CDD VAULT®
Complexity Simplified

Customer Case Study

Novalix

StarDrop™

optibrium™

"Thanks to StarDrop and CDD Vault … all the data from the pharmacology department, from ADME, DMPK, and cheminformatics, can be accessed in one place, representing a major time saving."
- Ruel Cedeno, PhD, Novalix Project Manager

Accelerating Early-Stage Drug Discovery: How Novalix Integrates CDD Vault and StarDrop for Smarter R&D

Founded in 2002 in Strasbourg, France, Novalix is today a premier contract research organization (CRO) dedicated to improving the critical early stages of drug discovery. The organization combines exceptional scientific talent and exclusive technology with a comprehensive portfolio of world-class chemistry, biophysics and pharmacology capabilities. Supported by innovative partnerships with leading instrument makers and academic institutions, Novalix works collaboratively with clients to meet complex scientific challenges.

Centers of Excellence

The firm's broad expertise is founded on what Laurent Saniere, PhD, Novalix Senior VP and Head of Drug Discovery, describes as a complete range of drug discovery services, from essential chemistry all the way through preclinical studies. Four centers of excellence include chemistry, biophysics, pharmacology and DMPK, and drug discovery.

Evolution of Novalix over the last five or six years - from a company rooted in structural biology and chemistry – has been supported by a series of strategic acquisitions and collaborations, explained Saniere. These include Novalix's acquisition, in 2022, of Sanofi's

pharmaceutical research facility in Strasbourg, now established as Novalix's headquarters and, 14 months later, the transfer to Novalix of Galapagos NV's research and discovery activities in Romainville, France, together with the exclusively related staff.

Laurent Saniere, PhD, Novalix Senior VP and Head of Drug Discovery

Supporting Early-Stage Discovery

Saniere commented, "With some 400 employees spread across three sites in France and a chemistry facility in Tunisia, we combine expert people with exceptional technology that allow us to manage the entire drug discovery project for our customers, supporting them from early discovery to candidate selection. As bringing new drugs to market has become more difficult and expensive, Novalix provides the expertise, flexibility, and efficiency required for early-stage pharmaceutical research. Together with our clients, we can increase the odds of success at each stage of a project."

A Central Repository for Data Management

To help achieve this, Novalix installed CDD Vault in 2021 as the central repository for managing the company's chemistry and assay data. The Vault represents a critical platform for the Novalix drug discovery, ADME, cheminformatics and (primarily in vitro) pharmacology teams.

The Vault's scalable, modular architecture and human-friendly user interface support more complete collaboration within and between departments, across geographies, and between project partners, or service partners and their clients, Saniere suggested. "The Vault offers us an efficient, user friendly and accessible data management tool, and a way for us to integrate in the same space, or location, data from different sources and departments, with a common index, around the compound itself."

Better Science Together

Using the Vault makes it easy to search and find data, as well as view and analyze different types of data within relevant analytical workflows, without loss of content or context. This can then maximize insight from collection date, to improve and speed decision making, and adds value for clients. "Ultimately, CDD Vault allows us to do better science together with our clients," Saniere commented.

Having diverse data in one centralized repository that is easily accessible to all departments is a major benefit across the board, explained Mariana Vaschetto, PhD, CDD Head of Operations EMEA/LATAM. "At CDD, our objective is to enable scientists to do their best work. Not only did we design CDD Vault to be

intuitive, we designed the software to serve as a scalable and secure data hub where collaborative research efforts make for great science. The combination of the modular features of the software are designed to pull together everyone's scientific expertise to improve and accelerate decision making."

CDD Vault Integration with StarDrop™

Novalix has integrated CDD Vault seamlessly with Cambridge, UK-based Optibrium's StarDrop™ platform, which provides an intuitive environment for molecular design and data analysis in hit-to-lead discovery and lead optimization workflows.

Adopted by Novalix in 2019, Optibrium's flagship compound design and optimization platform StarDrop empowers researchers to cycle iteratively through molecular design and data analysis, optimizing hit-to-candidate workflows through better, faster decision making.

Flexible and easily integrated with in-house databases and third-party tools, StarDrop's modules for in silico modelling, generative chemistry, and multi-parameter optimization generate actionable insights. Its interactive data visualizations combine with SAR analyses to help scientists understand relationships between compounds and within series. Researchers can then identify compounds likely to exhibit the optimal combination of activity, ADME and physicochemical properties.

In Silico Modelling and Design

"We want to give researchers the tools to target high-quality compounds for their project's objectives earlier in the discovery process," said Edmund Champness, Chief Scientific Officer at Optibrium. "StarDrop's comprehensive range of in silico modelling and design capabilities enables chemists to explore a wide variety of optimization strategies before focusing on the most promising candidates for synthesis and testing, improving efficiency and making better use of resources."

Integration via API

"Organizing and deriving contextualized results from diverse data would be a huge challenge without the Vault and StarDrop in combination. From a geographical perspective alone, as an organization with multiple sites that each generates its own data, it's really important that we can collate that data systematically and efficiently and make it user friendly to find and search."

- Ruel Cedeno, PhD, Project Manager, Cheminformatics, Novalix

CDD and Optibrium inked their collaboration to enable integration of StarDrop with the Vault back in 2016. The seamless integration via API means users can harness the two platforms' respective data management, visualization and analysis/design tools within and between projects, without the need to modify data for export/import and review. StarDrop users can search and query data directly in the Vault, and access results, formatted ready for visualization and analysis, directly in StarDrop.

"The API seamlessly linking CDD Vault and StarDrop means that we can access CDD Vault through StarDrop," commented Ruel Cedeno, PhD, Novalix Project Manager, Cheminformatics. "Before this direct integration it was a two-step process. We'd have to access the data in CDD Vault and then extract the CSV or SDF files. And then we would have to open those files in StarDrop." While this two-step process was still far more efficient and secure than using Excel files and emails, the API allows for a seamless connection between the two platforms.

