CDD VAULT®
Complexity Simplified

NVIDIA.

"We use computational modelling to generate starting structures where they don't exist. Even when there are structures, we can use tools like AlphaFold to look for different forms and to carry different protein models forward."

- Josh Pottel, Ph.D., President and CEO of Molecular Forecaster Inc.

Customer Case Study

molecular forecaster

MFI uses CDD Vault for Enhanced Collaboration and Efficiency in Data Management, Sees Opportunity in Integrations of NVIDIA NIMs

Situation

Molecular Forecaster Inc. (MFI) is a computational chemistry company with expertise in drug discovery, quantum mechanics, molecular dynamics, chemoinformatics, and artificial intelligence. Offering world-leading proprietary software, algorithms, and contract research services, MFI works with organizations looking to fast-track preclinical drug discovery, from start-up biotechs to established pharma.
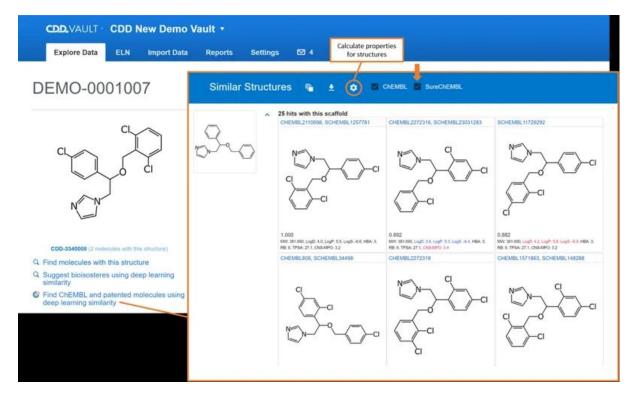
MFI's innovative software platforms are powered by chemistry-driven predictive tools, seamlessly integrating biophysics and machine learning. This enables tailored experimental design and workflow automation, all without relying on third-party applications.

MFI needed a better way to store and share data with its many collaborators across industry and academic institutions. As the company grew, it was no longer practical nor efficient to work with spreadsheets.

Solution

Molecular Forecaster Inc. deployed Collaborative Drug Discovery's CDD Vault, the hosted drug discovery informatics platform that securely manages both internal and external biological and chemical data.

While MFI considered other options, the company decided to go with CDD Vault.

"We did our due diligence," says Josh Pottel, PhD, CEO of Molecular Forecaster Inc. (MFI).

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The CDD Vault AI module generates bioisosteres to speed drug discovery.

"CDD Vault has a strong reputation with organizations we work with in Montreal and beyond. CDD is well known, and highly respected in all things data management and collaboration."

The collaboration element is especially important to MFI.

"Collaboration is one of our core values. We have that word written on the wall," Dr. Pottel says. "So having tools that help us interact more efficiently and effectively with our clients and partners, as well as helping us collaborate more efficiently internally, is extremely important to us."

Beyond CDD Vault providing a secure central repository for data and collaboration, MFI has started working with the CDD Vault AI module, which supports researchers managing and interpreting complex datasets, predicting compound behavior, and identifying potential leads with greater precision, and is directly integrated with the CDD Visualization module for multiparameter optimization.

The CDD Vault AI module includes Generative Bioisosteres and ultrafast deep learning similarity search within CDD Vault to suggest new molecules.

MFI also uses AlphaFold2, the deep learning model that reduces the time it takes to determine a protein's structure. CDD Vault integrates AlphaFold2 from NVIDIA's BioNeMo NIM microservices to provide seamless workflows between CDD Vault and AlphaFold2.

"We use computational modelling to generate starting structures where structures don't exist," Dr. Pottel says. "Even when there are

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structures, we can use tools like AlphaFold2 to look for different forms and to carry different protein models forward. This allows us more shots on goal in our research efforts."

Benefits

Molecular Forecaster Inc. sees potential in the combination of CDD Vault and NVIDIA technologies:

- CDD Vault provides a secure central repository
- Creates a strong collaboration environment
- Ideating using the CDD Vault AI module

CDD Vault Provides a Secure Central Repository

Molecular Forecaster Inc. subdivides its CDD Vault into separate vaults for each of the different projects it works on so data from one project can't be seen by researchers working on other projects.

"We have our vault configured so that each project has its own vault within the vault," Dr. Pottel says. "The central repository we have with CDD Vault is so much more efficient than tracking spreadsheets as we previously had to do."

Dr. Pottel notes that sharing spreadsheets can accumulate errors through copy and paste mistakes or problems with version control.

"Sending spreadsheets back and forth, the date changes, the name changes, you might end up sharing a file that somebody updated, but another person didn't update, so you're working off two different versions," Dr. Pottel says. "Data errors can encroach like a broken telephone quite easily in our world. So, any way

that you can improve on that is good. CDD Vault eliminates those problems."

Mihai Burai-Pătrașcu, Ph.D., Director Computer Aided-Drug Design at Molecular Forecaster, adds: "CDD Vault provides a way in which we can centralize all the data that we get from different assays, experiments, simulations, and other work, from our own efforts as well as those of our clients and partners."

