9.00 - 9.30	**Introduction to Mass Spectrometry facilities** The mass spectrometry induction session will introduce researchers to the Mass Spectrometry Research Facility, its staff, instrumentation and services and how you can access these. We will provide information about open Access mass spectrometers, trained-user instruments, including GC-MS and LC-MS, and advanced and specialised instrumentation and techniques. We will explain how the sample submission services work and provide details on how to sign up for a tour of the facility and open access training (bring your mobile phone to book during the session). *It is essential that anyone planning to use the Mass Spectrometry facilities attends this induction session.*	**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. *It is essential that anyone wishing to make use of the NMR facilities attend this induction session*	**Nick Rees & Harry Mackenzie**
10.15 – 10.30	***Break***	
	Introduction to Powder X-Ray Diffraction and Magnetometry Apologies I cannot be there today. If you're planning to use X-ray diffraction on powders or films, use SQUID magnetometry to assess magnetic properties, or measure thermal conductivity of a bulk sample then you'll want to use the Inorganic Materials Characterisation facility. Most resources and information to get you started can be found on the facility website https://imc.web.ox.ac.uk. A video talking you through the registration processes and where to look on the website for these can be found here.	**Simon Cassidy**
10.30 – 10.50	**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. It will explain how the instruments can be accessed and the training that is required to use them.	**Will Myers**

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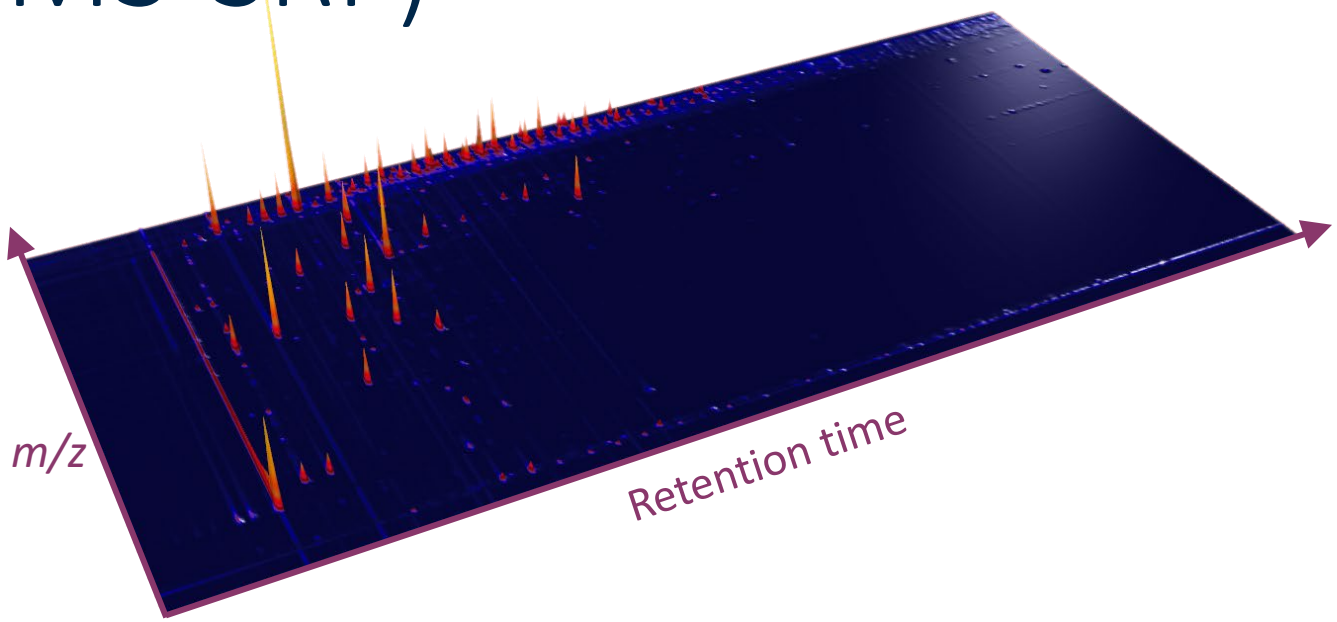
Introduction to the Mass Spectrometry Research Facility (MS-SRF)

Professor James McCullagh
Dr John Walsby-Tickle
Scientific Induction 2024



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

↓

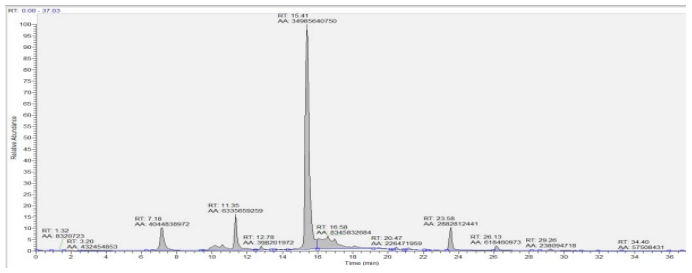
$C_6H_{13}O_9P$

↓

Glucose-1-phosphate

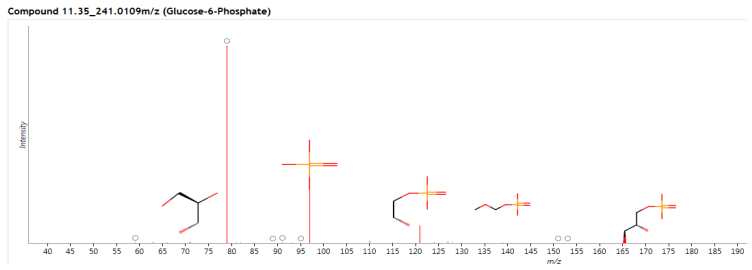
Separation & Quantification

Relative and absolute: LC-MS, GC-MS

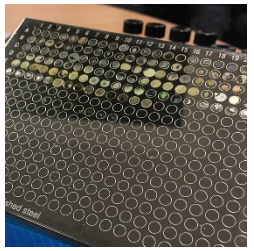


Structural analysis

Fragmentation studies using MS



'Omics', structural, synthetic and systems biology



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MS-SRF Staff

Ms Elisabete Pires
Research Associate in MS

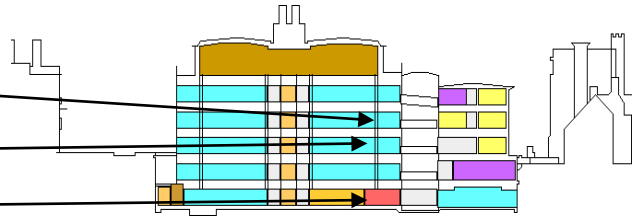
Dr Victor Mikhailov
Research Associate in MS

