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Magn. Reson. Discuss., author comment AC2
https://doi.org/10.5194/mr-2022-21-AC2, 2022

Reply on RC2

Da-Wei Li et al.

Author comment on "DEEP Picker1D and Voigt Fitter1D: a versatile tool set for the automated quantitative spectral deconvolution of complex 1D-NMR spectra" by Da-Wei Li et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2022-21-AC2, 2022

The procedure in this paper for esentially "peak picking" is quite good. My one comment is that while the peak fitting is very good, for the use in metabolomics one of the major issues is the identification of the peaks. They can have significatly different chemical shifts due to pH and ionic strenght differences. It would be good for the authors to suggest an approach to combinine their method with other methods using the AI approach for assignment of the fitted peaks.

Author response:

Thank you for the review. The final comment is similar to the last point of Reviewer #1. Peak annotation for the identification of known metabolites in complex metabolomics mixtures requires the pairing of the DEEP Picker1D and Voigt Fitter1D output with a metabolomics database along with a strong query engine for the analysis of cohorts of spectra that takes peak shifts into account. Such work is currently in progress.