NMR@CHEM.OX

Chemistry Research Laboratory

NMR Spectroscopy Facility Introductory Lecture

Dr Nick Rees
&
Dr Harry Mackenzie

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https://nmr.chem.ox.ac.uk/

Introductory Lecture

- NMR Facility Staff
- Magnet Hazards and Safety
- Sample Preparation
- Data Processing
- Facilities and Instrumentation
  - Open Access Facilities
  - NMR Submission Service
- Online Resources: NMR web site
- Future training courses

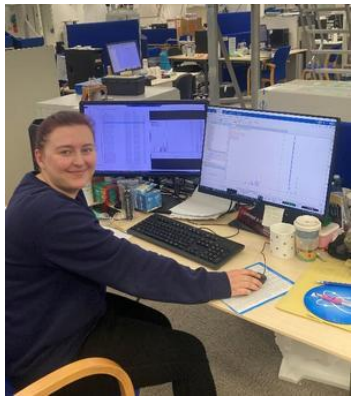
1. NMR Staff (2023)

- Facility Director:
  - Dr Nick Rees
- Service Manager:
  - Dr Coral Mycroft
- Research Technician:
  - Caitlin Salter
- NMR Officer:
  - Charlie Prentice

nmrstaff@maillist.chem.ox.ac.uk

Nick

Caitlin



Coral

Charlie

1. NMR Staff (2024)

- Head of Inorganic and Solid State NMR:
  - Dr Nick Rees
- Head of Organic and Biological NMR:
  - Dr Harry Mackenzie
- Service Manager:
  - Dr Coral Mycroft
- Research Technician:
  - Caitlin Salter

nmrstaff@maillist.chem.ox.ac.uk

Nick

Harry

Coral

Caitlin

Former NMR Staff

- Prof Tim Claridge

- Maria Marshall

- James Montgomery

- Charlotte Prentice

2. Safety in the NMR laboratories

- Very Strong Magnetic Fields!
- Hazards to:
  - heart pacemakers
  - magnetic bank or ID cards
  - watches (non-LCD)
- Stray fields in corridors!
  - especially ground floor NMR

Safety Rules

- No laboratory coats in NMR labs
- No metal objects to be taken into NMR labs
- Sample breakages must be dealt with immediately
  - Inform the NMR staff if in any doubt

Accessibility in the NMR laboratories

- If you require any assistance or adjustments in relation to training and/or using this facility or if you have any concerns you would like to discuss beforehand, contact

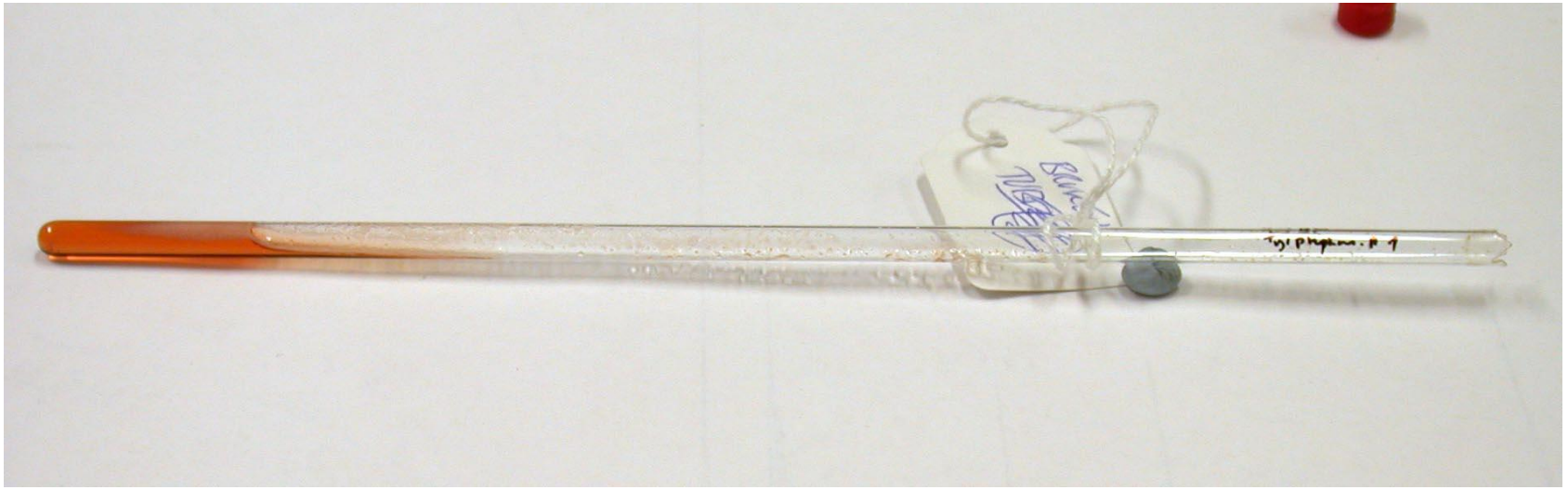
nick.rees@chem.ox.ac.uk

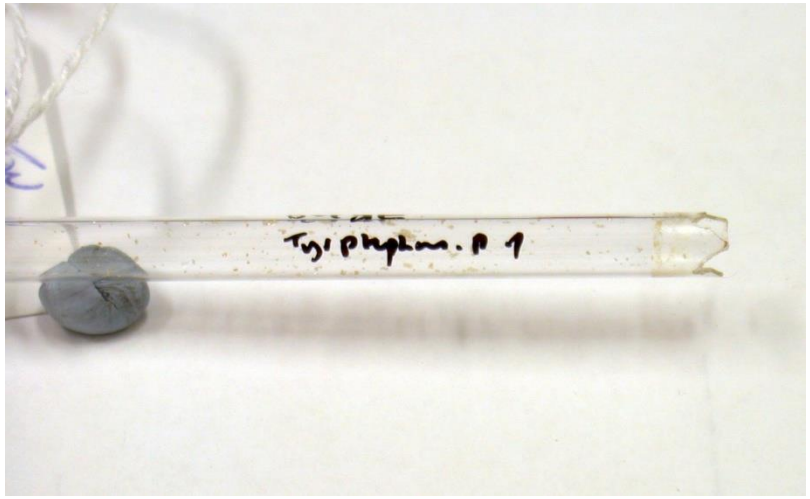
or

harry.mackenzie@chem.ox.ac.uk

3. Sample Preparation

- Tubes and *deuterated* solvents from stores
- Tubes must be “Wilmad 507” or “Norell S400” grade (or equivalent) at least
- Tubes must not be scratched or broken
- Label tubes very carefully (see future slide)
- Solutions must be correct depth (4 – 4.5 cm)
- Solutions must be free from particulates





3. Sample Preparation

- Tubes and *deuterated* solvents from stores
- Tubes must be “Wilmad 507” or “Norell S400” grade (or equivalent) at least
- Tubes must not be scratched or broken
- Label tubes very carefully
- Solutions must be correct depth (4 cm)
- Solutions must be free from particulates
- Dry tubes carefully; acetone rinse then:
  - Leave on vacuum line for some hours
  - Lay flat in oven, 1 hour @ 100 ^{o}C max

NMR Cap Colour and Tube Labelling Rules

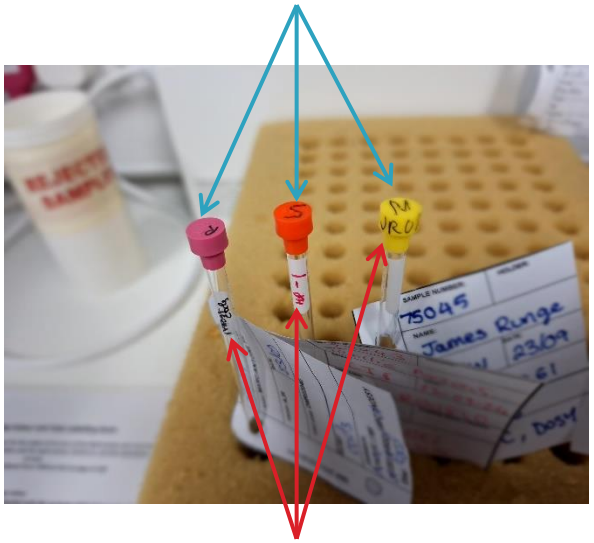
- The following rules are in place for the safety of all users of the NMR facility and must be followed. This includes NMR tubes used for open-access, hands-on, and the submission service.
  - Tube caps may be ordered from VWR on R12 as bags of 100.
- Rules:

- All groups must use their group cap colour
- The top of the cap must be clearly labelled with the surname initial of your group's academic
- Your own name/initials must be clearly labelled on the tube
- The solvent used must be clearly labelled on the tube
- If you are using a J Young's tube, you may use any colour cap but the full group initials must be written on, as well as the other above information

NMR Tube Cap Colours for Organic Chemistry and Chemical Biology groups

Research Group	Colour	Initial
E. A. Anderson	White	A
H. L. Anderson	Sky	A
H. Bayley	Pink	B
T. Brown	Blue	B
J. W. Burton	Yellow	B
S. J. Conway	Aqua	C
D. J. Dixon	Black	D
T. J. Donohoe	Purple	D
S. P. Fletcher	Sky	F
V. Gouverneur	Pink	G
I. McCulloch	Red	M
F. Probert	Purple	P
Y. Qing	Yellow	Q
P. Rabe	Red	R
J. Robertson	Orange	R
A. J. Russell	Fuchsia	R
C. J. Schofield	Orange	S
M. D. Smith	Blue	S
M. C. Willis	Aqua	W

Cap colour & Supervisor Initial

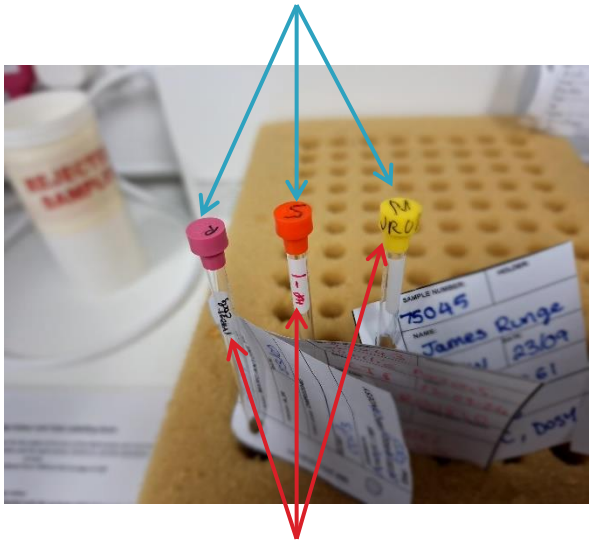


User Initials

NMR Tube Cap Colours for Inorganic Chemistry groups

Inorganic Group	Colour	Initial
S. Aldridge	Red	A
P. D. Beer	Sky	B
J. J. Davis	Blue	D
S. Faulkner	Red	F
J. M. Goicoechea	Aqua	G
G. L. Gregory	Fuchsia	G
M. J. Langton	White	L
M. Mehta	Orange	M
M. Neidig	Pink	N
D. O'Hare	Green	O
E. Tsang	Blue	T
K. Vincent	Purple	V
C. K. Williams	Yellow	W
L. L. Wong	Green	W

Cap colour & Supervisor Initial



User Initials

Sample masses required

- Rule of thumb for high-quality spectra (***minimum***):
- 400 MHz Open-access spectrometers:
  - Proton & 2D COSY: 2 mgs
  - 2D H-C HSQC: 10 mgs
  - 1D Carbon: 20 mgs
- Please weigh your samples!!

