# Noesy1d experiments with Vnmrj 4.2

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NOESY1D is the Varian implementation of the 1D NOE experiment using pulsed field gradients and selective pulses developed by Shaka *et al*. At the heart of the experiment is a double-pulsed-field-gradient-spin-echo (DPFGSE) pulse sequence that achieves selective spin inversion effectively and cleanly. It is important to recognize that NOESY1D is a transient NOE experiment, which differs from the traditional steady-state NOE experiment. NOESY1D employs a series of pulses and gradients to invert a particular spin, a mixing time to allow the NOE to develop, and a read pulse to obtain a NOE spectrum. Therefore, an equilibrium value for the NOEs is not obtained. NOEs obtained from transient NOE experiments are generally lower in intensity (38% max vs. 50%, for small molecules) and their relative intensities are not directly comparable to steady-state NOEs. So, This experiment is good at detecting the presence of an NOE, when two protons are close together in space ($\approx$3-5 Å apart), but is not good for determining the correct magnitude of the NOE.

Running the NOESY 1D experiment

- As usual, begin by acquiring a 1D proton spectrum in workspace.

  Type *jexp1*   (join experiment 1)

  Set up and run a standard ^{1}H experiment.

- Make sure the sample is properly shimmed and the spectrum is carefully phased.

  When the ^{1}H experiment is completed

  Type *mf(1,2)*   (move the 1H FID from exp1 to exp2)

  Type *jexp2*   (join experiment 2)

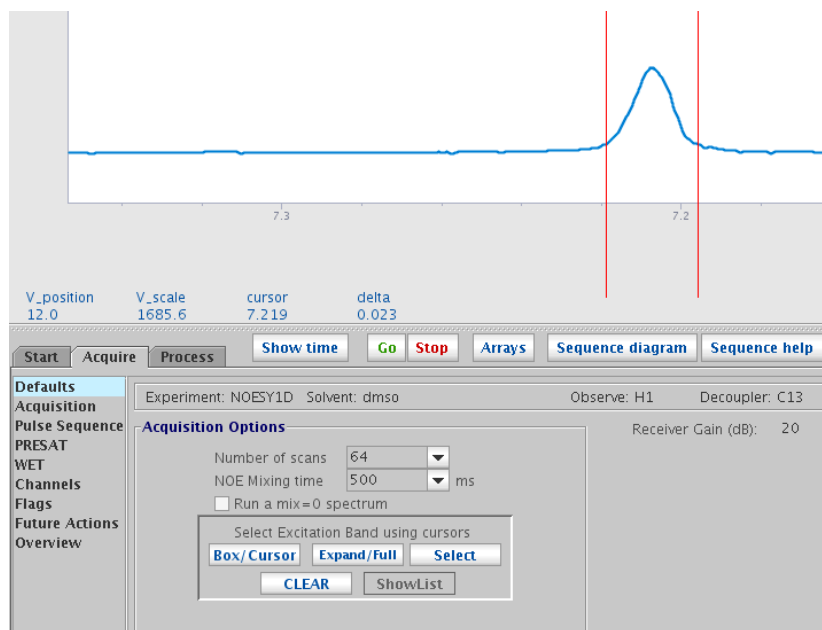 Type *wft ds*   (Fourier transform FID)
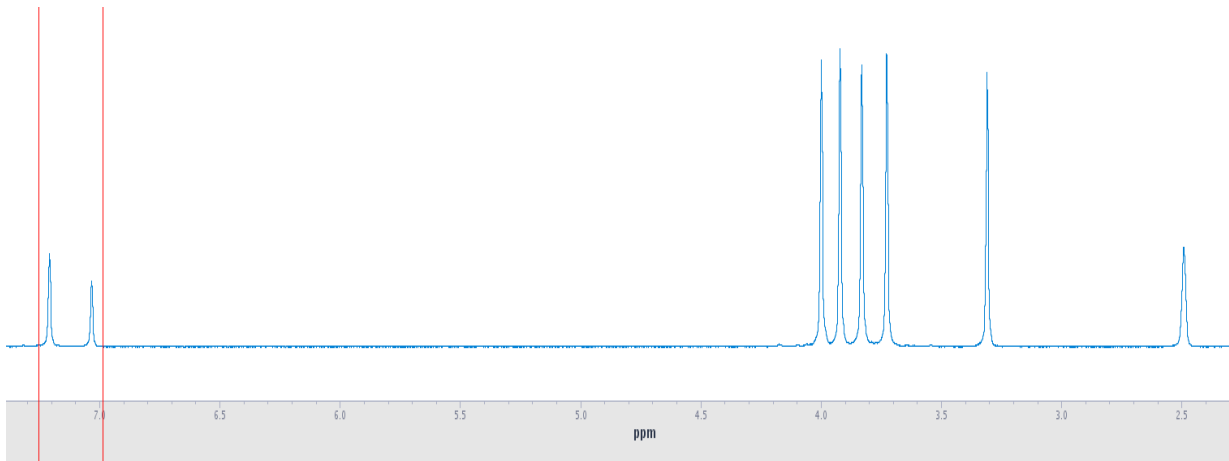
Expand around first resonance to be inverted.

