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UniSA Clinical & Health Sciences: Mass Spectrometry & Proteomics Facility Information Handbook

A Mass Spectrometry & Proteomics facility co-funded by the University of South Australia, the South Australian Government, and Bioplatforms Australia.

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1 Mass Spectrometry & Proteomics

The **Mass Spectrometry & Proteomics (MSP)** facility located within Clinical & Health Sciences at the University of South Australia provides expertise for Tissue Mass Spectrometry Imaging and proteomic analyses. MSP is a Proteomics Node for Bioplatforms Australia in South Australia that was established under the National Collaborative Research Infrastructure Strategy (NCRIS). We offer all types of proteomic services including quantitative proteomics, phosphoproteomics and glycomics. Furthermore, our facility offers, to a limited extent, lipidomics and metabolomics, in collaboration with the Australian Wine Research Institute (AWRI), which is a Metabolomics Node for Bioplatforms Australia, also located in South Australia.

Bioplatforms Australia's Vision:

Bioplatforms Australia enables Australian life science research by investing in state-of-the-art infrastructure and associated expertise in the specialist fields of genomics, proteomics, metabolomics and bioinformatics. Bioplatforms' proteomics partners offer leading edge infrastructure, expertise and advanced protein discovery services. A broad range of services are offered including mass spectrometry, monoclonal antibody production and drug screening.

Bioplatforms Australia's Mission is to support world class research and innovation in the life sciences by:

- Ensuring broad and efficient access to state-of-the-art biomolecular ('omic) platform capabilities.
- Facilitating greater multi-disciplinary integration in basic and translational bioscience.
- Contributing to research collaborations that address scientific challenges of national significance.
- Supporting industrial applications of biomolecular technology and scientific collaborations between researchers and industry.
- Expanding international research networks.
- Sustaining a national intellectual capability and capacity.

2 Introduction

This handbook provides a reference for users and supervisors who wish to access the Mass Spectrometry & Proteomics facility located within Clinical & Health Sciences at the University of South Australia. While every effort has been made to ensure that the information contained within this document is correct and current, the policies outlined below are subject to change in line with University policies and procedures.

3 Use of the Facility

3.1 Work Request Procedure

For all internal and external access and work requests, please send an email to mSP.bioplatforms@unisa.edu.au. For students, please ensure your supervisor is cc'd and has approved your request for access and/or work. You will receive an email response letting you know how to proceed. You may be invited to attend a short meeting to discuss your needs, or you may be directed to a staff member to begin training or analysis. There are two ways to carry out research using our instrumentation, either by getting trained and running the instrument yourself, or by having one of our staff members assist you. This is dependent on the platform you require to use as well as the 'omics' methodology you wish to employ. Please note that to qualify for training on some instruments, a minimum training session may be required, and this will be charged as a minimum number of hours as required.

4 Instrument Charges & Costings

A schedule of costings is provided as an appendix of this document and may change periodically. For specific workflows, such as Mass Spectrometry Imaging and label-free LCMS quantitation, pricing has been defined to account for required setup and replicate runs, respectively. Instruments are available to both internal and external academics in South Australia at the same cost, and staff time is only costed for sample preparation, data analysis, and reporting, as required. Commercial work is invoiced at full cost recovery, and this costing will be provided up-front before work begins. South Australian industry partners will have priority access to the facility as required.

5 Guests, Visitors & Tour Groups

Anyone who is entering the laboratory for the sole purpose of passive observation are allowed temporary access to the area under direct supervision of MSP staff members. Any PPE requirements of the laboratory must be adhered to while visiting the laboratory. No guests, visitors or tour groups should be left alone in the laboratory. Tour group supervisors should review the UniSA “Tour Safety Instructions” and follow the accompanying SOP to ensure tours are carried out safely and professionally.