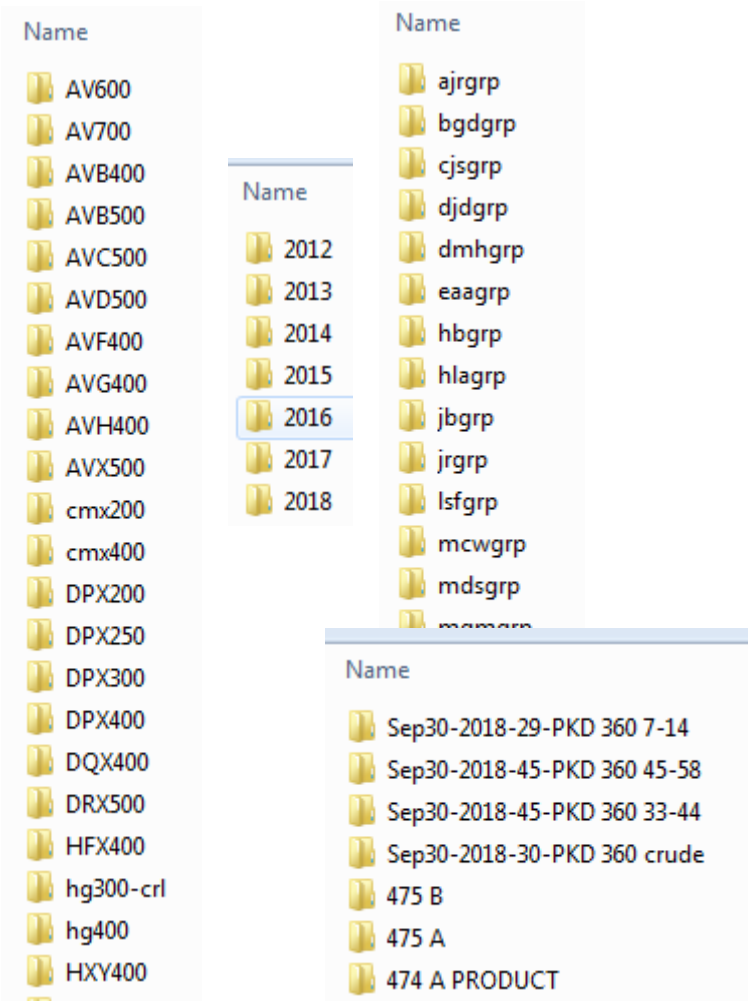
How much is 10 mg?

NMR tube cap
Glycine Camphor $CuSO_4$

4. Data Processing & Storage

- Data from all spectrometers can be downloaded *ONLY* from the on-line archive for off-line processing and local storage

- NMR Store & archive:
  - Chemistry domain file sharing:
  - \\chem.ox.ac.uk\SRF\NMR
  - Macs:
  - smb://chem.ox.ac.uk/SRF/NMR



Data Processing Software

- Windows and Macs:
  - **MestreNova:** 1D and 2D processing; platform independent
    - Chemistry site licence

- Windows and Macs:
  - **TOPSPIN**: Used on all spectrometers, 1D/2D NMR processing;
    - Free for academic use

Software installation

- Departmental PCs and Laptops:
  - **MestreNova**: Download latest version from Mestrelabs website. Copy and install licence from NMR server (\\chem.ox.ac.uk\SRF\NMR\NMR Software\Mnova\)
  - www.mestrelab.com
  - **Topspin**: Download from Bruker site and request licence:
  - https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html

5. How to use the facilities

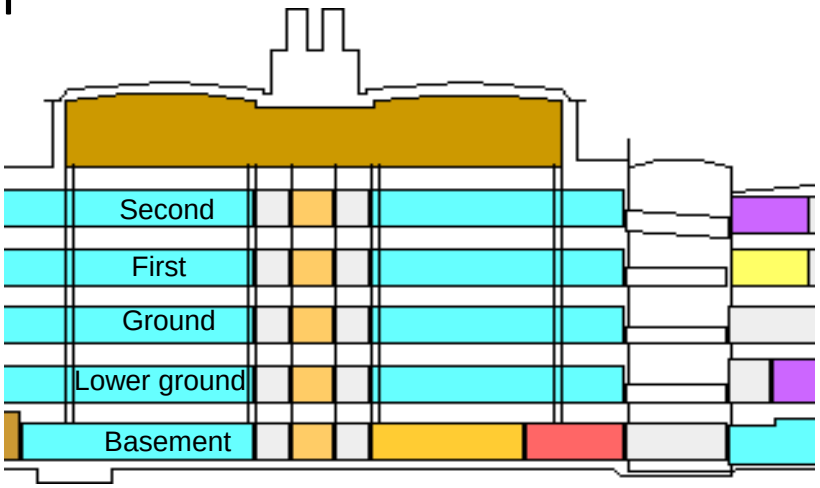
- Facilities operate at 4 levels:
  - "open-access": automated instruments for all to use
  - "hands-on": manual use of instruments for specifically trained users
  - "submission service": analytical service provided by the NMR staff
  - "research projects": collaborative projects involving the NMR staff/group

NMR in CRL

[Instrument nicknames shown]

Organic/Chem Biol Section

Inorganic Section



DPX200, AVF400
AVG400, AVH400

None

AVB400, AVB500, AVX500, NEO600, AV600, AV700

Venus400 +Mercury400

AVD500, Solids [HFX400 and HXY400]

Organic Chemistry and Chemical Biology

Instrumentation

- 10 research instruments @ 200-700 MHz
  - 1 @ 200 MHz: Open Access ^{1}H and ^{13}C
  - 3 @ 400 MHz: Open Access ^{1}H, ^{13}C, ^{19}F, ^{31}P & 2D
  - 1 @ 400 MHz: Hands on multinuclear and VT work
  - 2 @ 500 MHz: Hands on use & Service work
  - 1 @ 600 MHz: Service work (NEO)
  - 1 @ 600 MHz: Research projects & Service work
  - 1 @ 700 MHz: Research projects & Service work

Open access 200/400 MHz facilities

- Automated 200 and three 400s
- Provide rapid access to basic 1D & 2D ^{1}H and ^{13}C spectra, plus ^{19}F and ^{31}P
- Available to all research workers
- Spectra provided as PDF files and data on server

- Training ***must*** be given by a member of the Analytical staff:
  - Sessions will run Wednesday 2nd (pm), Thurs 3rd (pm) and Fri 4th (am): **Meet in CRL reception**
  - **Online booking and registration is required**

Automated AVIII400 [Ground Floor]

Known as the AVG400

^{1}H, ^{13}C, ^{19}F, ^{31}P
2D COSY
2D HSQC

file://chem.ox.ac.uk/SRF/NMR/AVG400/setup.html

Automated AVIII400 [Ground Floor]

Known as the AVH400

^{1}H, ^{13}C, ^{19}F & ^{31}P
2D COSY
2D HSQC

Faster for ^{1}H than AVF400 or AVG400

file://chem.ox.ac.uk/SRF/NMR/AVH400/setup.html

Automated AVIII 400 [1st Floor]

Known as the AVF400

^{1}H, ^{13}C, ^{19}F & ^{31}P
2D COSY
2D HSQC

Generally very busy- only submit experiments you are sure are essential!
Check ^{1}H only first

file://chem.ox.ac.uk/SRF/NMR/AVF400/setup.html

Semi-Automated DPX200 [1st Floor]

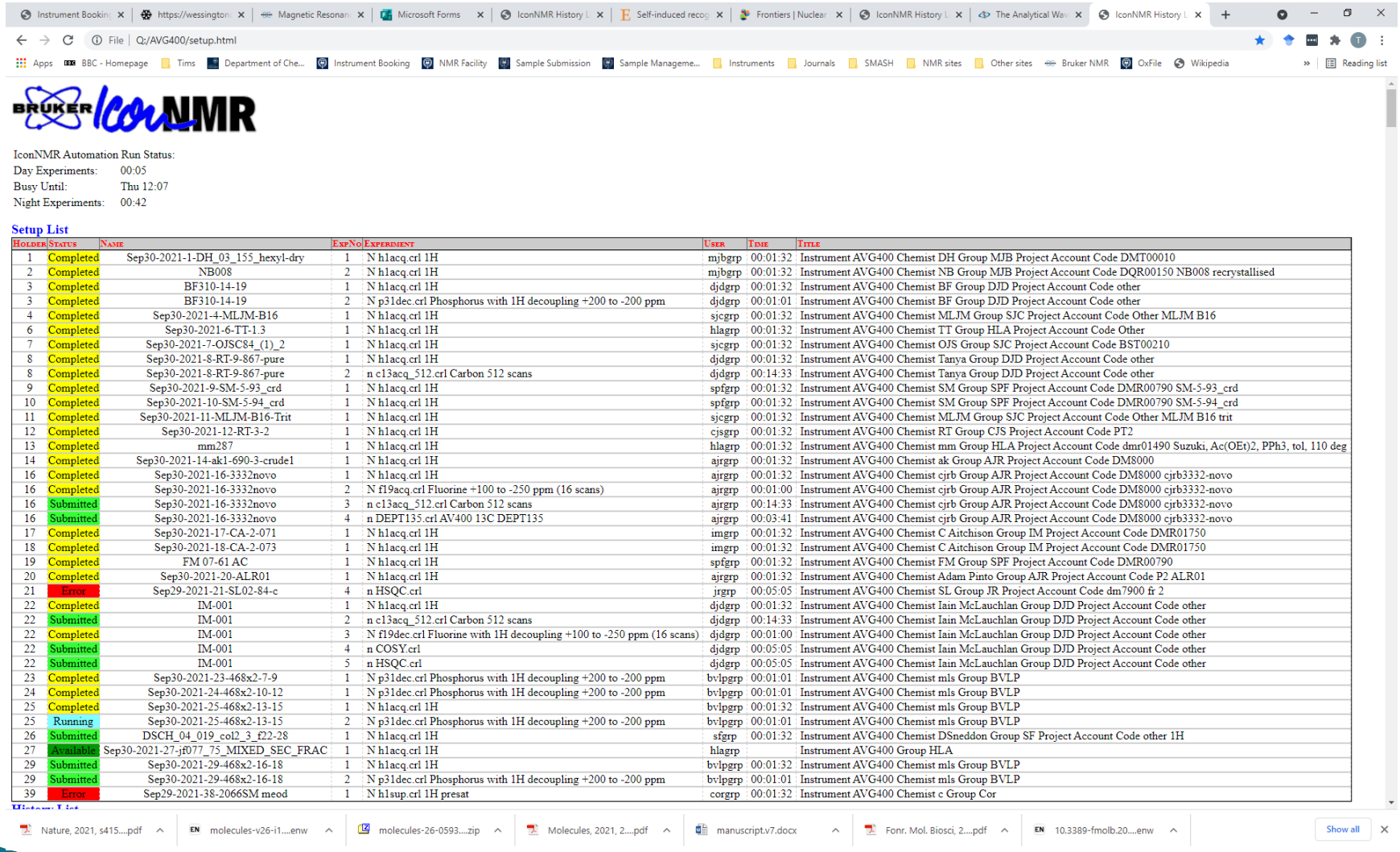
^{1}H NMR

Meant for fast ^{1}H screening- first come, first served.

