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Comment on mr-2021-56

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Referee comment on "Selective excitation enables encoding and measurement of multiple diffusion parameters in a single experiment" by Neil MacKinnon et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-56-RC1, 2021

The work by MacKinnon et al. describes a new concept for diffusion experiments, where multiple selective excitation/refocusing blocks are used not only to excite different segments of the spectrum, but also encode diffusion in a different way for each segment in a single scan. This is demonstrated here by using different gradient strengths for the diffusion encoding of the water and the MAS peptide signals, but indeed could be expanded upon towards other parameters such as gradient direction. This concept is useful, and one can indeed think of ways to apply this to other diffusion pulses sequences. It is certainly of interest for the readership of MR.

The authors mention that wider segments of the spectrum can also be selected, encompassing multiple signals. But what if the signals within one segment are coupled to one other? Would that not generate artefacts from non-refocused J-coupling evolution?

The SNR for the Ala methyl signal increased significantly for the selective experiment compared to the non-selective experiment (Table 1). This is unexpected, given the expected increased relaxation losses during the selective pulses. Is there an explanation for this? Is the same observed for the Methionine methyl signal?

The SNR and diffusion coefficient measured on the Methionine methyl group are not shown in Table 1, not discussed in the text, and the decay curves are not shown in Figure 3. Yet this was the third signal selected. It would be good to include this, to observe the consistency with the Ala signal.

Some remarks about the representation of the pulse sequence of Figure 1.

- It would be useful for the sake of clarity if the flip angles of the selective and hard pulses are indicated (90°, 180°). Also, it would be useful if it can be clearly indicated somewhere that the order of selective pulse frequencies in the encoding and decoding blocks are the same, as actually this is not strictly necessary (even though the effective â□□ would vary then).
- The way that the diffusion delay â□□ is indicated in the pulse sequence is misleading, since now the wrong suggestion is made that it is the delay between the last selective

pulse of the encoding block and the first selective pulse of the decoding block. The conventional definition of â□□ actually also requires including either the full encoding block (from the beginning of the first gradient pulse of the encoding block until the beginning of the first gradient pulse of the decoding block), or the full decoding block (from the end of the last gradient pulse of the encoding block until the end of the last gradient pulse of the decoding block).

- The pulse sequence also shows gradient pulse durations can be different for each selected frequency, i.e., $\delta_n/2$. In principle this is indeed possible, but not used here. In fact, looking at the Bruker pulse sequence code provided by the authors on zenodo, this appears hard coded to be the same for each block (p30). Here, it is in fact the gradient strength g that varies with n, and should be indicated as g_n in the figure to make it consistent with the demonstration in this work.
- Finally, it would be nice to also explicitly indicate τ from the ST equation (or perhaps as τ_n, if different 180° pulse durations are envisaged).

The Stejskal-Tanner equation (1) is valid for rectangular gradient shapes. The gradient shape is not mentioned in the experimental part. It would be good to confirm the gradient shape in the experimental part, since for Bruker these are standardly SINE or SMSQ shapes, requiring a slightly modified ST equation.

Also, it should maybe be explicitly noted that the value of τ is actually quite significant here to correctly take into account, since it also encompasses the long selective 180° pulse (14.7 ms). If different selective pulse durations would be used for each spectral segment (as is possible in the pulse sequence code provided on zenodo), the ST-equation will be significantly different for each segment.

Figure 3a shows the signal intensity as a function of k, while Figure 3b shows it as a function of gradient strength percentage. This inconsistency seems unnecessary to me.

On page 3, line 66, ledbpge2s1d should be ledbpgp2s1d.