

Magn. Reson. Discuss., referee comment RC1
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Comment on mr-2021-32

Anonymous Referee #1

Referee comment on "Application of multiplet structure deconvolution to extract scalar coupling constants from 1D nuclear magnetic resonance spectra" by Damien Jeannerat and Carlos Cobas, Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-32-RC1>, 2021

The manuscript entitled "Application of multiplet structure deconvolution to extract scalar coupling constants from 1D NMR spectra" presented by D. Jeannerat and C. Cobas proposes an efficient automated solution of the problem of coupling pattern description in 1D ^1H NMR and extensions to moderately strong couplings and to couplings with nuclei of $S > 1/2$. The manuscript was well prepared and is well written.

The doublet to singlet reduction process that constitutes the cornerstone of this manuscript is based on Figure 2 and some aspects of it are unclear to me. Convoluting a doublet with something that leaves a singlet at the end is unexpected. You will find attached a revised Figure 2 (left panel). My red "ovals" show Dirac functions that are not expected to be there, unless $M(J^*)$ is not made of 10 Dirac functions but of an "infinite" number of them, something that cannot be guessed from Figure 2 (left). What is reported in the right panel is not equivalent to what is reported in the left panel, unless I misunderstood the process you reported. Scanning through the data points and subtracting the current amplitude and the amplitude of the data point J^* Hz ahead in the original spectrum is a way to calculate a convolution product by an anti-phase doublet of Dirac functions. The convolution of an in-phase doublet(J) with an anti-phase doublet(J) provides an anti-phase doublet($2J$) and is not made a single positive peak, unless some removal of the negative part of the resulting spectrum is carried out. The present description of the "scrapper" procedure seems very close to the one of J-doubling, reported by R. Freeman and coworkers.

The only request of the reviewer to the authors is to make Figure 2 more precise and to describe the algorithm they use in a clearer and more detailed manner, at least when it deals only with weak couplings and $S = 1/2$ nuclei.

Please also note the supplement to this comment:

<https://mr.copernicus.org/preprints/mr-2021-32/mr-2021-32-RC1-supplement.pdf>