CDD VAULT®
Complexity Simplified

Customer Case Study

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- Adam Kallel, Senior Director of Computational Chemistry, Plexium

Plexium

Plexium Moves to CDD Vault, Reduces Admin from 3 Informaticians to Just 1 Part-Time, "Returning Them to Science"

Situation

Plexium is an emerging biotechnology company focused on discovering and developing protein degrading therapeutics to treat cancer and other serious diseases, utilizing the company's DELPhe platform to identify novel small molecules that redirect E3 ligases to targets of interest or induce degradation of targets by directly binding to them.

The company's interests include identifying E3 ligase-binding small molecules that redirect the immune system or increase its function in immunosuppressive environments. With an understanding of the relevant activating and inhibitory signals that impact immune cell function, Plexium identifies small molecules that will restore desired signaling and optimize beneficial immune cell responses.

Plexium's biologists, chemists, and engineers needed a central repository for storing and accessing entities. The software solution it was using was difficult to load, cumbersome to use, and limited in its ability to support searches. The company needed a better solution.

Solution

Plexium conducted a head-to-head test between its existing solution and Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both private and external biological and chemical data.

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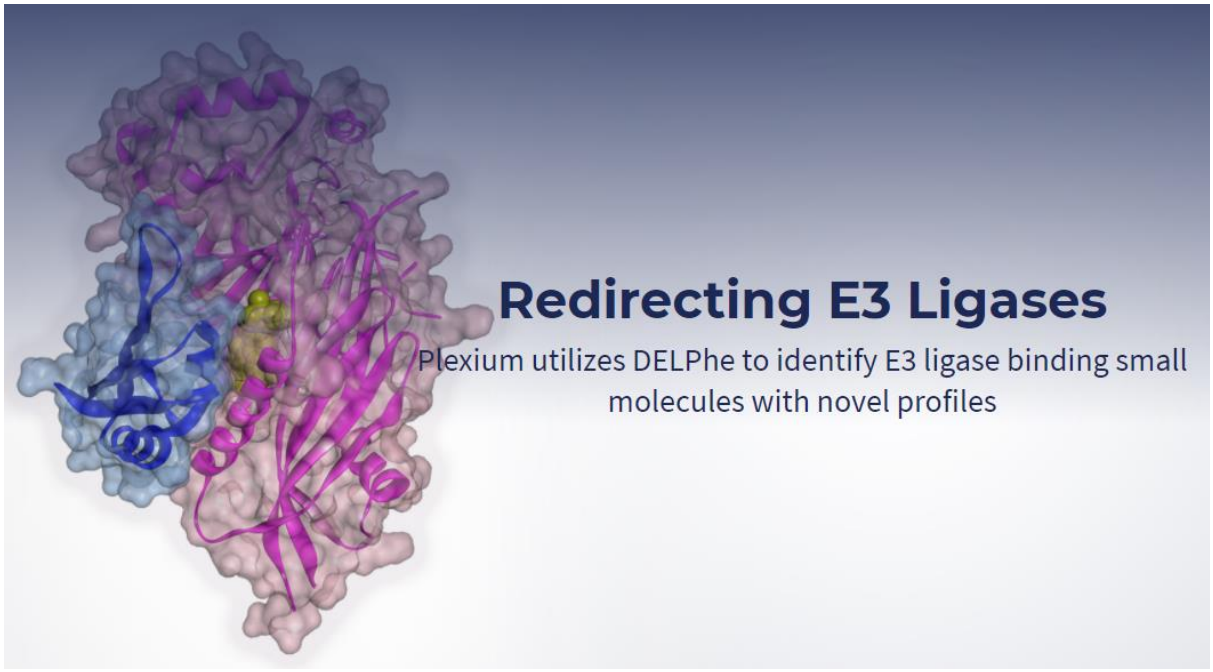


Plexium uses CDD Vault to support its pioneering work.

Kallel, Senior Director of Computational Chemistry at Plexium. "It was a unanimous decision, and we've all been extremely happy we made the change. Because of its ease of use and robust search capabilities, CDD Vault makes life easier for all of us."

About 25 Plexium scientists and engineers use CDD Vault, which is a complete informatics platform hosted through an intuitive web interface. Plexium takes advantage of CDD Vault's Multi-Vault capabilities to store some 300,000 entities across five different Vaults:

- Internal compound collection Vault, for individually synthesized compounds
- Reagents Vault
- Bulk compound combinatorial library Vault, for individual containers of collections of combinatorial compounds
- Individual compounds Vault, for the combinatorial libraries
- MolPort catalog Vault

Having a robust drug discovery informatics platform is especially important to Plexium in its work screening DNA-encoded small molecule libraries in picoliter to nanoliter volumes. The company's innovations enable both cell-based and biochemical assays, redefining high-throughput screening.

Experiments are performed in picowells with a signal bead coated with a given small molecule and associated DNA tag in each well. Small molecules can be released from the bead in a controlled dose. Cell lysates are analyzed in a multiplex manner across selected biological readouts, providing rich information on small molecule activity.

