CDD VAULT®
Complexity Simplified

Schrödinger

Customer Case Study

"You can support the full loop of the design/make/test cycle using CDD Vault and Schrödinger LiveDesign."
- Dr. Mary Mader, Vice President Molecular Innovation, Indiana Biosciences Research Institute

INDIANA BIOSCIENCES RESEARCH INSTITUTE

Indiana Biosciences Research Institute Enables Drug Discovery Using CDD Vault and Schrödinger LiveDesign

Situation

The Indiana Biosciences Research Institute (IBRI) is a leading translational research center that advances academic and industry science through collaboration to improve patient health outcomes. The IBRI supports translational research across a number of areas, including diabetes, Alzheimer's disease and pediatric rare diseases.

As part of its translational research efforts, the IBRI is committed to accelerating digital drug design. Using automated informatics workflows, incorporating in silico modeling and property predictions, and connecting data and teams to facilitate seamless collaboration are ways the IBRI is enabling accelerated drug design and research.

As these modern approaches leverage increasing amounts of complex data, there are significant challenges to ensure this information is accessible, usable, and updated in real-time for the scientists and project teams involved.

Dr. Mary Mader, Vice President of Molecular Innovation at the IBRI, explained that the institute recognized a need for an efficient drug discovery informatics platform that could seamlessly integrate visualization, physics, and 3D space modeling.

The Technology Solution

After evaluating a number of options, the IBRI deployed a solution using Collaborative Drug Discovery's CDD Vault and Schrödinger's LiveDesign. CDD Vault is the hosted drug

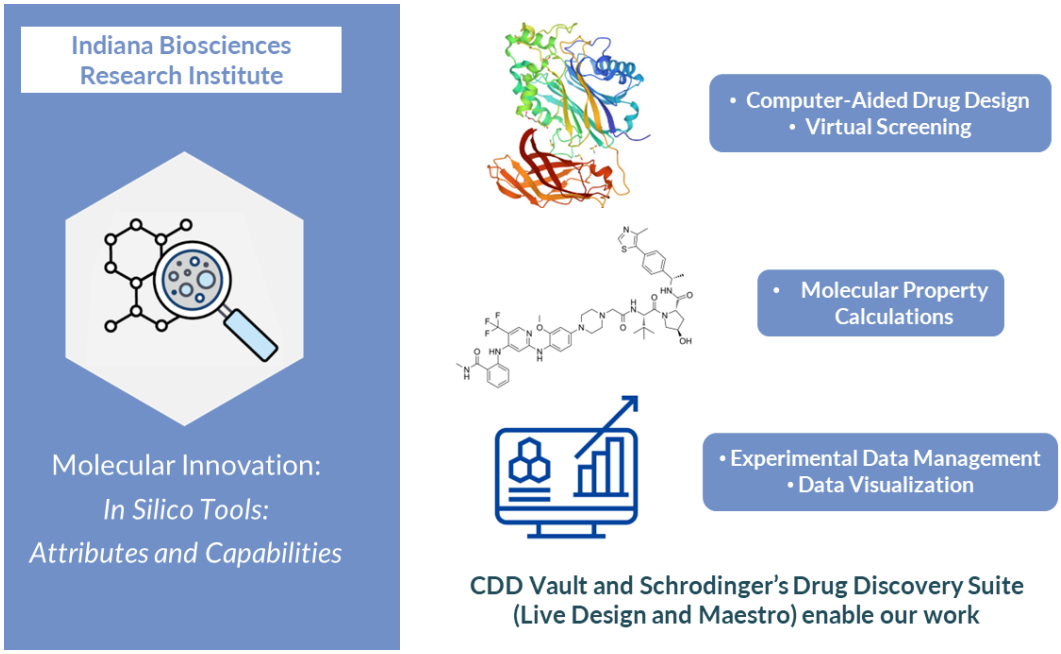
Indiana Biosciences Research Institute. Advancing academic and industry science through collaboration to improve patient health outcomes.

discovery informatics platform that securely manages both internal and external biological and chemical data. LiveDesign is a cloud-native enterprise informatics platform that enables teams to rapidly advance drug discovery projects by collaborating, designing, experimenting, analyzing, tracking, and reporting in a centralized platform.

“When we were initiating the Molecular Innovation Group, we were partnering with investigators at the Indiana University School of Medicine,” says Jay McGill, PhD, Chief Operating Officer and Executive Vice President of Administration at the IBRI. “We looked at various tools for specific parts of the process—including tools for sample registration and for doing molecular calculations. We brought a lot of these tools together for evaluation. We found the best solution for us was CDD Vault integrated with Schrödinger’s LiveDesign.”

“Experimental data capture and analysis are core to what we want to be able to do and to what we want our academic partners to have access to,” Mader says. “We’ve achieved this using CDD Vault in partnership with Schrodinger's Drug Discovery suite, including LiveDesign.”

