



Customer Case Study

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Dr. Christoph Sager, Senior Scientist, Head of Computational Chemistry & IT, leadXpro AG

leadXpro

leadXpro Combines CDD Vault with DataWarrior to Speed Drug Discovery

Situation

leadXpro AG is a biotechnology CRO specializing in structure-based drug discovery for membrane proteins, which are promising yet challenging drug targets. The company integrates advanced protein science, structural biology, and ligand design expertise to address these challenges.

Based in Villigen, Switzerland, leadXpro's research covers a range of membrane proteins, including GPCRs, ion channels, transporters, and enzymes. leadXpro acts as a research partner for a growing number of pharmaceutical, biotechnology and academic institutions.

In its lead discovery workflows, leadXpro uses DataWarrior, an open-source program for data visualization and analysis with chemical intelligence. More recently, leadXpro entered a partnership with Alipheron, whose founders Dr. Modest von Korff and Dr. Thomas Sander, were

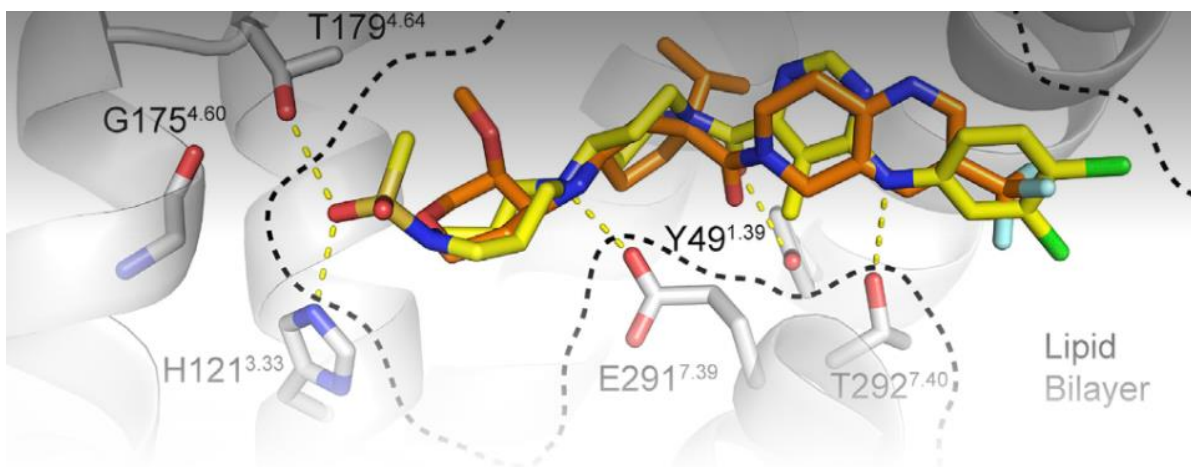
co-creators of DataWarrior, along with Joel Freyss and Christian Rufener. Alipheron's Pharos3D is a DataWarrior plug-in that provides 3-dimensional molecular modeling and search for drug analogues in ultra-large combinatorial libraries.

As DataWarrior isn't a database, leadXpro sought a powerful database to hold its research data that could seamlessly integrate with the workflow.

Solution

leadXpro deployed Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both internal and external biological and chemical data.

leadXpro has deployed multiple instances of CDD Vault: One Vault for its CRO business, a second Vault for leadXpro Therapeutics, its



leadXpro brings expertise in all aspects of membrane protein production, structural biology and lead discovery.

internal drug discovery business, as well as additional instances for collaborating with partners.

“Having separate CDD Vaults allows us to keep our CRO work strictly separate from our leadXpro Therapeutics work,” says Dr. Christoph Sager, Senior Scientist, Head of Computational Chemistry & IT, at leadXpro AG. “We also create separate Vaults for work with each collaboration partner.”

CDD Vault complements DataWarrior by enabling seamless data integration. Dr. Sager highlights its searchability and the Curves module, which simplifies data processing and visually represents complex trends.

Benefits

CDD Vault Provides a Secure Central Data Repository and a “Single Source of Truth”

CDD Vault provides leadXpro with a secure central repository for all of its research data.

The company uses CDD Vault to track chemical information, inventory samples, assays and other data, all of which can easily be pulled into their DataWarrior.

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The combination of CDD Vault and DataWarrior provides a classic Better Together story.

