NOMAD Instructions

The Nuclear Magnetic Resonance (NMR) facility at the Molecular Sciences Research Hub (MSRH) is now using the NMR Online Management and Database (NOMAD). This transitions has taken place in collaboration with *Alchemy* and Tomas Lebl (University of St. Andrews).

This browser-based application allows users to set up experiments, access data remotely and process NMR spectra in *NMRium*. NOMAD is an open-source platform hosted on GitHub and operates using a virtual machine hosted by ICL. *NMRium* is a browser-based application for NMR data visualisation and processing.

MSRH NOMAD server: https://aichemy-nmr.ch.ic.ac.uk/dashboard

Users will need connect to the Imperial network to access the NOMAD server, either on-site or via VPN.

Getting Started

Contact Stuart Elliott (s.elliott@imperial.ac.uk) with your finance code to arrange an induction and account set up.

Once your account is active:

- Go to: **https://aichemy-nmr.ch.ic.ac.uk/dashboard**
- Click the user symbol in the top right corner, then click: Reset Password
- Your username will be your short email prefix with no capitals or spaces, *e.g.*, sje123
- An email will be sent with a password reset link (this may take a few minutes)

Once you have set up your account, you are ready to log in and submit experiments to the open access machines (A, B and C) as long as it is available (green). Use the options in the top right corner to submit experiments or access data.

Sample Submission

To see a demonstration, watch the NOMAD video at:
https://www.youtube.com/watch?v=SRDQqJkQFXc

- Go to: **https://aichemy-nmr.ch.ic.ac.uk/dashboard**
- Click the user button to log in
- Click Book New Job in the top right corner
- Select a spectrometer from the drop down list*
- Specify the number of samples to be submitted
- Click Book Slots

**Please note that the list of spectrometers is not currently in order.*

Scroll down to see the slots you have been allocated. Beside each, populate the Solvent, Title (sample name) and Experiment (parameter set) fields.

To run additional experiments, click the + symbol under ExpNo.

The run time for each experiment is shown under ExpT, with an estimated total experimental time for the sample (including sample changeover and setup) shown beneath.

When all the relevant fields are completed, click Continue to add these experiments to the Pending list.

The home screen will be shown. After a short delay, the submitted experiments will be visible in the Pending Holders list (yellow icon in top left). **At this stage you must load your samples into the autosampler.**

When your samples are loaded, open the Pending list and select your experiments, then click Submit. You may be asked to verify your password at this stage. After a short delay, your experiments will be submitted to the queue.

Data Retrieval

- Go to: **https://aichemy-nmr.ch.ic.ac.uk/dashboard**
- Click the user button to log in
- Click Datastore => Search Experiments (top right corner)
- Use the filters as needed, then click Search. Your level of access to your group's data will be determined by your group settings.
- Select the experiments you want. Click either Download (to save the raw data to your computer) or Open in NMRium (top of page) as desired. You can expand the folders as required to view individual experiments.
- If opened in NMRium, you can make changes (peak picking etc.) and use the save button (top of the page). You can also export images for publication and much more - see the NMRium tutorials for details.