



# 5 Benefits of Signals Notebook



## Introduction

Recent trends in the pharmaceutical and biotechnology industries have influenced the evolution of electronic lab notebooks (ELN). Trends including IT budget allocations and an acceleration of outsourcing efforts have resulted in data collaboration beyond institutional boundaries. In addition, the efficient collection and security of ever growing volumes of data is more essential than ever given the realization that “Big Data” significantly improves the speed and outcomes of clinical development.

The implementation of an ELN has a transformative effect on the way research is conducted. Beyond ensuring that the needs of scientists are met with capabilities specialized for their discipline, the business needs to examine factors such as streamlining implementation and system costs. R&D organizations that adopt a cloud ELN can take advantage of immediate and long-term benefits. Cloud-native ELNs delivered as SaaS (software as a service) platforms enable scientists of all disciplines to easily document and find their work, collaborate within and across organizations, as well as enable IT to take advantage of more efficient, cost effective storage and performance with automatic updates and connectivity to other informatics platforms. In addition to the five core benefits cited below, cloud ELNs can be deployed quickly (environments can literally be set up in minutes), and have high adoption rates and a lower learning curve because of their browserbased, modern user experiences. This whitepaper will cover a blueprint to identify and expand on these benefits that impact both R&D organizations and individual users the most.

## Benefit 1 - Improved Collaboration

Scientific collaboration is more strikingly prevalent today than decades ago.<sup>1</sup> The trend in many areas of research is toward catalyzing collaborative efforts that bring together researchers with diverse scientific backgrounds. These alternate perspectives help address perplexing questions and solve complex problems that benefit from an interdisciplinary or multidisciplinary approach.<sup>2</sup>

Collaboration is central in your organization and can occur internally as well as with external commercial partners or academical institutes. The most important aspect of any collaboration is the value recognized upon the sharing of data, the fuel that powers your research. A siloed, disconnected informatics environment creates challenges in project management, reporting, and scientific data exchange that must be addressed if the team is to collaborate effectively and achieve business goals.

In absence of an ELN as a central data repository, research data and interpretations are shared in a non-confidential way often via email. Using an ELN to facilitate the sharing of data is more efficient and secure, as a consortium of collaborators can define who has access to which data while the data continues to be stored in a secure environment. Collaboration internal to an R&D organization may be as simple as being able to link experiments or allowing multiple people to contribute to or comment on the same work. Collaboration can also be more comprehensive. For example, you may require an ELN to facilitate how projects are spun up and down, how external partners access project related reports and documents, and how they communicate and share experimental data.

The screenshot displays the Signals Notebook interface. On the left, a 'Comments' sidebar shows a conversation between Ben Bracke, Linda Kewitsch, and Paul Kuhn. The main area shows a chemical reaction scheme with reagents [III] and [IV], and products [V] and [VI]. Below the reaction is a table of reactants with columns for Run ID, Reactant, MF, FM, MW, EM, Limit, Eq, Sample Mass, Moles, Molarity, Vol, d, % Wt, and Link To Reg.

Run ID	Reactant	MF	FM	MW	EM	Limit?	Eq	Sample Mass	Moles	Molarity	Vol	d	% Wt	Link To Reg
I	methyl (E)-3-cyclopropyl-2-methyl-3-(tosyloxy)acrylate	C <sub>15</sub> H <sub>19</sub> O <sub>5</sub> S	310.36	310.36	310.08749	✓	1	1.00 g	3.22 mmol					CL
II	(3-(benzyloxy)phenyl)boronic acid	C <sub>13</sub> H <sub>13</sub> BO <sub>2</sub>	228.05	228.05	228.09577		1.1	808 mg	3.54 mmol					CL
III	potassium phosphate	K <sub>3</sub> O <sub>4</sub> P	212.26	212.26	211.84454		3.00	2.05 g	9.67 mmol	1 molar	9.67 mL			CL
IV	precatalyst	C <sub>19</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub> P <sub>2</sub> PS	768.16	768.16	767.10042		0.1	248 mg	322 μmol					CL

Figure 1: Intuitive collaboration in Signals Notebook: add comments, tag colleagues and use hashtags to link to relevant experiments.

