NMR Safety Guidelines

Compliance with these rules is required in the NMR Facility!

WARNING

Accidents caused by carelessness near strong magnetic fields can cause serious injury or death and significant damage to personal property, equipment and data

1. **Individuals with medical devices that can be disrupted by magnetic or radio fields (e.g. cardiac pacemakers and metal prostheses) must remain outside the 5-gauss perimeter.**
2. **In the event of a "magnet quench" (a sudden, violent release of cold helium gas from the magnet), evacuate the facility immediately, and contact NMR personnel.**
3. **Ferromagnetic metal objects must remain outside the 5-gauss perimeter, marked on the floor around each magnet.** This includes most ordinary tools, electronic equipment, compressed gas cylinders, steel chairs, and steel carts. Only non-ferromagnetic materials should be used near the instruments.
4. **Do not look directly down the upper barrel of an NMR spectrometer while trying to eject the sample.** Refer any problems with sample ejection to facility staff.
5. **Do not exceed the boiling or freezing points of your sample; approach these temperatures cautiously, as the instrument may overshoot the selected temperature or the temperature display may be somewhat inaccurate. This can cause excessive pressure to build up and break the tube.**
6. **If you have a sample that is expected to have or generate internal pressure, test all operations with it in a hood and with suitable safety equipment before inserting it into an instrument. Cold samples will warm up significantly while they are being inserted into the instrument, even if the probe is precooled.**
7. **Keep your hands out of the path of the robotic arm of the SMS sample changers.** Broken NMR tubes and cuts to your hands could result.
8. **Wipe down NMR tubes and spinners with a Kimwipe before they go in the magnet and <u>after</u> you remove any lab gloves you have worn from your own lab. Don't wear lab gloves while handling spinner turbines or typing on shared keyboards.**
9. **Don't pipet or mix chemical solutions on the computer work tables—use the fume hood.** Lab gloves and eye protection should be worn for those operations, but remove the gloves before returning to the spectrometer.
10. **Cards with magnetic strips, cellular phones, laptops and mechanical watches should remain outside the 5-gauss perimeter.** Strong magnetic fields surrounding the NMR spectrometers can damage the strip of magnetic media found on credit cards, ATM cards, driver's licenses, and other kinds of cards, disk drives, and other susceptible devices.

I have received a copy of these safety guidelines, read them, and will abide by them.

Name of Facility User: _____ Date: _____

IMSS Username: _____ PTA #: _____

Email Address: _____ Advisor's name: _____

Status: Postdoc____ Graduate Student____ Special Student/Visitor____ Other_____

Undergraduate, here this summer only: ____ or continuing Caltech student: ____

I have trained the above user in the proper use of the facility instruments and proper safety guidelines.

Name of GLA: _____ Instrument: _____ Date: _____ Account made: _____

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Working with the SMS robots on hg3 and indy

- These robots only handle standard 8" tubes with caps—no other types. Tubes with broken or cracked ends should never be used. If you want to wait until you get to the NMR room to decide which instrument to use, prepare the sample in an 8" tube, or you have already decided not to use indy or hg3. You can use 8" tubes on any instrument and 7" tubes anywhere except indy and hg3.
- Some tubes are especially likely to break as the SMS robot arm handles them, Kontes NMR tubes in particular. You can buy these tubes for use on the other spectrometers, but avoid them with indy and hg3. Norell tubes are quite robust. Disposable Wilmad WG-1000 tubes are more likely to break than Norell tubes, but they are less breakable than Kontes tubes.
- Watch out for tubes which are loosely fitting in the spinner turbine, as the robot arm can pull them partly or completely out of the spinner. This could be from an undersize tube, or a spinner with a worn o-ring. If you find a spinner with an o-ring problem or there's broken glass in it, set it by the sink in the NMR room.
- Each instrument has a specific height for the sample in the depth gauge; these are slightly different on indy and hg3. If the sample gets picked up and put back by the robot, the tube height will probably change. If you want to put a sample back in the queue for additional experiments, recheck the tube position. If you want to use a liquid height in the tube which is shorter than recommended, this is up to you; spectrum quality may suffer. If you do this, pull the sample up in the spinner to center the liquid column around the probe center. **Do not reset the sample depth gauge, just your individual sample.**
- Make sure you are putting your sample in the numbered chute in the rack that the software tells you to use. The chutes are somewhat strangely numbered from the right side. It is very important not to put any sample into the rack in the position belonging to the sample coming out of the magnet. This could cause a collision between the samples, break one or both tubes, and even damage the robot.
- If you decide to resubmit a sample for additional experiments, move it to the new location assigned by software, but at the same time, re-check the sample height in the spinner. The robot will often push the sample tube down in the spinner as it replaces the spinner in the sample tray.
- Avoid using large gobs of parafilm around tube caps or any kind of tape where there is a sticky surface facing out towards the robot gripper fingers. The gripper fingers need to let go of the sample cleanly in order to put it first in the magnet and then back into the tray. Damage to the sample or robot may result from the sample remaining stuck to the gripper fingers.
- If a collision or any other robot malfunction occurs, **immediately press the red panic button connected to the robot.** Then get assistance from Dave or from a GLA.