Dr John Walsby-Tickle
MS Services Manager

Prof James McCullagh
Director of the MS-SRF

+ New Research Technician in MS
In recruitment

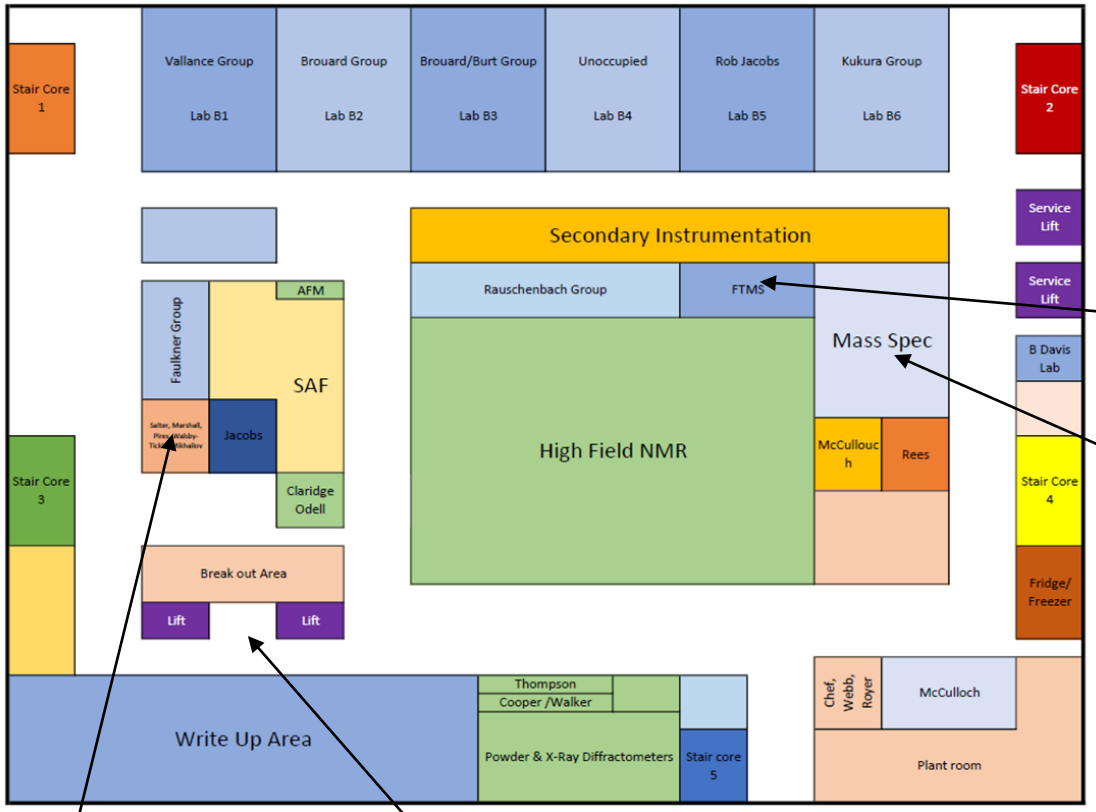
MS Labs

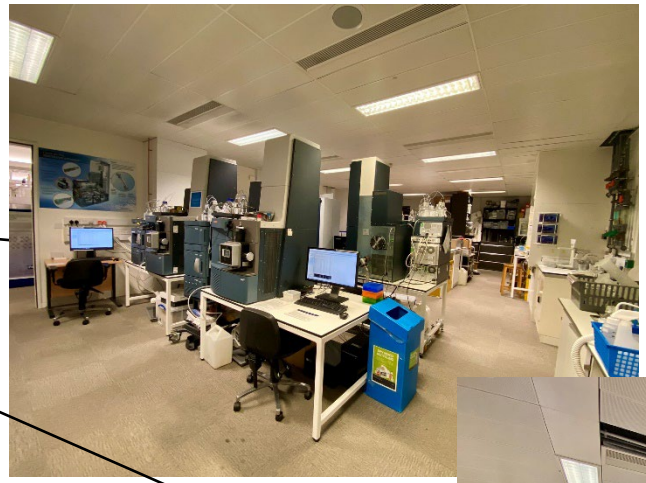


1st Floor: Submission service

Ground Floor: Open access MS labs

Basement: Main MS labs





MS staff offices

Scenic lifts

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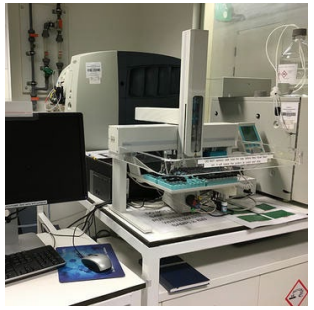
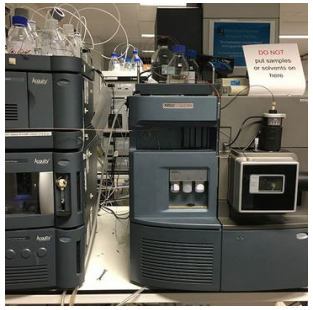
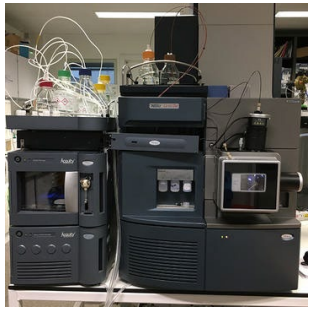
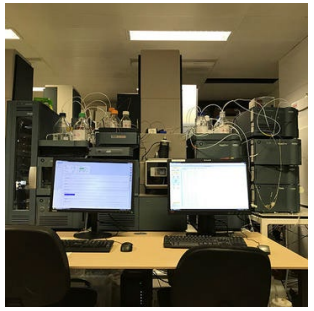
20+ Mass Spectrometers