It is imperative to define how to manage different types of data and data formats such as chemical structure and quality data, calculated and measured physicochemical properties, biological assay data and pre-clinical data describing the characteristics of active pharmaceutical ingredients across the partner landscape. In addition, there is the consideration of how to distribute and archive the data among partners when a project ends. Lastly, and arguably most important, how the IP is managed throughout the duration of the collaboration must be considered from the start. The immense challenge of data management and technology exchange becomes most apparent when one considers that a typical external collaboration can generate tens of thousands of data points throughout its duration.

With these challenges in mind, R&D organizations with many partnerships are turning to cloud-native collaboration workspaces that are accessible from anywhere with an internet connection and provide a level of business agility and security that is not available with server-based, on-premise ELNs.

## Benefit 2 - Connectivity

ELNs are the heart of scientific data documentation, processing, and compliance. At their simplest, they facilitate the capture of data and documentation of experiments. At their best, they assist the scientist and the business at every step of data generation and analysis along the R&D value chain and facilitate collaboration with external partners. ELNs that are easily accessible and designed to be the central integration point in the

informatics electronic lab environment will provide the most value.

As previously mentioned, research is ever more distributed, and scientists need to be able to access their information from many different locations at any time of day and potentially from different machines. Access to a cloud ELN is only limited by internet connection. As there is no application installed on the machine itself, scientists can review and enter data from any internet connected device. Cloud ELNs effectively allow scientists to work from anywhere and the heightened connectivity will improve efficiency and productivity.

In addition to better connectivity to the ELN platform itself, there is also the benefit of improved connectivity to other informatics systems. Scientists, regardless of their discipline, use many applications and tools essential to executing their daily work, and often the data generated from these other tools need to be incorporated into their experiments. Not only is the enterprise software landscape of internal systems strikingly different from one organization to the next, but there are also external systems to consider. Internal systems that the ELN may be required to integrate with can include, but is not limited to, chemical and biological registration and inventory applications, and laboratory information management systems (LIMS). In addition, valuable external databases exist with information on available chemicals, reaction planning, safety data, and sequence information etc. There is also the possible need to connect to digitized equipment including balances, pH meters, bioreactors or analytical instruments.

The screenshot displays the Signals Notebook interface. The main window shows a chemical reaction scheme with reactants [I], [II], and [III] reacting to form product [IV]. Below the reaction scheme, there are two tables: 'Reactants' and 'Products'.

Rxn ID	Reactant	MF	MW	EM	Limit?	Eq	Sample Mass	Moles	Molarity	Vol	d	% Wt
I	phenylmethanamine	C <sub>7</sub> H <sub>9</sub> N	107.16	107.07350		1.50	18.88 g	176.2 mmol		19.2 mL	0.961 g/mL	
II	isobutyl carbonochloridate	C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub>	136.58	136.02911		1.10	17.65 g	129.2 mmol		17.0 mL	1.04 g/mL	
III	4-methylmorpholine	C <sub>5</sub> H <sub>11</sub> NO	101.15	101.08406		1.10	13.07 g	129.2 mmol		14 mL	0.92 g/mL	
IV	((benzyloxy)carbonyl)-L-serine	C <sub>11</sub> H <sub>13</sub> NO <sub>3</sub>	239.23	239.07937		1	28.1 g	117 mmol				

Rxn ID	Product ID	Product	Compound Name	MF	MW	EM	Theo Mass	Actual Mass	Purity
V	P1	benzyl (S)-1-(benzylamino)-3-hydroxy-1-oxopropan-2-yl((carbam...		C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	328.37	328.14231	38.6 g	34.6 g	98 %

Summary statistics: Total Volume 800 mL, Total Reaction Molarity 147 mmolar, Limiting Moles/Solvent Ratio 157 mmolar.

Figure 2: Integration of Signals Notebook with ChemACX gives scientists immediate access to pertinent data around commercial availability of materials.

Cloud based ELNs are commonly built off RESTful API's which facilitate data trafficking between disparate systems. Using such modern standards for API development, the programmatic burden of integrating systems is significantly reduced. Integrations can access the APIs of an ELN by an external application to precipitate events such as automatically writing instrument data to an experiment. Alternatively, a service within the ELN can access a third-party API to access stored data about a sample from a LIMS or to check the safety and regulatory profile of a reagent from an external database. Whichever integrations are achieved, the greater agility offered by such modern applications allows the ELN to expand to provide the core of a connected electronic lab environment.

Cloud ELNs have enhanced connectivity that is inherent in the way they are designed and provisioned. There is no "one size fits all" ELN, therefore integration with other systems must be not only possible, but also streamlined.

