

Interactive comment on “ssNMRLib: a comprehensive library and tool box for acquisition of solid-state NMR experiments on Bruker spectrometers” by Alicia Vallet et al.

Anonymous Referee #2

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The manuscript by Vallet et al introduces a library of pulse sequences for Bruker spectrometers that enables the users to easily implement a wide range of experiments commonly employed for resonance assignments or probing dynamics in solid state NMR.

While ssNMRLib is not a novel experimental technique, it could be of great use for users with different levels of expertise in setting up solid-state NMR experiments. The features that I find useful are:

(1) Easy optimisation protocol for coherence transfer steps that are the building blocks for complex resonance assignment experiments. (2) The ease with which a new exper-

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iment can be added to the library. (3) The ease with which the experimental parameters can be retrieved, especially RF powers in kHz units.

I would like to ask the following questions to the authors:

(1) The authors implement a security feature that adds one more layer to the “Power Check” feature of Topspin, which is concerned with duration. A full proof security feature is probably difficult to set up, but could the authors please comment about switching to a “duty cycle” based security system?

(2) As the authors promise, indeed it would be great if on-the fly shape generation could be implemented. It would also be helpful if optimal control derived shapes are available in ssNMRLib. However, judging from the setup of ssNMRLib, this can be achieved with reasonable efforts also from the users.

(3) Like any other software, it would be great to have a “Troubleshooting” section that would help the beginners to address problems. In this regard, also an email discussion group among users would be beneficial.

(4) It is well accepted among NMR users that Topspin is not really well suited for performing quantitative data analysis. By integrating ssNMRLib with programs like nmrglue and matplotlib, the users can extend the workflow from setting up experiments to even reliable data analysis. Do the authors already plan to add features like this in ssNMRLib?

To conclude, I find the manuscript interesting and publishable in Magnetic Resonance.

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