No robot operation.

file://chem.ox.ac.uk/SRF/NMR/DPX200/setup.html

Instrument status web pages



BRUKER IconNMR

IconNMR Automation Run Status:

Day Experiments: 00:05

Busy Until: Thu 12:07

Night Experiments: 00:42

Setup List

Holder	Status	Name	ExpNo	Experiment	User	Time	Title
1	Completed	Sep30-2021-1-DH_03_155_hexyl-dry	1	N h1acq.crl 1H	mjbgrp	00:01:32	Instrument AVG400 Chemist DH Group MJB Project Account Code DMT00010
2	Completed	NB008	2	N h1acq.crl 1H	mjbgrp	00:01:32	Instrument AVG400 Chemist NB Group MJB Project Account Code DQR00150 NB008 recrystallised
3	Completed	BF310-14-19	1	N h1acq.crl 1H	djdgrp	00:01:32	Instrument AVG400 Chemist BF Group DJD Project Account Code other
3	Completed	BF310-14-19	2	N p31dec.crl Phosphorus with 1H decoupling +200 to -200 ppm	djdgrp	00:01:01	Instrument AVG400 Chemist BF Group DJD Project Account Code other
4	Completed	Sep30-2021-4-MLJM-B16	1	N h1acq.crl 1H	sjcgrp	00:01:32	Instrument AVG400 Chemist MLJM Group SJC Project Account Code Other MLJM B16
6	Completed	Sep30-2021-6-TT-1.3	1	N h1acq.crl 1H	hlagrp	00:01:32	Instrument AVG400 Chemist TT Group HLA Project Account Code Other
7	Completed	Sep30-2021-7-OJSC84_(1)_2	1	N h1acq.crl 1H	sjcgrp	00:01:32	Instrument AVG400 Chemist OJS Group SJC Project Account Code BST00210
8	Completed	Sep30-2021-8-RT-9-867-pure	1	N h1acq.crl 1H	djdgrp	00:01:32	Instrument AVG400 Chemist Tanya Group DJD Project Account Code other
8	Completed	Sep30-2021-8-RT-9-867-pure	2	n c13acq_512.crl Carbon 512 scans	djdgrp	00:14:33	Instrument AVG400 Chemist Tanya Group DJD Project Account Code other
9	Completed	Sep30-2021-9-SM-5-93_crd	1	N h1acq.crl 1H	spfgrp	00:01:32	Instrument AVG400 Chemist SM Group SPF Project Account Code DMR00790 SM-5-93_crd
10	Completed	Sep30-2021-10-SM-5-94_crd	1	N h1acq.crl 1H	spfgrp	00:01:32	Instrument AVG400 Chemist SM Group SPF Project Account Code DMR00790 SM-5-94_crd
11	Completed	Sep30-2021-11-MLJM-B16-Trit	1	N h1acq.crl 1H	sjcgrp	00:01:32	Instrument AVG400 Chemist MLJM Group SJC Project Account Code Other MLJM B16 trit
12	Completed	Sep30-2021-12-RT-3-2	1	N h1acq.crl 1H	cjsgrp	00:01:32	Instrument AVG400 Chemist RT Group CJS Project Account Code PT2
13	Completed	mm287	1	N h1acq.crl 1H	hlagrp	00:01:32	Instrument AVG400 Chemist mm Group HLA Project Account Code dmr01490 Suzuki, Ac(OEt)2, PPh3, tol, 110 deg
14	Completed	Sep30-2021-14-ak1-690-3-crude1	1	N h1acq.crl 1H	ajrgrp	00:01:32	Instrument AVG400 Chemist ak Group AJR Project Account Code DM8000
16	Completed	Sep30-2021-16-3332novo	1	N h1acq.crl 1H	ajrgrp	00:01:32	Instrument AVG400 Chemist cjrb Group AJR Project Account Code DM8000 cjrb3332-novo
16	Completed	Sep30-2021-16-3332novo	2	N f19acq.crl Fluorine +100 to -250 ppm (16 scans)	ajrgrp	00:01:00	Instrument AVG400 Chemist cjrb Group AJR Project Account Code DM8000 cjrb3332-novo
16	Submitted	Sep30-2021-16-3332novo	3	n c13acq_512.crl Carbon 512 scans	ajrgrp	00:14:33	Instrument AVG400 Chemist cjrb Group AJR Project Account Code DM8000 cjrb3332-novo
16	Submitted	Sep30-2021-16-3332novo	4	n DEPT135.crl AV400 13C DEPT135	ajrgrp	00:03:41	Instrument AVG400 Chemist cjrb Group AJR Project Account Code DM8000 cjrb3332-novo
17	Completed	Sep30-2021-17-CA-2-071	1	N h1acq.crl 1H	imgrp	00:01:32	Instrument AVG400 Chemist C Aitchison Group IM Project Account Code DMR01750
18	Completed	Sep30-2021-18-CA-2-073	1	N h1acq.crl 1H	imgrp	00:01:32	Instrument AVG400 Chemist C Aitchison Group IM Project Account Code DMR01750
19	Completed	FM 07-61 AC	1	N h1acq.crl 1H	spfgrp	00:01:32	Instrument AVG400 Chemist FM Group SPF Project Account Code DMR00790
20	Completed	Sep30-2021-20-ALR01	1	N h1acq.crl 1H	ajrgrp	00:01:32	Instrument AVG400 Chemist Adam Pinto Group AJR Project Account Code P2 ALR01
21	Error	Sep29-2021-21-SL02-84-c	4	n HSQC.crl	jrgrp	00:05:05	Instrument AVG400 Chemist SL Group JR Project Account Code dm7900 fr 2
22	Completed	IM-001	1	N h1acq.crl 1H	djdgrp	00:01:32	Instrument AVG400 Chemist Iain McLauchlan Group DJD Project Account Code other
22	Submitted	IM-001	2	n c13acq_512.crl Carbon 512 scans	djdgrp	00:14:33	Instrument AVG400 Chemist Iain McLauchlan Group DJD Project Account Code other
22	Completed	IM-001	3	N f19dec.crl Fluorine with 1H decoupling +100 to -250 ppm (16 scans)	djdgrp	00:01:00	Instrument AVG400 Chemist Iain McLauchlan Group DJD Project Account Code other
22	Submitted	IM-001	4	n COSY.crl	djdgrp	00:05:05	Instrument AVG400 Chemist Iain McLauchlan Group DJD Project Account Code other
22	Submitted	IM-001	5	n HSQC.crl	djdgrp	00:05:05	Instrument AVG400 Chemist Iain McLauchlan Group DJD Project Account Code other
23	Completed	Sep30-2021-23-468x2-7-9	1	N p31dec.crl Phosphorus with 1H decoupling +200 to -200 ppm	bvlpgrp	00:01:01	Instrument AVG400 Chemist mls Group BVLP
24	Completed	Sep30-2021-24-468x2-10-12	1	N p31dec.crl Phosphorus with 1H decoupling +200 to -200 ppm	bvlpgrp	00:01:01	Instrument AVG400 Chemist mls Group BVLP
25	Completed	Sep30-2021-25-468x2-13-15	1	N h1acq.crl 1H	bvlpgrp	00:01:32	Instrument AVG400 Chemist mls Group BVLP
25	Running	Sep30-2021-25-468x2-13-15	2	N p31dec.crl Phosphorus with 1H decoupling +200 to -200 ppm	bvlpgrp	00:01:01	Instrument AVG400 Chemist mls Group BVLP
26	Submitted	DSCH_04_019_col2_3_f22-28	1	N h1acq.crl 1H	sfgrp	00:01:32	Instrument AVG400 Chemist DSneddon Group SF Project Account Code other 1H
27	Available	Sep30-2021-27-jf077_75_MIXED_SEC_FRAC	1	N h1acq.crl 1H	hlagrp		Instrument AVG400 Group HLA
29	Submitted	Sep30-2021-29-468x2-16-18	1	N h1acq.crl 1H	bvlpgrp	00:01:32	Instrument AVG400 Chemist mls Group BVLP
29	Submitted	Sep30-2021-29-468x2-16-18	2	N p31dec.crl Phosphorus with 1H decoupling +200 to -200 ppm	bvlpgrp	00:01:01	Instrument AVG400 Chemist mls Group BVLP
39	Error	Sep29-2021-38-2066SM meod	1	N h1sup.crl 1H presat	corgrp	00:01:32	Instrument AVG400 Chemist c Group Cor

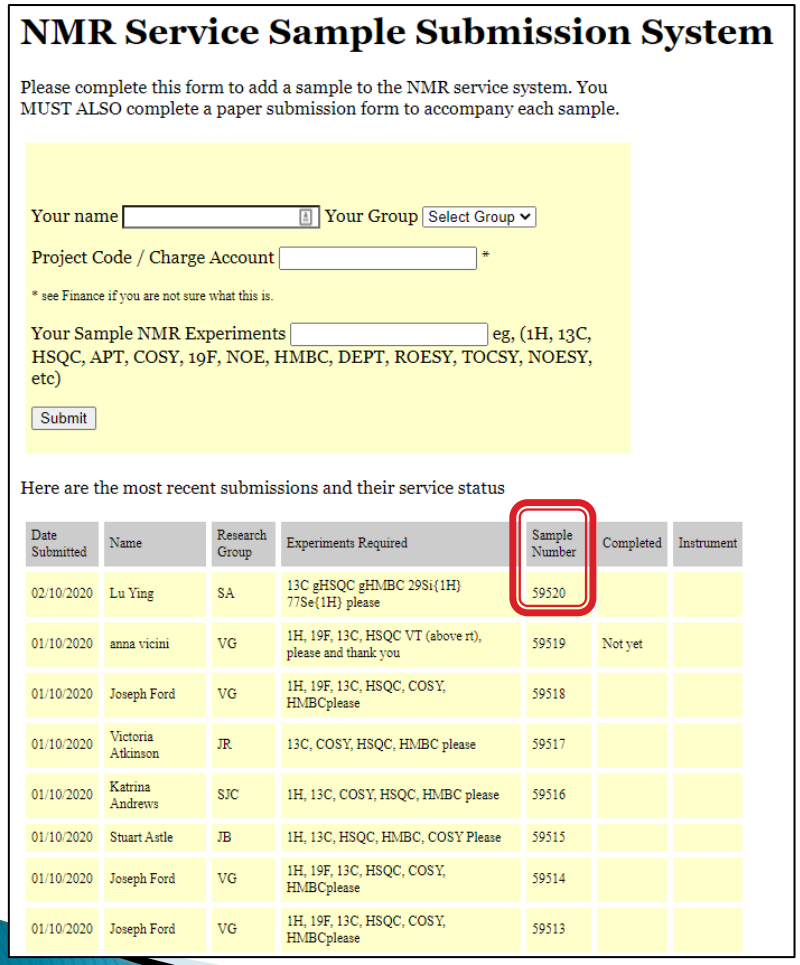
High-field facilities

- Basement high-field NMR lab
- 400 and 500 MHz instruments available for specifically trained users (“hands-on” use). 600/700 MHz for bio-projects
- Training must be given by NMR staff
- Please enquire with NMR Staff if you wish to be trained
- Online booking (intranet)- registration is required:
- https://nmr.chem.ox.ac.uk/hands

NMR Submission Service

- Many routine 1D and 2D ^{1}H, ^{13}C, ^{19}F, ^{31}P, & ^{11}B experiments can be performed using open-access 400 MHz
- Daily service provided by Dr Coral Mycroft and Caitlin Salter
- NMR Service uses 500 & 600 MHz instruments *not* 400
- Each sample must have electronic submission form (Word) and ^{1}H spectrum (PDF) *of same sample*

NMR on-line Submission



NMR Service Sample Submission System

Please complete this form to add a sample to the NMR service system. You MUST ALSO complete a paper submission form to accompany each sample.

Your name [ ] Your Group [Select Group]

Project Code / Charge Account [ ] *

* see Finance if you are not sure what this is.

