

Magn. Reson. Discuss., referee comment RC2
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Comment on mr-2021-52

Anonymous Referee #2

Referee comment on "Signal-to-noise ratio in diffusion-ordered spectroscopy: how good is good enough?" by Jamie Guest et al., Magn. Reson. Discuss.,
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In this article, Guest et al. analyse the effect of the signal to noise ratio in diffusion-ordered NMR spectroscopy (DOSY), and provide guidelines on a choice of sampling strategy (number of gradient increment, maximum attenuation, SNR) that provides good accuracy. The paper is very well written and contains a number of interesting and useful explanations on DOSY. The main message is enlightening and important for users of the method. I recommend publication in Magnetic Resonance, after the following minor points have been addressed.

It would be useful to clarify what is meant by "accuracy" in the text. Sometimes the word refers to systematic errors only, sometimes to a combination of systematic and random errors (https://en.wikipedia.org/wiki/Accuracy_and_precision). Here the latter seems to be used, but this would need to be explicit.

The conclusion reads "a trivial calculation will show both whether or not such experiments are worth attempting in the first place, and what limiting diffusion resolution is achievable". Does this calculation require knowledge of SNR_{lim}? How can this quantity be determined?

It would be useful to have guidelines on what to do in a fixed total experimental time. Is it better to increase the number of gradient increments, or the number of averaged scans? In which cases? The answer lies in the proposed equations, but this is so frequent a question that it may deserve a specific discussion. For example, it seems from Eq. 13, that increasing N will always increase accuracy, while increasing SNR is only useful up to a certain limit. Is it the case that one should increase N only as soon as the number of scans is sufficient for phase cycling purposes and peak detectability?

Overall, while all the tools are provided to guide readers in the choice of appropriate

parameters, the usefulness of the paper would be increased by the addition of a practical example.

The “inverse of the coefficient of variation” is introduced as “a convenient measure of resolution”. This choice should be justified. In spectroscopy, resolution or dispersion is usually quoted on an absolute, not a relative scale. Why use a relative scale here ?

In Eq. 4, the half sine shape seems to be accounted for in Δt , but not in the gradient area.

In Eq. 5, shouldn't a sum symbol be used instead of an integral symbol?

Also in Eq. 5: what is the variable t_i ? From Franconi et al., it should be ϵ_i ?

I could not find the reference to Recic et al. and Franconi et al. in the manuscript