



CDD Vault: Secure, Collaborative, and Integrated Data Management for Academic Research



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[CDD Vault - Free Evaluation Licence](#)

Advancing Research with Powerful Data Management, ELN, Inventory, and Analytical Solutions Ensuring Data Sustainability

Abstract

CDD Vault is a cloud-based data management platform tailored for academic research and drug discovery, offering secure, collaborative, and reproducible work-flows. Its comprehensive suite of tools includes compound registration, assay management, inventory tracking, an Electronic Lab Notebook (ELN), data visualization, and protocol management, all designed to enhance research efficiency and secure collaboration where required. The tool is agnostic to any type of research, including small molecules, nucleotides, peptides, antibodies, proteins, mixtures, etc.

Introduction

Academic research requires robust, secure, and collaborative data management systems, especially in drug discovery and life sciences. Traditional methods like pen and paper can hinder progress, leading to misplaced data, repeated experiments, and inefficient hand-overs between researchers. CDD Vault offers a scalable, modern solution to overcome these challenges, enabling researchers to securely document, analyze, and share data across institutions with ease.

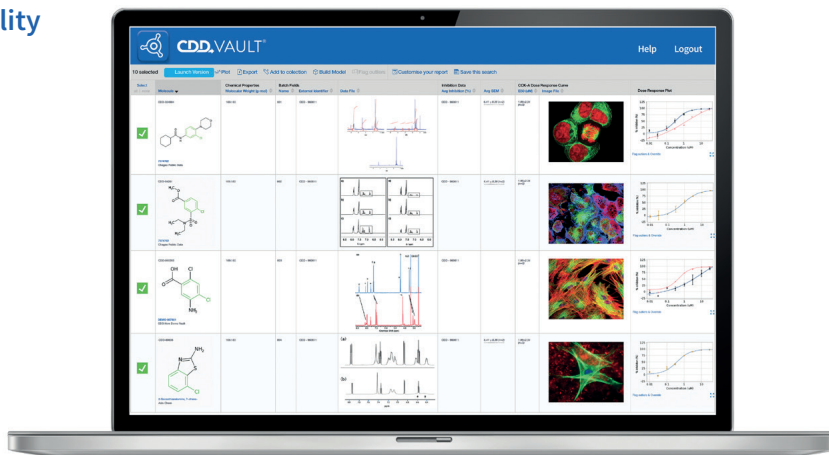
Explore how institutions using CDD Vault have improved compliance standards, safeguarded intellectual property, fostered cross-disciplinary collaboration, and significantly reduced costs through centralized, efficient data management.



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Complexity Simplified

I. Common Challenges Addressed

- Data Searchability and Accessibility
- Data Sustainability
- Private and Confidential Collaboration
- Novel Molecule Discovery and design efficiency
- Remote Data Access



Data Searchability and Accessibility

All research data is securely stored and indexed in a single location - Single Source of Truth. This simplifies searches by allowing researchers to filter through all uploaded data rapidly.

Data Sustainability

As all data is stored and kept in a single, secure location, no data is misplaced in lost paper notebooks, thumb drives, or laptops that leave the lab. This ensures that there is no more repeating of experiments but a smooth handover of projects when new researchers are on-boarded into the group.

Private and Confidential Collaboration

By facilitating seamless collaboration across departments and institutions, researchers can securely share datasets and insights in real-time, enhancing the efficiency of collaborative research projects. With access permissions and audit trails in place, you ensure that any modifications are tracked and all data is secure.

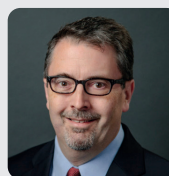
Novel Molecule Discovery and Design Efficiency

Enhance molecule design and streamline drug discovery work-flows as researchers can rapidly search databases like ChEMBL, SureChEMBL, Enamine, and CDD Public for similar structures without leaving CDD's secure environment.