### Benefit 3 - Performance at Scale

Whether you're a scientist, the head of IT, or an investor, you can benefit from the exceptional performance of enterprise software. An ELN user must be able to upload all different types data, quickly find historical data, and have access to the most modern, up-to-date functionality in a timely manner. The business supporting the ELN will be concerned with ease of implementation, accessibility or uptime, and scalability. Cloud ELNs fulfill all these needs as they are delivered in a matter of minutes, elastically scalable, updated automatically, and have guaranteed uptime.

A well-designed cloud-native ELN will be built on modern technology that on-premise ELNs cannot take advantage of. The architecture of traditional on-premise ELNs are either a single application process or a multi-tiered system of database, web server, and application tiers. A cloud-hosted solution of a traditional ELN is the same tiered architecture, just installed in the cloud. Both have upper performance limits and require additional cost, support, or services from IT to analyze the system and optimize it in order to scale. In contrast, a well-designed cloud-native ELN is built with a microservice based architecture, meaning each dedicated component can operate independently. If one component temporarily fails, others remain unaffected and the system is still usable. Microservices are resilient and self-healing. They are designed to auto recover from adverse events that may impact the database, application servers, or network services. This architectural approach has many other benefits, including immediate scalability during periods of rapid growth, and unrivaled search performance through hundreds of millions of entries thanks to modern storage and indexing technologies. This is simply not possible with an on-premise or cloud-hosted ELN built with traditional architecture.

Cloud ELNs delivered as a SaaS solution also have the advantage of elimination of "environmental" issues as well as a continuous release cycle that allows the pushing of new functionality frequently and, depending on the deployment, automatically. A well designed SaaS offering will allow internal administrators to configure their own unique workflows that are not impacted by these updates. Cloud ELNs also have guaranteed uptime, as the entire system is in a controlled environment and is not at the mercy of the many variables onpremise systems are.

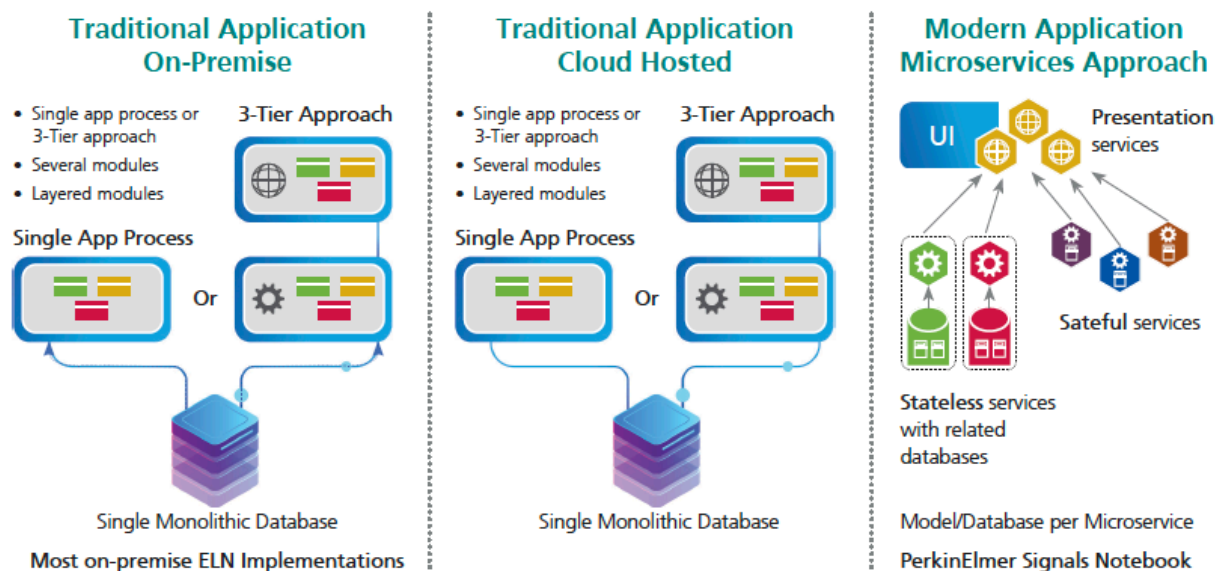


Figure 3: Benefits of a microservice architecture: services operate independently and utilization of best-of-breed for each type of technology.<sup>3</sup>

## Benefit 4 - Security

Protecting and securing your data is paramount. Often at larger institutions, entire teams are devoted to doing just that. Of course, this includes the data you generate in-house at your organization, but 25% of Pharma and Biotech work is now outsourced. Data needs to flow into and out of your organization every day and the right people need to see the right information on-demand.

