Acquiring Kinetics Data

Acquiring kinetic data with VNMRJ is easy and straight forward. More complex situations can also be accommodated, involving relatively complex acquisition schemes. All commands in **bold** should be entered in the command line.

1. Run a normal 1D spectrum. Choose your desired spectral width (keeping in mind where the product signals will appear) with the cursors and type **movesw ga**. This will acquire a spectrum with the reduced sweep width.

2. If you wanted to acquire a 32 scan proton spectrum every 10 min for 5 hours you will end up with 30 spectra for your kinetics experiment. These parameters will be used for the example.
Type **nt=32 time**. This will tell the acquisition time for a 32 scan proton experiment. For this example the experiment time is 1 min 37 sec (97 sec). Each spectra of 32 scans will take 97 seconds. To start each spectrum every ten minutes we need to subtract the length of the acquisition from the pre-acquisition delay. For this example

3. Type **array('pad',30,503,0)**. This will setup an array in which the *p*re-*a*cquisition *d*elay (pad) is setup. The first value after array **'pad'** tells the spectrometer that pad is the parameter to be arrayed. The **30** is the number of steps in the array (30 spectra, once every 10 min for 5 hours). The **503** is the length of the **pad** (this is the 10 min minus the 97 seconds for the acquisition (600-97=503). Finally the **0** is the array increment. For kinetics we want the same delay between each acquisition.

4. To change the first array value so that it doesn't wait 503 seconds to acquire the first spectrum. Type **pad[1]=0**.
   - If you do not want to acquire a spectrum with the same pre-acquisition between each you can program in the values that you want. For example, if you wanted to do 10 min for the first 2 hours then 30 min for the remaining 3 hours you would type **pad=0,503,503,503,503,503,503,503,503,503,503, ,503,1703,1703,1703,1703,1703,1703**. This will run 12 spectra for the first 2 hours (once every 10 min) followed by 6 for the final 3 hours (once every 30 min).

5. Prepare the sample for the kinetics run and insert the sample into the magnet.

6. Type **go** to start the acquisition. If you wish to see an individual spectrum type **wft(#)** where # is the number of the spectrum you wish to see. For example if you want to see the first spectrum type **wft(1)**. To see the fifth type **wft(5)**. This will allow you to integrate each spectrum.

7. To view all the spectra stacked vertically click on ArrayedSpectra in the upper left corner of VnmrJ. Make sure that Vertically is selected and click Transform.

ProcessPlot | ArrayedSpectra
Protocols | QuickSubmit | Frame | Viewport

ArrayedSpectra

Show
- ● Spectra ○ FIDs
- Horizontally ○
- Vertically ●
- Auto ○
- Custom ○
- Display 1D
- Numbers ☐
- Values ☐

Misc
- Transform
- Absolute ▼
- ☐ Drift Correct
- ☑ Show Scale
- ☐ Whitewash
- ☐ Color traces
- Redisplay
- Plot Page
- Plot Preview

Choice of Values
Start at #	1	Reset Values
Stop at #	54	Reset All
Step every	3	
Max. #	54	

Chart Dimensions
Horiz. Width	250.0	250	±1
Horiz. Pos.	0.0	0	±1
Vert. Height	3121.7	3121	±1
Vert. Pos.	0.0	0	±1

Numbers
Style	☐ Flip	auto ▼	
Horizontal	0	0	±1
Vertical	0	0	±1

Offsets
Horizontal	-0.00	0	±1
Vertical	6	6	±1
Cutoff ☐	200.00	200	±1

Exp:2   Seq: PROTON   Index: 1

9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 ppm