Safety

- Enclosed footwear must be always worn in all laboratories.
- Safety glasses must be always work in all laboratories. Safety glasses will be provided either at the start of the tour or as you enter a laboratory.
- You may enter operational laboratories. Please do not touch any surfaces, equipment or containers. If a demonstration has been organised, follow the directions of your tour guide or MSP staff member.

Emergency

- In case of an emergency, please follow the instructions of your tour guide, one of the emergency wardens or UniSA security. All buildings have a PA system to notify of emergency conditions.

Medical

- Do you have a pacemaker or are pregnant? Please advise your tour guide prior to tour commencement. Some laboratories have strong magnetic fields that may interfere with a pacemaker and some laboratories have chemicals that can affect the fetus.

Food or drinks are not permitted in any laboratories at any time.



6 Equipment & Laboratory Usage

6.1 Sample Preparation & Storage

Samples prepared by MSP staff will be stored in appropriate conditions within the MSP laboratories. After analysis, samples will be stored for 36 months, after which will be discarded. Samples brought into the instrument laboratory should be taken away by the researcher when their analysis is complete. Any samples left in MSP laboratories that have been brought in by a user may be disposed of if MSP staff haven't been informed to retain.

6.2 Instrument User Etiquette

- It is a laboratory requirement to be polite and courteous to our staff, as well as other laboratory users.
- You must follow all procedures and instructions, no exceptions.
- You must follow the data indexing system on each system used
- You must fill in the logbook for any system before you begin work.
- Instruments that can be used independently must not be modified by the user. The instrument PC must not be modified in any way except for the specific purpose of storing the data obtained by the instrument.
- Samples are not to be left in the laboratory or instrument.

7 Booking Instruments

For MS systems that do not require MSP staff to operate (e.g. MALDI-ToF MS, LC-Qq-ToF MS), all instrument bookings are made online using a system known as EZBooking. You will need to have a UniSA account to be able to use this booking system. For external users, please email msp.bioplatforms@unisa.edu.au to help you make a booking. Please note that you will not be able to make a booking until you become an approved user in our facility. Please follow this link to access the booking system:

https://ezbooking.unisa.edu.au/EZBooking/EZbooking/cgi-bin/ezb_frameset.cgi?goToAction=default

7.1 EZBooking Rules

The booking etiquette is as follows:

- Please attend the start of your session on time.
- Do not book a session for someone else in your name. The person named on the booking calendar must attend. Other students and staff may also attend the experiment if they wish, but they must all be authorised to enter the laboratory.
- Do not use an instrument if you have not booked it.
- Do not use an instrument if you have not been trained on it.

Please note that we use the booking system to count how many hours each instrument is used. This is extremely important because without an adequate level of usage, we cannot justify the expense of keeping all of our instruments running. Failure to use the booking system with integrity will result in a warning in the first instance, and in the second instance the Node Director may choose to remove your booking privileges.

7.2 Priority Booking

We are happy to provide additional assistance with extra bookings if you have some time pressure.

Examples of reasons that we may grant you a priority booking include:

- Having family commitments.
- If you are restricted to business hours.
- If you have time-sensitive experiments in progress.
- You are visiting us from another Institution.

7.3 Safety

It is a UniSA policy that all tasks are risk assessed before they are undertaken. It is the responsibility of researchers and their supervisors that this is carried out to an appropriate standard. The MSP staff require a risk assessment to be provided for all material being studied is a medium or high-risk material. Please discuss with MSP staff prior to use to ensure your sample/s can be analysed safely.

Laboratories within Clinical & Health Sciences are classified based on inherent hazards that have been determined by a risk assessment-based approach by Laboratory Coordinators and the Ops group. Clear signage at the entrance to each laboratory and/or appropriate colour coded lines on the floor indicate the status of a laboratory and areas within a laboratory. Laboratories with mixed risk level will have both requirements described on signage at the entrance

Laboratory classification:

- **GREEN** – hazards are similar to an office environment - no specific PPE requirements, no hazardous chemicals (beyond what would be found in a kitchen, etc)
- **ORANGE** – general laboratory
- **RED** – laboratory or area within a laboratory with a higher level of hazards, which has the potential to cause serious injury or death. – i.e. HF, LN2, radiation, etc. that requires specific PPE above that of an Orange laboratory.

