NMR self-service at IOCB

NMR SPECTROSCOPY
RESEARCH-SERVICE GROUP
IOCB PRAGUE

1. Instrumentation

"OLD"	**"PRODIGY"**
probehead: broad band 5mm	**probehead:** broad band 5mm nitrogen cooled cryo-probe
measured nuclei: ^{1}H, ^{19}F, ^{13}C, ^{31}P, ^{11}B	**measured nuclei:** ^{1}H, ^{13}C, ^{31}P, ^{11}B
sample changer: B-ACS for 120 samples	**sample changer:** Sample Xpress for 60 samples
Icon-Web access: http://ob-a401:8015	**Icon-Web access:** http://ob-a402:8015

2. General policy

- All users must pass a training course before they obtain their own access to the spectrometer. The training course takes place every Monday at 9:00 a.m. Please, arrange an appointment at NMR-400@uochb.cas.cz.

- The samples are run on a first-come-first-serve basis with all experiments longer than 35 minutes (OLD) or 30 minutes (PRODIGY) running at night. Night experiments start at 6:30 p.m. (18:30) and end at 8:30 a.m. (8:30). Weekends are treated as night days with day experiments priority.

- Clean the bottom part of the NMR tube and the spinner with provided paper napkins moistened by ethanol prior to placing the sample into the sample changer. Always use the calibration tool to ensure correct tube insertion depth in the rotor. Incorrectly inserted tubes can break when being dropped into the magnet.

- The experiments can be only submitted via the Linux workstations controlling the NMR spectrometers.

- Take your NMR tubes back ASAP after the measurement is finished. Samples that are not taken back will be discarded one month after the date of measurement.

- Users are asked to report damaged or improperly inserted sample tubes to the NMR Facility staff immediately in order to avoid needless down time and equipment damage!

- There is maintenance time every Monday morning (9:00 – 11:00 a.m.) reserved for the NMR Facility staff. **Entering the spectrometer room during maintenance time is forbidden** to ensure safety and prevent equipment damage.

- In the case of spectrometer failure, contact the NMR staff at NMR-400@uochb.cas.cz.

3. Before you start

- Samples for the measurement must be prepared in the user's laboratory.

- Special precaution for "OLD": Your NMR tube **must be at least 17.5 cm** (6.9 inches) in length and **must not be broken or cracked**! If your tube is shorter than 17.5 cm, it will not be grabbed fully by the sample changer and may fall and break on the floor or on the top of the magnet. Tubes with chipped tops are weakened and may be broken by the robotic arm pincers which grab the tube very firmly close to the top. Any tube shorter than 17.5 cm or with a chipped top submitted to the sample changer will be removed.

- Your NMR tube **must not have any label (paper, tape, sticker etc....) attached to it**. This may stop the sample changer from working properly and may result in sample breakage and equipment damage. Tubes can be labeled on the glass or the cap with permanent marker. Any tube with an attached label submitted to the sample changer will be removed.

- **Always use 0.5-0.6 ml of solvent** and make sure your sample is dissolved. Unsuitable solvent levels or non-homogeneous samples can lead to a bad shimming result and useless spectra. Moreover, using excess solvent increases the risk of equipment damage in case of a broken tube.

- Think of experiments you are going to submit and use the spectrometer time responsibly. **Do not submit both ^{13}C and APT for one sample.** Do not submit more than 3 samples with complete set of experiments in one submission.

4. Accessing and handling your data

- Status of the sample changer (information, if your sample has been already measured) can be viewed on-line using Icon-Web service simply by typing http://ob-a401:8015 (OLD) or http://ob-a402:8015 (PRODIGY) into your web browser. Submitting of experiments through Icon-Web is forbidden.

- Immediately after the experiment is completed, the data are stored at the Linux workstation in the directory opt/Bruker/Data/data/*username* and automatically archived at the SAMBA server in the directory 147.231.122.7/nmruser/data/*username* (OLD) or 147.231.122.7/nmruser/PRODIGY/data/*username* (PRODIGY) accessible through the IOCB network. **Please, backup your data! We do not take responsibility for your data!**

5. Mestrenova – process your data

- The latest version of NMR processing software Mestrenova can be downloaded from Mestrelab Software web pages: http://mestrelab.com/download/mnova/.

- The Mestrenova license files can be found at the SAMBA server in the directory: 147.231.122.7/nmruser/MestrecLic