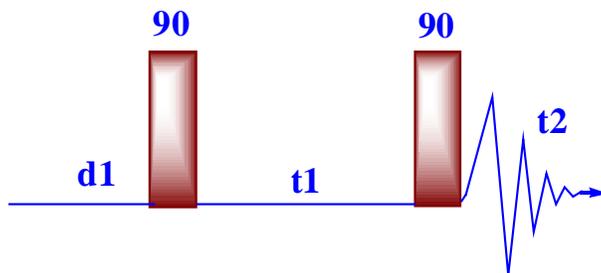


COSY experiment

There are 2 types of 2D NMR, phase-sensitive 2D NMR and non-phase-sensitive NMR. In phase-sensitive 2D NMR, phase is set to **phase=1, 2**. However, in non-phase-sensitive NMR, phase is set to **phase=1**. How do you know? It is easy. Type **phase?[return]**, you will see.

COSY, gCOSY, HMBC and gHMBC are non-phase sensitive. You do not need to phase, because they are acquired in magnitude mode.



COSY is one of the simplest and most useful experiments. It needs a minimum of 4 transients to have a conventional 2D NMR experiment. With the addition of gradients, the minimum transient number can ever be set to 1 meaning that this 2D experiment can be done in several minutes.

The pulse sequence of COSY experiment is composed of a first 90 degree pulse that creates magnetization in the transverse plane. During the evolution time, the variable delay t1 is incremented systematically in order to sample the spectral width indirectly. Following this variable time period, a second 90 degree pulse mixes the spin states, transferring magnetization between coupled spins.

The spectrum is then acquired during t2 (detection time). After double Fourier Transformation, a spectrum is obtained showing a diagonal component (for magnetization that did not exchange magnetization) and cross peaks (off-diagonal) for nuclei exchanging magnetization through scalar coupling. The data is usually symmetrical in respect to the diagonal and therefore the data can be symmetrized as part of the processing to improve the quality by typing **foldt** in the final data processing (care must be taken here to make sure that by getting rid of the non-symmetrical artefacts we are not also getting rid of precious information that might not be totally symmetrical). *The data is usually acquired in a phase insensitive (magnitude mode) manner, avoiding the difficulty to phase a 2D data set.* This phase insensitive mode gives rise to very broad lineshape that can be sharpen using sine-bell or pseudo-echo shaping processing method which can be done using weighting function window(**wti**) or by typing **pseudo** after acquisition.

Steps of doing COSY experiment

1. Run a 1-D ¹H spectrum and calibrate the pw90. Place the 2 cursors 0.5 ppm away at both sides. `movesw`↵
 2. Run 1D spectrum again. Reference the spectrum.
 3. `mf(1,3) jexp3`↵
 4. `COSY`↵
 5. `dg`↵
- you should see the parameters like these.