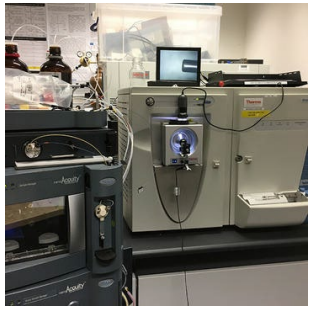






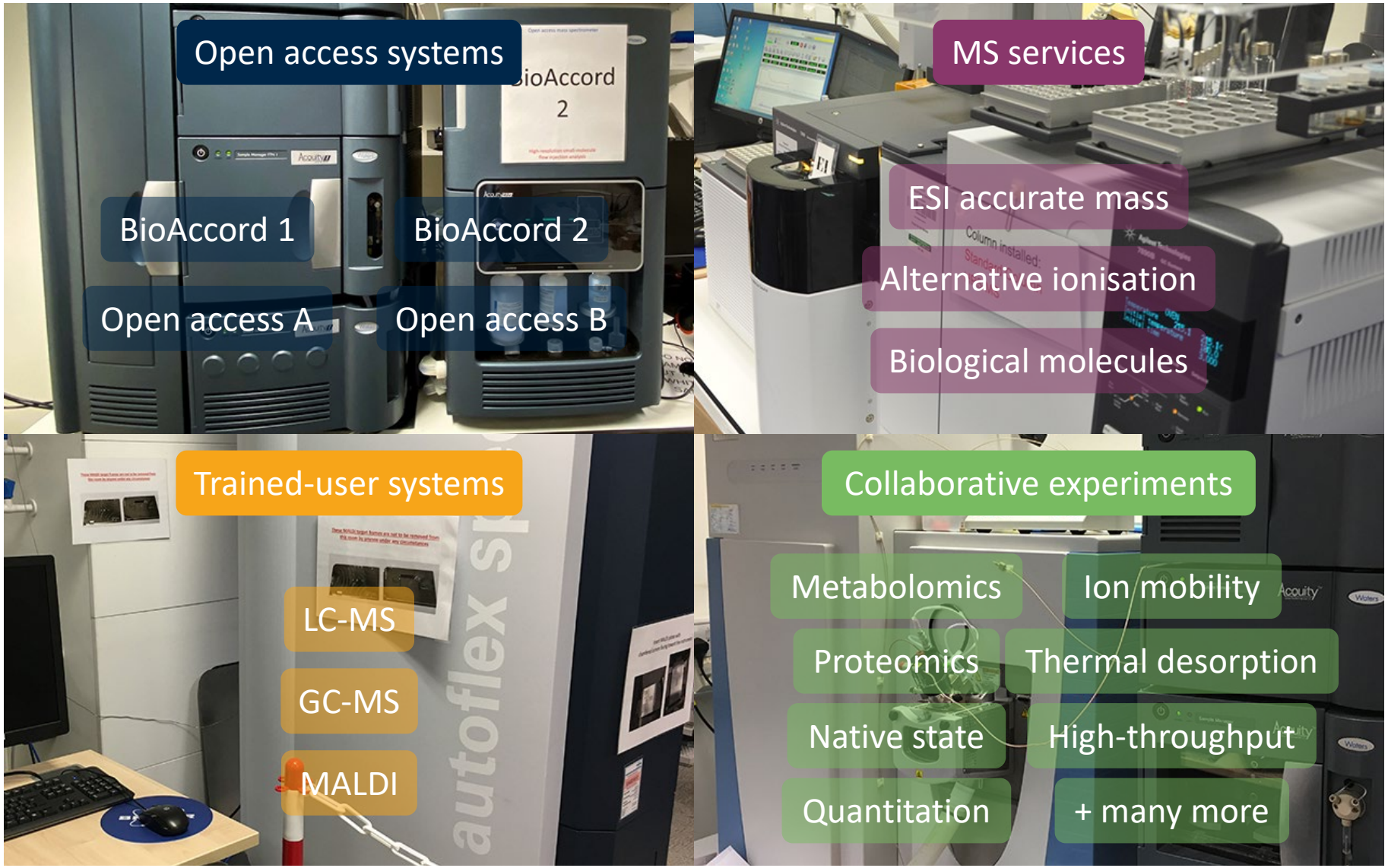






+

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

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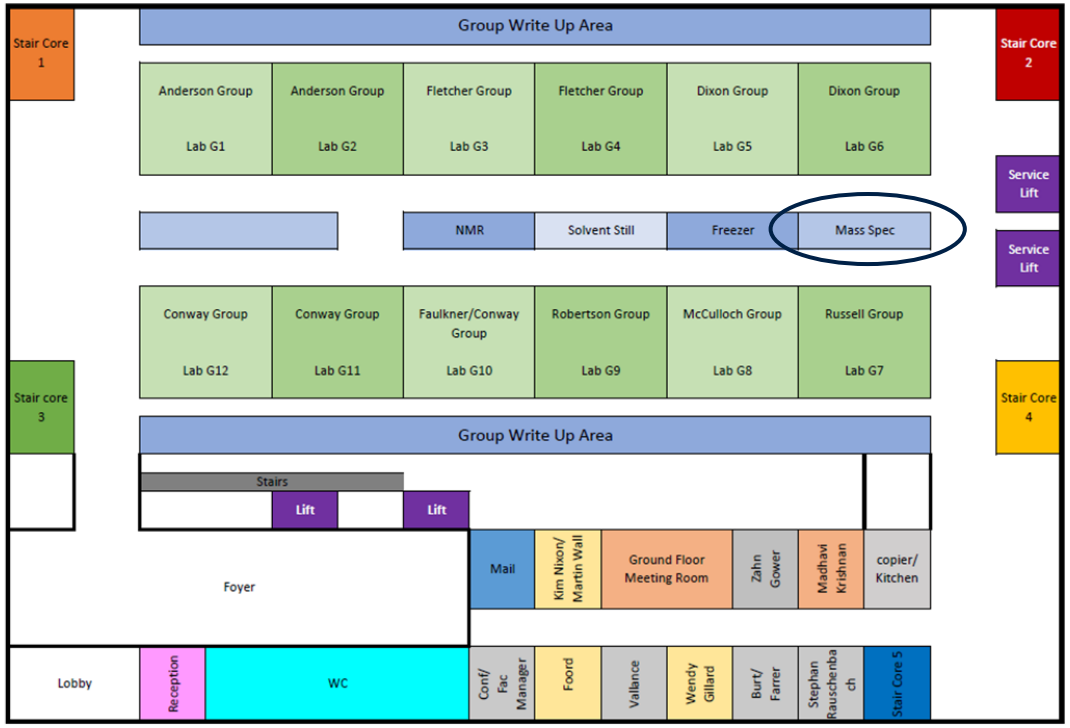
Open Access Systems

Victor Mikhailov

Research Associate in MS

Runs open access systems and small molecule services

Ground Floor



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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

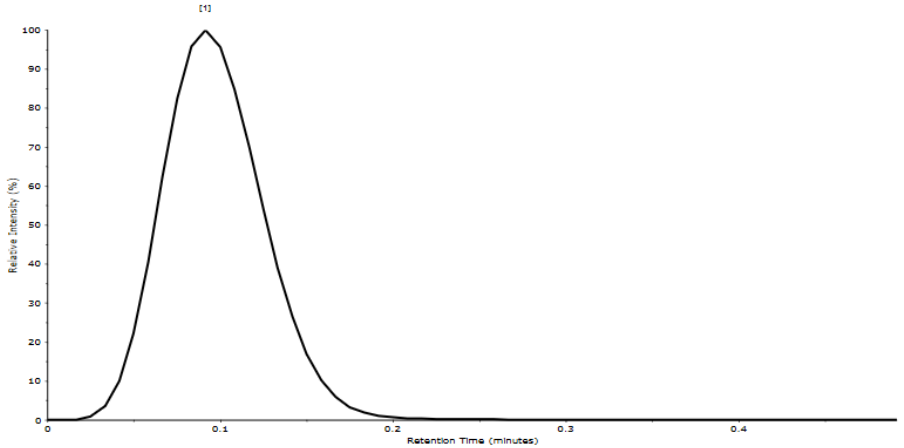
Submitter: John Walsby-Tickle
Project: BioAccord 2 - Accurate Mass Confirmation
