

# Increasing Research Throughput with an ELN for Chemists and Biologists

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**Lead<sup>o</sup>pharma**  
Discover Design Deliver





**Lead Pharma discovers and develops innovative therapeutics against cancer and autoimmune diseases.**

The company has unparalleled expertise in the discovery and optimization of first- and best-in class small molecules for challenging drug targets. Lead Pharma's drug discovery engine combines adept medicinal, structural and computational chemistry capability with complementary expertise in the fields of cell biology and omics technologies. The company's innovative approach enables isolation, purification and manufacture of target proteins and the development of biochemical, cellular, and functional reporter assays as well as biomarkers.

Lead Pharma's highly skilled workforce, many of which hold a PhD in Chemistry or Biology and have extensive experience across big pharma and biotech sectors, are based at state-of-the-art research laboratories at the Pivot Park in Oss, the Netherlands.



Sander Nabuurs is drug discovery project leader with experience in leading hit identification, hit-to-lead and lead optimization projects for various target families, including nuclear receptors, G-protein-coupled receptors (GPCRs) and epigenetic targets, in both immunology and oncology. He has co-authored more than 50 scientific publications and patents.



**Dr. Sander Nabuurs**  
Project Leader Drug Discovery  
& Head Computational  
Chemistry  
Lead Pharma

## The Challenge: Disparate Research Data with Increased Number and Complexity of Drug Discovery Programs

Lead Pharma's new entity discovery and development capability has grown significantly during recent years. In response, assay throughputs and analysis requirements have increased within the company's research functions and based on their experience within larger organizations, scientists at Lead Pharma were concerned about the limitations of traditional paper laboratory notebooks.

Paper-based cross-referencing of scientific information heavily relied on team knowledge and was consequently vulnerable to staff turnover. Industry processes also required laboratory journals to be checked and countersigned by a scientific colleague or supervisor; a procedure dependent on the timely availability of appropriate staff members. Paper notebooks were used in combination with conventional Microsoft software packages (e.g. Excel, Word) and digital databases, resulting in a labor intensive, mixed-media approach.

*Efficiency of workflows and accuracy of data are critical in an increasingly competitive field, incentivizing drug discovery organizations to seek electronic alternatives for data capture and reporting, freeing scientists to analyze experiments and make next-step project decisions.*



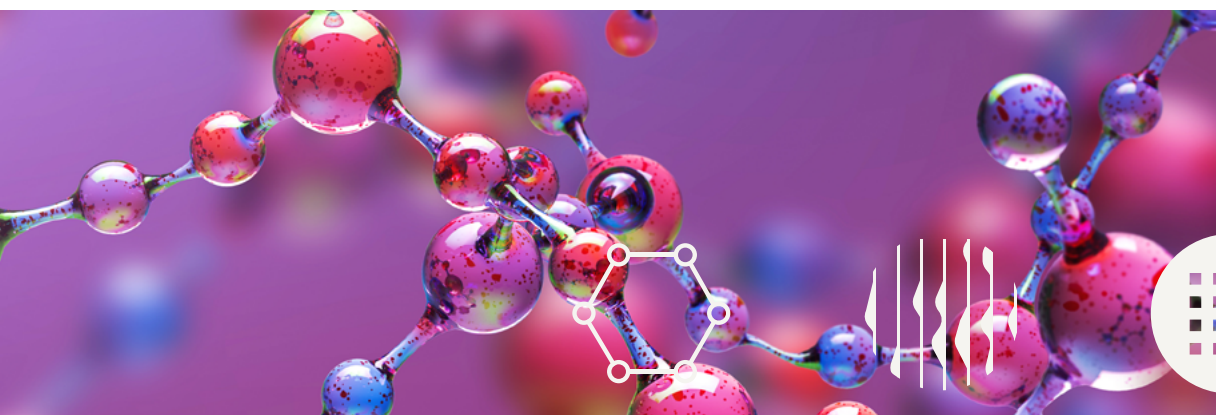
## The Approach: A Best of Breed Informatics Solution to Support Both Biology and Chemistry Functions

Lead Pharma sought an Electronic Laboratory Notebook (ELN) to replace their paper-based system that would also integrate with the company's existing internal project database; the primary data repository for all structural and assay data. A key requirement was an ability to support both chemistry and biological science functions across the business.

