

Magn. Reson. Discuss., referee comment RC1 https://doi.org/10.5194/mr-2022-22-RC1, 2022 © Author(s) 2022. This work is distributed under the Creative Commons Attribution 4.0 License.

Comment on mr-2022-22

Anonymous Referee #1

Referee comment on "Facilitating the structural characterisation of non-canonical amino acids in biomolecular NMR" by Sarah Kuschert et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-22-RC1, 2022

This article addresses an important and increasingly common problem, namely how to provide a standardised and highly automated procedure for handling non-canonical amino acids in NMR structure determination. The workflow of the software is clearly described and its performance convincingly demonstrated in the results section. Any remaining shortcuts are also honestly addressed. All in all, this work will greatly facilitate the work of many NMR groups and especially promote the study of ncAAs.