Instrument: BioAccord 2

Adduct: +H

Proposed Formula: $C_{28}H_{37}N_5O_7$

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		C14H27OSi, 1.8 Error (ppm), Target m/...
☐	2915	dmjc734C		C28H37O5, 2.1 Error (ppm) [S], C28H36...
☐	2914	dmjc734B		C26H41O5, 0.8 Error (ppm), C26H40O5...

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Open access systems

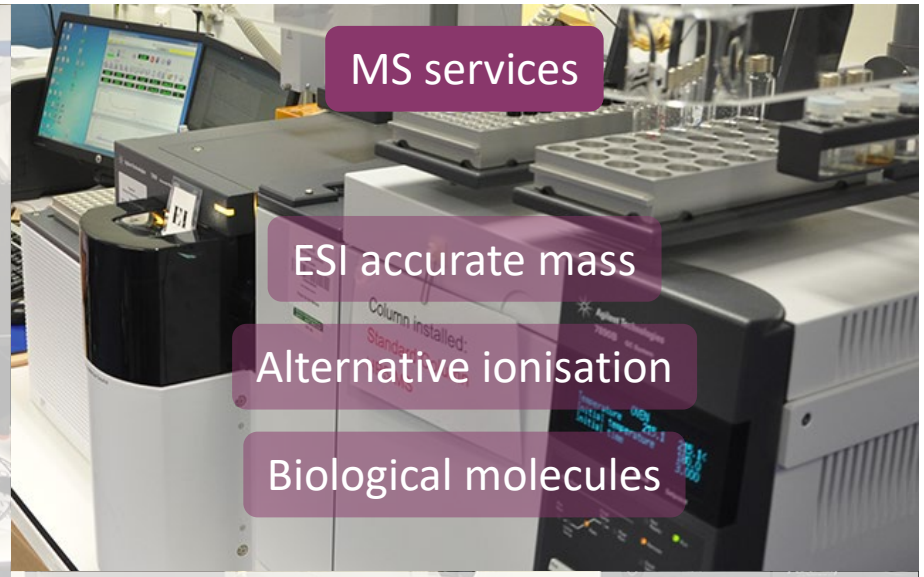
BioAccord 1

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

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Small molecule characterisation services
Organic and inorganic

