

9.00 - 9.30	Introduction to Mass Spectrometry facilities The Mass Spectrometry induction session will introduce researchers to the mass spectrometry facilities available to support research the Chemistry Department. It will explain how these can be accessed including Open Access Mass spectrometer systems, training to use LC-MS and GC-MS and how the sample submission services are arranged and run by the mass spec staff. <i>It is essential that anyone planning to use the Mass Spectrometry facilities attend this induction session.</i>	James McCullagh & John Walsby-Tickle
9.30 - 10.15	Introduction to NMR Spectroscopy facilities The NMR induction session will introduce the NMR staff, instruments, and facilities available to support research in organic chemistry, chemical biology and inorganic chemistry. It will explain how these can be accessed, the training that is required to use the instruments, and will introduce the NMR Submission Service provided by the NMR staff. <i>It is essential that anyone wishing to make use of the NMR facilities attend this induction session</i>	Nick Rees & Harry Mackenzie
10.15 – 10.30	Break	
10.30 – 10.45	Introduction to Powder X-Ray Diffraction and Magnetometry A brief introduction to the Inorganic Materials Characterisation facility which encompasses PXRD and SQUID magnetometry. An overview of the equipment and an explanation of the induction process will be given, relevant to all new starters undertaking synthetic work.	Simon Cassidy
10.45 – 11.15	Introduction to X-Ray Crystallography A short introduction to the single crystal X-ray crystallography service suitable for all Part II and new DPhil students. This session is relevant to chemists doing synthetic work in all sections of the Department.	Amber Thompson
11.15 – 11.35	Introduction to ESR Spectroscopy facilities The ESR induction session will introduce the ESR staff, instruments, and facilities available to support research in chemical biology and inorganic, organic, and physical chemistry. Application examples, instrument access and safety will be explained.	Will Myers

Walk-up NMR and MS training

Walk-up NMR and MS training will be arranged by the service managers. (Sign-up forms will be available on-line).

Laser Safety training

Compulsory for all students intending to use class 3 and class 4 lasers - please ask your supervisor

13.00 - 14.30	Laser Safety for Part II students Thursday 25 th September, ICL Lecture Theatre Please be respectful of other attendees and speakers. Compulsory for all students intending to use class 3 and class 4 lasers - please ask your supervisor	Lavina Snoek
11.45 - 13.15	Laser Safety for DPhil students Thursday 2 nd October, ICL Lecture Theatre Please be respectful of other attendees and speakers. Compulsory for all students intending to use class 3 and class 4 lasers - please ask your supervisor	Lavina Snoek

Electronic workshop in ICL open day:

Tuesday 7th October
2.00pm – 4.00pm

The workshop will be open for students and academic staff from all Sections to find out what facilities are available and the kinds of work that can be carried out.

Chemistry workshops in PTCL open day:

Wednesday 8th October
2.00pm – 4.00pm

All workshops will be open for students and academic staff from all Sections to find out what facilities are available and the kinds of work that can be carried out.

Workshops are as follows:

- Electronics Workshop;
- Mechanical Workshop;
- 3D Printing Facility

– all in PTCL. You are welcome to visit any, or all, of the workshops.

In addition, other induction sessions available include:

Liquid nitrogen, and gas regulators:

Additional training on these commonly used items will be given by your Building Manager.

Inorganic Materials Characterisation facility

Please note that all users of X-ray diffractometers must be registered with the Safety Office and attend the ['Safe use of X-ray generators, sealed sources and accelerators'](#) training at the first available opportunity (see below).

NB. A PXRD instrument in the CRL is run separately by Crystallography, training for that instrument should be arranged through them.

Compulsory Safety Office courses

Some students will be required to undertake additional, compulsory courses run by the University Safety Office due to the nature of their research.

To book onto a course you will need a University 'single sign-on'. Click on the relevant link below and complete the registration process via the University's CoSy Training Platform.

Enquiries should be emailed to training@safety.ox.ac.uk

PLEASE CHECK WITH YOUR SUPERVISOR IF YOU NEED THIS TRAINING, and please book on the course through [CoSy](#) (SSO needed):

Introduction to Laser Safety::

[An essential course for any individual operating a laser](#) where the beam is not fully enclosed (open). This might include both routine and non-routine operations (e.g. alignment, modifications, maintenance).
tbc

Radiation Safety for Laboratory Workers:

[New radiation workers intending to work with unsealed \(open\) radioactive sources, such as radioactive labelled compounds.](#)

Note: This session is relevant to use of unsealed radioactive sources e.g. U/Th compounds.

14th October, 1300 – 1500, ICL LT

Introduction to Biological safety and Genetic modification:

[For new students, workers new to Oxford University](#) and non-biologists undertaking (or planning to undertake) biological and/or genetic modification work.

For classroom teaching – An introduction – [check the website.](#)

[Pre-recorded Online Training Presentation in two parts.](#)

Safe use of X-ray generators, sealed sources and accelerators:

