

This quick guide describes how to use shaped pulses to selectively excite or suppress spectral features in NMR spectra. Shaped pulses are only available on the Varian 500 and the Varian 501.

Conventions used in this guide are as follows:

- **Boldface** type indicates commands that are typed into the VNMR input window or in a terminal window
- Italic [**Boldface**] type with square brackets indicates a button in the VNMR menu that is to be pushed.
- <**Boldface**> type surrounded by a bra and a ket (how quantum mechanical!) indicate keyboard strokes.
- **LMB** indicates the Left Mouse Button
- **MMB** indicates the Middle Mouse Button
- **RMB** indicates the Right Mouse Button
- Unless otherwise noted, all commands typed into the input window are to be followed by an <↵ Enter> keystroke.
- When a command, parameter, or macro is first introduced a full definition or description will immediately follow.

- 1) Collect and phase a 1D spectrum in the usual fashion. Make sure sample is shimmed as well as possible and it is also recommended that you not spin. If you would like to gradient shim your sample (recommended) a help sheet is available [here](#) (in .pdf format). You should also consider calibrating the 90° pulse. A 90° pulse calibration tutorial is available [here](#) (also in .pdf format).
- 2) Following the acquisition, record the 90° pulse width (**pw90**) and the RF transmitter power (**tpwr**). These values may be queried by typing **pw90?**, and then next typing **tpwr?** in the Input Window. Record these values, as they will be required shortly.

*Example:*

<b>pw90?</b>	pw90 = 8.2
<b>tpwr?</b>	tpwr = 56

- 3) Next, type **ds** (**display spectrum**) in the Input Window. This will allow access to Menu Button Window containing the Pbox (Pandora's Box) button. Click the [**Pbox**] button.
- 4) Click the [**90**] button. Then, using the **LMB** and then the **RMB**, select a region of the spectra you wish to selectively excite or suppress.
- 5) Click the [**e-burp1**] button. The selection process may be repeated as many times as desired, as several spectral features may simultaneously be selectively excited or suppressed.
- 6) When finished, click the [**close**] button and then the [**name**] button. At this point, the program will prompt you for a filename for the shaped pulse sequence you have just created. Enter a filename and then click [**Close**].

*Example:*

Shapefile name: **My\_nobel\_prize** [Close]

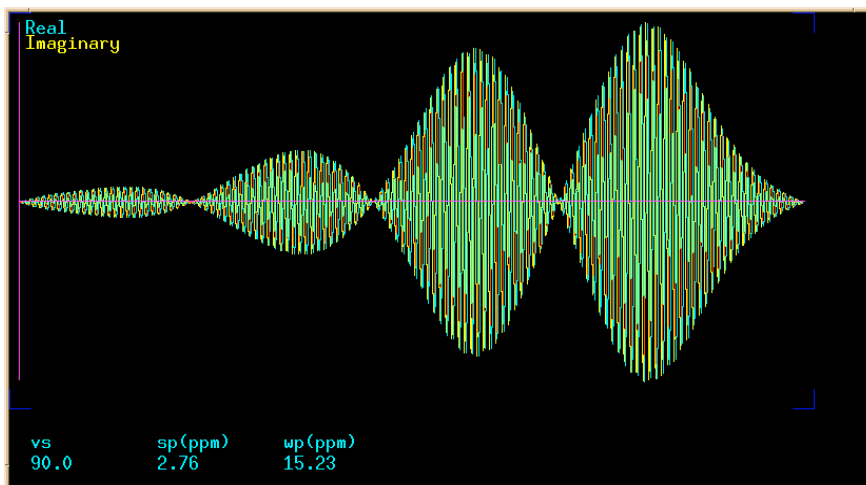
- 7) The program will now prompt you for the pw90 and tpwr values that you recorded in step (2) above. Note that the pw90 value must be entered in microseconds and the tpwr in dB.

*Example:*

Enter reference 90 degrees pulse width (usec): **8.2**

Enter reference power level: **56**

- 8) Your shaped pulse will now be displayed in the Graphics Window (shown below).



The corresponding pulse width and pulse power will be displayed in the Text Window (shown below).

```
Welcome to Pandora's Box!  
Version 5.2a (970130)  
  
Reading input data from :  
"/export/home/vnmr1/vnmrsys/shapelib/Pbox.inp" ...  
  
Saving waveform to :  
"/export/home/vnmr1/vnmrsys/shapelib/My_nobel_prize.RF" ...  
1560 Steps generated ...  
RF calibration data: ref_pwr=56, ref_pw90=8.20  
  
>>> Set pulse width to 55.6920 ms <<<  
>>> Set pulse power to 3 dB <<<  
  
Done.  
displaying data from /export/home/vnmr1/vnmrsys/shapelib/pbox.fid
```

The text window will contain two important numbers: the “set pulse width and the

“set pulse power” (in this example these values are 55.6920 ms and 3 dB respectively). Record these values, as they will be required shortly.

The following steps will be required for either selective excitation or selective suppression.

- (a) For selective excitation enter **selexMIT** in the Input Window.
- (b) For selective suppression enter **selsupMIT** instead.

- 1) After entering either selexMIT or selsupMIT in the Input Window, enter **selpw = set pulse width** recorded in step (8) above.

*Example:*

**selpw=0.0556920** Note that the selpw value must be entered in seconds!

- 2) Now enter **selpwr = set pulse power** recorded in step (8) above.

*Example:*

**selpwr=3**

- 3) Next, enter **pwpat = 'filename'**, where filename is the name you chose in step (6) above.

*Example:*

**pwpat='My\_nobel\_prize'** Don't forget the single quotes!

- 4) Finally, type **dps (display pulse sequence)** in the Input Window. Verify that the pulse width and filename are correct.

- 5) Type **ga (go acquisition)**.

Note:

It has been found that the best peak suppression occurs when the **transmitter offset (tof)** is centered on the peak that you wish to suppress. The transmitter offset can be moved using the **movetof (move transmitter offset)** macro.

To do this:

- 1) Acquire a spectrum in the usual fashion.
- 2) Using the **LMB** place the cursor on the spectral feature of interest.
- 3) Type **movetof ga** in the Input Window.
- 4) Follow the above steps to selectively excite (or suppress) the spectral feature of interest with your new *tof*!