



Customer Case Study

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- Jeffrey Albert, Ph.D., SVP of Medicinal Chemistry, X-Chem



X-Chem Finds CDD Vault's Ease of Use Slashes Weeks from CRO Project Times

Situation

X-Chem Montreal (formerly known as IntelliSyn) is among the leading independent providers of drug discovery support in North America. The company was formed by members of the AstraZeneca leadership team following the site closure in Montreal. The company's experienced scientists have in-depth understanding of all aspects of medicinal chemistry and the expertise to accelerate drug discovery of clinically viable, maximally de-risked drug candidates.

The company's state-of-the-art facility in Montreal is fully equipped to support all aspects of drug discovery, from hit ID to clinical candidate nomination. The company was formed to bring highly efficient capabilities and experienced personnel to rapidly advance clients' projects on a reliable, secure, and economical basis.

Jeffrey Albert, Ph.D., Senior Vice President at X-Chem, gained more than 20 years of experience in Medicinal Chemistry at AstraZeneca in the US and in Canada, serving as Section Head in the Lead Discovery Department and as Project Leader in the Neuroscience Department.

When forming X-Chem Montreal, they needed to choose a secure informatics platform flexible enough to support the company's fast-paced work.

Solution

X-Chem adopted Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both private and external biological and chemical data.

It was an easy choice.



X-Chem provides integrated drug discovery support

“We used CDD Vault at AstraZeneca, and it worked so well that we required some of our CROs to also use it,” Dr. Albert says. “CDD Vault is popular because of its flexibility and ease of use. So when starting our own company, it was natural to use CDD Vault, and we’re really happy that we did.”

About 50 X-Chem scientists use CDD Vault, which is a complete informatics platform hosted through an intuitive web interface. X-Chem uses CDD Vault to help its project teams manage, analyze, and present data for their biotech customers, to store some 500,000 compounds and about 75,000 fragments.

X-Chem values the tight security built into CDD Vault, including the ability for teams to provide granular, role-based access to data. CDD Vault also provides cross-discipline tools for both chemists and biologists. This helps chemical structures registered by chemists and assay

results captured by biologists to reveal structure-activity relationships.

“We use CDD Vault as a front end for database analysis, trend analysis, and building structure-activity relationships,” Dr. Albert says. “We also use CDD Vault as the underlying infrastructure to bring data into Spotfire and other analytic tools that allow us to interrogate the results and set up different mathematical models.”

X-Chem also likes the predictive models of CDD Vault.

“The CDD Vault predictive models are quite good,” Dr. Albert says. “We find the CRP model used is superior to the XRP that we find in other packages.”

Benefits

X-Chem has enjoyed a number of benefits since adopting CDD Vault, including ease of use,

faster implementations & customizations, powerful flexibility & agility, a great platform for organizing, cleaning, & analyzing data, and impressive support.

Ease of Use “I’m a Chemist, Not a Data Scientist ... I Find it Intuitive”

X-Chem has found that CDD Vault has ease of use—from deployment onward. The company especially values that the product is so easy to use that they no longer are dependent upon backend engineers for deployment and configurations—as had been the case at other companies that X-Chem scientists have worked with.

“CDD Vault is very robust in enabling our scientists to collect, curate, and utilize data from many, many databases,” Dr. Albert says. “And it is able to do all of this without requiring back end IT support. I’m a chemist. I’m not a data scientist, yet I find it quite intuitive.”

Throughout his career, Dr. Albert has been involved in setting up a number of different databases, including those specified by collaborators. He’s never found one as easy to set up, use, and modify as CDD Vault.

“I’ve worked with many databases, going back to RAS and to even before ISIS Base,” Dr. Albert says. “While databases today tend to have similar functionality, CDD Vault seems to be, in my assessment, unique in the sense that it doesn't require back end IT support.”

