

## ***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 #1**

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The manuscript **mr-2020-25, ssNMRLib: a comprehensive library and tool box for acquisition of solid-state NMR experiments on Bruker spectrometers** by *Vallet et al.* introduces a solid-state NMR pulse sequence library, accompanied by a setup tool specifically for Bruker spectrometers. Sadly, the NMR structural biology community is far behind other communities such as X-ray and EM in terms of automation. Therefore, the step towards more automation to save experimental time is in general commendable.

I have a few minor remarks:

1. The setup was tested on **AVIII** and **NEO** consoles. The authors should com-  
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ment, if or how their setup and pulse sequences are compatible with **AVII** consoles. Despite the fact that the support for **AVII** consoles is declining, they are still widespread within the NMR community.

2. How about compatibility on a spectrometer work station running **Microsoft Windows OS**?
3. Obviously, frequency units are more intuitive in the NMR perspective. However, from the technical point of view the use of power levels in Watts alerts the user more than using frequency units, as the nutation by  $X$  kHz can require very low or very high power, depending on the  $90^\circ$  pulse length. Can the authors comment on how their safety check traps this potential risk?
4. Along these lines, the authors implemented safety measures by checking for overshooting RF power for specific pulse elements. However, RF limits are given here in units of kHz, which might be risky as the absolute power integral is crucial. The authors should add more details on how exactly the safety checks are implemented as it is still unclear to the reader by which criteria the margins are set.
5. The setup tool presented in this work does not provide much novelty as it is very similar to the tools offered by the manufacturer, namely **TopSolids** and **bioTop**. The latter is largely for solution-state experiments, but the functionalities, such as creating experimental templates, is provided as well as an automated calibration function, and, I believe, solid-state setups are being currently included. Furthermore, **TopSpin** already provides a large and growing number of solid-state pulse sequences for biomacromolecules, but also for materials, which is not included in the library compiled by the authors. In my opinion, it would be more helpful to the NMR community to push the manufacturer to improve the tools that they already have to the desires of the users and provide them with state-of-the-art pulse sequences.

In conclusion, it is a nice attempt and the authors introduce some new assignment experiments, however, the setup is only a minor advancement compared to already existing tools. In my view, joining forces with Bruker would be much more fruitful in terms of an universal solution for the NMR community.

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