Scientists at the IBRI use CDD Vault for registration of compounds, data storage, and its visualization tools, including data curves, to perform initial analysis; meanwhile LiveDesign is used to perform computational modeling and further analysis on data, including for SAR analysis and 3D molecular modeling.



Scientists at the IBRI drive their drug discovery workflows by integrating CDD Vault and Schrödinger's Drug Discovery Suite (LiveDesign and Maestro).

Benefits

The IBRI has found a number of benefits since adopting this multi-tool approach, including:

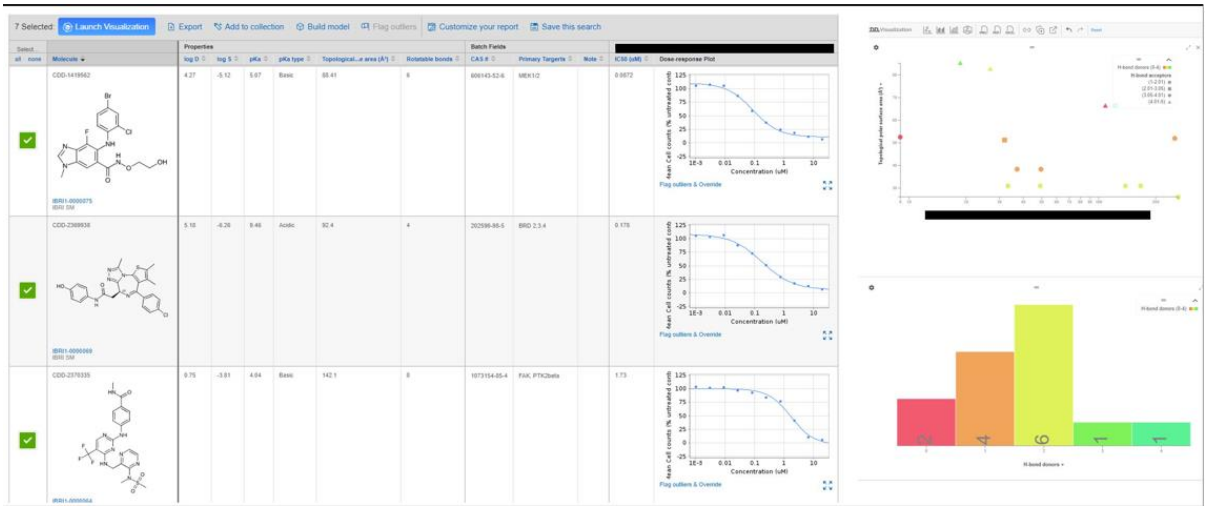
- Supporting a "single version of the truth"
- Streamlining workflows through integration of complementary solutions
- Integrating the full Design-Make-Test-Analyze cycle

Supporting a "Single Version of the Truth"

The IBRI's dedication to speeding the translation of scientific research into health care advances required a drug discovery informatics platform that could serve as a secure central data store and provide what Mader refers to as "a single version of the truth."

"When you're trying to share data across a number of different partners in different departments and different institutions, Excel spreadsheets aren't scalable," Mader says. "Several of us here at the IBRI came from an industrial background where storage of data into a data repository, and then having a common platform for data sharing, was something that we expected. But not all of the partners that we now work with have been accustomed to that. CDD Vault helps us achieve our vision of the IBRI both partnering with academic institutions, as well as providing a place to house startup companies and potential partners to come to Central Indiana and work in our lab space."

Mader values the flexibility CDD Vault provides in hosting diverse data types. "CDD Vault serves as a repository for all of our drug discovery needs, including cell lines, sequence



The IBRI team uses CDD Vault to archive and visualize calculated properties and essential data.

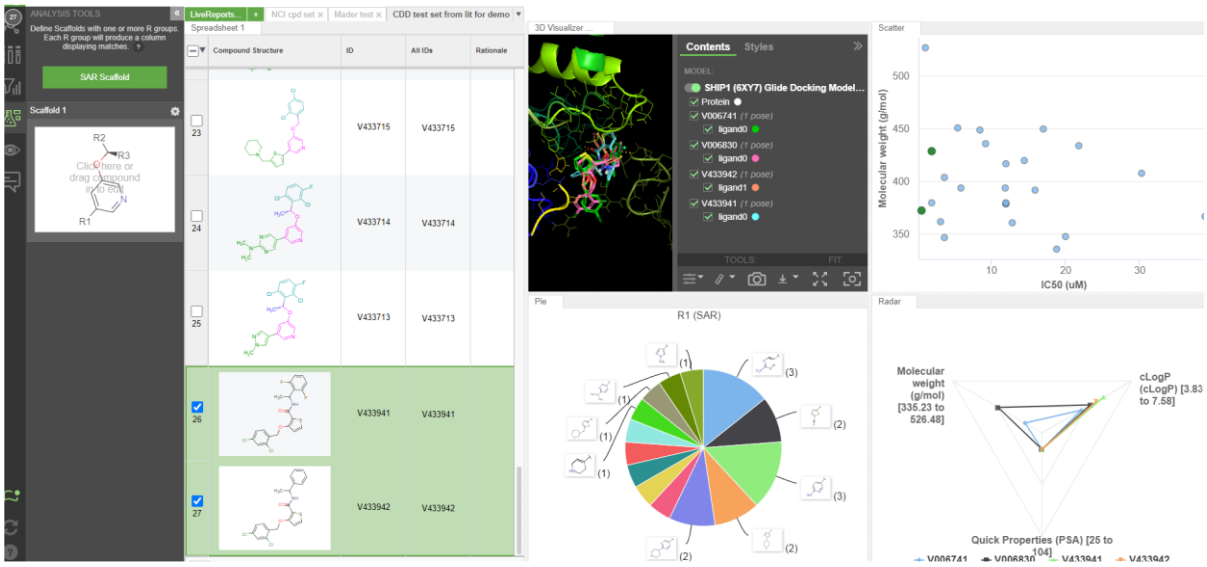
information, and differentiation protocols for iPSCs," Mader says. "Having a common place of data storage for members of the team to be able to access is extremely useful for us. It enables us to share data with our partners and keep everyone on the same page."

