Magn. Reson. Discuss.,
https://doi.org/10.5194/mr-2020-32-AC2, 2021

Open Access MAGNETIC RESONANCE Discussions

Interactive comment on "Extending the applicability of P3D for structure determination of small molecules" *by* Alain Ibáñez de Opakua and Markus Zweckstetter

Alain Ibáñez de Opakua and Markus Zweckstetter

mzwecks@gwdg.de

Received and published: 6 January 2021

There are some discrepancies in the sucrose data that should be clarified. In figure 5 the numbering of the sucrose structure (a) and the notations in the table (b) don't agree. CH vectors with numbers 1,2,3 and 4 in the structure displayed are nearly parallel and should have very similar RDCs. The data appear to come from the Ndukwe reference, which does show this trend. In the manuscript table RDCs with the Ndukwe values are numbered 5,9, 10 and 11.

Reply: Thanks for detecting this mistake. We corrected the numbers in the revised version of the manuscript.

Printer-friendly version

Discussion paper

Also, it is not clear where the populations are coming from. These appear to be fitted parameters? The text seems to suggest that the populations are consistent with free ender estimates on line 315. They are not. Also, some comment might be made in comparison to water MD simulations (Case) where only M1 and M2 are highly populated with a difference of only 0.3kcal, something more in line with populations.

Reply: The populations of Fig. 5 come from the Ndukwe reference and the populations of Fig. 6 are fitted. We added a comment to the figure legend to avoid this confusion. The populations are based on the three conformations present in the M1 (called S3-i, S3-iii and S3-iv in that paper). The structures were taken from table S14. The description of the populations is just a short summary of the work from Ndukwe et al. We are not trying to suggest that the free energy from DFT explains the calculated populations. The information is just descriptive.

There are a few places that the text could be improved for clarity: Line 31 – not clearly worded. Maybe: “alignment requires a minimum concentration of lyotropic medium and then often aligns strongly at this concentration, resulting in ..”

Reply: Thanks, we changed it to: "Alignment requires a minimum concentration of lyotropic medium and often aligns strongly at this concentration, which limits the tunability of the alignment strength."

line 87: RQ might be defined here as opposed to much later.

Reply: Changed.

Interactive comment on Magn. Reson. Discuss., https://doi.org/10.5194/mr-2020-32, 2020.

Printer-friendly version

Discussion paper