Your Sample NMR Experiments [ ] eg, (1H, 13C, HSQC, APT, COSY, 19F, NOE, HMBC, DEPT, ROESY, TOCSY, NOESY, etc)

Submit

Here are the most recent submissions and their service status

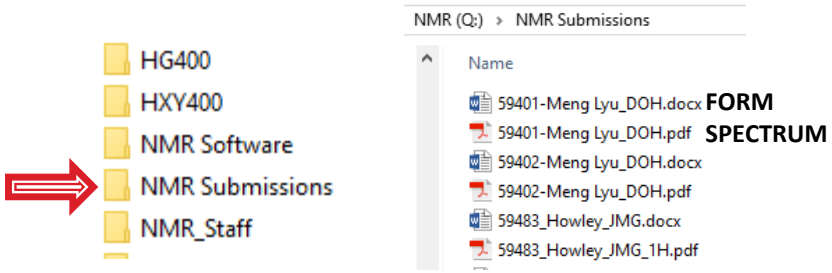
Date Submitted	Name	Research Group	Experiments Required	Sample Number	Completed	Instrument
02/10/2020	Lu Ying	SA	13C gHSQC gHMBC 29Si{1H} 77Se{1H} please	59520		
01/10/2020	anna vicini	VG	1H, 19F, 13C, HSQC VT (above rt), please and thank you	59519	Not yet	
01/10/2020	Joseph Ford	VG	1H, 19F, 13C, HSQC, COSY, HMBCplease	59518		
01/10/2020	Victoria Atkinson	JR	13C, COSY, HSQC, HMBC please	59517		
01/10/2020	Katrina Andrews	SJC	1H, 13C, COSY, HSQC, HMBC please	59516		
01/10/2020	Stuart Astle	JB	1H, 13C, HSQC, HMBC, COSY Please	59515		
01/10/2020	Joseph Ford	VG	1H, 19F, 13C, HSQC, COSY, HMBCplease	59514		
01/10/2020	Joseph Ford	VG	1H, 19F, 13C, HSQC, COSY, HMBCplease	59513		

https://web.chem.ox.ac.uk/samples/

Sample Number is unique for every NMR sample tube submitted and is used to track samples- every tube ID tag must be labelled with this number (at least)

Part IIs should enter: p2

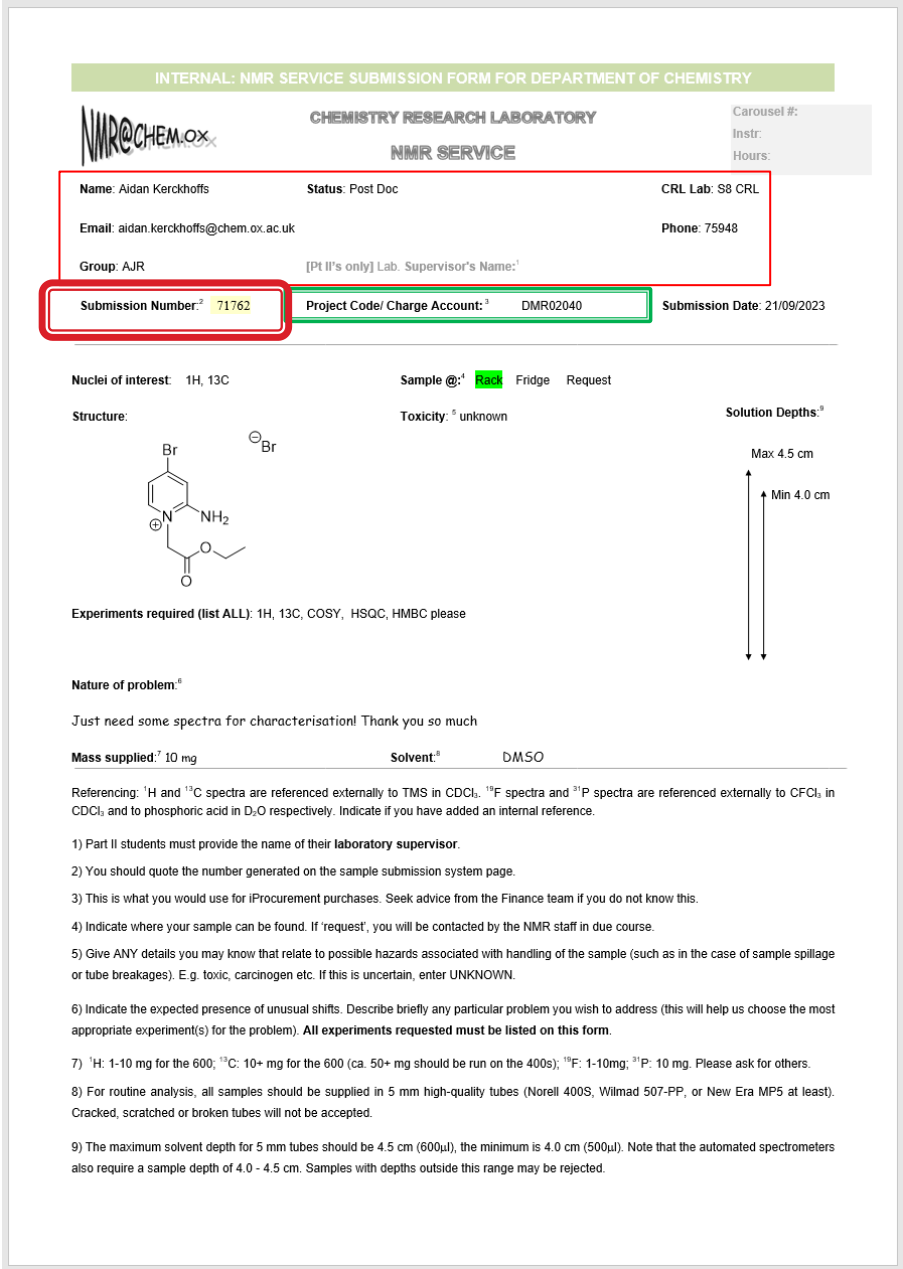
Sample Submission Form: Word document



FORM

SPECTRUM

The sample submission process will also be explained to you as part of your open-access training…



INTERNAL: NMR SERVICE SUBMISSION FORM FOR DEPARTMENT OF CHEMISTRY

NMR@CHEM.OX

CHEMISTRY RESEARCH LABORATORY

NMR SERVICE

Carousel #:
Instr:
Hours:

Name: Aidan Kerckhoffs **Status**: Post Doc **CRL Lab**: S8 CRL

Email: aidan.kerckhoffs@chem.ox.ac.uk **Phone**: 75948

Group: AJR [Pt II's only] Lab. Supervisor's Name:[1]

Submission Number:[2] 71762 **Project Code/ Charge Account:**[3] DMR02040 **Submission Date**: 21/09/2023

Nuclei of interest: 1H, 13C **Sample @:**[4] Rack Fridge Request

Structure: **Toxicity**:[5] unknown **Solution Depths**:[9]

Max 4.5 cm

Min 4.0 cm

Experiments required (list ALL): 1H, 13C, COSY, HSQC, HMBC please

Nature of problem:[6]

Just need some spectra for characterisation! Thank you so much

Mass supplied:[7] 10 mg **Solvent**:[8] DMSO

Referencing: ^{1}H and ^{13}C spectra are referenced externally to TMS in $CDCl_3$. ^{19}F spectra and ^{31}P spectra are referenced externally to $CFCl_3$ in $CDCl_3$ and to phosphoric acid in D_2O respectively. Indicate if you have added an internal reference.

1) Part II students must provide the name of their **laboratory supervisor**.

2) You should quote the number generated on the sample submission system page.

3) This is what you would use for iProcurement purchases. Seek advice from the Finance team if you do not know this.

4) Indicate where your sample can be found. If 'request', you will be contacted by the NMR staff in due course.

5) Give ANY details you may know that relate to possible hazards associated with handling of the sample (such as in the case of sample spillage or tube breakages). E.g. toxic, carcinogen etc. If this is uncertain, enter UNKNOWN.

6) Indicate the expected presence of unusual shifts. Describe briefly any particular problem you wish to address (this will help us choose the most appropriate experiment(s) for the problem). **All experiments requested must be listed on this form**.

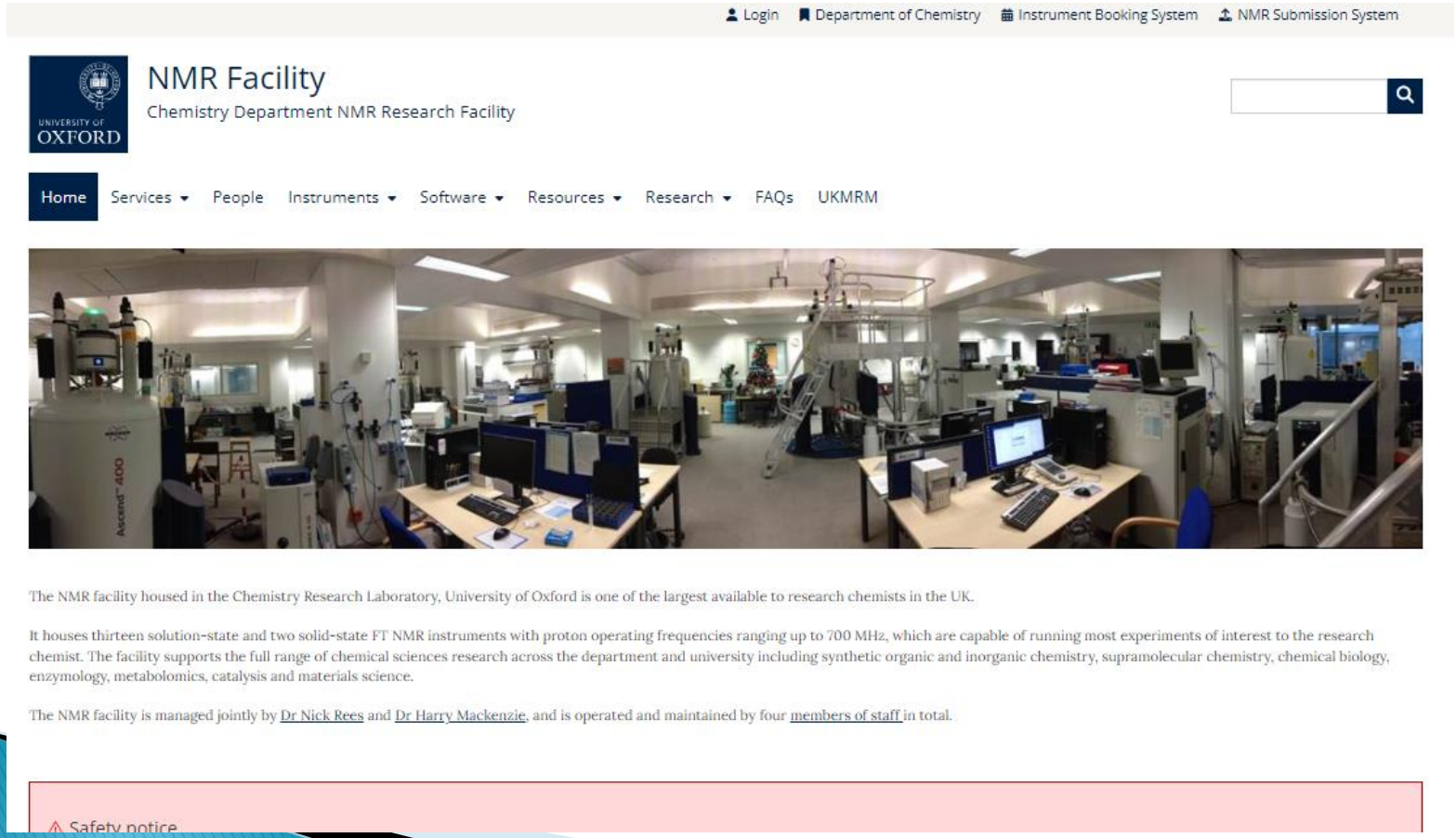
7) ^{1}H: 1-10 mg for the 600; ^{13}C: 10+ mg for the 600 (ca. 50+ mg should be run on the 400s); ^{19}F: 1-10mg; ^{31}P: 10 mg. Please ask for others.