As data storage in the cloud is elastically scalable, cloud ELNs can be automatically backed up daily and those backups can be stored for an extended period. Organizations that implement a well-designed cloud ELN will benefit from business continuity and a disaster recovery plan that has been vetted by a large number of customers, as opposed to an on premise system that may have less scrutiny.

Not only are there multiple copies of your data at any given time at one data center, but cloud ELNs also provide the benefit of data redundancy. Current best practice for cloud ELN infrastructure is to have it deployed and maintained in at least two physical and geographic locations to mirror your data and guarantee maximum availability if hardware or network issues were to occur. In the incredibly unlikely event that a disaster occurs at one data center, the other can continue delivering the ELN service without interruption or loss of data.

Cloud ELNs often have several deployment models that can include multi-tenant and private cloud environments. A cloud vendor should ensure security infrastructure is equally robust, regardless of deployment model, though the perception that private cloud offerings have better security often leads organizations to that option. Regardless of the deployment model, data is always encrypted in transit to and from the cloud as well as when it is "at rest" in the system. With any cloud platform, the vendor should ensure access to the system is based on a well-defined role based policy, such that designated people only have access to particular subsystems and conduct regular proactive security assessments at the network, host, and application level, remediating all vulnerabilities in a timely fashion.

## Benefit 5 - Total Cost of Ownership

In the late 1980s, Gartner popularized the term "total cost of ownership" (TCO) to define the long-term cost of maintenance in addition to the upfront capital investment in enterprise technology. It is imperative to consider what total cost of ownership means when selecting an electronic laboratory notebook for your R&D organization and how it could influence your decision. The component most people are typically concerned about is the initial capital investment required when selecting and implementing a solution. Let's say your organization has reviewed multiple vendors for their functional capabilities and the scientists are satisfied with the technical aspects. Next, you begin to evaluate the costs.

The complexity of the underlying IT infrastructure and maintenance for a cloud ELN as a service, is all handled by your cloud ELN vendor. Neither the end users or your organization's IT department must worry about hardware maintenance, upgrades to the application, or what versions of underlying databases are compatible etc. A cloud ELN is managed by the vendor experts who developed and understand the application inside and out. They are familiar with all operations of the application and can make changes to the cloud deployment to ensure maximum levels of performance and robustness. Cloud ELNs are quickly scalable and can grow with your organization as capacity needs increase. With most traditional software, you are not guaranteed on how well it will perform when installed on your local infrastructure given all the variables at play (database, servers, network, end user machines, etc.). With a cloud ELN you are, and most vendors will guarantee that your application will be up and available 99% of the time.

As mentioned previously, cloud ELNs eliminate the cost for data backup, redundancy and recovery because these costly and timely services are provided by the ELN vendor, but they also eliminate sunken opportunity cost. Cloud ELNs can be updated more frequently because everyone is on the same source code and vendors don't have to release unique fixes for highly customized ELNs. These more frequent updates ensure that the functionality continues to be improved and modernized. Cloud ELNs also provide the benefit of predictable costs for both licenses and administration. Licenses are typically sold as yearly subscriptions, so during periods of rapid growth you will have a clear idea of what your costs will be.

## Talk about performance! Sub-second structure searching in Revvity's Signals™ Notebook

Chemical substructure and similarity searching is the cornerstone of most cheminformatics systems and a critical feature in electronic lab notebooks. However, as the scale of cheminformatics systems has grown, scientists are often frustrated with the performance of their chemical queries. Mature ELNs in production for well over a decade at global pharmaceutical and chemical companies currently store tens of millions of chemical structures and reactions.

Revvity has been the industry leader in adopting modern NoSQL technologies to build the next generation cloud-native ELN and scientific computing platform, Signals™ Notebook. Chemical structure searching in Signals™ Notebook is facilitated by Revvity's ChemSearch NoSQL chemistry cartridge, the first chemical search cartridge compatible with scalable, NoSQL systems. ChemSearch offers exact, substructure, and similarity search capabilities with performance at scale. This new search engine is based on the open source and battle-tested Elastic Search

technology- the search engine used by most online shopping, airline, hotel reservation, and social media sites. Elastic Search is an index, not a database, that consumes documents and other electronic content, parses it, and organizes it in a way that makes it easier to find.

