



Customer Case Study

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- Fernando Martinez, Ph.D., Founding Scientist, Topos Bio



Connecting AI and Experimental Data: CDD Vault Helps Topos Bio Target “Undruggable” Proteins

Situation

Topos Bio is an AI-powered biotechnology company developing therapies for intrinsically disordered proteins (IDPs). Headquartered in San Francisco, the company's platform integrates physics with generative AI to target disordered proteins across disease areas such as neurodegeneration and oncology.

The company recently introduced two new AI foundation models. The first is Topos-2, built to predict how IDPs, which are dynamic in nature, move and change shapes. The second is Topos-Bind, a first-of-its-kind model designed to predict how these dynamic proteins interact with potential drug molecules. Together, these models represent a significant advancement in AI-driven drug discovery, addressing a class of

disease-causing proteins historically difficult to study and target.

Topos Bio's mission is to build foundation models to drug historically “undruggable” targets, disease-causing proteins that resist traditional drug therapies and tools. These targets, comprising close to two-thirds of all proteins in humans, are major drivers of the most aggressive cancers and neurodegenerative diseases including Alzheimer's, Parkinson's, ALS, and Huntington's. The company needed a secure central repository for its research data.

Solution

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

company's biologists, chemists, and computational chemists.

Additionally, Topos Bio uses CDD Vault's Electronic Lab Notebook and Inventory modules.

As the company was formed some two years ago, choosing to deploy CDD Vault was an easy decision.

"Some of our team had experience using CDD Vault at other organizations, and it was agreed that it's the best platform anyone had used for chemistry and small molecules," says Fernando Martinez, Ph.D., Founding Scientist at Topos Bio. "I've used seven or eight different repositories, and believe CDD Vault is by far the best for any kind of small molecule discovery."

A solid, secure central repository is essential to the work of Topos Bio.

"We're trying to understand the dynamics of the IDPs and the IDRs [intrinsically disordered regions]," says Dr. Martinez. "Unlike a crystal structure or a structured protein, the structure is more like a video than a snapshot because the IDR, the IDP is constantly moving around. We're using a combination of biophysics, AI, and traditional molecular modeling to generate that video, so to speak, for an IDR or an IDP, and then determine how we can fit a small molecule onto the frames of the video."

All of this generates a lot of data, which the company stores in CDD Vault.

Benefits

Topos Bio has enjoyed a number of benefits through use of CDD Vault, including:

- CDD Vault provides a "single source of truth"
- CDD Vault stores simulation and computational data
- CDD Vault for chemistry-aware registration "The best I've seen"
- Ease of use "All of us can set up our own assays"
- Using CDD Vault to register plasmids and DNA constructs
- CDD Vault ELN helps ensure complete documentation and audit trail
- Easier to demonstrate SAR
- CDD Vault supports faster time to discovery
- CDD Vault "Helps establish and protect our IP"
- CDD provides great customer service

CDD Vault Provides a "Single Source of Truth"

Topos Bio stores the large volume of data it generates in CDD Vault, which the team values as its single source of truth.

"We use CDD Vault to keep a record of pretty much everything," Dr. Martinez says. "We do a lot of medicinal chemistry, and all of our small molecules go in CDD Vault. For the biophysics, we use a lot of protein constructs that we've made, and we keep track of all of those in CDD Vault, along with their associated data, and the same with our plasmids."

CDD Vault plays a role in the day-to-day work of the company's scientists.

"We rely on it extensively," Dr. Martinez says. "Every week we look at which new medicinal compounds have been registered, and see if any of these compounds are missing assay data, or if any assays need to be repeated. Based on this we can see what needs to be done. CDD Vault helps us plan our work for the week."

Throughout all of their work, CDD Vault serves as a valued central repository.

“CDD Vault provides a rock-solid record of what’s been made, everyone’s experimental data, and what’s been done,” Dr. Martinez says. “It’s what everyone searches when they need to examine assay data for a specific compound. Without this central repository we could have people working on slightly different versions of molecules, differing assays. It removes inefficiencies by providing us with a single source of truth.”

CDD Vault Stores Simulation and Computational Data

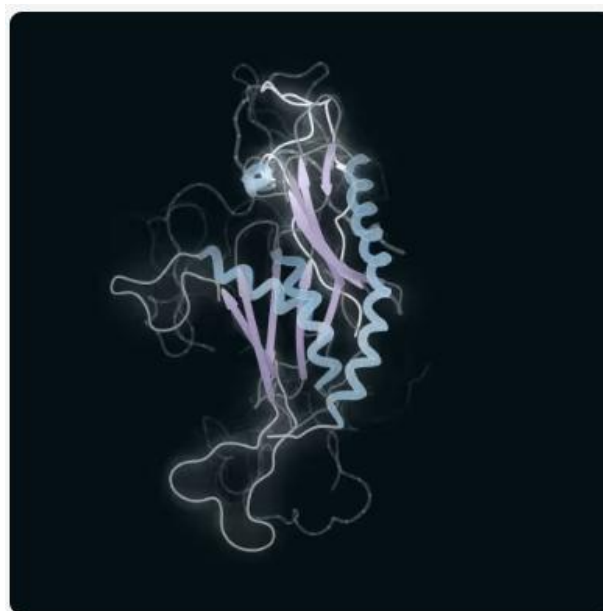
CDD Vault seamlessly unites Topos Bio’s AI-generated data with its experimental data.

