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Call for a crystallization ontology

Howard Einspahr[a]* and Manfred S. Weiss[b]*

[a]PO Box 6483, Lawrenceville, NJ 08648-0483, USA, and [b]Helmholtz-Zentrum Berlin für Materialien und Energie, Macromolecular Crystallography (HZB-MX), Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

This issue introduces a new category of publication in *Acta Cryst. F*: Scientific Comment. Scientific Comments can address any scientific topic deemed of interest to the readership of the journal. The inaugural Scientific Comment (Newman *et al.*, 2012), the first article of this issue, reports conclusions drawn and commitments made as the result of a meeting in 2011 of a select group of macromolecular crystallization scientists whose objective is to enable better use of all results of screening experiments. This includes both successes and failures, or positive and negative results, as currently defined solely on the presence or absence of crystals. The outcome of the meeting is a commitment to develop a precisely defined language, ontology in the modern computer-science sense of the word, for description of the results of macromolecular crystallization experiments.

Almost from the dawn of the age of macromolecular crystallography, it was clear that a major limitation to applications of X-ray diffraction techniques was the preparation of crystalline samples sufficient for structure determination. This limitation was widely decried, bemoaned, mourned, and regretted in publications (and no doubt countless grant applications) over the years until it is now known widely as 'the bottleneck'. Despite major advances in preparation of proteins and other macromolecules and in the systematic search for crystallization conditions, despite crystallization successes numbering in the tens of thousands, the perception is that the limitation remains a challenge undiminished. One might even consider the several Nobel Prizes awarded to macromolecular crystallography over the last decades as acknowledging fundamental advances against this limitation.

As noted in the article, a number of scientists have recognized that in current practice most of the results of crystallization experiments, both positive and negative, are under-utilized during the course of the campaign and are ignored and discarded once success has been obtained. A seminal paper by Carter & Carter (1979) described an incomplete factorial method for incorporating results other than crystals into a landscape from which likely crystallization conditions could be inferred. Subsequently, a seminal screen was developed to provide initial results upon which the methods could be applied (Jancarik & Kim, 1991). The principal reason that the method has never been properly applied has always been the difficulty in usefully describing results other than crystals in a quantitative or semi-quantitative way.

The purpose of the article is to announce an effort by the authors to overcome that difficulty once and for all. It is hoped that the effort will stimulate discussions and contributions from other macromolecular crystallization scientists. A crystallization ontology would permit precise description of results of experiments and foster communications and discussions of results among crystallization scientists. Ontology development will not be an easy task, but the deluge of results from robotic crystallization campaigns that the authors handle on a daily basis should help coalesce consensus descriptions of results. That same deluge also accents the need for this ontology to enable automated evaluation and scoring of results. One can hope that development of additional methods for observation of results, such as UV microscopy and dynamic light scattering, for example, will further enhance quantitative descriptions.

This effort will be a challenge, but it is overdue. We wish them success.

References

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