Saving Time and Supporting Collaboration

The quality of service offered by Novalix is supported by the complementary capabilities of the Vault and StarDrop, the combined use of which not only help to ensure maximum value from data across departments, but also routinely save Novalix scientists hours or potentially days of work refining, interrogating and reporting data, explained Cedeno. "Organizing and deriving contextualized results from diverse data would be a huge challenge without the Vault and StarDrop in combination. From a geographical perspective alone, as an organization with multiple sites that each generates its own data, it's really important that we can collate that data systematically and efficiently and make it user friendly to find and search."

Prior to CDD and StarDrop that data would be largely held in Excel files, and even finding and distributing data could represent a huge headache, Cedeno further acknowledged. "Thanks to StarDrop and CDD Vault this has changed. All the data from the pharmacology department, from ADME, DMPK, and cheminformatics, can be accessed in one place, representing a major time saving." The Vault gives Novalix a user-friendly platform from which to view, compare and analyze data, making it possible to generate the intelligence required to show clients, Cedeno suggested.

Built in Analytical Tools

Vaschetto further commented, "The built-in analysis tools in the CDD software allow customers to maintain high fidelity of their data. Organized, structured data means having the ability to simplify tasks such as generating reports and creating data visualizations within the platform itself with just a few clicks."

Added Cedeno, "Without CDD Vault, we'd have to email the other departments and ask for specific data, which they would then have to search for in their hard drive, and once found, check if it's in the correct format before sending it to us. And unless that data is downloaded immediately, then its retrieval in the future may require a trawl through historical emails. This might not appear too problematic at first sight, but when data accumulates in email trails, the time spent hunting for those emails and then organizing or formatting the data that they contain, can be significant."

Integral Lab Notebook

Dhoha Triki, PhD, Novalix Senior Scientist, Molecular Modelling, noted, "In my role I primarily use StarDrop to visualize the data, perform histograms and do clustering and R group analysis. In comparison to other platforms, like open-source tools I've used previously, StarDrop offers the convenience of being able to visualize data without the need

for any coding. We also calculate ADME properties prior to synthesis and testing using the ADME QSAR module. The lab notebook that is integral to CDD Vault means that experimental data can be connected to the Vault, and this will add context, save time and aid collaboration."

A "Bigger Picture"

Yaelle Fischer, PhD, Novalix Research Associate, further stated, "we also use StarDrop to create the radar plots for physicochemical properties, and to generate histograms for additional visualization when building our DNA-encoded libraries. We use the clustering function here a lot too." The ability to see dose response curves adds key insight, Cedeno suggested. "We don't just see the final value that we report, we attach evidence to that. And being able to analyze that bigger picture of the data, not just the final value itself, is a huge benefit."

> ***"The API means we can simply click and access data from CDD Vault in StarDrop to perform our analyses using different models."***
>
> *- Dhoha Triki, PhD, Novalix Senior Scientist, Molecular Modeling*

Triki explained, "As Ruel mentioned, we integrate all the DMPK, biological and biochemical assay and experimental data generated at our different sites into CDD Vault." The drug discovery team can then use this data, via StarDrop, to visualize 3D structures, carry out clustering, and other tasks. Triki continued, "The API means we can simply click and access data from CDD Vault in StarDrop to perform our analyses using different models. For example, with SeeSAR we're able to understand and analyze the interactions between ligand and protein in 3D, to identify the key interactions driving binding affinity. We can then save the StarDrop folder or session and send that to the medicinal chemists for further design. So having CDD Vault and StarDrop together enables all the teams to connect and accelerate the whole process."

A Global View of Data

Edmund noted, "We understand that researchers need to use a whole suite of tools in their drug discovery workflows. That's why we've built StarDrop to connect easily with in-house and third-party informatics platforms. Our direct integration with CDD Vault is a great example of this. Teams can operate within their custom workflows, incorporate their own models and algorithms, and get a global view of their data for better and faster decision making."

CDD Vault has been designed to simplify the generation and export of reports, saving time and ensuring that data can be relayed to colleagues and clients fast and in the optimum format. Novalix works with clients who themselves use CDD Vault for data management, as well as with clients who are not Vault subscribers. Saniere explained that exporting data from CDD Vault to clients that also use the Vault is seamless, and for clients that don't have CDD Vault, a conversion step allows for data export in formats that are compatible with other platforms.

Easy Onboarding

Importantly, onboarding is relatively easy. “I’d not used CDD Vault before joining Novalix, but for me it was very user friendly,” Cedeno said. For both Cedeno and Triki, two or three interactions with the system were enough to get a feel for it, and learn how to export data as well as search for and visualize data. “And the good thing, is that everything is automatically updated in real time,” Triki commented. “We just have to connect to see the most recent results.”

Vaschetto pointed out that CDD was designed with scientists in mind. “The onboarding process can take as little as half a day and allows us to quickly set up a system that fits with our customers’ needs. Using CDD Vault as a central repository where data is organized and managed - because at CDD we strongly support all FAIR principles - we believe lends itself well to being part of an integrated solution. We’re committed to our customers’ success because when they succeed, the whole world benefits.”

Headquarters Novalix SAS in Strasbourg, France

“The integration of CDD Vault and Optibrium’s StarDrop within Novalix has improved the way teams collaborate, access, and analyze data. By centralizing diverse datasets and enabling seamless visualization, researchers across departments and sites can work efficiently and insightfully. This connected approach not only saves time but also empowers scientists to make faster, more informed decisions, ultimately delivering better science, together.”

- Laurent Saniere, PhD, Novalix Senior VP and Head of Drug Discovery

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.