

Magn. Reson. Discuss., author comment AC1
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Comment on mr-2022-3

Henry W. Orton et al.

Author comment on "Localising nuclear spins by pseudocontact shifts from a single tagging site" by Henry W. Orton et al., Magn. Reson. Discuss.,
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We thank the reviewer for careful reading and helpful comments!

1) We agree that *complete* structure determinations based on PCSs only may not yield highly accurate structures. Structure refinements of specific sites in proteins of known 3D fold, however, can yield very precise structural information that for all intent and purpose appears to be accurate too, as we have shown recently with IMP-1, where we deployed flexible tags at three different tagging sites (Orton et al., 2022). PCSs from flexible tags deliver accurate structural information provided the fitted effective DeltaChi tensors predict the PCSs accurately in the immediate vicinity of the site of interest, as pointed out in lines 250 to 255 and lines 299 to 303.

We propose to amend the second part of the sentence in the abstract:

"and PCSs generated from multiple tagging sites have been shown to enable highly accurate structure determinations at specific sites of interest even when using flexible tags, provided the fitted effective DeltaChi tensors accurately back-calculate the experimental PCSs measured in the immediate vicinity of the site of interest."

Points 2 - 7: We agree and will amend accordingly.

Reference:

Orton et al., Magn. Reson. 3, 1-13, <https://mr.copernicus.org/articles/3/1/2022/>, 2022.