

Accelerating Formulation Innovation with Connected R&D Intelligence

WHITE PAPER

Published: August 20, 2026



Unleash that big, beautiful science.

Introduction

Formulation science is crucial for ensuring the performance, stability, and quality of products across industries from specialty chemicals, coatings, and additives to cosmetics, food, pharmaceuticals, and other innovation-driven sectors. Each of these sectors has unique product performance requirements, regulatory standards, and ingredient characteristics, making formulation science both diverse and highly specialized.

Many research and development (R&D) teams still rely on legacy tools like spreadsheets for formulation project planning and data tracking. Those tools aren't designed to handle the complex, multivariable challenges of modern formulation work. Some R&D workflow focused software, such as electronic laboratory notebooks (ELNs) and laboratory information management systems (LIMS), offer advanced features, higher efficiency, and greater scientific robustness for tackling the unique challenges faced by formulators in optimizing specialty chemicals, cosmetics, food products, and pharmaceuticals. However, these systems are often built primarily for data capture and compliance rather than formulation-centric data analytics, and many remain complex or unintuitive for scientists to use directly within their daily formulation workflows.



Specialized software offers advanced features, higher efficiency, and greater scientific robustness for tackling the unique challenges in formulation science.

Understanding the Evolving Role of R&D Software in Formulation Science

Formulation scientists design and adjust the balance of ingredients to create functional, stable, and cost-effective products. They work in a wide variety of industries, each with unique performance requirements and regulatory standards.

- In specialty chemicals, formulators focus on developing customized chemical blends with specific functionalities, such as corrosion resistance or conductivity, for commercial applications.
- Personal care sectors (cosmetics, beauty, and fragrance) balance esthetics, skin compatibility, and shelf life.
- Food technologists face challenges related to taste, texture, and preservation.
- In pharmaceuticals, formulators determine the optimal dosage form and combine active pharmaceutical ingredients (APIs) with excipients to ensure stability and bioavailability.

The products are distinct, but they all need to meet precise performance criteria under challenging environmental or operational conditions, requiring deep knowledge of materials science and process engineering. Despite the differences between sectors, all formulation scientists share similar todo lists, such as selecting ingredients, proportioning, processing, testing, optimizing, and eventually manufacturing formulas.

Limitations of Traditional Tools for Formulation Development

Formulation science has grown more sophisticated in recent years with advances in nanotechnology, controlled-release systems, 3D printing, and smart materials. However, the digital tools still used by many formulators do not have the capabilities to meet new, more nuanced requirements.

General-purpose design: Tools like Microsoft Excel and Google Sheets offer flexibility for general data organization, but they don't have the domain-specific functionalities that formulators need.

Basic data management: Spreadsheets can struggle with high-dimensional data, especially with the high number of variables, constraints, and interactions that today's formulations include. They are not scalable or meant for handling the large, complex datasets that formulation science requires.

Static and open to human error: Legacy systems, especially on-premises software, can lead to version control issues and data integrity concerns. They don't have the transparency, collaboration, and traceability of cloud-based solutions. Plus, when chemists set up formulas manually in spreadsheets, they can make mistakes that compromise the experimental results and decisionmaking.

Addressing the Challenges of Formulation Science with Specialized Software

Modern R&D data software offers powerful capabilities, in a user-friendly format, to meet the high demands that formulators face today when optimizing products like specialty chemicals, cosmetics, and foods. These solutions address the inefficiencies and limitations of traditional tools by unifying experimental design, inventory integration, collaboration, and analytical power in a single environment. They provide capabilities that go far beyond what spreadsheets can achieve without custom programming or add-ins, which are often cumbersome and error prone.

