Comment on mr-2022-21

Milo Westler (Referee)

Referee 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-RC2, 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.