

# Self-correcting science at work

In this Editorial we reflect on post-publication discussions and corrections, and look at some recent examples from *Nature Catalysis*.

Disagreement and dissent are an important part of any healthy scientific discourse. Every discipline is familiar with its own internal debates and the literature — as a quick web search can testify — is rich in articles whose titles refer to misconceptions and pitfalls within a specific area; such manuscripts recurrently focus on topics for which a consensus has not yet been reached or best practice rules have not been formulated.

The essence of such form of debate is captured by peer review. However, it is only when a manuscript — or its message — starts circulating through to the whole community that it gets available for deeper scrutiny. Conferences — and to a certain extent social media — play an important role in this regard, but the true change of pace has come with the use of preprints, which render the details of a work immediately accessible and allow discussions to rapidly kick off. Thus, analysis, validation experiments and reproduction by independent laboratories will determine if the findings or a given technology will be adopted by other researchers. Occasionally, further investigations reveal limitations or inaccuracies within a study, which can then result in commentaries or changes to published papers. This form of scrutiny is a precious resource for the community and is essential to preserve the integrity and value of the scientific record.

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In this issue of *Nature Catalysis*, Hua-Jian Xu, Hai-Zhu Yu and colleagues retract an article published in January 2021 that reported the ability of an amine organocatalyst to promote the Suzuki–Miyaura-type coupling of aryl halides with arylboronic acids (*Nat. Catal.* **4**, 71–78; 2021). The retraction of this work testifies to the effectiveness of the mechanisms highlighted above, and came off the heels of new evidence produced by different

laboratories (*Nat. Catal.* <https://doi.org/10.1038/s41929-021-00709-8>; 2021, and *Nat. Catal.* <https://doi.org/10.1038/s41929-021-00710-1>; 2021, and *Nat. Catal.* <https://doi.org/10.1038/s41929-021-00711-0>; 2021) as well as the original authors that rendered the main conclusions of the study questionable.

Upon publication of the paper there were very different reactions by the community. A method for the construction of C–C bonds that can be applied to the synthesis of bioactive compounds and does not require the use of toxic metals was hailed as a breakthrough by some, considering the potential for the production of pharmaceuticals. At the same time, a wave of genuine scepticism arose on social media, and many researchers questioned the results.

Between February and April, *Nature Catalysis* was contacted by different teams that expressed criticisms and submitted validation studies related to the work by Xu, Yu and colleagues. Nature Portfolio values such contributions and considers them in the form of Matters Arising articles — a peer reviewed format that provides a forum for discussion and further inquiry related to published research papers. Accordingly, we initiated the process to formally evaluate the collected evidence. At the same time an editorial note was published to alert our readership that the conclusions of the paper were subject to criticisms that were being considered by the editors.

Matters Arising articles are carefully evaluated by editors and reviewers, and are taken forward for publication when judged of exceptional interest for the community. Moreover, they are generally accompanied by a reply by the authors of the original article. In all cases, the editorial office invites the criticising researchers to contact the authors and discuss the concerns before the process is formally initiated, as simple clarifications can often solve a controversy. Because it can take time to clarify the issues, we encourage the deposition of preprint versions of Matters Arising articles in public repositories to facilitate early awareness of the issues under debate by the community.

Since the release of the first preprints, we have been in touch with the authors of the

original article and asked them to clarify the issues raised by the community. Eventually, three Matters Arising articles were submitted to the journal, and all supported the idea that the observed cross-coupling activity, while reproducible, can be explained by the presence of trace amounts of Pd in the reaction mixtures. Similar concerns had been raised during peer review and initially addressed with tests that seemed to rule out metal contribution. The evidence contained in the Matters Arising articles, however, provided a different interpretation implying that the experiments included in the published manuscript could be only seen as an indication rather than a conclusive proof. Moreover, reproduction of the trace metal analysis estimated higher Pd quantities than initially reported. At this point, we agreed to give Xu, Yu and their team time to engage in a series of experiments with the aim to review the issues and the received criticisms objectively. Someone may perceive this procedure as unnecessarily long considering the urgency for clarity that certain issues demand. However, post-publication debates must be moderated in a context of impartiality; therefore, it is important that the authors of the original article are given the opportunity to base a potential response on supporting experimental results.

After a few months of investigation, and thanks to the feedback provided by independent reviewers, the contour of the story has become clear. A consensus has in fact emerged between the authors of the original article and the criticising authors about the nature of the actual catalysts for this process, which was confirmed to be the Pd metal initially employed for the preparation of the amine organocatalysts. Accordingly, Xu, Yu and colleagues have agreed that the article should be retracted as the substantial amount of collected evidence supersedes their initial findings and we have supported this course of action.

The three Matters Arising articles and the related retraction carry an important message: the many researchers involved in the process have indirectly reaffirmed crucial criteria for the study and validation of metal-free reactions and they have pointed to the need of designing appropriate control

experiments in order to exclude the effect of false positives — or false negatives. The knowledge generated will certainly be useful to those continuing in the endeavour of developing methods for cross-couplings that do not rely on metals.

More generally, the history of these articles reminds us that scientific knowledge can only be generated by dealing with doubt and uncertainty: by questioning and validating facts, the members of a community set in motion that

form of self-correcting mechanism that contributes to the generation of the scientific consensus. □

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