

1. Presaturation of Solvent Resonance.

This technique involves irradiating at the precise solvent frequency with a long (~ 1 sec.) low-power signal to saturate (equalize populations) the solvent protons meaning that the number of magnets at the lower energy level is equal to that at the higher level ($N_{1/2} = N_{1/2}$). There is no transition for the solvent protons. Then a normal high-power (non-selective) pulse is immediately delivered to excite the solute nuclei and obtain an FID. The solvent protons have no population difference ($M_z = 0$) at the time of the high-power pulse and therefore produce no magnetization in the x-y plane and no signal in the FID.

2. VNMR discreption.

The **presat** macro sets up a standard two-pulse sequence with optional composite observe pulse.

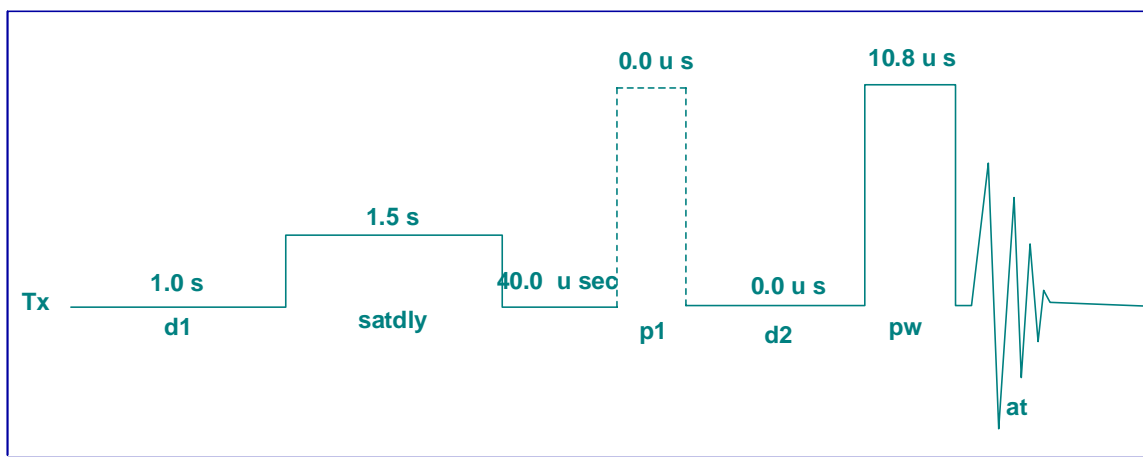
satmode='y', gives observe transmitter saturation at “**satfrq**” with “**satpwr**”.

sspul='y' does *trim(x)trim(y)* to destroy all magnetization.

composit='y' uses composite 90 for **pw**.

presat is executed only if **satdly>0**(**satflg** not active)

3. presaturation pulse sequence



4. The default parameter list for a water-containing sample.

	acquisition	sample	processing	flags
sfrq	399.73	date may 8, 2004	lb	1 il n
tn	h1	solvent D ₂ O	sb	not used in n
at	3.744	file exp	gf	not used dp y
np	44932	decoupling	fn	not used hs nn
sw	6000	dn	math	f saturation
fb	3000	dof 0		sspul n
bs	16	dm nnn		satpwr 2
ss	0	dmm c		satfrq 0
tpwr	63	dmf 11148		satdly 1.5
pw	10.8	dpwr 42		satmode ynn
p1	0			
d1	1.000		werr	
d2	0		wexp	
tof	-154.5		wbs	
nt	1		wnt	
ct	0			

5. The instructions

Text in **bold** is typed on the command line with [return] after each line.

- Set up the experiment as you normally would, lock and shim the sample
- **dn='H1' dm='n' nt=1 ss=0 gain=0 ga**
- When the spectrum is displayed set the cursor on the solvent signal (here is water).
- **nl** , which moves the cursor exactly at the water peak.
- **movetof**
- **presat** to set up the presaturation experiment.
- **dps** to take a look at the pulse sequence.
- **satdly=1.5** you can change it to another number, normally more than 1 sec.
- **satfrq=tof**, if it is 0, you need change it to the number of **tof**.(**tof** is obtained by placing the cursor at the water peak with a command of **movetof**. You might need to type **dg** to get the number on the text window in the previous **s2pul** experiment.
- **satmode='ynn'** is the saturation mode which has been automatically set to 'ynn'.
- **sspul** - set to 'n' (**sspul** is an extra pulse to remove residual X-Y signals. Set this to 'y' if desired.).
- **satpwr** - saturation power, this is dependent on sample, 2-10 dB
- **d1=0** Collect 1 transient to test.
- Optimize the parameters for best suppression. Parameters that may be altered to improve the saturation include checking the saturation frequency (**satfrq**). This

parameter can be arrayed around the starting value to find an optimum. Also, increasing **satpwr** may help. Be sure to increase the gain, use steady state scans (**ss=32** optimum) and collect at least 8 transients for the final spectrum. A well-suppressed sample can often achieve a **gain=30,40** or 50 without a receiver overflow

