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Complexity Simplified

Customer Case Study
University-Wide Licensing

***"We wanted to remove the barrier of individual labs having to make budgetary decisions … We alleviate that through the university-wide license."***
- Peter Toogood, Ph.D., Director, Michigan Drug Discovery, University of Michigan

**Michigan Drug Discovery**
**University of Michigan**

# Michigan Drug Discovery Deploys University-Wide Licensing for Data Management System

## Situation

Michigan Drug Discovery (MDD) is a university-spanning collaborative program established at the University of Michigan to mentor, support, identify, and coordinate resources for investigators with an interest in pursuing drug discovery research, and to accelerate the process of drug discovery.

Peter Toogood, Ph.D., Director of Michigan Drug Discovery,[1] wanted to support students and faculty researchers in their drug discovery efforts by providing linked electronic laboratory notebooks (ELNs) and centralized, secure data storage. The need was underscored by publication of the 2023 NIH Data Management and Sharing Policy, which promotes the management and sharing of scientific data generated from NIH-funded or conducted research.

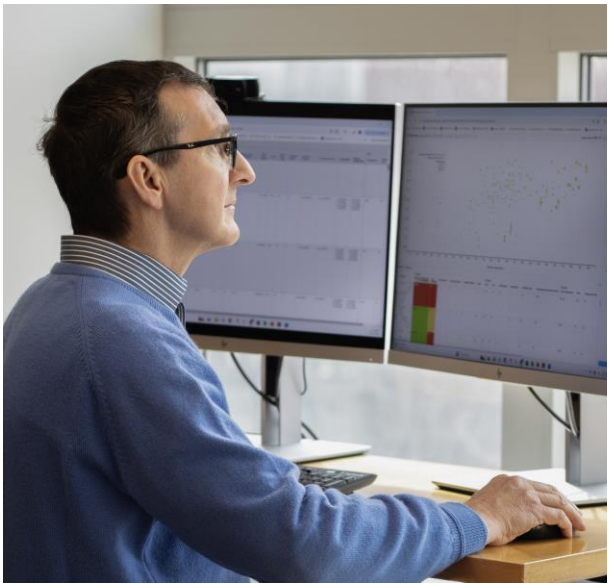
## Solution

To this end, MDD licensed Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both internal and external biological and chemical data. Deployment includes CDD university-wide licensing, freeing individual labs and researchers from having to purchase separate licenses, while providing a unified solution for secure electronic data storage and ELNs.

[1] *Title provided for identification purposes only. The views and opinions expressed are those of the individual only and do not necessarily reflect the positions of the University of Michigan.*

"So far we've seen 12 labs with about 60 researchers deploy CDD Vault and the ELN," Dr. Toogood says. "And we are expecting adoption of CDD Vault to grow. I spent 20 years in industry before I came into my current role, so I'm very familiar with the value of electronic lab notebooks and cloud-based data storage systems."

Each lab has deployed its own instance of CDD Vault, with one lab deploying two Vaults. "We didn't impose any restrictions on CDD Vault deployment, but I think there's a certain convenience for each lab to deploy their own," Dr. Toogood says. "And you can obviously have multiple projects within a Vault."



**Peter Toogood, Ph.D., Director, Michigan Drug Discovery, University of Michigan, using CDD Vault.**

## Benefits

Dr. Toogood has seen a number of benefits since adopting CDD Vault with university-wide licensing, including:

- University-wide licensing ensures all researchers can have secure, centralized data storage & an ELN.
- University-wide licensing provides a unified data storage platform facilitating collaboration.
- Easier CDD Vault administration with university-wide licensing.
- CDD Vault provides "A Single Source of Truth."
- Using electronic lab notebooks helps ensure data capture and availability.
- Providing electronic tools helps prepare the next generation of research scientists.
- Protecting the integrity of institutional intellectual property.
- CDD Vault supports collaboration.
- Supports secure remote access.
- Preserves the value of legacy data.
- Provides visualization tools to explore data.
- Embraces FAIR Data Principles.

### University-Wide Licensing Ensures All Labs & Researchers Can Have Secure, Centralized Data Storage & an ELN

Adopting university-wide licensing for CDD Vault helps ensure that all labs and researchers can have secure, centralized data storage with integrated ELNs.

