

## Procedure for NMR analysis on the 500-MHz with SAMPLE CHANGER, Broadband (BB) probe, and Automatic Tuning and Matching (ATM)



Figure 1



Figure 2

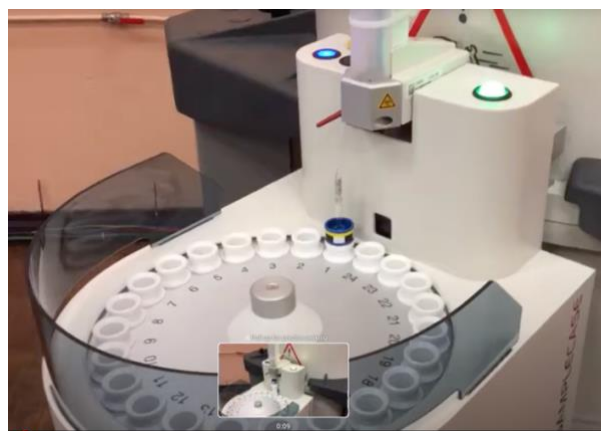


Figure 3

- 1) The Sample Changer (Bruker's SampleCase-24) is shown in **Figure 1**; there are 24 slots in which you can insert your sample (see **Figure 3**). **Get the BLUE spinner from the box (Figure 2). The Sample Changer must be used with the BLUE spinner designed specifically for this model of Sample Changer.**
- 2) Insert your sample into the blue spinner, adjusting its position with the Bruker gauge.
- 3) Choose ONE position inside one of the slots of the Sample Changer (**for example, position 10**). Put your sample **INSIDE** this position.
- 4) Type at the TopSpin command line, **SX 10 (SXspace10) <enter>**. The Sample Changer will rotate clockwise until it lines up with the tube that will shuttle the sample toward the magnet, inserting it. Before that, the Sample Changer will EJECT the "dummy" sample (D2O/H2O) on its "default" position, which was established to be **slot 1**.

Once the sample is inserted, proceed the NMR session as usual, with the following instructions:

- 5) Load the nucleus parameters (*e.g.* PROTON), either from:
  - a. Typing at the Bruker's TopSpin command line: **rpar PROTON all <enter>**
  - b. **Loading one previous experiment (*e.g.*, PROTON) by dragging and dropping the respective folder into TopSpin's graphics window.**
- 6) Type **edc <enter>** at Bruker's TopSpin command line to edit the template to determine the new name for the sample, the kind of experiment (PROTON, Carbon, etc.), the title of the sample, and check whether the directory path established on the template is correct (*i.e.*, showing the name of your professor), as your NMR data will be saved there. Click on the **Save** button.
- 7) **\*\*\*IMPORTANT\*\*** - type **getprosol <enter>** at the TopSpin command line – the probe has changed, and this command loads the specific parameters for this probe.

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- 8) **\*\*\*IMPORTANT\*\*** - type **ATMA <enter>** at the TopSpin command line. **Wait for the tuning DIP to be automatically CENTERED** (for those NMR users who used to manually tune the probe by reaching the capacitors underneath the magnet, **this step is NOT necessary anymore!**)
- 9) **\*\*\*IMPORTANT\*\*** - lock on the **Deuterated Solvent** of your sample.
- 10) **\*\*\*IMPORTANT\*\*** - type **topshim <enter>** at the TopSpin command line. **Please wait until the process informs you that it is finished.**
- 11) Spin the sample by typing **ro <enter>** at the TopSpin command line. **Left-click** on the **Start rotation** button.
- 12) Type **rga <enter>** at the TopSpin command line. Please wait until the process informs that it is finished.
- 13) Type **zg <enter>** to start the acquisition.
- 14) **For QUICK data processing only:**
  - a. Type **efp <enter>** at the TopSpin command line.
  - b. Type **apk <enter>** at the TopSpin command line.
- 15) If the spectrum has good **Signal/Noise** and **resolution**, the experiment is finished, and one may save the data in a **USB flash drive** inserted into the host computer.
  - a. **Please note the USB flash drive icon is on the monitor's desktop folder.** To remove the USB flash drive from the computer, **right-click** the USB icon and choose **UNMOUNT by left-clicking** on this option. Please do not remove the USB flash drive before this step, as it might corrupt the Linux file system.
- 16) type **SX 1** (see step 4), to eject the sample. Your sample will be ejected, re-inserted into slot **10**, and the carousel of the Sample Changer will rotate to **slot 1** and insert the DUMMY sample again into the magnet. Lock in D<sub>2</sub>O/H<sub>2</sub>O, and make sure the sample is NOT spinning.
- 17) Once step 16 is complete, your Session finishes and you may LOGOUT from the FOM calendar reservation.

**Questions or comments on the 500-MHz operation:**  
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