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Using structural genomics depositions in undergraduate teaching of protein crystallography: everybody wins

Jon Agirre*

York Structural Biology Laboratory, Department of Chemistry, The University of York, York YO10 5DD, United Kingdom.
*Correspondence e-mail: jon.agirre@york.ac.uk

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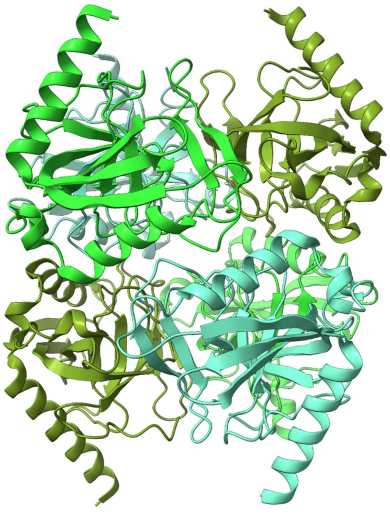
Doing protein crystallography is easier than it has ever been thanks to advances in mechanics automation and software methods, but there is one step that remains tricky: obtaining crystals. Teaching the complete protein crystallography workflow requires having or growing crystals. And while some proteins do crystallize quite predictably within the time frame of almost any course, they are at this point almost devoid of the exhilaration that comes with stepping into the unknown. In this issue of *Acta Cryst. F, Structural Biology Communications*, a group led by Professor Krystle J. McLaughlin (Assistant Professor of Chemistry at Vassar College, New York, USA) shows how deposited but uninterpreted protein models from structural genomics consortia can be harnessed in undergraduate teaching to give students real-world research experience. The three leading authors on the article (Moorefield *et al.*, 2023) were undergraduate students at her course, and produced all the biochemical data and structure interpretation work presented there.

Professor McLaughlin is passionate about making the protein crystallography experience accessible to undergraduate students with a special focus on minorities currently underrepresented in research, all through the CURE (Course-based Undergraduate Research Experience) programme (McLaughlin, 2021). In the context of a biochemistry course underpinned by BASIL teaching modules (https://www.basilbiochem.org), McLaughlin got in touch with the Seattle Structural Genomics Center for Infectious Disease (SSGCID, funded by NIAID, NIH) in the USA to identify suitable targets for study. A good match right from the outset, the SSGCID specializes in microbial proteins, and wants to partner up with structural biologists to provide useful context to their structures. With their depositions currently sitting at 1656 structures (Fig. 1), they are sure to continue providing targets for generations of students to come. The SSGCID provided pure protein for the students to analyse; moreover, they would have supplied plasmids too, should they have been required for the study.

Several undergraduate student groups took part in the course, but the one integrated by Moorefield, Konuk and Norman (lead authors on the article) managed to get the best data on the activity of their target enzyme, a family I inorganic pyrophosphatase from



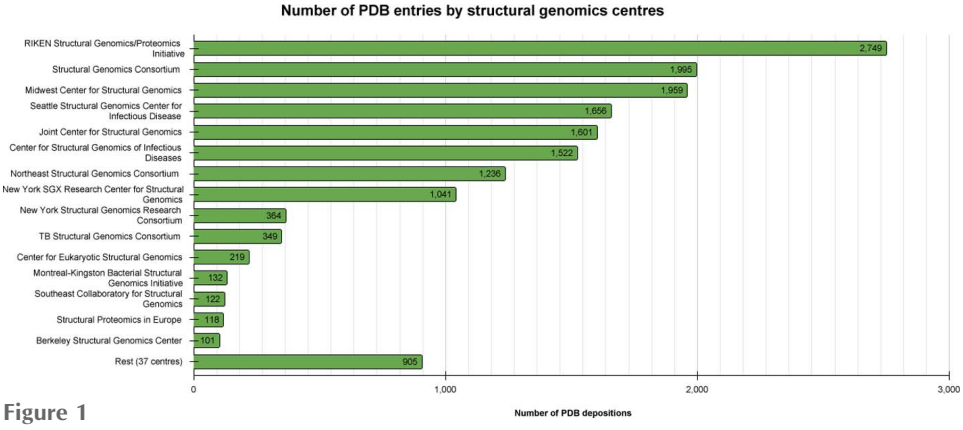


Figure 1
PDB depositions by 52 structural genomics centres around the world. Only centres with more than 100 depositions are named. Data: https://www.pdb.org.

Figure 2
Professor Krystle J. McLaughlin (Vassar College, New York, USA).

Legionella pneumophila. The ultimate deliverable of the research course was to produce a draft article in the style of *Structural Biology Communications*, which they did – McLaughlin fact-checked the draft and made some minor corrections prior to submission.

There are a number of important side-effects from this study. The importance of providing a controlled but meaningful research experience to undergraduate students comes across as critical to help avoid the disappointment some graduate researchers experience after starting a PhD; crucially, it might give students sitting on the fence a welcome push towards STEM research – this could be helpful in motivating students from disfavoured backgrounds who may feel discouraged by the current scarcity of visible role models. Underrepresentation of minorities is a problem that is most evident after the formative stage of career progression; bringing the *first article* event of scientific life forward by a few years – as opposed to doing it at the middle or end of a PhD – can only help increase diversity at the other end of the undergraduate-to-graduate gap. When asked about the aspirations of the three lead authors, McLaughlin sounded positively optimistic.

The model presented here provides an excellent blueprint for establishing more collaborations between academia and any of the 52 structural genomics centres that have deposited structures in the Protein Data Bank, 15 of which are named in Fig. 1. However, this is just one way young researchers can contribute: another one could be submitting topical reviews by graduate/masters students who routinely survey the literature in support of their research project; or short software methods papers from those scripting workflows at their labs.

I should like to emphasize that *Structural Biology Communications* is open for business when it comes to processing submissions including undergraduate/masters students, and will handle and showcase their research the best it can. Finally, I would like to thank outgoing Section Editor Janet Newman (University of New South Wales, Australia), who championed the idea of encouraging younger authors to contribute their articles to this journal, and edited McLaughlin's manuscript.

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