoft Excel or a company's LIMS, can be directly integrated in the ELN. There's no need to switch between applications — everything can be done with the same interface, saving scientists time and effort.

This interconnected working environment also ensures data integration. Instruments from around the laboratory can be interfaced with the ELN, so that experimental data is fed into the electronic notebook as work is carried out. Data from other programs or databases can also be incorporated easily. Having all the data in one place creates a single source of truth, making researchers' work easier and more efficient.

Different types of devices can also be connected. If permitted by internal corporate rules, users can access a cloud-based ELN from mobile devices like tablets and phones, for smooth connectivity throughout laboratory, research, and even remote settings. Mobile devices can also be set up with new features, for example, using voice-entry of experimental data to increase efficiency in laboratory environments where typing is difficult.

With cloud-based ELNs, the ease of software integration also provides a limitless ability to expand capabilities as technology advances. For example, the latest AI technology can be quickly rolled into a cloud-based ELN, giving users seamless access to powerful new tools—without any new installation or software upgrade required.

This digital integration provides scientists with a well-rounded, intuitive, efficient, and secure research environment. Having all the data, software, and tools in a single interface — a single ecosystem — allows researchers to make the best use of their time and energy, so they can focus on ideation and product development.

Collaborative Communication

Collaboration is another cornerstone of chemical research. Digital transformation with cloud-based ELNs can assist in putting collaboration at the forefront.

"Research and development isn't done by one person," Gosalvez says. "There are collaborations across the organization and around the globe, so sending data between people can help move the project forward in an interconnected way, driven by the electronic systems in place."

The latest cloud-based ELNs can become a communication and collaboration hub for research teams.

For instance, scientists developing a new catalyst to produce a polymeric plastic can record their data in the ELN and associate searchable keywords such as "catalyst research" or "polypropylene" with the data.

They can then tag other colleagues — much like tagging friends on a social media post. Colleagues will be alerted and can view the data or start a chat within the ELN interface to respond to a question in real time, getting feedback to researchers quickly (Figure 2).

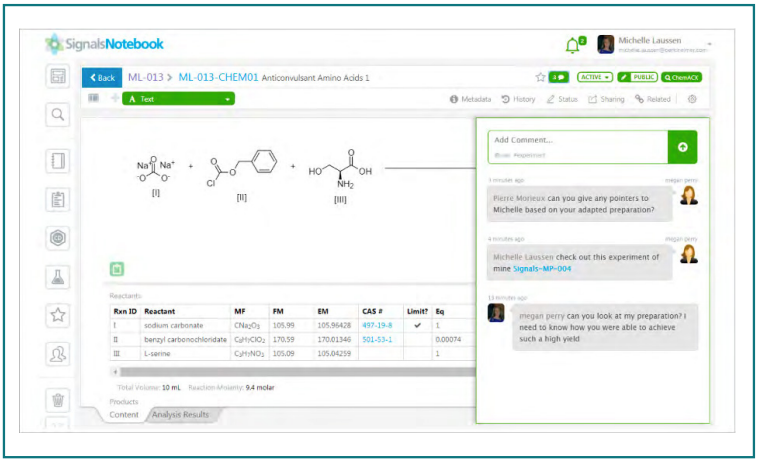


Figure 2. *A user in Signals Notebook draws a chemical reaction in the notebook using ChemDraw. Cloud-based communication lets the user add comments and tags to link relevant experiments or bring attention to a team member. Communication can happen within the ELN interface in real-time in a chat format, giving the user instant feedback.*[1]

Increased Data Security and Compliance

Of course, with broader collaboration, both inside an organization and with external collaborators, robust security and compliance measures are essential.

"As data becomes more available and accessible around the globe, we have to make sure our system of allowing broader access and collaboration is also in compliance with regulations related to data sharing between companies and countries," Feng says. "The challenge is achieving data sharing without risking noncompliance."

Advanced ELNs circumvent this hazard by allowing selective data sharing. As an example, Signals Notebook lets users control which data is included when sharing a notebook with other parties. Companies can filter access based on specific criteria, providing an added layer of security for sensitive data they may want to keep private because of regulatory or intellectual property concerns.