Enhanced Capabilities and Built-In Calculations Tailored for Formulation Science

Spreadsheets are still commonly used in formulation workflows. Many scientists like these tools, because they are familiar and offer flexibility to run formulation math, adjust inputs, and calculate ratios or percentages. Statistical analysis software, such as Design-Expert, JMP, or Formulator Software, provide more advanced features for formulation development, such as regression modeling, solubility predictions, ingredient compatibility checks, and property optimization. However, these tools are often optimized for expert statisticians rather than R&D scientists, with steep learning curves and limited support for intuitive, day-to-day formulation workflows.



A more advanced data management software combines flexibility, ease of use, and powerful functionality with a unified data infrastructure and a user-friendly interface designed for scientists. For example, Signals One™ from Revvity Signals enables formulation cloning, embedded formulas, dynamic tables, and error-checking. This cloud-native R&D data management software features native ChemDraw integration, so every step of formulation lives in a single streamlined workflow. With ChemDraw embedded directly in the platform, formulators can draw, edit, and reference chemical structures inline without exporting files, switching between applications, or losing the link between a structure and its associated experimental data. This keeps molecular detail tied to the rest of the record as scientists collaborate and capture chemical composition, ingredients, inventory, testing, and equipment data in one unified environment. In addition, such a formulation system does more than handle formulation experiments and data. Signals One allows formulation scientists to structure data so it can be organized, manipulated, and interpreted, with customizable table templates, variant tables, and hierarchy tables that help standardize data entry. Structured data also enables the use of machine learning and artificial intelligence applications.

Design of Experiments (DoE) for Statistical Rigor

Effective formulation software helps scientists implement and improve traditional design of experiments (DoE) a systematic approach to planning, conducting, and analyzing controlled tests that evaluate the relationships between multiple formulation variables and their outcomes. This approach helps formulation scientists optimize ingredient combinations, understand key performance drivers, and reduce the number of experiments needed. It is especially valuable in complex product development, where interactions between ingredients or process parameters can affect stability, efficacy, or cost. When DoE capabilities are included, scientists can define variables, specify design targets, build experiment matrices, and automatically populate test conditions across multiple formulations.

Modern R&D data management platforms also provide the foundation for statistical analysis and predictive modeling tools that help scientists draw meaningful conclusions from DoE results.

Formulation teams can use the system's built-in analytics, visual dashboards, and collaboration features to help them optimize trial-to-success cycle and make data-informed decisions.

An advanced R&D data management system can efficiently handle complex, multivariable formulation designs so users can visualize response surfaces, optimize multiple criteria simultaneously, identify robust formulations, and perform factorial design or inverse design with statistical rigor. This capability is particularly important in highly competitive industries such as specialty chemicals because it helps accelerate product development cycles and reduce costs by minimizing the time scientists spend on trial-and-error experimentation.

Robust Data Infrastructure and Seamless Integration

The foundation of high-quality formulation software is a strong data infrastructure. A modern R&D data management software solution structures data in a way that's machine-readable, query-able, and future-proof, to support long-term value extraction from R&D activities. This includes establishing links between experiments, materials, test results, and project timelines that enable better traceability, auditability, and integration with broader enterprise systems such as Laboratory Information Management System (LIMS), Enterprise Resource Planning (ERP), or Product Lifecycle Management (PLM) software.

Improved Management of Ingredients and Materials

Modern formulation platforms provide centralized databases, automatic versioning, and secure access controls, significantly reducing the risk of errors and improving collaboration across teams. The integration of an inventory and material management system enables formulation scientists to know which raw materials are available, while providing information about their properties, expiration dates, storage locations, and regulatory status. With a built-in inventory management system, users can automatically track material usage while performing experiments and avoid using missing or expired materials. This not only makes it easier for scientists to do their work, but it also improves traceability, forecasting, and resource management.



Standardized Data Entry for Error Prevention and Data Integrity

Signals One brings together experiment documentation and formulation management in a single, unified environment where scientists can also capture critical data such as ingredient identities, concentrations, process parameters, and performance attributes such as pH, stability, and viscosity.

