1D Selective NOESY with Topspin

Reference Spectrum

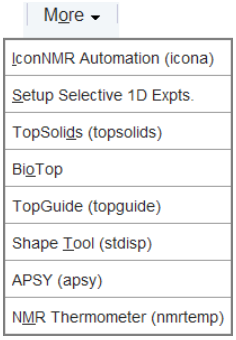
Run a 1D Proton spectrum, following the instructions in the short Bruker manual.

Set up the 1D selective NOESY

The selective pulse regions are set up using the integration tools. Power and duration of the shape pulses are calculated using the hard 90° pulse in the prosol table.

1. Stay in the reference spectrum, on the menu bar,click **Acquire**.

On the **More** button, click the **drop-down** arrow to see more options.

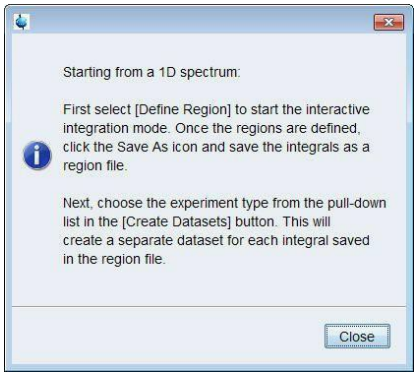


2. In the list, select **Setup Selective 1D Expts**.

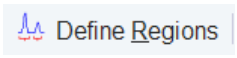
The Workflow button bar changes for setting up the 1D selective experiment.

3. On the Workflow button bar, click **1D Selective Experiment Setup**.

4. In the message window, click **Close**.



There is no other function to this button then the instruction displayed above.
Expand the spectrum region having peaks you are interested in doing NOE.

5. On the Workflow button bar, click **Define Regions**. 

The Define Regions toolbar is displayed:

6. Integrate the peak (multiplet) that you will irradiate to observe the NOE.

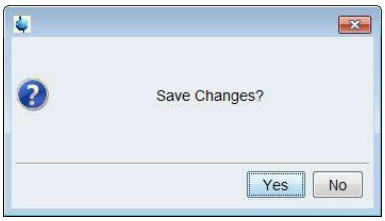
If desired, other peaks can be integrated and a separate dataset will be created for each integral saved in the region file.

7. On the toolbar, click **Save/export regions**  .

8. In the list, select **Save Regions to 'reg'**.

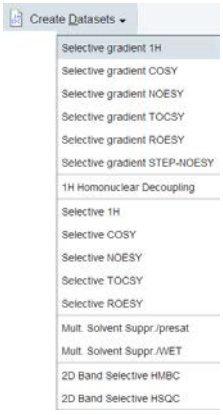
9. On the toolbar, click **Return do NOT save regions!**. 

10. In the message window, click **No**.



11. On the **Create Dataset** button, click the **drop-down** arrow to see more options.

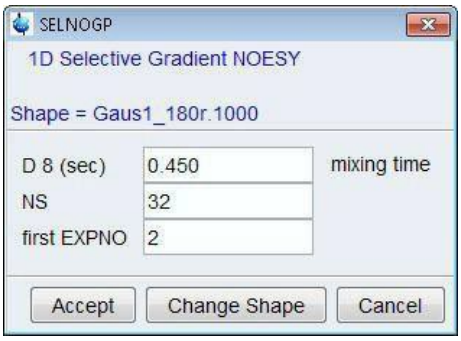
12. In the list, select **Selective gradient NOESY**.



The default parameters are taken from the standard parameter set **SELNOGP**. The mixing time **D8** is dependent on the size of the Molecule and the magnetic strength. It can vary from a large Molecule to a small one from **100 ms** to **800 ms**. If desired, the **Gaus1_180r.1000** pulse can be changed by clicking on the **Shape** button in the above window. Number of scans (NS) should be determined based on your sample concentration.

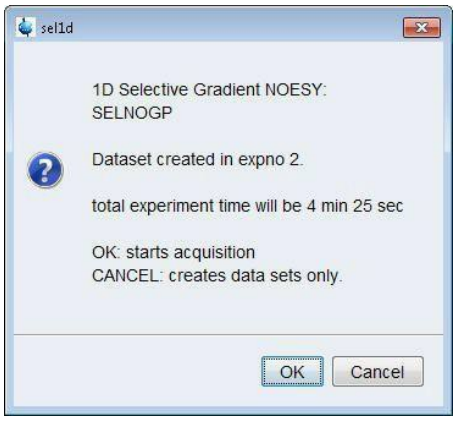
13. Enter:
D8 = **0.450**
NS = **32**

14. In the SELNOGP window, click **Accept**.



The new dataset is created and all parameters are automatically set.

15. In the sel1d window, click **OK** to start the acquisition.



If you click “cancel”, dataset will be created but not run. You can make further changes and then start acquisition.

Display 1D NOESY together with 1D proton spectrum

1. Display the selective NOESY spectrum.

2. On the toolbar, click **Multiple display**.  The Multiple display toolbar is displayed:

3. Drag the Reference spectrum (1D proton) into the spectral window.