Crystalline

The newsletter of The Cambridge Crystallographic Data Centre

The Chinese Connection

CCDC has throughout 2012 been making a focussed effort to raise our profile in China. It will not come as news to most of our readership that the Chinese economy has been growing at a huge pace, a rate which exceeded 9% in 2011 [1]. But did you also know that Chinese scientists have risen from 6th to 2nd world-wide by publication volume? [2] There are at present 821 academic institutions teaching natural sciences in China and CCDC plans to connect to more and more of them. The boom in China has also brought in multinational chemical and pharmaceutical firms which sit alongside thriving domestic counterparts, all fitting within CCDC's standard user-base.

We are aware of a strong appetite for both the data offered in the CSD and our software tools (as seen in e.g. existing users of our online access to the CSD, WebCSD, Figure 1). We understand the mutually beneficial relationships offered between many new scientists, crystallographers and/or depositors and our existing user-base through the CSD and CCDC's scientific activities.

To facilitate a strong foothold in China in June 2012 we established a new agreement with HongCam, one of China's largest distributors of chemical software, based in Beijing. As with CCDC's distributors in other territories, HongCam are well positioned to provide sales, marketing and native-language scientific and technical support. Our activities in China have in 2012 consisted of attending both national (Chinese speaking) and international (English speaking) conferences, holding software workshops and visiting our existing academic and industrial customers.

CCDC employees Bing-Bing Waterman and Yu Gan have been key in co-ordinating CCDC's activities in China, assisted throughout the year by a number of other CCDC staff. In April this year a trip was made to Nanjing to present the CSD System to scientific librarians at the E-resources training course at the National Science Library. This also provided a good opportunity to visit HongCam in Beijing.

As part of the initiative, together with our designer, new Chinese language conference marketing materials (e.g. pop-up banners and posters) have been produced, and with the help of a postgraduate student reading chemistry at the University of Cambridge, a number of CSD System tutorials have been translated. The task is currently being expanded to incorporate product flyers, tutorials and other materials for our full range of software. These materials have already proved invaluable during the visits.

August proved to be a busy month which saw a ten day trip with visits in both Beijing and Xi'an. During the first leg in Beijing, Yu Gan and Peter Galek took the opportunity to see the Great Wall of China at Badaling, which was an hour's journey from our hosts at the National Institute of Biological Sciences.

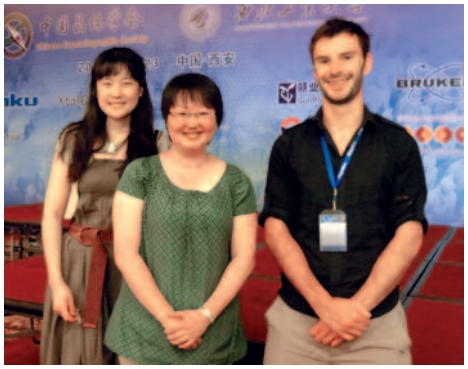

Figure 2. Miss. Huan (HongCam), Yu Gan and Peter Galek (both CCDC) at the 5th general assembly of the Chinese Crystallographic Society

Xi'an was the host city for the fifth general assembly of the Chinese Crystallographic Society (Figure 2), a busy meeting which generated much interest at our stand. Yu and Peter also attended and presented a talk at an international satellite workshop on New Developments and Methods and Software for Protein Crystallography.

In October, Yu Gan and Dave Bardwell ran a very well attended and received CSD System workshop during the Chinese Chemical Society's 6th National Structural Chemistry conference in Suzhou.

We are now also planning our future activities in China for 2013, where we intend to build on CCDCs progress during 2012 in this most dynamic, progressive, industrious and vibrant of nations.

Peter Galek

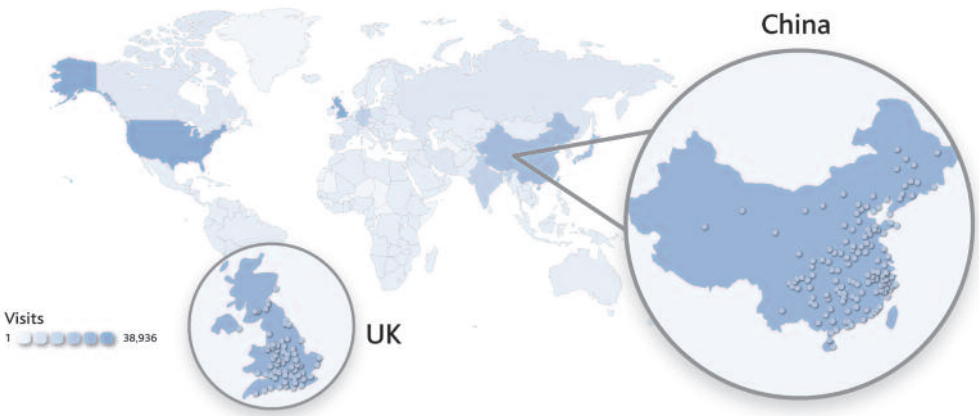

Figure 1. Usage statistics to end Dec 2011 show a globally significant rate of Chinese users accessing WebCSD

