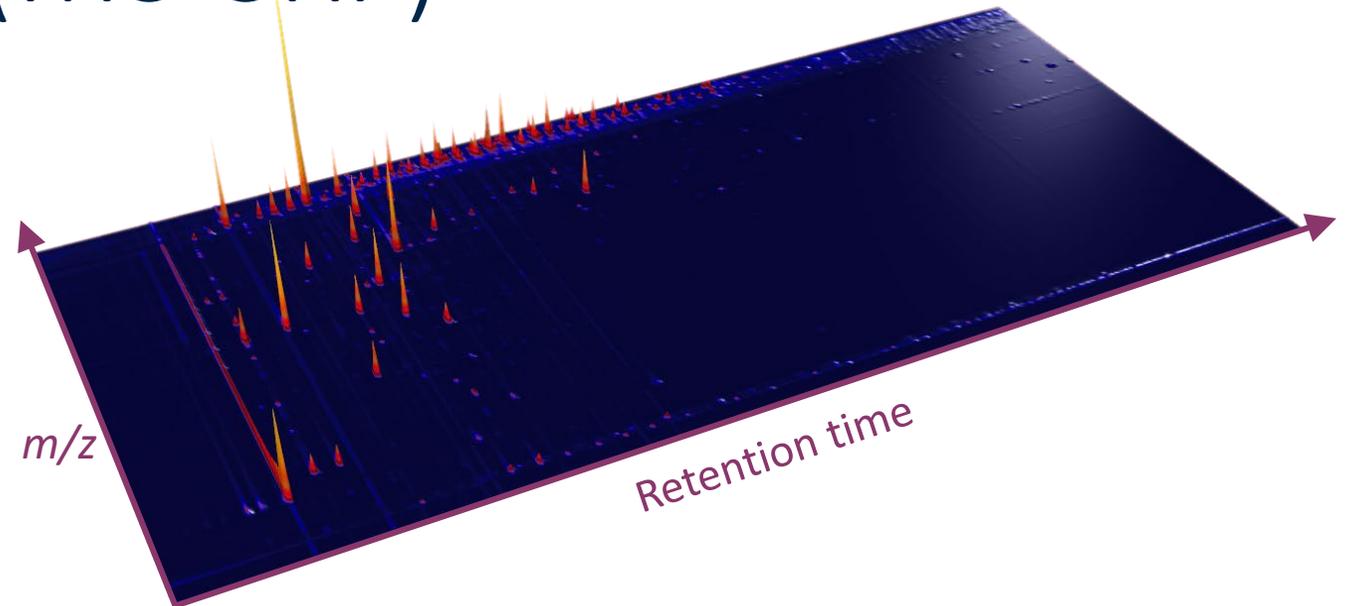


9.00 - 9.30	Introduction to Mass Spectrometry facilities The mass spectrometry induction session will introduce researchers to the Mass Spectrometry Research Facility, its staff, instrumentation and services and how you can access these. We will provide information about open Access mass spectrometers, 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). <i><u>It is essential that anyone planning to use the Mass Spectrometry facilities attends this induction session.</u></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><u>It is essential that anyone wishing to make use of the NMR facilities attend this induction session</u></i>	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

