

Magn. Reson. Discuss., author comment AC1 https://doi.org/10.5194/mr-2021-11-AC1, 2021 © Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.

Reply on RC1

Timothy J. Keller and Thorsten Maly

Author comment on "Overhauser dynamic nuclear polarization (ODNP)-enhanced twodimensional proton NMR spectroscopy at low magnetic fields" by Timothy J. Keller and Thorsten Maly, Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-11-AC1, 2021

Please find our reply to the reviewer's comments marked as **RESPONSE**:

Possible corrections:

- line 152: do you mean Tecmag, not Techmag, correct?
 RESPONSE: Yes, this is correct, we were referring to Tecmag. This mistake will be corrected in the revised version of the manuscript.
- In Figure 4a, shouldn't the x-axis be labeled "J-coupling (Hz)"?
 RESPONSE: This mistake will be corrected in the revised version of the manuscript.

Suggested comments to address:

 It seems from the technical details that 2D acquisitions presented took about 30 mins. What are the limitations of the proposed method? Could it be applied to non-monotonic drift? Could the method be applied for much longer acquisition times particularly when the samples are not neat compounds?

RESPONSE: In the two examples presented here the field drift can be modeled using a 4th order polynomial (we will add the coefficients to the SI in the revised version of the manuscript). In these experiments, the field drift was always monotonic so we can only speculate about the performance of our field correction method. We do believe, as long as a function can be found that adequately models the field drift it will be possible to correct for the drift even for non-monotonic drifts (e.g. oscillations). In the case of sudden field jumps, it should still be possible to correct for such disturbances. This should allow for measurements that would require much longer acquisition times.

What applications would benefit most from such instrument/method? Compared to more traditional compact NMR spectrometers?
 RESPONSE: In recent years many more vendors offer bench-top NMR spectrometers. In our system, we demonstrate, as a proof-of-concept, that high-resolution NMR spectroscopy can be combined with ODNP. While we can foresee/speculate many different applications, one particular application, the measurement of hydration dynamics stands out as the method that would most benefit from the described

instrument. Currently, ODNP measurements for hydration dynamics are performed by adding DNP capabilities to an EPR spectrometer. However, the homogeneity of the electromagnet is often not ideal, hence the off-signal (the signal recorded without microwave radiation) is often weak and broadened due to field drift/instabilities. While an EPR magnet can be equipped with active shims, a system based on a compact permanent magnet will have a much smaller footprint compared to a floor-model EPR spectrometer. In addition, there are several new diagnostic techniques that rely on low-field NMR measurements (e.g. methods developed by T2 Biosystems, WaveGuide Corp., Synex Medical e.g.). These methods often rely on measurements of relaxation parameters because of the inhomogeneous magnetic field. These methods can potentially benefit from ODNP too. We will add this discussion to the revised version of the manuscript.