A cloud-based ELN also increases data security by taking advantage of the expertise of providers whose primary focus is safe data storage. Rather than relying on their own organization's overstretched IT team, companies using cloud-based ELNs can rely on specialized cloud security experts who follow every new development.

Cloud-based ELNs also increase data security through the ability to quickly upgrade software to protect against new threats, without waiting for a corporate IT rollout. Data are also always backed up, for business continuity and disaster recovery. With cloud-based connectivity, researchers also avoid using non-confidential methods, such as email, to share data.

The ease of software upgrades in cloud-based ELNs also ensures software consistency among all users, eliminating version incompatibility that can lead to data loss. If assistance is needed with the software, the ELN's service team can provide remote diagnostics and support, if the company wishes to grant this access.

Summary

Only with the newest digital tools can chemists truly harness the benefits of digital transformation to drive product development and innovation. With the most advanced, cloud-based ELNs like Signals Notebook, researchers access all their data and software tools in a single interface that can extend connectivity across devices. Chemists in R&D labs communicate easily across teams and organizations, sharing data and ideas securely and efficiently, and readily harnessing information from colleagues' past and current experiments. Features like templating and tagging save time and ensure maximum use of existing data. The advantages provided by these tools enable researchers to focus on the most important aspects of their work: product innovation.

Advantages of Advanced, Cloud-Based ELNs

Search functions	Search text across various file formats, plus additional filtering by content creator, data tag, or time stamp
Chemical structure search	Search using whole or partial chemical structures; no text or chemical names required
Specialized tools	Specialty software such as ChemDraw can be used directly within the ELN interface
Integration with other software	Other software can be used within the ELN interface; no need to switch between programs
Data migration from other systems	Data can be linked and integrated directly into the notebook interface
Internal and external data sharing	Global teams, including external partners, can reference and share experimental data in a timely, traceable, and secure fashion
Real-time collaboration	Real-time updates and chat options allow easy and fast communication among colleagues within the ELN interface
Full control over data sharing	Companies can control access according to specific criteria, to ensure protection of confidential data while promoting collaboration
Access from mobile devices	Can be set up to allow access from tablets and phones, for smooth connectivity between office and laboratory settings
Software Simplicity	There are no on-site installation or data storage requirements, reducing demands on information technology departments. Software updates are automatically rolled out as they're introduced, so all researchers have the most current software
Future-proofing	The simplicity of updating the software means that new tools, like the latest AI technology, can be rolled out quickly as they evolve.
Enhanced Security	Data is backed up and secured by professional data-storage experts. Quick software updates protect against new threats. Researchers avoid sharing data via unsecured means like email.
Cost	Cloud-based storage is a cost-effective way to store and maintain data long term compared with using local storage.

SOURCES

1. "Signals Research Suite," Revvity Signals website, n.d., https://revvitysignals.com/products/research/signals-research-suite

CHAPTER 3

LEVERAGING THE LATEST TECHNOLOGY FOR MORE EFFICIENT DECISION-MAKING

The chemical development process progresses over familiar ground—a hypothesis will be developed, experiments designed, and potential candidates will be rigorously tested. After the results are carefully documented, scientists are left with datasets. The data needs to be digested and analyzed to extract meaning and guide decision-making.

The data that comes out of an instrument during experimentation "isn't the scientific result," says David Gosalvez, Executive Director of Science and Technology at Revvity Signals. "You don't inherently know how to proceed with the experiment, project, or product until you process the data."

Only a few of the tested product permutations will advance to further testing or introduction to the market. Researchers need to correlate the raw experimental data with desirable product traits to choose which chemical, material, or formulation to move forward with.

Selecting the best candidate for a given application involves processing and understanding the data across a large number of parameters. Which of the tested catalysts produced a plastic polymer with the desired flexibility and tensile strength? Which of the synthetic dyes produced the proper pigment while maintaining water solubility? The experimental phase of product development will yield data and observations about the applicable properties for each variation of the novel products.

