2H (deuterium) NMR experiments require the use of non-deuterated solvents: oddly enough, you will be acquiring a form of no-D NMR spectrum (so the write-up for no-D is similar to that below). On all our spectrometers, we use the simplest method for 2H observation by using the lock channel. Sensitivity is best on cryoprobes (esp. callisto), but will be adequate in most cases on other spectrometers and probes.

A. Initial Setup:
1. Read in parameter set probename_H2lk.sUW. The parameter set will be probe specific so make sure to choose the correct one.
2. In the acqu tab set lock to: LOCK-OFF
3. Do NOT tune and match (atma). The instrument will try to tune and match on the X-channel, not the lock channel that is used for acquisition.

B. Shimming:
1. In TopShim, set options: 1h lockoff o1p=<value in ppm> selwid=0.5
2. If topshim says it’s reducing the echo time, add convcomp to the line above (always use convcomp with the Prodigy and DCH cryoprobes).
3. Staff prefers selwid=0.5 in the above, which changes from the default 1 ppm selection width to 0.5 ppm. If that doesn’t work, find us….

C. 2H NMR in IconNMR run on Callisto:
To perform 2H NMR on callisto, get cgf to add the DCH_2Honlock experiment to your list. Then change all four setting in the lock panel shown below.

Know your protonated solvent: you must know the value for o1p to shim (see section A in the no-D page if you don’t).

Click the Change Lock icon and do the following:

a) Lock Program to: LOCK-OFF.

b) Shim Program to: TOPSHIM convcomp 1h lockoff o1p=?? selwid=0.5

where ?? is the chem. shift of your protonated solvent as found in section A above.

c) IT IS CRITICAL(!) to click both 1H and X Channel Tuning/Matching to No (see fig). Failure to do so will interrupt proper locking for other queued samples.