Open Access MAGNETIC RESONANCE Discussions

Magn. Reson. Discuss., editor comment EC1
https://doi.org/10.5194/mr-2021-30-EC1, 2021

Comment on mr-2021-30

Jörg Matysik (Editor)

Editor comment on "Insights into Protein Dynamics from ^{15}N-^{1}H HSQC" by Erik R. P. Zuiderweg, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-30-EC1, 2021

Dear Eric,

Unfortunately, after consulting several editors, we cannot accept your paper for publication in MR.

Conceptually your idea to use sensitive 15N-1H HSQC spectra for dynamics analysis of proteins is very nice and could be very useful for a large number of biological applications. Thus, the software you developed for that would be a valuable contribution. However, the results still show a poor correlation between predicted (cf Fig. 4 and 6) and measured relaxation properties and are therefore not convincing yet. Therefore the dynamics analysis still remains very qualitative in the end. As various experts indicated, there can be several reasons for this, such as slow dynamics/exchange and indirect saturation transfer effect. Since good methods exist to study those, the current paper seems to be premature.

Whereas the current manuscript cannot be accepted, we encourage you to progress these studies, to investigate improvements via, e.g., MD simulations and to obtain more convincing data in particular. We think that this could lead to a balanced publication that gives credit to your software and its theoretical analysis. We know that you will be disappointed not to add an accepted manuscript to the Special Issue for Robert Kaptein. When you want, it is possible to leave your current manuscript as a contribution to MR Discussions and in that case it would still be connected to this SI, as indicated by Dr Bodenhausen. Since our task as guest editors for this SI will end, you can also enquire with the executive editors how this contribution could be merged into a full publication later on.

With kind regards
Jörg (Matysik)