

# NMR Facility Newsletter



5 February, 2013

## Disruptions of NMR Service

There are several events that will result in some disruptions to NMR service over the next several weeks. The exact dates may change so be sure to check the NMR website for the latest information. We are attempting to stagger the events so that NMR access will always be available.

## UofA Cryo-Recycling Centre



(Photo of helium recovery at Photonics Inc: [www.photonics.com](http://www.photonics.com)).

The VP-R is sponsoring the rejuvenation of the University of Alberta helium recovery system (formerly operated by the Department of Physics).

The new helium re-liquefaction infrastructure (low pressure collection, high pressure storage, and helium liquefier) was attained via a government of Alberta equipment grant and support of the VP-R's office. The facility is located in the Li Ka Shing building, and requires the repair and extension of the cross campus helium recovery lines. The restoration of the lines has now extended into the Department of Chemistry. Former small (*i.e.* 0.5-1.25 inch) copper lines are being replaced with 2 inch diameter lines throughout both east and west chemistry buildings. During this first week of February workers will be drilling holes

and mounting recovery lines in EB-44 (home of the v700, u500, and i500 spectrometers).

**Please inform your lab members that copper lines, equipment, and workers will be present and may impeded access. Everyone is asked to be extra careful during these times to avoid injury.**

During the past several weeks lines in the hallways have been upgraded. New lines to all spectrometers will be run and may temporarily impede access during the coming weeks to the other instruments. Instruments in the sub-basement, 1st floor of West Chemistry, and on the 3rd floor of East Chemistry are all scheduled for new lines.

In addition to NMR spectrometers, the Mass Spectrometry facility will also be connected to the recovery system, as will other groups utilizing liquid helium such as Arthur Mar's and John Klassen's laboratories. Extension of the system will also include the new CCIS building, though there is presently no schedule for that portion of the project.

# i300 upgrade

The Inova 300 NMR spectrometer (circa 1997) located in SB-3E is scheduled for replacement. Starting March 8<sup>th</sup> the magnet will be de-energized and the system removed preparing for the new spectrometer on March 15<sup>th</sup>. The new system is scheduled to enter service April 29<sup>th</sup>. Special thanks to: Todd Lowry for spearheading the initiative, and the Alberta Glycomics Centre, and the Department of Chemistry for making this much needed upgrade possible. The final preparatory steps are detailed below.

## Rerouting of Airlines



In order to prepare for the new system requirements, there will be a disruption to the i600, i300, and i400 high pressure and low pressure air lines on [February 11<sup>th</sup>](#). High pressure airlines will need to be re-routed from SB-3F (600 room) into SB-3E (300 and 400 room).

The re-routing of airlines should only take a day, but will require pressurized air shutdown for all 3 instruments and therefore the spectrometers will not be available for use during this time.

## De-Energization of i300 Magnet

The de-energization of the 300 is scheduled for [March 8<sup>th</sup>](#) so that we have time to then warm and remove the spectrometer, and clean the room in anticipation of the installation the following week.

The de-energization should not disrupt i600 access but will prevent access for the day to the i400 for safety reasons.

Our commercial clients normally utilizing the i300 and i400 in the early morning hours have been tentatively rescheduled for i400 access: [March 8 to April 29](#) - Mon 7-9 am, Tue 7-11 am, Wed 7-9 am, Thu 7-10 am, Fri, 7-10 am, and Sat 8-9 am.

Please let us know if you have any concerns and we will work to make other instruments available, or re-schedule if major issues arise.



## Installation of mr400

The new spectrometer is scheduled for installation on March 15<sup>th</sup>. The instrument will need to be unpacked (elevator limits can't accommodate the entire shipment), moved to the room, assembled and energized. The new spectrometer will take approximately a week to settle after energization. The shims will then be mapped, and extensive console acceptance testing begun. We are hoping to have the instrument fully online by the end of April. We will attempt to keep the instrument booking schedule updated to indicate when access to the i400 may be restricted during the installation and when the new instrument is ready for use.

Should anyone be interested in the cooling and energization process please let the NMR staff know so that we can organize time for safe size limited groups to observe the processes.



