

DQFCOSY

Experiment setup.

- *Tune the proton channel of probe.
- *Calibrate the 90^0 pulse according to the [“Calibration of \$90^0\$ pulse”](#) menu
- *Record the proton spectrum according to [“Short instruction of basic operation of Bruker NMR spectrometer.”](#) Limit the “sw” of the spectrum to the important peaks. This will save you experiment time.
- *Measure the spin-lattice relaxation time of the slowest peak according to [“Measurement of spin-lattice relaxation time \$T_1\$ ”](#)
- *Type “rpar” and load the “dqfcosy.BBI” parameter file.
- *Go to “EDA” menu. Insert the exact “sw” value as the same for both dimensions. Insert “O1p”
- *Insert “p1” according to 90^0 pulse calibration.
- *Set up “D1” = $1.27 T_1$
- *Take “rg” from 1D experiment multiply by factor of 1.5 and insert it.
- *The number of experiments in second dimension depends on the required resolution and the experiment time you would like to take. In most cases 128 spectra is enough. If, your sample has a large “sw” 256 might be necessary.
- *number of scans “ns” needs to be 8n. Very often 8 scans are enough. If sample has a smaller concentration more scans might be required.
- *Check the experiment time “exptime” .
- *type “zg” to start acquisition.
- *type “xfb” for Fourier transformation. Type “abs1” and after is finished “abs2”
The spectrum can be checked anytime during the experiment. Experiment does not need to be finished if one is satisfied with the spectrum.
- *to symetrize the spectrum type “sym”. However, this might introduce artificial peaks, so caution is needed.
- *The default phasing is set to “mc” mode. However, if one would like to take advantage of phase, in the “EDP” menu the PH_mod needs to be set to “no” for both dimensions. After “xfb” is finished you will need to phase the spectrum according to “Avance user’s guide” pp. 144.
- *Adjust contour levels “+/-“ if negative peaks are not visible.
- *Enter “abs1” and “abs2”. The “symba” might be used for symetrization.
- *To add projections to the spectrum type “edg” and click “EDPROJ1” to the F1 parameters. Edit as follows:
PF1DU -disk partition one of (/w, /x or /m)
PF1USER- username
PF1NAME – filename
PF1EXP- experiment #
PF1PROC – processed data #
Repeat the procedure for F2 dimension.
- *Save the optimum display parameters by clicking on “DefPlot”.
- * “View” and plot the spectrum.