Solvent Suppression

The most straightforward way for solvent suppression is with presaturation of the solvent resonance.

Presat

1) Setup H1 1D experiment

2) Normally, acquire H1 1D. If sample is in 90% protonated solvent, set:
gain = 0
then acquire:
ga

3) Process the data, put the cursor on the solvent resonance, then type:
movetof
[this will move the tof (transmitter offset, the center of the spectrum) to the solvent resonance]

4) Convert H1 1D to presat experiment, type macro:
presat

5) The macro will setup the presat experiment and set the frequency to suppress in the center of the spectrum. The parameter for suppression frequency is satfrq. It will also set the length of time of suppression, satdly and the power to suppress peak, satpwr as well as the number of scans, nt, the time between scans, d1.

6) For protonated solvents, you normally need satdly of 2-5 seconds. The satpwr could be increased a few units beyond the default value (usually satpwr is ~2 but that instrument specific). The higher the power the larger the frequency range the peak is suppressed.

7) You might want to optimize the satfrq value. The value set by movetof is usually close but often a few Hz off of the best value. First confirm what the satfrq is set to, type:
satfrq?
This gives you a starting point. On the 600, typically the optimum value is slightly more negative that what the movetof command set the satfrq to.

To optimize, array the value for satfrq:
array('satfrq',10,-230,1)
This would set satfrq to 10 values from -230 increasing by 1 Hz, so -230,-229,-228…-221

On the 600 at room temperature and neutral pH, the optimum value is often between -226 and -229.

To run the arrayed experiment, set nt = 1, gain = 0, then start the acquisition:
ga
To process the data from arrayed experiment, type:
wft f av vsadj dssh

This will do Fourier Transform, show the full ppm (you could zoom on solvent resonance instead), do absolute value of spectrum (av), scale to the largest resonance (vsadj) and show all spectra (dssh)

Find the spectrum with the lowest intensity solvent peak, then choose that value of satfrq.

8) To acquire the full presat experiment, increase the value of gain as the higher the gain value the higher the signal to noise. You can autoset gain by setting:
gain = 'n'

9) Once you have set the gain value, set the number of scans, and if you need to change the time between scans for relaxation, change d1.

10) Start acquisition, type:
go

11) For processing, if you arrayed the satfrq value, you will need to switch out of dssh and av modes, to do this type:
wft f full ph

The command full removes the dssh display and the ph command goes back to phase mode from av mode.

12) Process the data as you would a normal 1D. Sometimes autophase does not work well, so you might need to manually phase.

For more signal to noise, you might use linebroadening of ~0.5 Hz, so in VNMRJ type:
lb = 0.5
wft

13) Save the data, export to MNova.