8) For routine analysis, all samples should be supplied in 5 mm high-quality tubes (Norell 400S, Wilmad 507-PP, or New Era MP5 at least). Cracked, scratched or broken tubes will not be accepted.

9) The maximum solvent depth for 5 mm tubes should be 4.5 cm (600µl), the minimum is 4.0 cm (500µl). Note that the automated spectrometers also require a sample depth of 4.0 - 4.5 cm. Samples with depths outside this range may be rejected.

Online resources

- NMR web pages:
  - https://nmr.chem.ox.ac.uk/
  - or through ***Intranet*** link to ***Facilities*** then ***Instrument booking and analytical services*** on Chemistry homepage.



Future training courses

- Use of the Open-Access NMR Spectrometers & Service
  - ***Running this week- meet in CRL reception***
  - *Compulsory sessions- you must attend before using instruments or the NMR submission service.*
- Mnova NMR Software Introductory Lecture
  - Single online lecture introducing main software features
- Modern NMR Spectroscopy for the Research Chemist
  - 8-lecture course providing overview of NMR techniques
  - **This course can be found on the Oxford Canvas site at: https://canvas.ox.ac.uk/courses/54457**
- CDT students
  - *NMR training courses in Jan 2025: DO NOT SIGN UP FOR TRAINING THIS WEEK*

Inorganic Chemistry
Instrumentation

- 5 research instruments @ 400-500 MHz
  - 1 @ 400 MHz: Open Access multinuclear
  - 1 @ 400 MHz: Open Access multinuclear
  - 1 @ 500 MHz: Hands on & Service multinuclear and VT work
  - 1 @ 400 MHz: Service **Solid State** HXY
  - 1 @ 400 MHz: Service **Solid State** HFX, microimaging & diffusion

  - Access to 600 MHz: Service

Automated AVIIIHD400 [2nd Floor]

Known as the Hg400

- 60 place autosampler
- ^{1}H, ^{19}F, ^{31}P to ^{13}C
- ^{1}H–^{1}H, ^{1}H-^{13}C gradient selected 2-D experiments

Meant for fast daytime turnaround & longer overnight experiments

file://chem.ox.ac.uk/SRF/NMR/HG400/setup.html

Automated AVIII400 [2nd Floor]

Known as Venus400

- 60 place autosampler
- ^{1}H, ^{19}F, ^{31}P to ^{13}C
- ^{1}H–^{1}H, ^{1}H-^{13}C gradient selected 2-D experiments

Meant for fast daytime turnaround & longer overnight experiments

file://chem.ox.ac.uk/SRF/NMR/venus400/setup.html

Hands on AVIII500 [basement]

Known as the AVD500

- 24 place autosampler
- ^{1}H, ^{19}F to ^{109}Ag
- ^{1}H–^{1}H, ^{1}H-X gradient selected 2-D experiments
- VT work

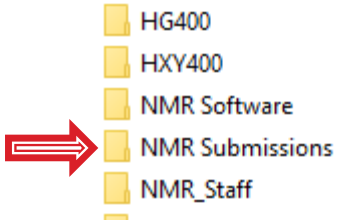
Booking required (online system)

Solid state NMR

- Service provided by Dr Nick Rees
- Stable samples provided as a solid (c.a. 200mg)
- Unstable samples can be packed in glove box
- Consult Nick Rees **before** submitting samples
- nick.rees@chem.ox.ac.uk
- Submit samples via the sample submission service
- Stable samples should be placed in the box through the basement NMR lab hatch
- For unstable samples provide email address on submission form.

Solid state NMR

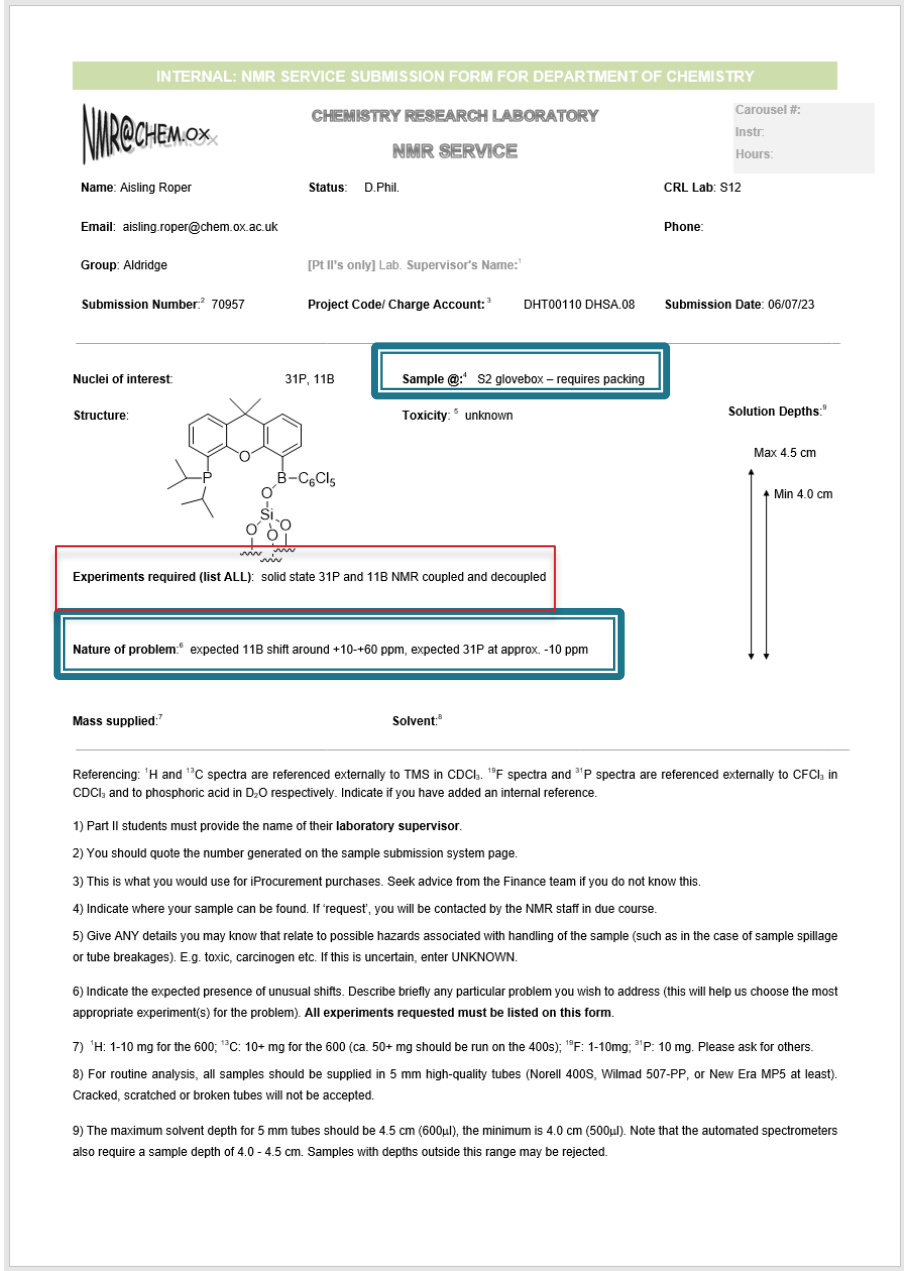
Sample Submission Form: Word document



List experiments
And specify SSNMR

If needs to be packed in glove box give contact email address

The sample submission process will also be explained to you as part of your open-access training…



INTERNAL: NMR SERVICE SUBMISSION FORM FOR DEPARTMENT OF CHEMISTRY

NMR@CHEM.OX

CHEMISTRY RESEARCH LABORATORY

NMR SERVICE

Carousel #:
Instr:
Hours:

Name: Aisling Roper **Status**: D.Phil. **CRL Lab**: S12

Email: aisling.roper@chem.ox.ac.uk **Phone**:

Group: Aldridge [Pt II's only] Lab. Supervisor's Name:[1]

Submission Number:[2] 70957 **Project Code/ Charge Account:**[3] DHT00110 DHSA.08 **Submission Date**: 06/07/23

Nuclei of interest: 31P, 11B **Sample @:**[4] S2 glovebox – requires packing

Structure: **Toxicity**:[5] unknown **Solution Depths**:[9]

Max 4.5 cm
Min 4.0 cm

Experiments required (list ALL): solid state 31P and 11B NMR coupled and decoupled

Nature of problem:[6] expected 11B shift around +10-+60 ppm, expected 31P at approx. -10 ppm

Mass supplied:[7] **Solvent**:[8]

Referencing: ^{1}H and ^{13}C spectra are referenced externally to TMS in $CDCl_3$. ^{19}F spectra and ^{31}P spectra are referenced externally to $CFCl_3$ in $CDCl_3$ and to phosphoric acid in D_2O respectively. Indicate if you have added an internal reference.

1) Part II students must provide the name of their **laboratory supervisor**.

2) You should quote the number generated on the sample submission system page.

3) This is what you would use for iProcurement purchases. Seek advice from the Finance team if you do not know this.

4) Indicate where your sample can be found. If 'request', you will be contacted by the NMR staff in due course.

5) Give ANY details you may know that relate to possible hazards associated with handling of the sample (such as in the case of sample spillage or tube breakages). E.g. toxic, carcinogen etc. If this is uncertain, enter UNKNOWN.

6) Indicate the expected presence of unusual shifts. Describe briefly any particular problem you wish to address (this will help us choose the most appropriate experiment(s) for the problem). **All experiments requested must be listed on this form**.

7) ^{1}H: 1-10 mg for the 600; ^{13}C: 10+ mg for the 600 (ca. 50+ mg should be run on the 400s); ^{19}F: 1-10mg; ^{31}P: 10 mg. Please ask for others.

8) For routine analysis, all samples should be supplied in 5 mm high-quality tubes (Norell 400S, Wilmad 507-PP, or New Era MP5 at least). Cracked, scratched or broken tubes will not be accepted.

9) The maximum solvent depth for 5 mm tubes should be 4.5 cm (600µl), the minimum is 4.0 cm (500µl). Note that the automated spectrometers also require a sample depth of 4.0 - 4.5 cm. Samples with depths outside this range may be rejected.