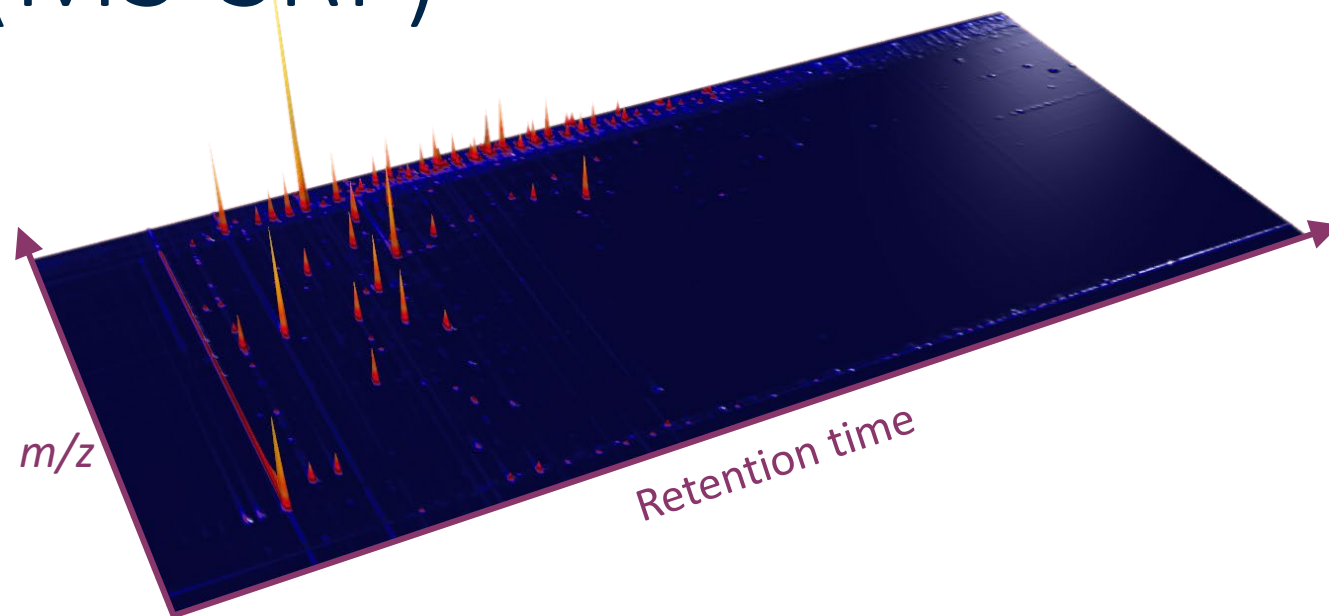
[For new radiation workers](#) intending to work with sealed (closed) radioactive sources or ionising radiation generators.

Note: This session is relevant to x-ray single crystal and powder diffraction.

22nd October, 1400 – 1600, ICL LT

Introduction to the Mass Spectrometry Research Facility (MS-SRF)

Dr John Walsby-Tickle
Scientific Induction 2025



Mass Spectrometry (MS)

- Mass spectrometers measure the mass to charge ratio (m/z) of ions in the gas phase

Elemental composition and Identification

260.02972

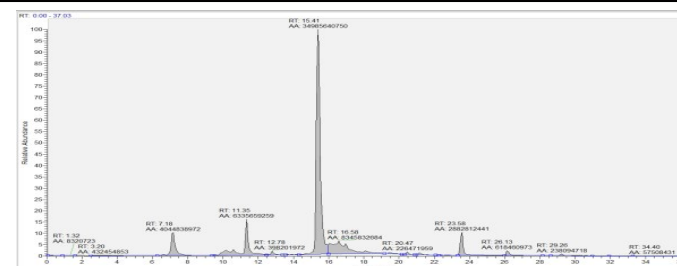


$C_6H_{13}O_9P$



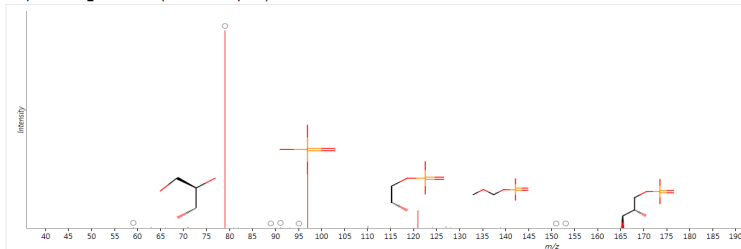
Glucose-1-phosphate

Separation & Quantification Relative and absolute: LC-MS, GC-MS

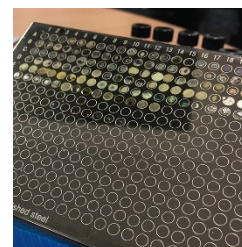


Structural analysis Fragmentation studies using MS

Compound 11.35_241.0109m/z (Glucose-6-Phosphate)