First Floor

Dr Victor Mikhailov
Research Associate in MS

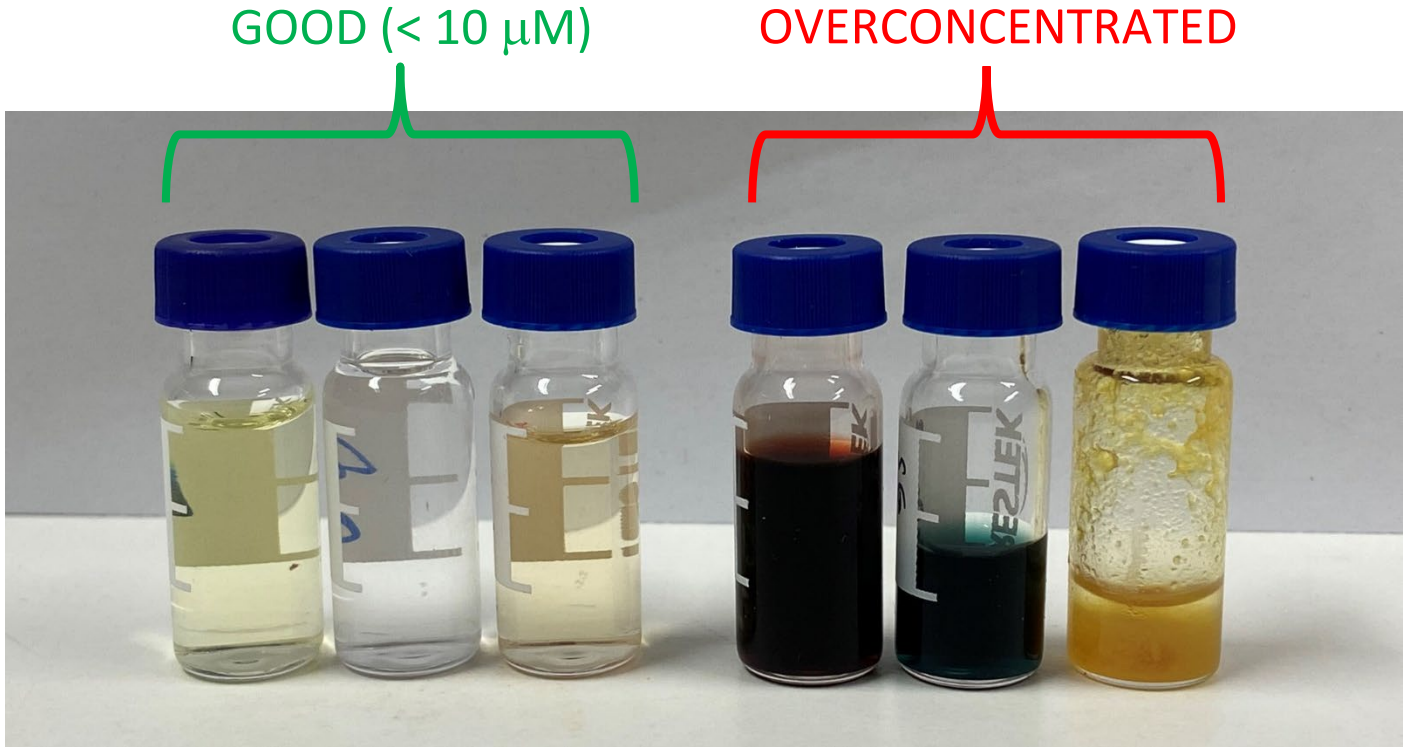
Dr John Walsby-Tickle
MS Services Manager

- 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

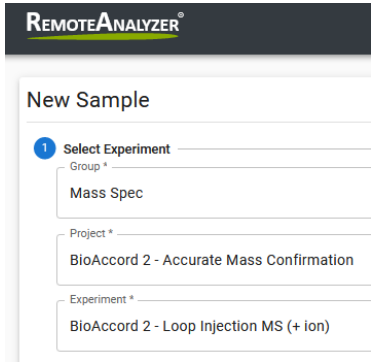


BioAccords: https://massspec.chem.ox.ac.uk/files/spp-ba-targetconfirmation

ESI Service: https://massspec.chem.ox.ac.uk/files/esi-servicespppdf

Small molecule characterisation services
Submission process

ESI SERVICE:
Submit sample details online

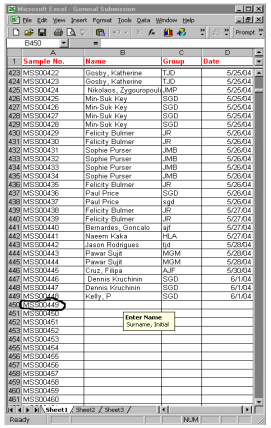


Confirm sample using tablet

Label sample vial

Place labelled samples in correct tray in sample submission fridge

AI SERVICE:
Complete white excel spreadsheet



Complete sample submission form including the MSS number and submit on the 'Q: drive'
https://massspec.chem.ox.ac.uk/alternative-ionisation

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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
Mansfield road, Oxford
Telephone: +44 (0)1865 275
james.mccullagh@chem.ox.ac.uk

Reset Form | Print Form

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/spectroscopy/mass-spec/index.html

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

Sample Information

Sample Type: Digest (in sol) Digest (in gel) Cell lysate Gel band Purified prot

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:

e.g. samples in hexane/ thermally unstable, air sensitive, etc.

* 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 CRL 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