Solid State AVIIIHD400WB [basement]

Known as the HXY400

- 4 & 1.9 mm Triple Magic Angle Spinning Probes (^{1}H, ^{19}F, ^{31}P to ^{15}N)
- 4mm Low Gamma (^{13}C to ^{109}Ag) Magic Angle Spinning Probe
- Wideline Deuterium Probe
- Goniometer probe for oriented samples
- Variable temperature capable (-150 to 150C)

Solid State AVIIIHD400WB [basement]

Known as the HFX400

- 3.2mm HFX Triple Magic Angle Spinning Probes (^{1}H, ^{19}F, ^{31}P to ^{15}N)
- 30mm Micro-imaging probe
- Diffusion probe
- Variable temperature capable (-150 to 150C)

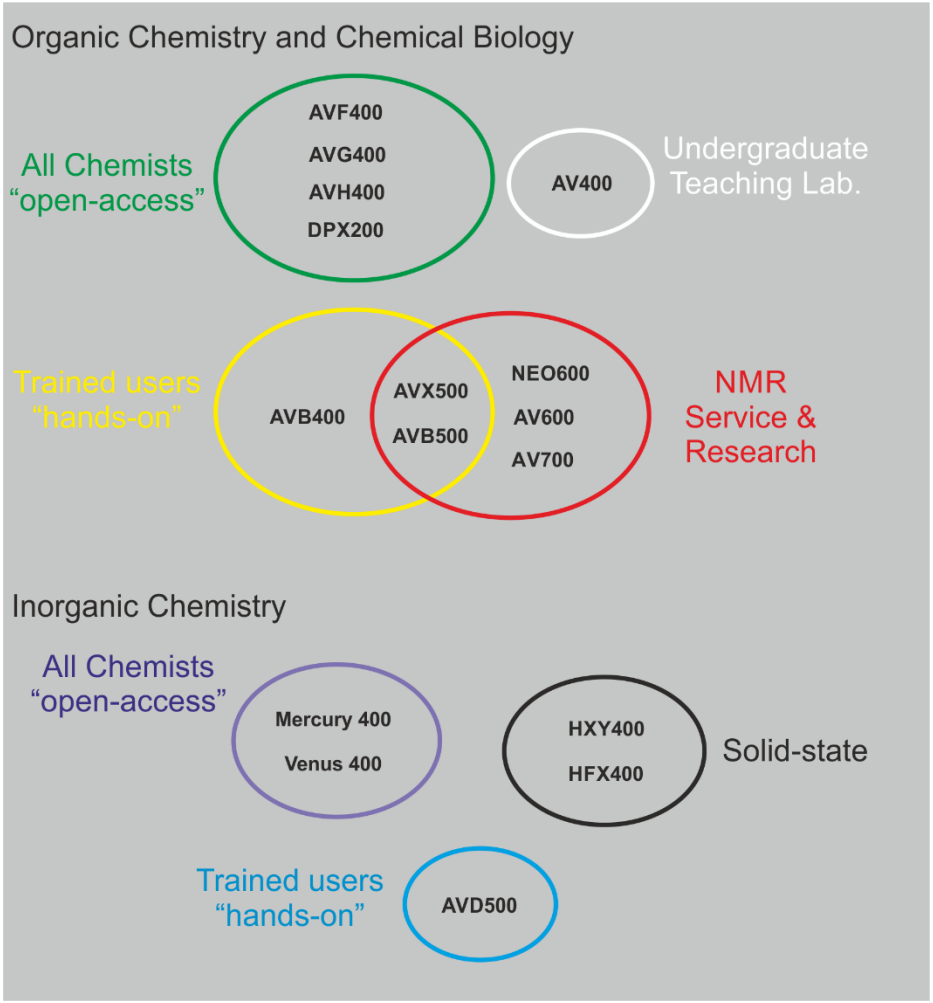
Inorganic Open-Access training:

- Use of the Open-Access NMR Spectrometers & Service
  - ***Running this week- meet in CRL reception***
  - *Compulsory sessions- you must attend before using instruments or the NMR submission service.*
  - Sessions will run Wednesday 2nd (pm), Thurs 3rd (pm) and Fri 4th (am): **Meet in CRL reception**
  - **Online booking and registration is required**

- Mnova NMR Software Introductory Lecture
  - Single on-line lecture introducing main software features

- CDT students
  - *NMR training courses in Jan 2025: DO NOT SIGN UP FOR TRAINING THIS WEEK*

Instrumentation Access



NMR training for new researchers

1: Register as an Organic Section NMR user:

https://forms.office.com/e/sYyFxBKJ7e **or**

1: Register as an Inorganic Section NMR user:

https://forms.office.com/r/h30g6LxEsT

2: Sign up for a training session

Select **Organic Section NMR:**

https://outlook.office365.com/owa/calendar/SRFInductions2024@UniOxfordNexus.onmicrosoft.com/bookings/s/bgg8DtMOmEmNP7fT42ZQhQ2

or Inorganic Section NMR:

https://outlook.office365.com/owa/calendar/SRFInductions2024@UniOxfordNexus.onmicrosoft.com/bookings/s/Cf0I_LTuLk2LQKJEyn2onw2

Meet for training in CRL reception

To arrange training external users should email: nmrstaff@maillist.chem.ox.ac.uk

All the above links can be found at:

https://massspec.chem.ox.ac.uk/book

QR for training sign-up sheets

OPEN ACCESS TRAINING: NMR SERVICE

Coral Mycroft
NMR Service Manager

NMR Facility – 4 Levels Of Analysis

Open Access

- Walk up use at any time of the day
- Common 1D/2D experiments: ^{1}H, ^{13}C, ^{19}F, ^{31}P, COSY, HSQC
- Fast turnover and hence rapid sample throughput
- Ground/first floors: Organic
- Second floor: Inorganic

NMR Service

- A submission service where researchers may submit samples for the NMR staff to run on the basement instruments.

Hands on

- Users can book the basement systems for manual/automated operation.

Research Projects

- Collaborative projects involving the NMR staff/group

A Typical Procedure Of Analysing A Sample Using NMR

Check the sample quality

- Open-access spectrometers to collect a basic 1D ^{1}H NMR spectrum
- Check structure corresponds to what you expect, as well as the integrity and quality of the sample

Collect further data

- Open-access spectrometers to characterise the molecules: 1D and 2D spectra
- Always assess the ^{1}H NMR spectrum first

Further experiments (if necessary)

- If the data collected is insufficient, you can consider submitting the sample to the NMR service / use the hands-on instruments (if trained)

Why Use The NMR Service?

Availability of experiments

- Other nuclei: ^{2}H, ^{7}Li, ^{27}Al
- 2D experiments: HMBC, NOESY, ROESY
- More specialised experiments: DOSY, variable temperature, pure shift, selective and more

Dilute samples

- Walk-up instruments do not allow you to adjust any experiment parameters
- The NMR service will adjust experiment parameters so acceptable spectra is obtained.

Higher field spectrometers

- 500 – 700 MHz

Solid state samples

Six Steps To Use The NMR Service for Solution-State NMR

(solid-state mentioned later)

Step 1: NMR Sample Preparation

Sample Tubes

- 5 mm high-quality tubes: Norell 400S, Wilmad 507-PP, or New Era MP5 at least
- Cracked, scratched, short or broken tubes will not be accepted

Solvents

- Use a deuterated solvent
- Solvent depth for 5mm tubes should be between 4.0 - 4.5 cm (500 - 600 μL)

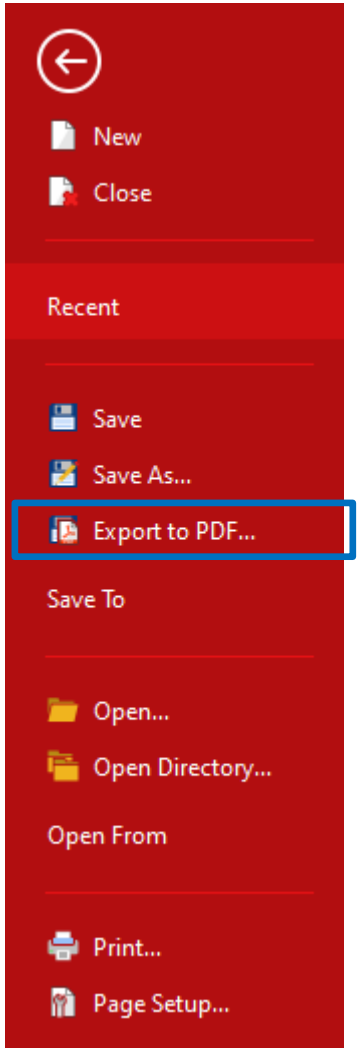
Quantity of sample

- ^{1}H / ^{19}F: 1-10 mg for the 600 MHz
- ^{13}C: At least 10+ mg for the 600 MHz (ca. 50+ mg should be run on the 400s)
- ^{31}P: 10 mg

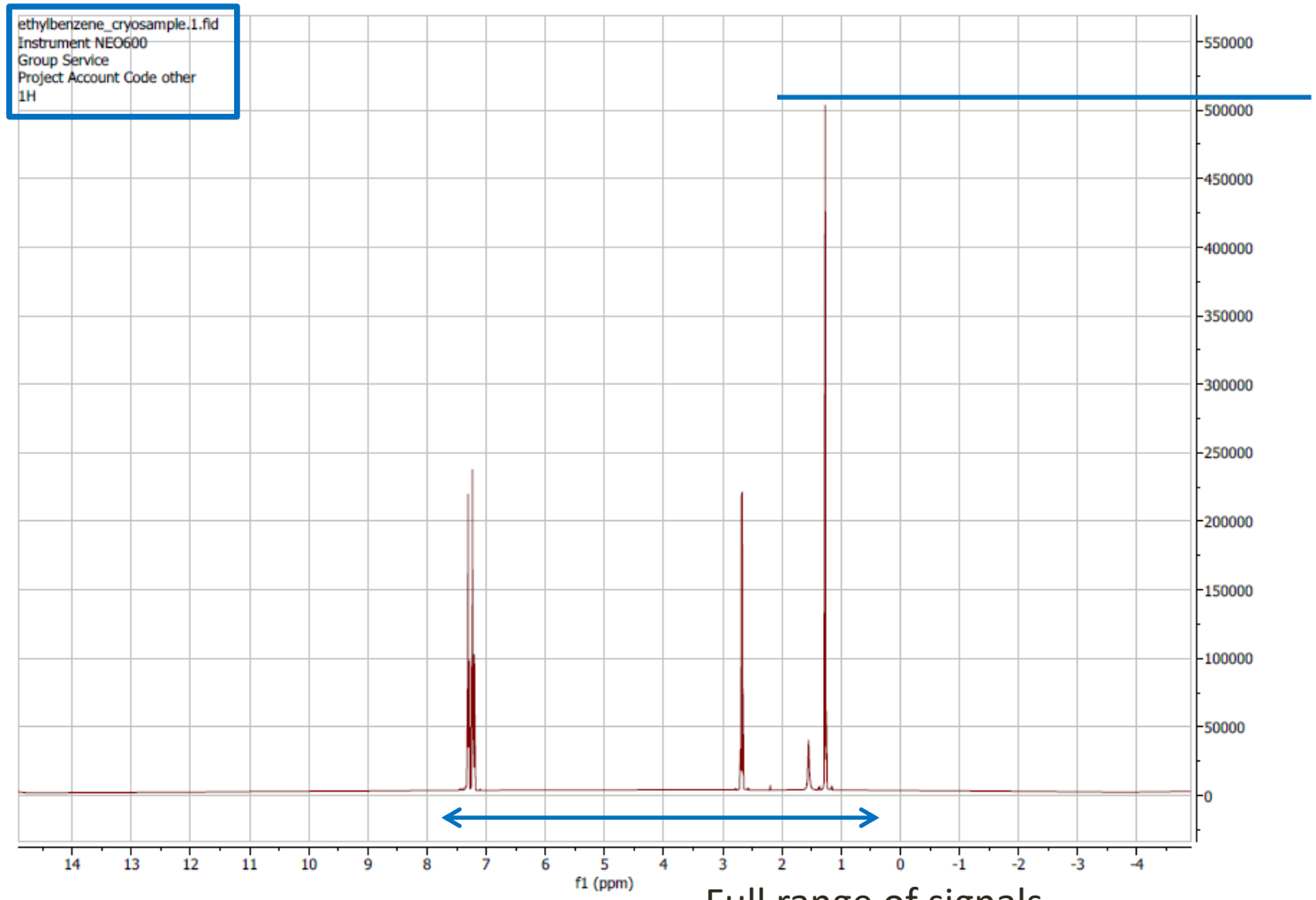
Labelling of NMR tube

- Use the correct NMR cap colour
- Label cap/tube with initials, solvent and group

Step 2: Acquire A ^{1}H NMR And Convert Spectrum To A PDF.