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

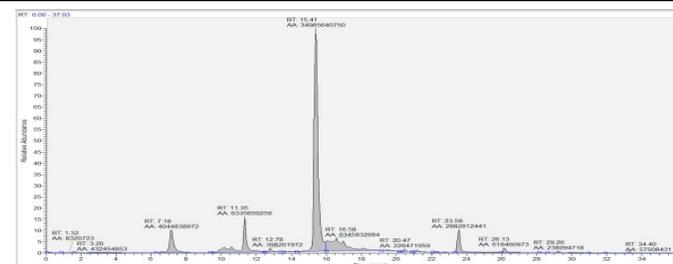


$C_6H_{13}O_9P$

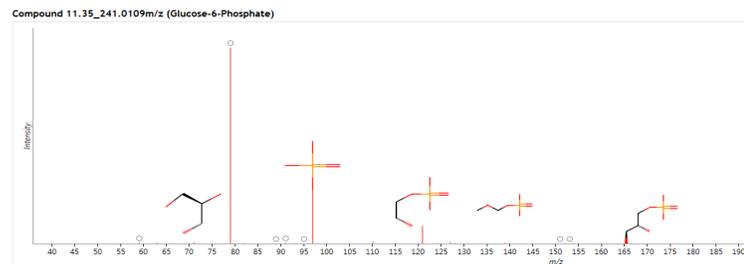


Glucose-1-phosphate

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



Structural analysis Fragmentation studies using MS



'Omics', structural, synthetic and systems biology



MS-SRF Staff



Ms Elisabete Pires
Research Associate in MS



Dr Victor Mikhailov
Research Associate in MS



Dr John Walsby-Tickle
MS Services Manager

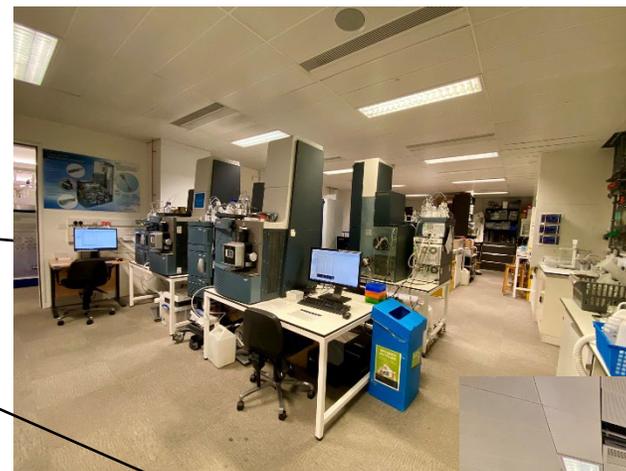
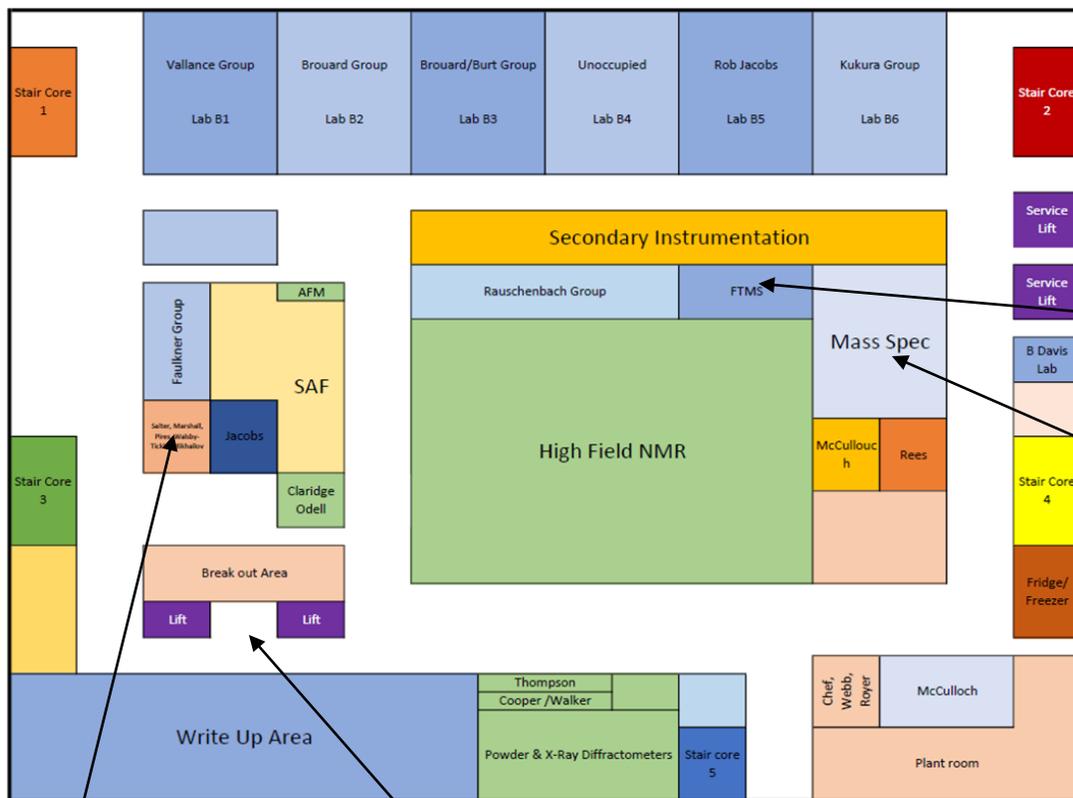
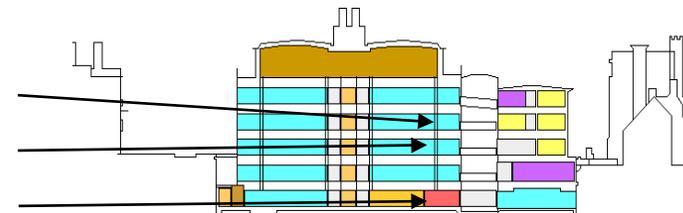


Prof James McCullagh
Director of the MS-SRF

+ New Research Technician in MS
In recruitment

MS Labs

1st Floor: Submission service
 Ground Floor: Open access MS labs
 Basement: Main MS labs