Fully enclosed footwear with a broad, low heel must be worn at all times in all laboratories green, orange and red. This applies to laboratory users and tour groups. Wearing gloves may be required to protect the skin and may also be required to keep samples clean while they are being handled. In all cases, the choice of gloves, and when they are to be used, should be indicated by your risk assessment in consultation with the instrument coordinator.

Breaches of safety are quite serious. UniSA policy stipulates that all safety breaches and near misses are reported at <http://w3.unisa.edu.au/safetyandwellbeing/default.asp>. Any staff member can ask a researcher to stop-work-for-safety. It is procedural that any user's online booking privileges be temporarily suspended during a stop-work-for-safety. You will be able to recommence your work when you have satisfied all UniSA policy requirements.

7.4 Building Emergency Evacuation

If you hear a continuous alarm bell or tone or are requested by an Emergency Warden/Security to evacuate the building, you must:

- Follow their instructions.
- Leave the building immediately by the nearest safest exit stairs – do not hesitate.
- You are not allowed to use the lift; you must use the stairs and keep to the left.
- Proceed to the assembly point.
- Remain at the assembly point until advised the emergency is over.
- Do not re-enter the building until advised it is safe to do so by the Emergency Evacuation Officer or Security. Do not try to re-enter just because the alarm has stopped.

In the event of a fire:

- All equipment must be left behind.
- All doors must be closed to prevent spread of fire.

Unless instructed otherwise stay with the group at the assembly area after reporting to the Building Evacuation Officer. The all clear to return to the building will only be issued via Building Evacuation Officers or Deputy Building Evacuation Officers (Security or campus services may give the message but only if the Evacuation Officers are not available) with a direct message - do not re-enter the building unless this has been given. As part of your laboratory induction the closest emergency assembly area will be pointed out to you. These are as follows:

Building	Assembly Point	Assembly Point Number
MM	Grassed area south of building MM	7
X	Grassed area between Q & R	23
HB	SAHMRI Courtyard, North Terrace	3
	Corner North Tce and Morphett St (outside Convention Centre)	8

7.5 After Hours Access

After hours include: weekdays before 7 am and after 7 pm, weekends, public holidays and other periods when the university is closed. After-hours access may be permitted to UniSA staff and students and requires permission from both the Technical Services Manager and the Instrument Co-ordinator. All requests for after-hours access must be submitted in writing to msp.bioplatforms@unisa.edu.au.



8 Instrument Damage & Malfunction

In the event of an instrument malfunction, or if you are unsure if the instrument is functioning normally, please contact a MSP staff member by phone, email (misp.bioplatforms@unisa.edu.au) or direct contact. Staff details can be found in section 12.5 Staff Contacts. Staff will instruct you with what to do next. Please do not attempt to fix, re-boot or modify the instrument. Record your observations in the logbook.

Any repair costs for damage caused by wilful misuse by a researcher will be charged back to the research group or company of which the user is a member.

9 Data Management & Integrity

Instrument users are responsible for the archiving of their data. Users are strongly encouraged to retrieve their data during the booked hours. The loss of any data is not the responsibility of the instrument co-ordinator or MSP staff member.

It is the responsibility of the user to ensure academic and scientific integrity of all data, data analysis and interpretation. Although instrument co-ordinators and MSP staff members may provide some advice regarding analysis and interpretation, all responsibility for scientific accuracy and integrity remains with the individual researcher.

10 Acknowledgement

All users are required to acknowledge use of the instrument in any research output derived from the images and data obtained. For the purpose of collecting the research output obtained from the facility, all users must report any research output involving use of these instruments.

