

1D TOCSY

S console, walkup mode, VNMRj 2.1A

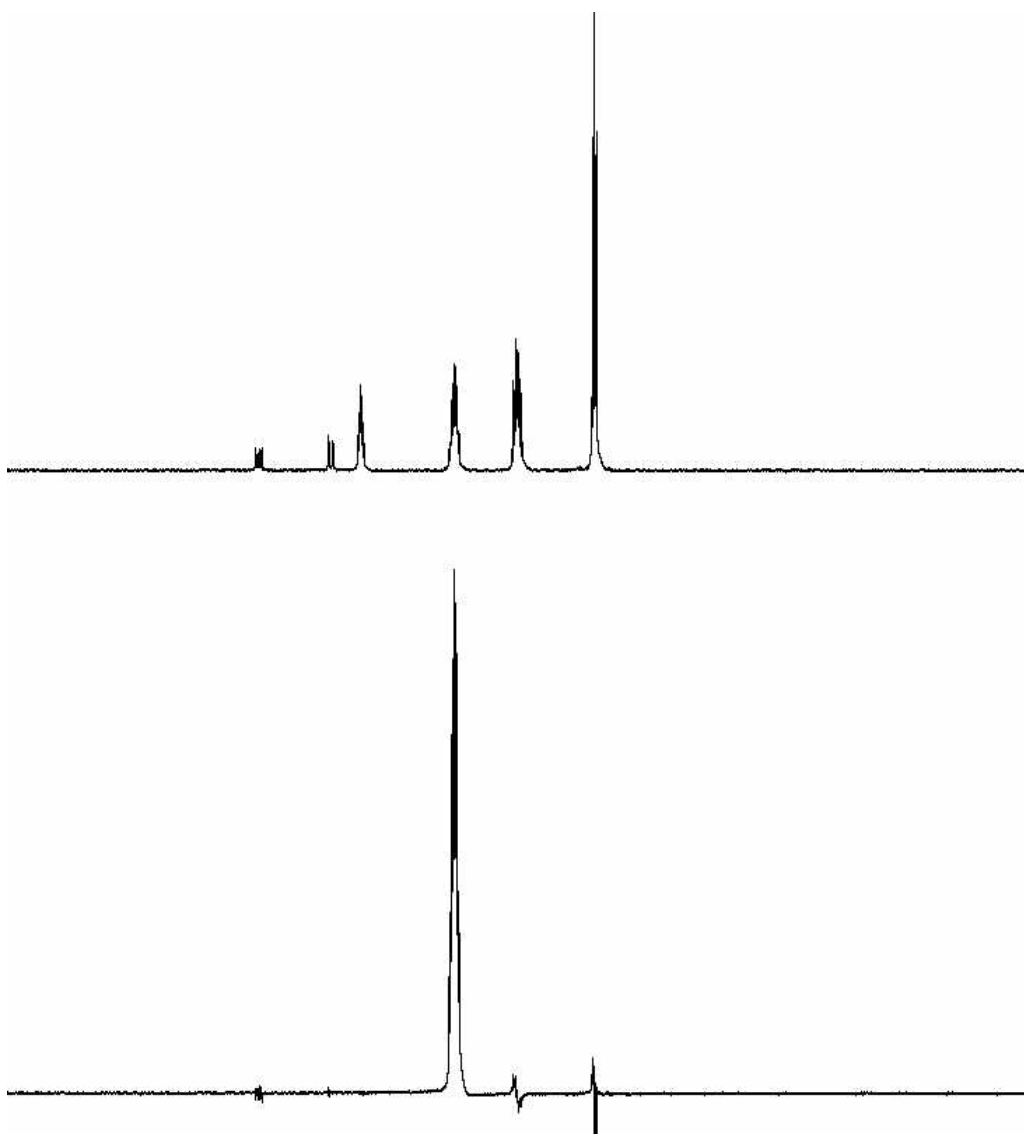
1. Run a 1-D proton in study queue with the same window in ppm required for the 1-D TOCSY.
2. Leave a processed 1-D spectrum on the screen.
3. Select 1-D TOCSY from the study queue menu. Double click the parameters for this experiment. Go to the Acquire → Default menu. *Be sure to keep the spectral width unchanged from the 1-D proton to the 1-D TOCSY!*
4. In the middle of the panel will be buttons labeled [Select] and [Proceed]. Place the cursors around the peak to be investigated and choose [Select] then hit [Proceed].

The screenshot shows the VNMRj 2.1A software interface. At the top, there are tabs for 'Start', 'Acquire', 'Process', 'Stop' (highlighted in red), and 'Show Time'. Below the tabs is a sidebar menu with options: 'Defaults' (highlighted in yellow), 'Acquisition', 'Pulse Sequence', 'Channels', 'Flags', and 'Future Actions'. The main panel is titled 'Tocsy1d' and contains the following parameters and controls:

- Spectral Width [ppm]:** 14 -> -2 (dropdown menu)
- Downfield:** 14.0 (text input)
- Upfield:** -2.0 (text input)
- Pulse Width [degrees]:** 90 (dropdown menu)
- Enter pulse angle:** 90 (text input)
- Relaxation Delay [sec]:** 1 (dropdown menu)
- Number of Scans:** 16 (dropdown menu)
- Mixing time [ms]:** 80 (dropdown menu)

On the right side of the panel, there are three buttons: 'Display Sequence', 'Select' (under the heading 'Select Excitation Band Using Cursors'), and 'Proceed'. A 'CLEAR' button is located at the bottom right.

5. Change any of the other parameters necessary. Then submit the study.
6. The spectrum should be automatically processed and displayed. The first spectrum will be the spectrum of the shaped pulse only and the 2nd spectrum is the 1-D TOCSY information.



1-D NOESY

The 1-D NOESY is setup identically to the above protocol except for the number of scans and mix times.

1. Run a 1-D proton in study queue with the same window in ppm required for the 1-D NOESY.
2. Leave a processed 1-D spectrum on the screen.
3. Select 1-D NOESY from the study queue menu. Double click the parameters for this experiment. Go to the Acquire → Default menu. *Be sure to keep the spectral width unchanged from the 1-D proton spectrum.
4. In the middle of the panel will be buttons labeled [Select] and [Proceed]. Place the cursors around the peak to be investigated and choose [Select] then hit [Proceed].
5. Change any of the other parameters necessary. Remember that the NOE can be a weak interaction so more scans may be necessary (recommended 64). Also, check the mix time. The default is 500 ms that should be ok for most samples (range 500-800 ms). Then submit the study.

6. The spectrum should be automatically processed and displayed. The 1-D NOESY has only one spectrum where the peak selected should be negative and the peaks with corresponding NOEs should be positive. The spectrum may need to be phased to properly present this spectrum.