

Solution Story: Building a one-stop platform for chemistry information

How Lundbeck and Elsevier are collaborating to maximize the accessibility and value of the available data



Lundbeck, a global pharmaceutical company that specializes in diseases of the brain, is collaborating with Elsevier on an ambitious project to integrate their internal data with content from Reaxys and Reaxys Medicinal Chemistry in a one-stop platform for chemistry and pharmacology information.

“The potential to integrate Reaxys content and our data is very attractive.”

—Dr. Ludovic Tranholm Otterbein,
Director of Research Informatics & Operations, Lundbeck

Introduction

Lundbeck is a global pharmaceutical company that specializes in diseases of the brain. For over 70 years, the company has been at the forefront of neuroscience research, working to fulfill the promise of a better life for people living with brain diseases.

At Lundbeck, there is a clear recognition of the parameters for success in data-driven pharmaceutical R&D.

“Our goal is to develop therapies for complex brain diseases,” said Ludovic Tranholm Otterbein, Director of Research Informatics & Operations at Lundbeck. “To achieve this, we need to break down our data silos and increase data interoperability.”

To this end, they recently partnered with Elsevier to create a comprehensive database of chemistry content. This project involves working together to integrate Reaxys and Reaxys Medicinal Chemistry into Lundbeck’s existing research ecosystem, making it possible to access internal and external data through a single, seamless interface.

We recently met with Dr. Otterbein to discuss the project.

Challenge

Dr. Otterbein heads a department that supports over 250 scientists engaged in every stage of pharmaceutical development, from early discovery to production. “My department supports all the applications and IT services for our scientists. We develop scientific computing algorithms and visualization tools where commercial solutions are not available or suitable. And we have a key role in data capture, integration, management and supply to the scientists.”

The fragmented nature of modern pharmaceutical R&D, where labs are located across the globe, leads to challenges with managing a company knowledge base. “We had contracts with organizations around the world for synthetic chemistry, including some big players in China and India. Each internal lab and contract CRO used its own electronic lab notebook (ELN) and recorded information in different file formats. Obviously, there were difficulties in using the full potential of the information: finding it, comparing it, and so on. Our extensive chemistry knowledge was in completely separate silos.”

Added to this was the challenge with integrating internal and CRO data with content from commercial databases. “For some time, we’ve been considering a cheminformatics platform that could stand as one unique point of access for chemistry and pharmacology data. **When we looked at Reaxys, the potential to integrate its content with our data was very attractive.**”

Solution

A trial of Reaxys and Reaxys Medicinal Chemistry followed. “We engaged with our scientists, who performed comparisons of the Elsevier solutions with another tool we had been using to access external content. During that trial phase, discussions about the value of integrating our data with Elsevier’s data began. **The potential to improve productivity with a one-stop platform for chemical and bioactivity data was undeniable.**”

Dr. Otterbein’s team started the project to integrate Reaxys, Reaxys Medicinal Chemistry and their own data with an important needs assessment. “We consulted with our own heads of chemistry groups to ensure full awareness of what the platform should do well.”

After that, they began working alone and then with Elsevier’s Professional Services team, starting with the reaction data that were important to synthetic chemists. “First, we created our own reaction-centric data lake, taking the time to look at the educated data model and ensure that things were structured the way we needed them. Having that structure in place made it easier make the ELN-to-platform and Reaxys-to-platform connections. Then we proved that there were more opportunities with this new integrated platform than with any systems or tools we’d used before.”

The success of that initial integration has encouraged the team to look into more such possibilities. “We’re still working with Elsevier’s Professional Services team on further integrations. For example, we’re creating a unique database of reagents available in our own stock, through our CROs and from Enamine. We’re also ensuring that the direct link from Reaxys to eMolecules functions through our platform, so people can stay in one environment and place reagent orders. These integrations streamline stock lookup and ordering, making the synthetic chemists’ jobs much easier.”

The role of Reaxys Medicinal Chemistry at Lundbeck is also coming into focus. “The way that the pharmacology data points have been normalized using the pX values is excellent. It gives a really fast and efficient way to get the overview of one target being hit by one substance. If people had to do that by themselves, they would have to go through all the papers, create spreadsheets, normalize the structure–activity relationships themselves, and then try to create a ranking. That’s a huge benefit that we certainly intend to explore.” They also have plans to perform the same de-siloing and integration exercises for their own pharmacological data in the near future.

Business impact

Dr. Otterbein is very satisfied with the results of the collaboration. “The work with Reaxys has been extremely positive. We’ve provided a platform for all our scientists to access our internal and external data. And it was relatively fast: in a few months, we were able to break apart the data silos at Lundbeck and create the integration with our ELNs.”

He reserves particular praise for the Professional Services team. “We’ve received great support from Elsevier. The training and follow-up has helped reassure scientists who were nervous about the new platform. And we’re impressed with the flexibility and customer focus that Elsevier has, particularly being open to discussing any concerns or improvement requests from our side. Elsevier is open to finding a collaborative way forward.”

Scientists at Lundbeck are also happy, in his opinion. “When I drop in on any of the synthetic, medicinal, process or computational chemists, they’re satisfied. They’ve quickly adopted the platform and there are plans to integrate access to more internal data and to look at some new visualization tools to address more of their needs.”

Ultimately, Dr. Otterbein feels that Reaxys was the best choice for integration with their system. “One reason that we chose Reaxys is how it captures chemistry **and** contains so much in vitro pharmacology information. There are a lot of tools out there that do not really capture the chemistry properly. To the best of my knowledge, **Reaxys is the only chemistry-centric database that enables users to access reactions, informational substances, and documents covering the in vitro and in vivo spaces.**”

Reaxys

Reaxys helps customers drive successful early drug discovery by providing chemists with the shortest path to relevant substance properties, experimental procedures, literature and patent information. Reaxys Medicinal Chemistry helps customers achieve more efficient hit identification and lead optimization with normalized substance–target affinity data and comprehensive pharmacological profiles.

For more information about solution name, visit elsevier.com/reaxys.

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