Benefits

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

- Ease of use.
- Ease of administration, allowing system administrators to be reduced from 3 full-time informaticians, to just one part-timer, freeing them to return to science.
- User friendly ELN, enabling 100% compliance.
- Central repository to ensure everyone is dealing with the most recent data.
- Multi-Vault storage and searchability.
- Enjoying CDD as a great company to work with, and exceptional customer support.

Ease of Use

Plexium values the ease of use that CDD Vault has brought to their operations, as their previous system was difficult to learn, and difficult to use—including loading data for storage.

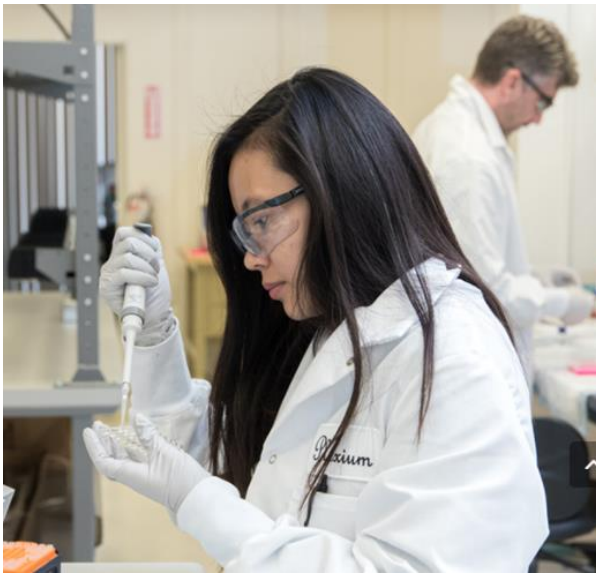
"Our old system had a three-day training for the full database management, and even after that it was extremely difficult to use," Kallel says. "When we moved to CDD Vault, we had a one-hour training, and that's all that was required."

Onboarding new users is also a snap.

"I can onboard a new user in about 15 minutes, and they are ready to go," Kallel says. "With our old system it would take hours, and it was so complicated that people were reluctant to use it."

Ease of use extends to performing queries.

"Performing queries was overly complicated in our old system, especially using Boolean logic," Kallel says. "Queries are so much easier in CDD Vault, including operations such as a substructure query coupled with a query across an assay type, for example. Everything is just easier."



Plexium scientists appreciate CDD Vault's ease of use.

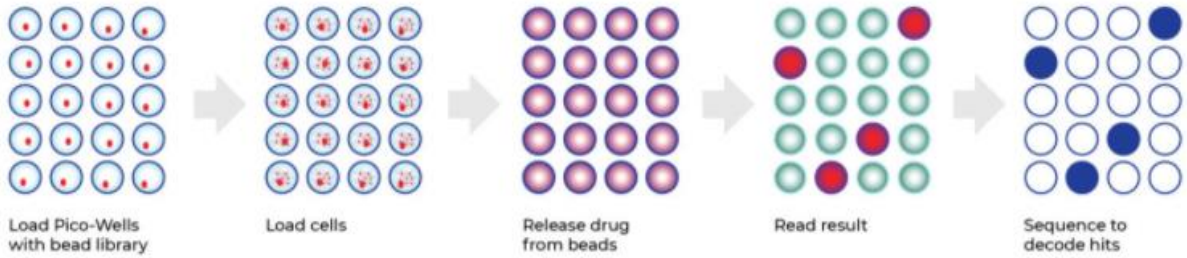
Plexium also values the CDD Vault assay system, including its assay tracker.

"We use CDD Vault to store formulas, assay data, and associations with compounds," Kallel says. "If you have ADME data, you can write the formula into the assay system and store your ADME data. We also use the ELN system to store our study reports, and any other information that may be useful."

User Friendly Electronic Lab Notebook Means Better Compliance

The overall ease of use of CDD Vault includes its electronic lab notebook—something that is greatly appreciated by Plexium.

"The CDD ELN system is so much easier for our people to use," Kallel says. "Our previous ELN system was very formalized and required the chemists to use it in a specific manner, so everyone, including the biologists, appreciate that CDD Vault allows them to just drag and drop spectra as PDF files. It lets them put in the



CDD Vault makes it easy for Plexium scientists to store and retrieve data on their DNA beads.

reaction scheme just by sketching it in with Marvin. And it's much easier for compliance. Our previous ELN system was so cumbersome and difficult to use, that not all of our ELNs were always up to date. With CDD Vault, our compliance has gone up to 100%."

Kallel notes that ELN compliance is especially important for patent data and protection of intellectual property.

"100% ELN compliance means that our intellectual property is protected, whereas before, it sometimes wasn't," Kallel says. "You have to be able to show documentation for patent protection, and some of our scientists weren't keeping their notebooks up to date—just because the old ELN was so difficult to work with. Having everyone in 100% compliance is a great relief for all of us. I really appreciate the ease of use that CDD brings to ELNs because as part of my responsibilities I used to have to serve as the ELN police, running around making sure everyone was in compliance."

