**Document Title:**

# Chemistry NMR Access Guide

**Document No.:**

**6100-NMR-Guide**

## 1 Purpose

This guideline aims to provide users information how to access the Chemistry NMR managed by TrACEES platform, as well as data access and management.

## 2 Access

### 2.1 Access steps

a. New users submit Training request (section 2.5).
b. Users get trained.
c. Users' accounts will be created (section 2.6).
d. Users request access to share drive (section 4).
e. Users access and operate NMR.

### 2.2 Access time

Bookings are not required. However, there are several limitations.

| | | |
|---|---|---|
| Day | 8:00 - 19:00 | Each experiment <10 min, Max 1 hour per user |
| Night | 19:00 - 8:00 (next day) | Each experiment <3 hrs, max 6 hours per user |
| Weekend | Sat - Sun | Same as night operation |

### 2.3 Experiment

| | |
|---|---|
| Standard | 1H, 13C, 19F, 35Cl, 11B, 31P |
| Allowable | 13C DEPT135, COSY, HMBC, HSQC |
| Others | Request Bio21 NMR facility |

Experiment will be setup through ICON software. Instruction is provided in a separate document.

### 2.4 Samples and tubes

| | |
|---|---|
| NMR tube | 7 inch only |
| Solution height | Min. 4cm |
| Coloured cap | • Each group will use own coloured cap<br>• Labels are up to individual group |

### 2.5 Training

| | |
|---|---|
| Training request | Training request shall be submitted through TrACEES iLab NMR training request form.<br>https://unimelb.ilab.agilent.com/service_center/show_external/4561/melbourne_tracees_platform<br>under "Equipment booking" - > Chemistry node -> NMR -> Initiate |
| Frequency: | At the beginning of each semester, and upon request at other times |
| What involved | Induction, OHS, cleaning tubes and house keeping |
| Instructor | Dr Alex Duan, Dr Milena Czyz |
| Trainee | School of Chemistry and Chemical Engineering researchers or students who access NMR in a daily basis.<br>Note: Training is not required for postdoc and/or senior researchers with previous Bruker NMR and ICON experiences |

### 2.6 NMR ICON Account

At the completion of the training, the user's ICON account will be created.
Username: [Surname][initial of first name] (e.g. **smithj** for John Smith)
Temporary password: 1234

***How to change user's password***

In ICON window, go to "Options" (menu tab) -> change additional user password -> Enter "1234" then enter new password and again.

## 3 House keeping

Users shall keep PC desk clean and free of any NMR tubes.
All spinners, sample tubes shall be kept at the workstation. Workstation is the area users can insert samples tube into spinners, adjust tube height and find completed sample tubes.

| | | |
|---|---|---|
| NMR tube collection | Day operation | By the end of the day |
| | Night operation | By 10am of the next day |
| | No collection by end of the week | Group will be charged |

## 4 Data management and transfer

**Important:**

**USB is NOT allowed** to transfer data or files at any time.

Users are not permitted (unless approved) to use NMR PC to process their data.

Please refer to ***Management of Research Data and Records Policy (MPF1242)***.

### 4.1 Results and data

- At the completion of each experiment, the user will receive results (*.pdf) via email.
- All NMR data are stored in the University's share drive \\research-cifs.unimelb.edu.au\6100-nmr
- Request to access the share drive shall be submitted through the following link: http://go.unimelb.edu.au/eek6

### 4.2 Data processing software

Users who would like to further process their data shall copy and paste the data to own local hard drive.
TopSpin software can be downloaded at Bruker's website.
Academic license is free for any university staff and students. Other software may also work. Please consult senior member in your group.

## 5 Acknowledgement

Users shall acknowledge Melbourne TrACEES Platform for the technical support in their publications.

## 6 Version Control

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|---|---|
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