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Using CDD Vault to Manage Redbrick Molecular Ltd. Catalogues: Case Study



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Redbrick Molecular has a rapidly growing library of novel building block and chemical scaffolds for Medicinal Chemistry from a variety of sources. They needed to track compounds, properties, availability, and customer feedback in a secure database system that would be easy for users. Andy Hogben, MD of Redbrick Molecular, tells us about their challenges and how they made use of the CDD Vault to implement a complex catalogue in a simple way.

Redbrick Molecular manufactures and delivers novel building blocks and chemical scaffolds for medicinal chemistry. Set up in 2017 by the Universities of Sheffield and Leeds, the company is built on an innovative business model that combines in house chemistry synthesis expertise with unparalleled access to novel synthetic organic chemistries developed by top UK universities. Redbrick has strong relationships with the pharmaceutical industry, and dedicates all profits to fund further academic research.

We are continually growing our stock of unique compounds produced using pioneering methodologies developed by our member

universities, and we also manufacture larger batches of compounds on a contract basis. Details of these exciting new materials are provided to customers in a standard electronic catalogue, from which medicinal chemists can order compounds to complement their own research programs.

Our ability to execute this innovative business model hinges on the management and mining of strategic information, such as: structures, concepts, stocks, sales, licenses and feedback from customers (Figure 1).

Handling diverse data from multiple sites in real time is a key challenge.



Figure 1: Redbrick data components to manage

Selecting a Data Management System

Redbrick needed a chemically intelligent, secure database system that was easy to share either in part or in its entirety, and offered intuitive, user-friendly features.

Key considerations included:

- Ease of registering and maintaining a record of structures
- The ability to search by more than one parameter at the same time

- Ease and speed of data export
- Assurance of data security through the control of users and data access

After assessing multiple commercial and freeware solutions we opted for a short trial of Collaborative Drug Discovery's (CDD's) cloud-hosted CDD Vault, and subsequently chose the system as our database and informatics platform.

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Accessed through a user-friendly web interface, CDD Vault allows us to manage all our compound and client data securely. The platform is affordable, doesn't require any IT expertise on Redbrick's part, and is maintenance-free. As a hosted system, CDD Vault is also fast, and our in-house computing power doesn't get slowed down. The team at CDD provided all the training required to set up and start using the software, and they also offer training sessions when needed. Support staff at the rapid response helpdesk are always on hand to answer queries and provide practical help.

Most importantly, CDD Vault allows us to store information in easy to search, view and analyse formats, including text-based and numerical information, images and structural data. The platform is also highly forgiving of information source; if the data can be put into spreadsheet, then it can probably be stored in CDD Vault.

A key feature for Redbrick is that the Vault lets us easily insert new text and numeric user-defined fields, so that we can add data associated with compounds and collections, as well as link compounds to our relationships with and licenses from the university originators.

Building Redbrick Molecular Catalogue in CDD Vault

CDD Vault captures all of Redbrick's chemistry and operational data. Compounds under development and catalogues of virtual and in-stock structures, including their location, are easily searched and updated (Figure 2). Using CDD Vault we can upload bulk and individual packets of data and images. The system confirms that newly added structures are unique to the database – an alert will flag up duplicate structures – and auto-generates catalogue numbers.

CDD Vault also tracks our complete inventory, including compound source, stock and pricing. The platform manages our interaction with our university partners, tracks sales and administrative tasks, and collates all customer feedback. This gives us a holistic view of how we operate as a business and helps us to manage internal purchasing and manufacturing.

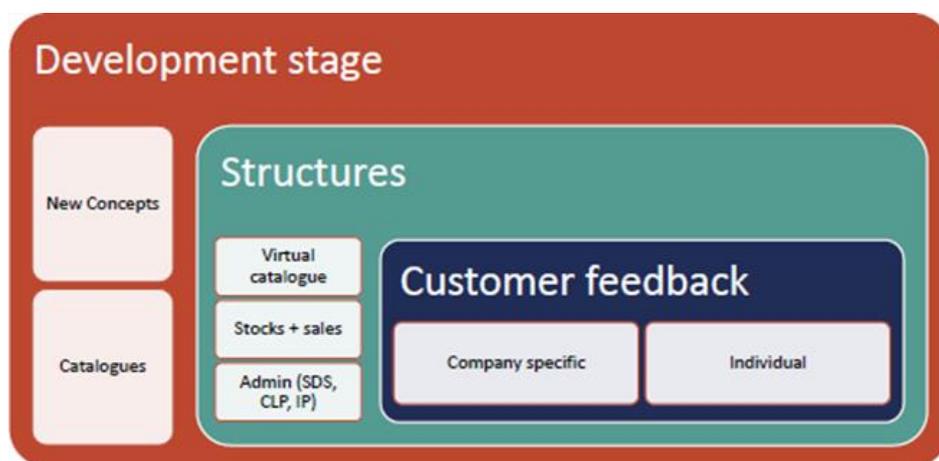


Figure 2: Information captured in CDD Vault.