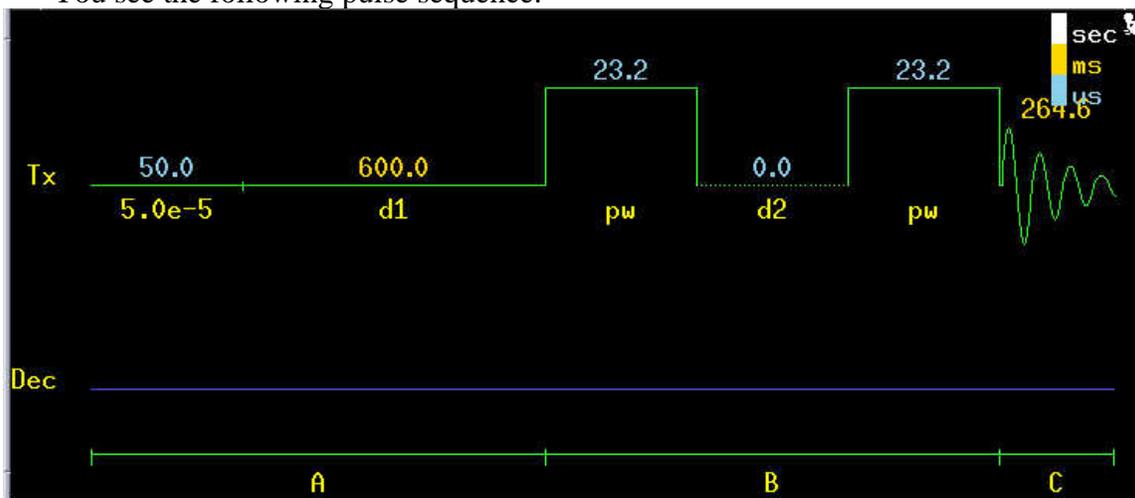
ACQUISITION		TRANSMITTER		PRESATURATION		PROCESSING	
seqfil	COSY	tn	H1	satmode	n	sb	-0.066
sw	3870.0	sfrq	399.729	satfrq	0	sbs	not used
at	0.265	tof	-403.2	satdly	0	fn	2048
np	2048	tpwr	57	satpwr	0	2D PROCESSING	
ss	32	pw	23.250	FLAGS		sb1	-0.070
d1	0.600	DECOUPLER		hs	nn	sbs1	not used
nt	2	dn	H1	sspul	n	proc1	lp
ct	0	dm	nnn	SAMPLE		fn1	2048
2D ACQUISITION		SPECIAL		date	Mar 3 2004	GRADIENTS	
sw1	3870.0	temp	not used	solvent	CDC13	PFGflg	y
ni	400	spin	not used	sample	undefined	hsglv1	4854
		gain	20			hsgt	0.005000

In this table $np=fn=fn1$; $sw=sw1$ (they are required to do symmetry processing). `pw` is the 90 pulse of proton which you should calibrate first before doing 2D experiment. `sw` is the sweep width of the standard 1D spectrum in which you optimize the `sw` by placing the two cursors at both side with 0.5 ppm away from the side peaks. `np=2048`↵ (to the power of 2), the computer will automatically change `at = 0.265` at the `sw=3870.0`.

$$np=2*at*sw \text{ or } at=np/(2*sw)$$

6. `dps`↵

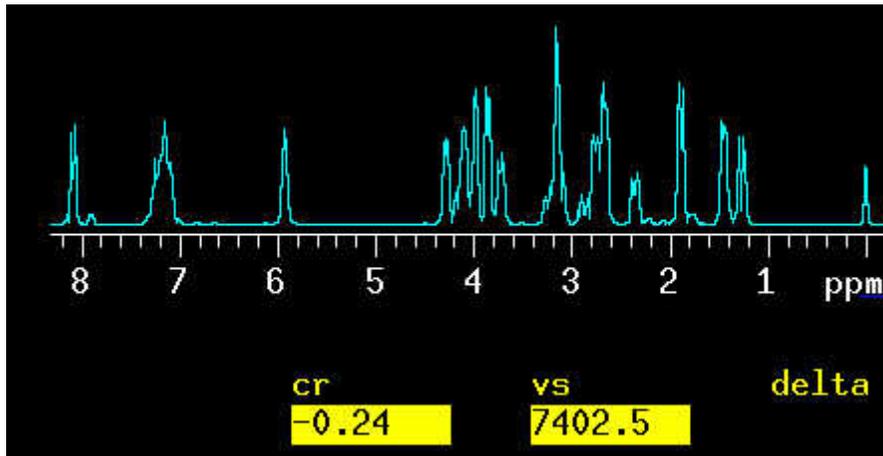
You see the following pulse sequence.