The company values the efficiency they've gained using CDD Vault as a central repository.

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"CDD Vault increases our efficiency in communicating and knowing where to go for analyzing data," Dr. Pottel says. "The central repository becomes more important the more people and projects and data that you bring together."

Creates a Strong Collaboration Environment

Collaboration is central to MFI's drug discovery work, especially given the number of projects in works on and the breadth of its work.

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"We work with quantum chemists to structural biologists, and everything in between," Dr. Pottel says. "With CDD Vault, researchers with different expertise can look at the same data differently. The more we can share all the information, the better we can derive the most knowledge from it."

Having CDD Vault as a collaboration tool makes it easy for everyone to have secure access to the same data across time and geography.

"We currently have a use case where we are working on a public-private grant partnership with McGill University," Dr. Pottel says. "We are working with CROs doing some of the experimental work. We're doing computational prediction. Synthesis happens in the academic institution, and then biochemical assays are being run by another partner, TransBioTech, based out of Quebec City."

"Lots of data is generated: binding data, functional data, other parameters like solubility," Dr. Pottel continues. "We all need immediate access to all this data. It's all part of the DMTA—design, make, test, analyze cycle. All these parties to share information, so having our common central repository for information is essential."

Ideating Using CDD Vault AI Module

MFI sees the CDD Vault AI module's generative bioisosteres function as a source of new ideas and insights when evaluating molecules. The company also likes that the AI module includes within-vault access to resources including the ChEMBL and SureChEMBL databases of bioactive molecules, and to Enamine, the chemical supplier.

"If you do an initial virtual screening and have hits, it is great to have the AI module's bioisosteres to get like a quick glance of what other molecules could be of potential interest," Dr. Burai-Pătrașcu says. "We can look for close analogs and compare different properties and then suggest better compounds for further SAR testing. Its integration with ChEMBL, SureChEMBL and Enamine also helps determine what can be synthesized or purchased."

Integration of AlphaFold2

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"A client might come to us for help with a protein that, for example, is of interest in treating Parkinson's disease," Dr. Pottel says. "They might have reason to believe that a biological mechanism might go through protein A, and they want to interact with that in some way, to either inhibit it or activate it or do something else. That protein A may have a crystal structure, it may have a cryo-EM structure, or it may have no reported structure at all.

"In every single case, AlphaFold2 has something to bring as a tool," Dr. Pottel continues. "In the case where there is no known structure, AlphaFold2 will generate you one. There are other tools. You can use a homology model and base it off of a similar target, but AlphaFold2 is another way to get a starting point and perhaps a different perspective."

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.

About NVIDIA

NVIDIA (NASDAQ: NVDA) is the world leader in accelerated computing.

Certain statements in this press release including, but not limited to, statements as to: the benefits, impact, availability, and performance of NVIDIA's products, services, and technologies, including NVIDIA AI Foundry, NVIDIA NIM microservices, NVIDIA Blueprints, NVIDIA RAPIDS, NVIDIA AI Enterprise software platform, NVIDIA BioNeMo, NVIDIA MONAI, NVIDIA DGX B200 systems, NVIDIA Blackwell architecture, and NVIDIA DGX Cloud; NVIDIA's partnership and collaboration with third parties, and the benefit and impact thereof; third parties adopting NVIDIA's products and technologies, the benefits and impact thereof, and the features and performance of their offerings; and the combination of NVIDIA's AI and accelerated computing capabilities with the expertise of industry leaders being poised to usher in a new era of medical and biological innovation and improve patient outcomes worldwide are forward-looking statements that are subject to risks and uncertainties that could cause results to be materially different than expectations. Important factors that could cause actual results to differ materially include: global economic conditions; our reliance on third parties to manufacture, assemble, package and test our products; the impact of technological development and competition; development of new products and technologies or enhancements to our existing product and technologies; market acceptance of our products or our partners' products; design, manufacturing or software defects; changes in consumer preferences or demands; changes in industry standards and interfaces; unexpected loss of performance of our products or technologies when integrated into systems; as well as other factors detailed from time to time in the most recent reports NVIDIA files with the Securities and Exchange Commission, or SEC, including, but not limited to, its annual report on Form 10-K and quarterly reports on Form 10-Q. Copies of reports filed with the SEC are posted on the company's website and are available from NVIDIA without charge. These forward-looking statements are not guarantees of future performance and speak only as of the date hereof, and, except as required by law, NVIDIA disclaims any obligation to update these forward-looking statements to reflect future events or circumstances.

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About Molecular Forecaster Inc. (MFI)

Molecular Forecaster Inc. (MFI) helps organizations make smarter decisions in drug design. We've spent six years democratizing computer-aided drug design via our highly collaborative research-as-a-service model. Today, we're integrating what we've learned into new and improved software tools. Our goal? To become the go-to partner in small molecule drug design, combining proprietary technology, our expertise and know-how, and our all-in approach to collaboration that sets our partners up for success.

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