System Administrators Reduced from 3 Fulltime to 1 Part Time

The same ease of use that makes CDD Vault simple for scientists to learn and use also translates to an extreme reduction in the efforts required to administer the system.

"With our old solution we had three informaticians working full time to manage it," Kallel says. "Now we are down to just me, and it is an extremely part-time effort. The other two informaticians are freed to work on important experimental and instrumentation projects and they're able to concentrate on bioinformatics and help the engineers work on automated routines to pick hits from the screening."

For Kallel, the ease of managing CDD Vault has enabled him to return to doing science.

"Managing CDD Vault requires so little effort, that I've been able to return to my modeling work," Kallel says. "I'm a card-carrying computational chemist, so it is great to be able to spend more of my time on computational chemistry."

One reason systems administration has become just a part time task is that the ease of use of CDD Vault means that scientists can do their own self-servicing.

"With our old system if a biologist wanted to set up an assay, it would require an hour of my time to program in the assay, and this wasn't something you could just teach the person and expect them to do," Kallel says. "In contrast, now I can teach a biologist how to add an assay in just 15 minutes."

Kallel continues: “People can also self-service for registering compounds, upload libraries, and perform all manner of other tasks that used to require help. The CDD Vault assay protocol is insanely flexible and easy to use. We track how RXN degrades DNA on beads, and were able to easily set up the protocol for that.”

Central Repository Ensures Everyone Dealing with Most Recent Data

CDD Vault has given Plexium a central repository into which it can store all information—whether coming from its chemists, biologists, or engineers.

“We now have the ability to put all of the data in one place,” Kallel says. “And it doesn't matter what kind of information we’re storing. We can store PDF files, Excel spreadsheets, PowerPoints, assays, DNA bar codes, all of these things, and they all get indexed, and they're all searchable. The ability to store whatever we need, and have it all searchable is hugely important, greatly enhancing efficiency.”

The previous system made it difficult to load information, so too often data was held in noncentralized locations. The problem was multiplied by the fact chemists, biologists, and engineers had their own storage needs and methods.

“Having a central repository means we no longer have to go searching through folders on different network drives,” Kallel says. “CDD Vault is a one-stop shop that people can go to and find all their information.”

This eliminates what Kallel says was an ongoing concern about working with the most recent data.

“When people used to store data on Excel spreadsheets and on shared drives, the big concern was always: Is this the most current data set? Or is it sitting on somebody’s hard drive,” Kallel says. “With CDD Vault we know exactly where to find our data and we can know it is the most recent version.”

CDD Vault has also made it easy for Plexium scientists to store and retrieve data on their DNA beads.

“We have DNA encoding on the beads, and the sequencing is stored on DNA bar codes,” Kallel says. “We store all of this in the vault, which makes it simple to search across and access the DNA bar code information. This is something we couldn’t do with our previous system.”

Multi-Vault Storage & Searchability

Plexium, as noted earlier, uses five different Vaults within CDD Vault. The Multi-Vault capability provides storage for specialized interests, while the Multi-Vault searchability of CDD Vault means that all data is visible for search and queries.

The company also likes the ease with which they can customize search tables, something they couldn’t do within their previous system.

“I’m a big fan of the customizable search that CDD Vault provides because it allows you to tightly tailor searches to meet your precise needs,” Kallel says. “For example, I do a lot of QSAR, so when I search for a particular assay type, I don't want to see the dose response curve. I don't want to know all the other assays. I just want to get the structure so I can get the SD file and the geometric mean of the IC50. With CDD Vault, I can just have that set up as the default search, which is great.”

Kallel also values CDD Vision, which provides powerful and intuitive visual analysis and plotting features, and seamlessly integrates with CDD Vault.

“Let’s say someone wants to run a logD among chemical properties,” Kallel says. “They can just use Vision to plot it and start looking for correlations.”

The storage and searchability of CDD Vault also makes it easy to work with combinatorial libraries.

“If a screener wants to do something such as going back to validate a hit, they need to be able to easily find out the exact location of the vial containing the beads,” Kallel says. “In terms of being able to search for reagents, if you're searching for boronic acid, for example, you want to be able to eliminate things that we already have in our collection, so we aren’t buying duplicates. We save a few thousand dollars a month by avoiding duplicate purchases. All of this makes the ability to search across multiple Vaults a big deal.”

Great Company to Work With: “We Get Almost Instant Response … Our Old Company Could Take Days”

Plexium has found CDD Vault to be a great company to work with.

“We get almost instant response,” Kallel says. “I've never had to wait more than a half an hour or so. If an issue is complex, they will put me directly in touch with a developer. Our old solution was a nightmare for support, they could take days to get back to you.”

Kallel also appreciates the solid, well-tested, code that CDD Vault puts out when releasing updates.

“We’ve never seen CDD roll out a patch or a new version and have it break something,” Kallel says. “With our previous solution, their new releases would frequently break something. And sometimes the fixes they released would break something else. So we appreciate the effort that CDD puts into testing before release.”

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.