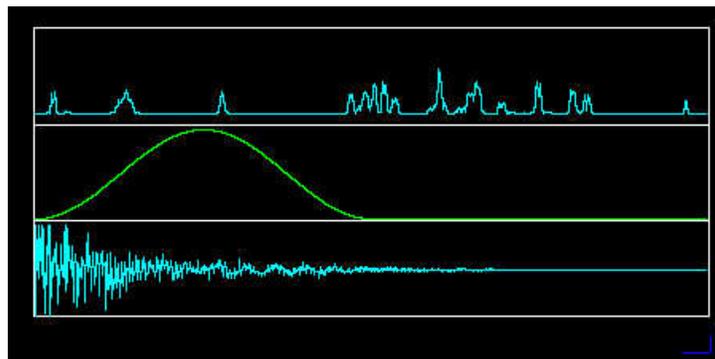
7. `go`↵ (do not type ga)

After the experiment is done, you need to process the data.
(Please save the original FID first and then process the data. You could start at any time in the future)

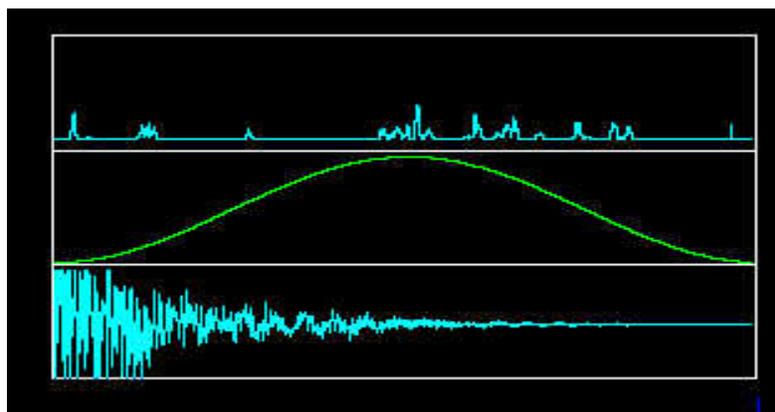
8.1 wft(1) ↵



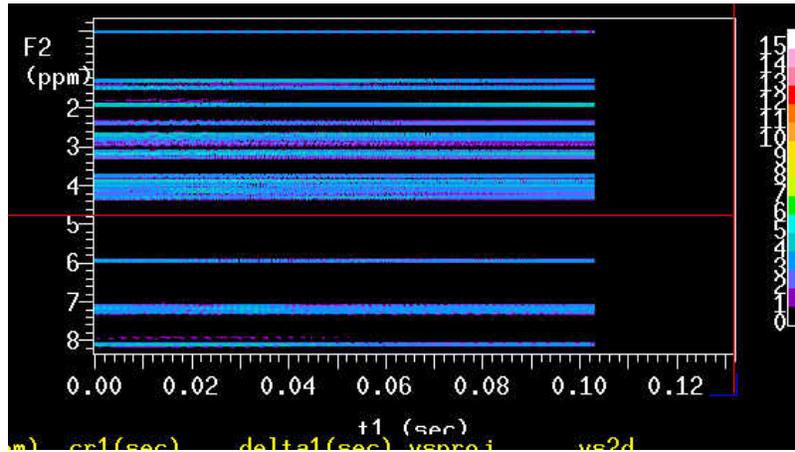
8.2 wti ↵



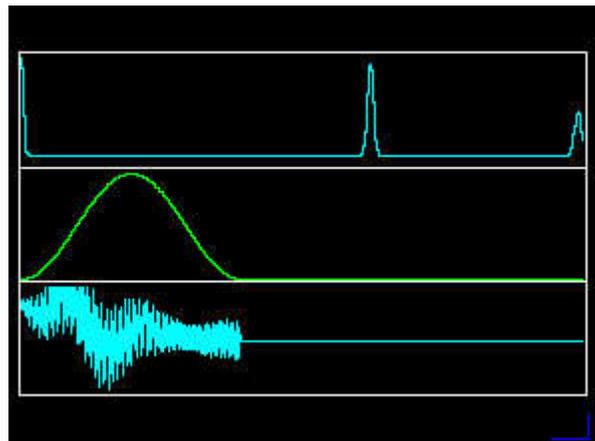
8.3 adjust the sine bell to the end of the window as shown below



