

Policies

1. NMR Facility equipment

Agilent Mercury-300 MHz “Routine” NMR Spectrometer

The Agilent Mercury 300-MHz spectrometer is equipped with two probes, two rf channels with pulsed field gradient. On the routine, it is equipped with an AutoSwitchable four-nucleus probe which allows the operator to switch the resonance frequency (^1H , ^{13}C , ^{31}P , or ^{19}F) from the computer terminal without any manual adjustment of the probe. A 10 mm Broadband probe is also available upon request for high sensitivity X channel observation on the inner coil. The probe is available in a number of broadband frequency ranges, each optimized for the highest performance in that tuning range.

Agilent Inova-400 MHz “Routine” NMR Spectrometer

The Agilent Inova system is equipped with an Indirect Detection Probe, two RF channels and pulse field gradient, which offers a routine and robust way to do multidimensional (2D) experiments. Because of the pulse field gradient capability, data are produced faster and cleaner with one scan per increment since the time consuming phase cycling is eliminated. With the inverse detection pulse field gradient probe, CH correlation experiments like GHMQC and GHMBC provide greater sensitivity enhancement over conventional hetero type experiments and even HMQC experiments.

Brucker AVANCE III 600 MHz NMR Spectrometer

The Brucker AVANCE III 600 MHz NMR Spectrometer is equipped with two probes, with four RF channels for generation of phase, amplitude and frequency. The instrumentation shall generate 1D/2D/3D spectroscopic data for full state of the art elucidation of molecular solution structure. This feature makes the instrument especially suited for experiments that have low sensitivity and on samples that are limited in quantity. This new system will significantly enhance the sensitivity for study of large proteins and DNA in water and limited amounts of sample from natural product extraction, drug metabolites and a long/complex synthetic procedure

Inverse quadruple resonance (**QXI**) probe for observation of ^1H while decoupling ^{13}C , ^{15}N , and ^{31}P . The inner coil is double tuned to observe ^1H with ^{31}P decoupling. The outer NMR coil is double tuned for decoupling on ^{13}C and ^{15}N . All four channels can be operated simultaneously.

Multinuclear broadband observe (**BBO**) probe with digital tuning covering the range from ^{15}N to ^{31}P with ^1H decoupling, ^1H channel tunable to ^{19}F .

Spectrometer is also equipped with **BCU-05**, pre-cooling and stabilization accessory, for ultra-precise temperature control from near ambient conditions down to 0 °C sample temperature.

2. Access to instruments

Instruments are accessible to anyone who has been trained by the NMR facility staff. You should plan your training at least one week in advance. The training forms are available from the NMR facility and web site. Complete the training form and return it to the NMR Facility Director. *No unauthorized training!*

Each authorized user group is given an account on the instruments. Please use a secure password and do NOT let anyone else use your account.

3. General policies

No food or beverages near the spectrometers.

Do not leave your NMR tube in the NMR facility.

If a sample breaks in the magnet, contact the NMR facility Director immediately (by phone or in person) so the probe can be cleaned. Minimum information needed: name and structure of the compound if known, or at least class of compound, name of solvent, toxicity of material, and other solvents which dissolve it, special precautions in handling if it is toxic. Please leave a note on the instrument keyboard warning users not to use the instrument. This will minimize probe damage.

Repairs for any damage to the probes resulting from user error will be charged to the user group.

If there is problem, leave a note or contact the NMR facility Director if it cannot be resolved by following **Troubleshooting FAQ**.

DO NOT TOUCH HARDWARE or REBOOT INSTRUMENT.

All users must lock and shim on the dummy sample and LOGOUT from your account when finished with the spectrometer. The dummy sample on the instruments is CDCl_3 . If the dummy sample breaks, contact the NMR facility staff so that we can replace it.

READ THE MANUAL! You will find most of your questions are addressed in the 1D instruction manual.

4. Restrictions on usage

ON 300 MHz NMR:

Monday - Friday: 9:00 am-6:00 pm: 4 slots/user (15minutes/slot), reserve within a week. Cancellation must be made at least 1 hour in advance.

Monday -Thursday Overnight, 6:00 pm-9:00 am, reserve within two weeks. Cancellation must be made at least 5 hrs in advance.

Weekends and Holidays: Reserve within a month. Cancellation must be made at least one day in advance.

Non-standard experiments (VT work, exotic nuclei, 10mm BB probe) must be scheduled with the NMR facility Director one week in advance.

ON 400 MHz NMR:

Reservation for Minutes and less than 5 hours, reserve within a week. Cancellation must be made at least 1 hour in advance.

Reservation for more than 5 hours & overnight, reserve within two weeks. Cancellation must be made at least 5 hrs in advance.

Days, Reserve within a month. Cancellation must be made at least one day in advance.

ON 600 MHz NMR:

In order for the high-end instrument to effectively service faculty/students with their research needs and bring great benefits to Department/VCU/, the training/usage on 600 NMR will be based on your special request on your “real sample / research project”. Please email me if you need to use 600 NMR. Then I will discuss with you and schedule training.

If you reserve time, it is your responsibility to be there during that time and also to be finished at the proper time unless problems are encountered. If you cannot be present for your reserved time, it is your responsibility to cancel it from the time slot. It will be charged to your account for non- or late-cancellation.

5. Charging for instrument time

Rates for spectrometer usage vary from the time periods and users. All accounting is done automatically with spectrometer logins. There is no charge for usage of the data workstation.

Instrument	academic users	Non-academic users
Bruker AVANCE III 600 MHz	\$15/hr \$200/day	\$100/hr
Agilent Inova 400 MHz	\$10/hr 7:00-19:00 \$5/hr night & holidays	\$100/hr
Agilent Mercury 300 MHz	\$10/hr 7:00-19:00 \$5/hr night & holidays	\$100/hr

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