



## Customer Case Study

*“CDD Vault has significantly boosted data intelligence from our in-house projects and the value chain for our partners and collaborators.”*

- Dominique Audenaert, Head of the VIB Screening Core



# Digitalization of VIB’s Biomedical Research with CDD Vault

For any research-based organization in the life sciences arena, experimental data is the key to deriving biological and biochemical insight and understanding, and ultimately driving product development. The ability to manage, access, share – where appropriate - and analyze data is thus critical at all levels of research, from discovery, through development and into the clinic.

And with vast volumes of information being generated through diverse experimental workflows, and the need to manage huge numbers of samples and compound libraries and screening results, for example, managing all these different datasets using paper- or even spreadsheet-based approaches is untenable. At VIB, a major non-profit research institute in Belgium, the group of scientists who carry out high throughput screening (HTS) assay development and HTS campaigns for both in house and partnered projects, implemented

Collaborative Drug Discovery’s CDD Vault registration system and electronic laboratory notebook (ELN) as the central data management infrastructure that helps to maximize the value of the institute’s key compound library assets, track and compare experimental workflows, access data for analysis and comparison, and reduce repetition.

VIB is an entrepreneurial research institute focused on strategic basic research in life sciences. The organization and its 1500 or so scientists work in close partnership with the five universities in Flanders – Ghent University, KU Leuven, University of Antwerp, Vrije Universiteit Brussel and Hasselt University – to expedite research and biological/biomedical innovation. It’s a strategy that has resulted in some groundbreaking discoveries, leading to the spinout of multiple companies to commercialize new platforms and technologies.

VIB has established core facilities to provide support in a wide array of technologies with the aim to advance science and accelerate breakthroughs explained Dominique Audenaert, head of the VIB Screening Core. “We have, for example, a Nucleomics Core that supports transcriptomics research, a Proteomics Core, an Imaging Core, and also the Screening Core that I lead. The small group of scientists in this Screening Core are focused on assay development – primarily to aid miniaturization and automation of bench-top assays – and carry out the HTS programs”, Audenaert continued. “We run a broad diversity of screening assays, ranging from low-complexity biochemical assays to assess enzymatic activity up to high-content imaging assays to evaluate the expression, localization and functionality of a protein in a cellular context.”

The VIB Screening Core historically managed its compound libraries – the internal VIB collection spans about 45,000 compounds – using spreadsheets, but relating any insight from screening programs back to those structures was a major headache, Audenaert continued. “The Excel spreadsheets and basic database that contained the structures of the molecules didn’t allow us to annotate any of the biological data coming from the screens to those



structures,” Audenaert noted. “And this meant that there was no way to immediately see, compare or otherwise analyze relational data in the context of these compound structures.”

Realizing that a better platform was needed to support its operations, in 2016 the VIB Screening Core adopted CDD Vault as a secure repository for its compound data. Importantly, the vault made it easy to tie key screening and other experimental data to the chemical structures. “We carried out trials to assess different software packages, and CDD Vault stood out as an easy-to-use, web-based application,” Audenaert explained. “As a small team of biologists, not chemists, it was important to have a relatively simple, plug-and-play tool that was straightforward to implement and roll out. CDD offered a streamlined product and great support to make this a reality.”

“Having CDD Vault as our compound repository means that now, when we have finished a screen and generated the data, we can link that data to the structures, to facilitate additional cheminformatics analyses, say, clustering or similarity analyses between lead compounds.” Centralizing all the data also makes it more convenient to cross-reference across different screens, he noted.

Importantly, CDD Vault is easy to manage on a daily basis. “Data can be exported manually out of the vault as files for sharing with chemists and other scientists.” This process can also be automated through the API, which is something CDD will be working on with VIB.

The VIB Screening Core’s expertise has evolved from carrying out primarily plant-based screening in small model plants and plant cell cultures, to mammalian cell-based assays, and now high-content screens, Audenaert explained. “We started out performing primarily relatively simple, plate-reader-based assays, but have more recently been completing high-content imaging screens, and that was actually quite a big step, with new scientists brought on board.” High-content screens also set more of a challenge with respect to data storage and curation, he continued. “We need to store and manage high volumes of images and image data, which adds another layer of complexity. We currently use PerkinElmer’s Columbus™ image data storage and analysis system to manage datasets.”

One of the next potential steps for VIB will be to connect the Columbus platform with CDD Vault, so that the image data can be linked directly back to the compound structures. This is something that can be done using CDD Vault API.



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The VIB Screening Core has also, more recently, implemented the CDD Vault ELN, so that the scientists can securely and easily record and report experiments and laboratory workflows, Audenaert noted. “The Vault represents the repository for our screening data, but we also want the ability to track the experiments that are carried out during assay development. We can now put these experiments and workflows directly into the ELN. The ELN is a relatively recent implementation, but the benefits are evident. Our scientists no longer have to rely on remembering when or how a past experiment was carried out and can search and access the ELN easily. All experimental data and workflows can thus be tracked, we can learn from past projects through a complete trail of activity and documentation, use the information to translate past experiments into new studies, and ensure that we don’t repeat past work unnecessarily.”

The CDD Vault registration system and ELN have formed a key infrastructure that is allowing the VIB Screening Core to digitalize its laboratory,

streamline and maximize the value of data emerging from assay development, and HTS campaigns. “These new tools have significantly boosted our efficiency and the intelligence and insight derived from our in-house projects and assay development efforts, as well as maximized the depth and breadth of data and value chain, for our external partners and collaborators,” Audenaert stated. One of VIB’s key strengths is its flexibility to work with partners in a wide range of fields. “We apply our expertise to many different fields of research and experimental goals,” he continued. “We can work with industry on a collaborative basis to generate shared IP, but can also offer our expertise on a fee-for-service basis. The business and commercial support of VIB allows us to tailor partnerships on an individual basis. CDD Vault and its ELN represent key tools that can only aid that flexibility, and help to maximize value chain from our research carried out by our own scientists, and on behalf of and in partnership with an increasing number of collaborators and clients who access our expertise.”

## About Collaborative Drug Discovery

Collaborative Drug Discovery provides a modern approach to drug discovery informatics that is trusted globally by thousands of leading researchers. Our CDD Vault is a hosted informatics platform that securely manages both private and external biological and chemical data. It provides core functionality including chemical registration, structure-activity relationship, inventory, visualization, and electronic lab notebook capabilities. For more information, visit us at [www.collaborativedrug.com](http://www.collaborativedrug.com).