NOAH2_BS experiment

The NOAH2_BS experiment is a combined acquisition of ^{1}H-^{13}C HMBC and HSQC. It is measured on all service spectrometers whenever both heteronuclear experiments are submitted. Due to the combined acquisition, a considerable amount of measurement time can be saved (or alternatively more scans per sample can be measured). The NOAH2_BS experiment roughly takes the same measurement time as an HMBC with equivalent parameters, and an HSQC with superior quality to the usual setup is measured at the same time.

NOAH2_BS experiment in the Open Acces

The NOAH2_BS is also available in the Open Access at the ASC400 spectrometer (right side). It should be favoured over individual acquisition of ^{1}H-^{13}C HMBC and HSQC to save measurement time. There is a short version as day measurement (equivalent to standard HSQC, but inferior quality compared to standard HMBC, only for concentrated samples) and a long version as night measurement (superior compared to standard HSQC, equivalent to standard HMBC).

Data structure and processing

The NOAH2_BS experiment has been given the name BS, so the corresponding folder will be called e.g. XYBS001A. As usual, inside this main directory there is the experiment folder 10 which contains the raw data. Due to the combined acquisition, these raw data cannot be processed with `xfb` as usual. Instead, there is an au program in Topspin that deconvolutes the data into two separate data sets and performs the respective correct processing. In this way, folders 10001 (HMBC) and 10002 (HSQC) are generated. This au program is evoked from the command line with the command `splitx_au`.

Warning: Do not process the raw data (folder 10) with `xfb` as usual. The result does not correspond to any correct data! Also, do not reprocess the generated HMBC or HSQC spectrum (folders 10001 and 10002) with `xfb`. This command will use some default processing parameters that are not in accordance with some acquisition parameters of the NOAH2_BS experiment. You will see some spectral result with intensity roughly in the correct positions, but the processing is really incorrect and your data quality considerably reduced! If you do this by accident, you can always repeat `splitx_au` on the raw data and all wrongly processed data in folders 10001 and 10002 will be overwritten.

If you are not satisfied with the way `splitx_au` processes the data and would like to reprocess by yourself, please contact us for further information.

Getting and running the au programs

If you have Topspin 4, all required au programs are contained in the installation (if you have executed `expinstall` initially). Simply type `splitx_au` in data set 10 and the processing will start. When you execute `splitx_au` for the first time, it will take several seconds and result in some popup windows. This is normal and due to the fact that `splitx_au` and several other au programs have to be compiled on your computer.

If you use Topspin 3, you first have to copy the required au programs (provided in zip-file upon request) in the Topspin#/exp/stan/nmr/au/src/user folder where Topspin# is your Topspin installation directory. Afterwards everything should work as described above.

NOAH2_BS experiment in MestreNova

MestreNova can read the Topspin-generated HMBC or HSQC data sets (folders 10001 and 10002) without problem. The best option is to load them with import of processing parameters. To do so, tick the corresponding options under Preferences/NMR/Import (apodization, zero-filling, linear prediction). If you do not want to perform the `splitx_au` in Topspin prior to loading the data into MestreNova, you can also load the raw data (folder 10) directly, as MestreNova is able to do the splitting on its own. However, in this case, load the data without importing the processing parameters from Topspin (untick the corresponding options under Preferences/NMR/Import). Otherwise the result will be wrongly processed (weird anti-phase type peaks in the HSQC, doubling of signals in the f1 dimension in the HMBC). When you do not import the processing parameters, the result will be correct, but not necessarily beautiful. Depending on your individual processing templates, you might have to apply some apodization (e.g. qsine window function) in MestreNova in order to have optimally processed data.

If you have NOAH2_BS data from the 600 MHz machine (file name ending on letter A or B), then these were recorded using non-uniform sampling (NUS). Note that NOAH-NUS data sets are currently not supported by MestreNova. This means that you do have to do the splitting in Topspin. If you try to load the raw data of a NOAH-NUS data set into MestreNova, the result will be completely wrong, something that looks mostly like t1 noise and nothing else.