

NJIT NMR Lab

Acquiring an NMR spectrum

(Quick instructions for Topspin 3.0, Bruker AVIII-500-MHz)

Preparation:

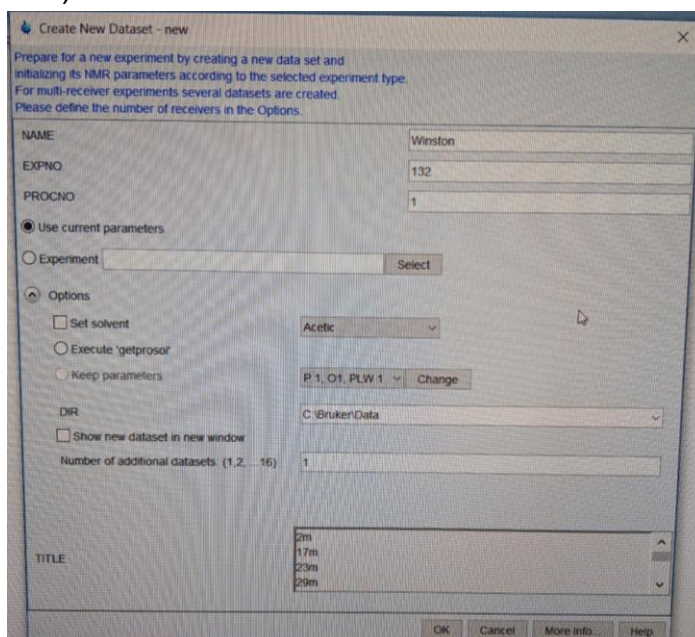
- 1) Clean the NMR sample tube with a Kimwipe
- 2) Insert the NMR sample tube into a blue spinner and measure height with the provided measuring gauge
- 3) Type *ej* <enter> at the TopSpin (TS) command line (or press the LIFT button on the external BSMS)
- 4) Insert the sample into the probe, by placing it on top of the magnet while the eject air is blowing. **The sample will be floating on top of the magnet**
- 5) To insert sample, type *ij* <enter> at the TS command line (or press the LIFT button again on the external BSMS)

Create a new experiment:

- 1) Type *new* <enter> (at the Topspin command line)
- 2) Type *PROTON* <enter> (for ^1H experiment)
- 3) Select solvent
- 4) Click on “**Execute ‘getprosol’**”
- 5) Choose the right folder (PI’s last name)

Creating a new experiment from an existing one:

- 1) Drag an experiment folder into the display window
- 2) Type *edc* <enter> (a new following window pops out, see picture on the right)
- 3) Click on “**Use Current Parameters**”
- 4) Click on “**Set solvent**”
- 5) Write details about your sample and experiment, date, etc.



Setting up the experiment (type followings in the topspin command line):

- 1) Type *lock* <enter> at the Topspin command line
- 2) Select the appropriate solvent and wait until it is completed
- 3) Check the tuning by typing *wobb* <enter> at the Topspin command line
- 4) Type *topshim* <enter> at the Topspin command line to shim the sample **automatically**
- 5) Change the number of scans (ns) as required (default # is 16)
- 6) Type *rga* <enter> at the Topspin command line
- 7) Type *zg* <enter> to start the experiment

Processing the data (type followings in the topspin command line):

((the following are basic TS processing commands for you to inspect the quality of the data just acquired – the bulk of NMR data processing should be done off-line using the software of preference. The NMR Laboratory recommends MNova from Mestrelab))

- 1) Type *efp* <enter>
- 2) Type *apk* <enter> (correct the spectrum manually if the automatic phasing does not work perfectly)
- 3) Type *abs n* <enter> at the Topspin command line
- 4) Type *ej* <enter> (to eject sample from the magnet)

Please note: the AVIII-500-MHz is online. You mail email the NMR data to yourself (after zipping the NMR data directory) or bring a USB flash drive to transfer your data to it.

Should you require assistance, please contact:

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