Selective 1D Proton Experiments

Bruker has an easy tool to setup various selective 1D experiments using Topspin 3.5 (not on the 300wb). A selective experiment is where one proton is chosen and its interaction with other protons is measured. The following 1D experiments can be setup with the tool:

1D NOE
1D ROE
1D TOCSY
1D $^1$H-$^1$H homonuclear decoupling (one proton only)
1D solvent suppression (one or more solvents!)

Procedure:

1. First run a 1D proton spectrum. ns=1 is usually sufficient. Process normally.

2. Go to the [Acquire] menu and select [More].

   ![Acquire Menu]

   Choose [Setup Selective 1D Experiment] under the drop down menu.

   ![Setup Selective 1D Experiment]

   A new menu will appear and flash briefly:

   ![Setup Selective 1D Experiment Setup]

   select [Define Regions]

3. Select integration mode. Integrate the peak of interest, then select and [Save Regions to ‘reg’], then exit [Back]. Answer [no] to the question about saving regions.

4. Select [Create Datasets] and choose the desired experiment from the list.
Always choose the gradient version of the selective experiments. For solvent suppression, chose the Mult. Solvent Suppr. WET as it works better.

If you have integrated several peaks in the previous step, separate datasets will be created for each peak, in the case of every experiment except solvent suppression. These separate experiments are then to be run sequentially. For solvent suppression, however, a special shaped excitation pulse is created that attempts to suppress all solvents peaks (2 is the practical maximum) at the same time in a single experiment.

You will get a window asking for parameters. For a selective gradient NOESY, you will get the window on the left.

5. Adjust the values (d8 ranges from 0.1 to 0.8 s depending on the size of your molecule) as desired and click on [Accept]. For TOCSY, the mixing time is usually 0.120 sec.

6. Clicking [OK] in the window on the right will start the experiment in the INDICATED experiment number (not the current one). Type re (expno) to change to the active experiment.