Spectrum information



Top of the most intense signal can be seen

Full range of signals

Step 3: Generate Submission Number

- Unique number associated with a NMR sample
- Three distinct samples = three unique numbers

NMR Facility Website
https://nmrchem.web.ox.ac.uk/home

NMR Service Sample Submission System

Please complete this form to add a sample to the NMR service system. You MUST ALSO complete a paper submission form to accompany each sample.

Your name Coral Mycroft Your Group OTHER

Project Code / Charge Account DMT12345 *

* see Finance if you are not sure what this is.

Your Sample NMR Experiments 1H, 13C, COSY, HSQC eg, (1H, 13C, HSQC, APT, COSY, 19F, NOE, HMBC, DEPT, ROESY, TOCSY, NOESY, etc)

Submit

Here are the most recent submissions and their service status

Date Submitted	Name	Research Group	Experiments Required	Sample Number	Completed	Instrument
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71800		
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71799		
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71798		
28/9/2023	Zhuxin Zhang	CJS	1H, 13C, HMBC please	71797		
27/9/2023	Marta Serafini	SJC	1H, 13C, COSY, HSQC, HMBC please	71796		
27/9/2023	Nicoleta Lazar	JR	1H, 13C, COSY, HSQC, HMBC	71795		

NMR Service Sample Submission System

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Your name Coral Mycroft Your Group OTHER

Project Code / Charge Account DMT12345 *

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Your Sample NMR Experiments 1H, 13C, COSY, HSQC eg, (1H, 13C, HSQC, APT, COSY, 19F, NOE, HMBC, DEPT, ROESY, TOCSY, NOESY, etc)

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28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71798		
28/9/2023	Zhuxin Zhang	CJS	1H, 13C, HMBC please	71797		
27/9/2023	Marta Serafini	SJC	1H, 13C, COSY, HSQC, HMBC please	71796		
27/9/2023	Nicoleta Lazar	JR	1H, 13C, COSY, HSQC, HMBC	71795		

NMR Service Sample Submission System

Please complete this form to add a sample to the NMR service system. You MUST ALSO complete a paper submission form to accompany each sample.

Your name Your Group Select Group

Project Code / Charge Account *

* see Finance if you are not sure what this is.

Your Sample NMR Experiments eg, (1H, 13C, HSQC, APT, COSY, 19F, NOE, HMBC, DEPT, ROESY, TOCSY, NOESY, etc)

Submit

Here are the most recent submissions and their service status

Date Submitted	Name	Research Group	Experiments Required	Sample Number	Completed	Instrument
28/9/2023	Coral Mycroft	OTHER	1H, 13C, COSY, HSQC	71801		
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71800		
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71799		
28/9/2023	Maddie Hindson	MDS	1H, 13C, COSY, HMBC, HSQC pls	71798		
28/9/2023	Zhuxin Zhang	CJS	1H, 13C, HMBC please	71797		
27/9/2023	Marta Serafini	SJC	1H, 13C, COSY, HSQC, HMBC please	71796		

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+ Expand All

Internal samples (i.e. researchers in Chemistry)

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1. Visit the **sample submission webpage** and fill in the form. This form will assign you a **submission number** — note this down.
2. Download and complete the NMR submission form [Word], using the submission number assigned previously. Please feel free to provide any extra details here if necessary, such as unusual chemical shifts.
3. Place the completed form in the "**NMR Submissions**" folder in the NMR data server; this can be accessed at **\\chem.ox.ac.uk\SRF\NMR\NMR Submissions** (please see here for instructions on how to access this folder if needed). Forms should be named in the following manner:
   <submission number>_<name>_<supervisor initials>.
   Note that paper forms will not be accepted!
4. In the same folder, place a PDF copy of the 1D ^{1}H spectrum of the same sample you are submitting, using the following name:
   <submission number>_<name>_<supervisor initials>_1H.pdf
5. Bring the sample down and place it either on the sponge rack or inside the small fridge as per the location indicated on the submission form. Both of these can be accessed via the hatch to the side of the NMR lab entrance.
   If your sample is unstable or requires special attention, choose "Request" as the location and do not bring down the sample; a member of the NMR staff will contact you to arrange for this.

After a sample has been submitted, you will find the following:

1. Your submission form has been removed from the NMR Submissions folder. This is normal and indicates that it has been processed by a member of the NMR staff.
2. The completion status on the submission webpage is updated to "Yes", and the spectrometer(s) used to run the sample indicated next to it.

AutoSave Off nmrsubmissionforminternal2021docx(3).docx - Word Search Coral Mycroft CM

File Home Insert Design Layout References Mailings Review View Help Nuance PDF Share

Paste Cut Copy Format Painter | Arial 10 | Clipboard Font Paragraph Styles Editing Find Replace Select

AaBbCc ¶ Heading 1 | AaBbCcDc ¶ Normal | AaBbCcDc ¶ No Spac... | AaB Title | AaBbCcD Subtitle | AaBbCcDc Subtle Em... | AaBbCcDc Emphasis | AaBbCcDc Intense E... | AaBbCcDd Strong | AaBbCcDc Quote | AaBbCcDc Intense Q... | AABBCCDI Subtle Ref... | AABBCCDI Intense Re... | AaBbCcDc Book Title

INTERNAL: NMR SERVICE SUBMISSION FORM FOR DEPARTMENT OF CHEMISTRY

NMR@CHEM.OX

CHEMISTRY RESEARCH LABORATORY

NMR SERVICE

Carousel #:
Instr:
Hours:

Name:	**Status**: Pt II D.Phil. Post Doc	**CRL Lab**:
Email:		**Phone**:
Group:	[Pt II's only] Lab. Supervisor's Name:[1]	
Submission Number:[2]	**Project Code/ Charge Account:** [3]	**Submission Date**:

Nuclei of interest:

Sample @:[4] Rack Fridge Request

Structure:

Toxicity: [5]

Solution Depths:[9]

Max 4.5 cm

Min 4.0 cm

Experiments required (list ALL):

Nature of problem:[6]

Mass supplied:[7]

Solvent:[8]

Referencing: ^{1}H and ^{13}C spectra are referenced externally to TMS in $CDCl_3$. ^{19}F spectra and ^{31}P spectra are referenced externally to $CFCl_3$ in $CDCl_3$ and to phosphoric acid in D_2O respectively. Indicate if you have added an internal reference.

1) Part II students must provide the name of their **laboratory supervisor**.

2) You should quote the number generated on the sample submission system page.

3) This is what you would use for iProcurement purchases. Seek advice from the Finance team if you do not know this.

4) Indicate where your sample can be found. If 'request', you will be contacted by the NMR staff in due course.

5) Give ANY details you may know that relate to possible hazards associated with handling of the sample (such as in the case of sample spillage or tube breakages). E.g. toxic, carcinogen etc. If this is uncertain, enter UNKNOWN.

6) Indicate the expected presence of unusual shifts. Describe briefly any particular problem you wish to address (this will help us choose the most appropriate experiment(s) for the problem). **All experiments requested must be listed on this form**.

7) ^{1}H: 1-10 mg for the 600; ^{13}C: 10+ mg for the 600 (ca. 50+ mg should be run on the 400s); ^{19}F: 1-10mg; ^{31}P: 10 mg. Please ask for others.

8) For routine analysis, all samples should be supplied in 5 mm high quality tubes (Norell 400S, Wilmad 507 PP, or New Era MP5 at least)

Personal information

Sample and experiment information (mostly)

Guidance on filling out the submission form

Page 1 of 1 353 words Focus 100%

Inbox - coral.mycroft... Re: NMR training link... Submission service | ... nmrsubmissionformi... Documents Mail - Coral Mycroft -... NMR Service - Open ... 11:53 am

INTERNAL: NMR SERVICE SUBMISSION FORM FOR DEPARTMENT OF CHEMISTRY

NMR@CHEM.OX

CHEMISTRY RESEARCH LABORATORY

NMR SERVICE

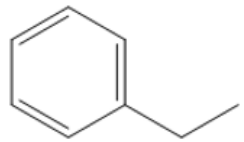
Carousel #:
Instr:
Hours:

Name: Coral Mycroft	**Status**: Pt II D.Phil. Post Doc	**CRL Lab**: B00.120
Email: nmrstaff@maillist.chem.ox.ac.uk		**Phone**: 12345
Group: VG / CJS / HLA / DOH	**[Pt II's only]** Lab. **Supervisor's Name:**[1] D.Phil/Post Doc name	
Submission Number:[2] 71801	**Project Code/ Charge Account:** [3] DMT12345	**Submission Date**: 28/09/2023

Nuclei of interest: 1H, 13C

Sample @:[4] Rack Fridge Request

Structure:



Toxicity: [5] FLAMMABLE. HARMFUL.

Solution Depths:[9]

Experiments required (list ALL):

1H, 13C, COSY, HSQC

Nature of problem:[6]

Standard structure assignment of new compound. Sample too dilute for 13C and HSQC on open access spectrometers.

Mass supplied:[7] < 1 mg

Solvent:[8] $CDCl_3$

Step 5: Place Completed Form And PDF In The NMR Submissions Folder In The NMR Data Server

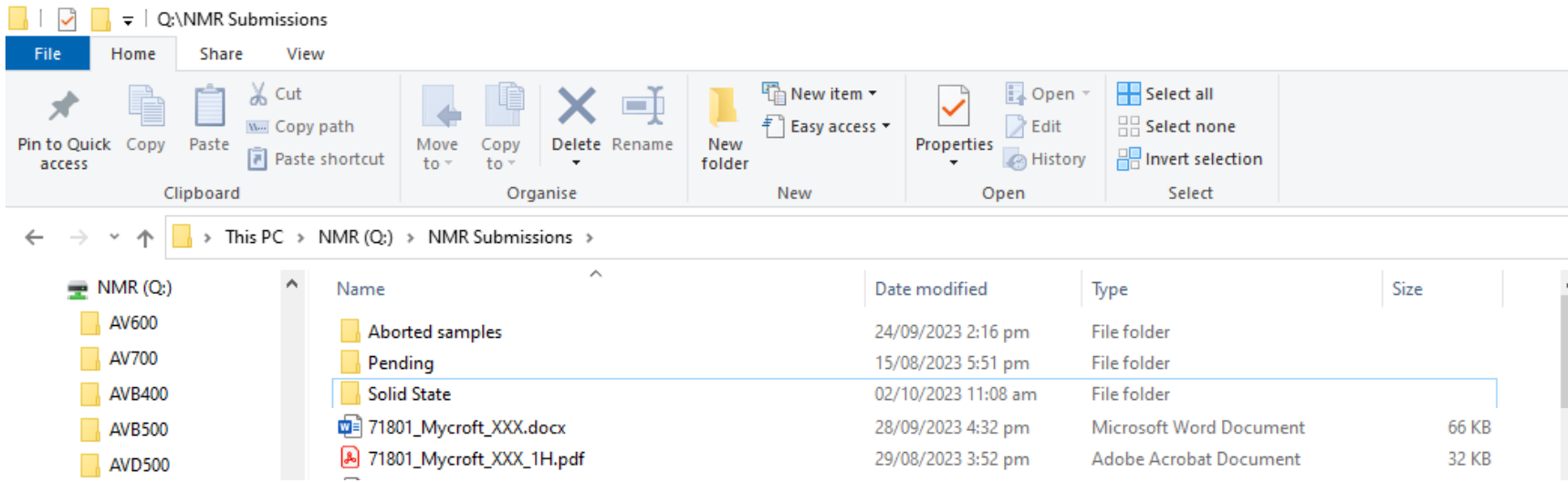
Word: <submission number>_<name>_<supervisor initials>

71801_Mycroft_XXX

PDF: <submission number>_<name>_<supervisor initials>_1H.pdf

71801_Mycroft_XXX_1H

Solid-state samples: Place word document in the *'Solid State'* folder. No PDF required.