'Omics', structural, synthetic and systems biology



MS-SRF Staff



Ms Abigail Dixon
Research Technician in MS



Dr Victor Mikhailov
Research Associate in MS



Ms Elisabete Pires
Research Associate in MS



Dr John Walsby-Tickle
MS Services Manager



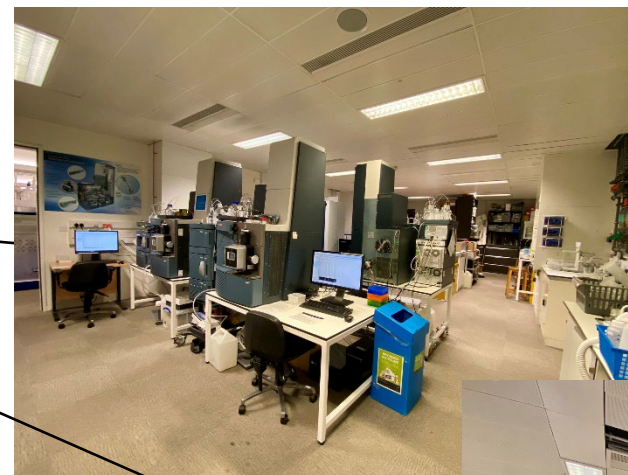
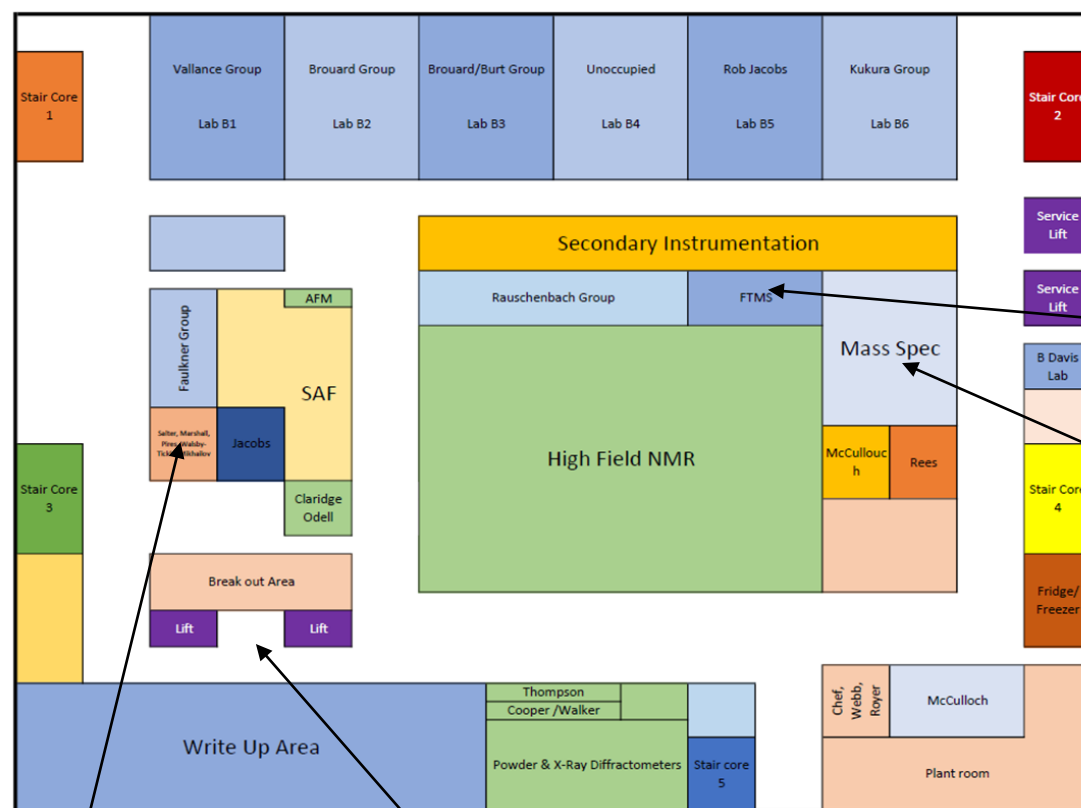
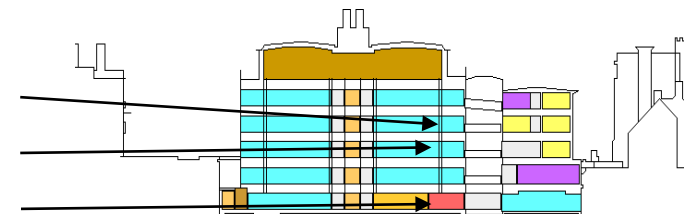
Prof James McCullagh
Director of the MS-SRF

