**New CCDC Website Launched**

CCDC are excited to announce the beta launch of our new website, which went live on 25th April, and is now available from the web address beta-www.ccdc.cam.ac.uk.

The new website is just part of our commitment to provide our user communities with the most accurate and up-to-date service and product information. We also hope it will help strengthen research partner relations and allow us to share more effectively our knowledge and expertise in the fields of structural chemistry and crystallography.

Our solutions section contains detailed information about the products and services we offer, whilst an interactive solutions matrix enables visitors to easily locate solutions based on their area of science or specific application need. The website also features new types of rich content in the form of articles, case studies, videos, interviews, presentations and teaching resources. This material is hosted in a dedicated resources section and can be queried based on scientific application, product, and resource type.

During the development of the site particular attention was given to the implementation of a new fully searchable support database. In addition to addressing a range of technical installation and configuration issues the database also features advice from our applications scientists on the most effective usage of our tools. As this database grows it will provide an increasingly valuable resource for resolving specific issues as well as helping users gain maximum benefit from their software.

In addition to this service and product information, a new blog provides insights into the activities and personalities of the research scientists, software developers and editorial staff who comprise the CCDC. In fact, this blog is just part of our recent efforts to better inform and interact with our depositors and users. For example, you can now also follow us on twitter (@ccdc_cambridge) or Facebook (www.facebook.com/ccdc.cambridge), where we report the very latest views, news and developments.

The new CCDC website has been built using the Microsoft SharePoint 2010 content management system with a SQL Server database back-end. A specialist SharePoint developer was brought in-house to implement the website based on the wireframe designs produced by our graphic designers. A number of bespoke customisations were applied in order for us to deliver the features and user-experience our visitor’s desire. This technology is a huge departure from that used by the previous generation website, which was built using the more traditional Apache/PHP platform.

One of the attractions of SharePoint was its ability to integrate efficiently with other Microsoft server technologies currently being implemented at the CCDC, including Dynamics CRM, which has been selected as the platform for our new internal user relations management system. Our ultimate goal is to provide a service portal on our public website which will allow visitors to interact directly with their accounts and to manage their deposited structures, subscriptions and software licenses. We believe SharePoint will provide the foundations for developing these exciting new services.

The views and opinions of our users are crucial as we continue to develop the website. Please let us know what you think by filling in our feedback form which is accessible from a link at the top of every page.

*Gary Battle, Marketing and Communications Manager*

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1. The website offers a new layout and refreshed content to allow users to efficiently find the information they require.  
2. Information on CCDC software is integrated with links to case studies, documentation and support pages.  
3. The new website covers the whole range of CCDC activities, from research initiatives to the latest news on upcoming software releases and conference visits.  
4. The new support database enables users to quickly find assistance to their queries regarding CCDC software and services.
Our stand at the recent Spring ACS in San Diego  
The terrace at the San Diego convention centre  
Educating a budding young crystallographer!

www.ccdc.cam.ac.uk
A few years ago the development sector of the agrochemical and pharmaceutical industries was identified as an area where an expanded use of the CSD would be beneficial. The development sectors are fundamental cogs in the “molecule to market” machine and they take the active molecule and turn it into the saleable product – a tablet or a sprayable herbicide for example.

Broadly speaking, this means taking the active ingredient and finding the “right form”; the most stable polymorph, the best salt, the most appropriate coformer which turns that initial material into a solid that has the right stability, the right bioavailability or efficacy, and the right processability. The chosen solid form then has to be formulated for delivery. For pharmaceuticals that may involve ensuring that the active ingredient can be compressed for tableting without compromising any of the required properties. For the agrochemical industries formulations are designed which can easily transform a settled solid into a sprayable suspension. These are complex problems and the science and ingenuity employed by the chemists and engineers is impressive.

Very simplistically, many of the problems faced when turning the active ingredient into a product come down to how that molecule interacts with other molecules in the crystalline environment. Polymorphism for example is an expression of the different ways a molecule can interact with itself in a 3D lattice. Screening successfully for a new cocystal can be targeted through consideration of how the active ingredient might interact with the coformers.

Preventing crystals from growing into hard-to-process needles can be achieved by poisoning a fast growing face with a “blocker” molecule. We have a database of small molecule crystal structures covering millions and millions of intermolecular interactions, a resource that could be put to good use by those scientists developing active ingredients. We felt it was a good time to start to talk.

