



Customer Case Study

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- Christopher Michael McBride, Director, 858 Therapeutics



858 Therapeutics Uses CDD Vault and its ELN for “Supporting Research Efforts from Concept to Clinic”

Situation

858 Therapeutics is a biotechnology and drug discovery company developing a portfolio of small molecule drugs that act on novel therapeutic targets in oncology, including proteins that regulate RNA and the innate immune response.

858 was founded by a veteran team who together bring a track record of success in pharma and biotech drug discovery. Building from its collective experience in the fields of epigenetics, single-cell genomics, and innate immunity, 858 Therapeutics scientists are dedicated to the company’s mission to discover innovative therapeutics for the treatment of cancers that are resistant to current therapies.

Headquartered in the biotech hub of San Diego, CA, the company maintains lab operations in

both San Diego and New York City, providing proximity to leading investigators and scientific talent on both coasts of the US.

858 needed a drug discovery informatics platform that was comprehensive, yet user friendly—for its internal scientists, as well as for CROs it works with around the globe. High on the want list was a powerful electronic lab notebook (ELN) to enhance collaboration and to help establish and protect its intellectual property. The company also wanted a system that made it easy to register and track new compounds.

Solution

858 Therapeutics deployed Collaborative Drug Discovery’s CDD Vault, the hosted drug discovery informatics platform that securely

manages both internal and external biological and chemical data.

The choice was guided by two of its scientists who had used CDD Vault at other organizations.

“The database we had at our earlier company was very clunky and made things difficult when it came time to write up our proposals for development candidates and stage ourselves for IND preparation,” says Chris McBride, Director at 858 Therapeutics. “Our scientists who had previously worked with CDD Vault at another organization made a strong case for it. We tested CDD Vault, saw that it provided everything we were looking for and deployed it.”

So far 858 Therapeutics has deployed four instances of CDD Vault:

- **Corporate Vault.** The Corporate Vault is the company’s main repository, holding experimentals describing the synthesis of promising compounds that the scientists have created along with associated biological data and inventory tracking.
- **Virtual Vault.** The Virtual Vault is used for exploration and generation of ideas. It is used heavily by chemists for prioritizing and tracking potential products while providing separation from the company’s compounds of more immediate interest.
- **Chemical Inventory Vault.** The Chemical Inventory Vault is used to store intermediates and related data for inventory tracking. Inventory is tracked in-house and across multiple CROs.
- **Sandbox Vault.** The Sandbox Vault was created for storing conceptual data and compounds that could be of interest further into the future.

The company uses CDD Vault across its research efforts, including for:



- **Collaboration.** 858 uses CDD Vault as a collaboration center for all of its research employees—including CROs. “CDD has tight security settings so we can precisely share data with a CRO on a project basis, while completely restricting access to all other Vault data,” McBride says.
- **Registering Compounds.** All compounds acquired or synthesized for 858 discovery programs are registered into CDD Vault.
- **Tracking Work with the ELN.** All work performed by 858 internal scientists, as well as work performed by its chemistry CROs, is recorded in the CDD Vault ELN. So far, the company has made more than 18,000 ELN entries. Time-stamped entries in the ELN help the company document the discovery process and establish intellectual property rights. McBride says: “The CDD ELN is crucial for us as chemists, and we like that it is integrated with all the biological data which is viewable with just a click.”
- **Data Visualization.** 858 takes advantage of the data visualization built into CDD—a process that with their previous solution required exiting to a 3rd-party application.



CDD Visualization. 858 Therapeutics uses CDD Vault’s dynamic analysis tool to visualize drug discovery data.

858 Therapeutics initially rolled out CDD Vault for use by 10 of its scientists and soon afterwards expanded its use throughout the company. Cross-Vault searchability enables 858 to seamlessly search for data across its four CDD Vaults as if they were one.

Benefits

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

- Providing a “One-stop shop supporting research from Concept to Clinic”
- Intuitive ease of use
- Easy to administer
- Built-In data visualization
- Documenting with the ELN to establish and protect intellectual property
- Streamlining work with CROs
- Security & Vault segmentation

- Easier reporting

Providing a “One-Stop Shop Supporting Our Research from Concept to Clinic”

858 Therapeutics finds CDD Vault to be a complete drug discovery informatics platform, freeing it from the expense and frustration of assembling a collection of separate applications.

“CDD Vault provides a one-stop shop for us, supporting our research efforts from concept to clinic,” McBride says. “We can use CDD Vault from the conception of ideas, through synthesis and into biological and ADME assays, into animal studies, through the preparation of an IND and the supporting documents needed to move things forward.”

This is a welcome relief from previous solutions that consisted of a collection of separate special-purpose applications.

“Before you might have a product for the biological data, another for your ELN, another for biologists to work with data uploaded into the database, another product for visualization, and maybe another for your inventory,” McBride says. “CDD has done a really good job of integrating all of these features into a one-stop shop. This makes life easier for our scientists, and you always know exactly where your data is.”

Intuitive Ease of Use

858 Therapeutics is pleased with the ease of use they’ve found with CDD Vault.

CDD Vault also makes it easy for 858 to integrate operations with their CROs.

“With CDD Vault, it's very easy for the chemists to highlight the compounds they want to go out for ADME screening at a CRO or whatever other tasks we need performed,” McBride says. “The ELN is so easy to use that it helps ensure that everyone stays current on documenting their work.”

CDD Vault’s integration with the CAS numbers also provides ease of use. “You can just type in CAS numbers and it’ll pull up structures for you when you’re drawing reaction schemes,” McBride says. “This makes it easy to put together a reaction scheme and minimizes errors in drawing structures.”