“We register our simulation and computational data, alongside the experimental data including affinity and potency,” Dr. Martinez says. “This helps us see what computational methods correlate with the experimental data.”

CDD Vault for Chemistry-Aware Registration “The Best I’ve Seen”

Topos Bio also values CDD Vault’s chemistry awareness, which begins the moment a compound is registered and catches issues generic repositories miss, such as duplicate compounds and untraceable salts.

“We like that CDD Vault does so well with physical and chemical properties such as salt stripping, duplicate detection, and substructure search,” Dr. Martinez says. “All of that is the best I’ve seen. I’ve worked with a lot of the more bio-focused repositories, and they don’t enable much chemistry at all, which makes it



A sequence of Topos-2 ensemble predictions for various proteins across the ordered-to-disordered spectrum.

really hard for any kind of small molecule development.”

The lack of a chemistry-enabled repository also introduces inefficiencies.

Dr. Martinez says: “I’ve worked in other places where the repository didn’t support chemistry, and people were making or buying duplicates of the same compound, or we ended up with a lot of different salts that nobody really understood because it couldn’t be tracked.”

Ease of Use “All of Us Can Set Up Our Own Assays”

Scientists at Topos Bio enjoy the ease of use of CDD Vault, which means everyone can do their own registrations and set up their own assays.

“With CDD Vault everyone can upload their own data, register molecules, and download data,” Dr. Martinez says. “All of us can set up our own assays.”

The company also used the CDD Vault API to automate data uploads.

“We interface programmatically with CDD Vault, using the API,” Dr. Martinez says.

“Another way we get good use from the Vault is we process our lab data with custom scripts into a form that CDD Vault can ingest on its own. This gives us an automated pipeline uploading data from our lab to CDD Vault.”

Using CDD Vault to Register Plasmids and DNA Constructs

Topos Bio uses CDD Vault to register its biologics, including plasmids and DNA constructs.

“We especially like that we can register our own plasmids and DNA constructs,” Dr. Martinez says.

The ability to easily register plasmids improves efficiency in the lab, including ordering, cloning, and custom synthesis.

“Prior to the Vault and the ability to register plasmids, we had an issue with accumulating a lot of different constructs, where it was sometimes unclear where they came from or what the sequence was,” Dr. Martinez says.

“Now we make sure that everything is in CDD Vault, prior to any orders going through. This has saved us a lot of time, a lot of money, and a lot of confusion. Now everyone can see what a sequence is and what it is for.”

The ELN Helps Ensure Complete Documentation and Audit Trail

Topos Bio uses CDD Vault’s ELN to enhance efficiency and to ensure complete documentation across its research efforts,

“It’s impressive how quickly you can see and communicate your SAR. I’ve used other products, and I haven’t found another that lets people communicate as well what their SAR is for a chemical series. In my experience, CDD Vault is the best for that.”

- Fernando Martinez, Ph.D., Founding Scientist, Topos Bio

including biological assays and chemistry workflows.

“With all of our scientists using the CDD Vault ELN, it provides the entire team with a disseminated single source of truth, as opposed to everyone keeping separate documents,” Dr. Martinez says. “This central source of lab entries and protocols benefits the entire team. And its integrated audit trail shows whenever a change has been made, and who made it, which enhances efficiency.”

Easier to Demonstrate SAR

Topos Bio finds that CDD Vault makes it easier to demonstrate SAR.

“It’s impressive how quickly you can see and communicate your SAR,” Dr. Martinez says. “I’ve used other products, and I haven’t found another that lets people communicate what their SAR is for a chemical series. In my experience, CDD Vault is the best for that.”

“The fact that you can create a table with your chemical series and the assay data right from CDD Vault, adding whatever measurements you want, and then create a report, enables you to quickly demonstrate SAR,” Dr. Martinez says. “You can see, for example, if we add charge groups to one part of the molecule, we get more activity or less activity. It provides a quick and definitive way to demonstrate the SAR to yourself and others.”

CDD Vault Supports Faster Time to Discovery

The many benefits of CDD Vault combine to support a faster time to discovery.

“CDD Vault provides a platform for us to identify our most promising molecules and their associated data,” Dr. Martinez says. “Part of the pathway to faster discovery is understanding what you've got and how good it is. We're sorting through a lot of different molecules trying to understand their properties and whether they can do what we want. CDD Vault makes it faster and easier to sort through what we've made, and understand what's good and what's not, and then make a decision about what we should make next.”

CDD Vault “Helps Establish and Protect Our IP”

CDD Vault plays an important role at Topos Bio in protecting the intellectual property it generates.

“ELN documentation as part of our CDD Vault also helps establish and protect our intellectual property,” Dr. Martinez says. “That's how the molecules get documented and patented. Whenever we speak to our attorneys, we rely on structures and reports from CDD Vault to

communicate what we've made. They use the structures, the synthesis schemes, and the assay data from CDD Vault when they draft our IP.”

CDD Provides Great Customer Support

CDD provides Topos Bio with exceptional customer support. The company appreciates the depth of knowledge and the speed with which requests are met.

“CDD customer service is great,” Dr. Martinez says. “They provided clear guidance when I was working with the API, and they helped another of our scientists with his SPR data. Questions are usually answered the same day, and they have deep knowledge of the product and of the drug discovery process.”

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 <https://www.collaborativedrug.com/>.