"Digital tools can help give the human brain that additional help to think about what the data really means."

— Sharon Feng, Director of Science and Technology and Global Analytical Sciences at PPG Industries

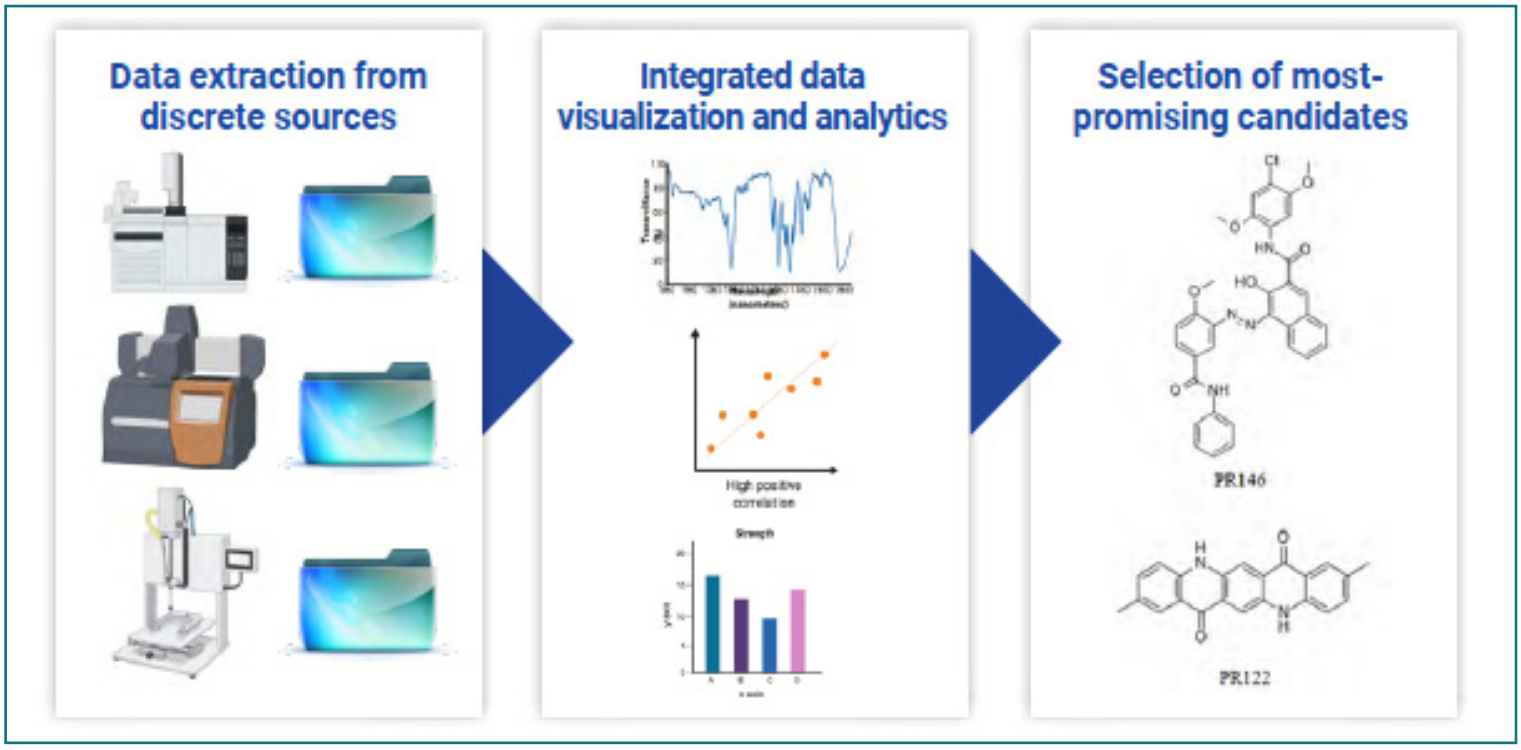


Figure 1. *Advanced digital tools can transform the decision-making process by making data analysis easier and more efficient. Raw or processed data can be imported from various file formats or instrument types. The data are then processed in a user-defined manner. Visual representation of data within a single integrated interface allows researchers to identify which chemical product candidates to move forward with.*

The Cost of Selecting the Wrong Product

Selecting the most desirable product gives chemical companies a competitive edge in the marketplace.[1] Advanced data analysis as part of the decision-making process can therefore have a significant impact.