MS Labs

1st Floor: Submission service

Ground Floor: Open access MS labs

Basement: Main MS labs



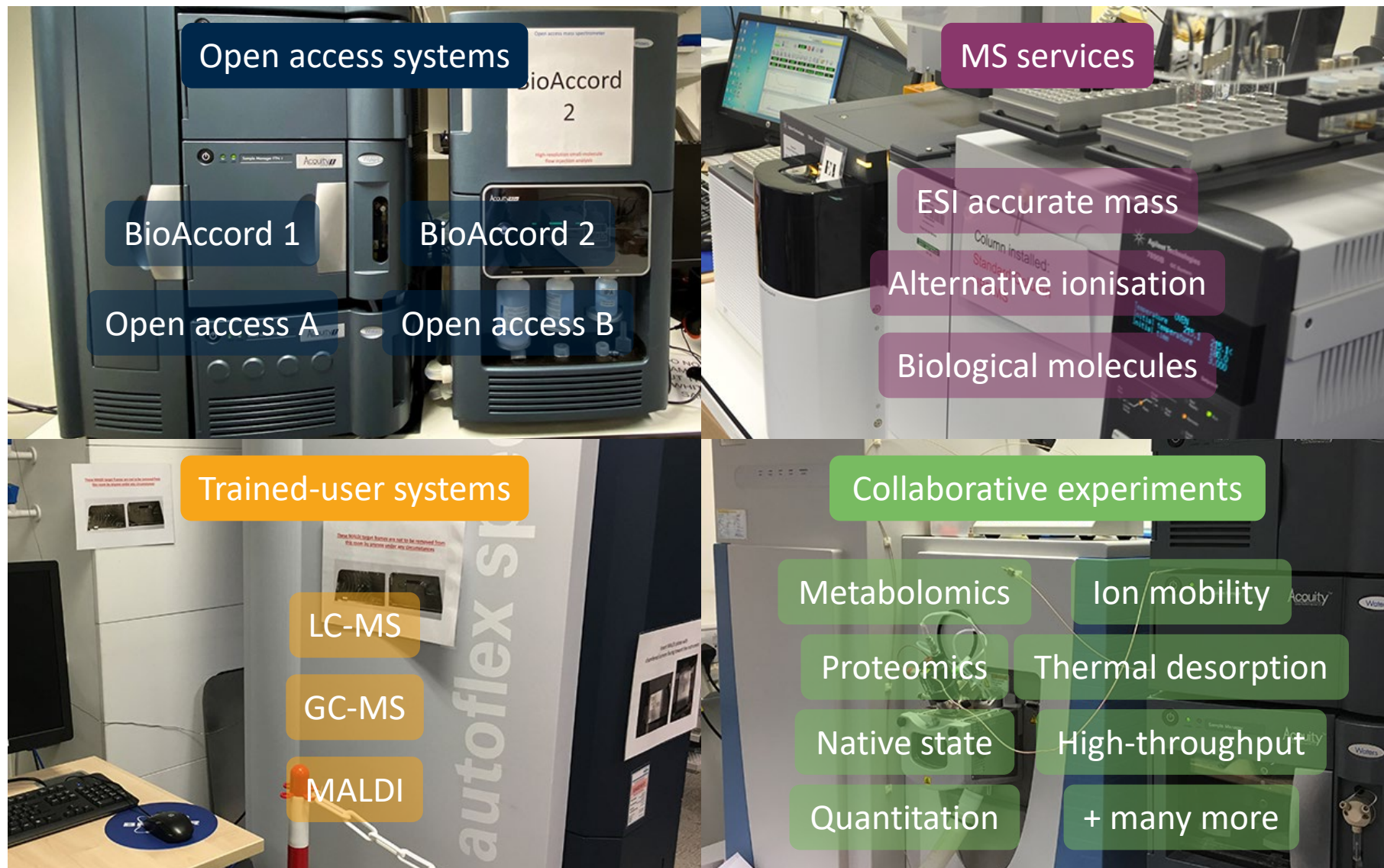
MS staff offices

Scenic lifts

20+ Mass Spectrometers



<https://massspec.chem.ox.ac.uk/instruments>



Open access systems

BioAccord 1

BioAccord 2

Open access A

Open access B

MS services

ESI accurate mass

Alternative ionisation

Biological molecules

Trained-user systems

LC-MS

GC-MS

MALDI

Collaborative experiments

Metabolomics

Ion mobility

Proteomics

Thermal desorption

Native state

High-throughput

Quantitation

+ many more

Open Access Systems



Victor Mikhailov

Research Associate in MS

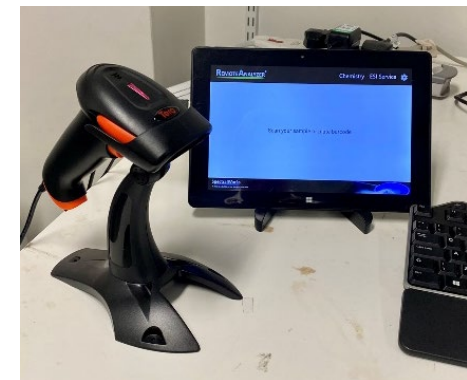
Runs open access systems and small molecule services

Ground Floor



<https://spectralworks.chem.ox.ac.uk>

SpectralWorks



Target Confirmation Report

Sample ID: LeuEnk
Group: Mass Spec
Acquisition Date: 03/08/2022 08:44:30
Experiment: BioAccord 2 - Loop Injection MS (+ ion)
Filename: Mass_Spec_JWT_LeuEnk_1575_C28H37N5O7_(+H)+.pdf

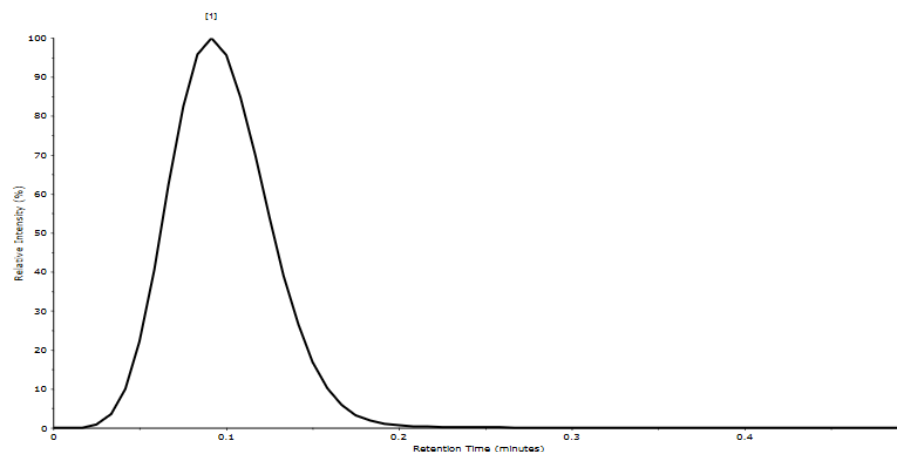
Submitter: John Walsby-Tickle
Project: BioAccord 2 - Accurate Mass Confirmation
Instrument: BioAccord 2

Adduct: +H

Proposed Formula: C₂₈H₃₇N₅O₇

Additional Comment:

EIC m/z=556.2766 +/- 0.0500, Target Mass and BasePeak Peaks Align, 1 Peaks Detected, NL 6.868E06



REMOTEANALYZER[®]

☐	↓ ID	Sample Refere...	Status	Result
	🔍	🔍		🔍
☐	2921	OMP040-C	■■■■■■■■	Target m/z 334.1562 not found, Target ...
☐	2919	JTW-3-045-Ax	■■■■■■■■	C96H119N12O2, 3.3 Error (ppm)
☐	2918	EF001A	■■■■■■■■	C26H51N4O6, 3.5 Error (ppm), C26H50...
☐	2917	SM-8-41	■■■■■■■■	C24H39BF3O3Si, 1.7 Error (ppm), C24...
☐	2916	SM-8-35	■■■■■■■■	C14H27O5Si, 1.8 Error (ppm), Target m/...
☐	2915	dmjc734C	■■■■■■■■	C28H37O5, 2.1 Error (ppm) [S], C28H36...
☐	2914	dmjc734B	■■■■■■■■	C26H41O5, 0.8 Error (ppm), C26H40O5...

