

Magn. Reson. Discuss., referee comment RC1  
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## Comment on mr-2021-48

Anonymous Referee #1

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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

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An approach for virtual decoupling ( $^1\text{H}$ - $^{13}\text{C}$ ) of  $^{13}\text{C}$ - $^1\text{H}$  HSQC NMR spectra of metabolic mixtures is presented in the manuscript by Charlier et al. With the approach presented it is possible to obtain  $^{13}\text{C}$ - $^1\text{H}$  correlation spectra with very high resolution in the directly detected  $^1\text{H}$  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  $^1\text{H}$  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  $J(^{13}\text{C}$ - $^1\text{H})$  may vary from site to site. The authors should briefly describe how varying  $^1J_{\text{CH}}$  could affect the presented virtual decoupling approach.