"One of the biggest advantages, from my perspective, is that we can offer this to faculty, essentially for free," Dr. Toogood says. "The university pays one price, meaning that individual faculty and labs don't have to bear the cost. We wanted to remove the barrier of individual labs having to make budgetary decisions on whether they could subscribe. We alleviate that through the university-wide license with a single point that's paying the bill."

## University-Wide Licensing Provides a Unified Data Storage Environment

University-wide licensing of CDD Vault helps provide a unified electronic data storage environment for drug discovery research across the University of Michigan.

“Having a university-wide license means that we can always be in the same environment,” Dr. Toogood says. “When there are collaborations between faculty on campus, they can be working within the same electronic data storage environment. The data may be in different vaults, but they can share information without security concerns. We are all behind the same firewall, protected by the same vault security.”

## Easier CDD Vault Administration with University-Wide Licensing

The university-wide licensing for the University of Michigan simplifies site administration, Dr. Toogood says.

“We can administer CDD Vault from a single point, which means we don't have multiple faculty members having to deal with invoices and purchase orders and pricing,” Dr. Toogood says. “This also makes it easier for labs who might still be using spreadsheets and other non-centralized data systems to deploy CDD Vault within their lab environments.”

Dr. Toogood says ease of use was a big factor in choosing CDD Vault.

“One of the major criteria for us in selecting CDD Vault was ease of use, because even though I describe myself as sort of the primary point of contact, I don't want to spend my time being a fulltime research informaticist, troubleshooting everybody else's vault platform,” Dr. Toogood says. “There are some tools out there that require a full-time person who's knowledgeable about the guts of the system, but we didn’t want that. CDD Vault is much easier to use, which lowers the barrier to entry. That means the individual faculty can maintain their own vault, they can add and remove users, they can set up protocols. If they want to add a collaborator, they can add a collaborator, they don't have to go to CDD Vault to ask them to do it for them. CDD Vault has terrific support, but you don’t need it. Everything is very straightforward. I think that that's a huge benefit.”

## CDD Vault Provides “A Single Source of Truth”

Researchers using CDD Vault for centralized, secure, data storage benefit from having what is sometimes called “a single source of truth.” This provides a more efficient form of data storage than using spreadsheets and other methods where version control and searchability can be challenging.

“Historically, data has been deposited into some form of spreadsheet, like an Excel file,” Dr. Toogood says. “With spreadsheets you lack the ability to search by things like chemical structure, which for people doing chemistry is a high priority.”

Data access—and updates—can also be an issue with spreadsheets.

“Data on spreadsheets may not be accessible to others in real time, and may not get updated,” Dr. Toogood says. “When doing the kind of work that I do, which is medicinal chemistry, where we're essentially associating a chemical structure with a biological activity—with that

activity expressed in a numerical value—that's exactly the kind of data CDD Vault handles extremely well. Good practice entails determining that value more than once. If it's a compound that you're evaluating multiple times, the precise number is going to vary, and updating that in an Excel spreadsheet format can be very cumbersome, but within CDD Vault, it just happens essentially on the fly."

Toogood notes: "CDD Vault has some very good tools that allow you to interpolate measures such as the 50% inhibition concentration."

CDD Vault makes it easy for researchers to dig deeper into data when needed.

"One of the strengths of the system is that I can go back and look at what the value was the first time I measured it, see the value the second time I measured it, as well as the dates associated with those measurements," Dr. Toogood says. "We can actually associate those measurements with individual batches of protein, and so forth. So, there's meta data associated with those determinations. While we might use the average of seven determinations as our true value, we can always dig a little deeper into the layers and go: 'Were there any outliers? When did they occur? Did the compound have the same level of purity every time we measured it?' So, there's a lot of other information that's available that that might get lost otherwise."

## Using Electronic Lab Notebooks to Ensure Data Capture and Availability

With its university-wide licensing, it is easy for researchers and students at the University of Michigan to take advantage of the efficiencies of the CDD Vault Electronic Lab Notebook.

"Traditionally, faculty and student researchers have written down their experimental procedures and findings by hand into hardcopy lab notebooks," Dr. Toogood says. "That's great, as far as it goes, but it's not searchable. And it also is less readily monitored in real time, as in: Are they actually writing up their experiment, and doing so in a way that is clear and easy to follow for other people? Do other people who are working on the same project have access to that information in real time? Is the information available for someone to reproduce the work? All of those things are limited when you have a hardcopy lab book."