Open access systems

BioAccord 1

BioAccord 2

Open access A

Open access B

MS services

ESI accurate mass

Alternative ionisation

Biological molecules

Trained-user systems

LC-MS

GC-MS

MALDI

Collaborative experiments

Metabolomics

Ion mobility

Proteomics

Thermal desorption

Native state

High-throughput

Quantitation

+ many more

Small molecule characterisation services

Organic and inorganic

First Floor



Dr Victor Mikhailov
Research Associate in MS



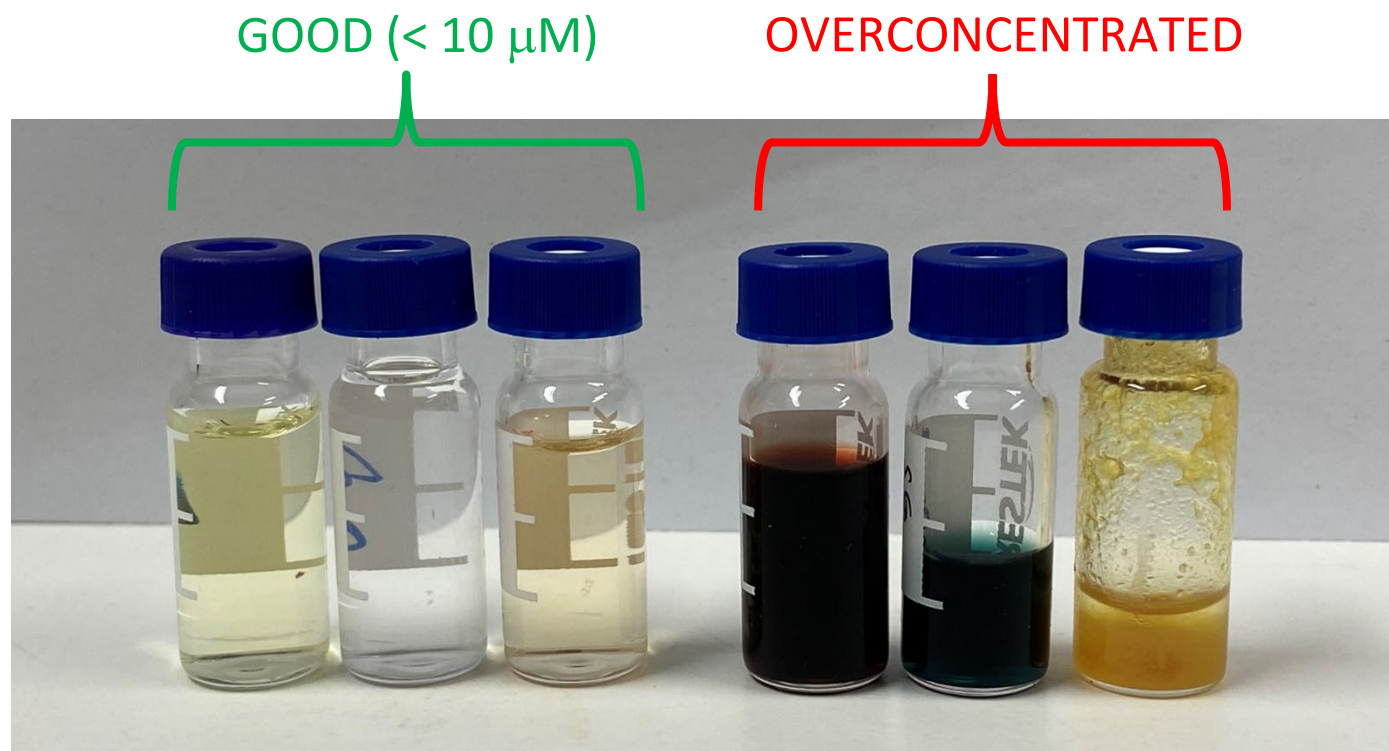
Ms Abigail Dixon
Research Technician in MS

- ESI Accurate Mass Service
- Alternative Ionisation Service (APCI, EI, MALDI)

NB. Samples must be analysed using an OA system before submitting to the services

<http://massspec.chem.ox.ac.uk/services>

Sample preparation



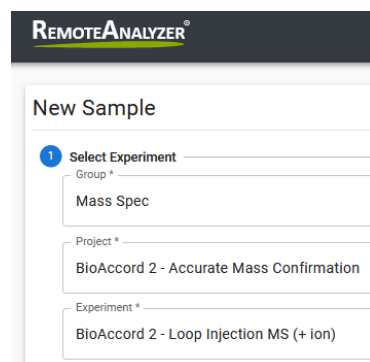
BioAccords: <https://masspec.chem.ox.ac.uk/files/spp-ba-targetconfirmation>

ESI Service: <https://masspec.chem.ox.ac.uk/files/esi-servicespppdf>

Small molecule characterisation services

Submission process

ESI SERVICE:
Submit sample
details online



REMOTEANALYZER

New Sample

1 Select Experiment

Group *

Mass Spec

Project *

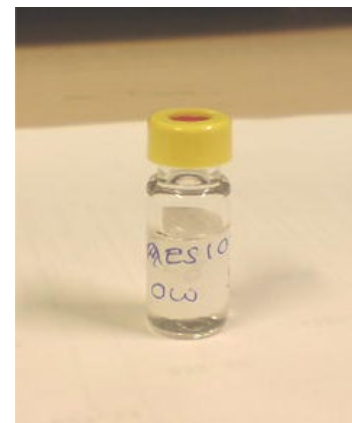
BioAccord 2 - Accurate Mass Confirmation

Experiment *

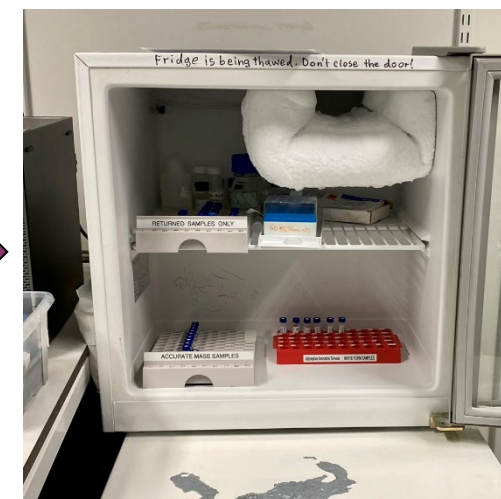
BioAccord 2 - Loop Injection MS (+ ion)