Revvity Signals instructed Elastic Search how to perform chemical searching and now ChemSearch allows Signals Notebook to provide sub-second response time on databases with hundreds of millions of molecules and reactions. Indexing systems are also very efficient at assigning relevance to results, as it is not enough to return results quickly. The results must be valid, and the most important ones should be returned first. The second step in chemical searching is to evaluate which of the screened molecules is really a valid substructure of the query molecule. This is a complex and computationally expensive process akin to a pass/fail relevance test. Matching molecules are assigned a high relevance, failing ones are dropped from the list of results. The good news again, is that Elastic Search is particularly well suited to scoring the results via a relevance function. It efficiently

parallelizes the scoring process by allowing hundreds or even thousands of small computers to each handle a fraction of the results to score. The net result is a system that is vastly more scalable and performant than older SQL Cartridges found in many on-premise ELNs.

## Conclusion

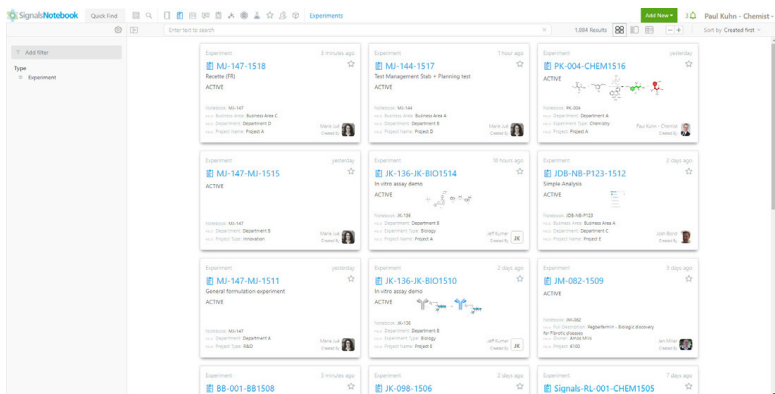
A successful ELN implementation must meet the criteria of and provide benefits to both the technical and business sponsors. The ELN must enable scientists to quickly and easily narrate their experiments, enter and analyze data, and more importantly, share and collaborate on that data to move projects forward. Project managers should be able to track experiment and project progress and gauge efficiency. Investing in a cloud ELN will kickstart your organization's digital transformation, lower the barrier for cross institutional collaboration, and increase R&D efficiency.

Revvity Signals™ Notebook is the next generation cloud ELN and scientific collaboration platform for today's

scientists. One of the most intuitive ELNs on the market, it looks and feels like modern consumer apps used every day. Signals Notebook employs a cloud-based micro-service architecture with advanced data lake storage technologies for document storage and indexing. Revvity has architected Signals Notebook to grow with organization's needs and is quickly scalable. Collaboration is supported with social media-like commenting and notifications and creating contextual relationships between experiments. Signals Notebook is a SaaS ELN and as such Revvity owns all the system maintenance and updates, which deliver new functionality and bug fixes every 3-6 weeks.

# More about Signals Notebook, Cloud ELN

Signals Notebook's intuitive user experience enables rapid user adoption – get your organization up and running in no time with an ELN that looks and feels like modern consumer applications.



Signals Notebook is the intuitive, searchable, scalable, and secure platform designed to increase productivity, enhance collaboration, and reduce risk. Request your 30-day free trial today and get started using it tomorrow to see for yourself.

ChemDraw, the world's leading chemical drawing software, is embedded in Signals Notebook for seamless support of synthetic chemistry workflows and reaction planning.