# Additional News

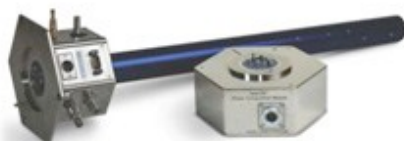
## Spectrometer Selection Process

The selection process involved many people from Supply Management Services (SMS), the Department of Chemistry, and the NMR facility. Initially both major vendors were asked to submit proposals for a spectrometer console and probe upgrade, however 7 Tesla (300 MHz) spectrometers are relatively rare today making the request excessively expensive to support a 16 year old magnet (magnet life spans are typically 20-30 years). The cost of a new 9.4 Tesla (400 MHz) magnet, console, and probe proved to be a far more cost effective/long term purchase. A scoring system was devised based on factors such as price, performance, space requirements, shipping dates, warranty, etc. and applied to full proposals from major NMR vendors. Several instrument configurations and packages were offered, but one in particular substantially stood out based on performance. The 400 MHz DD2 Agilent Spectrometer equipped with "One-Probe" and the automated ProTune was by far the best option.



## Agilent One-Probe and ProTune

The Agilent One-Probe specifications were substantially better than all other proposed spectrometer configurations. This particular NMR probe has the advantage of excellent  $^{13}\text{C}$  signal detection while maintaining the  $^1\text{H}$  sensitivity. The improvements over the i300 include a 4.5 fold increase in  $^1\text{H}$  sensitivity, and nearly a 17 fold increase in  $^{13}\text{C}$  detection. Other nuclei such as  $^{19}\text{F}$ ,  $^2\text{H}$ , and  $^{31}\text{P}$  down to  $^{15}\text{N}$  are also included with excellent performance.



The ProTune module allows for rapid and automatic tuning/matching of the system to whatever nuclei is desired without the requirement for cable changes, exchange of tuning rods, or manual alteration of

the probe circuitry. Several ProTune modules are presently in use on other instruments. Together these components will result in an extremely efficient and robust "work-horse" ready for the many NMR challenges users will encounter.

## Replacement of 700 MHz NMR

The 700 MHz magnet is scheduled for replacement early this spring and the new magnet has already arrived on campus (the new magnet is in storage at shipping and receiving). The present 16.4T magnet was discovered to have an unstable cryogenically cooled z1-shim. While this shim can be temporarily compensated by the user with the room temperature z1 shim, long term experiments suffer from signal degradation over time. In addition, as the cryo-shim moves it will eventually exceed the compensation capacity of the room-temperature shim. Agilent has agreed to replace the



magnet free of charge to the department and we are presently awaiting a large enough liquid helium supply to begin the installation.

## New NMR Website



We are in the process of switching the existing NMR website over to the university standard content management system (CMS). The CMS provides a standardized format for presenting university based information, media, documents, and links. This not only provides a common professional look and feel to the website, but also dramatically simplifies how the information is entered into the website itself for presentation to the site visitors. There is less need for explicit familiarity of coding using HTML, and secure remote access to the server, The primary advantage is the increased efficiency for updating existing content on typically static pages.

In addition, forms can easily be created making tracking necessary information far more efficient. We are planning on first using the forms for outside department sample submissions.

The university uses a web browser based system called Proshop or Site-Core to build and populate the webpage content, and most other faculty pages have either already been switched over or in the process of being converted. We will keep you posted as the new site develops and will send out links later for beta-testing. If you have suggestions on additional content for the new site please let us know so that we can incorporate suggestions early on.

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## NMR Service Contact information:

Ryan McKay - NMR Facility Supervisor (E3-17A) Office: (780) 492-9950

[ryan.mckay@ualberta.ca](mailto:ryan.mckay@ualberta.ca)

Mark Miskolzie - Spectroscopist (WB-13) Office: (780) 492-2573

[mark.miskolzie@ualberta.ca](mailto:mark.miskolzie@ualberta.ca)

Nupur Dabral - Spectroscopist (WB-13) Office: (780) 492-2573

[nupur.drabal@ualberta.ca](mailto:nupur.drabal@ualberta.ca)