Confirm sample
using tablet

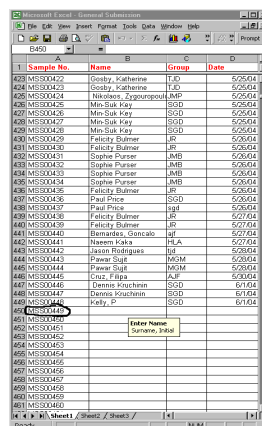


Label sample vial

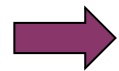


Place labelled samples in
correct tray in sample
submission fridge

AI SERVICE:
Complete white
excel
spreadsheet



Sample No.	Name	Group	Ion
429 MS30042	Gosky, Katherine	TD	5/25/04
424 MS30043	Gosky, Katherine	TD	5/25/04
426 MS30044	Nichols, Zeynep	MD	5/25/04
428 MS30045	Min Suk Kay	SD	5/25/04
427 MS30046	Min Suk Kay	SD	5/25/04
429 MS30047	Min Suk Kay	SD	5/25/04
428 MS30048	Min Suk Kay	SD	5/25/04
430 MS30049	Felcity Sumner	JD	5/25/04
431 MS30040	Felcity Sumner	JD	5/25/04
432 MS30041	Felcity Sumner	JD	5/25/04
433 MS30042	Felcity Sumner	JD	5/25/04
434 MS30043	Felcity Sumner	JD	5/25/04
435 MS30044	Felcity Sumner	JD	5/25/04
436 MS30045	Felcity Sumner	JD	5/25/04
437 MS30046	Paul Price	SD	5/25/04
438 MS30047	Paul Price	SD	5/25/04
439 MS30048	Felcity Sumner	JD	5/25/04
440 MS30049	Felcity Sumner	JD	5/25/04
441 MS30040	Bernardo, Goncalo	JD	5/25/04
442 MS30041	Heaven Kaka	MSA	5/25/04
443 MS30042	Jason Rodriguez	JD	5/25/04
444 MS30043	Pravin Sult	MSA	5/25/04
445 MS30044	Pravin Sult	MSA	5/25/04
446 MS30045	Paul Price	SD	5/25/04
447 MS30046	Denise Kirschner	SD	5/25/04
448 MS30047	Denise Kirschner	SD	5/25/04
449 MS30048	Paul Price	SD	5/25/04
450 MS30049	Paul Price	SD	5/25/04
451 MS30040	Paul Price	SD	5/25/04



MASS SPECTROMETRY RESEARCH FACILITY

Small Molecule Sample Submission Form

This form is for the submission of small molecule samples for MS analysis. It must be completed and submitted to the MSS number and sample details. Please ensure that the sample is correctly labeled and that the form is filled out accurately. The form is to be submitted to the MSS number and sample details. Please ensure that the sample is correctly labeled and that the form is filled out accurately.

Sample Information

Sample Name: [Blank]

Sample ID: [Blank]

Sample Weight: [Blank]

Sample Volume: [Blank]

Sample Concentration: [Blank]

Sample Purity: [Blank]

Sample Solvent: [Blank]

Sample Storage: [Blank]

Sample Handling: [Blank]

Sample Analysis: [Blank]

Sample Results: [Blank]

Sample Comments: [Blank]

Sample Date: [Blank]

Sample Time: [Blank]

Sample Location: [Blank]

Sample Operator: [Blank]

Sample Reviewer: [Blank]

Sample Status: [Blank]

Sample Notes: [Blank]

Sample Instructions: [Blank]



Complete sample submission form including the MSS number
and submit on the 'Q: drive'

<https://massspec.chem.ox.ac.uk/alternative-ionisation>

Large molecule characterisation services



Ms Elisabete Pires
Research Associate in MS



Dr Victor Mikhailov
Research Associate in MS

- Proteomics
- Oligonucleotides
- MALDI - peptides and proteins

- Native state proteins
- MALDI - polymers



<https://massspec.chem.ox.ac.uk/proteomics-service>

Large molecule characterisation services

Submission process



Elisabete.pires@chem.ox.ac.uk

If you have not used biological service before you must first discuss your research requirements with Elisabete Pires.



MASS SPECTROMETRY RESEARCH FACILITY

Department of Chemistry
University of Oxford
MassSpec mass. Oxford
Telephone: +44 (0)1865 275
james.mccoy@chem.ox.ac.uk

MS Facility Sample Submission Form:
Proteomics samples

Please complete 1 form per sample
This form can be found at: <http://www.chem.ox.ac.uk/massspectrometry/mass-spec/index.htm>

Name/Company name: _____ Telephone: _____
Group: _____ email: _____
Project Code/Charge Account*: _____ Date: _____

Sample Information

Sample Type: ☐ Digest (in well) ☐ Digest (in gel) ☐ Cell lysate ☐ Gel band ☐ Purified post

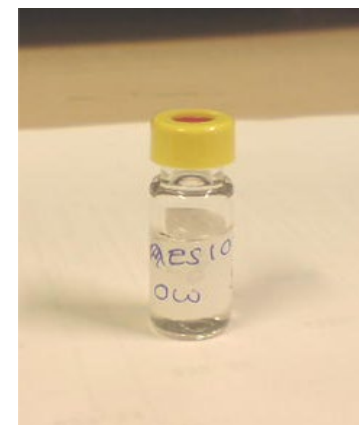
Sample ID: (5 characters or less and as appears on vial) _____
Enzyme used for digestion: _____
Sample volume supplied: _____
Amount of protein digested: _____
Protein name: _____
Sample/buffer solvent: _____
Organism protein is from: _____

Analysis Type **Analysis Required** **Please send/bring amino acid sequence for data analysis**

☐ Untargeted MS/MS (default method)
☐ Targeted MS/MS (please provide precursor (target) mass)
Other information or special instructions: _____

* Note a Project code or Charge account is now compulsory as of 5th Aug 2015. If you do not know which project code to use please discuss with your supervisor or the CHL Finance team. Samples WILL NOT be analysed without a valid code being entered.

Complete PDF proteomics sample submission form



Bring sample and completed form down to basement MS lab and submit to Elisabete in person. There is a freezer for storage of samples.



It can take up to 4 weeks to analyse samples. You should contact Elisabete to check your analysis has completed successfully.