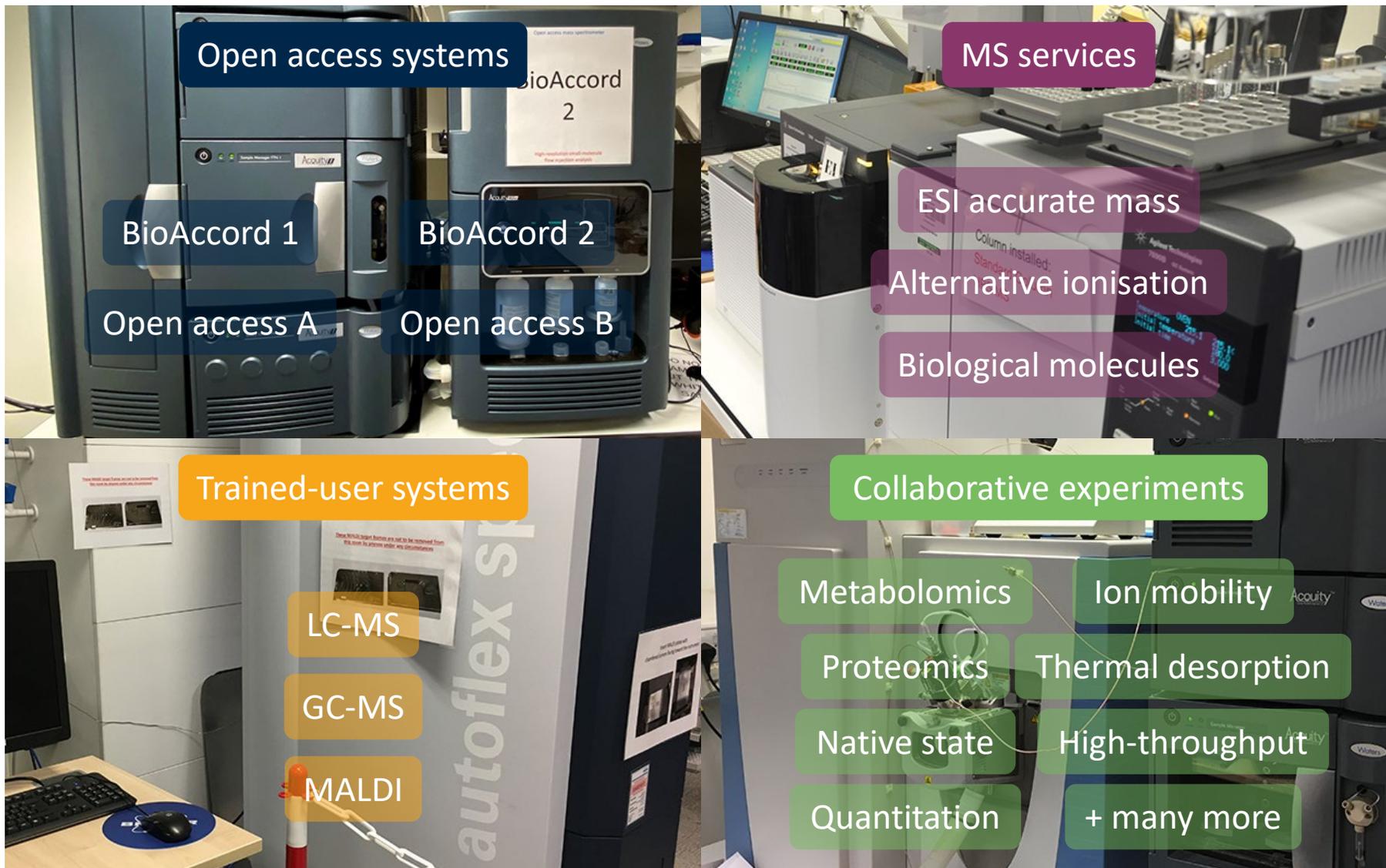


MS staff offices

Scenic lifts

20+ Mass Spectrometers





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

<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

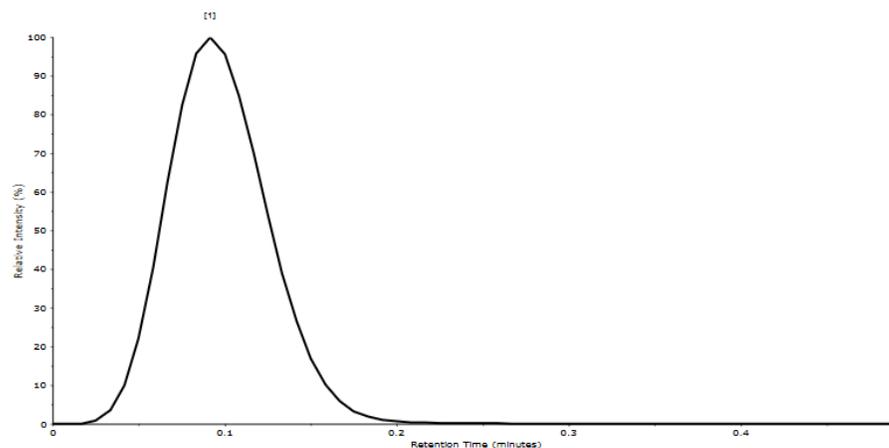
Submitter: John Walsby-Tickle
Project: BioAccord 2 - Accurate Mass Confirmation
Instrument: BioAccord 2