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Developing Teaching and Self-Study Support Materials Using WebCSD

For many years, CCDC have been aware of the visual impact of chemical 3D chemical structures and their ability to aid teaching at all levels. We made contact with a similarly enthused individual, Prof. Greg Ferrence, Illinois State University, USA at an American Chemical Society (ACS) Meeting a few years ago and with his help we have a well-established undergraduate teaching initiative in the USA (see http://bit.ly/ccdcpublications for an up to date list of publications), however our presence elsewhere and at other teaching levels is less well established.

In 2010 CCDC attended the Variety in Chemical Education Conference (ViCE), a UK-based and organised conference enabling opportunities to present curriculum developments and research investigations and to share best practices within the discipline. While there we ran a workshop on WebCSD (http://bit.ly/webcsdccdc) and the teaching materials created in collaboration with Greg. One of the attendees, Dr Peter Hoare from Newcastle University, asked "Have you ever thought about using this for outreach?", to which the answer was, "Yes, but we know little about teaching curricula and schools...". It transpired that Peter, originally a school teacher with 20 years experience and more recently an RSC School Teacher Fellow and currently Chemistry Outreach Officer at Newcastle University, considered WebCSD to be the ideal tool to develop computational chemistry exercises to compliment his laboratory-based outreach activities. His dedicated Chemistry Outreach Laboratory at Newcastle consists of a state-of-the-art laboratory area with an adjacent classroom equipped with PCs and appropriately pitched exercises that use WebCSD would enable him to make use of both rooms simultaneously with twice the number of students. Please see Peter's website for more information http://www.ncl.ac.uk/chemistry/outreach/.

Following the ViCE conference in 2010, CCDC joined forces with Peter to initially produce A-level appropriate University outreach materials. However, we soon realised a much wider potential use – both for post-16 learning in schools/colleges around the world and as review/revision exercises for early years chemistry undergraduates too. We have provided Peter with access to the CSD System and have met with him at regular intervals to trouble-shoot and to keep up with progress. Peter has used our existing teaching materials as a starting point for his work and then used his knowledge of current A-level specification to establish which topics were missing from the exercises we already have. He has secured Nuffield bursary funding for four AS-level chemistry students who have devised examples that introduce concepts such as E/Z isomerism of alkenes, shapes of transition metal complexes, optical isomerism, aromaticity and VSEPR theory, all of which use WebCSD.

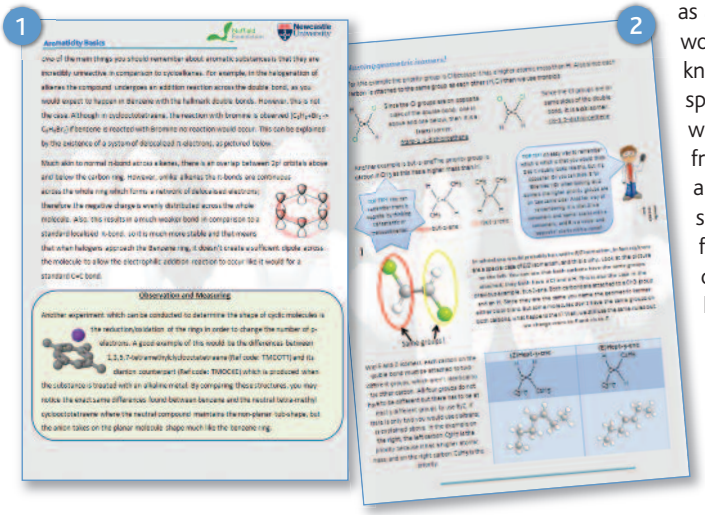
The format for each topic is a theory summary sheet followed by a basic worksheet and one or more extension worksheets, all complete with answer sheets. All sheets are maximum 2 sides of A4, thus making them easy to use next to your PC or laptop.

