Shimming on non-deuterated solvents ("no-D")

Automatic Shimming

+ First run a one scan 1D proton spectrum without locking, so that you know where the solvent peak occurs. Use ns of 1 and ds of 0. Do [tune], [prosol], [gain], [go].

The following procedure will tell the instrument to not lock on deuterium, but use the proton signal instead for shimming.

- + Open the BSMS window by selecting or
- + In the [Lock/Level] tab, turn off both sweep and lock.
- + Enter topshim gui on the command line.
- + Check the Parameters box and enter:

lockoff 1h o1p=# where # = chemical shift of the solvent in ppm
or

lockoff 1h solvent="acetone" if your sample is in acetone

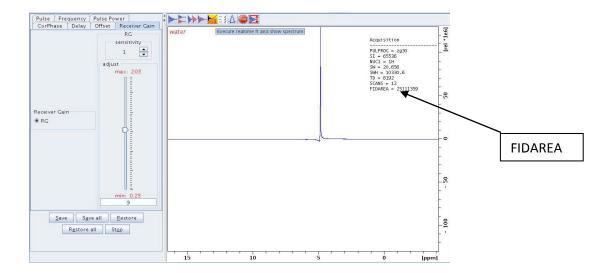
Alternatively, you can type **topshim lockoff 1h o1p=#** in the command line

If Topshim fails, add *ordmax=3* (default is 5) to the above commands.

If you have more than one solvent peak, add selwid=0.5

Manual Shimming

- + First run a one scan 1D proton spectrum without locking, so that you know where the solvent peak occurs. Use ns of 1 and ds of 0. Do [tune], [prosol], [gain], [go].
- + Go to the [ProcPars] tab and change ph_mod to "pk"
- + Type *gs* and the following windows will open:



- + Select to see the spectrum collected in real time. The upper right hand corner shows the FIDAREA. Monitor either of these while you shim to increase the FIDAREA number or improve the lineshape.
- + Open the BSMS window by selecting or or
- + Select Z and use the +/- buttons (or the mouse scroll wheel) to improve the shape of the spectral peak and increase the FIDAREA number. Continue with Z^2 , etc.
- + Select in the gs window when you are finished.

Solvent Suppression (one peak)

- + Run a 1D spectrum to find where your solvent peak occurs. Use ns of 1 and ds of 0.
- + Reference your solvent peak.
- + Shim. If your solvent is non-deuterated, use the "Shimming on non-deuterated solvents" method.
- + Create a new dataset using the experiment: WATER
- + Click on [prosol]
- + Type xaua

This macro will run 2 experiments—the first one finds where the solvent peak is (default 4 scans), the second one will do the suppression (16 scans).

To change the number of scans, wait for the first spectrum to complete, and the second one to start. Then type **halt**, change **ns**, and resume by typing **go**

Multiple peak suppression using WET

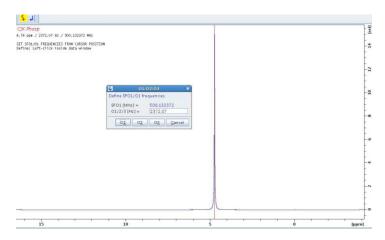
- + Run a 1D spectrum to find where your solvent peaks occur. Use ns of 1 and ds of 0. Do [tune], [prosol], [gain], [go]
- + Reference your solvent peaks.
- + Shim. If your solvent is non-deuterated, use the "Shimming on non-deuterated solvents" method.
- + Create a new dataset (or iexpno).
- + Read in parameters for SOLVSUPWET (under /user directory].
- + getprosol
- + Type xaua

This macro will run 2 experiments—the first one finds where the solvent peaks are (default 16 scans), the second one will do the suppression (64 scans), for a total of ~10 min experiment time. Do not try to process it before it is complete.

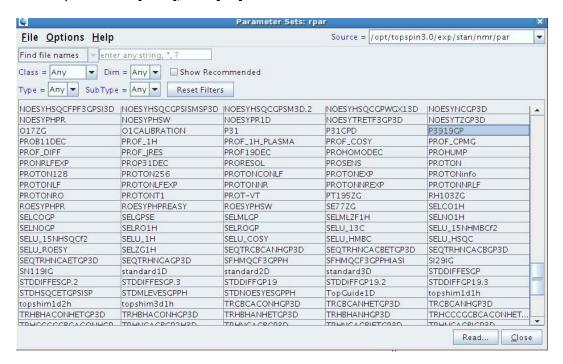
The default experiment is set up to suppress two peaks. Use the parameter **L30** to change the number of peaks to suppress.

Watergate

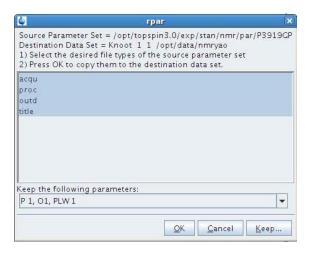
- + Run a 1D spectrum to find where your solvent peaks occur. Use ns of 1 and ds of 0. Do [tune], [prosol], [gain], [go]
- + Click on , then identify the peak to be suppressed by left-clicking on it and choosing [o1] in the new dialog box.



+ Under the [Start] menu, select and choose P3919GP from the list in the /par directory and select [Read], then [OK].



Under "Keep the following parameters:" select P1, O1, PLW1



Do [Prosol], [Gain], [Go].

To fine tune, do pulsecal under [Prosol] menu.

Use these parameters for the getprosol: getprosol 1H pw dB, e.g., getprosol 1H 14.02 -11.8

Type **gs** and adjust [Offset] tab by moving slider to get lowest possible FID area.