



Show me how it's done: introducing *Protocols*

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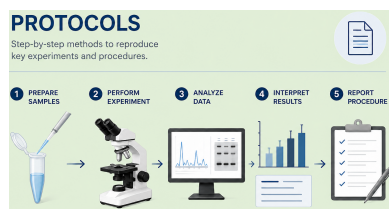
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Methodological papers have always been an important part of structural biology research: they enable major biological discoveries through improvements in sample preparation and crystallization, instrumentation, computation, refinement, validation, and data interpretation and presentation. IUCr Journals are fortunate – and, as society journals, also proud – to have published some of the most consequential methods papers in the history of structural biology (French & Wilson, 1978; Read, 1986; Schneider & Sheldrick, 2002; McCoy *et al.*, 2007; Garman, 2010; Chen *et al.*, 2010; Cipriani *et al.*, 2012; Terwilliger *et al.*, 2023).

While early methods papers often described mathematical formulations, they have over time diversified to now include software algorithms, descriptions of user-interface logic and pipelines. In many cases, such papers are also accompanied by the release of new or updated software, or novel devices.

Our journals have adjusted over the years to offer paper categories that are suitable for most methodological studies, such as *Methods Communications*, but we feel it is time to provide an additional category that addresses a current gap. The existing categories of contribution offer a venue for methodological innovation, but the descriptions are often on such a high or abstracted level that it can be difficult for the broad readership to apply or reproduce the methods. For example, it may be difficult to reproduce algorithms from the descriptions because the paper does not leave enough space to describe all shortcuts or assumptions. Alternatively, the description of new software or devices provides an overview of what the tool can do, but there is typically no opportunity to describe useful practical information (for example, what settings may be useful in which context). The challenge is not limited to computational methods. Experimental procedures often rely on tacit knowledge that is difficult to capture in a conventional *Materials and Methods* section, such as sample-preparation strategies, crystallization optimization, specimen preparation for cryo-EM, instrument configuration, or troubleshooting steps that can critically influence success. Enter *Protocols* articles at *Acta Crystallographica Section F: Structural Biology Communications*. The purpose of this new category is to provide to the reader procedures that are sufficiently detailed so other researchers can reproduce the described workflow. This may include critical experimental parameters, troubleshooting considerations, quality-control steps or recommendations for best practices. The description of a new device could be accompanied by a video illustrating its set-up and use. Software protocols could benefit from screenshots of the graphical user interface or the complete list of nondefault options and settings for various use scenarios.

Protocols may be prepared as a standalone submission, but it will also be possible to complement a longer-format research article that has been submitted to an IUCr journal, either by expanding on the *Materials and Methods* section, or by submitting a standalone *Protocol* first and citing it in the longer-format research paper. In any of these joint or sequential submission scenarios, we would highly recommend discussing the publication timeline and strategy with Mark van Raaij, our new Commissioning Editor.



Like all other kinds of articles, *Protocols* will be reviewed by at least two experts in the field and handled by a specialist Co-editor. Upon submission of a *Protocols* article to *Acta Crystallographica Section F*, authors will be able to select a specific Co-editor from our growing roster of methodology specialists, which at the moment includes Dorothee Liebschner for crystallography methods and software, Michael A. Hough for serial and room-temperature crystallography and fragment screening, Stephen P. Muench for cryo-electron microscopy and Kyeong Kyu Kim for nucleic acids. Beyond methodology, all co-editors can be found along with their respective expertise on our journal page (<https://journals.iucr.org/f/services/editors.html>).

In this editorial, we would like to invite you to share protocols that will be useful to the community, and help maintain *Acta Crystallographica Section F* and the other IUCr Journals as important references for how structural biology research is performed.

A full description of the *Protocols* category can be found in our recently updated *Notes for Authors* at <https://journals.iucr.org/f/services/notesforauthors.html>.

References

- Chen, V. B., Arendall, W. B., Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S. & Richardson, D. C. (2010). *Acta Cryst. D* **66**, 12–21.
- Cipriani, F., Röwer, M., Landret, C., Zander, U., Felisaz, F. & Márquez, J. A. (2012). *Acta Cryst. D* **68**, 1393–1399.
- French, S. & Wilson, K. (1978). *Acta Cryst. A* **34**, 517–525.
- Garman, E. F. (2010). *Acta Cryst. D* **66**, 339–351.
- McCoy, A. J., Grosse-Kunstleve, R. W., Adams, P. D., Winn, M. D., Storoni, L. C. & Read, R. J. (2007). *J. Appl. Cryst.* **40**, 658–674.
- Read, R. J. (1986). *Acta Cryst. A* **42**, 140–149.
- Schneider, T. R. & Sheldrick, G. M. (2002). *Acta Cryst. D* **58**, 1772–1779.
- Terwilliger, T. C., Afonine, P. V., Liebschner, D., Croll, T. I., McCoy, A. J., Oeffner, R. D., Williams, C. J., Poon, B. K., Richardson, J. S., Read, R. J. & Adams, P. D. (2023). *Acta Cryst. D* **79**, 234–244.