Especially in a university environment, hardcopy lab books can create challenges for storage and retention.

"With hardcopy lab books you've got the issue of storing them," Toogood says. "What happens when someone changes buildings, or changes institutions? There's always the potential for the lab books getting lost. Sometimes students leave and take their lab notebooks with them."

These problems are solved with an ELN.

"Moving lab notebooks into an electronic environment with an ELN addresses a lot of those issues," Toogood says. "You've got a networked system where others can securely access the information. The ELNs are searchable. You no longer have to worry about researchers moving, because the data stays securely stored in the cloud."

## Providing Electronic Tools to Help Prepare the Next Generation of Research Scientists

Educating the next generation of research scientists is an important part of a university's

function. Providing students with access to CDD Vault and its ELN helps prepare them for their professional careers.

“Providing students with CDD Vault provides a layer of professionalism,” Dr. Toogood says. “Part of the consideration we put into selecting CDD Vault was that this is a tool that is used by many of the companies to which our students may go when they graduate from here and look for full time employment.”

Working with electronic data storage benefits students even if they go to a company or other organization that is using a different product.

“We want our students to have a state-of-the-art experience, exposing them to tools that they're going to be using when they get into the workplace,” Dr. Toogood says. “When our students move into jobs in biotech or pharma, they will be already familiar with CDD Vault. If that's the tool that that company is using, it will be a seamless transition. If the company is using another platform, they will at least be familiar with the concepts. And it will be less of a transition for them because they'll have used an ELN in the past and they will be familiar with cloud-based data storage practices. They won’t be starting from ground zero.”

## Protecting the Integrity of Institutional Intellectual Property

One of the goals of Michigan Drug Discovery is to work with the University of Michigan’s Innovation Partnerships team to grow the university’s impact on the local and state economy, by identifying opportunities and partners for licensing University of Michigan discoveries and forming startup companies that can advance these discoveries through clinical development.

All of this makes it critically important to protect the intellectual property created along the path to drug discovery.

“For my colleagues and I who are working in medicinal chemistry, our ultimate customer is likely to be a startup biotech or an existing pharmaceutical company that has the interest and the wherewithal to be able to license the compounds and the intellectual property that we generate, and then take it to the next level,” Dr. Toogood says. “These companies aren’t going to be interested in making that kind of investment if they don't think that we have done a good job of maintaining the integrity of our data and making sure that it's been kept confidential. The value of any intellectual property would be completely undermined if its confidentiality has been breached.”

Using CDD Vault helps demonstrate dedication to protecting intellectual property.

“We need to maintain the same level of data security that an external partner would maintain with their own data,” Toogood says. “One way that we can demonstrate our rigorous security to potential partners is to show them that we're using a state-of-the-art secure data store that requires granular permissions to access data. You can’t say: ‘We keep it in spreadsheets laying around my desk and email it to people, even though my email can be hacked.’ That doesn’t fly. Instead, we can say we are using CDD Vault, which is often the same platform they are using, and even when not, they respect it as being secure.”

## CDD Vault Supports Collaboration

CDD Vault serves as a collaboration platform. Dr. Toogood sees collaboration happening at three levels:

- **Between scientists within the same lab**: "Within the lab, the students who are working on the same project have access to the same data [stored in CDD Vault] and each other's electronic lab notebooks," Dr. Toogood says. "This enables them to see things in real time. They know where the data are, they can contribute to those data, they can help maintain the electronic database to ensure that it's current. And so, within a group, the platform enables a level of ongoing collaboration."
- **Between teams from different labs**: "Cross-group collaboration is important to our efforts," Dr. Toogood says. "If you have a chemist and a biologist working together, oftentimes the biologist is producing the data, and the chemist is making the compounds. By facilitating collaboration through our use of CDD Vault we can gain acceleration as you get more data that helps improve the design of the compounds and get more compounds that generate more data and so forth. That's the kind of dynamic that accelerates our efforts in drug discovery."
- **Between institutions**: "A third level of collaboration comes when working with researchers beyond our institution," Dr. Toogood says. "Sometimes a project requires giving secure access to colleagues beyond the University of Michigan, so they have access to the same real-time data. CDD Vault makes it easy to provide them with secure access on a granular basis so everyone can work with and contribute to the same data. CDD Vault makes it trivially easy to securely share data."