Working with the other users of the instrument

- The VnmrJ software will not allow you to submit experiments lasting more than an hour during the day queue. However we also expect that you won't string several long experiments together in a row (even though the software won't stop you from doing this). If you use indy for an hour during the day, you can use it again later the same day, but allow at least one hour before you submit anything else. On hg3, keep your usage down to about half an hour at one time.
- Unless you have a very concentrated sample, don't do ^{13}C NMR on hg3. It's very slow compared to other instrument choices including indy, and it just slows down the queue for everyone else.
- Experiments which would keep the instrument running for hours at a time should be put in the night queue. The night queue is the only time you need to make an advance reservation to use the instrument (using the webcal scheduling software). The night queue hours are 11:30 pm to 8 am on indy.
- If you remove someone else's NMR tube from a spinner, put that tube in the appropriate position in the sample rack where the other user can find it, just like you want other people to treat your samples. For very valuable samples, the sooner you retrieve them from the instrument, the better.

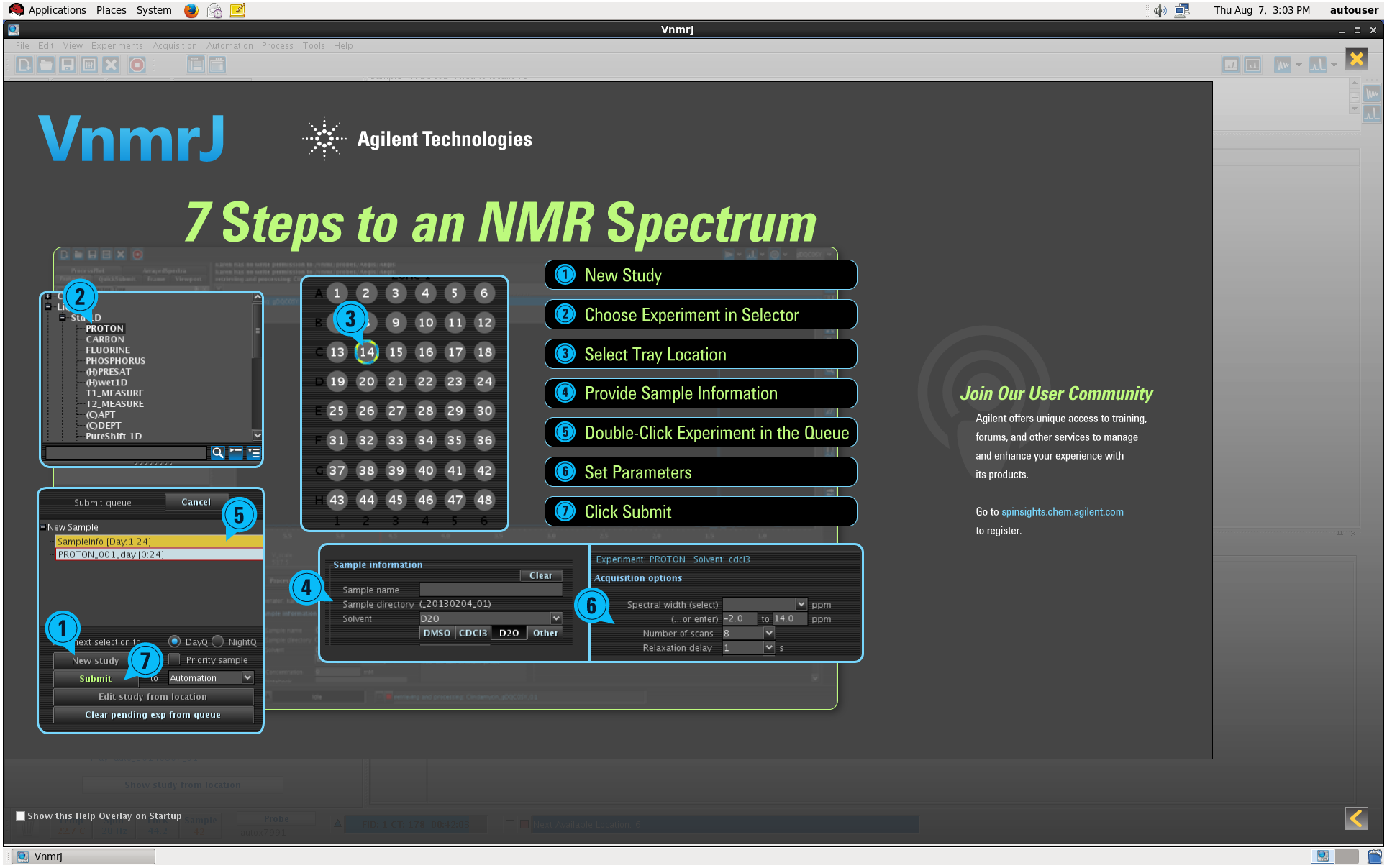
Choosing experiments

- VnmrJ has a standard list of experiments which looks the same on every instrument. Not all of them work, or work well, on every instrument. Indy does ^{1}H, ^{13}C, and their 2D combinations only, no other X nuclei. Hg3 does ^{1}H, ^{13}C, ^{19}F, and ^{31}P, and is mostly intended for 1D spectra.
- The Common tab on each instrument shows the top eight or so experiments done on that instrument. The rest of the VnmrJ experiment library (about 80 experiments total) is available through the Liquids tab and its submenus. Refer to the VnmrJ experiments guide (PDF or printed version) for more information.

Submitting a sample

- Refer to the Agilent graphic "7 Steps to an NMR Spectrum."
- As you complete the 7 steps, pay attention to the software's response and wait for it to complete one step before moving to the next one. You can't make it go faster by clicking faster, but you can lock up the software that way, which will slow you down.
