

Magn. Reson. Discuss., referee comment RC4 https://doi.org/10.5194/mr-2022-6-RC4, 2022 © Author(s) 2022. This work is distributed under the Creative Commons Attribution 4.0 License.

Reply on CC2

Paul Schanda (Referee)

Referee comment on "Imatinib disassembles the regulatory core of Abelson kinase by binding to its ATP site and not by binding to its myristoyl pocket" by Stephan Grzesiek et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-6-RC4, 2022

I fully support the view expressed by Dorothee.

In the present case of the Abl kinase, the problems extend further, beyond the JMB paper. Anyone who digs into details of the associated paper in Science (10.1126/science.abc2754) may make their opinion about the quality of those NMR structures. The number of NOE restraints there is rather low, and in some biologically important parts (e.g. A loop) there are hardly any restraints. Moreover, three states were simultaneously present in that sample, exchanging with a kex of 50 s-1, which raises serious questions what one actually seens in NOESY experiments with 150 ms mixing time.

I think transparency is key to scientific progress, and in the mentioned paper(s) there is a lack of transparency. The contribution by the Grzesiek group to point out these issues is, thus, important to correcting the literature views. Of course, the best place to publish them is in JMB, where the authors of the original paper would be forced to reply (or to retract the paper altogether).

From my experience, it is often very difficult to publish data which demonstrate that published data are incorrect or incorrectly interpreted. We have made such an experience during a rather long struggle at NSMB where we and an independent group showed serious flaws in published research, including erroneous data fits, omission of data (cherry-picking their data) and omission literature data that contradicted their data (https://www.nature.com/articles/nsmb.3059). It took us almost two years to get our correction published, despite clear-cut reviewers' assessements.

An underlying problem in scientific publishing practices is that nobody wants to see that sometimes the scientific publication process fails. Reviewers may miss important details --simply because it takes a lot of time to dig into details and they do it for free; and editors may miss them, too. Authors presumably do their best to avoid errors or misinterpretation, but errors can happen. These failures are understandable and simply can happen. However, it is absolutely crucial that the scientific community corrects for these errors. In this sense, I find the contribution by the Grzesiek group important.