The AI solutions prioritize synthesizable molecules, supporting a focus on practical and actionable outputs. An innovative bioisosteric suggestion algorithm improves molecular potency and pharmacokinetics, accelerating the development of new therapies.

Remote Data Access

CDD Vault's cloud-based platform allows students to securely access, review, and analyze experimental data from anywhere, ensuring they remain productive regardless of their location. By organizing data into a centralized system with intuitive tools for analysis and visualization, CDD Vault simplifies the process of interpreting results and gathering insights. This streamlined workflow enables students to focus on writing research papers efficiently, even when they are away from the lab or campus. With its reliable remote access, CDD Vault supports students in maintaining progress on their research and academic writing without interruption.



"Electronic data storage is so important to drug research that you need to lower the barriers for entry ... School-wide licensing helps reduce the barriers."

Paul Carlier, Ph.D.

Director, University of Illinois Centre, Hans W. Valteich Chair in Medicinal Chemistry, Professor for Pharmaceutical Sciences and Chemistry, University of Illinois



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II. Methods and Features

1. Core Features Included

- **Registration:** Manage compound/sample registration
- **Activity:** Capture and manage assay and screening data
- **Parser:** Direct data ingestion from instruments, minimizing data manipulation
- **Assay Management:** Additional features for organizing assay data
- **Protocol Forms:** Ontology-driven management of assay protocols
- **Visualization:** visualization to analyze assay data visually

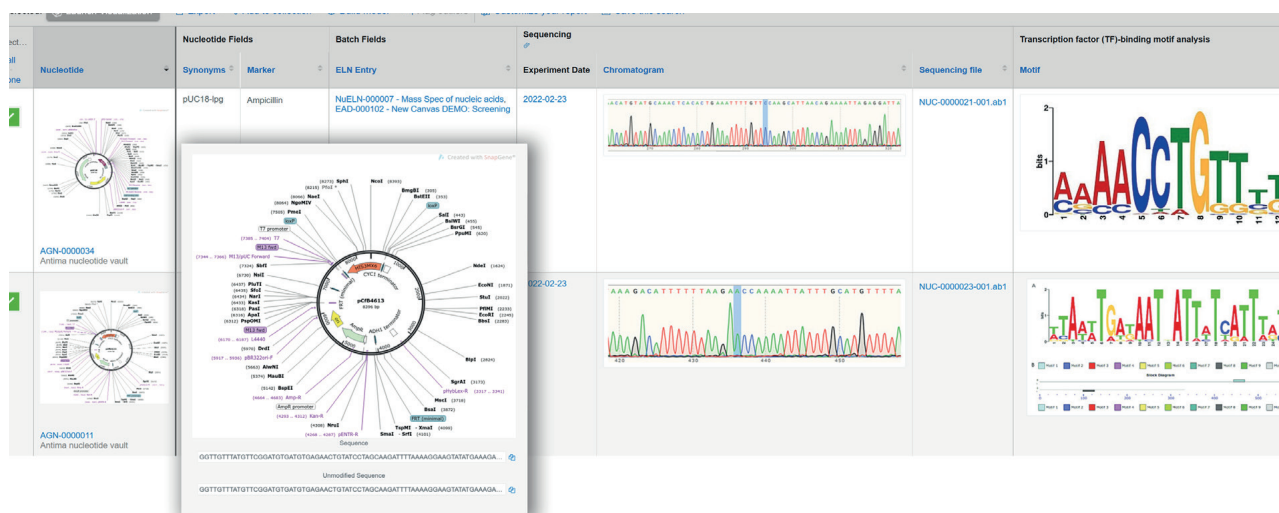
2. Additional Features (Optional Add-ons)

- **Electronic Lab Notebook (ELN):** Digitize and streamline lab notes and experimental data
- **Advanced Inventory:** Track samples with detailed location features (racks, freezers, etc.)
- **AI:** Advanced tool for identifying similar structures and generating bioisosteres, integrating ChEMBL, SureChEMBL, Enamine, and CDD Vault Public datasets
- **Curves & Analytics:** Plot various graphs, including time-dependent variables
- **Automation/API:** Access programmatic integration with CDD Vault using KNIME, R, Python, and Pipeline Pilot
 - Pre-built connectors for DataWarrior and Star Drop by Optibrium are available

Registration and Activity – Organize, Search, and Collaborate

Efficiently register, organize, and search research data in a secure, centralized platform. CDD Vault supports workflows for compound registration, bioassay management, and sample tracking.