Proteomics protocols and submission form can be found on the website:

<https://massspec.chem.ox.ac.uk/proteomics-service>

Open access systems

BioAccord 1

BioAccord 2

Open access A

Open access B

MS services

ESI accurate mass

Alternative ionisation

Biological molecules

Trained-user systems

LC-MS

GC-MS

MALDI

Collaborative experiments

Metabolomics

Ion mobility

Proteomics

Thermal desorption

Native state

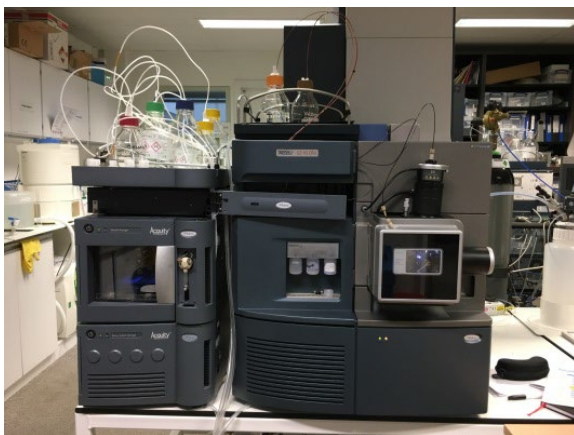
High-throughput

Quantitation

+ many more

Trained-user systems

LC-MS



Waters UPLC – Xevo G2-XS QTOF

- Small molecules
- Complex mixtures
- Peptides
- Proteins



Waters UPLC – Xevo G2-S QTOF

- Small molecules
- Complex mixtures
- Peptides
- Proteins



Waters UPLC – Xevo G2 QTOF

- Oligonucleotides

Training available on request: <https://massspec.chem.ox.ac.uk/trained-user>

Trained-user systems

MALDI



Bruker Autoflex Speed TOF-TOF

- Peptides
- Proteins
- Oligonucleotides
- Polymers
- Small molecules > 450 Da

GC-MS



Agilent 5977B

- Volatile small molecules
- Complex mixtures amenable to EI

Training available on request: <https://massspec.chem.ox.ac.uk/trained-user>

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Native state

High-throughput

Quantitation

+ many more

Collaborative experiments



Nanospray

Quantitation



Metabolomics

Air-sensitive



GC-FID

Native state

Ion mobility



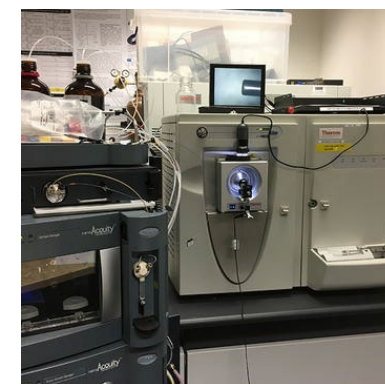
High throughput screening

ASAP



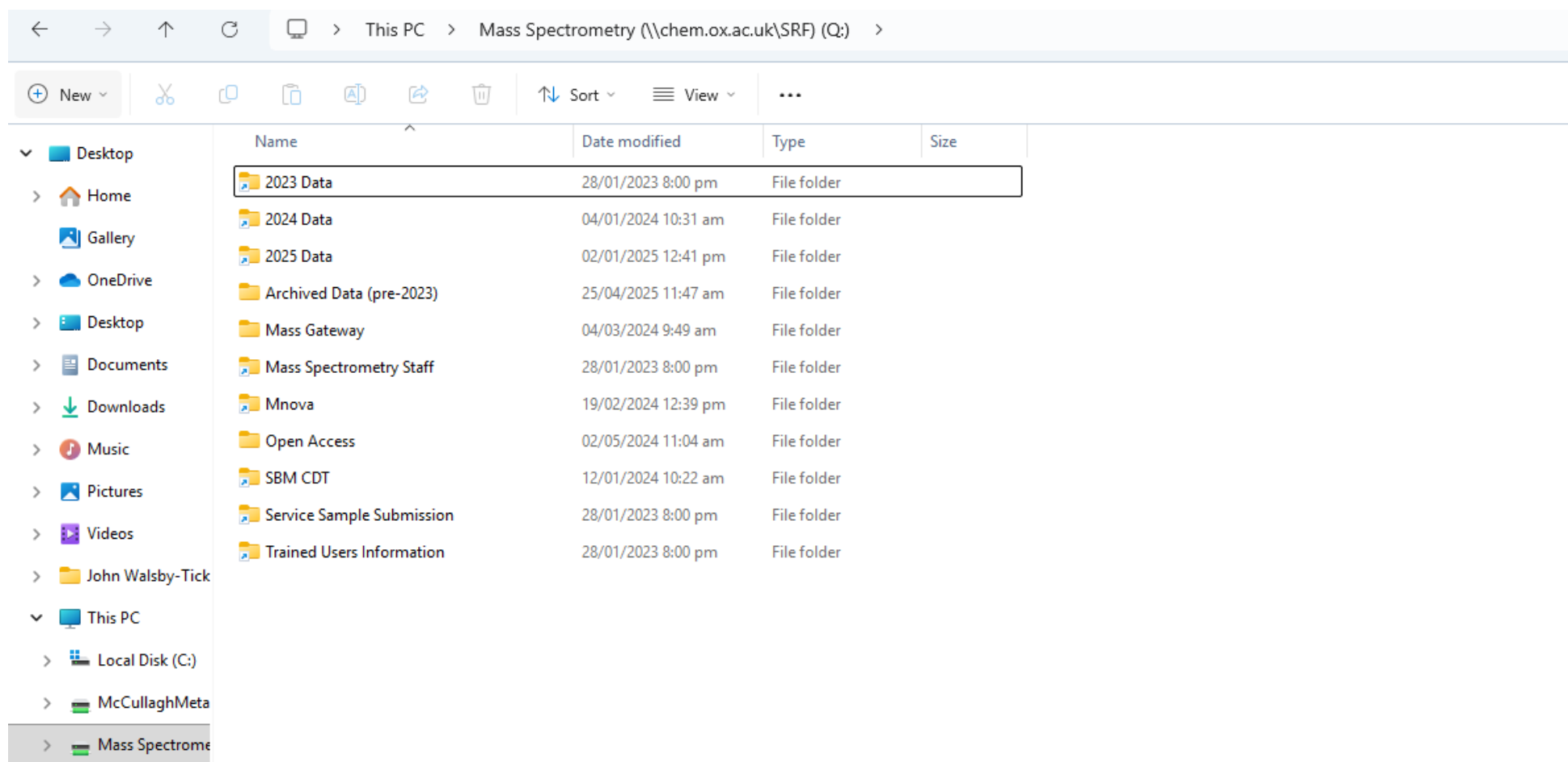
Thermal desorption

Live-cell assays



Proteomics

Data storage (Q: drive)



