"This (CDD Vault) gives our clients the freedom to mine and explore that data themselves, allowing us to work collaboratively with them so that they can see the data in the same way that we see it.

- Andy Carr, Director of Chemistry Operations

Supporting RxCelerate to Accelerate Drug Discovery and Development Programs

CDD is pleased to highlight our collaboration with RxCelerate, an outsourced drug discovery and development company, based in Cambridge, UK, dedicated to delivering scientific excellence to a global client base within the biotech and pharma sectors.

They offer a comprehensive suite of services including *in silico* design, antibody discovery, synthetic and medicinal chemistry, bioanalysis, *in vitro* and preclinical services, and project management. Clients also benefit from proprietary platforms such as RxNfinity™ for rapid in silico screening, the Galaxy® platform for generating diverse 'clinic-ready' antibodies, and ProQuant® for precise bottom-up proteomics. For more information, visit www.rxcelerate.com or contact info@rxcelerate.com.

We spoke to three team members at RxCelerate to discuss their approach to drug discovery and

how CDD is supporting this with our flexible data repository and management platform.

Tailored Services and Expertise

Unlike traditional CROs that offer fixed, off-the-shelf assays and services, RxCelerate has built a business model focused on partnering with clients to design and deliver flexible, tailored services. Kate Willetts, RxCelerate's Head of Assay Development, explained, "Many of our

clients are early-stage, virtual or semi-virtual companies, so we become part of their project team and go beyond a traditional CRO service model, by offering scientific input and expertise, alongside access to our toolkit of technologies and services, to really help guide them along the drug discovery road."

> *"Having the Vault also means that if we're having an issue with one particular molecule, it's not synthetically accessible for example, we can apply that knowledge across multiple projects without inadvertently rediscovering the same issues."*
>
> Andy Carr, Director of Chemistry Operations, RxCelerate

Dr. Rebecca Clayton, Chemistry Project Manager, added, "Our size and integrated teams mean we can be very agile with how we approach each project, to ensure both efficiency and cost-effectiveness, this is important for small and virtual startups looking to validate their projects across cost, as well as scientific priorities, when looking to secure staged funding. We strategically implement the right assays at the right time to generate key results appropriate for each stage of the pipeline, to avoid unnecessary activities and ensure focused and efficient progress. If there is a pause in a project for weeks, months, or even years, we can pick it up again with the customer when they are ready."

Scalable Data Management with CDD Vault

In 2023, RxCelerate selected CDD Vault as their data repository and management platform for small molecule programs. Dr. Rebecca Clayton explained, "We needed a scalable, reliable, and user-friendly platform that would be accessible by people across departments and disciplines within RxCelerate." CDD Vault has provided RxCelerate with the tools to store, visualize, and manage assay and project data effectively, supporting their broad-ranging laboratory and project management capabilities.

Andy Carr, Director of Chemistry Operations, highlighted the benefits of the Vault, saying, "Having the Vault also means that if we're having an issue with one particular molecule, it's not synthetically accessible for example, we can apply that knowledge across multiple projects without inadvertently rediscovering the same issues."

Data Security and Accessibility

The CDD Vault platform is set up to compartmentalize data for each project, ensuring security and confidentiality.

Andy Carr explained the benefits of this, "This makes it easy, but safe, when sharing data with clients, while allowing RxCelerate's internal chemists and biologists the appropriate level of visibility internally. The user-friendly interface also means that functionality is more easily

added and navigated, while new personnel accessing our CDD Vault find it relatively hassle-free to learn how to use the platform."

Support and Implementation

CDD supported RxCelerate through an extensive demo and trial process of our platform. Dr. Rebecca Clayton noted that setting up the Vault with CDD's support was relatively straightforward, and ongoing support from the CDD experts is always available to the RxCelerate team.

Kate Willetts also added, "We've found all of the CDD team to be incredibly helpful, and they usually respond to and help us with any query within the day. If it's something really tricky, we can video call and tackle an issue in real time."

Data Upload and Management

Uploading historical data into the Vault involved setting up a suite of protocols and parsers to make the data compatible with the Vault structure. Kate Willetts acknowledged, "There was quite a lot of manipulation required to present the data correctly, but now we have those templates sorted the process is much quicker."

At the start of 2024, CDD updated its import data wizard to introduce a flexible parser that accommodates various data file formats, including plate layouts. Saved parsers can then be shared across Vault.

Kate Willetts explained "We appreciate the ability to set up mapping templates and parsers, making data uploads straightforward, as long as users select the correct parser and mapping template."

Dr. Rebecca Clayton added, "We are also uploading into the Vault data that we've generated with external CROs. This makes it easier to create a more complete and insightful package of data for each client."

Real-Time Data and Visualization

CDD Vault offers RxCelerate a suite of data visualization and analysis tools, adding valuable insight and connectivity to data across its clients' projects and pipelines. Dr. Rebecca Clayton highlights the value of the visualization tool, stating, "We can use the visualization tool on our data to evaluate trends in SAR and other key parameters. This tool removes the need to manually input data to create graphs for clients, saving critical time and aiding in timely decision-making."

Future Growth

RxCelerate is keen to try out new features and modules for the Vault as they are released, to evaluate their potential use both now, and going forward. For example, the Curves module makes it possible to automatically plot and compare curves across entities and protocols for potency, selectivity, ADME, toxicity, PK, and PD. A new PK module for the Vault is something that is of particular interest to RxCelerate. "We are really excited about that," Kate Willetts told us.

RxCelerate is also evaluating additional Vault functionality and modules, such as managing inventory beyond compounds. "The extent to

which the company will utilize Vault for more widespread inventory management is still being evaluated," Kate Willetts acknowledged, "but we have, for example, begun to get quite creative and use Vault to track and calculate how much material is used or left after weighing out to replenish stocks." Some simple protocols can make those calculations, giving us useful information that wasn't possible to derive using spreadsheets."

CDD Vault offers customers a suite of modules and functionality that can be added at any time.

Client Communication and Advice

RxCelerate uses a mix of approaches when communicating data to clients. Historically, data was abstracted and communicated offline from the Vault, but recently, clients have been given direct access to their data. Andy Carr notes, "This gives our clients the freedom to mine and explore that data themselves, allowing us to work collaboratively with them so that they can see the data in the same way that we see it."

Andy Carr was asked 'When considering data management, what advice would RxCelerate offer to newly established CROs, or to emerging pharma and biotech enterprises.'

He said, "Get your informatics solution sorted early," emphasizing the importance of scalable data management solutions.

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.

Benefits of Using CDD Vault for RxCelerate

Scalable and Reliable Platform: CDD Vault provides a scalable and reliable data management solution that grows with RxCelerate's needs.

User-Friendly Interface: The platform is accessible to users across departments, enhancing collaboration and data sharing.

Integrated Data Management: Allows for the integration of databases, visualization of results, and evaluation of trends across multiple studies.

Real-Time Data Access: Ensures that authorized users have real-time access to data, aiding in timely decision-making.

Secure Data Compartmentalization: Ensures data security and confidentiality while allowing internal teams to navigate and link molecules and assays.

Comprehensive Support: CDD offers extensive demo and trial processes, along with ongoing support to ensure smooth operations.

Collaborative Drug Discovery – RxCelerate Case Study