



## Customer Case Study

*“CDD Vault expedites drug discovery by giving you the ability to quickly visualize your data, and then propose the next molecule to make.”*

- Roopa Rai, PhD, Founder & CEO, Isosterix



# Isosterix Uses CDD Vault to Expedite Drug Discovery & Securely Collaborate

## Situation

Roopa Rai is the Founder and CEO of Isosterix. With over 25 years of experience, Roopa has held leadership positions in discovery research in various therapeutic areas including oncology. She has a successful track record of driving programs from discovery to IND-ready compounds including six clinical candidates. Past positions include SVP, Discovery Research at Myoforte Therapeutics and Senior Director of Chemistry at Medivation and Assembly BioSciences. She is a co-author/inventor on 70+ patents and publications. She has a Ph.D. in Organic Chemistry from the University of Illinois at Urbana-Champaign and has done postdoctoral research at Cornell University and Stanford University.

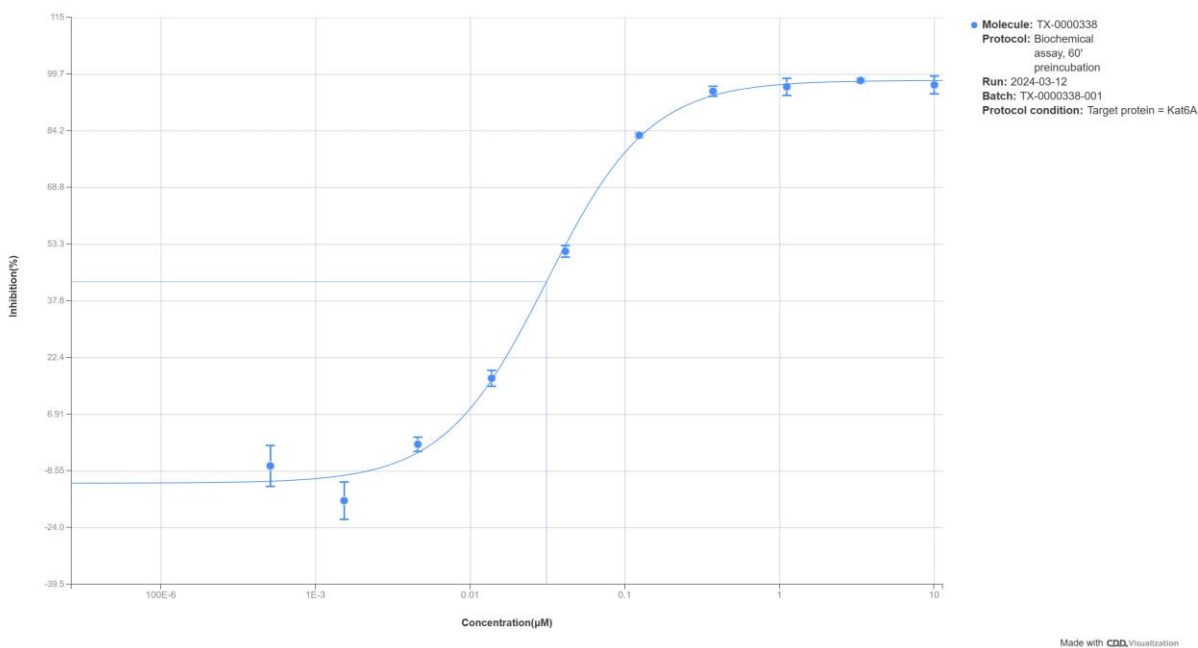
Rai founded Isosterix to develop small-molecule inhibitors of KAT6A, an epigenetic oncogene that is implicated in multiple cancers including breast, prostate, lung, ovarian and

hematological cancers. KAT6A/B are histone acetyl transferases (HATs), a new class of epigenetic regulators. KAT6A is a promising new oncology target particularly in endocrine-resistant breast cancer. Isosterix has inhibitors that are selective for KAT6A over other HAT family members, including its paralogous protein Kat6B.

## Solution

As Rai created her new company, she deployed Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both internal and external biological and chemical data.

This was an easy decision, as she had been using CDD Vault for more than a decade while working at other biotech companies. Rai has also consulted with companies that don't use CDD Vault, which reminds her of how much she values it.



**Drug Discovery.** Isosterix values CDD Vault as a mission-critical tool in its drug discovery efforts, including for biochemical assays, as shown above.

“I have used CDD Vault for years and couldn’t do the work that I do without it,” Rai says. “CDD Vault helps speed time to discovery.”

Isosterix uses CDD Vault to store some 350 compounds. Rai uses CDD Vault to register compounds, view assays, perform data searches, SAR analysis, and to securely collaborate with the company’s consultants and offshore CRO.

## Benefits

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

- Providing a “single source of truth”
- Speeding time to drug discovery
- Serving as a powerful tool for startups
- Supporting collaboration with consultants and CROs

- Protecting intellectual property

## Providing a “Single Source of Truth”

Having worked widely within the world of pharmaceutical research, Rai appreciates the significance of CDD Vault providing what many refer to as a “single source of truth.”