“DataWarrior is not a database,” says DataWarrior co-creator Dr. Sander. “It is a visualization tool with chemical intelligence, which means that beyond simple visualization DataWarrior understands chemical molecules and reactions. DataWarrior perceives and visualizes chemical molecules in two and in three dimensions. It can take molecular structures and experimental data from CDD Vault, and the user can extract knowledge from this data by calculating molecular properties of the compounds and by correlating the data with data from external sources.”

Dr. Sander notes that Alipheron recently released a plug-in that unlocks additional investigative power, as it directly links DataWarrior with Alipheron's Pharos3D to search ultra large combinatorial libraries for three-dimensional structure motifs.

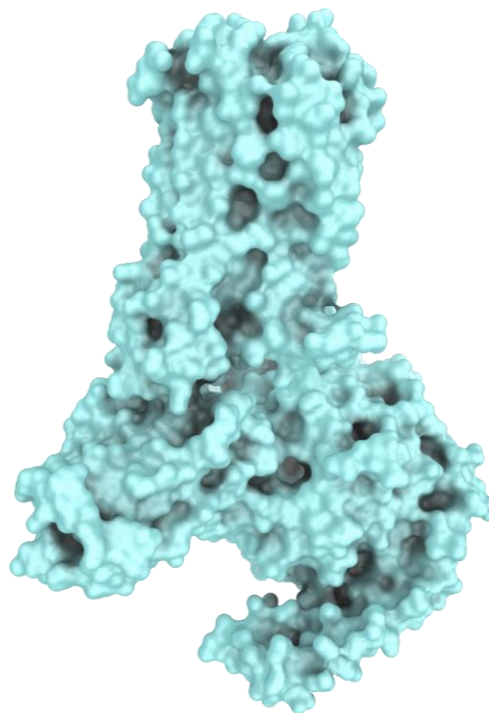
CDD Vault provides leadXpro with what's often referred to as a single source of truth, removing the potential headaches of trying to verify who has the most recent spreadsheet or other data collection.

Dr. Sager recalls his experiences at an earlier drug discovery company where they attempted to create their own repository to provide a single source of truth.

"The connection between CDD Vault and DataWarrior is very close to what we wanted to have back then," Dr. Sager says. "Now we have a single source of truth."

Noting the need for a secure central repository that provides a continuously updated single source of truth, Dr. Sager recalled the frustration of going through spreadsheets and PowerPoint presentations before weekly meetings.

"I remember how before weekly meetings we had to pull data from PowerPoint files," Dr. Sager says. "But the day after we had the meeting, the data was already outdated. Sure, you could still go and look it up on SharePoint, but it would already be out of date as work continued in the lab. This is not the way to do drug discovery. We need to use tools that enable us to see the full picture in an easy way, so we can make decisions on actual live data."



leadXpro specializes in structure-based drug discovery for membrane proteins.

Integration with DataWarrior

DataWarrior co-creator Dr. Sander says that early in the project a DataWarrior plug-in for CDD Vault was created in response to requests from users. Alipheron has since released an updated version of the plug-in providing even tighter integration.

"The updated plug-in allows users to directly search CDD Vault from DataWarrior so they can do structure searches and download chemical structures together with experimental result data into DataWarrior, unleashing advanced cheminformatics methods and chemistry aware

visualization methods to convert raw data into knowledge”, Dr. Sander says.

Visualization “Our Chemists Love CDD Vault Curves”

While leadXpro chemists continue to use DataWarrior for visualization, they have also integrated use of CDD Vault visualization and analysis tools, including the Curves module. Curves enables users to plot and analyze a wide range of data utilizing a variety of curve fits, custom calculations, curve customization, and plot customization options like overlays.

“We’ve had Curves enabled, thankfully for a couple of months now, and it’s great,” Dr. Sager says. “This is one of the CDD Vault features that our chemists love. We like it because we can have multiple measurements in the same plot and directly compare to the reference. We no longer have to go and separately look up IC50 values and a range of other data. It’s very intuitive. Seeing data visually represented provides an extra layer of confidence.”

Robust Searchability

Researchers at leadXpro appreciate the robust searchability of CDD Vault.

“It is really important to us that with CDD Vault we can search for compound structures as well as sub structures,” Dr. Sager says. “We like that we can also search by name because our medicinal chemists have their own naming schemes for the compounds they are designing. CDD Vault ensures we can find all data that has ever been recorded for each compound.”

leadXpro researchers also value the security of CDD Vault, enabling them to safely search for

“The updated plug-in allows users to directly search CDD Vault from DataWarrior so they can do structure searches and download structure data, and perform other operations directly against the data in CDD Vault.”