Adduct: +H

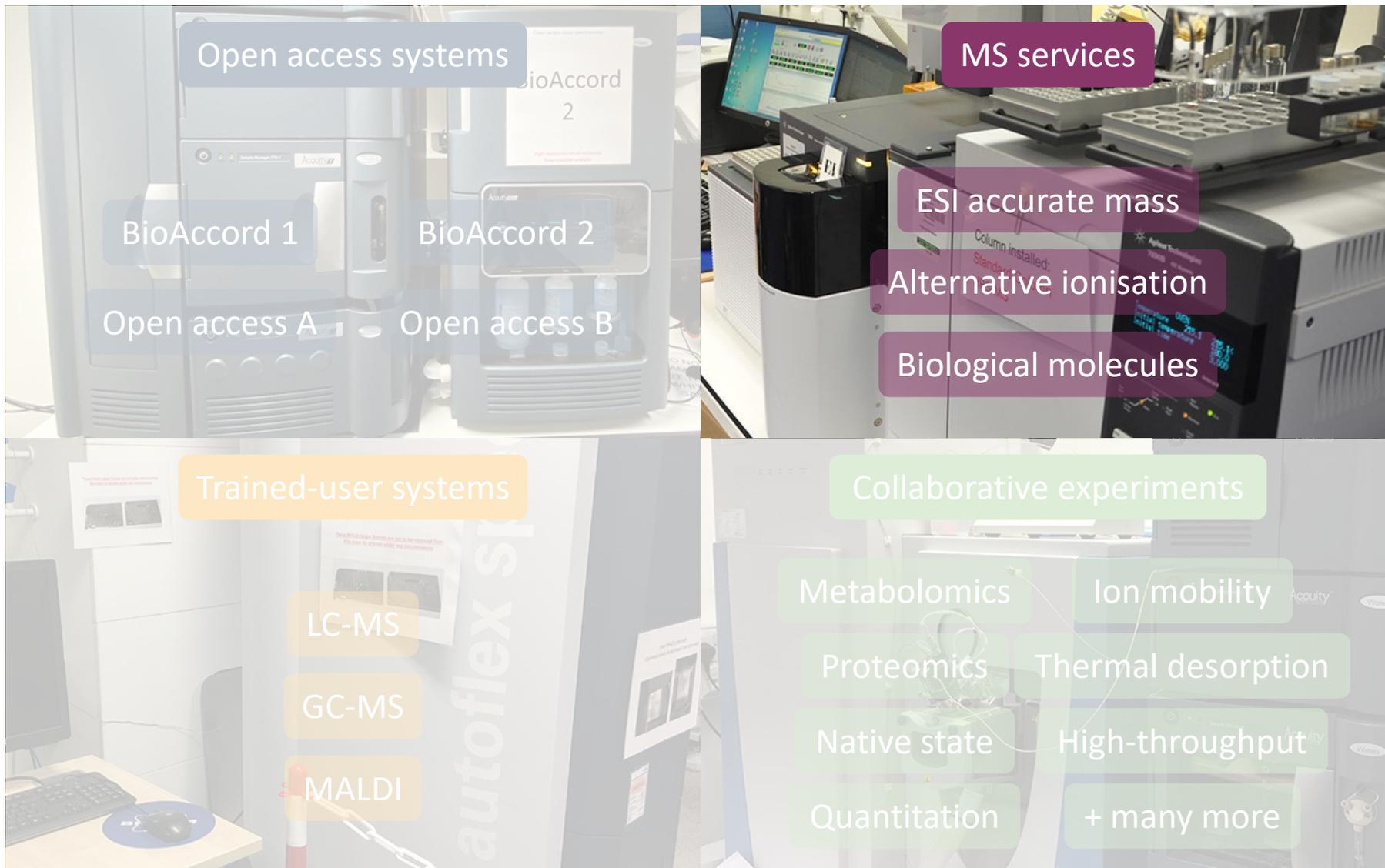
Proposed Formula: C₂₈H₃₇N₅O₇

Additional Comment:

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



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



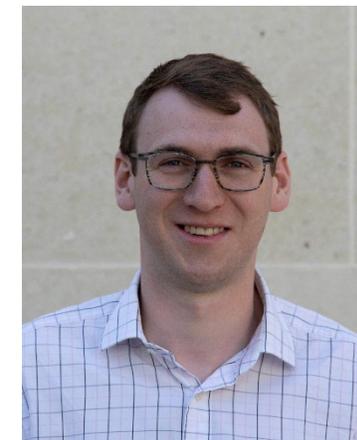
Small molecule characterisation services

