Bio-NMR user Training Procedure on Bruker AVIII HD 800 and 700:

1. Open topspin
2. Start → Create Dataset (new)
    - Check Experiment and select ZGPR; Select solvent (H2O+D2O) for 90%H2O/10%D2O buffer; check 'getprosol'.
3. Acquire →
    - Sample (ej & ij) --- wipe and clean nmr tube and handle spinner and sample gage properly. (sx 3 or sx 16 for the sample in # 3 or # 16 position.)
    - Lock (lock) --- wait till "lockn: done."
    - Tune manually (atmm) for samples using 90%H2O/10%D2O. (atma) --- automatically tuning.
    - Spin (ro off; ro on; ro); don't spin for protein samples.
    - Shim (topshim; topshim tune tunea)
    - Prosol (getprosol);
    - for ZGPR, use (pulsecal) to calibrate 1H 90° pulse -- P1; set rg = 1 and (gs) to find O1, which is the center of the spectrum, and water peak position too.
    - Gain (rga) — automatically rg adjustment.
    - Go to "AcquPars tab" to change 'NS'; and click "clock" to show total experiment time.
    - Go (zg);
    - load ZGESGP, update P1, O1, and set proper NS, and then zg.
    - HSQCETFPF3GPSI is a good one for 2D N15 HSQC…
4. Process →
    - Proc. Spectrum ('proc1d y' or efp)
    - Adjust Phase (apk)
    - for 2D: use (xfb – 2D FT); (rser 1 – read first FID) (efp, apk, .ph)
    - Calib. Axis (.cal)
    - Pick peaks (.pp); Integrate (.int); Correct baseline (absn)

Note:

1) Always **PATIENTLY** wait till "tune or other process done or finished" shown up and then go to next step! Important!
2) must do **TUNE** again if you use other nuclei (C13 /N15) besides H1.
3) always go through the above procedure once again for every new sample.
4) Drag previous data folder in, and "use current parameters" …
5) Upload your data from (/opt/topspin3.5pl5/data/your_nmr_username/nmr --- on B800 and B700) into your OneDrive.
6) Always ask Hongwei first before you run any new things.