*“A key selection criteria for us was the ability to support both chemistry and biology within the one system. Initial investigations revealed few platforms with the ability to effectively support both of these important functions.”*

*Dr. Sander Nabuurs*



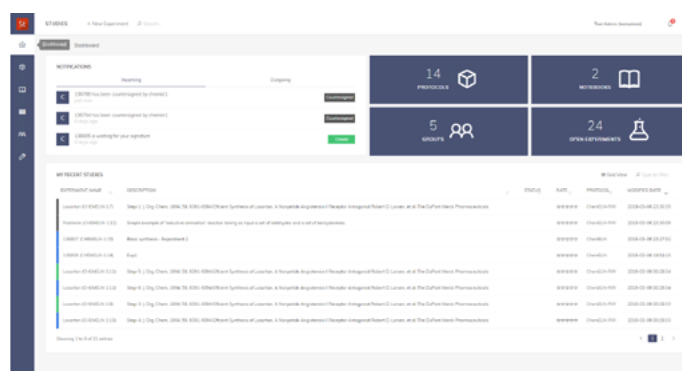


## The Solution: A Web-based Platform for ELN with Advanced Data Visualization and Analytics

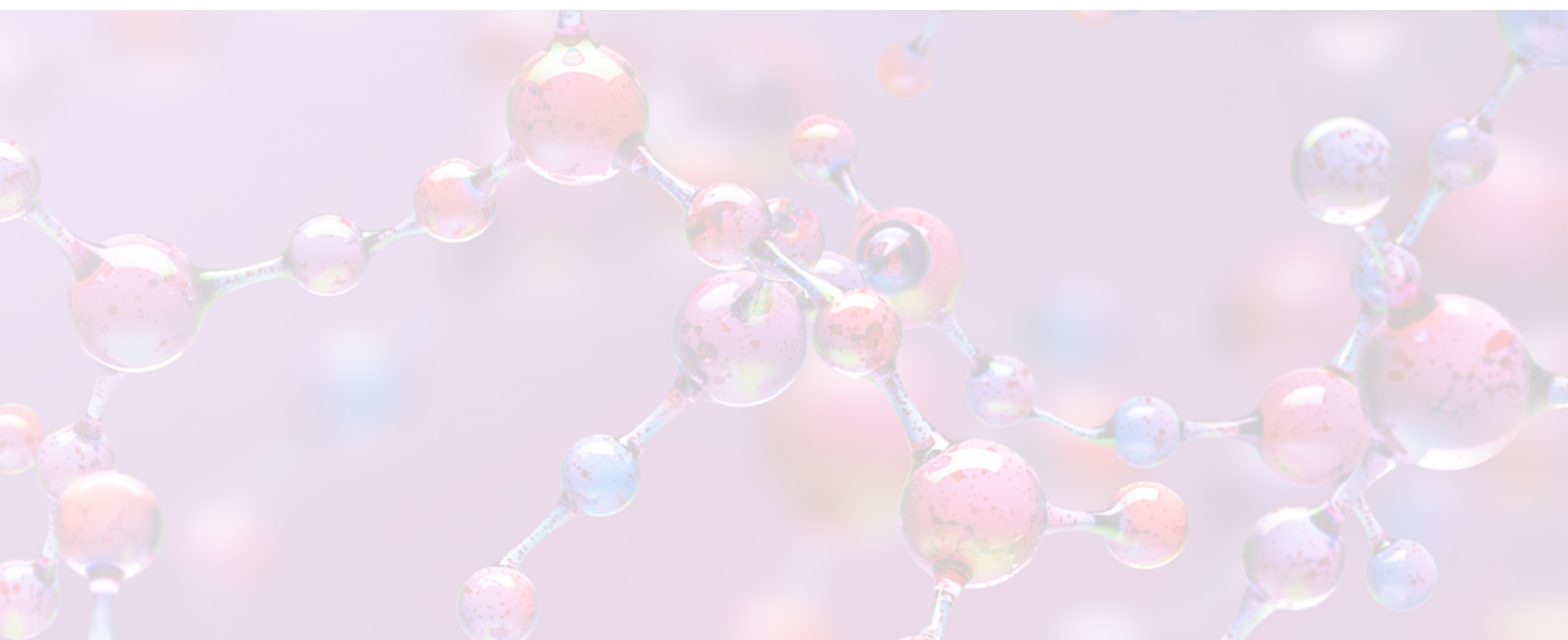
**After a full market review, the Dotmatics Platform was selected. The Studies Notebook ELN addressed each of Lead Pharma's specific challenges, with features and tools that offered value for chemists and biologists across the organization.**

