

## Welcome to the NMR Facility in the Chemistry Department

### NMR Instruments available:

Name	<sup>1</sup> H Freq.	Preferred Uses	Room
1. Varian Gemini-200	200 MHz	Undergraduate priority	OC 118
2. Bruker AM-250	250 MHz	Routine <sup>1</sup> H and <sup>13</sup> C, short time periods	OC 121A
3. Varian Unity-300	300 MHz	Routine and low temperature, <sup>19</sup> F, <sup>31</sup> P	OC 122
4. Bruker DRX-500	500 MHz	Best for organic 2D experiments	OC 121C
5. Bruker DRX-600	600 MHz	For complex molecules and biological 2D	OC 121B
6. Varian Inova-600	600 MHz	Biological 2D and 3D (cryogenic probe)	OC 121D

The Bruker instruments and the Varian Inova-600 are located in the NW corner of the first floor of Old Chemistry (room 121) and the lower-field Varian instruments are located in the opposite (SE) corner (rooms 118 and 122). All instruments are available for "hands on" use after appropriate training is completed. Funding for a new 400 MHz instrument for routine <sup>1</sup>H, <sup>13</sup>C, 2D and undergraduate teaching has been approved, and we expect to install this instrument in summer 2009.

**Computer Support:** The Campus Wide NMR Server ([uanmr.chem.arizona.edu](http://uanmr.chem.arizona.edu)) is a Gateway Linux server with an Intel Xeon processor at 3.0 GHz with a front side bus speed of 1333 Mhz, 4GB RAM and MegaRaid and SAS hard drives. This "nerve center" of the NMR facility has most of the hard disks of the NMR spectrometers mounted on it remotely (via the network) so that NMR data can be processed and plotted on paper without using or paying for the NMR instruments. Two different NMR software packages (Bruker "XWinNMR" and Accelrys "Felix") are available and both can be accessed from an IBM or Mac personal computer via the network. This means that you can process and plot NMR data from your own office or laboratory anywhere on campus. The workstation also serves as a scheduler for NMR reservations on all of our instruments. In addition, the Varian Unity-300 has two Sun UNIX satellite workstations for data processing and plotting using the Varian VNMR software.

### NMR Facility Staff:

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**Where to Start:** You must be in the departmental database to use the NMR instruments. Go to the Chemistry Department main office. Then see Neil Jacobsen or one of the Graduate Assistants.

**How much does it cost?** We charge \$10.00 per hour of instrument time on all of the instruments, with the exception of the Inova-600 with cryogenic probe, which costs \$15.00 per hour. If you do not wish to use the instruments yourself, an additional charge of \$40.00 per hour of operator time is charged for the NMR Facility personnel. These rates apply to the entire campus community; outside users are charged three times these rates. Hands-on use is not limited to the Chemistry Department;

anyone on campus can get training and use the instruments. For hands-on use, each instrument requires a login ID and password and keeps track of the time used.

**NMR Training:** Everyone must have a “driver’s license” for a specific instrument to have hands-on access to that instrument. The license is obtained when you successfully complete training for that instrument. There are two “tracks” for NMR training: the Varian track and the Bruker track. If you already have experience with Bruker, for example, it will be easiest to start with the Bruker track. Eventually if you use NMR regularly you will want to learn both Bruker and Varian to have the greatest versatility. If you have extensive experience with the Varian Unity or the Bruker DRX you may be able to start with these UNIX-based instruments, but most people start with the Varian Gemini or Bruker AM systems and work their way up to the more modern instruments.

There are two simple ways to get NMR training: individual training and training workshops. Training workshops are short classes which include lectures, demonstrations and individual training at the instrument. Each participant is given a two-week “practice account” on the instrument(s) covered by the workshop. A bound workshop book includes a general description of NMR acquisition and processing parameters as well as detailed instructions for using the instruments. The “driver’s test” involves obtaining a  $^1\text{H}$  and  $^{13}\text{C}$  spectrum of a standard sample. In more advanced workshops this can also include advanced 1D or 2D experiments. A take-home written test covers the parameter names, concepts and hardware of the NMR instrument. After going over the spectra and written test with Dr. Jacobsen, you get a “permanent” driver’s license. Workshops for the Gemini-200 and AM-250 instruments (basic workshop) are once a year in March and cover only 1D  $^1\text{H}$  and  $^{13}\text{C}$ . Workshops for the Unity-300 and DRX-500 are given in the summer and cover advanced 1D (DEPT, 1D NOE) and basic 2D (HSQC) experiments as well as basic 1D. Since the DRX-600 is essentially identical in software and operation to the DRX-500, there are no workshops specific to this instrument.

Individual training is available at all times with the understanding that the next available workshop will be attended. For example, if you get a license to use the Bruker AM-250 by getting a small group demonstration and completing the “driver’s test”, you will still need to attend the basic NMR training workshop (lecture and written test) the next time it is given. We require a group of at least 3 students to give a training demonstration, so you may have to wait.

A third way to get NMR training is to attend Chemistry 534A (Practical NMR Spectroscopy Laboratory), a 3-credit graduate laboratory course. This course is given in the Fall semester of each even-numbered year and covers all of the common 1D and 2D experiments used for elucidation of structure in solution. Upon successful completion of this course you will have a license for hands-on operation of the Varian Unity-300 and Bruker DRX-500 and DRX-600 instruments. Chemistry 534B, which is taught in the Fall semester of odd-numbered years, is a 3-credit lecture course covering NMR theory.

**The Reservation System.** NMR time must be reserved beforehand using a computerized reservation system. Each instrument has rules which govern the amount of time you can reserve and how far ahead of time you are allowed to reserve an instrument. These rules are designed to maximize the efficiency of use of each instrument and are subject to change as needs and pressure change. As soon as you receive a driver’s license you will be entered into the reservation system and permitted to reserve time on that instrument. To reserve time simply SSH to uanmr, logging on as “reserve” (get the password from Neil). To get an overview of the reservation schedule, log on as “schedule”.

**NMR Tubes.** Only Kontes 33-220 or Wilmad 507-PP 5-mm glass tubes, or better quality, can be used on Facility instruments. These are available in the stockroom for about \$10.00 each. For undergraduate class work, we allow Wilmad “Thrifty” tubes on the Gemini-200.

**Keys.** To get keys, you must be “licensed” on the appropriate instrument. Everyone in the Chemistry Department (Graduate Students, Postdocs, Visiting Faculty) should have a building key. This gets you into the Old Chemistry building (building 41) after hours and also opens the door to room 118 (Varian Gemini-200) and room 121 (Bruker AM-250). These doors are locked at all times except from 8 a.m. to 6 p.m. Monday-Friday. If you are an undergraduate or from another department, you will need to get a building key if you wish to use the NMR facility after hours. In addition, the doors to room 122 (Varian Unity-300 and the SGI workstation “UANMR”), room 121C (Bruker DRX-500), room 121B (Bruker DRX-600) and room 121D (Varian Inova-600) are locked all times and require special access keys. The same key opens rooms 121B, 121C and 122. To get keys, go to the Chemistry departmental office (room 221 Old Chem.) and pick up a Key Request Form. Fill this out and get a signature from Neil Jacobsen in room 119, then bring the completed form back to the Chemistry Office with your Cat Card and your Room Privilege Card. They will give you the paperwork for the new key(s). Bring this to the Key Desk (North of Speedway: 1533 E. Helen St., hours 7 a.m. – 3 p.m.) and pick up your key(s).