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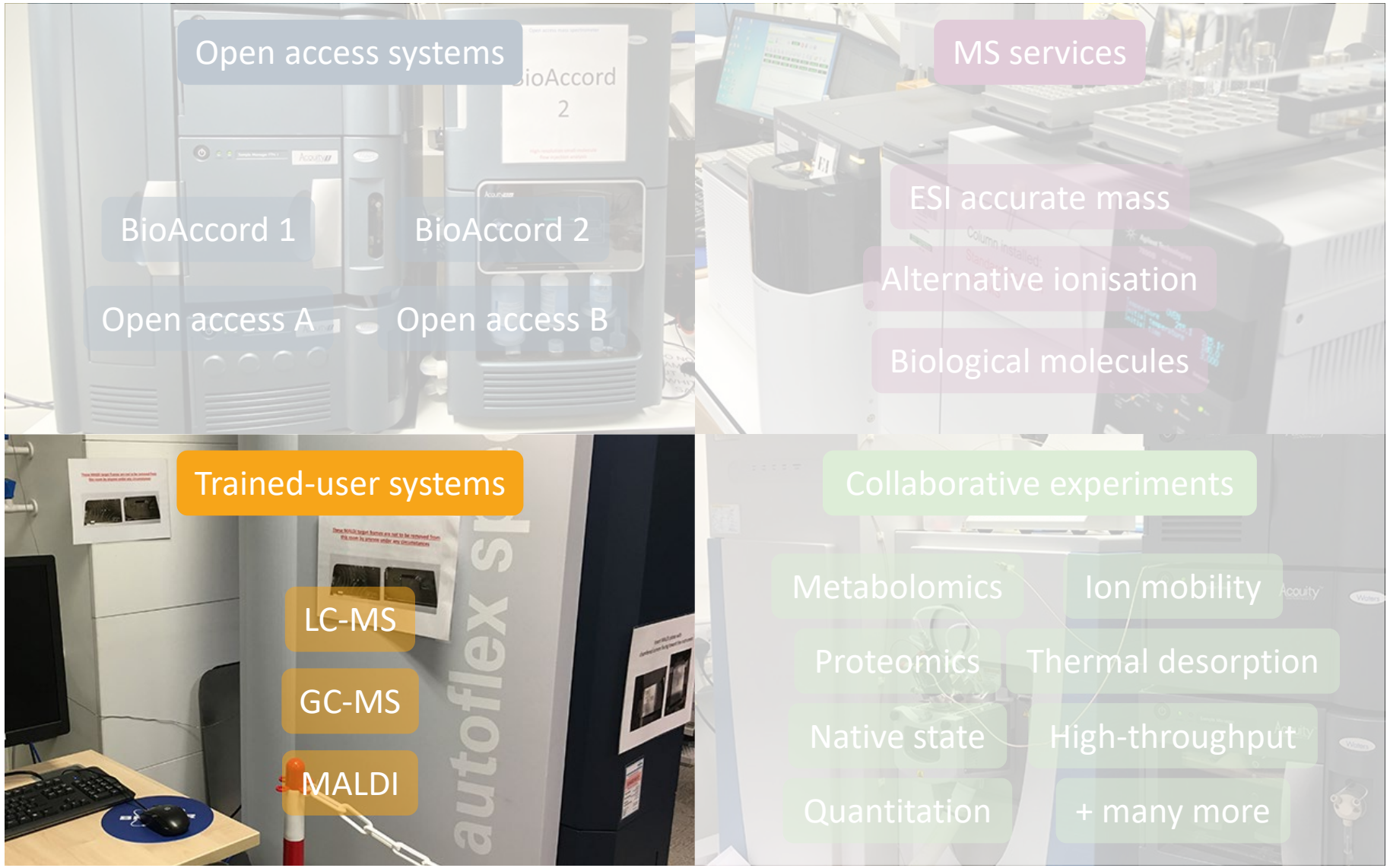

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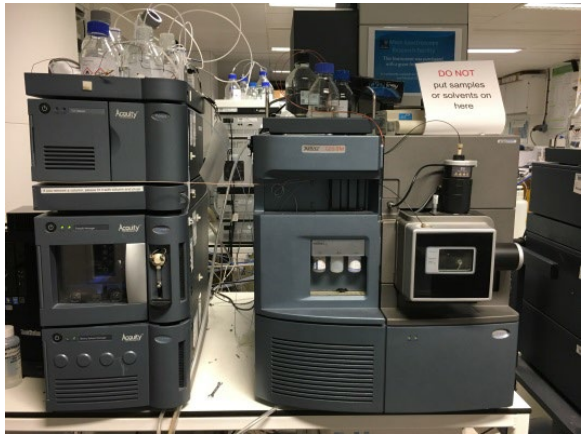
Trained-user systems
LC-MS

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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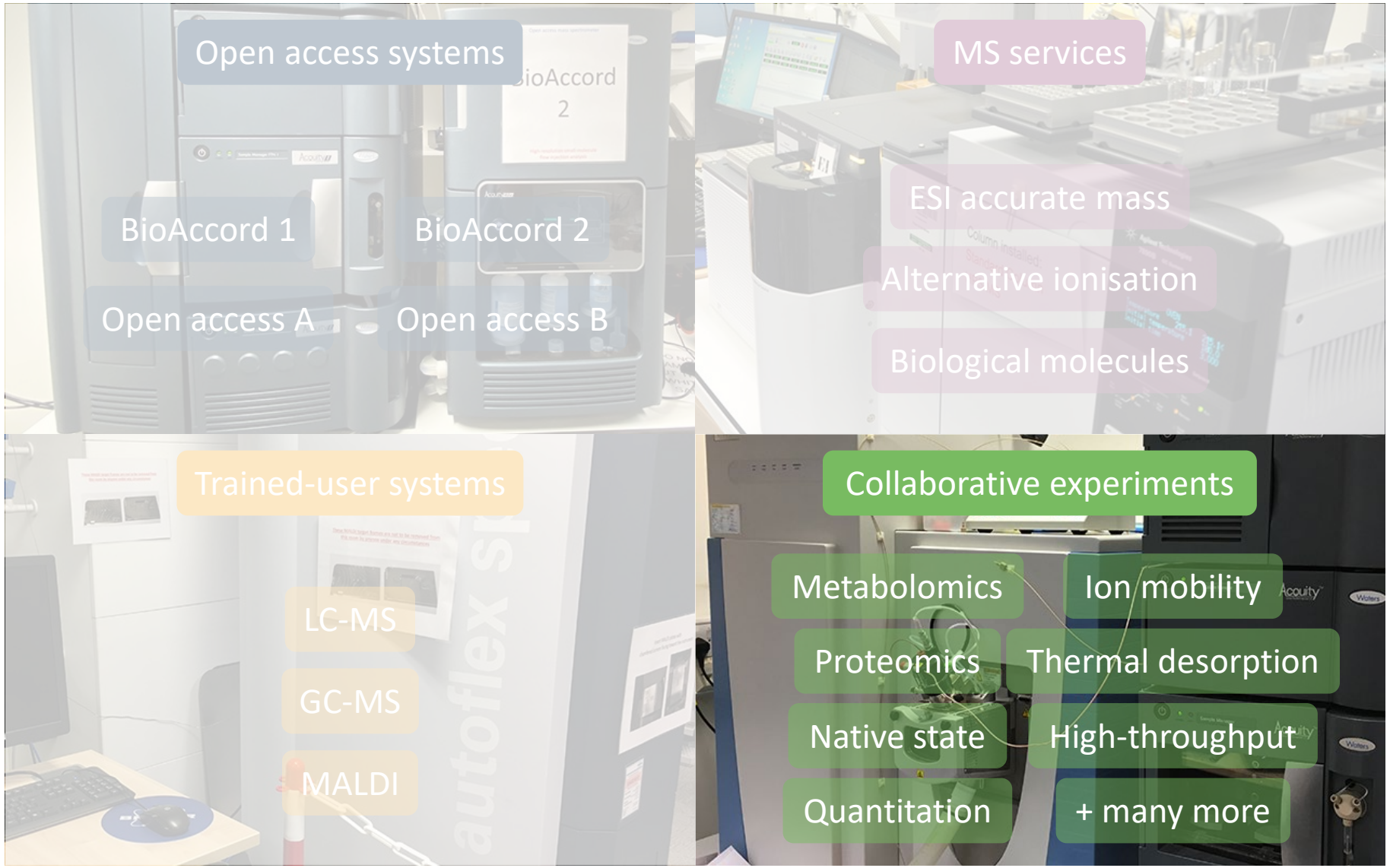


