

Nuclear Magnetic Resonance is an enormously powerful and versatile technique for investigating the structure and dynamics of molecules.

NMR Center News

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Molecules are inconveniently small, it is too small to be observed and studied directly. One therefore needs a spy, capable of relaying information on the structures, motions, and chemical reactions of molecules without significantly modifying those properties, and versatile enough to report on a wide range of molecules in a variety of situations. The spies are atomic nuclei. The NMR is the media between the nuclei

APT experiment on INOVA400

APT—**A**ttached **P**roton **T**est is designed to produce decoupled ^{13}C spectra with C-H multiplicity discrimination. It is useful alternative to off-resonance decoupling and it is greatly better than that method for molecules with a large number of carbons.

To set up the experiment, type **apt** in the command window. The apt macro sets up the experiment either by modifying an existing ^{13}C experiment parameters or by using default ^{13}C parameters. It also sets the *tau* delay to 7 ms, which gives CH's CH₃'s down and C's, CH₂'s up.

tau — Specifies a delay which determines the relative intensities of the signals from C, CH, CH₂ and CH₃. If set tau = 3 ms, only C's are observed. If set tau = 7ms, C's and CH₂'s signals are up and CH's and

It is Cheap Enough to Use NMRs

We found that most of our graduate students are capable of acquiring a proton spectrum within 10 minutes, including processing and plotting. The current NMR usage rate is \$3.60 per hour during the day. That is 60¢ per proton spectrum.

Cheap enough!!

The Other Facts:

The plot paper for QE300 is \$18.25 per pack (250 sheets). It is about 7.3¢ per page. The cryogen consumption is about 50¢ per hour whenever

the instrument is in use or not. The plotter pen is \$1.75 each. The 5mm NMR tube is \$5.50 each (Stockroom). The average

graduate student pay is \$8.00 per hour.

Although the NMR time is cheap, we found some NMR users still try to save pennies for their boss by "late login" or "early logout", even "forgot login" on the accounting computer.

According to the NMR Center User's Policy, they should login to the

accounting computer before starting to use the instrument, and after they finish experiment then logout.



Official Clock for NMR Time

Our accounting computer has recorded some users who only used one minute to acquire their NMR data. That is incredibly fast! If he/

QE300 Usage Time (August 97)	Used 586 times
NMR Used less than 3 mins	42 times
Used 3 to 5 mins	61 times
Used 5 mins or more	483 times

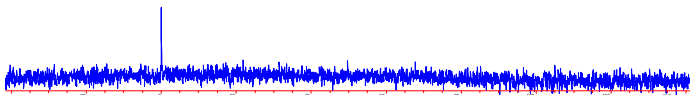
If you need to perform a special NMR experiment, such as multinuclear NMR or 2D NMR, please feel free to ask us.

¹⁸³W experiment on UNITY400 is Available now

After several months hard work, finally we are able to acquire ¹⁸³W spectrum on both of UNITY400 and INOVA400. The sensitivity of ¹⁸³W is only 0.00001 relative to 1H and the observe frequency is very low (16.663 MHz). The chemical shift range is about -4000 ppm to 2000 ppm and T1 from 0.3 to 50 seconds. The

chemical shift standard is 1.0M Na₂WO₄ in D₂O. One scan, the signal noise ratio is 9.2. 0.5 Hz line broadening was used. The T1 of Na₂WO₄ in D₂O is 45 seconds. The 90 degree pulse is 70 micro seconds at transmitter power 58 dB. The *rof2* was set to 40 and the *alfa* was set to 20 micro seconds. Isfid was set to 1. A normal ¹⁸³W sample with concentration above 0.1M, 12 hours should be enough to acquire a good spectrum.

You have to believe it. That is a 183W signal of Na₂WO₄ in D2O.



NMR Center Staff Responsibilities

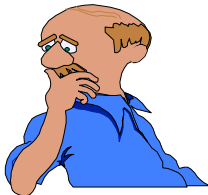
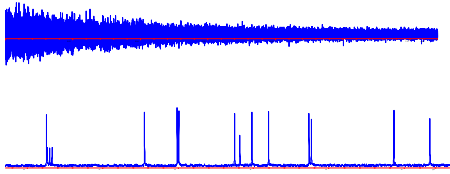
Shaoxiong Wu (7x6621): Over all maintenance and development of NMR Center. Training new users on Omega600 INOVA400 and UNITY400 and certifying all NMR users. Develop new techniques to meet research needs.

Collaboration with internal and external NMR users. **Shubao Chen**(7x2493): Order and refill cryogen for all NMRs. NMR usage accounting and administrate all NMR logs and documentation. Help NMR users to perform different NMR experiments. Tainting

users on INOVA400 and GN500. Order NMR Center supplies.

Jenna Siracusa (7x4416): Training QE300 users and giving NMR test to new NMR users.

Huadong Zheng(7x4419): Training GN500 users and



INOVA 400 NMR Usage	Prime Time (Hours)	Off -Time (Hours)
May, 1997	154.92	116.40
June, 1997	232.11	73.29
July, 1997	245.60	153.90

When you are running a dilute C13 spectrum, please try this one:

DO NOT SKIP AHEAD. Read the message ONE LINE AT A

TIME and just do what it says. You will be glad you did. If not, you'll feel like an idiot and wish you had listened.

- pick a number from 1-9
- subtract 5
- multiply by 3
- square the number
- add the digits until you get only one digit (i.e. 64=6+4=10 or 10 = 1+0 = 1)
- if the number is less than 5, add five. Otherwise subtract 4.
- multiply by 2
- subtract 6
- map the digit to a letter in the alphabet 1=A, 2=B, 3=C, etc..
- pick a name of a country that begins with that letter.
- take the second letter in the country name and think of a mammal that begins with that letter.

you have a 20% chance of picking a mammal from the alphabet

12) think of the color of that mammal.

This exercise is very