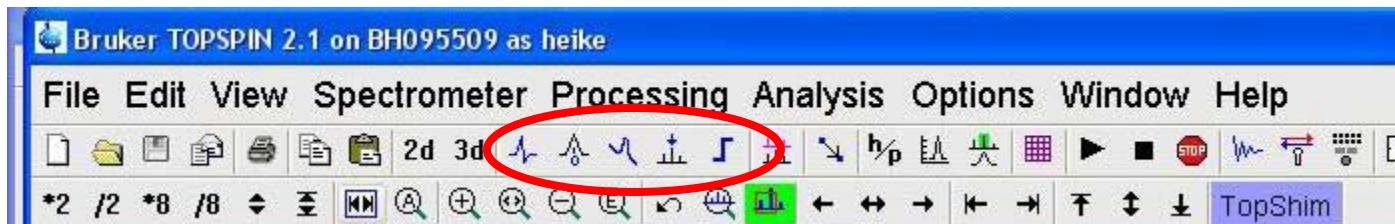


## WORKING GUIDE for

### 300/500 MHz NMR

- log on to the NMR computer, enter you user name and password and double click the TOPSIN 2.1 icon on the desktop to open the TopSpin program.
- Into the command line type **edc**, then enter dataset name (NAME), and experiment number (EXPNO) and save.
- In the command line enter **rpar**, chose the desired experiment from the list of parameter sets. When the rpar window opens, click on Copy All.
- On the BSMS control suite (this window will open when you start TopSpin., but might be in the taskbar)
  - 1) turn off **Lock**
  - 2) **Lift** sample (make sure the lid is off)
- The sample will lift out of the magnet. Put your sample into the sample holder and adjust its position using the depth gauge. Insert the sample holder into the top of the magnet.
- Press the **Lift** button which will lower the sample into the magnet.
- type **lock** and select the right solvent from the list.
- Type **atma** for automatic tuning and matching (make sure you have the right parameter set selected). atmm allows you do manually tune and match.
- Start the **Spin** on the BSMS.
- Type **topshim** (or use the colored button in the lower toolbar). This will automatically shim your sample.
- Set receiver gain by typing **rga** into the command line. Wait until rg is established (rga : finished).
- **zg; efp** will start data acquisition and then process the data. The default number of scans **ns** is 8. To change this, type ns and enter the desired number into the window.
  - **apk** – automatic phase correction
  - **abs n** – automatic baseline correction without integration

- Move on to the spectrum tabs:



- Phase: click on button **phase** . Use automatic peak selection or manually select toggle point, then correct **PH0**, **PH1**, **save & return**.
- If necessary, **calibrate** using the solvent peaks, according to the list located near the NMRs. Pay attention to the temperature dependence of the solvent's shift. Be consistent: calibrate on the same solvent peak (e.g. on THF - left peak on 3.57).
- If necessary, use baseline correction .
- Peak picking** : use the box function or manual peak picking . Save and return will take you back into the 1D window.
- Integration** : mark integration limits by placing the mouse on the left side of the peak, press the left mouse key and move the mouse to the right side. Release the mouse key. Each peak or group of peaks can be integrated separately, or the entire spectrum can be integrated at once and then separated using the key.
- Define spectral region: zoom into the spectrum, once you have chosen the appropriate region, right click into the spectrum and save display region to F1/F2. Ok to save.
- Set the title in the title tab
- Type plot, the editor will open and you can print the spectrum from there.
- Type prnt, this will just print the window and file location.

To finish, take off the **lock**, stop **spinning** and **lift** tube. Remove your sample and insert the D<sub>2</sub>O sample. **Lock** the sample. Make certain that the sample is locked before you exit TopSpin. Log off your account.