## Supports Secure Remote Access

Dr. Toogood appreciates the ease with which CDD Vault enables secure remote access to data—whether a researcher is working from home or traveling.

"Whether you're traveling or just working from home, we've found CDD Vault to be very easy to use in securely accessing needed data," Dr. Toogood says.

The same simplicity applies when securely accessing data from CDD Vaults deployed in different organizations.

"I do a certain amount of consulting outside the university, and many of the companies that I've worked with also employ CDD Vault as their primary data store," Dr. Toogood says. "When they are asking me to look at their data or make decisions based on their data, they're providing me access to their CDD Vault. At different points in time, I might have access to three different CDD Vault systems—maybe for a different university, and for a couple of different companies. It's been really easy for me to access those systems in a completely confidential way. There's no bleed from one to the other. I know which system I'm in. I know whose data I'm looking at. There's no crosstalk between any of them. And that's beautiful. It works so well."

## Preserving the Value of Older Data

The university-wide licensing at the University of Michigan makes it easy to protect the value of not just current data, but also of previously acquired data.

This is important as availability of data tends to decrease over time. A study published in *Cell* is headlined "The Availability of Research Data Declines Rapidly with Article Age." The authors wrote, in part: "For papers where the authors gave the status of their data, the odds of a data set being extant fell by 17% per year. In addition, the odds that we could find a working e-mail address for the first, last, or

corresponding author fell by 7% per year. Our results reinforce the notion that, in the long term, research data cannot be reliably preserved by individual researchers."

Dr. Toogood sees CDD Vault as helping to preserve older data in two ways:

- **Avoiding data loss from turnover**: "In an educational environment you are dealing with constant turnover of personnel," Dr. Toogood says. "Every time a student or faculty member leaves, you lose some institutional knowledge. To the extent that you can capture what they have done in an electronic format, you're doing the best job possible of trying to retain at least the information content—maybe not the experience and the know-how that they've developed—but at least the information and data that they generated during their time. This makes it available to the next generation, and hopefully people can build on that work going forward."
- **Avoiding data loss from uncentralized storage**: "Researchers have used various storage systems over the years, going from tapes to disks to CDs and other devices. I've got plenty of data stored in different formats that I'm not sure I can access any more. For instance, I've got data on CDs, yet don't have a CD ROM reader anymore. With our use of CDD Vault, I think we're at a state where the data that we're storing now in the cloud, which gets replicated and backed up, will mean that we can trust and rely on those data being available to us for many, many years to come."

## Visualization Tools to Explore Data

CDD Vault includes powerful visualization tools that all students and faculty can access for free as part of the university-wide licensing. This is significant because visualization is such a powerful research tool.

"I use the CDD Vault visualization tools all the time because I think that anytime you're looking at data, being able to interrogate it graphically is a huge bonus," Dr. Toogood says. "In chemistry and medicinal chemistry, in particular, it is very much about identifying trends. Whether looking for trends or for outliers, it's helpful to be able to look at datasets in a graphical way."

Having visualization tools built into CDD Vault makes them easier for researchers to access.

"Prior to the introduction of the graphical display tools within CDD Vault, you would have had to export the data, import it into some other application, which may or may not cost you something," Dr. Toogood says. "There are some very good free graphical display tools, but there are multiple steps involved in exporting and re-importing. So having visualization capability within a single platform makes it easy to use. If you find you are missing a piece of data, you can just grab it and replot it. Including visualization tools was a big step up for CDD that I was really glad to see."

## Embraces FAIR Data Principles

As noted in *Nature*, "There is an urgent need to improve the infrastructure supporting the reuse of scholarly data," which gave rise to the FAIR (Findable, Accessible, Interoperable, Reusable) Data Principles. CDD Vault embraces FAIR, as core to its Assay Registration system. The resulting standardized ontologies, with annotation flexibility, enable consistent query results, saving time and costs, bringing efficiency to research, collaboration, and preparation of publications and patents.

## 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.