- Select from the Menu "Experiments > Selective Excitation Experiments > 1D NOESY (dpfgse)".
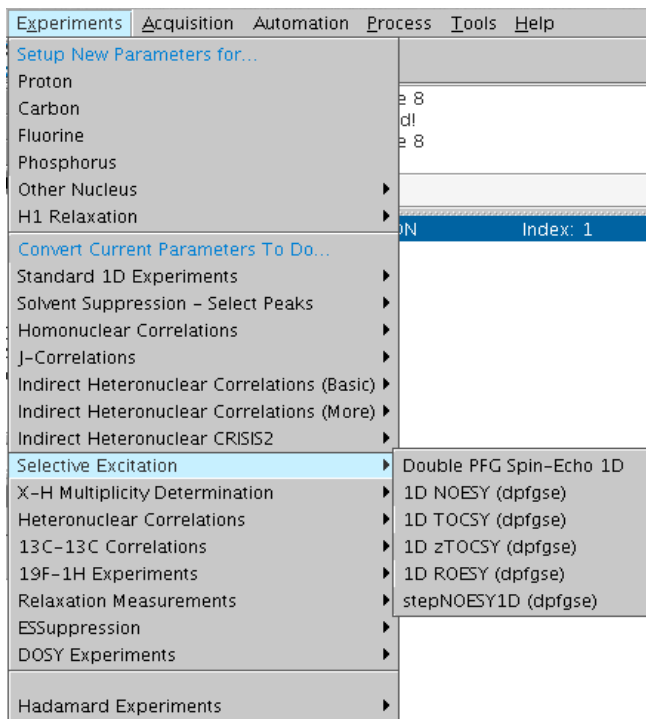
- Display the "*Acquire, Defaults*" panel if not already displayed.

- Expand around the region of the spectrum you want to irradiate. Place the cursors around the peak to irradiate and click the <Select>button.

- The cursors should contain the peak entirely, starting at the baseline and should be symmetrically positioned around the middle of the peak.

- If you make a mistake during peak selection, click the <CLEAR> button to delete the last defined peak.

- Type **nt=128** or desired number, this set number of scans. Must be a multiple of 8. The number of scans can also be set with pull down menu in the Acquire/Default panel.

- Select **NOE mixing time** from the Acquire/Default panel show above. Mixing time=500 ms is the default value and is optimal for short-range interactions of small to medium sized molecules. If you are looking for long range interaction, mixing times comparable to the 1H T1's can be used.

- Make sure the sample is not spinning as gradient selected experiments like NOESY1D do not work with spinning.

- Click on the green <GO> bottom at acquire tab, do not just type go or ga. The pulse sequence requires that the shape of a selective pulse be calculated and this is done only when the <GO> button is clicked.

- When the experiment is done type ***wft ds***, this does Fourier transform and display the spectrum.
- In NOESY1D spectrum, the irradiated peak is negative and very large. NOE peaks are generally positive and smaller in amplitude than the irradiated peak, but they can also be negative. Protons that are scalar coupled (on adjacent carbons) may show a peak with positive and negative segments. The NOE spectrum below shows that two protons with resonances near 4 ppm are close in space to the one with resonance above 7 ppm.
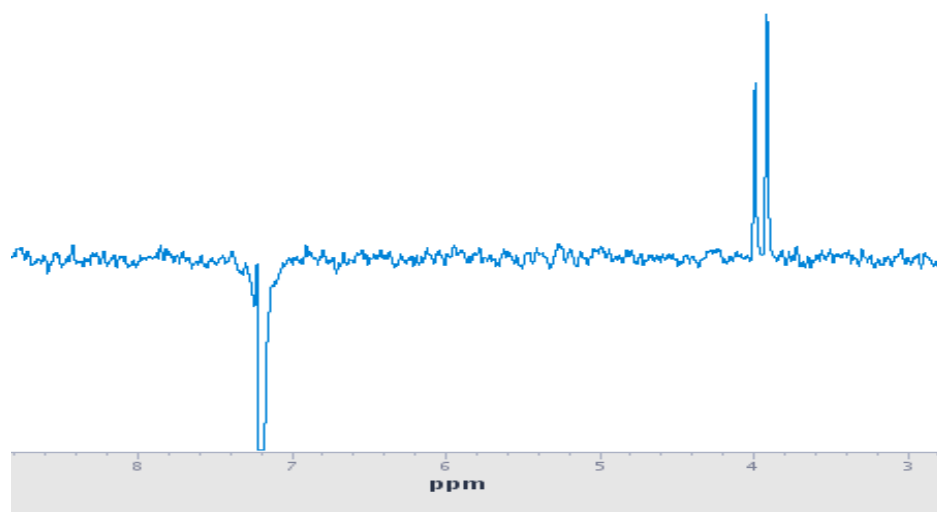
- To save the spectrum type ***svf*** enter a file name and click ***<Ent>***

Printing your NOESY1D spectra

- Type ***pl pscale page***, this does print spectrum, and scale.