Deciding which product to bring to market has become more complex. One reason for this is shifting customer and market demands.[2] Another is the technological advances in instrumentation that have led to an explosion in the amount of data and observable properties that can be recorded in a single experiment.[1,2] Relying on the ability of experienced professionals to mentally juggle all the factors is no longer a viable approach.

"Digital tools can help give the human brain that additional help to think about what the data really means," says Sharon Feng, Director of Science and Technology and Global Analytical Sciences at PPG Industries. "What are these 40,000 data points really telling me? Understanding that question can inform decision-making and speed up project timelines."

Failure to properly summarize all the available data — possibly because there are too many factors for the human brain to fully consider at once — could lead to choosing a second-rate product that is not the most competitive in the market. That has a real cost.

To this end, digital transformation can help specialty chemical companies adopt data-driven and mathematically rigorous approaches to product decisions, enabling them to select the most competitive product.

Efficient Data Analysis Workflows

The first step in analyzing data is getting access. With the latest cloud-based tools, researchers can access company-wide data stores in seconds. Much as they do in the ideation process, researchers can "shop" for the data they want using key search terms or chemical structures. Data tagging, as enabled by the latest digital tools, also helps make this phase more efficient. This allows researchers to quickly narrow down the entirety of experimental results to the targeted subset needed for the product analysis and decision-making.

Once the necessary data is found, it needs to be analyzed. The selected files can be imported into a data analysis system that uses mathematical modeling and statistics, such as Signals Inventa data analytics solution, and then undergo processing. Signals Inventa is powered by the scientific data analytics engine Spotfire®, licensed exclusively by Revvity Signals[3].

Using customizable data-processing workflows, chemists can begin to make sense of their multiparametric data. Say a team of chemists is trying to design a formulation for a new polymer-based surface coating for the aerospace industry. Researchers will identify key metrics that the formulation needs to meet, such as being sufficiently hard, resistant to scratching or deformation, and sufficiently dense, which can help determine drying times and coverage area.

The researchers could upload their experimental results from tests on multiple permutations of formulations into Spotfire®. Key metrics can be selected to illustrate how each formulation performed. In this case, scatter plots of hardness and density metrics can be simultaneously visualized and correlated (Figure 2).[4] Outliers in the data set can be quickly identified and filtered out or kept in the analysis.

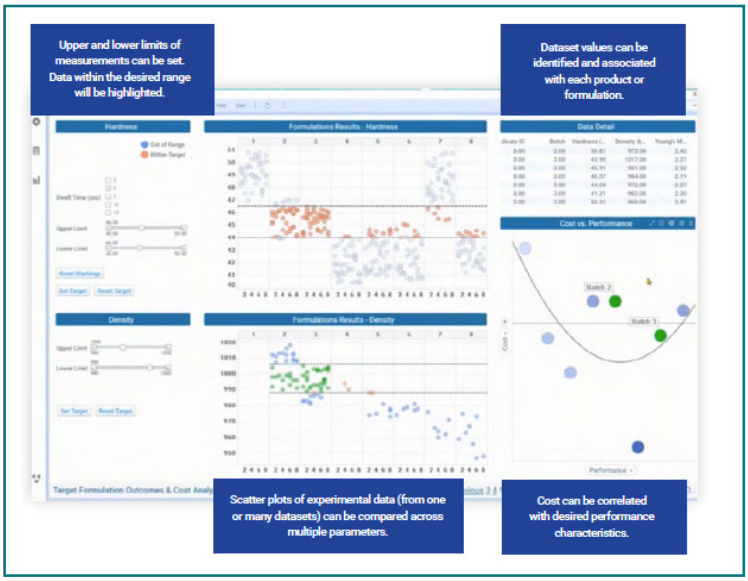


Figure 2. *Analysis in Spotfire® incorporates visual analytics to allow researchers to identify viable product options. Data measurement thresholds can be set to identify optimal products, which can then be coupled to cost analysis.[4]*