Organic and inorganic

First Floor



Dr Victor Mikhailov
Research Associate in MS



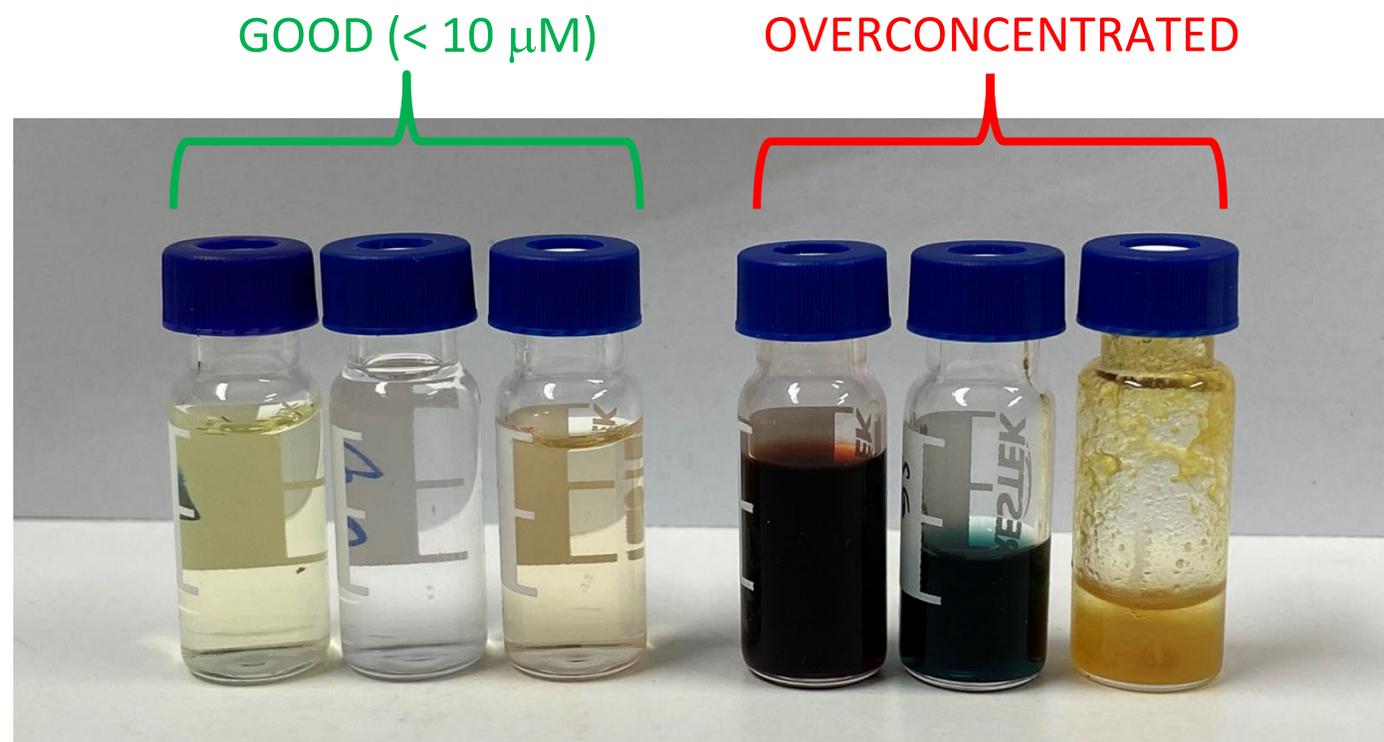
Dr John Walsby-Tickle
MS Services Manager

- 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

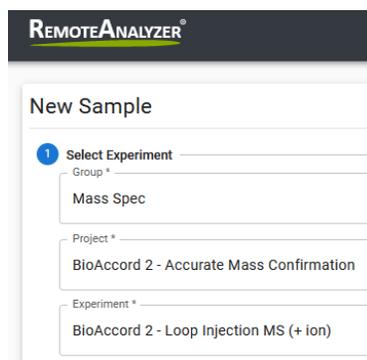


BioAccords: <https://masspec.chem.ox.ac.uk/files/spp-ba-targetconfirmation>

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 *

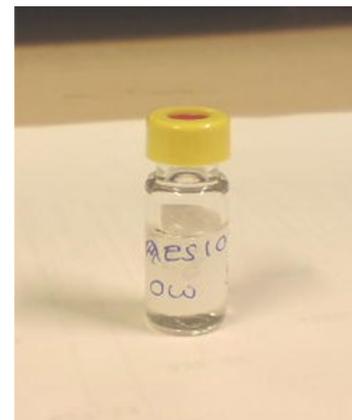
BioAccord 2 - Accurate Mass Confirmation

Experiment *

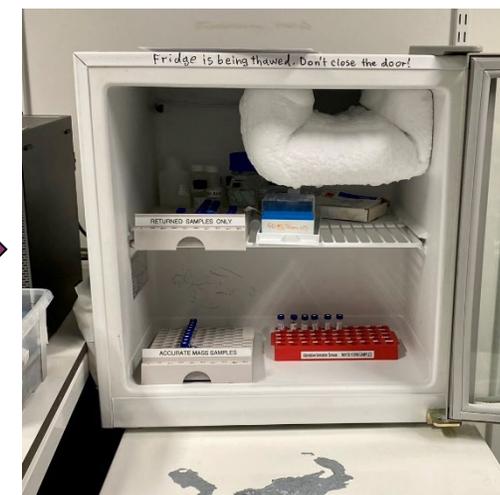
BioAccord 2 - Loop Injection MS (+ ion)



