s1.m2.p2 **Crystal Structure EPrints: Publication @ source through the open archive initiative.** Simon Coles,[a] Jeremy Frey,[a] Michael Hursthouse,[a] Leslie Carr[b] and Christopher Gutteridge[b], [a]*School of Chemistry, University of Southampton, Southampton. SO17 1BJ, UK, and* [b]*School of Electronics and Computer Science, University of Southampton, Southampton, SO17 1BJ, UK. E-mail: s.j.coles@soton.ac.uk*

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Advances in crystallographic instrumentation and computational resources have caused an explosion of crystallographic data, as shown by the recent exponential growth of the CSD [1]. However, even this is considered to be lower than expected, following the introduction of area detection. The reason for this is clearly identified as a publication bottleneck, which can only become even more severe with developments in high throughput crystallography [2]. As a result of this situation, the user community is deprived of valuable information, and the funding bodies are getting a poor return for their investments! Unlike the mathematical and electronic sciences, the chemical sciences have been reluctant to embrace the 'preprint concept' [3]: the one exception has been the efforts of rapid electronic communications journals. This poster outlines a pre-print procedure for the rapid and effective dissemination of structural information to the scientific community which removes the lengthy peer review process that hampers traditional publication routes, but provides an alternative mechanism. Crystallographic EPrints are built on a concept developed in the Computer Science community [4] whereby an author may reveal to the public archives of information. An EPrint makes available all raw, derived and results data from a crystallographic experiment via a searchable and hierarchical system. At the top searchable level this metadata includes bibliographic and chemical identifier items which allow access to a secondary level of searchable crystallographic items which are directly linked to the associated archived data. Hence the results of a crystal structure determination may be disseminated in a manner that anyone wishing to utilise the information may access the entire archive of data related to it and assess its validity and worth.

[1] F.H. Allen, CCDC, Cambridge, UK. http://www.ccdc.cam.ac.uk/products/csd/statistics
[2] M.B. Hursthouse (2004), *Crystallogr. Revs*,. In press.
[3] L.R. Garson (2004), *Acc. Chem. Res*., ASAP Article; DOI: 10.1021/ar0300017, **Web Release Date**: February 10, 2004.
[4] C Gutteridge (2002), *Proc. 11th Panhellenic Academic Libraries Conf.* (http://eprints.ecs.soton.ac.uk/archive/00006840/).

s1.m2.p3 **Winners and Losers - Ranking Crystals from Diffraction Images.** A.R. Criswell, R. Bolotovsky, T. Niemeyer†, R. Athay, J.W. Pflugrath. *Rigaku/MSC, Inc., 9009 New Trails Dr., The Woodlands, TX 77381 and †where's Thad?. E-mail: mf@rigakumsc.co.uk*

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With the advent of automation, many home labs and beamlines have developed robotic systems for high-throughput evaluation of crystal samples. Ideally, an automated system should provide methods to identify desirable samples. However, most of these systems still depend on human intervention to judge the quality of crystals. We have implemented a method in d*TREK software to evaluate the quality of diffraction images and assign a rank per sample. This ranking procedure evaluates images in terms of several rules and calculates an award or penalty for each rule. The awards and penalties are then summed and updated on a per sample basis. Samples can then be ranked according to these values, and data collected in descending rank order. In general, the ranking rules include the number of Bragg reflections per resolution shell, the <I/sig(I)> of reflections per shell, the spot sharpness, the presence and sharpness of ice rings, crystal mosaicity and unit cell refinement results. We discuss the usefulness of these rules in the evaluation of diffraction images, and highlight those rules which seem most important for ranking of crystals.