The company also enjoys the ability to customize CDD Vault.

“We can develop protocols to do things like charting our inventory as a living entity—rather

“Everybody has found CDD Vault to be very intuitive and user-friendly.”

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858 Therapeutics**

than just a static registry,” McBride says. “We use CDD Vault to track things in real-time.”

Easy to Administer

CDD Vault has proven to be an easy drug discovery informatics platform for the company to administer. McBride and one of his colleagues handle CDD Vault administration on a part-time basis.

“At a previous company with about double the headcount, we had an informatics group to administer all of the applications,” McBride says. “There were so many different licenses and so many different applications that everyone had to be trained on, that it was definitely a full-time job. CDD Vault requires very little time to keep up and running.”

Built-In Data Visualization

The data visualization built into CDD Vault makes it easy for scientists at 858 Therapeutics to identify significant variables, without having to go into a separate visualization application.

“Very often in medicinal chemistry, the performance—especially in ADME or tox assays—is dictated by one of a few physico-chemical properties,” McBride says. “Being able to chart those against performance in different assays is very useful when we’re trying to predict the next set of compounds we should make.”

Data visualization can make significant relationships pop into view, compared with studying columns of data.

“When you put these things in a table, points of interest may not be readily apparent,” McBride says. “But significant relationships can jump out at you when you put them in a histogram or scatterplot, which is very easy to do with the CDD Vault visualization tools. Visualization can make it very apparent that there's maybe a cutoff in tPSA, or molecular weight, or in other chemical descriptors that we like to use. CDD Visualization is a very nice feature, and it is seamless to use. We don't have to move data to another application.”

Documenting with the ELN “To Make Things Like IP Clear Cut”

The CDD Vault ELN is helping 858 Therapeutics document its current scientific work and discovery.

“When it comes to time to do things like documenting inventorship for IP and that sort of thing, it's very clear cut when people have been drawing pictures in their ELN,” McBride says. “All entries in the CDD ELN are timestamped, so we have a registration date. This documents when people were thinking about things and what they contributed. You want to make things like IP clear-cut.”

McBride encourages scientists to work with an ELN page open at all times, and to drag and drop things into the CDD Vault.

“Whenever they have ideas around something, whenever new data comes out, whenever they see something that might inspire a new analog, we encourage them to just go ahead and draw

it out in the ELN, maybe make a couple of comments.”

He says the CDD Vault ELN makes all of this easy. “You can just take a snapshot and drag and drop it into the ELN, along with any other supporting information, literature, or other data,” McBride says. “If you do a search, it's really easy to pull in any routes and just drop them in there. This enables the synthesis and helps build the case for inventorship.”

All of this helps the scientists keep their eye on the prize.

“At the end of the day, our goal is to file an IND, and that process can be extremely painful,”

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McBride says. “Anybody who has gone through that process knows just how laborious it is to pull all of the data out and bring everything together. This is why our use of the ELN is so important. We may also at some point need to undergo due diligence, whether it's from potential partners or buyers. Using CDD Vault and its ELN will make it easier to pull together all of the data we need.”

Streamlines Working with CROs

858 Therapeutics has found that CDD Vault greatly streamlines working with its CROs around the world. CROs enter their work

directly into the ELN, providing great visibility into project progression.

“It used to be that our CROs typically used paper notebooks,” McBride says. “The CDD Vault ELN is so intuitive and easy to use, that we just give our CROs an hour of training and they are up and running using the ELN. And after we train one person in a CRO, they train others who come onto the project.”

Moving CROs from paper notebooks to the ELN has simplified project tracking and record keeping.

“We’ve gone from a situation in which CROs would send us these giant boxes of paper notebooks, to them entering data directly into the ELN,” McBride says. “With everyone inputting data to the ELN, we can monitor efforts on a day-to-day basis, and ensure they’re capturing all the information that we’re going to need to support the scale-up of lead series and intellectual property filings. The ELN is a powerful tool for managing CRO efforts as well as our own internal work.”

The company appreciates the ease with which its internal and external scientists can make ELN entries and share data with others on a project.

“CDD Vault makes it easy to attach data to share with others,” McBride says. “People can just drag and drop files. The ease of use means there’s really no excuse for not putting all your supporting data into the ELN. This includes anything a scientist has generated along the way that might help us later with efficiencies of reactions, side products, or anything else that could be of value. It’s just so convenient.”

Security & Vault Segmentation

CDD Vault provides multi-layered security for its informatics platform, including the use of TLS encryption for data in transit, as well as dual firewalls. CDD Vault also allows precision Vault segmentation, so scientists, including CROs, can only access project areas for which they are given specific access.

“With CDD Vault, I can give a CRO access to the specific projects they’re working on,” McBride says. “For example, we have a CRO in India that might be working on multiple projects, but they can’t see any data outside of the segmentation we’ve created for them with CDD Vault. This

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gives us all the advantages of having a centralized data-sharing platform, while maintaining strict controls on data access and security.”

Easier Reporting

Having CDD Vault as a central repository for research data simplifies creating custom reports.

“I’m constantly having to communicate with people about what direction we need to hit next, and CDD makes it extremely convenient to create things like SAR tables to make the case,”

McBride says. “In the past, you would have to go mine the data, and then you'd have to get ChemDraw out and create a bunch of structures. Then you'd have to create a table in PowerPoint and populate all the data yourself. CDD allows you to do all of this easily without leaving the platform.”

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.