Standardized data entry ensures consistency and reproducibility, making it easier for scientists to compare experiments, identify trends, and reuse successful formulations.



Signal One has built-in validation and guided workflows that help reduce mistakes. It often includes audit trails and documentation templates, helping scientists prepare for inspections and regulatory submissions.

Time and Cost Savings

R&D data management software automates many repetitive data processing and analysis tasks that would take hours in Excel, ultimately freeing scientists to focus on innovation rather than data wrangling. Over the course of a formulation project, the time saved through improved workflow integration and decision-making accuracy translates to faster time-to-market and lower development costs.



Analytical Validation, Tracking and Trending

Formulation success depends on experimental validation, and Signals One allows users to input raw measurements, link them to specific formulations or process conditions, and track performance over time. It can also provide visualizations, identify trends, and assist with statistical analysis to help scientists make quick decisions.

Capturing the Full Scientific Picture with Context and Structured Data

Rich text and embedded media, alongside structured inputs and metadata, ensure context to make sure the story behind the data is not lost. This qualitative information supports knowledge transfer, training, and deeper interpretation of experimental outcomes. The system can capture information from a wide range of file types:

- Text - Microsoft Word documents, Google Docs, plain text files
- Images - PDFs, JPGs
- Spreadsheets - Microsoft Excel, Google Sheets, CSV files
- Instrument outputs - EZreader (rst), and Flow Cytometry (fcs) files

Comprehensive data capture, from all input formats, allows scientists to include all the relevant information in one place, keeping valuable experimental knowledge accessible and interpretable, even as projects and teams evolve over time.

Smart Search, Filter, and Sorting Capabilities

In an R&D setting, scientists often need to sift through large volumes of experiments, formulations, and material records. Signals One includes advanced search, filtering, and sorting functionalities. Formulators can search by ingredient name, property value, test result, date, or keyword in notes to find exactly what they need in seconds. Tagging, metadata indexing, and customizable views transform historical data into a usable resource, enabling machine learning algorithms to identify trends and accelerate product development.



Modern Design for an Intuitive User Experience

Scientific users need tools that are easy to use so they can focus on exploring the intricacies of formulas. A modern ELN includes intuitive functions like copy-paste, undo-redo, drag-and-drop, and keyboard shortcuts, allowing scientists to quickly duplicate experiments, reuse previous formulations, and navigate through large datasets without getting bogged down by cumbersome software.

Collaboration and Knowledge Retention

Cloud-based R&D data management allows large and dispersed teams of scientists to work on the same platform, share data and templates, leave comments, and track changes in real time, anytime, from any location. A unified environment enhances transparency, fosters innovation, and ensures that institutional knowledge is preserved and accessible even through staff turnover and as teams evolve to become distributed across the globe.

This collaborative capability also plays a crucial role in attracting and retaining talented employees. Today's formulation scientists expect to use sophisticated software to complete their work, and R&D organizations that invest in high-quality digital tools will be able to recruit top talent.

Conclusion

Catalyze Innovation with Modern Formulation Software

While spreadsheets are useful and familiar tools, they don't sufficiently address the technical, statistical, and collaborative demands of formulation science. Modern R&D data management software provides a superior alternative for formulation development by enabling deeper insights, better data management, reduced risk, and faster innovation.

Signals One is far more than a digital replacement for paper notebooks or spreadsheets. It is a connected, intelligent system that supports every stage of product development from raw material selection to final analysis. By combining structured data capture, flexible calculations, inventory integration, test result management, intuitive user experience, narrative context, and intelligent data retrieval, advanced formulation software helps scientists innovate faster, reduce errors, improve reproducibility, and quickly create formulations that meet their industry's unmet needs.

Upgrade your formulation tools now to gain a competitive edge.
[Explore Signals One](#) to discover how to boost your R&D work today.





77 4th Avenue
Waltham, MA 02451 USA
(800) 762-4000
(+1) 203-925-4602
revvitysignals.com



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