The principal function of the database is to handle all the chemical structures (either in virtual or real catalogues), their associated properties, as well as stock levels (Figure 3). Chemical properties pinned to the structures include standard calculated

descriptors, such as structure in SMILES (simplified molecular-input line-entry system) or InChI (the IUPAC International Chemical Identifier), and predicted physicochemical properties, such as LogP, LogD, MW.



Overview | Batches: 1 | Plates: 0 | Protocols: 0 | Collections: 0 | Projects: 1 | Files: 1

Definition [Edit definition and structure](#)

Name: RBM-000412

Synonyms: (no synonyms)

User-defined Fields [Edit user-defined fields](#)

University:	2
Academic:	4
Project:	2
Item:	1
H2W catalogue number:	2-4-2-1

Owner: Andy Hogben
Created: August 11, 2017
Updated: August 11, 2017

Figure 3: Example of a Redbrick compound

Projects in CDD Vault are used to separate New Concepts, Intermediates and the actual Catalogue Compounds.

Projects are kept consistent, so information can be moved easily from one project to another without losing any details

Figure 4: Redbrick Projects

Catalogue Distribution

We have found that many customers expect to have catalogue data imported into their internal purchasing systems, so they can search and review, and purchase directly.

Complete catalogues or collections of fragments with the relevant fields can be easily exported from CDD, or alternatively, we could give customers access to the online live system (Figure 5).

Export Selected Results

File format:
 XLS - Excel
 Monochrome printer friendly
 CSV - Comma-Separated Values
 SDF - Structure-Data File

[Export](#) or [cancel](#)

	A	B	C
1	Molecule Name	SMILES	RBM catalogue number
2	RBM-0000413	CC(C)(C)OC(=O)N1[C	1-1-3-10
3	RBM-0000413	CC(C)(C)OC(=O)N1[C	1-1-3-10
4	RBM-0000412	CC1=C2C=CNC(=O)C2	2-4-2-1

Figure 5: Exporting collections of compounds or catalogue for customers.



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Gathering Customer's Feedback

Objective qualitative and quantitative feedback from customers about compounds, data content, and interaction with Redbrick helps us to ensure that we are efficient, and deliver what our customers are looking for. We needed a straightforward process for incorporating that feedback – which is key to shaping the catalogue content – into our working processes. The import data wizard in CDD Vault makes it easy to achieve

just that (Figure 6). We created a protocol for gathering customer feedback. Based on responses and comments, one can easily assess the commercial attractiveness of each compound in the catalogue, which helps us to prioritize compound synthesis (Figure 7). Feedback from customers, which is also searchable, can be passed back to the academic teams.

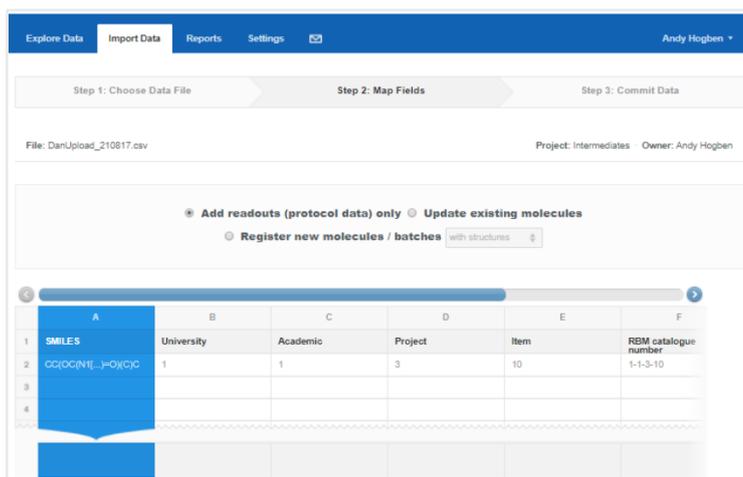


Figure 6: Adding the customer's feedback with the import data tool is easy and quick.

Molecule	Batch	Plate	Well	Customer Number	Attractiveness	Comments 1	Comments 2	Customer internal ref
REB-0000175	001			1.0	5			
REB-0000149	001			5.0	3			
REB-0000144	001			2.0		bifunctional scaffold	desirable	
REB-0000146	001			2.0		bifunctional scaffold	desirable	
REB-0000149	001			2.0		bifunctional scaffold	desirable	

Figure 7: Tracking feedback from Redbrick Molecular's customer.

Conclusions

Redbrick selected CDD Vault because it fulfilled all our technical specifications, was user-friendly and inherently flexible. At both the technical and operational level, CDD Vault has provided the optimum set of features so that we can work with

our academic partners to commercialise their innovative chemistry and methods, and provide customers with novel chemistry that one day may be developed into new medicines.

Contact

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