She notes that the alternative too often is a collection of spreadsheets or other forms of decentralized data stores which can make it difficult and time consuming to determine where the most recent data resides.

“With CDD Vault, the freshest data is always just a click away,” Rai says. “The moment new data is uploaded into CDD Vault, it’s available to all scientists registered on your CDD Vault.”

This immediacy of data availability, combined with CDD Vault searchability and SAR analysis helps drive discovery.

“New data elicits new ideas, such as how the next molecules might be made,” Rai says. “As a central data repository, everyone on the team can securely access the newest data to guide their work.”

With her long background working with CDD Vault, Rai finds it frustrating when working with organizations that don't have a centralized repository.

“I'm consulting with a company now that doesn't have CDD Vault and a lot of time can be wasted looking for data that would be just a click away with CDD Vault,” Rai says. “I recently spent 30 minutes pulling together data that I could have had within moments using CDD Vault. So it can be frustrating to work without it.”

## Speeding Time to Drug Discovery

The powerful SAR analysis and robust searchability of CDD Vault helps speed time to discovery.

“The SAR analysis in CDD Vault helps you to think of new molecules and generate new hypotheses for whatever problem you are trying to solve,” Rai says. “In drug discovery you go through iterative cycles of structure, activity relationships. You look for trends. You might say: I need a hydroxy group, but at another position on the molecule. That's my next hypothesis. We improve whatever it is we're trying to improve in that particular cycle of SAR.”

“CDD Vault expedites drug discovery by giving you the ability to quickly visualize your data,

and then propose the next molecule to make,” Rai says. “CDD Vault helps in the thinking process. It gives you the ability to sort data and ask questions, and to quickly propose the next, most promising, molecule to make. This saves you from having to make 50 molecules to get to the next iteration of improvement in potency or improvement in oral bioavailability. CDD Vault helps you get to the next step more quickly by querying the data and getting the answers.”

## CDD Vault is a Powerful Tool for Startups

After working for a number of biotechnology companies, Rai decided to create her own,

***“CDD Vault helps in the thinking process. It gives you the ability to sort data and ask questions, and to quickly propose the next, most promising, molecule to make.”***

**- Roopa Rai, PhD, Founder & CEO, Isosterix**

initially with just herself as the sole employee, augmented by consultants and a CRO.

From this experience, she suggests that every biotech startup make CDD Vault part of their work foundation, or at least to do so by the time they begin to do their research.

“CDD Vault is a great organizer,” Rai says. “It should be an essential part of any new drug discovery venture because otherwise the data becomes overwhelming in a hurry. You are tracking multiple kinds of data for each compound, and that complexity grows with each new compound. The moment you start

making compounds and gathering data, which is what drives your progress, that's when you need CDD Vault. I couldn't do without it."

### **CDD Vault Is Easy to Use: "I Don't Have Any IT Specialists. With CDD Vault, I Don't Need Any."**

CDD Vault has long been praised for its ease of use, which is especially important for startups and other small biotech businesses that might not have IT specialists on staff.

"CDD Vault is extremely easy to use," Rai says. "I don't have any IT specialists. With CDD Vault, I don't need any. When I have a question, I just contact CDD and they respond almost immediately, providing all the help and guidance I might need."

Rai also appreciates built-in protections to ensure data integrity, including automated duplication protection which prevents registering the same compound twice.

Registration of new compounds is simplified through use of custom templates that CDD creates for clients.

"I just send CDD a description of my current program and they create a custom template for me," Rai says. "With the template, it's just a few clicks and your compounds are registered into CDD Vault."

### **Supporting Collaboration with Consultants and CROs**

Rai has long valued the ease with which CROs can be given secure, granular access to CDD Vault, enabling them to directly upload their work, making it immediately available to others from anywhere around the world.

"Working with biotechs prior to starting my own business I might have one CRO doing biology and another CRO doing chemistry, and I would set them up with licenses so they could directly interact with permissioned areas of CDD Vault," Rai says. "This is a very efficient way to collaborate across the world."

Now with her own company, Rai has found that even without providing licenses to her CRO, she is able to simply upload their data through the CRO's use of the CDD Vault template she sends them.

"My CRO returns the template and with just a few clicks I can register new molecules and related data into CDD Vault," Rai says. "I also use CDD Vault to provide access to my consultants. For example, if a biologist needs a molecular weight or something, they can get the data immediately."

### **Protecting Intellectual Property**

The tight, granular, security of CDD Vault helps protect intellectual property, which is absolutely essential for successful drug discovery.

As Isosterix prepares to license a compound to a pharmaceutical company, it is able to demonstrate IP protection through its use of CDD Vault.

Along the way, the company can securely grant specific data access on an as-needed basis to collaboration partners.

Rai also likes that using CDD Vault makes it easy to securely share data rather than sending material as attachments.

"I communicate with one of my consultants every day through emails," Rai says. "If I want

her to see a certain SAR, I just send her a link from CDD Vault. She can click on the link and securely see the data from within CDD Vault, because she's a registered member. This means we can share data in a confidential way without sending structures attached in an email.”

## 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).