Faster Implementations and Customizations

The user-friendly design of CDD Vault, which has freed the X-Chem team from having to

route change requests through an IT department or service provider means scientists can do their own implementations and customizations in real time.

CROs pride themselves in being fast and efficient. So, it can be frustrating when administrative complexity gets in the way.

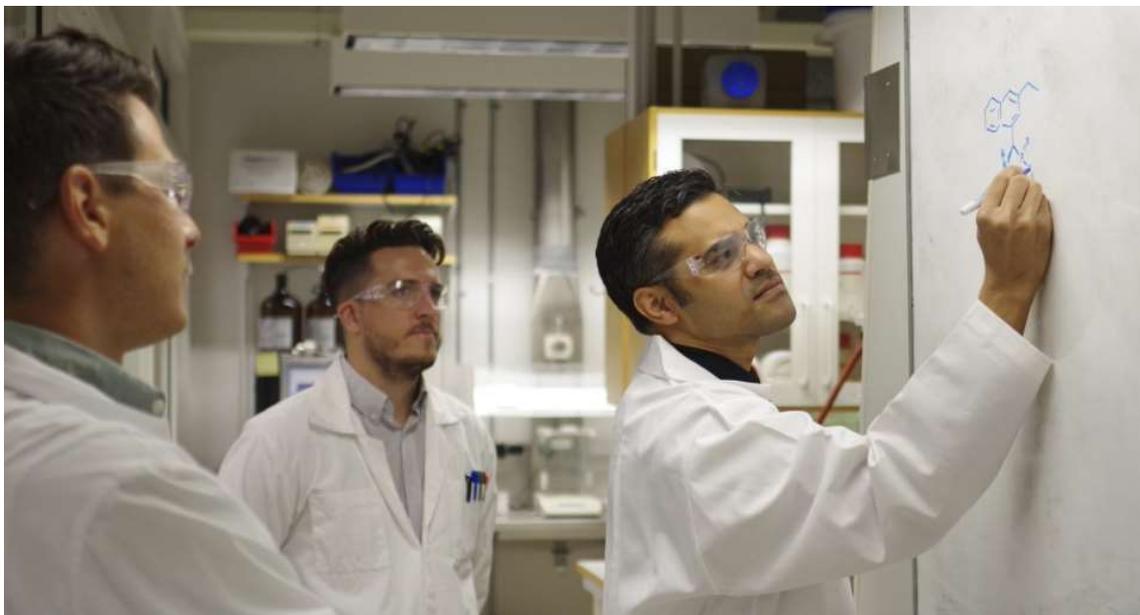
“Implementation speed is always of interest,” Dr. Albert says. “With CDD Vault we can import data for a new project that has hundreds of

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“For example, if we want to set up a new model or even a new collaboration, we don't need to have dedicated IT infrastructure, which also means we don't have to wait a week or more to get things set up,” Dr. Albert says. “We can do it ourselves in real time, and the resulting output is pretty close—or identical—to the capabilities



X-Chem also provides process improvement and scale-up excellence.

that we had when working inside major pharma.”

This contrasts with having to work with some customers with less flexible systems, in which change requests had to be routed through layers of IT support groups.

“In cases like that the lead time between identifying a problem and getting a solution could run anywhere from a week to never,” Dr. Albert says. “This is frustrating when you know you could do the same thing with CDD Vault in a matter of minutes, or at longest a single day.”

Powerful Flexibility & Agility to Support Fast-Moving Collaboration

The flexibility of CDD Vault gives X-Chem the agility it needs to support the fast-moving collaborations it has with companies on the leading edge of pharma R&D.

“We’re working with some of the fastest moving companies in the industry, and it’s important that we stay at the leading edge in terms of collecting, curating, and sharing data in a very fluid and interactive way,” Dr. Albert says. “CDD Vault gives us the ability to analyze data sets in very flexible ways, as well as the ability to securely share our findings in real time.”

Providing just one example of how X-Chem uses the flexibility of CDD Vault, Dr. Albert pointed to fingerprinting compounds.

