



## Customer Case Study School-Wide Licensing

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**UIC** COLLABORATIVE ENGAGEMENT IN NOVEL THERAPEUTIC RESEARCH AND ENTERPRISE

# University of Illinois Chicago’s UICentre Enhances Collaboration and Data Integrity with School-Wide Licensing of CDD Vault

## Situation

The University of Illinois Collaborative Engagement in Novel Therapeutic Research and Enterprise (UICentre) is the campus-wide drug discovery initiative at the University of Illinois, Chicago that utilizes existing resources to leverage the expertise of scientist and clinician teams across campus in collaborative engagement in translational research in drug discovery and development.

The mission of UICentre is transformative: to instill a scientific culture, and build accompanying technological and educational infrastructure that overcome the obstacles to translational drug discovery at UIC. The expertise of UICentre ranges from target validation and bioassay development to high-

throughput screening analysis of novel compound libraries to medicinal chemistry incorporating structure-based, ligand-based and chemo-proteomics assisted drug design, in addition to pre-clinical drug metabolism and pharmacokinetic studies.

The specific aim of the UICentre is to create and support multidisciplinary collaborations that transform basic science projects into team-based drug discovery initiatives at UIC and across the Chicagoland academic community with the long-term objective of improving human health by creating novel drug candidates that can be translated into commercialized therapeutics.

## Solution

## UICentre | UIC's Campus-wide Drug Discovery Enterprise



**The University of Illinois Centre.** UICentre takes advantage of school-wide licensing of CDD Vault to enhance collaboration and data integrity.

The UICentre deployed Collaborative Drug Discovery's CDD Vault, the cloud-based scientific data management system that securely manages both internal and external biological and chemical data. Deployment includes CDD school-wide licensing, freeing individual labs and researchers from having to purchase separate licenses, while providing a unified solution for secure electronic data storage and electronic laboratory notebooks (ELN)s.

UICentre and associated labs have deployed five instances of CDD Vault. UICentre's CDD Vault stores more than 20,000 compounds.

### Benefits

The University of Illinois Centre has found a number of benefits since adopting CDD Vault with school-wide licensing, including:

- Providing labs with a "single source of truth"

- Enhanced collaboration between chemists and biologists
- Meeting NIH requirements for data management and protection
- Ensuring data integrity and supports deep exploration
- Substantial savings versus individual licensing
- Protecting intellectual property
- Electronic Notebooks enhance research efforts and help prepare students for industry

### School-Wide Licensing Provides Labs with a Single Source of Truth

UICentre values the ability of CDD Vault to provide researchers with a secure centralized data repository that provides what is often referred to as "a single source of truth."

"With CDD Vault, everyone is looking at the same data," Dr. Carlier says. "You don't have one person looking at an Excel spreadsheet

from a month ago, and another looking at one from last week, while you are trying to discuss the most current findings.”

“The confusion that comes from poor version control is very frustrating,” Dr. Carlier says. “Using CDD Vault we have all our data stored in a central data repository that our whole team and collaborators can look at. A secure, centralized repository is enabling. It helps keep a team focused on what are the latest findings and best hits.”



**Drug Discovery.** CDD Vault helps serves as a data repository for UICentre’s campus-wide drug discovery efforts.

## School-Wide Licensing Enhances Collaboration, Including Between Chemists and Biologists

School-wide licensing of CDD Vault makes for easier collaboration, including between chemists and biologists, Dr. Carlier finds.

“UICentre is the drug discovery center of the University of Illinois, Chicago, and we are funded by many stakeholders across the university,” Dr. Carlier says. “Our goal is to encourage collaborations with principal investigators from across the College of Medicine, the College of Pharmacy, and the College of Chemistry. We started using CDD Vault in the Fall of 2022 and it was quite clear that this platform could be transformational in creating collaborative teams. It makes it easy for chemists and biologists to work closely together.”

Dr. Carlier notes that the completeness of the data that can be stored in CDD Vault enables looking at old data in a new way.

“It is critical that we be able to see not just the data that we like and remember, but also the data that we didn't understand and sort of put on the backburner,” Dr. Carlier says. “Having all of the data in one repository allows you to go back with high fidelity to reinvestigate your hypothesis. One of the benefits of CDD Vault is that you can ask questions of big datasets, that help refine your conclusions. It helps us to not just look at the beautiful molecules that test positive in our assays, but at the ugly ones as well, to see what we can learn from them.”

## School-Wide Site Licensing Helps Meet NIH Requirements for Data Management and Protection

The NIH [introduced](#) its Data Management and Sharing Policy as part of its longstanding commitment to making the results of NIH-funded research available. The NIH writes: “Responsible data management and sharing has many benefits, including accelerating the pace of biomedical research, enabling validation of

research results, and providing accessibility to high-value datasets.”

UICentre has found that its use of CDD Vault makes it easy to comply with the NIH Data Management and Sharing Policy.