Streamlining Workflows through Integration of Complementary Solutions

"Because CDD partners with LiveDesign, researchers can draw from the data in CDD Vault when designing compounds in LiveDesign, to have all properties depicted in one view," Mader says. "You're not having to flip between two different pieces of software."

"Capturing synergy data depictions with LiveDesign and CDD Vault is powerful. We can have an image file stored of the synergy scoring protocols that we use so that we're aligned on the data analysis. We're all seeing the same information consistently across the project," says Mader. "Schrödinger's LiveDesign greatly enables compound analysis, including plotting SAR space, and understanding the SAR space associated with compounds that you have designed relative to existing compounds."

The seamless integration between CDD Vault and Schrödinger LiveDesign eliminates difficulties researchers previously had when shifting to other visualization tools – allowing teams to make better use of the tools they had at their fingertips. Mader noted, "Both of these tools have very good data visualization capabilities built within them, and you can work back and forth between them without interruption. Unlike tools I've worked with in the past, CDD Vault and Schrödinger LiveDesign allow you to create standardized views of ways that you want to analyze data or ways that you'd like the team to think about analyzing the data. This enables consistency in how a team sees a depiction of data, while also allowing them to create their own views, and share that information through CDD Vault. "



The IBRI team uses LiveDesign for real-time design iteration and detailed analysis, accessing data stored in CDD Vault.

Integrating the Full Design-Make-Test-Analyze Cycle

The IBRI has found that the combination of CDD Vault and Schrödinger LiveDesign supports the full Design-Make-Test-Analyze (DMTA) cycle of drug discovery.

"As you move into designing compounds, the ability to pull data from CDD Vault into LiveDesign to create new compounds is enormously powerful," Mader says. "Once in LiveDesign, you can create a workflow within data generation and compound design, and use docking tools, MPO scores, and a number of other parameters that are calculated for you. You can support the full loop of the design/ make/test cycle using CDD Vault and Schrödinger LiveDesign."

"If you have a body of data against target X from the literature, you can import that data and create a docking model to serve as the basis of design," Mader says. "You can use that model to try to identify new parts and pieces of a molecule that you might want to make. This sort of workflow for the designing, making, and testing of compounds gives you a larger picture of designed, potential molecules. From there you are able to select for characteristics of interest, see which meet the many criteria that you may be applying to your design hypothesis,

"We believe that our use of CDD Vault and Schrödinger LiveDesign will help speed this process. The value of these two tools comes in how they enable the drug discovery process."

- Jay McGill, PhD, Chief Operating Officer and Executive Vice President of Administration, Indiana Biosciences Research Institute

and then solve for within SAR. So, the workflow and access to the data tools that are available within these two pieces of software have accelerated this full loop process."

Combining Tools to Enable Drug Discovery

"Ultimately, for all of us, our success is measured by how many molecules we produce that become drugs that have a positive impact on patient health," McGill says. "We believe that our use of CDD Vault and Schrödinger LiveDesign will help speed this process. The value of these two tools comes in how they enable the drug discovery process."

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 Schrödinger

Schrödinger is transforming the way therapeutics and materials are discovered. Schrödinger has pioneered a physics-based computational platform that enables discovery of high-quality, novel molecules for drug development and materials applications more rapidly and at lower cost compared to traditional methods. The software platform is licensed by biopharmaceutical and industrial companies, academic institutions, and government laboratories around the world. Schrödinger's multidisciplinary drug discovery team also leverages the software platform to advance a portfolio of collaborative and proprietary programs to address unmet medical needs. Founded in 1990, Schrödinger has approximately 800 employees and is engaged with customers and collaborators in more than 70 countries. To learn more, visit us at https://www.schrodinger.com.