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Magn. Reson. Discuss., referee comment RC1
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# Comment on mr-2021-52

Anonymous Referee #1

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Referee comment on "Signal-to-noise ratio in diffusion-ordered spectroscopy: how good is good enough?" by Jamie Guest et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-52-RC1, 2021

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An important problem in DOSY is how well differences in diffusion coefficient can be resolved. In older literature, a "rule of thumb" can be found stating that (in case of non-overlapping signals and good signal-to-noise ratios) the diffusion coefficients have to differ by at least 30% to be distinguished, but the reality is of course more complex. This work presents a very welcome quantitative assessment of how the signal to noise and sampling of gradient strengths affect the diffusion resolution. These new insights can indeed help practitioners to assess beforehand whether it will at all be feasible to resolve different molecules in the diffusion dimension, using for instance also tools to predict diffusion coefficients (based on molecular weight, by the same research group).

I do have some questions that the authors may wish to clarify or consider commenting on.

The final equation (13) illustrates that in practice improving the diffusion resolution by increasing the signal-to-noise ratio has its limits. The same equation seems to suggest that an increase in the number of gradient values N, rather than increasing the number of transients, could indefinitely improve the diffusion resolution. Figure 2 indeed shows no deviation from the linear behaviour of $R_D$ as a function of $\sqrt{(N-1)}$. Do the authors think that in reality there is also here a limit to be reached, for instance due to gradient hardware limitations, or environmental changes as a function of time or gradient strength?

The value of $SNR_{lim}$ in equation (13) appears to be determined by systematic errors in signal intensity, which, besides hardware and environment fluctuations, will probably depend on the pulse sequence used. The authors rightly mention that in general more rf-pulses in the sequence or additional unwanted coherence transfer pathways will result in more systematic 'noise'. I wonder if $SNR_{lim}$, which can be determined experimentally in the way described in the paper, could serve as a means to compare the performance of various DOSY pulse sequences, comparing it to, for instance, the value measured for the oneshot sequence on the same spectrometer and sample?

Figure 2 shows that the data points obtained for low values of N (10 (black) and 17 (grey)) deviate somewhat more from the fitted curve than all the other data points. Does this imply that equation (13), combined with equation (11) and Table 1, approximates reality less well for lower values of N?

Some further technical comments that should be fixed:

In equation (3), the gradient shape factor for half-sine shapes, (2/π)^2, has been forgotten.

Equation (5), expression for B, shows $t_i$ before the exponent. I guess this should be $\varepsilon_i$.?

There are problems with the references. Some citations in the main text do not feature in the reference list (I spotted Brihuega-Moreno 2003, Franconi 2018, Reci 2020 and Power 2016 to be lacking). The reference to Mehlkopf et al. lacks the title.