“As NIH-funded researchers we need to document our data management plan to the NIH when submitting our grant proposals,” Dr. Carlier says. “The NIH is very concerned that you have some way to track all your data and that you're not going to lose it. In our NIH applications, we state that we have CDD Vault, explain how we use it, and that all of our data is stored within the Vault so we can go back to reprocess it at any time.”

Even before the NIH issued its data management requirements, other research partners were requiring use of electronic data storage.

“Prior to UICentre’s adoption of CDD Vault, our sister institute, the Institute for Tuberculosis Research, was mandated to use CDD Vault by one of its chief partners,” Dr. Carlier says. “When organizations provide funds for research they want to make sure that the data is well managed and its value preserved.”

## **CDD Vault Helps Ensure Data Integrity and Supports Deep Exploration**

UICentre uses CDD Vault to store all raw data to help ensure the integrity of its findings, and to help ensure findings can be replicated.

“An experiment might measure drug response across several concentrations, and we'll capture mid-curve data in terms of IC50 or EC50 or some other measure,” Dr. Carlier says. “These

are numbers that we would typically report in journal articles, but it's much better if you can capture all the raw data, which is what we can do with CDD Vault. We can also see how many times an experiment was done, how many technical replicates, how many biological replicates. All of this can be precisely tracked through the assay dates.”

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original data in new ways.

“We might screen 10,000 compounds for a particular biological activity, and we would naturally focus on the small percentage of compounds that performed well in our testing,” Dr. Carlier says. “We then might draw conclusions based on the activity and the structures of those compounds that tested positive. If we see they all have a methyl group, benzene ring, or some other common structure, we might want to go back and look at the other 99% in our raw data to see how common the structure is to help gauge the significance. With

all or our raw data stored in CDD Vault, this type of deeper exploration is very easy to do.”

## School-Wide Licensing Provides Savings Vs. Individual Licensing

School-wide licensing makes it easy for researchers at UICentre and other campus labs to integrate CDD Vault into their work.

Speaking from his experience at earlier sites in his career, Dr. Carlier says the absence of school-wide licensing turns adoption of electronic data storage into a financial decision made one researcher or one lab at a time. He also finds that school-wide licensing lowers the price point per user, which also encourages adoption of this technology that can enhance drug discovery.

“Electronic data storage is so important to drug research that you want to lower the barriers for entry for all who can benefit from it,” Dr. Carlier says. “School-wide licensing helps reduce the barriers.”

## “Protecting IP is Absolutely Essential ... This is Another Area Where CDD Vault Really Shines”

The granular security of CDD Vault helps UICentre and other campus labs protect intellectual property.

“Protecting IP is absolutely essential, and this is another area where CDD Vault really shines,” Dr. Carlier says. “Within UICentre we have people working on different projects. One might be an NIH-funded grant, another might be a Gates Foundation grant. People on one team have access to their own data in the Vault, but unless there is a need, and they are given access, they can’t see data for another team’s

work. CDD Vault also provides levels of access, such as the ability to just read data, or to interact with it.”

“In addition to being director of UICentre, I’m PI for my malaria therapeutic lab in the Department of Pharmaceutical Sciences,” Dr. Carlier says. “The people in my malaria lab can’t see data from projects in the UICentre, and researchers in the UICentre can’t see data from the malaria lab. Keeping data firewalled like this helps protect IP.”

Dr. Carlier also sees CDD Vault value for holding

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all of the data needed for filing a patent.

## Electronic Lab Notebooks Enhance Research Efforts, and Great for Students

The searchability of electronic lab notebooks enhance research efforts, and use of an ELN also helps prepare students for work in the private sector.

“Searchability is one of the biggest benefits provided by something like the CDD Vault Electronic Lab Notebook, which is why I encourage everyone in our labs to use one,” Dr. Carlier says. “It is difficult to go searching

through a traditional paper notebook. Using an ELN also allows you to store all the confirmatory data used in establishing proof of structure and purity.”

“Without something like an ELN and CDD Vault, searching for data even when electronically stored can be difficult,” Dr. Carlier says. “Is the data on a hard drive on a server somewhere? What happens if you forget to backup your data and it gets lost? Is all of your data on the same computer? This is why something like CDD Vault and its integrated ELN is so valuable to the drug discovery process.”

Dr. Carlier also believes it is important for students to become accustomed to using an ELN because this is what they will likely be asked to do when working in the private sector.

“Even if they go to work for a pharmaceutical company with its own proprietary system, using CDD Vault prepares them for working with electronic data storage,” Dr. Carlier says.

## Ease of Use

UICentre researchers have found CDD Vault to be easy to use, which makes for an easier transition to electronic data storage.

“We don’t have an IT staff member to manage CDD Vault, because we don’t need that support,” Dr. Carlier says. “It took about five minutes for me to learn how to upload my own data. We have colleagues who will say: ‘Hey this is great, let me show you how we use it.’”

Coupled with ease of use are safeguards built into CDD Vault that prevent data from being improperly loaded. “You don’t have to worry about accidentally loading data into the wrong column or something, because the system flags errors to protect the data. CDD also has

excellent help and troubleshooters when needed.”

## CDD Vault 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](http://www.collaborativedrug.com).