Furthermore, Peter's summer chemistry intern, Kate Leary (who graduated this summer and is now doing a PhD at Imperial College) also developed parallel exercises focussing on intermolecular interactions, especially hydrogen bonding, using both WebCSD and IsoStar, to be used either as on-campus outreach activities or for undergraduate teaching support.

All these activities are available for download via a secure webpage for trial by anyone interested (www.ncl.ac.uk/chemistry/outreach/trial). Please contact Peter directly at peter.hoare@ncl.ac.uk for the access username and password. Feedback on the content and presentation of the activities would be very welcome – details of how to provide this via an online questionnaire are on the webpage. Peter also has a final year MChem project student who is trialling the activities with local schools and Universities across this academic year and will analyse and evaluate all the feedback received.

In the second half of 2013 we will be officially launching these teaching and learning support activities at various conferences around the UK, and potentially further afield. Visit the events page on our website http://bit.ly/ccdcevents to ensure you don't miss us! For further information or to test out these exercises for us, please contact either teaching@ccdc.cam.ac.uk or Peter direct at peter.hoare@ncl.c.uk.

Susan Henderson and Peter Hoare



1: Screenshot of the aromaticity worksheet by Gabriel Bramley.
2: Screenshot of page 2 of the E/Z isomerism worksheet by Emma Burnett

Events

Over the coming months you can come and meet us at various meetings and events around the world.

Date	Conference, meeting or event	Venue	Activity
11 Nov 2012	Protein Structure Determination in Industry	Paris, France	Attendance
30 Nov 2012	Young Modeller's Forum 2012	London, UK	Attendance
1 Dec 2012	AsCA	Adelaide, Australia	Talk
11 Dec 2012	Chemistry: Synthesis	Karnataka, India	Talk
14 Dec 2012	Biological and Medicinal Chemistry Symposium	Cambridge, UK	Attendance
2 Jan 2013	Association of Science in Education	Reading, UK	Workshop
23 Jan 2013	Quality by Design	London, UK	Attendance
5 Mar 2013	Fragments 2013	Rutherford Appleton Lab, Oxfordshire, UK	Talk
19 Mar 2013	Conference of the German Crystallographic Society	Freiberg, Germany	Attendance
21 Mar 2013	Molecular Interactions in Drug Discovery	Cambridge, UK	Talk
7 Apr 2013	Spring ACS	New Orleans, USA	Exhibition, Talks
Apr 2013 TBC	XIV Durham Crystallography School	Durham, UK	Workshop

How did GOLD perform in a standardised docking test?

A two-day symposium at the 241st American Chemical Society meeting (Anaheim, September 2011), organised by Greg Warren of OpenEye and Neysa Nevins of GSK and entitled Docking and Scoring: A Review of Docking Programs, gave all suppliers of docking packages the opportunity to present the results of running their software using the same set of protein and ligand structures. The use of standardised test sets under standardised conditions not only allowed us to assess GOLD's performance, it also allowed us to compare the four different scoring functions provided with GOLD (GoldScore, ChemScore, ChemPLP and ASP (Astex Statistical Potential)). All involved parties subsequently published their findings. [1]

The test was separated into two different parts: one that assessed pose prediction and another that assessed virtual screening performance. The Astex Diverse Set [2] of protein-ligand complexes was used as a basis for the first part; the ligand was docked back into the cognate protein and the resultant pose assessed based on RMSD from the cognate ligand's pose. The DUD/Active Decoy set [3] of 40 diverse targets was used for virtual screening and the enrichment success measured using the total area under the Receiver Operating Characteristic (ROC) curve.

In general GOLD performed very well. In the pose prediction part of the test we were delighted to learn that GOLD is one of the most accurate docking programs available, with 81% of the top ranked solutions being within 2Å RMSD of the cognate ligand and 59% within 1Å RMSD (ChemPLP function). In the virtual screening part of the test GOLD achieved an average Area Under the ROC Curve of 0.70 (ChemPLP), very similar to the results achieved by competitor programs using the input structures supplied by the organisers. ChemPLP was found to be the highest performing GOLD scoring function. A more detailed summary of the test conditions, GOLD's performance and other conclusions that we were able to draw from this standardised test are provided elsewhere [3,4,5].