Confirm sample
using tablet

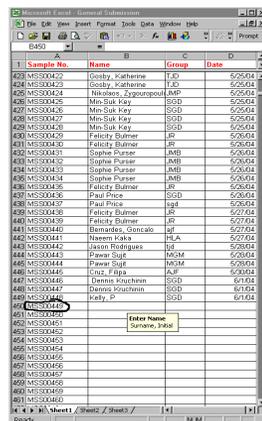


Label sample vial



Place labelled samples in
correct tray in sample
submission fridge

AI SERVICE:
Complete white
excel
spreadsheet



Sample No.	Name	Group	Date
423	MS30042	Gosky, Katherine	15/05/2014
424	MS30043	Gosky, Katherine	15/05/2014
425	MS30044	Nikolaev, Zvezdana	15/05/2014
426	MS30045	Min Suk Kay	15/05/2014
427	MS30046	Min Suk Kay	15/05/2014
428	MS30047	Min Suk Kay	15/05/2014
429	MS30048	Min Suk Kay	15/05/2014
430	MS30049	Falcu, Sumner	15/05/2014
431	MS30050	Falcu, Sumner	15/05/2014
432	MS30051	Falcu, Sumner	15/05/2014
433	MS30052	Sophie Purser	15/05/2014
434	MS30053	Sophie Purser	15/05/2014
435	MS30054	Sophie Purser	15/05/2014
436	MS30055	Falcu, Sumner	15/05/2014
437	MS30056	Paul Price	15/05/2014
438	MS30057	Paul Price	15/05/2014
439	MS30058	Falcu, Sumner	15/05/2014
440	MS30059	Falcu, Sumner	15/05/2014
441	MS30060	Bernalda, Goncalo	15/05/2014
442	MS30061	Naveen Kalia	15/05/2014
443	MS30062	Jason Rodrigues	15/05/2014
444	MS30063	Praveen Staff	15/05/2014
445	MS30064	Praveen Staff	15/05/2014
446	MS30065	Gov. Pappa	15/05/2014
447	MS30066	Dennis Anthonissen	15/05/2014
448	MS30067	Dennis Anthonissen	15/05/2014
449	MS30068	Georg D.	15/05/2014
450	MS30069	Georg D.	15/05/2014



MASS SPECTROMETRY RESEARCH FACILITY

Small Molecule Sample Submission Form

Name: _____

Group: _____

Date: _____

Sample Information

Sample Name: _____

Sample ID: _____

Special instructions: _____

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

Large molecule characterisation services



Ms Elisabete Pires
Research Associate in MS

- Proteomics
- Oligonucleotides
- MALDI - peptides and proteins



Dr Victor Mikhailov
Research Associate in MS

- Native state proteins
- MALDI - polymers



<https://masspec.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
Maxwell Road, 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/submit.htm>

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

Sample Information

Sample Type: Digest (in vial) 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: _____

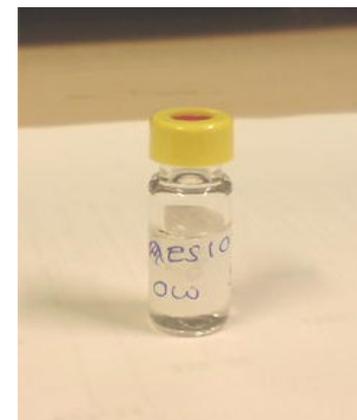
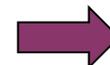
Analysis Type **Analysis Required** **Please send/bring amino acid sequence for data analysis**

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

© 2015 Proteomics Research Group, Oxford University

* 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 ORL/Inhouse team. Sample 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.

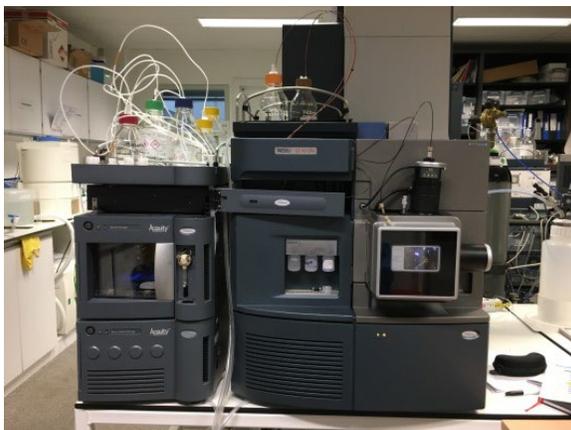
Proteomics protocols and submission form can be found on the website:

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



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://masspec.chem.ox.ac.uk/trained-user>