- Use your software assigned chute number. These numbers reset with the first user who arrives after 8 am each day. This could cause the splash screen to display a high number at first, which reverts back to 1. In this case, not using location 1 will lead to an error.
- Avoid using spaces or special characters in sample names, or re-using a name that only differs from an old name in capitalization. The network drives won't be able to distinguish the difference in capitalization.
- You need to log in on the VnmrJ splash screen, and click the logout button within VnmrJ to return to that screen. If you don't close that out, you are inviting other people to run their samples as you, at your expense. Do not entirely close VnmrJ or log out of the Linux desktop, as you won't be able to get back in.
- Before the robot puts the sample into the magnet, you can right click the circle for that sample and edit any of the sample information, add or modify experiments, etc. You must resubmit the sample to the same location in order for your edits to take effect.
- If the sample has already been placed in the magnet, and the experiments are started, your choices are to let it proceed as submitted or to abort the acquisition.

10/19/17


Applications Places System
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VnmrJ
File Edit View Experiments Acquisition Automation Process Tools Help
VnmrJ
Agilent Technologies
7 Steps to an NMR Spectrum
1 New Study
2 Choose Experiment in Selector
3 Select Tray Location
4 Provide Sample Information
5 Double-Click Experiment in the Queue
6 Set Parameters
7 Click Submit
PROTON
CARBON
FLUORINE
PHOSPHORUS
(H)PRESAT
(H)wet1D
T1_MEASURE
T2_MEASURE
(C)APT
(C)DEPT
PureShift 1D
Submit queue
Cancel
New Sample
SampleInfo [Day:1:24]
PROTON_001_day [0:24]
New study
Priority sample
Submit
Automation
Edit study from location
Clear pending exp from queue
Sample information
Clear
Sample name
Sample directory (_20130204_01)
Solvent
D2O
DMSO CDCl3 D2O Other
Experiment: PROTON Solvent: cdcl3
Acquisition options
Spectral width (select)
(...or enter) -2.0 to 14.0 ppm
Number of scans 8
Relaxation delay 1 s
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