

m45.o04

Promoting science through art - the Chem-moo-stry Project

Gordon Barr, Andy Parkin

WestCHEM, Department of Chemistry, University of Glasgow. E-mail: cow@chem-moo-stry.org

Keywords: chemical education, education, research

The general public perception of crystallography and chemistry as dull, old-fashioned and uninteresting is one of the most difficult problems that we have to deal with on a day-to-day basis.

The CowParade [1] is the largest public art event in the world and was in Edinburgh, Scotland from 15th May - 23rd July 2006. The idea behind CowParade is that artists are given a unusual canvas - one of 150 life-size 3-dimensional fibreglass cows - to decorate as they see fit, which is then displayed on the streets of Edinburgh.

By sponsoring a cow to represent chemical research in Scotland we had a unique opportunity to showcase some of the best research being undertaken to a much more varied audience than we could ever hope to reach otherwise. The cow generated positive publicity and interest across Scotland and beyond, reaching an international audience. It is a very conservative estimate to say that the cows was seen by tens of thousands of people - the Chicago Visitor and Convention Bureau estimated that the CowParade attracted an additional 3 million visitors to the city when it was held there in 1999.

By including a web address as part of the name of our cow, we were able to encourage people to find out in more detail about the chemistry represented by having an accompanying website. When visiting www.chem-moo-stry.org the public were given a chance to 'understand the science behind the cow'.

This was the first time that the CowParade has been used to promote chemistry and the public understanding of science. By making a visually striking statement with our cow, we began to challenge the myth that science cannot be important and cutting edge as well as fun.

[1] <http://www.cowparade.com>

m45.o05

eCrystals: A Route for Open Access to Small Molecule Crystal Structure Data

Simon Coles^a, Michael Hursthouse^a, Jeremy Frey^a, Andrew Milsted^a, Leslie Carr^b, Monica Duke^c, Traugott Koch^c and Elizabeth Lyon^c

^aSchool of Chemistry, University of Southampton, UK, ^bSchool of Electronics and Computer Science, University of Southampton, UK, ^cUKOLN, University of Bath, UK. E-mail: s.j.coles@soton.ac.uk

Keywords: electronic publishing, crystallographic databases, computer networking

Recently the funding councils in the UK stated that '*the data underpinning the published results of publically-funded research should be made available as widely and rapidly as possible*'.

Thirty years ago a research student would present about five crystal structures as their PhD thesis, however with modern technologies and good crystals this can now be achieved in the timespan of a single morning. This increase in pace of generation further exacerbates a problem in the communication of the results. Additionally, the general route for the publication of a crystal structure report is coupled with and often governed by the underlying chemistry and is therefore subject to the lengthy peer review process and tied to the timing of the publication as a whole. This bottleneck in the dissemination of crystal structure data hinders the potential growth of databases and the data mining studies that are reliant on these collections. Just 500,000 small unit cell crystal structures are available in the CSD, ICSD & CRYSMET databases, while it is estimated that at least twice this number have been determined in research laboratories and are likely to remain unpublished. In addition, publication in the mainstream literature still offers only indirect (and often subscription controlled) access to this data.

The work of the eBank-UK project (<http://www.ukoln.ac.uk/projects/ebank-uk/>) has addressed this problem by establishing an institutional data repository that supports, manages and disseminates metadata relating to the crystal structure data it contains (i.e. all the files generated during a crystal structure determination). This process alters the traditional method of peer review by openly providing crystal structure data where the reader or user may directly check correctness and validity. The repository (<http://ecrystals.chem.soton.ac.uk>) makes available all the raw, derived and results data from a crystallographic experiment with little further researcher effort after the creation of a normal completed structure in a laboratory archive. Not only does this approach allow rapid release of crystal structure data into the public domain, but it can also provide mechanisms for value added services that allow rapid discovery of the data for further studies and reuse, whilst ownership of the data is retained by the creator.

The details of the preparation of data, upload process, files supported and automatic report generation will be presented. Additionally, the process whereby metadata relating to each archive entry is disseminated, using current Digital Libraries technologies, for discovery and reuse by will be summarised. Strategies for the installation of archives at new sites, the construction of harvesting and aggregator services and the interaction with crystallographic data holding bodies, such as IUCr and CCDC, will also be outlined.

Additionally links to educational tools, specifically the Schools eMalaria project (<http://emalaria.soton.ac.uk>), will also be presented.