9.1 wft1d ↵

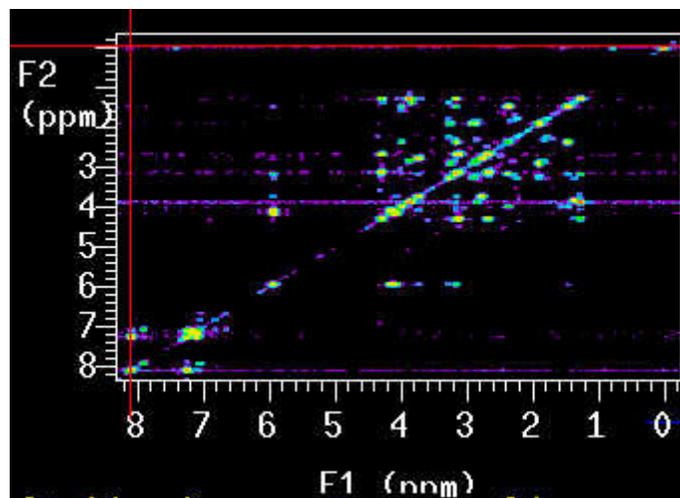


9.2 select a trace and type wti ↵

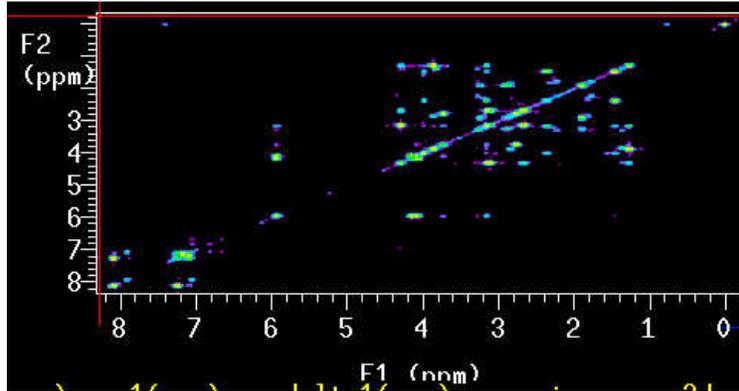


move the sb1 to the end of the fid in t1 dimension.

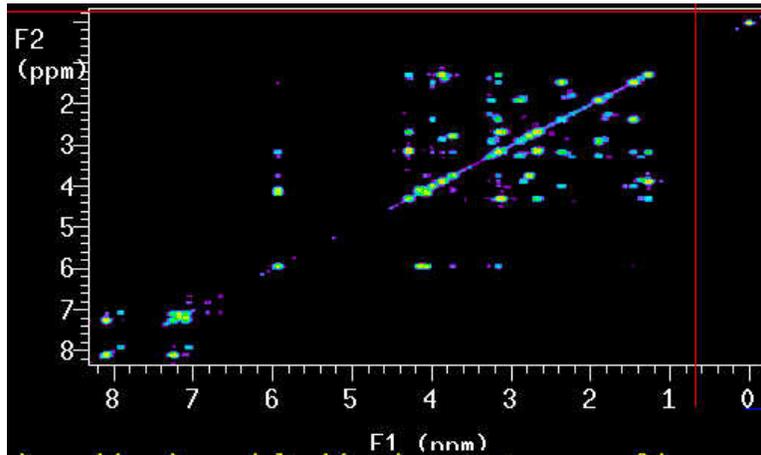
10.1 wft2d ↵



10.2 adjust the vs



10.3. foldt ↵



11 If you are not willing to do window function, then do this:

- `sb=-at/2, sb1=-ni/(sw1*2), sbs='n', sbs1='n'`
- `wft2d`
- `adjust vs`
- `foldt`

12. Data Display

- `dconi('dpcon', positive or negative, number of contours)` [eg. `dconi('dpcon',8,1.3)` gives 8 contours with a spacing factor of 1.3. `dconi('dpcon','pos',8,1.3)` shows 8 positive contours. `dconi('dpcon','neg',8,1.3)` shows negative contours.)
- to print, `pcon('pos',8,1.3) page`