Acta D/F meeting

Euroforum Infantes, San Lorenzo de El Escorial, Spain

20 August, 09:00-13:00, 21 August 09:00-10:30, Sala07

CHAIR: Ted Baker

Attendees: Terese Bergfors, Howard Einspahr, Elspeth Garman, Mitchell Guss, Janet Newman, Bernard Rupp, Robyn Stanfield, Se Won Su, Manfred Weiss

IUCr staff attending: Louise Jones

VALIDATION REPORTS AND ACCESS TO DATA

Provision of validation reports by authors appears to be working satisfactorily. The PDB task force on validation has recently completed its work and has published recommendations. It has been suggested that the report will contain a numerical assessment of the structure and any concerns will be raised. There will be a meeting in September when the PDB will decide whether to adopt the task force's suggestions and when to implement a new form of validation report. All journals will then be approached to require such reports.

Some co-editors thought that not all reviewers look at the validation reports and so it was suggested that an extra question be added to the reviewers questions or a tick box be added to show that the reviewer had looked at the report. Also the invite letter to the reviewers could ask the reviewers to examine the validation report. When the paper is accepted the acceptance e-mail to the Editorial Office could ask co-editors if they have checked the validation report (similar to the question on PDB codes).

The question of availability of data was raised as it was felt that validation reports at present do not supply enough information and it would be useful to have access to the data before they are released by the PDB. It was suggested that if the data were available we could provide an online view of the structure and the density (*e.g.* the EDS server could be used to check ligands). There is currently a link from the PDB site to the EDS server and perhaps the URL could be provided to reviewers. It was suggested that the PDB be approached to see if they would be willing to provide access to the data *via* a secure mechanism. In the meantime, if the reviewers or the co-editor wanted to see the data, the co-editor could ask the authors. It was felt that few authors would refuse the co-editor as if they did the co-editor may reject the paper. It was suggested that a standard letter be added to the submission system e-mails to ask the authors for their coordinates and data. (A meeting was held with the PDB at the Madrid Congress and they were asked to consider providing a secure server for journals to access the data before release. They were reluctant to do this for security and financial reasons.)

Some other journals do not accept papers until the data have been released by the PDB and it was asked if this should be adopted by Acta D and Acta F? It was felt that such a requirement was too complicated and asking the authors to provide evidence of release of their structures by the PDB could cause delays. Instead it was suggested that the status of the PDB entry was checked to make sure it was HPUB before publication.

Also it was felt that that no release delay should be allowed after publication and that this should go in the Notes for Authors. In addition, the IUCr Commission on Biological Macromolecules should be asked to update their policy on this and publish new guidelines. (The Commission chair was approached in Madrid and asked to put this to the Commission and, if agreement was reached, to write some new guidelines for publication in Acta D and F.)

DIFFRACTION IMAGES

The PDB is unwilling/unable to archive diffraction images although data quantity is not felt to be an issue. At present the TARDIS project archives data at the Australian synchrotron and there are also two other TARDISes at Sydney and Brisbane. Newer projects save much richer metadata including protein production data. It was felt that this was a Commission matter rather than a journals problem for now.

NEUTRON DATA

There have been some neutron-based papers submitted to Acta F that were submitted as crystallization communications but were not really suitable for this category as they contained neutron-density maps, presupposing structure refinement. However, they only contained preliminary data and so were not suitable for the structural communications category either. It was suggested that we should ask Paul Langan for some guidelines on what we should publish for these preliminary and other neutron studies (similar to NMR) and maybe have a joint Acta D/Acta F workshop on

requirements for publications that use a neutron source.

SAXS

A draft report on biological SAXS guidelines has been prepared and made available to the Co-editors. It was agreed that this should be adopted and mentioned in the Notes for Authors. Mitchell was also asked to write a paper on this. It was also felt that Arwen Pearson may a person to contact about this.