- Dr. Thomas Sander, Lead Developer & Founder, Alipheron, and Co-Creator of DataWarrior

data, ensuring sensitive data can only be viewed by those with appropriate permissions.

“Each of our chemists can have their own saved search for what they think is important for designing the next round of compounds,” Dr. Sager says. “Of course we can also pull data from these searches into DataWarrior with ease.”

Enhanced Collaboration

CDD Vault enhances collaboration within leadXpro and with external CROs and partners in its leadXpro Therapeutics efforts.

“When we outsource to CROs, we can flexibly and securely give them granular access to our CDD vault,” Dr. Sager says. “CROs can upload data, we look at it and share it with other collaborators. CDD makes collaboration easy and flexible.”

CDD Vault is proving its value with leadXpro’s recently announced partnership with Cumulus Oncology, based in Edinburgh, Scotland. The companies have signed a research collaboration focused on the discovery and development of

small molecules targeting GPR68 a novel cancer-focused G protein-coupled receptor acting as a proton sensor.

“CDD Vault is valuable to our partnership with Cumulus because they are sitting in the UK, we are in Switzerland, and we have CROs doing chemistry all around the world,” Dr. Sager says. “It’s essential that all parties have secure access to the same data at the same time, which is what we are able to do with CDD Vault. This truly facilitates collaboration.”

Alipheron CEO Dr. von Korff sees the collaboration enabled by CDD Vault as being the wave of the future.

“CDD Vault is a great tool, as teams today are often disparately located across much of the planet,” Dr. von Korff says. “With CDD Vault for storage, data can be accessed worldwide, for example, via DataWarrior. From there you can use Alipheron’s services Hyperspace and Pharos3D to search commercial ultra large combinatorial libraries in 2D and 3D to discover your next accessible and patentable lead compound.”

Do-It-Yourself Ease of Use

The intuitive, ease of use of CDD Vault is valued by leadXpro and its chemists and biologists.

“Big pharma companies have data scientists to handle uploads and other functions, but you can do all of that yourself with CDD Vault,” Dr. Sager says. “Uploads are easy. You can do template mapping. Vault automatically recognizes data that looks similar to previous things and suggests how to put it in the database.”

“With CDD Vault for storage, data can be accessed worldwide, for example, via DataWarrior. From there you can use the services for Pharos3D and perform hyperspace search on ultra large combinatorial libraries.”

- Dr. Modest von Korff, CEO & Founder, Alipheron, and Co-Creator of DataWarrior

Dr. Sager recalls recently spending an hour with a biologist, introducing her to CDD Vault, and showing her how to upload data.

“I briefly walked her through the process,” Dr. Sager says. “And in the afternoon, she was uploading data herself.”

Protecting Intellectual Property

Protecting IP is essential throughout the drug discovery process, which is why leadXpro appreciates the tight security built into CDD Vault.

“It is very reassuring that once you come to the step of patenting and protecting your IP, you know you have all of your data stored within CDD Vault,” Dr. Sager says. “And you know it is secure.”

He also appreciates how easy the transfer of IP and supporting data is at the end of a project.

“Once you know the project has come to the right stage, we can off license it, and hand over the Vault,” Dr. Sager says. “You essentially hand

the keys to the Vault over to the next person, which is easy to do. This is very appealing.”

CDD Is a Great Company to Work With Going into the Future

Dr. Sager sees CDD Vault as a valuable part of what he sees as a future in which a network of companies and services will emerge as ever more powerful participants in drug discovery.

“I believe we are seeing a paradigm shift,” Dr. Sager says. “I see a network of software companies, service providers, CROs, chemistry, biology, pharmacology, growing into a space where not one company does everything, but we help each other out.”

“The benefits for drug discovery are much greater when you can pull in experts from all the areas that you need for a project,” Dr. Sager continues. “CDD Vault is important for the storage of the molecules and ideas. leadXpro is important for protein structures. DataWarrior is important for visualization. Pharos3D is powerful for 3D modeling and massive searches. At leadXpro we have expertise in protein structures, biophysical data, lead discovery with computational chemistry and project management, and then we have CROs for additional chemistry and biology support.”

“Big pharma will always exist,” Dr. Sager says. “However, networks of specialists combining their expertise are becoming increasingly

valuable for accelerating and enhancing 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.