Collaborative experiments

Quantitation

Air-sensitive

Native state

Nanospray

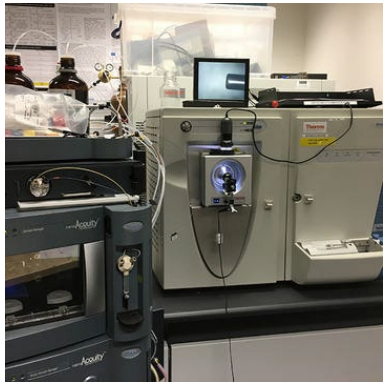
Metabolomics

GC-FID

Ion mobility

ASAP

Live-cell assays



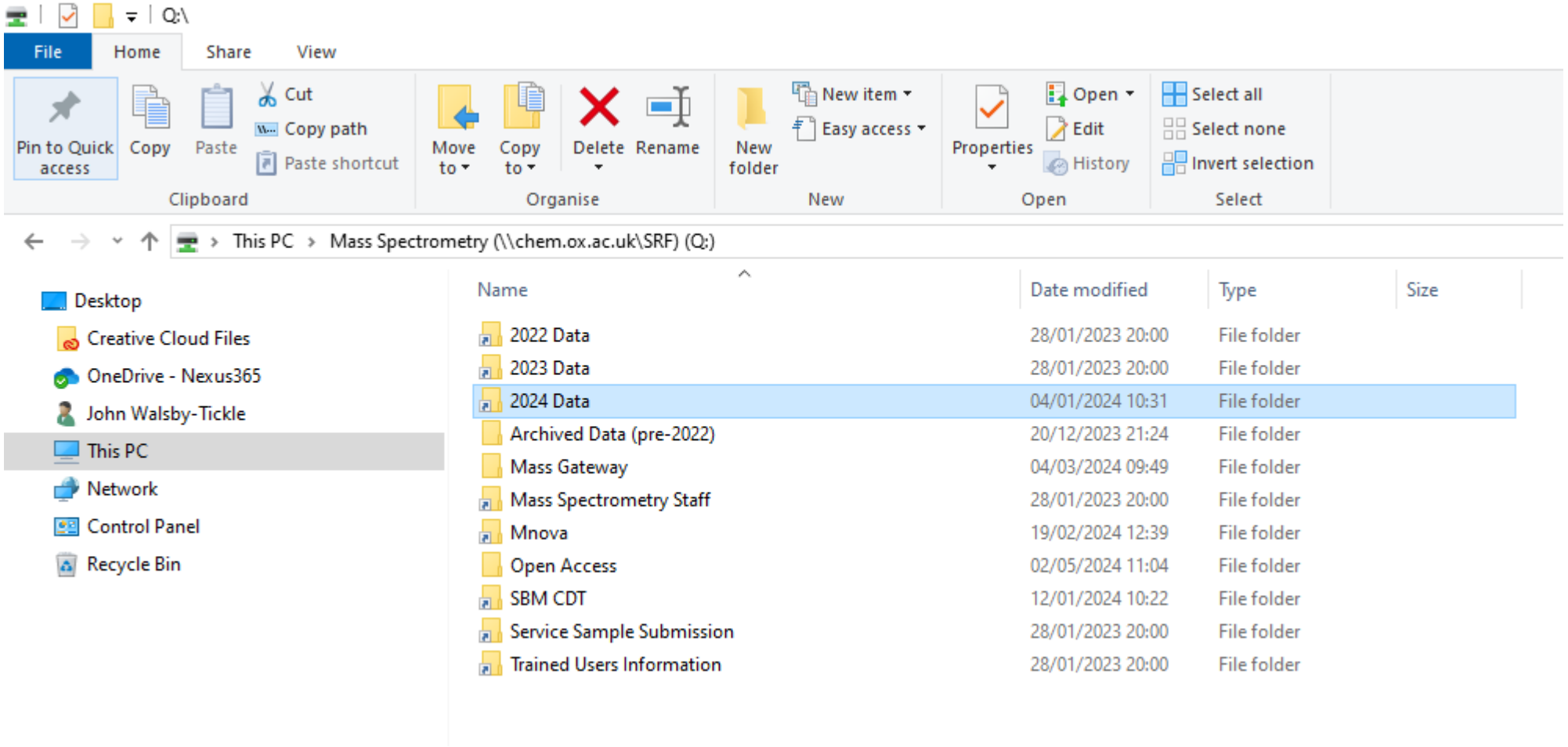
High throughput screening

Thermal desorption

Proteomics

https://massspec.web.ox.ac.uk/collaboration

Data storage (Q: drive)