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+ Expand All

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4. In the same folder, place a PDF copy of the 1D ^{1}H spectrum of the same sample you are submitting, using the following name:
   <submission number>_<name>_<supervisor initials>_1H.pdf
5. Bring the sample down and place it either on the sponge rack or inside the small fridge as per the location indicated on the submission form. Both of these can be accessed via the hatch to the side of the NMR lab entrance.
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2. The completion status on the submission webpage is updated to "Yes", and the spectrometer(s) used to run the sample indicated next to it.

Archiving NMR data

Spectra acquired on all NMR spectrometers are initially stored on the hard disks of the individual computers attached to the spectrometers, and *cannot* be accessed directly this way.

To obtain your NMR data, the spectra must be transferred to a central server (sometimes called the 'archive') which you can then access.

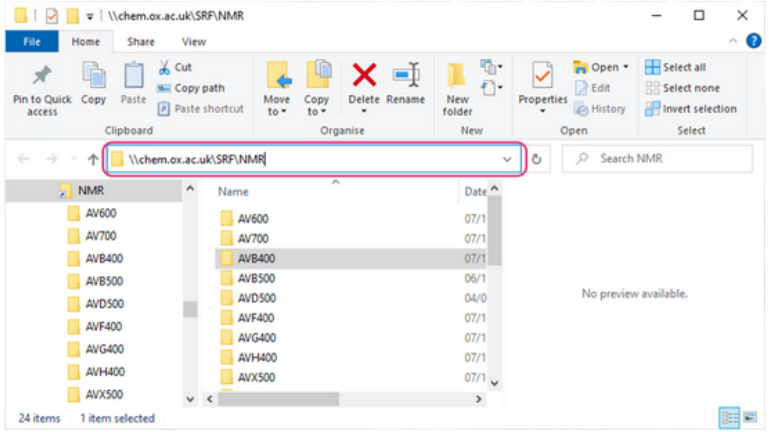
- **Open-access:** this is automatically done
- **Submission service:** this is automatically done, please email nmrstaff@maillist.chem.ox.ac.uk if you cannot find your data
- **Hands-on:** this is automatically done if you ran your experiments under IconNMR automation. If you ran them manually, then you must use the *archive* TopSpin command on each individual dataset in order to transfer them to the server.

Accessing the NMR server

On university computers (including group computers) — Windows

1. Log into Windows as any user in the CHEM domain. This can be done with either your own account (usually *firstname.lastname*) or a group account (usually *xyzgroup*).
2. Open any folder, click on the address bar (see screenshot below) and enter: **\\chem.ox.ac.uk\SRF\NMR**

You will then see a list of spectrometer data folders, from which you can obtain your spectra.



Includes how to access on university and own computers (Windows/macOS)

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+ Expand All

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1. Visit the **sample submission webpage** and fill in the form. This form will assign you a **submission number** — note this down.
2. Download and complete the NMR submission form [Word], using the submission number assigned previously. Please feel free to provide any extra details here if necessary, such as unusual chemical shifts.
3. Place the completed form in the "**NMR Submissions**" folder in the NMR data server; this can be accessed at **\\chem.ox.ac.uk\SRF\NMR\NMR Submissions** (please see here for instructions on how to access this folder if needed). Forms should be named in the following manner:
   <submission number>_<name>_<supervisor initials>.
   Note that paper forms will not be accepted!
4. In the same folder, place a PDF copy of the 1D ^{1}H spectrum of the same sample you are submitting, using the following name:
   <submission number>_<name>_<supervisor initials>_1H.pdf
5. Bring the sample down and place it either on the sponge rack or inside the small fridge as per the location indicated on the submission form. Both of these can be accessed via the hatch to the side of the NMR lab entrance.
   If your sample is unstable or requires special attention, choose "Request" as the location and do not bring down the sample; a member of the NMR staff will contact you to arrange for this.

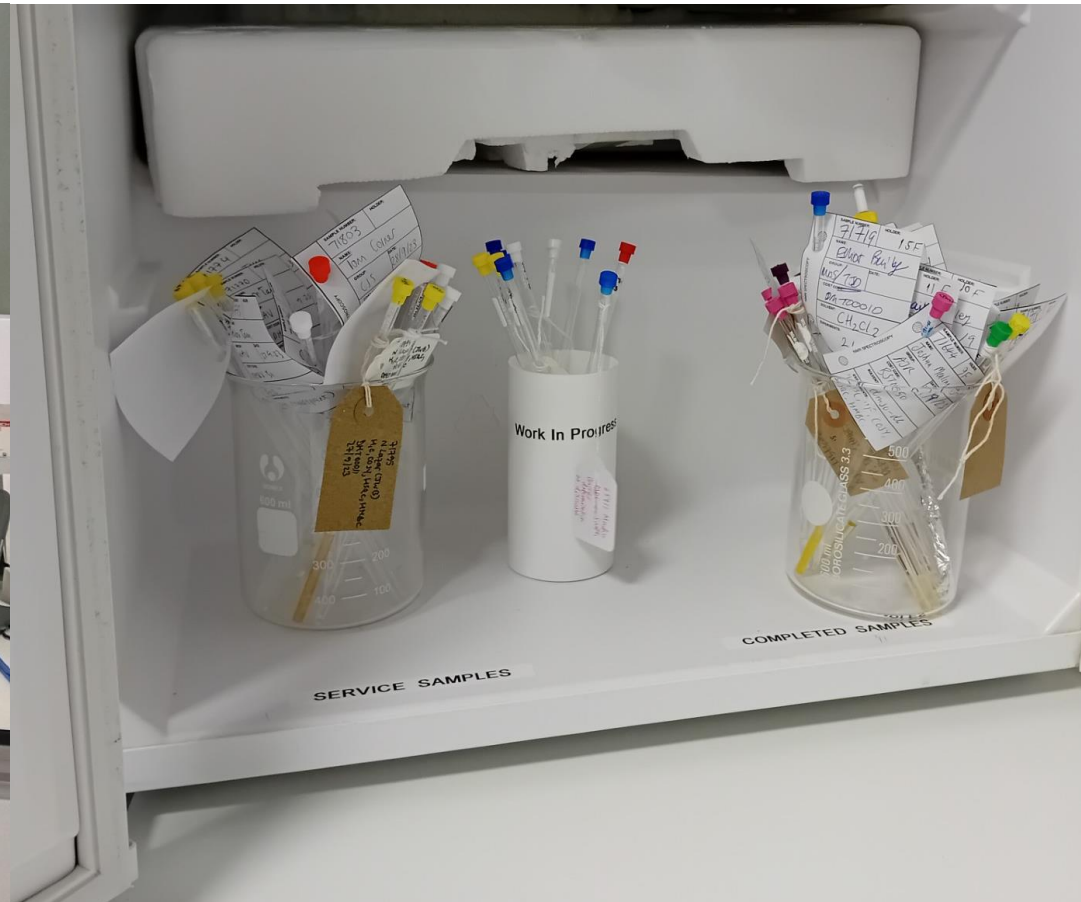
After a sample has been submitted, you will find the following:

1. Your submission form has been removed from the NMR Submissions folder. This is normal and indicates that it has been processed by a member of the NMR staff.
2. The completion status on the submission webpage is updated to "Yes", and the spectrometer(s) used to run the sample indicated next to it.

Step 6: Bring The NMR Sample Down To The Basement With A Completed Label

Solution-state incoming and completed

Solid state incoming and completed



Step 6: Bring The NMR Sample Down To The Basement With A Completed Label

NMR Spectroscopy

SAMPLE NUMBER: 71801	HOLDER: FOR NMR SERVICE ONLY – LEAVE BLANK
NAME: Coral Mycroft	
GROUP: HLA/ HB/ SJC	DATE: 28/09/2024
COST CODE: DMT12345	
SOLVENT: $CDCl_3$	STORAGE (RACK / FRIDGE): Rack
EXPERIMENTS: ^{1}H, ^{13}C, COSY, HSQC	

Six Steps To Use The NMR Service for Solid-State NMR

1. Consult Nick Rees before submitting samples
   - Nick.rees@chem.ox.ac.uk
2. Prepare the NMR sample
   - Stable samples provided as a solid (c.a. 200 mg)
   - Unstable samples can be packed in a glove box
3. Generate a unique submission Number *via* the NMR Facility Website
4. Complete submission form
5. Place submission form in the Solid-State submission folder on the Q drive
6. Stable samples should be placed in the box through the basement NMR lab hatch

https://nmrchem.web.ox.ac.uk/

Next Steps: NMR Facility Staff Take Over

The NMR facility will check the sample, paperwork and PDF of the submitted sample

- Everything is correct: schedule the analysis
- Issue with sample/paperwork/PDF: analysis will not be scheduled

When analysis is being run, the submission form and PDF will be removed from the NMR Submissions folder

Turnover is dependent on the current demand of the NMR Service and the analysis requested

Once complete, the status on the submission webpage is updated to “Yes”, with details of which spectrometer was used to run the sample

Date Submitted	Name	Research Group	Experiments Required	Sample Number	Completed	Instrument
28/9/2023	Coral Mycroft	OTHER	1H, 13C, COSY, HSQC	71801	Yes	AVX500

Next Steps: NMR Facility Staff Take Over

At this point you can obtain the data from the NMR data server. This data is organised by instrument and then by your research group initials. Each individual dataset is then named according to the following:

<initials> <five-digit submission number> <date in DDMM format>

cm718012909

The sample will be placed in the returns rack/fridge (solution) or completed tub (solid)

Why Hasn’t My Sample Been Run?

Check the submission system

If no information, the sample has yet to be run

- Service is very busy
- Analysis requires a specific spectrometer

If system says aborted, either an element of the paperwork or sample is incorrect

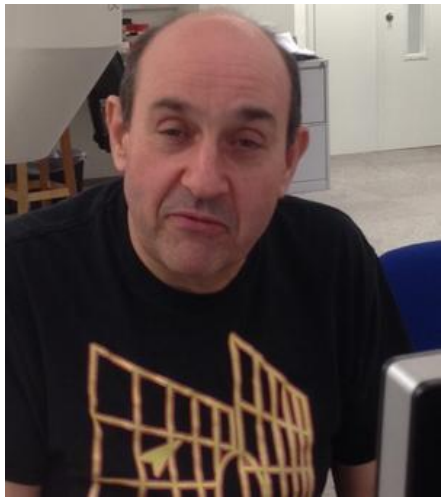
- Correct the error and re-submit the sample/paperwork
- Depending on how busy the service is, we may email you stating what is incorrect for you to fix

If it’s been >1 week and you’ve requested only conventional 1D and 2D experiments, you can email us: nmrstaff@maillist.chem.ox.ac.uk

NMR Facility Members

nmrstaff@maillist.chem.ox.ac.uk

Nick



Head of NMR

Caitlin

NMR Research Technician

Coral

NMR Service Manager

Charlie

NMR Officer

Training And Other

Providing you have registered, you are now trained to the open access NMR spectrometers on the relevant floors

- Ground/first floors: Organic
- Second floor: Inorganic

Use of the basement spectrometers in ‘hands on’ mode?

- Requires a separate 60-90 minute training
- Part 2 users are not allowed, unless their project has a significant NMR element

Slides for the NMR Introductory lecture and NMR Service are available on the NMR Facility homepage

Talk to us in person, or contact the NMR staff mail list for all enquiries.

nmrstaff@maillist.chem.ox.ac.uk