Trained-user systems

MALDI



Bruker Autoflex Speed TOF-TOF

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

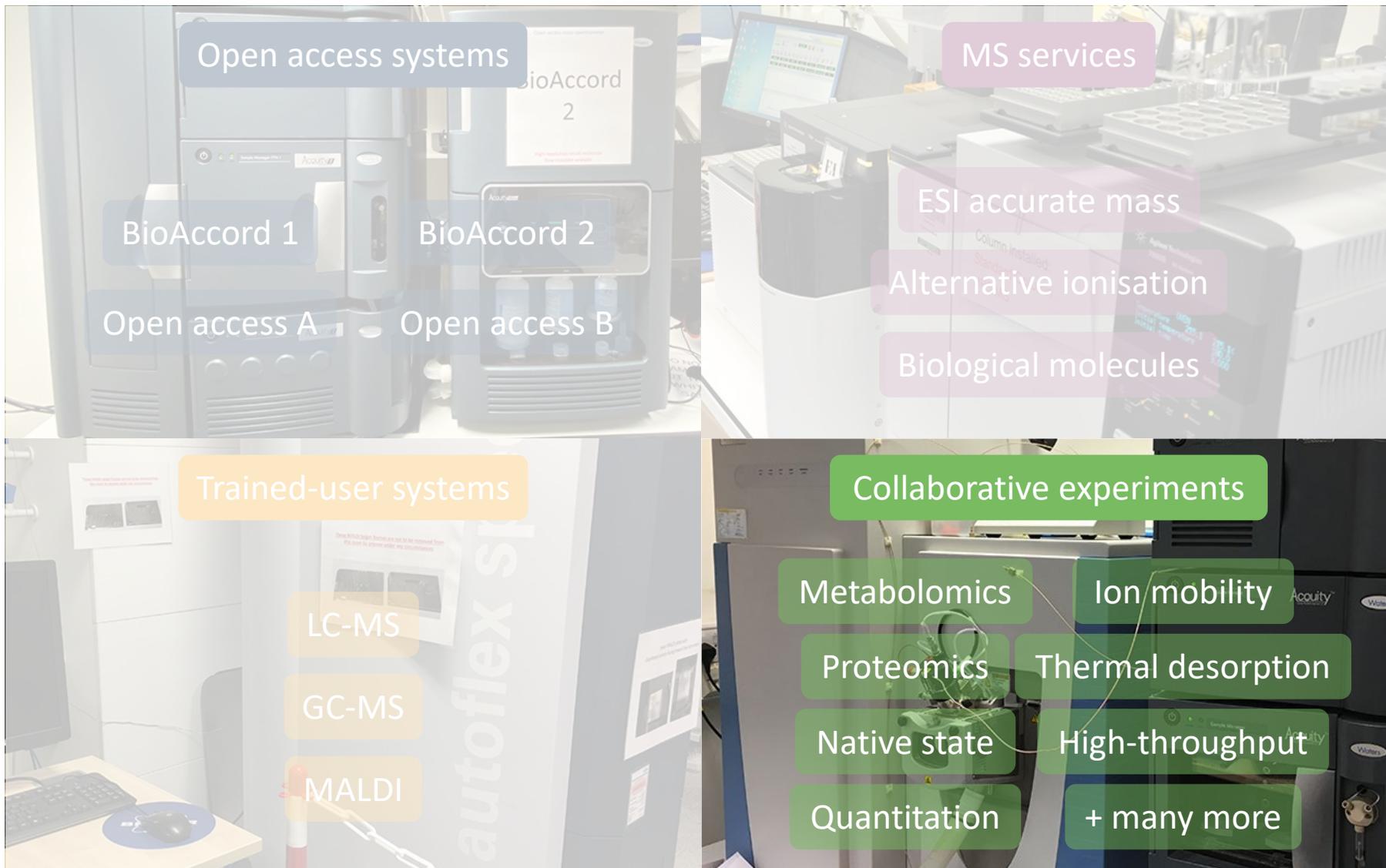
GC-MS



Agilent 5977B

- Volatile small molecules
- Complex mixtures amenable to EI

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



Collaborative experiments



Nanospray

Quantitation



Metabolomics

Air-sensitive



GC-FID

Native state

Ion mobility



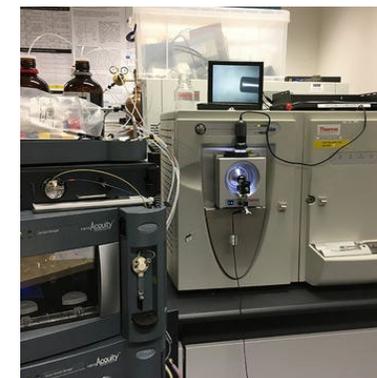
High throughput screening

ASAP



Thermal desorption

Live-cell assays



Proteomics

Data storage (Q: drive)

The screenshot shows a Windows File Explorer window with the address bar set to 'This PC > Mass Spectrometry (\\chem.ox.ac.uk\SRF) (Q:)'. The ribbon includes 'File', 'Home', 'Share', and 'View' tabs. The ribbon buttons are organized into groups: Clipboard (Pin to Quick access, Copy, Paste, Cut, Copy path, Paste shortcut), Organise (Move to, Copy to, Delete, Rename), New (New item, Easy access, New folder), Open (Properties, Open, Edit, History), and Select (Select all, Select none, Invert selection). The left sidebar shows navigation options like Desktop, Creative Cloud Files, OneDrive - Nexus365, John Walsby-Tickle, This PC, Network, Control Panel, and Recycle Bin. The main pane displays a list of folders with columns for Name, Date modified, Type, and Size. The '2024 Data' folder is selected.

Name	Date modified	Type	Size
2022 Data	28/01/2023 20:00	File folder	
2023 Data	28/01/2023 20:00	File folder	
2024 Data	04/01/2024 10:31	File folder	
Archived Data (pre-2022)	20/12/2023 21:24	File folder	
Mass Gateway	04/03/2024 09:49	File folder	
Mass Spectrometry Staff	28/01/2023 20:00	File folder	
Mnova	19/02/2024 12:39	File folder	
Open Access	02/05/2024 11:04	File folder	
SBM CDT	12/01/2024 10:22	File folder	
Service Sample Submission	28/01/2023 20:00	File folder	
Trained Users Information	28/01/2023 20:00	File folder	

High resolution MS data is LARGE

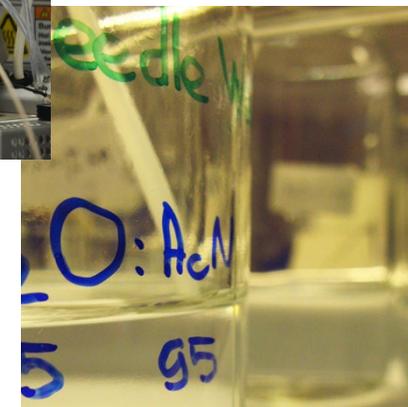
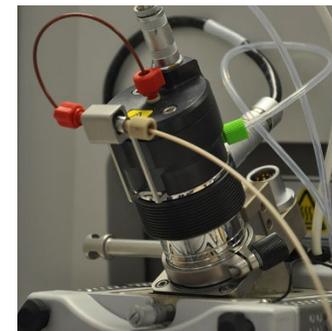
>150 TB RAID array