High resolution MS data is LARGE

>150 TB RAID array

Networked storage

Research group subfolders

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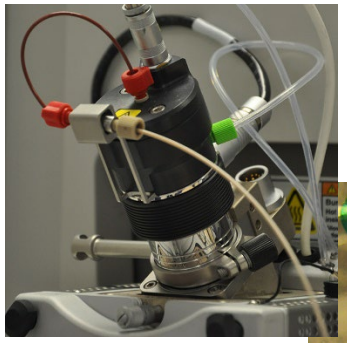
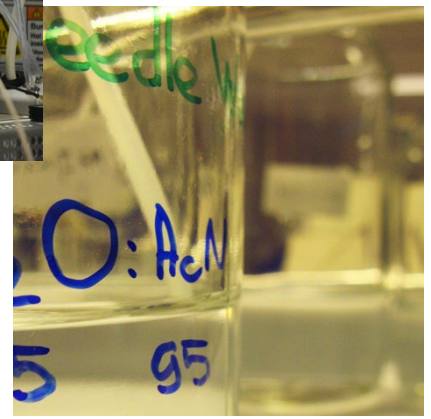
Safety in the MS labs





- 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#booking-rules

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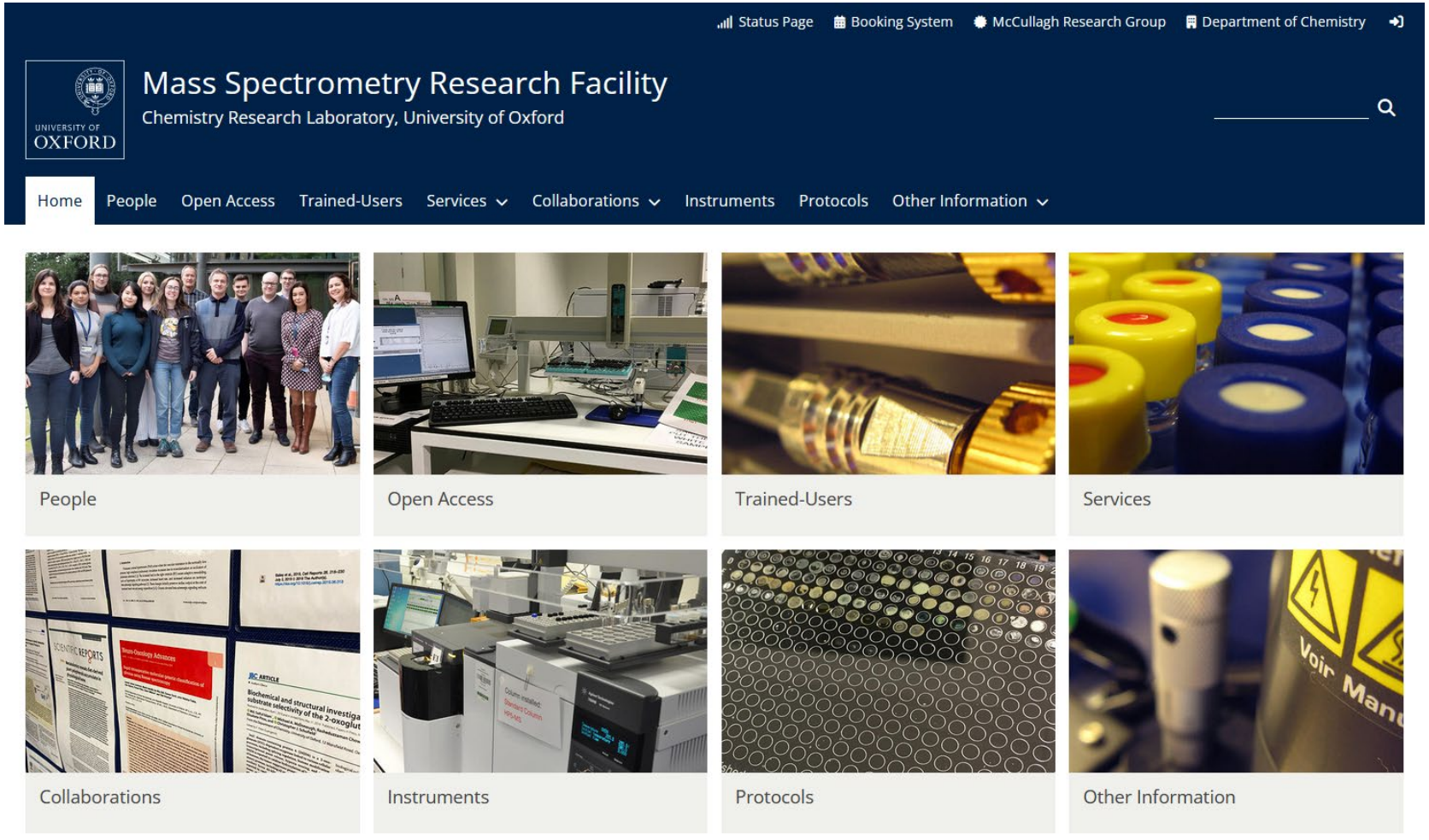
MS-SRF Website https://massspec.chem.ox.ac.uk/



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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

Wednesday 2nd October - 1pm, 2pm, 3pm

Thursday 3rd October - 1pm, 2pm, 3pm

Friday 4th October - 9am, 10am, 11am

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.

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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
Probe MS
MS services

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

Dr John Walsby-Tickle
Mass Spectrometry Services Manager
Tel: 85025, john.walsby-tickle@chem.ox.ac.uk

Areas of focus
Manages training & maintenance
Small molecule analysis
Metabolomics
Infrastructure
IT and software for MS

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

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QR for MS training

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