The settings can then be adjusted to focus in on target performance characteristics. For example, by setting upper and lower boundaries for acceptable hardness and density measurements, researchers can quickly identify formulations with values that fall in the acceptable range (illustrated in orange in Figure 2). They can then select the most promising formulations and conduct a cost analysis. By understanding the commercial factors that influence product viability, they can determine which product is most feasible. They can also understand how products will behave during the manufacturing process, which is another important factor to consider when selecting a product to take to market.

If the data analysis software is also cloud-based, like Signals Research Suite, a collaboration platform for R&D from Revvity Signals, the analysis can be shared in real time. A team member may view the analysis window and decide to make changes to the desired thresholds of the measured parameters. Instead of having to wait for the analysis data file, the scientist can change the parameters and immediately review the new results when given access.

Without the latest digital tools, researchers may have to sequentially analyze the hardness and density parameters in spreadsheets. Cost analysis would also have to be done separately and team members or supervisors would have to provide feedback via email or a meeting, extending the time it takes to analyze the data and delaying decision-making.

Data processing done with individual software, which is siloed, might have costs in terms of consistency, reproducibility, and sharing of results and processes, according to Gosalvez. “Having sharable and flexible tools that take the raw data and generate useful results can help improve interpretation and will be critical for product development,” he says.

Leveraging Technology to Spur Innovation

In addition to meeting customer specifications or improving chemical products, advanced digital tools can help scientists advance their research through product innovation. Statistical analysis, data mining, machine learning, and artificial intelligence can be leveraged in advanced software to help chemical researchers identify potential areas of growth.[1]

The human-driven product decision process has historically operated within the confines of the knowledge of the researcher analyzing the data. Yet even the most advanced and experienced researcher has blind spots that will bias the process. Optimization of product ideation using advanced statistics and algorithms reduces this human bias and allows for quicker analysis and innovation.

PPG's Feng says this innovation will be key to expanding industries and addressing new needs. "Needs that are currently unmet in the market aren't normally addressed by the conventional approaches used to develop new solutions or products," she says. "You have to go outside of that space to meet these needs, and you can come up with some really interesting inventions by doing so."

"Statistical analysis, data mining, machine learning, and artificial intelligence can be leveraged to discover new and disruptive solutions."

In her experience with water-based coatings, Feng says, most changes in product advancement are incremental. Many revolutionary advances or inventions come about by accident and aren't always logical, but scientists can't rely on happy accidents to move their research forward. Instead, software that lets researchers quickly analyze and visualize data can help them identify product candidates that may have unique properties.

For example, chemists can graph their data on a scatter plot of two parameters of interest using tools such as Spotfire®. They can then quickly identify outlier data points that are distinct from most of their data set. Traditionally, researchers

Multiparameter Optimization

Balancing the considerations of potential new products can be aided by advanced digital tools. Spotfire® can produce multiparameter optimization radar charts (right side of figure) to collectively analyze various candidates. This type of analysis optimizes multiple input parameters to provide an overview of the success of a chemical compound in relation to the desired properties.

The different plot axes represent different parameters or measurements, and algorithms can be used to analyze the data collectively to reveal correlations and trade-offs, helping researchers concentrate on the most promising new product and accelerate the decision-making process.

Spotfire® can be used to collectively analyze data through the use of visuals including multiparametric optimization radar charts.[5]

may have ignored or discarded outlier products or materials. But as changes in chemical markets demand creative solutions, these outliers may provide opportunities for innovation (Figure 3).