Acknowledgement:

“The authors acknowledge Bioplatforms Australia, the University of South Australia, and the State and Federal Governments, which co-fund the NCRIS-enabled Mass Spectrometry and Proteomics facility at the University of South Australia.”

11 Instruments & Locations

11.1 Instrument Locations

Instrument/Service	Building - Room
Autoflex Speed MALDI-ToF/ToF MS	HB8-48
Agilent 6495B LC-QqQ MS	MM2-11
Agilent 6550 LC-Qq-ToF MS	HB8-48
Thermo Orbitrap exploris480 MS	HB8-48
Bruker timsTOF fleX MS	HB8-48

Campus maps are provided in the Appendices of this document.

11.2 AutofleX Speed MALDI-ToF/ToF MS



The AutofleX Speed Matrix-Assisted Laser Desorption/Ionisation (MALDI) Time-of-Flight (ToF) MS system is a highly sensitive instrument that is suitable for multiple applications. The system can analyse multiple types of analytes, including (but not limited to) drugs, metabolites, lipids, glycans, peptides, proteins, and polymers. This system is configured as a Biotyper platform which allows the fast and reliable high-confidence identification and taxonomical classification of microorganisms, such as bacteria, yeasts and fungi.

11.3 Agilent 6495B LC-QqQ MS



The Agilent 6495B LC-QqQ MS system is the highest performance triple quad available and is ideally suited for targeted quantitation of metabolites and peptides as well as samples that are low in concentration and require high sensitivity. The combination of utmost sensitivity, extended mass range, ease of maintenance, and the power and flexibility of MassHunter makes this the system of choice for demanding applications, such as the quantitation of PFAS compounds which are very persistent environment contaminants that break down slowly over time.

11.4 Agilent 6550 LC-Qq-ToF MS



The Agilent 6550 LC-Qq-ToF MS system provides high accurate mass analysis of complex samples and multiple types of analytes. Agilent's iFunnel technology provides a level of robustness unmatched in the industry by preventing the transmission of uncharged species. This system offers qualitative and quantitative characterisation of samples, including metabolites, lipids, and peptides. The instrument is supported by Agilent's MassHunter software which allows the streamlined identification of metabolites and lipids. The instrument can be configured for low (nano) or high (analytical) flow rates to deal with various sample types and amounts.

11.5 Thermo Orbitrap Exploris 480 MS



The Thermo Orbitrap Exploris 480 MS system joins the family of next-generation Thermo Scientific mass spectrometers built on a common architecture with the guiding principle of ultimate performance and ease of use. Combined with the Thermo Easy-nanoLC 1200 and ProteomeDiscoverer software, the platform is the latest generation of accurate mass and high-resolution technology for proteomics analysis. The system is configured for label-free nLC-MS/MS of peptides from complex protein samples and can be used for high-throughput characterization of serum, plasma, and other complex sample types. The system is equipped with the Thermo Scientific™ FAIMS Pro™ interface, which minimizes co-isolation of isobaric peptides, increases the number of unique peptides identified, and improves signal-to-noise to sample low-abundance peptides.

11.6 Bruker timsTOF fleX MS



The Bruker timsTOF fleX MS system is a super-fast and highly sensitive ESI instrument for metabolomic, lipidomic, glycomic and proteomic analyses with an the integrated MALDI source used for rapid Tissue Mass Spectrometry Imaging applications. Built on the standard for shotgun proteomics, the timsTOF fleX combines the best in 4D-Omics using robust ESI measurements, along with Bruker's cutting edge MALDI Imaging technology to spatially resolve a wide range of molecules directly from tissue, all in one single platform. Changing from ESI to MALDI occurs within a matter of seconds. No complicated changeover means making zero compromises in productivity and the ability to move effortlessly from world class Omics identification and quantification workflows to creating high-definition molecular maps of tissue sections to visualise your analyte of target.

12 APPENDICES

12.1 FAQs

I don't know if my samples are compatible with the system or will work, who should I talk to?