Networked storage

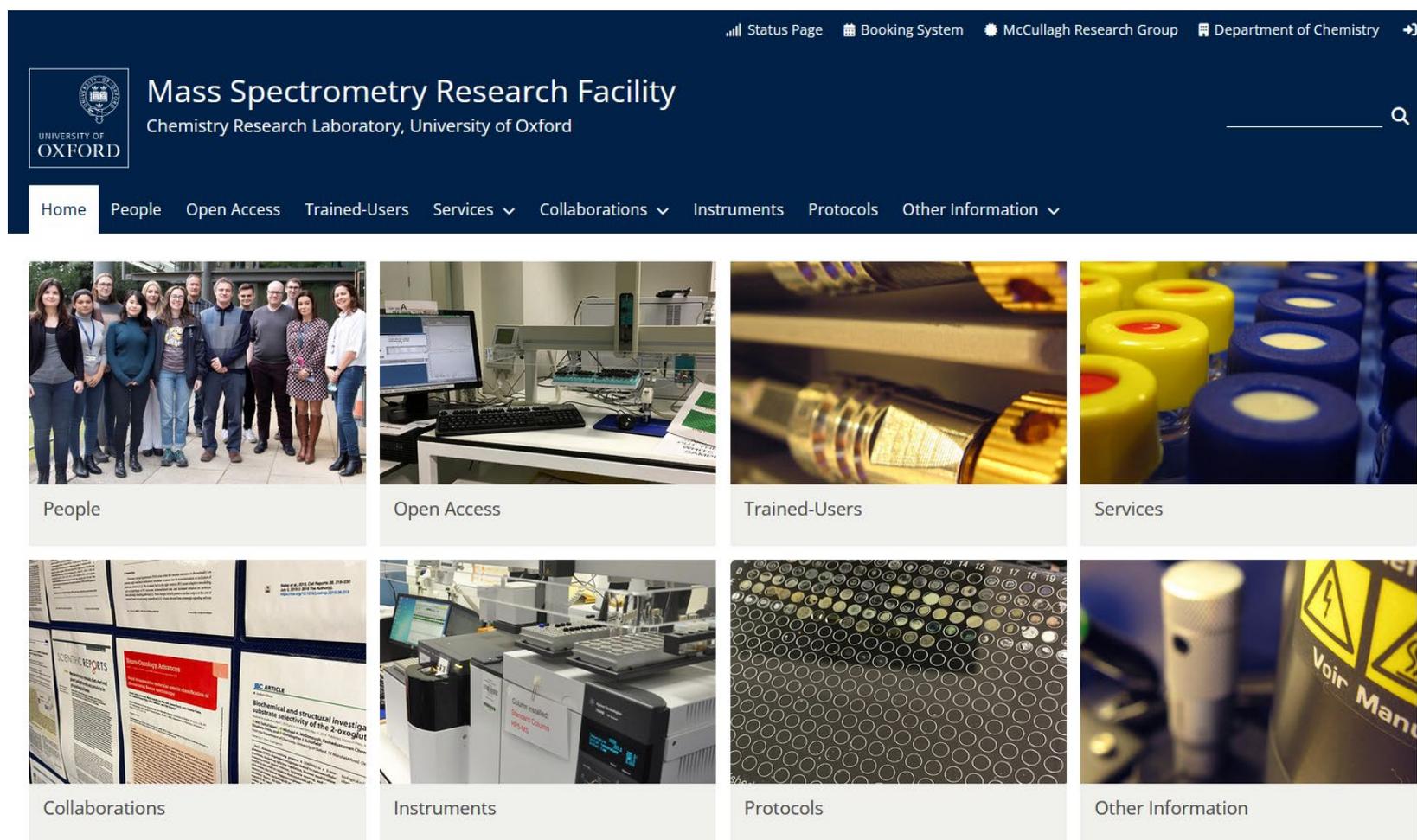
Research group subfolders

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#booking-rules>



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



The screenshot shows the homepage of the Mass Spectrometry Research Facility (MS-SRF) website. The header is dark blue with the University of Oxford logo on the left and navigation links for Status Page, Booking System, McCullagh Research Group, and Department of Chemistry on the right. Below the header is a navigation menu with links for Home, People, Open Access, Trained-Users, Services, Collaborations, Instruments, Protocols, and Other Information. The main content area features eight image-based tiles, each representing a different aspect of the facility: People (a group photo), Open Access (a computer workstation), Trained-Users (a close-up of a mass spectrometer component), Services (a row of vials), Collaborations (scientific posters), Instruments (mass spectrometer hardware), Protocols (a microplate), and Other Information (a warning sign).

Mass Spectrometry Research Facility
Chemistry Research Laboratory, University of Oxford

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

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.

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

QR for MS training



DEPARTMENT OF
CHEMISTRY



UNIVERSITY OF
OXFORD

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