ONLINE JOURNALS

Virtual journals or issues were felt to be a good idea if based on a topic or area of research. "Playlists" of papers were suggested and it was thought that each co-editor should be asked for their playlist. These virtual issues could be publicised on the CCP4 bulletin board. Also features such as "you may also like" could be added to the journals searching. Concern was raised over highlighting and links to databases in case we were seen to approve some and not others. BMRB, PDBsum and SWISSPROT were thought to be OK and it was better to link to databases rather than application servers.

ACTABIOSTANDARDS

Actabiostandards has been inactive for some time but it was felt that a mailing list such as this is preferable to a forum as a forum would need someone actively monitoring it. The CCP4 and Phenix bulletin boards were thought to be other places which fullfil the need for discussion in the community.

SUBMISSION AND REVIEW

Poor language

There are still problems with authors who do not have English as their first language. The editors all put some effort into improving the English or asking the authors to do so before sending the paper to the reviewers. It was asked if the received date should be the date on which a paper is ready to be sent to reviewers.

If details of an English language service could be provided more prominently this would be welcomed. It was also thought that it may be useful to have a list of common expressions which authors could use to replace poor expressions. It was asked if the IUCr would consider sponsoring a course on how to write papers, for PhD students for instance. It was felt that is may not be the role of the IUCr but perhaps the IUCr journals could provide some links to teaching aids or a reading list to help would-be authors. A link to examples of well written articles may also be useful. It was suggested that the journals website could be a better resource for authors.

It was thought that some reviewers may not know that a paper will be technically edited and thus worry too much about the spelling *etc*. It was suggested that a statement about technical editing be included in the e-mail to the reviewers saying that the main thing they need to concentrate on is that the work is scientifically clear. An online spellcheck when the paper was submitted was also suggested *i.e.* the incorrect spellings are highlighted as in Word documents.

Other points raised included questions on whether comments in PDFs could be anonymised; could the e-mails sent be improved as special characters are getting lost in some; templates for other citation managers as well as Endnote would be useful *e.g.* Zotero, Mendeley, Papers.

Transfers

It was felt that co-editors should consider if an article is suitable for other journals when editing a paper. In some cases could co-editors be more proactive in saying is this more suited to ...? Is the journal appropriate? Could you suggest an alternative? It was thought that overlap will occur between journals but is not a big problem.

Most transfers are from Acta D to F. Not all co-editors know all the criteria for both journals and may not consider a transfer so all the co-editors need to be made aware of the criteria. Also the wording in Notes for Authors may need to improved. To make referees aware of the criteria it was thought that a question could be added to the referees questions *e.g.* does this article provide new insights into biology, chemistry or structure?

The Section Editors on both journals need to be consulted about transfers. The question of co-submission to Acta D and F was raised but thought to be a bad idea. There was also a discussion about where crystallization methods papers should go and about the length of papers. It was felt that current journal policies should continue, i.e. articles reporting more limited methodological points will not be accepted be Acta D and should be submitted instead to Acta F.

ENHANCED FIGURES

It was thought that most people don't take the time to create these.

PROMOTION

It was felt that there could be more promotion between Acta D and F and it was suggested that e-alerts contain the latest contents of the other journal appended at the bottom. Printed leaflets were seen to be less popular than postcards, post-it notes and posters.

It was thought that it was good for the journal to be seen to set standards. It was suggested that we could perhaps publicise this by having some sort of seal of approval.

PUBLICATION TIMES

The editors suggested that the time limit for revisions for Acta F of one month seemed to be widely ignored. Automatic reminders to the co-editors were thought to be a good idea; however, it was emphasised that reviewers should not be chased using automatic reminders. A better summary on the co-editor's status page was thought to be one way to remind editors what to do next. In writing to authors it was felt that co-editors could imply that the deadline would be enforced and the paper withdrawn (even though it isn't), *e.g.* "you have four weeks to ensure that your paper remains in the system". The use of withdrawal followed by resubmission to the original Co-editor was also discussed as a way of reducing publication times, particularly for articles where major revisions are required.