“If we need to generate fingerprints across a database of 10,000 compounds, I can generate the fingerprints in 10 different styles, roll them all back into CDD, and then use structure searching to integrate all of that together,” Dr. Albert says. “I can add data and customize and tailor things in a very flexible way and use CDD to host all of that without cluttering the key core repository of information. This gives use

the flexibility to add things that we may want to change at some point in the future.”

Without CDD Vault, he notes that such work would be difficult to do. “You could do it in Excel, but then it would no longer be available for anyone in the future, because they wouldn't know which version was used, and the findings would be shared via e-mail or something. But if it's not captured in the database, it essentially doesn't exist.”

The flexibility of CDD Vault also helps ensure readiness for future needs.

“We tend to be involved in fast-moving collaborations, so that flexibility in being able to share data with various stakeholders and to be able to present that, interrogate it in a flexible way is essential,” Dr. Albert says. “We don't know how we'll be analyzing some of our data next year or a year from now, so we need to have that flexibility. We now have future-proofed flexibility that we can count on being able to split tests, or combine tests, or reanalyze things as future needs require.”

Great Platform for Organizing, Cleaning, & Analyzing Data

X-Chem has found CDD Vault to be a robust platform for organizing, cleaning, and analyzing data—while integrating easily with other tools.

“We use CDD to bring in significantly large numbers of compounds, and it does an excellent job of identifying tautomers and different stereogenic centers,” Dr. Albert says. “CDD Vault works seamlessly with other systems. I can go back and forth between CDD and generating SD files or Spotfire files, smoothly using these tools in an integrated way.”

Each new project begins with pulling data into CDD Vault. “A company might come to us with an academic asset and \$40 million in biobucks and three years to make their milestone,” Dr. Albert says. “They will have lots of data, but it can be in spreadsheets and data stores and they don't have a clear vision of how to begin their exploration.”

“We tell them we'll have it uploaded and ready on Monday,” Dr. Albert continues. “They are always delighted. Suddenly they see their data organized in a database repository, where they can begin doing structural searches and other functions.”

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CDD Vault proves especially valuable in cases in which a customer comes to them with a tangle of data from multiple systems and sources that needs to be cleaned and unified.

“One large, well-established company came to us with some specific problems, seeking our assistance to help them advance past some hurdles that they were having with their in vivo data,” Dr. Albert says. “They were using one of the large, well-known databases, but were unable to segregate out the data that they needed us to have access to. We solved the problem with CDD Vault and took over



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management of those data moving forward in the project.”

Another project involved analysis of fragment libraries from multiple sources to identify replicates and other characteristics.

“I was able to upload 500,000 compounds into CDD Vault and was done within a few hours,” Dr. Albert recalls. “Working in other environments, with other databases, this would have required going to IT experts and scheduling the task, which could have taken days or weeks. We don’t have time for that in this fast-moving business.”

Great Company: “I Feel Like CDD Support People are Just Like Me”

While it isn’t often that X-Chem needs to contact CDD support, Dr. Albert says it is a welcome change from what he has experienced with other companies.

“I’m continuously impressed by the professionalism and knowledge of the CDD support team,” Dr. Albert says.

This stands in sharp contrast to what Dr. Albert and his colleagues have experienced with other companies.

“Others will first ask you to write up a web request, which goes into the queue, and then you get a low-level person, who is trying to do their job, but the technical issues we bring them are not going to be solved by restarting the computer,” Dr. Albert says. “So, you gradually escalate to somebody who actually gets it, and then they need to make a use case, and then it may get done within a

month or so. But by that time, we probably don’t even need the data. The opportunity is gone.”

This is why CDD is so much appreciated.

“When I contact CDD, I get immediate results,” Dr. Albert says. “I feel like CDD people are just like me. Their support staff know what I want from informatics and articulate it better than I can. No other company comes even close.”

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.