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Reply on RC1

Jens D. Haller et al.

Author comment on "SORDOR pulses: expansion of the Böhlen–Bodenhausen scheme for low-power broadband magnetic resonance" by Jens D. Haller et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-1-AC1, 2022

Dear Philippe,

Thank you very much for the detailed reading and constructive comments. Please find in the following in which way we addressed your suggestions, which also involved the re-recording of quite a number of experiments. The manuscript was certainly improved considerably with your comments. We are confident that you will now find it acceptable for publication.

Sincerely yours,

Jens D. Haller, David L. Goodwin, Burkhard Luy

This article presents the application of a class of broadband Universal Rotation pulses, so called SORDOR pulses. The particularity of these pulses is that the rotation axis depends quadratically on the offset frequency and that they have low RF power requirements. By matching the different pulses in a sequence, SORDOR pulses can be used in virtually any experiment (although sometimes quadratic phase-corrections need to be applied in the data processing). The power of the method is demonstrated on a very demanding “19F-project” experiment. The concept described in this article could have a very wide applicability (even if a, as the authors acknowledge, the pulses still need to be improved) and are of much interest for the readership of *Magnetic Resonance*. I recommend its publication after the following comments have been addressed:

- Figure 4. The profile of the echo sequence with hard pulses seems to be much broader than the one of the of the 90 degree pulse, probably because the coherence pathway selection is not ensured. Usually, it is more instructive to look at a sequence which ensures the correct coherence selection pathway (by gradients or EXORCYCLE for example).

>>> We very much thank you for this comment! The performance of the hard pulses in the original manuscript did not take the coherence pathway selection into account. We re-recorded corresponding experiments with gradient-based coherence selection (see new Figure 4) which much more demonstrates the advantages of SORDOR pulses compared to the hard pulse approach!

- Figure 4. The amplitudes for the SORDOR profiles vary quite a bit, which is exacerbated for the echo sequence. The authors should quantify these variations. What are the consequences for an experiment with multiple echos (like the project sequence)?

>>> By re-recording the offset profiles with gradient-based coherence order selection also the offset profiles turned out to have much less variation, actually corroborating theoretical offset profiles. We added values for upper relative variations in the text.

- Figure 5. “Clearly the relaxation of all signals can be easily followed using up to 128 perfect echoes”. This figure on its own is not very instructive. Is the decay exponential (clearly not the case for the signal around -110ppm)? How much of the decay is due to imperfections of the pulses (see previous comment) or imperfect homonuclear decoupling? How close is the decay rate to the actual R2?

>>> We apologize that we did not show signal decays and also did not give any characterization of the PROJECT experiment. We re-recorded the spectra and included the decays for the 19F-PROJECT experiment in the SI. The signal decay for most signals is indeed exponential, only signals with expected 19F-19F second order artefacts deviate significantly, which is to be expected. We tried to compare the results with a hard pulse version of the 19F-PROJECT experiment for verification of exponential decay rates, but the hard pulses could not cover sufficiently the chemical shift ranges of coupled nuclei in the used sample. Resulting hard pulse PROJECT spectra resulted in highly distorted multiplets from which extraction of exponential decays was not at all possible. This made us aware that the PROJECT experiment in general does not lead to specific R2 rates of a single signal, but to relaxation rates determined by the inphase coherence transfer under planar mixing conditions of the full 19F spin systems. In addition, SORDOR pulses will lead to a (small) contribution of longitudinal relaxation. We rewrote parts of the experiment description accordingly. To test the performance and have a comparison with the hard pulse version of the PROJECT experiment, we measured the decay on a doped D2O sample and included the resulting exponential decays for the different versions in the SI.

- Line 162: “A disadvantage of the SORDOR pulses arises in heteronuclear experiments when pulses on different nuclei need to be applied simultaneously.” This also applies for homonuclear experiments. For example, does the fact that the coupled nuclei are not touched simultaneously has any effect on the perfect echo?

>>> The answer to this comment turns out to be quite complex. While adiabatic pulses due to the defined frequency sweep indeed show strong effects to coupled nuclei with considerable chemical shift difference, SORDOR pulses do not have an explicit frequency sweep, but a much more complicated trajectory during the pulse. An examination of the SORDOR pulses using average Hamiltonian theory shows (data not shown) that homonuclear coupling evolution is generally very low. Only nuclei with very small chemical shift differences close to the strong coupling limit will experience significant effects. We add a comment concerning strong coupling evolution within the context of the 19F-PROJECT experiment. In addition, we considerably changed Figure 3 showing now the quadratic phase behavior rather than the linear phase sweep, as your comment made us aware that this representation might be misleading.

-Sometimes the writing is a bit sloppy and imprecise (in particular in the introduction). For example: “With the advent of 1.2 GHz NMR spectrometers practically all common heteronuclear experiments require the use of amplitude- and phase-modulated pulses due to the enlarged bandwidths that need to be covered...”. The need of broadband pulses has only to do with the bandwidths that need to be covered, not whether the experiment is heteronuclear or homonuclear. A very common 15N/1H HMQC (or even an HNCO) does probably not need shaped pulses even at very high fields, while many homonuclear 13C experiments do.

>>>Indeed, an HNCO experiment can be run with hard and selective shaped pulses. In case of the 1H,15N-HMQC, however, broadband pulses are utterly needed for most samples. Nucleic acids, for example, contain amino and imino nitrogens, making it impossible to cover all resonances in a single experiment using hard pulses and conventional probeheads. And even in well-behaved proteins the N-terminal NH2-group is usually not covered with hard pulses. We rephrased the wording to “… a large number of experiments requires …”.

-Finally (this is more a comment to the editors of the journal, since the authors are not to blame): the format of the citations makes some parts of the article virtually unreadable (for a striking example see the second paragraph of the introduction). I think many readers would appreciate a change in format.

>>> We agree that citations using numbers would lead to less distraction when reading the text. But we leave any decision regarding the format to the Journal.