NMRlib 2.0: User-friendly pulse sequence tools for Bruker NMR spectrometers

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We present an updated version (2.0) of our pulse-sequence-tool software NMRlib that allows easy setup, running, and sharing of complex NMR experiments on Bruker spectrometers. Each experiment consists in a combination of python setup scripts and a Bruker pulse-sequence program. In particular, shaped pulse parameters are computed on the fly within the pulse sequence from user defined input values (in ppm) for the desired excitation band, that makes the experimental setup independent from the magnetic field strength. The different experiments are accessible via a graphical user interface (GUI) powered by Java swing classes included in the Bruker acquisition software TopSpin. The GUI provides a convenient way of personalizing and classifying the experiment library.
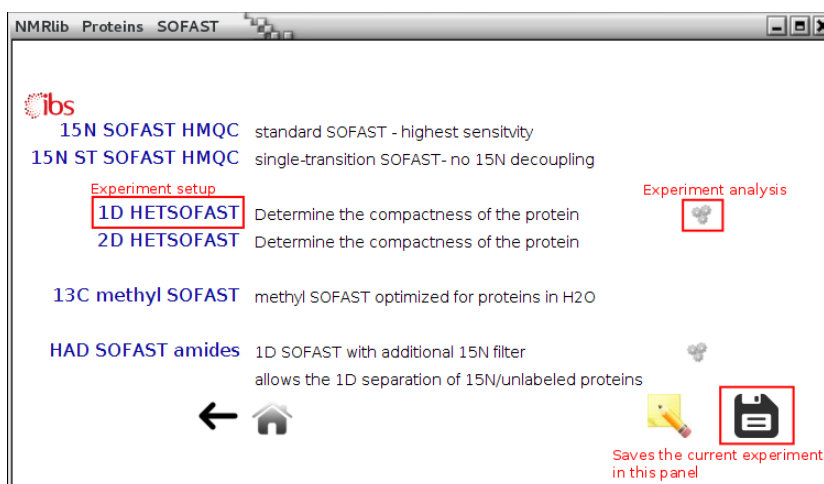

Figure 1: Example of the NMRlib GUI panel enabling the setup and analysis of SOFAST type experiments.

A new experiment is set-up by simply clicking on the corresponding button of the NMRlib GUI. In some cases, pop-up windows will open that allow the user to define the most important parameters for the experiment, or choose among different options, e.g. constant time and conventional frequency editing.

Interestingly, NMRlib also provides a tool that allows to save any interesting experiment as a NMRlib-type python script, and add a corresponding button in the NMRlib GUI. NMRlib is compatible with TopSpin versions 3.2 and 3.5. The software is freely available for academic users from the IBS web page (http://www.ibs.fr/science-213/scientific-output/software/pulse-sequence-tools/).

References
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[2] - P. Schanda, E. Kupĉe & B. Brutscher, SOFAST-HMQC experiments for recording two-dimensional heteronuclear correlation spectra of proteins within a few seconds. J. Biomol. NMR 33, 199-211 (2005).