

Chem NMR Facility – Fire Sprinkler Project

Changeover to 500s and 600 on Sunday Oct 25 at 1pm

→ continuing through Nov 8

I. Choosing the correct spectrometer

NMR staff will not have the time to choose spectrometers for you for the wide variety of samples heading toward us during this stage of operations. **Please think carefully, based on the information provided below, about which spectrometer you choose to submit your samples to.**

- **Callisto 500:** has the best ^{13}C sensitivity ($\sim 150\times$ faster than 400s) and very good ^1H sensitivity. ^1H and ^{13}C only.
- **Phoebe 600:** has the best ^1H sensitivity ($\sim 300\times$ faster than 400s) and very good ^{13}C sensitivity (about $4\times$ slower than callisto). ^1H and ^{13}C only.
- **Persephone 500:** has a broadband probe installed, with sensitivity a bit better but overall fairly similar to the 400s
 - use for all nuclei other than ^1H and ^{13}C , such as ^{19}F and ^{31}P
 - use for any sample that is strongly paramagnetic
 - use for any sample that has high (>9) or low (<5) pH
 - use for any sample that has high ($>100\text{mM}$) salt content

→ There will be little tolerance for users that submit samples to callisto that cause ATM (automatic tuning) errors. Samples that are strong paramagnetic, have “odd” pH, or high salt may do this. Such ATM errors stop the queue, and are difficult to correct. Submit samples that cause the problem twice and we’ll stop running your samples on callisto and phoebe during this portion of the fire sprinkler project. **If your sample is “odd”, submit it to persephone.**

→ Samples that are too concentrated ($> 30 \text{ mM}$) will have degraded ^1H resolution on callisto and phoebe. The simplest thing to do is to dilute the sample for the ^1H sample submission.

→ NMR staff may modify spectrometer selections. In particular, if callisto gets too busy, we may move samples to the 600, and vice versa.

→ See next for a new 6 sample submission limit for this phase of operation.

II. Robots controlling automation: sample submission limits

- The 400s have 600 sample positions available on each of them.
- The 500s+600 have 100 sample positions *total* available between them.

Persephone 500: 24 sample SampleCase robot
Callisto 500: 60 sample SampleXpress robot
Phoebe 600: 24 sample SampleCase robot

- So the number of samples at any one time is at a premium:
 - **submit a maximum of 6 samples per spreadsheet and container:**
i.e., each set of ≤ 6 samples must have their own container and associated spreadsheet
 - any user can submit multiple 6 sample spreadsheets+containers, but turn-around will be slowed after the 1st set

- **7" tubes only!**

- Any cap style is OK

→ Submissions with more than 6 samples, or with 4" tubes, will be returned to the user to be corrected and resubmitted.

→ *What happens if a user submits 18 samples in three batches, using 3 containers and 3 spreadsheets?*
We will prioritize the first batch of 6 samples, and get them onto the appropriate spectrometer as quickly as possible. If the robots are more than half full, the 2nd batch of 6 samples will wait until the first batch is finished before we will submit them. And the 3rd batch will wait for the 2nd batch to finish.

III. Queues and data archiving

- Queues for persephone, callisto and phoebe are available on the Chem NMR website at:
<https://nmr.chem.wisc.edu/spectrometer-calendars/>
- Users must track their sample submissions themselves. Note that NMR staff may move samples from the requested spectrometer, depending on how busy the queues are. We will not inform you about this: please interrogate all three queues before asking us about your samples.
- With the 400s, the spectrometers are nearly identical and provide nearly identical data quality. So during the earlier phase of the fire sprinkler project, all data was placed into the av400 folder, even if run on eos.

For the two 500s and the 600, various aspects of the data will be changed depending on the spectrometer used. So all data during this phase of operations will be archived to the spectrometer the sample was run on: i.e., data will end up in

`/castor/username/public_html/persephone`
or `/castor/username/public_html/callisto`
or `/castor/username/public_html/av600`