Capacity for up to 2 million samples, compounds, and mixtures.







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III. Sample Workflows

1. Compound Registration and Structure-Activity Relationship (SAR) Analysis

Register New Compounds:

- Chemists or researchers log in to CDD Vault and use the Registration module to input new compound structures, including SMILES or InChI notations.
- Each compound receives a unique identifier and automatically calculated chemical properties, including but not limited to molecular weight, Log P, and pKa.
- Additional details such as synthesis date, batch information, purity etc., as well as activity data can be added by the user(s).

Organize Compound Data:

- Registered compounds can be categorized by properties such as compound type, target, and activity range, facilitating the easy retrieval of specific groups of compounds.
- Compounds can also be organized by project to streamline collaboration between teams or institutions.

Search and Analyze Compound Data:

- Researchers can use the multi-parameter search feature to look up sets of compounds by specific properties, including (sub)structures, activity data (e.g., IC50 values), and chemical properties, to analyze structure-activity relationships (SAR) with the help of the CDD Vault visualization tool.
- Within the visualization tool, compound results and parameters can be plotted using various plot types, such as scatter plots, histograms, and R-group decomposition, as well as a cluster analysis tool to help identify trends and relationships between structure and biological activity, aiding lead optimization.

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2. Bioassay Data Management and Analytics

Input Bioassay Data:

- After running an assay, scientists enter raw and calculated results into the Bioassay Management module, linking assay data to specific entities.
- The assay protocol, conditions, and data, such as IC50/EC50 values, are standardized and stored within the platform to ensure consistency across assays.

Organize and Annotate Results:

- Each assay can be tagged with information like target, cell line, or organism, enabling organized results tracking over time.
- Annotations and comments on assay performance or specific data points can be added, supporting communication among team members.

Analyze and Visualize Assay Data:

- The platform's visualization tools allow for trend analysis and comparisons across different assays, helping researchers prioritize entities based on efficacy.
- Customizable reports and automated data workflows can be configured for periodic analysis, streamlining ongoing screening campaigns.



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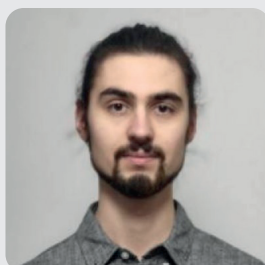
IV. Proven Impact on Academic Research



"After a brief introduction, I was immediately convinced that CDD was ideal for my project, where I need to keep track of a large molecular library. I was particularly impressed by the option of filtering for structural fragments. Creating a comparable setup myself would have taken an unmanageable amount of time. In addition, you can always rely on the outstanding customer support."

Leah Glanzmann

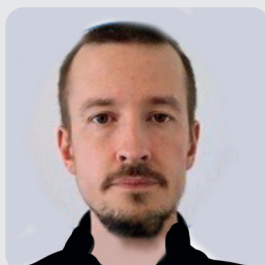
Doctoral Researcher, Universität Heidelberg



"I believe many of us will no longer want to do without the Volt and will encourage its use in our institutes as an alternative to cluttered folder structures on networks."

Leonard Trau

M.Sc. Candidate in Biotechnology, Universität of Munster, iGEM



"CDD was love at first sight for me. It is so intuitive to use that I picked it up in one day before I even received any training. The system is great for managing both structured and unstructured data."