Name	Date modified	Type	Size
2023 Data	28/01/2023 8:00 pm	File folder	
2024 Data	04/01/2024 10:31 am	File folder	
2025 Data	02/01/2025 12:41 pm	File folder	
Archived Data (pre-2023)	25/04/2025 11:47 am	File folder	
Mass Gateway	04/03/2024 9:49 am	File folder	
Mass Spectrometry Staff	28/01/2023 8:00 pm	File folder	
Mnova	19/02/2024 12:39 pm	File folder	
Open Access	02/05/2024 11:04 am	File folder	
SBM CDT	12/01/2024 10:22 am	File folder	
Service Sample Submission	28/01/2023 8:00 pm	File folder	
Trained Users Information	28/01/2023 8:00 pm	File folder	

High resolution MS
data is LARGE

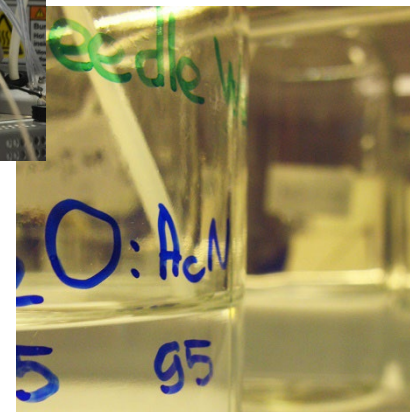
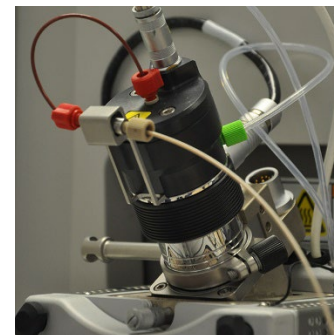
>150 TB RAID array

Networked storage

Research group
subfolders

Safety in the MS labs

- No lab coats to be worn in any of the MS labs.
- Never remove or modify any part of the mass spectrometer, sample inlet system or software.
- If something is not working properly or appears to be broken please report it to a member of the MS Facility staff.
- Please read safety information on the mass spectrometry website and all information provided on laminated sheets around the instruments.
- Follow the booking rules outlined on the intranet: <https://unioxfordnexus.sharepoint.com/sites/CHEM-Facilities/SitePages/Instrument-booking-and-analytical-services.aspx#mass-spectrometry>



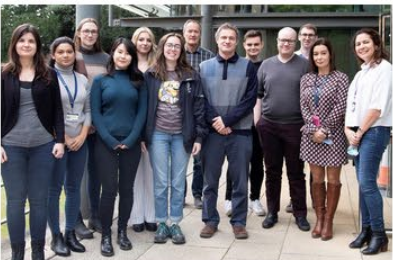
MS-SRF Website <https://massspec.chem.ox.ac.uk/>



Mass Spectrometry Research Facility
Chemistry Research Laboratory, University of Oxford

[Status Page](#)
[Booking System](#)
[McCullagh Research Group](#)
[Department of Chemistry](#)

[Home](#)
[People](#)
[Open Access](#)
[Trained-Users](#)
[Services](#)
[Collaborations](#)
[Instruments](#)
[Protocols](#)
[Other Information](#)



People



Open Access



Trained-Users



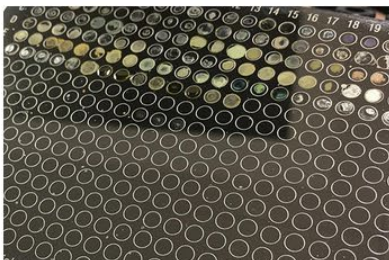
Services



Collaborations



Instruments



Protocols



Other Information

Induction and training

Open Access systems

To start using the MS open access systems and submission services you will need to complete some online training followed by short in-person induction session. You must complete the training before using open access MS instrumentation and services.

In-person inductions

Thursday 2nd October - 1pm, 2pm, 3pm [Ptilis ONLY]

Friday 3rd October - 9am, 10am, 11am, 1pm, 2pm, 3pm

Monday 6th October - 9am, 10am, 2pm, 3pm

Tuesday 7th October - 9am, 10am

Other instrument training

See website for information on trained user instruments and how training is organised. If you require training please contact John Walsby-Tickle.
john.walsby-tickle@chem.ox.ac.uk



QR code takes you to the booking forms for the training sessions.

Here to help you



Dr Victor Mikhailov

Research Associate in MS

Tel: 75687, victor.mikhailov@chem.ox.ac.uk

Areas of focus

MALDI, accurate mass analysis, native state proteins, open access, direct probe MS & MS services



Dr John Walsby-Tickle

Mass Spectrometry Services Manager

Tel: 85025, john.walsby-tickle@chem.ox.ac.uk

Areas of focus

Training & maintenance, small molecule analysis, metabolomics, infrastructure, IT & MS software



Ms Abigail Dixon

Research Technician in MS

Tel: 85024, abigail.dixon@chem.ox.ac.uk

Areas of focus

Quantitation, LC-MS
Sample preparation



Ms Elisabete Pires

Research Associate in Biological MS

Tel: 75942, elisabete.pires@chem.ox.ac.uk

Areas of focus

Proteomics, metabolomics, biological MS, LC-MS, MALDI (biological) & sample preparation



Prof James McCullagh

Director of the Research Facility

Tel: 75657, james.mccullagh@chem.ox.ac.uk

Areas of focus

LC-MS, metabolomics, isotope tracer experiments, orbitrap MS & quantitation

QR for MS training



DEPARTMENT OF
CHEMISTRY



UNIVERSITY OF
OXFORD

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