

Policies and Guidelines for NMR Usage

General

New Users –Users are required to undergo a basic training before they can operate the instrument and collect data by themselves.

- Please fill in the training form available in the *Services* web page, get signed by your supervisor and forward it to one of the staff members. The training will not be conducted until the form is submitted
- New users will be trained on Avance-300, DPX-300 or DRX-400, which involves manual shimming, first before on any other spectrometer
- When the new user has learned how to operate the Spectrometer, another staff member will schedule a check-out session. After successful completion of this session, the new user will receive a login name and password for the web reservation system
- Undergraduate students will be trained not more than two spectrometers and they have to choose instruments accordingly

Access –The NMR spectrometers are housed in three locations of the Chemistry Building and the rooms use either traditional locks requiring keys or AMAG cards.

- You can get access to an instrumentation room only after you get trained at least one of the spectrometers in that room.
- To get access fill in the key form available in the *Services* web page, get signed by your supervisor and forward it to one of the staff members.

Logbook entry- The users are required to make logbook entries, when they use any of the facility instruments or off-line processing computers. The primary reasons of using logbooks include but not limited to: a) computation of monthly billing, b) tracking maintenance, trouble-shooting and repair of the instrumentation and c) following usage patterns and statistics

- Users should sign-in the logbook before putting their sample in the magnet. Times should be recorded based upon a 24 hour clock (i.e. 8:00am is 08:00 and 5:00 p.m. is 17:00)
- Use your full last name to make entries. Do not use initials.
- The starting and ending date and time should be included clearly in the logbook entry. If the starting and ending date and time are not recorded properly, you may be overcharged
- Please use the correct MFK account number
- Users should enter any problems they encounter during their usage in the logbook. This will allow the staff members to resolve the problems as quickly as possible.
- Users should make an entry of any damage (e.g. breaking of NMR sample tubes) happened during their usage. Ignoring this policy can lead to disciplinary action including the termination of usage privileges

Web-based reservation

The sign-up and cancellation policies are only applicable to four spectrometers of the NMR facility, Avance-300, DPX-300, DRX-400 and Avance-400.

Sign-ups

Schedule for next 7 days is available at the NMR web page, (<http://nmr.chem.uiowa.edu/NMRshed.html>).

Avance-300, DPX-300 and DRX-400

Walk-on time slots (Avance-300 and DPX-300): 10-minute blocks identified by the term *walk*, marked blue and generally for short-term data collection

- There will be an initial *limit of four 10-minute* time blocks *per user* per day.
- There will be an initial *limit of ten 10-minute* time blocks per research *group* per day.
- Individual and group limits may be relaxed when the Spectrometer would sit idle, with the understanding that time should be made available to other users when requested.
- Variable temperature and long-term measurements are generally not allowed during walk time slots

Walk-on time slots (DRX-400): 10-, 20-, and 30-minute blocks identified by the term *walk* and are generally for short- and medium-term data collections. The longer time blocks are included to accommodate ^{13}C runs.

- There will be an initial *limit of 2 hours* per research group
- If a user or group has utilized their limit of walk-on time and if there is still time blocks available, then they may continue using the Spectrometer with the understanding that they will stop their usage as soon as someone else needs to use the Spectrometer.
- Do not sign-up for more time blocks than you will need. Users who routinely sign-up for significantly more time than they need will be billed for the unused NMR time that they reserved.
- Walk-on time should not be used as a way to extend an overnight data acquisition.
- Variable temperature and long-term measurements are generally not allowed during walk time slots
- NMR staff will periodically review the sign-ups, if users abuse the signup limitations, then staff may cancel signups to make time available to other users. Repeated abuse of signup limitations may result in signup privileges being temporarily canceled.

Evenings, nights and weekends (Avance-300, DPX-300 and DRX-400): Identified by the term *open*, marked green and generally for long-term data collection.

- When the instrument is used for long-term runs during weekday's evenings and nights, the ending time should not exceed 8:00am the next day. This will allow the short-term users to perform their experiments without difficulty.

Avance-III-400

This spectrometer has a higher priority for instructional over research usage. In the web-reservation system, the time blocks are not only marked with *walk* and *open*, but also by *not-available* and *available-on-request*. The walk and open time blocks have the same meaning as in

the other spectrometers of the Low-Field NMR Resource. “*Not-available*” refers to the anticipated use of the instrument by one of the undergraduate courses. “*Available-on-request*” refers to the requirement that the use is restricted to users who are approved by the undergraduate laboratory administrator; this restriction has been in effect since 2008.

Walk-on time slots: 10- and 30-minute blocks identified by the term *walk* marked blue and generally for short-term data collection. The usage policies are the same as those of the DRX-400 spectrometer and are meant to only for research use.

Evenings, nights and weekends: Identified by the term *open* or *available-on-request* and are generally used for long-term data collection

- The blocks marked *open* have the same meaning and usage policies as that of the DRX-400 spectrometer
- Contact Earlene Erbe, the undergraduate laboratory administrator, if you would like to use the “*available-on-request*” long-term run time blocks

Paper-based reservation

Paper-based Reservation is used for Fourier-300, Avance-500, Avance-III-500 solids and Avance-III-600 spectrometers. The primary reason for using paper reservation system is that the existing web reservation system cannot handle the time-reservation of more than four spectrometers and this system will be expected to continue until the web-reservation system is overhauled to accommodate additional spectrometers. The users are requested to use the time sheets posted on the instrumentation room doors for reserving time for the respective spectrometers.

Sign-ups

Schedule for next 2 weeks is available to sign-up on the doors of the NMR rooms.

Fourier-300 and Avance-500

The reservation and cancellation policies are the same as those of DRX-400 spectrometer, but the signups and cancellations are done on paper instead of on online. The usage policies of the DRX-400 are all applicable to the Fourier-300 and Avance-500 spectrometers.

Avance-III-500 solids and Avance-III-600

As these spectrometers are utilized by a fewer number of research groups and more often used for long-term spectral runs, users may reserve relatively large blocks of time (typically days) on these spectrometers either using the paper reservation sheets posted on the room door or by emailing to one of the staff members. There is additional usage and precautionary policies in using these instruments, and please consult with a staff member in case you have never used them before and would like to run samples.

Cancellations

Cancellation policies are introduced to minimize unused instrumentation time and wastage of resources. Users have been reserving time and then canceling at last minute, not showing up to use the reserved block of time, or signing up several time blocks and then only using a few

minutes. This prevents other users from planning for their NMR experiments and creating confusion and dismay.

Evenings, nights and weekends:

- If you reserved NMR time on a previous day, cancel 24 hours in advance
- If you reserved NMR time on the current day, cancel by 16:00
- If you do not follow these cancellation guidelines, you will be billed for the reserved time instead of actual used time

Walk-on time slots:

- If you reserved NMR time on a previous day, cancel at least 2 hours in advance. If you do not show up in the first 15 minutes of a reserved walk-on Time Block(s) or have not left word that you have been delayed; then if other users have need for NMR Time, they may use your time & you will lose the privileges for that time block and any sequential time blocks associated with your login reserved time.