Susan Henderson

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[1] *J. Comput. -Aided Mol. Des.* (2012) **26**, 675-799 10.1007/s10822-012-9551-4

[2] Hartshorn et al, *J. Med. Chem.* (2007) **50**, 726-741 10.1021/jm061277y

[3] J. W. Liebeschuetz et al, J. Comput. Aided Mol. Des. (2012) 26, 737-748 10.1007/s10822-012-9551-4

[4] http://beta-www.ccdc.cam.ac.uk/Lists/ResourceFileList/workcase_posepred.pdf

[5] http://beta-www.ccdc.cam.ac.uk/Lists/ResourceFileList/VS_workcase.pdf

CCDC: A Charitable Company!

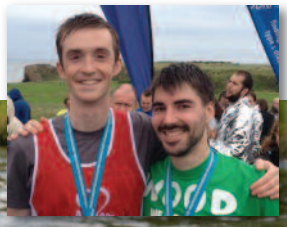
The CCDC is a registered charity (charity no. 800579), dedicated to the advancement of chemistry and crystallography for the public benefit through providing high quality information services and software. However, it's not just the organisation that is charitable.

Over the course of 2012, CCDC employees have been involved in a number of charitable activities, both in-house and in their own time. To begin with, every year the CCDC holds a coffee morning for Macmillan Cancer Support. This year we raised £250 by selling home-made cakes and second-hand books, and through a "guess the staff member from the baby photo" competition! Elna Pidcock was the winner there, correctly guessing 8 out of the 14 photos and winning a fruit box donated by the Cambridge Fruit Company.

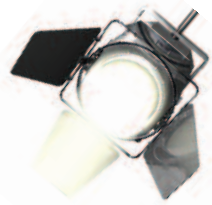
On September 8th, 9 CCDC staff members and their friends and family formed "The Space Group" team for the 2012 Cambridge Dragon Boat Festival. While they didn't win any of their races, they were recognised for raising more than £1200 for the festival's charity, East Anglia's Children's Hospices, one of the largest amounts of the day.

And on September 16th, CCDC research scientist Pete Wood ran the Great North Run, raising more than £1500 for Macmillan Cancer Support. Pete only started running in earnest a year earlier, and managed to finish in a spectacular time of 1:45:41! This was possibly not great news for the friends who offered to sponsor him an extra £5 for every minute he finished under his target time of 1:55:00, but was great news for Macmillan!

Lauren Thomas



Spotlight *on the CCDC's Communications*



Where can I find out more about the CCDC?

Whilst you most likely already know about the CCDC's Facebook and Twitter profiles, as well as our YouTube channel, you may not know that we also have a company profile on LinkedIn and a blog on our new website. Essentially, the more ways we use to communicate to our users what the CCDC is doing and thinking, the more of you we can reach.

Why are you on LinkedIn?

Most people are connected to at least one form of online networking, whether it is Facebook, Twitter or LinkedIn. Whilst Facebook and Twitter are seen as "social" networking sites, LinkedIn is seen as a "professional" networking site. This means it is best suited to updates about careers, research and publications that the CCDC is both involved in and interested in. Every networking site that we have a profile on increases our reach to our users, whether they prefer a more social or more professional environment to engage in.

Why have you decided to add a blog to your new website?

The CCDC has around 50 staff members, all working on different projects, attending conferences around the globe and publishing exciting papers. While Facebook and Twitter are great for short statements and quick updates, our blog allows us to go into greater detail, and give lots of different staff members the opportunity to introduce themselves to our users. We can engage in more in-depth discussions, and are hoping to add user comments to the blog in the not too distant future.

What if I would like to submit something to the CCDC's blog?

We're always looking to work with our users, so if you think you might have something of interest that our scientific community would like to read about, please send a message to admin@ccdc.cam.ac.uk, or contact us through one of our networking profiles!

Where can I find your LinkedIn page and blog?

Just go to http://bit.ly/CCDCLinkedIn for our LinkedIn page and http://bit.ly/CCDCBlog for our blog. Alternatively you can just scan the QR codes below with your smartphone!

Lauren Thomas

CCDC Publications *May 2012 to Oct 2012*

The CCDC team frequently publish results of their research, which is often the work of collaboration with industrial or academic scientists.

You can find the full list of our publications at www.ccdc.cam.ac.uk/publications.

Here are our most recent titles, published since 1st May 2012.

Validating and understanding ring conformations using small molecule crystallographic data
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Acid-base crystalline complexes and the pKa rule
A. J. Cruz-Cabeza, *CrystEngComm* (2012) **14**, 6362-6365. 10.1039/C2CE26055G

On the Trail of Chemistry in the Garden
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Up the garden path: a Chemical Trail through the Cambridge University Botanic Garden
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