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Comment on mr-2021-48

Anonymous Referee #1

Referee comment on "Virtual decoupling to break the simplification versus resolution trade-off in nuclear magnetic resonance of complex metabolic mixtures" by Cyril Charlier et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-48-RC1, 2021

An approach for virtual decoupling (1H-13C) of 13C-1H HSQC NMR spectra of metabolic mixtures is presented in the manuscript by Charlier et al. With the approach presented it is possible to obtain 13C-1H correlation spectra with very high resolution in the directly detected 1H dimension, without introducing heating from broadband decoupling techniques.

Overall, the manuscript presents an interesting application of virtual decoupling which also, combined with J-resolved spectra, provides valuable information for the assignment of complex 1D 1H spectra. As such, it is my impression that the manuscript will be of interest to the NMR field, in particular to those with an interest in characterisations of metabolic mixtures. A few comments below:

Comments:

- The process of virtual decoupling is not fully clear from the manuscript. The authors refer to their software, which indeed can be downloaded from GitHub, and they provide a very brief explanation on line 180 – 189, but more details should be included in the manuscript, for example in the method section. Specifically, it is not clear if just one multiplet is 'decoupled' at a time (and how) or if the standard IPAP approach is used, with sum and differences of IP and AP followed by frequency shifts (see e.g. Figure 6 of https://doi.org/10.1016/j.pnmrs.2009.07.004).
- The one-bond J(13C-1H) may vary from site to site. The authors should briefly describe how varying 1JCH could affect the presented virtual decoupling approach.