

scientific computing world

Whitepaper

CRUK Cancer Therapeutics Unit at the Institute of Cancer Research – Case Study Part IV: A Dotmatics Project Environment

By Dotmatics

Since 2005, The Cancer Research UK Cancer Therapeutics Unit (CTU) at The Institute of Cancer Research, together with its collaborators, has discovered 17 preclinical development candidates; seven of which are currently in clinical trials. This paper details why the CTU – the largest academic cancer drug discovery and development group worldwide – ensures that all its drug discovery projects are managed through the Dotmatics integrated suite of scientific informatics solutions.

When Julian Blagg, Deputy Director and Head of Chemistry for the CTU at the Institute of Cancer Research, joined the Unit in 2007 he brought with him a wealth of knowledge accumulated during his career in industry. At the time, there was no cheminformatics platform in place at the CTU to consolidate and provide quick and easy access to data, which had led to only certain people having full access to the project data landscape.

‘There are organisational cultures, both in academia and in the commercial world, that restrict what some scientists working on a project can access, but there are many advantages in ensuring that everyone involved can see all the data in real time without delay,’ commented Blagg. ‘You really can’t underestimate the impact of being able to freely access data, analyse it, see the correlations, and then being able to use those correlations to determine what direction to head in – all in real time. Moreover, it gives everyone the opportunity to review the data, challenge discrepancies, spot outliers and have input into what that next step should be.’ Blagg added that the Unit has an important remit to teach and train the next generation of scientists in cancer research and drug discovery, and that this training should include experience with state-of-the-art data handling, analysis and interpretation.

By 2008, the 13 team leaders at the CTU had all been experiencing the gap that comes from not having a comprehensive informatics platform in place, and so several providers were

brought in to demonstrate their solutions. Dotmatics was selected to begin a six month pilot, and the benefits of the platform soon became apparent. 'Dotmatics' solutions enable us to store documents and data, and have project-related repositories all within the same platform,' said Blagg. 'It's critical that only one set of data is used because as soon as data begins to be replicated in multiple places the danger grows that one person in one team is looking at slightly different data to what another scientist is seeing. You can then end up with multiple scientists on a project, all using variations of the same data.'

The research teams that make up the CTU, and in particular the Chemistry department within the Unit, all rely heavily on the Dotmatics informatics platform. Serving as the central point of convergence for the 163 people who staff the Unit, Dotmatics Gateway is a document management solution that holds all project information and standard operating procedures. All project data is managed by and accessible through Dotmatics Browser, a flexible web-based query and reporting tool that consolidates all disparate databases into one central resource. The CTU currently holds 115 seats for Browser, with levels of access that vary from full, director-level access to read-only access for specific projects.

Because this access can be defined on a project-by-project basis, Browser greatly facilitates the relationship between the CTU research teams and their many external collaborators. 'A fundamental part of setting up any scientific relationship with an external collaborator is the ability to share data confidentially and in real time. This is especially true for commercial partners,' Blagg explained.

Within the Dotmatics platform, setting the parameters for that exchange is straightforward: the CTU can assign a set number of seats to named collaborators within the external organisation who are then provided with a security code. This code means that only specific projects and their associated data and documentation can be accessed by the external organisation, and both the named collaborators and the assigned level of project access can be easily amended by the CTU at any time.

When new assay data comes in to the CTU it is immediately uploaded via Dotmatics Studies, a web-based data management solution that enables the creation, capture, analysis and storage of scientific data. That data is then accessible through Browser, and collaborators on any given project can then see it instantly. Unlike many other solutions that require a bespoke format for data upload and a subsequent change in work practice, the Dotmatics platform has a very flexible upload system.

'To ensure a smooth upload, we do provide all our collaborators with a template of how we need the data to be delivered,' commented Blagg, 'but we rarely experience any problems. For example, we're engaged in a long-term collaboration that involves a weekly data exchange with a commercial partner in Germany, and that process of data exchange is routine. Having the Dotmatics platform not only enables us to work closely with collaborators, it means that there is one single repository for all data, regardless of whether it's been generated at the

CTU or externally.’ Blagg added that having web-based access to the data has also been critical to facilitate flexible access and use of Dotmatics.

Deployment of the Dotmatics platform including the Vortex data analysis suite, has increased efficiency and enabled state-of-the-art data analysis in CTU, which in turn has driven improved medicinal chemistry design and decision making. ‘It’s essential that the academic drug discovery community is practising and teaching data- and hypothesis-driven medicinal chemistry design,’ said Blagg. ‘With limited synthetic chemistry resources it is important that we make optimal compounds – this is what commercial collaborators, funders and potential licensing partners expect, and we are doing this routinely.’ He continued by saying that it’s increasingly the case that academia is taking on some of the higher risk biological targets and moving them forward to a point where commercial partners come on board to collaborate or license those projects when they’ve been de-risked.

‘When a potential commercial partner or licensee evaluates our programmes it is important they can see we have an industry-standard cheminformatics package in place with appropriate, data integrity, analysis and storage. Solutions like Dotmatics are enabling organisations like ours to raise the academic game to another level,’ he concluded.