Dotmatics Studies Notebook enabled signing and countersigning of experimental work, facilitated collaborative working and provided a fully searchable system that was easy to navigate via the interactive dashboard. The ELN allowed assay scientists to flexibly record experiments, new compounds to be recorded as individual studies in the system and experiments could be cloned to simplify protocols for production of compounds synthesized from a common reaction.

In addition, Lead Pharma chose to license the Dotmatics Vortex product for advanced data visualization and analytics.



Dotmatics' Flagship ELN - Studies Notebook



## The Outcome: How to Extract Data from Value

**Workflows have been streamlined by integrating the Dotmatics Platform with Lead Pharma's existing chemistry database.**

Key benefits of the Studies Notebook ELN:

- Processes and checks are simplified and may be conducted online
- The need for manual transcriptions is removed
- A digital and remotely accessible countersigning process is provided
- Colleagues are able to collaborate and share results or insights with ease
- Templates are provided for assay experiments – allowing more efficient set-up
- Historical results are readily available and searchable
- Experiments may be cloned to allow efficient re-use of methods

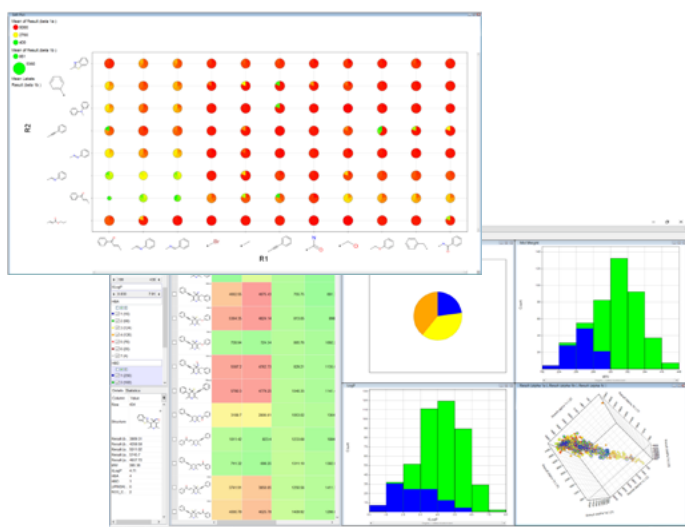
Lead Pharma's computational scientists (from both biology and chemistry functions) now have easy access to an ever-increasing volume of data and the means to conduct advanced analytics via Vortex, enabling visualization of sequencing data, structure-activity relationship (SAR) analysis and compound selection.

Lead Pharma's scientists recognized the benefits an ELN would bring to their working lives and so were very positive about the project, which was a significant factor in its success. Implementation of the Dotmatics platform has released staff members from many manual daily tasks, giving them more time to focus on scientific aspects of their research work.

*“Our lead programs have continued to increase in number and the ability to search and retrieve information across historic data is very important. We couldn't have continued with this pace of increase without a comprehensive informatics solution.”*

*“Our computational chemists and biologists were accustomed to a similar expert tool when at a previous organization and they have found Vortex to be a powerful data analytics and visualization tool.”*

*Dr. Sander Nabuurs*



Data Visualization Using Dotmatics Vortex



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**Dotmatics**