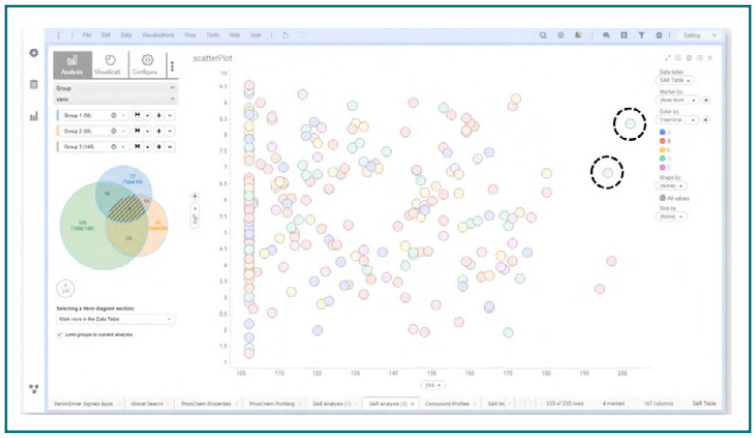


Figure 3. *Identification of outliers may help spur product innovation. By globally analyzing related products using known metrics, researchers can quickly identify outliers that may create new or unexpected solutions.*

"These tools will help us discover some of those really new and disruptive solutions that will add a lot of value," Feng says. "Having better digital tools will open more possibility for innovation during our product development process, including in space along the value chain."

Artificial intelligence and machine learning are also ushering in a new age of innovation in the chemical sciences. The iterative design-and-test process for chemicals and chemical products takes time, money, and other resources. Accurately predicting the properties of hypothetical molecules can allow scientists to focus on only the most promising candidates.

AI and machine learning use algorithms to predict chemical properties such as solubility and melting points based on existing experimental data. Each algorithm is trained using existing molecules and their known properties, thereby improving predictive power as more data are collected. Digital tools incorporating AI and machine learning, such as Signals Inventa, can help researchers accelerate research and development by predicting successful chemical candidates from the start.

The Digital Future

The chemical industry is poised to embrace digital transformation. By incorporating digital tools throughout the product development cycle, companies can make research and development more efficient and spur innovation. Ujwal Chejerla, Director of PPG's Artificial Intelligence and Machine Learning Center of Excellence, says he can envision how digital transformation will revolutionize the research and development process.

"Data and results are available faster and are more readily accessible," Chejerla says. "With digital tools, we can leverage this data to identify what we have, refine and test our formulations, and decide which product to move forward, helping protect our stakeholders and improving the products we produce."

As market demands continue to shift, chemical companies need to remain nimble to develop products that meet these needs.[2] Digital technology has become more advanced and cloud-based data storage has become more affordable. The question is no longer whether a chemical company can afford to start the digital transformation journey; it's now, can they afford not to?

For more information visit: revvitysignals.com

SOURCES

1. Knut Alicke et al., "End-to-End Digital Transformations for Chemical Companies," McKinsey & Company, Aug. 25, 2020, https://www.mckinsey.com/industries/chemicals/our-insights/end-to-end-digital-transformations-for-chemical-companies

2. Florian Budde et al., "The State of the Chemical Industry—It Is Getting More Complex," McKinsey & Company, Nov. 10, 2020, https://www.mckinsey.com/industries/chemicals/our-insights/the-state-of-the-chemical-industry-it-is-getting-more-complex

3. Spotfire: Transform Your Data into Actionable Insights," Revvity Signals website, n.d., https://revvitysignals.com/products/exclusive-reseller/tibco-spotfire

4. "Improved Decision Making in Material Science Innovation," Revvity Signals, https://revvitysignals.com/sites/default/files/2023-12/rs-brief-scientific-decision-support-for-advanced-materials%20-research-12042023v2.pdf

5. "Enterprise Scientific Research Solutions: Signals Research Suite," Revvity Signals, video posted to YouTube on Dec. 7, 2020, https://vimeo.com/886495906

Revvity Signals Software, Inc
940 Winter Street | Waltham, MA 02451 USA
P: (800) 762-4000 or (+1) 203-925-4602
revvitysignals.com/company/contact

Copyright ©, Revvity, Inc. All rights reserved. Revvity™ is a registered trademark of Revvity, Inc. All other trademarks are the property of their respective owners.