

# NMR NEWS

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## MNova Site License



Our free 3 month evaluation has ended and we now need feedback. Negotiations for a possible site license will begin shortly so please let us know what you thought. The more you can tell us the better we can decide. See Pg.2 for details.

## WebSite Updates

Colour changes and re-organizations have been introduced to make scheduling NMR time easier and more intuitive. Spectrometers are organized in the summary view by building location now. Let us know if you have further suggestions.

## Lab Coats and Gloves in the NMR Lab

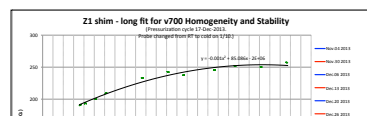


A reminder for everyone's safety that **lab coats and gloves are not allowed in the NMR labs**. Samples should be sealed and properly transported, and any breaks are to be dealt with on-site.



## 700 Status Update

In our last update we detailed the monitoring of the new 700 MHz magnet. We are very happy to report substantial settling of the magnetic field.



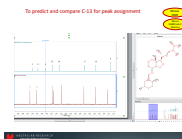
Special thanks to Knut Mehr at Agilent for all his help evaluating the performance. The magnet is fully functional and we are now confident that it will meet all researcher requirements. We also mentioned that we were monitoring room environmental aspects such as pressure, temperature and external temps. We are extending the investigation to other spectrometer rooms so don't be surprised if you see monitoring units.

Lastly please see Pg. 3 regarding some exciting changes to 700 access on Tuesdays.



## MNova Software

**Software License:** During the summer MestraLab (creators of MNova) were kind enough to offer the department a 3-month, 100 seat trial license for their chemistry NMR software. A local site license managing program was set up on our department web server (thanks Mark!) and licenses distributed to any departmental request. Instructions were documented and sent around to all staff, students and researchers. If you participated in the site license trial and/or have previous experience with MNova please let us know your feedback by Nov. 15<sup>th</sup>. Negotiations for a departmental license, number of seats, and the optional packages will commence shortly. Software is not cheap and despite the excellent capabilities of the program and additional packages we need some departmental consensus in order to proceed. If you would like to see what MNova has to offer please see their website list at <http://mestrelab.com>

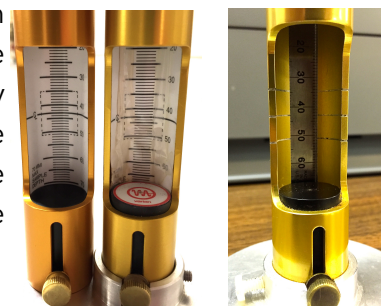


## Spinners and Depth Gauges - *please don't clean*

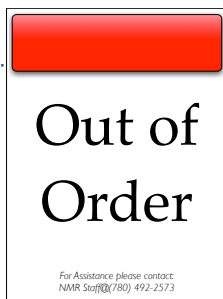


The NMR spinners are ceramic, breakable, and very expensive (~\$316 each). With Agilent no longer selling NMR products they are now even more precious. The black band with white dots is used to determine the spinning rate. **If you break a sample in the spinner and/or depth gauge please contact the NMR staff and do NOT clean the spinner.** Ethanol (and other common solvents) coupled with wiping damages the paint. In the inset figure you can see a new spinner (right) and one repainted (left). This requires specific paint, several careful sanding sessions, and a lot of time.

Along that subject please be careful with the NMR sample depth gauges. In the figures on the right you can see a new depth gauge (left) along side one seeing some use (middle). The label is badly damaged from rinsing with solvents when a sample is broken in the gauge. Eventually it has to be completely removed. The Machine Shop was kind enough to modify a very badly damaged gauge (right), providing meticulous etching in the metal itself.



**If you break an NMR sample please inform staff immediately and let us help handle the situation.**



## Out of Order Signs

When the spectrometers are not functioning properly please put the Out-Of-Order signs up in front of the keyboard and screen, then go get facility assistance. It is important that someone else does not start using the instrument while you are seeking help. This is especially important on the weekends and during the evening when it might be sometime before staff can resolve the problem.

The signs are either behind the monitors, or on a shelf nearby. If you can not find the sign please use a piece of spare paper to leave a message on the keyboard to prevent escalating problems.

## 700 MHz Access on Tuesdays

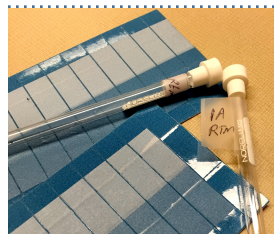
The 700 MHz NMR spectrometer (known affectionately as the v700) is reserved for complex biomolecular spectroscopy or specific requests for high resolution experiments. In an effort to make our flagship instrument more accessible and give researchers an opportunity to see what higher field and cryo-probe sensitivity can do, we are opening up access on Tuesdays after the cryogen fills. Please contact NMR staff for website login and instrument access and don't forget the group will need to get a key for Room EB-44b from Laura. We'd like to start with 1 or 2 designated people from each lab and assess how things go before releasing full general access due to the added vulnerability of the cold probe and no auto-sample handling robot on the v700. Let us know if you have questions and make sure to bring your most challenging problems.

## Changes to Door Access (EB-44a)

We've had an interesting incident with a hooded, sun-glass wearing, large back-pack carrying "student" looking for the bathroom in the spectrometer room. With the increased foot traffic through Chemistry to CCIS this was bound to happen and security through obscurity only gets one so far. We've therefore moved to locking WB-13 and EB-44a any time staff is not present. While we appreciate that some well intentioned students are unlocking the mechanism trying to be helpful (i.e. they are not aware of the change), **please do not unlock the mechanism during business hours.** We will be closely monitoring the situation and please let us know if you have any concerns or have noticed similar incidents in the NMR rooms.



## NMR Tube Labels



NMR tubes are cheap, relatively robust and unfortunately pretty hard to identify. Even different colour caps don't help much to identify samples. The present solution is to use a piece of folded scotch tape with a name or sample identification written down (see inset - right tube). The drawbacks to this method occur when people don't fold the tape back over itself cleanly (i.e. labels stick to each other and other tubes) or when using a robot sample handler. The robots hate tape, and we therefore have people remove labels. The vast majority of users are diligent when removing samples and carefully re-apply the tape to the sample for their colleagues. However, errors happen and occasionally high value samples are misplaced, sometimes permanently. Another clever solution in use is to write the information on the NMR tube cap itself. This requires the caps to be disposable with a large reserve, while the tube is retained for future use.

Another alternative is NMR tube labels (figure - left tube and sheets) that provide space for sample name/identification and then fold around the NMR tube with a clear protective layer on the label. This helps prevent label damage during solvent spills. The formal labels are a few pennies a label and come in sheets of 26 (25 sheets per pack Sigma-Aldrich). If you'd like to try some please drop by and see Ryan in Room E3-17.