REFEREE REPORTS

It was thought that all the referee reports for a paper could be made available to all the referees at the point of acceptance, if appropriate. Also if a paper needed to be re-reviewed the reports could be made available. The editors suggested an option to have all the reviews available as an attachment to the standard e-mail that can be sent to reviewers to let them know of the decision made about a paper. As a long-term idea, it was thought that it would be nice to be able to do this automatically at the point of acceptance/rejection/withdrawal, but with the ability to opt out if required.

IMPROVING IMPACT FACTORS AND ATTRACTING GOOD PAPERS

Acta D was thought to have found its niche but maybe can include more commentaries or editorials and a question arose as to whether such articles are included in ISI. However, it was thought that it still needs more structure papers where the paper is the first publication of a structure. J. Mol. Biol. was thought to be reducing the number of structure papers so this may be beneficial to Acta D and Acta F.

Citations in supplementary materials were still thought to be important to our impact factors. After publication of the joint editorial in our journals showing how citations are lost, it was hoped that other publishers would do something about this. It was suggested that both *Nature* and *Science*, formerly two of the worst offenders, had taken action, but it was agreed that we should verify that this was actually the case for all relevant journals.

It was suggested that online enhancements for Acta F should be exploited more. For example, there could be more movies with voiceovers on topics in Laboratory Communications. Papers demonstrating techniques *etc.* (*e.g.* greasing plates) could be encouraged. These were thought to be good for the journal but may not enhance its impact factor.

Publicising the Acta D impact factor was discussed. It was suggested that a logo on all papers showing that the structures in Acta D/F papers have undergone quality checks may attract papers (*c.f.* Michelin stars). To further show the quality of a structure, the online version could also link to Astex viewer. It was thought that validation reports are not yet required by other journals so are a selling point for Acta D/F which are the first journals to require them. (A subsequent meeting with the PDB showed that they are encouraging other publishers to use validation reports but other publishers are not enforcing their submission at present.)

It was agreed that the quality of papers needs to be maintained and authors need to be informed of what is required and what is acceptable. A discussion on some guidelines for authors ensued and it was suggested that some crystallization papers do not have enough information on the crystallization and also the protein design may need to be described, *i.e.* the construct should be given. The diffraction limit should be given and this and other values were thought to be important. It was felt that a standard table could help authors provide the required values.

In order to ease submissions of structural papers to Acta F it was suggested that the format could be shortened in a fashion similar to Acta E *i.e.* have a more rigid format with less text. The content of the shortened papers was discussed and it was suggested that a slimmed down list of items might be workable with the understanding that if the referees or the co-editor asked for more information it would be provided by the authors. publBio, which can already produce tables from mmcifs, could be developed to produce such papers. Also, mmcifs of unpublished structures in the PDB could be used for publication, but flexibility to accept non-mmcif files was also needed. It was questioned whether publication of old structures is necessary since the PDB summary provides relevant information on the structures, but it was felt that authors still require publication of their work and a PDB entry is not a publication and it is not peer reviewed. (In the meeting with the PDB at the Madrid Congress other possible options for publication mechanisms were discussed.)

To get more authors to publish their unpublished work it was thought that an invite could be sent out to authors of unpublished structures in the PDB. One possible author was suggested and others are known to the Editors. It was felt that if publBio was developed further it could be tested by these authors before being released more generally. Also a number of new style papers could be published to advertise the new format. Advertising slogans including decluttering or "put more structure in your life" were suggested.

SPECIAL ISSUES

It was felt that these did not always contain articles typical of the journals they appeared in and may not have high impact. It was felt important to make these issues as focused as possible. The area of protein production was covered in some special issue papers so it was asked if this be covered in general. The number of these papers is low at the moment and it was not thought necessary to have a specific co-editor but co-editors should try to choose suitable referees and contact Section Editors if they are having problems with such papers.

Special issues are also seen as a lot of work and can increase publication time statistics. It was suggested that special issues are published in parallel with regular issues but it was also realised that this could cause problems for the Chester staff. In spite of these comments it was felt that special issues were well received and some are very good, notably the structural genomics ones. Future topics were discussed and free-electron lasers were thought to be something to keep an eye on.