Iwan Grion

Lab Manager, Universitätsklinikum Tübingen



"Continuity is a big issue in academia with so much knowledge being lost due to lab member turnover. With CDD Vault ELN, we have easy access to experiments from 5 years ago without digging through endless notebook pages. CDD is a launching pad that brings new scientists up to speed and gives them the freedom to focus on creative thinking."

Digamber Rane

Senior Researcher, Ohio State University



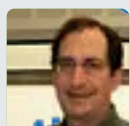
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V. Case Study

University of Illinois Chicago's UI Centre Enhances Collaboration and Data Integrity with School-Wide Licensing of CDD Vault

The University of Illinois Centre (University of Illinois Chicago) has found several benefits since adopting CDD Vault with school-wide licensing, including:

- Providing labs with a single source of truth
- Enhanced collaboration between chemists and biologists
- Meeting NIH requirements for data management and protection
- Ensuring data integrity and supporting deep exploration
- Substantial savings versus individual licensing
- Protecting intellectual property
- Electronic Notebooks enhance research efforts and help prepare students for industry



Brian Roth
Bryan Roth University of North Carolina School of Medicine | Pharmacology

"The CDD Database is an extremely elegant platform. I highly recommend it for anyone generating drug discovery data."

VI. Data Security and Compliance

Rigorous Data Security, Regulatory Compliance, IP Protection

- **User Permissions & Data Control:** Granular access controls for users, permissions, and data visibility.
 - **Communication Encryption:** SSL encryption secures all browser communications with CDD's websites.
 - **Application Security Testing:** Automated security testing ensures isolated access between vaults to prevent unauthorized data access.
 - **Firewall Protection:** Dual-layer firewall ("defence in depth") setup with both hardware and software protection for sensitive servers.
- More details in our Security White Paper, upon request.*
- With CDD Vault's audit trails and version control, researchers can validate experimental workflows and ensure research reproducibility.

CDD Vault: Europe-Specific Deployment

To meet the needs of our European customers, CDD Vault will offer a dedicated EU instance. Please contact info@collaborativedrug.com for additional information.

- **Data Residency Guaranteed:** Your data stays within the EU, ensuring compliance with GDPR and regional data regulations.
- **Enhanced Performance:** Reduced latency for European users.
- **Compliance You Can Trust:** Included in our SOC 2 Type II certification.
- **Seamless Experience:** Same functionality, security, and support as our global deployment.



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VII. Conclusion: Key Benefits of CDD Vault for Academic Research

- Secure, cloud-based data storage optimized for research
- Advanced visualization tools for data-driven insights
- Fully integrated ELN for comprehensive data documentation
- Streamlined collaboration across teams and institutions

CDD Vault empowers academic researchers with a secure, scalable, and user-friendly platform that enhances data management, collaboration, and discovery.

From streamlined work-flows to advanced visualization tools, it ensures that research teams can focus on innovation rather than data logistics.

By adopting CDD Vault, institutions can meet compliance standards, safeguard intellectual property, and foster cross-disciplinary collaboration, all while reducing costs through efficient, centralized data management.

Join the growing number of academic institutions leveraging CDD Vault to advance their research and experience the benefits of an integrated platform designed for modern challenges in drug discovery and life sciences.

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CONTACT INFORMATION:



cddvault.com

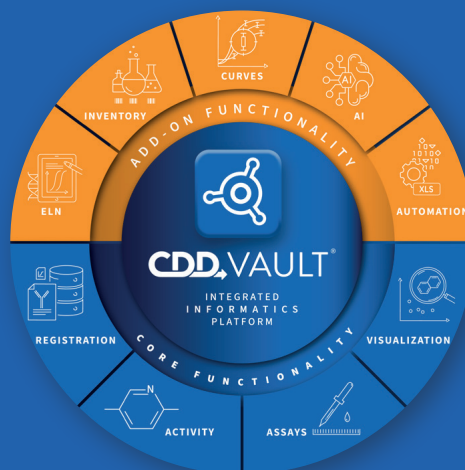


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