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Another case of fraud in structural biology

The first article in this month's issue (Rupp, 2012) is a Scientific Comment revealing another instance of scientific misconduct in the literature of macromolecular crystallography. The first such instance was uncovered just a few years ago. It effectively terminated a whole sequence of fraudulent activities and resulted in the retraction of about a dozen structures and associated publications. Although the act of one individual, it tarnished several reputable journals, several reputable institutions and many reputable colleagues. It was also a very public injury, the subject of news articles and editorials, including a joint editorial by the Editors of *Acta Cryst. D* and *F* (Baker *et al.*, 2010*a,b*). The second painful insult, disclosed in this issue, was also the act of a single individual. While it seems to be limited to one structure, one journal, one institution and fewer colleagues, and may or may not attract the same amount of attention as the first, it is no less painful, no less disappointing.

The subject of this comment (Zaborsky *et al.*, 2010) was discovered as the result of a routine search of the *PDB_REDO* database (Joosten *et al.*, 2011). It raised suspicions for a number of reasons. A determined effort at analysis confirmed those suspicions as does the response from the authors (Zaborsky *et al.*, 2012).

What motivates these hoaxes? It seems clear that the pressures on scientists early in their careers are so severe that a few are compelled to risk their careers in order to further them. The dilemma is perhaps more fathomable when one considers the publication and citation metrics academic departments now use to evaluate staff, the difficulties crystallographers face in attracting funds early in their careers, and the seemingly inexorable march toward commoditization of the crystallographic product. Can this be changed any time soon?

So, once again, we must rely on ourselves and ask how we can protect our science by minimizing recurrences. We do have the advantage that crystallography is richer in hard experimental data than most areas of science, and should therefore have more powerful tools for detecting fraud. The new recommendations of the Validation Task Force are a major, positive step forward (Read *et al.*, 2011). Where scientific publication is the concern, however, their impact will only be fully effective if all relevant journals follow the path of IUCr Journals and require that validation reports as well as coordinates and structure factors be made available for peer review upon submission. It is equally important that all relevant journals include at least one expert crystallographer among the referees for all submissions that describe crystallographic structure determinations, even if those structures are but one aspect of the paper. In the current case, however, validation by re-refinement and electron-density evaluation seems to have been the key. To do this on a routine basis will put an extra burden on crystallographers who serve as referees, making development of tools to ease that burden another worthwhile contribution.

It is important to note, however, that in neither of these cases was a single frame of data collected. Not one. This alone demands a redoubled effort to produce a universal system for deposition and storage of original diffraction images.

References

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