Through our involvement in the Pfizer Institute of Pharmaceutical Materials Science we have benefited from the focus on real problems that Pfizer Global R&D brought to our software development. To expand on this collaborative approach we established a Crystal Form Consortium in 2008 with 11 industrial partners from around the world in the agrochemical and pharmaceutical sectors. We held our first meeting in early 2009 and established our first software development goal: to provide a tool to help with risk assessment for polymorphism. Three years later we have come to the end of the first phase of the Consortium and it has been enjoyable as well as successful. We have built strong, trusting relationships with our Consortium members, we have delivered useful software and have received even more valuable feedback. The second phase of the Consortium, will start later this year. There is a move away from achieving quality through testing and towards designing quality into the products. As a Consortium we will focus on providing tools to help achieve this. The team here at CCDC is delighted to be joined by Dr Neil Feeder, formerly of the Materials Science group at Pfizer Global R&D who will bring highly valuable insight from the pharma industry to the CCDC. We are looking forward to the next phase of the Consortium and the puzzles and challenges it will bring.

_Elna Pidcock, Senior Research and Applications Scientist_

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**Solid Form Informatics in the Front Line**

Although historically considered to be a specialised research tool, the Cambridge Structural Database (CSD) System is fundamentally a library of accurate 3D molecular structures. As such, this unique database is finding increasing application as a general purpose chemical information resource.

Currently, one of our biggest goals at the CCDC is to broaden the use of the CSD and to make structures accessible and comprehensive to all of our users, particularly to students and teachers. We also have a role to play in promoting scientific literacy and a broader understanding of structural chemistry. In order to achieve these goals, we have focussed our efforts on encouraging site wide licensing and distribution of the CSD via university libraries. Our intention is to enable teachers and students at all levels to fully utilise this unique source of 3D structures.

Approximately 1200 academic institutions support the CSD through a licence, and increasing numbers of these institutions are now switching over to unlimited site-wide licensing (a 21.5% increase in the last year alone).

WebCSD, the online search interface to the database received over 25000 unique visitors from the 1st April 2011 to the 31st March 2012, an increase of 13% on the same period a year earlier. Figure 1. Shows the demographic breakdown of visitors at sites based in Illinois, to show how extensively WebCSD is being used. From the 1st April 2011 to the 31st March 2012, we received 1666 visits from 49 cities in this state.

The value of the CSD as a chemical information resource has recently been recognised by the Chemistry Division of the Special Libraries Association and ACS Division of Chemical Information in their publication "Information Competencies for Chemistry Undergraduates: the elements of information literacy. 2nd ed. Sept 2011.”

[http://units.sla.org/division/dche/il/cheminfolit.pdf](http://units.sla.org/division/dche/il/cheminfolit.pdf)

The key information competencies outlined in this publication encompass the skills and knowledge that undergraduates should have by completion of a bachelor’s degree in chemistry.

_Gary Battle, Marketing and Communications Manager_
Why does the CCDC have a YouTube Channel?
The CCDC has a global user base, and while we would love to be able to give all of our users one-on-one training, with an institute of less than 50 employees this is a big ask. So, we thought that by having our own YouTube channel, we would be able to provide our users with webinars and "How-To" videos that would enhance their use of our products, and enable them to get the best out of them.

What sort of videos will I find there?
So far we’ve posted webinars, teaching demos and how-to videos using Mogul and Mercury, such as “How to visualise the void space of a functional structure in Mercury”, but we have plans to post many more, covering our entire product base.

Will they take me ages to watch?
Whilst the webinars are around 30 minutes long, the "how-to" videos are only around 1 minute long, and the demos are around 8 minutes on average.

Can I request a video on a specific subject?
Of course! The purpose of our YouTube channel is to provide you with the material you want to see, and to help you understand how to make the most out of the product you’ve purchased. You could request demos and tutorials by commenting on the current videos, emailing admin@ccdc.cam.ac.uk or by getting in touch via our Facebook page (www.facebook.com/ccdc.cambridge) or on Twitter (www.twitter.com/ccdc_cambridge).

How will I find you on YouTube?
Just search for ccdc.cambridge and you’ll find us. Make sure you’re following us on Facebook and Twitter and that you subscribe to our channel to be the first to know when a new video is posted!

Lauren Thomas, Account and Marketing Manager

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