

Customer Case Study

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- Cen Gao, Ph.D., Computational Chemist & Drug Designer, Acerand Therapeutics



Acerand Therapeutics Uses CDD Vault Across Two Sites and Multiple CROs in Search for New Drug Candidates

Situation

Acerand Therapeutics, founded by industry veterans with Lilly Asian Ventures (LAV), is an innovative biotech company focusing on the discovery and development of novel best-inclass and/or first-in-class drug candidates for clinical development. The company has operations both in Shanghai, China as well as Indianapolis, U.S., to reflect its overall global strategy and business intents.

Founded in June 2020, the company's chemists and biologists are focused on creating new drugs for oncology and autoimmune diseases.

"All of us are drug hunters, so we don't typically have to worry about all the scientific infrastructure that supports our efforts," says Dr. Cen Gao, Computational Chemist & Drug Designer at Acerand. "Many of us came from large pharmaceuticals with internal systems and support staff. As a startup, we knew we needed a solid scientific informatics platform to support our work."

Acerand's chemists and biologists needed a central repository for storing and accessing its small molecules, assays, and related data. It also needed an informatics system that would work well with the CROs the company works with in the U.S. and China.

Solution

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



Acerand Therapeutics uses CDD Vault for its exploration of therapeutic agents.

It was an easy choice to make because several Acerand scientists had either used CDD Vault before, or had colleagues—within the industry and academia—who used the product and spoke of it enthusiastically.

"We were also impressed that all of the CROs we work with were familiar with CDD Vault," Gao says. "The CROs were either using it inhouse for their own efforts, or had experience working with it because it was used by companies they contracted with. Everyone has good things to say about CDD Vault, so it was an easy decision."

Acerand deployed two Vaults—a production Vault shared by the company's two locations, and a sandbox Vault used for testing. While the two locations share a Vault, they use individual Projects to completely separate the data to protect the intellectual property of each group as they pursue separate projects and therapeutic targets.

Benefits

Acerand has found a number of benefits since adopting CDD Vault, including:

- Ease of use & easy to manage
- Easy collaboration with CROs
- Tight security to protect IP
- Visualization of overlay assay curves
- Support for remote workers
- Great customer support

Ease of Use & Easy to Manage

Acerand is impressed with how easy CDD Vault is to use—and to manage.

"Our biologists and chemists can use CDD Vault comfortably after minimal training—just an hour or so," Gao says. "It's browser-based, with a very logical interface, which definitely helps in usability."



Acerand Therapeutics: "All of us are drug hunters."

Gao knows how easy CDD Vault is to use because he's the person his colleagues come to when they have a question.

"As a small biotech, we don't have a dedicated IT staff. I'm a computational chemist, so if there are any questions, they come to me," Gao says. "Early after deployment a few questions came up, but soon after the questions stopped. Everything comes very naturally with CDD Vault."

Gao says CDD Vault proved to be exactly what the company needed.

"We're an early-stage drug discovery company," Gao says. "We have specific needs such as storing assay data and registering compounds. What CDD offers is simple to use and just exactly what we need. We also require tight security, which CDD provides. I'm sure CDD Vault offers functionalities that we don't use, but what CDD offers is perfect for the needs of an early biotech startup like ours."

Easy Collaboration with CROs "They Knew CDD Vault Better than Us"

A pleasant surprise for Acerand was the ubiquity with which CDD Vault is used across the chemistry and biology CROs it works with in the U.S. and China.

"It seems like all the major CROs are either using CDD Vault themselves, or at least have a deep knowledge of CDD from working with others," Gao says. "When we first started out, the CROs knew CDD Vault better than we did.

They would give us suggestions on how to optimize different tasks."

All of this makes for easy collaboration with the company's numerous chemistry and biology CROs.

"The CROs load data directly to our CDD Vault, so they are loading it from their own CDD systems, or already have a process to convert their internal data into a CDD-ready format for the uploading," Gao says. "The ability for CROs to load their own data is a time saver for us so we don't have to spend our own time doing it. CDD Vault has definitely helped our collaborative process. We plan to add more CROs to meet workflow demands, and it is good to see that onboarding more CROs will be an easy process."

Tight Security to Protect IP

As a drug discovery company, protecting intellectual property is mission-critical to Acerand. The multi-layered security of CDD Vault is one of the reasons Acerand chose it as its informatics platform.

CDD has several layers of security, including the use of TLS encryption for data in transit, as well as dual firewalls—one in hardware, the other in software.

"The security of CDD Vault means that one of our chemistry CROs can register a compound to our Vault, while a Biology CRO can upload assay data on the compound, with each party tightly restricted in what they can see and do," Gao says. "The Structure Masking feature of CDD Vault means a biology CRO, for example, only sees the compound ID, but does not see the chemical structure."

The same data compartmentalization capability also provides a barrier between Acerand's two sites. As part of its organizational structure, each site works on its own projects, pursuing different targets.

"CDD Vault has nicely kept our projects, data, and IP separated within one vault," Gao says. "We can only see our own data. When sharing data with a CRO or other party, we can do so in an extremely granular fashion. This helps us protect our IP, which is the most important thing for an early discovery company like us."

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Visualizing Overlay Assay Curves

Acerand scientists appreciate the visualization capabilities of CDD Vault, including the ability to dynamically overlay assay curves, including when creating half maximal inhibitory concentration IC50 tables.

"Our biologists use CDD Vault Visualization to fit curves, generate IC50 tables, and perform similar analytical tasks," Gao says. "With CDD visualization, we can overlay multiple assay curves for a single compound into one graph. This allows us to see the assay variability of the

same compound between different runs, or to compare the behavior of multiple compounds in different runs. Using different colors for each run, we can easily see the difference, and identify patterns."

CDD Visualization is effective—and easy to use.

"The overlay curves are automatically generated when you query the data in the aggregated manner," Gao says. "Without CDD Vault visualization, it would be very hard to compare curves when they're in two different pictures, especially when they are in different scales or have other formatting differences. We like this feature a lot."

Support for Remote Workers

"When your company is launched in the midst of a pandemic, support for remote workers is mission-critical—as all of Acerand's employees began their efforts through working remotely, and a year later, as the COVID-19 pandemic drags on—continue to do so."

"We haven't been in the office since pretty much day one," Gao says. "Starting in the middle of the pandemic, we had to learn how. to do everything virtually. CDD Vault is pretty much the only way we share the real data. We can put data on a slide, but when we want to see something like the real IC50 curve, our biologists feed their data into CDD. Our chemists log into CDD to look at their data. Without CDD Vault, I don't know how we would have been able to do this."

Great Customer Support

Acerand is impressed with the quality and speed with which CDD delivers its customer support.

"We sometimes send emails after work, and we still get a response within a couple of hours," Gao says. "Sometimes working late, we'll be amazed to receive a reply in the middle of the night. CDD provides the best customer service we've seen, including the use of interactive video sessions."

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.