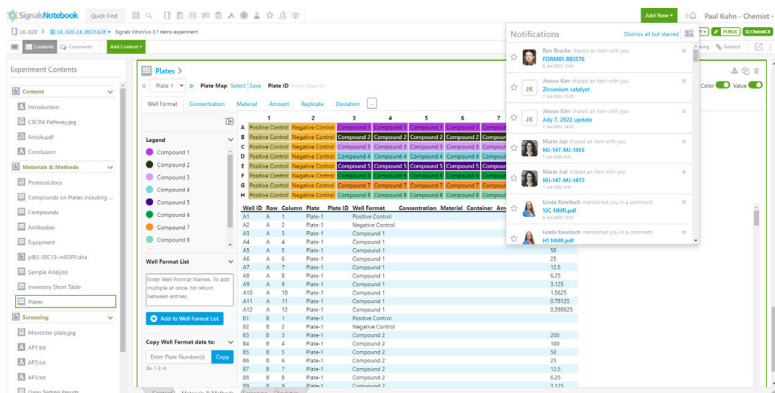
The screenshot shows the Reaction scheme interface. It features a chemical reaction scheme with reagents and conditions. Below the scheme is a stoichiometry grid with columns for Run ID, MF, IUPAC Name, MW, EM, FM, Limit, % Wt, Eq, Sample Mass, Moles, and Vol. A table of suppliers is also visible on the right side.

Run ID	MF	IUPAC Name	MW	EM	FM	Limit	% Wt	Eq	Sample Mass	Moles	Vol
I	C <sub>16</sub> H <sub>19</sub> NO <sub>2</sub>	tert-butyl 4-hydroxypiperidine-1-carboxylate	261.27	201.19449	201.27	✓		1	10.0 g	48.7 mmol	
II	CH <sub>2</sub> Cl <sub>2</sub>	methanechloroform	146.04	119.9523	116.04			9	17.5 g	140 mmol	
III	CH <sub>3</sub> N <sub>2</sub>	N,N-dimethylhydrazine	122.17	122.0840	122.17			1.1	6.66 g	54.7 mmol	
IV	C <sub>4</sub> H <sub>11</sub> N	triethylamine	101.19	101.12045	101.19			1	5.03 g	48.7 mmol	

The screenshot shows the Procedure interface. It includes a text area for the procedure description, a reaction scheme, and a stoichiometry grid. The procedure text describes the synthesis of a product from phenylmethanamine and isobutyl carbonochloride.

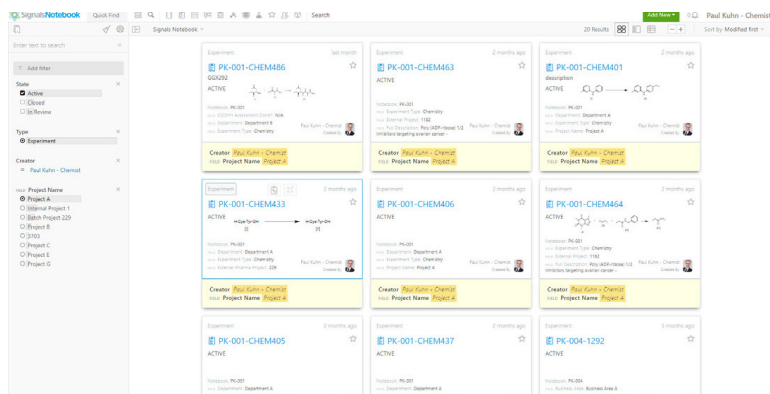
phenylmethanamine (18.88 g, 19.2 mL, 1.50 Eq, 136.2 mmol) was added portion wise to a stirred solution of isobutyl carbonochloride (17.65 g, 37.0 mL, 1.18 Eq, 129.2 mmol) in [SOLVENT] at [CONDITION]. The resulting mixture was stirred for [CONDITION] at [CONDITION], and [REACTANT] was then added. The resulting mixture was then heated to [CONDITION] for [CONDITION]. The reaction was quenched with water and the aqueous portion was extracted with [SOLVENT]. Several times eluting with the [SOLVENT]. PRODUCT was obtained as a white solid.

Quickly document your procedures and protocols by using quick keys to insert auto-text snippets and lists, as well as materials or reaction properties linked to the stoichiometry grid.



Signals Notebook has many capabilities to facilitate collaboration within and across organizations. Teamwork is instantaneous with social media like commenting, the ability to link multiple experiments and notifications delivered in app or via email.

Searching has never been faster or easier. With syntax free text and property search and proprietary ChemSearch functionality for structure searching, Signals Notebook delivers the exceptional search experience scientists can't live without.



## References

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2. Weeks, W. B., Wallace, A. E., & Kimberly, B. C. (2004, Nov). Changes in authorship patterns in prestigious US medical journals. *Social science & medicine*, 1949-1954.
3. Image adapted from <https://msdn.microsoft.com/en-us/magazine/mt595752>