

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.

Manuel Hora

manuel.hora@ub.tum.de

Received and published: 21 October 2020

The authors present a tool box for simple setup of ssNMR experiments on Bruker spectrometers. ssNMRLib comprises a large variety of experiments both for calibration and for analysis of protein samples, e.g. for assignment, distance restraints or dynamics. In my opinion, ssNMRLib provides several benefits both for individual scientists and for the scientific community:

1) The library of already implemented experiments is valuable especially for beginners to get an idea, which experiments are available and might be used. A collection of pulse programmes is also useful for scientists who want to try new types of experiments, but

C1

cannot write pulse programmes (yet) on their own.

2) Power levels in kHz are convenient to quickly check resonance conditions or duty cycles.

3) The recap files are helpful for reporting experimental parameters. Unfortunately, it still happens in papers that important NMR parameters are not reported or not reported in a meaningful manner. The recap files could (maybe in parts) be reported in supplementary information of research articles to facilitate assessment of results or reproducibility of experiments.

4) For the same reason, I support the author's invitation that other scientists should add their (newly developed) experiments to the library. Doing so has a chance to accelerate spreading new pulse programmes among different labs.

To conclude, I consider ssNMRLib a useful tool for training of new NMR spectroscopists, for documentation and for spreading new techniques in a standardised way.

Interactive comment on Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2020-25>, 2020.

C2