Please contact any MSP staff member, who will advise you about the system and sample compatibility. We prefer people to ask questions, rather than waste their time or damage an instrument. If in doubt, please ask us to help you out.

Who should I contact for training?

Please contact MSP staff members directly.

How do I gain laboratory access?

All UniSA users are required to complete compulsory UniSA and WHS online modules. After completion, users must send copies of their completion certificates to the MSP Team (msp.bioplatforms@unisa.edu.au). No activity in any lab can commence until these modules are complete. You will then need to complete a local laboratory specific induction before we can grant you access.

My access card stopped working, what do I do?

Please contact the MSP Team (msp.bioplatforms@unisa.edu.au) detailing your problem.

Can I use equipment myself?

For certain MS infrastructure, including the MALDI-ToF MS and LC-Qq-ToF MS platforms, you can be trained to use the system yourself. Specific equipment, such as the Exploris480 and timsTOF fleX, is only managed by MSP staff members and not setup to be used independently.

12.2 Fee Schedule

The instrument access fee schedule below is subject to change. Pricing is reviewed on an annual basis. Although every effort is made to update the information below, please contact MSP for an official quotation.

STAFF FEE					
SERVICE	INFORMATION	UNIT	INTERNAL RATES*	EXTERNAL ACADEMIC*	INDUSTRY RATES*
MSP Staff Time	Sample preparation, data analysis and reporting for all types of analyses	Per hour	\$70	\$110	\$180

MSP Pricing Structure – Main Services

Effective September 2022

QUALITATIVE ANALYSIS					
SERVICE	INFORMATION	SAMPLE NUMBER	INTERNAL RATES*	EXTERNAL ACADEMIC*	INDUSTRY RATES*
LC-MS					
LC-MS/MS Analysis for Protein Identification	Trypsin digestion, clean-up, nanoLC-MS/MS data acquisition, database search and reporting	1-5	\$180 per sample	\$240 per sample	\$300 per sample
		6+	\$130 per sample	\$190 per sample	\$250 per sample
LC-MS/MS Analysis for Small Molecule Identification	Small molecule extraction, clean-up, LC-MS/MS data acquisition, database search and reporting	1-5	\$180 per sample	\$240 per sample	\$300 per sample
		6+	\$130 per sample	\$190 per sample	\$250 per sample
MS Analysis of Purified Intact Proteins	Direct injection, MS data acquisition and reporting	1-5	\$130 per sample	\$190 per sample	\$250 per sample
		6+	\$100 per sample	\$160 per sample	\$220 per sample
Data Independent Analysis (DIA-PASEF) using the timsTOF fleX	PoA				



MALDI-MS					
SERVICE	INFORMATION	SAMPLE NUMBER	INTERNAL RATES*	EXTERNAL ACADEMIC*	INDUSTRY RATES*
MALDI-MS Analysis for Protein Identification (from gel spot)	Trypsin digestion, clean-up, MS data acquisition, database search and reporting	1-5	\$180 per sample	\$240 per sample	\$300 per sample
		6+	\$130 per sample	\$190 per sample	\$250 per sample
MALDI-MS Biotyper® Analysis	Microbial identification of isolates and reporting with sample preparation completed by the client	1-50	\$100 minimum (\$2 per sample)		\$250 minimum (\$5 per sample)
MALDI-MS Analysis using the Autoflex Speed	MS data acquisition, data analysis and reporting with sample preparation completed by the client	1-10	\$100 setup fee		\$250 setup fee
MALDI-MS Analysis using the timsTOF fleX	MS data acquisition, data analysis and reporting with sample preparation completed by the client	1-10	\$250 setup fee		\$400 setup fee
MALDI Imaging using the timsTOF fleX	Sample preparation, enzyme application, matrix deposition, MS data acquisition, data analysis and reporting	(PoA for large cohort)	\$800 per slide	\$1100 per slide	\$1500 per slide
GC-MS					
GC-MS Analysis	PoA				

QUANTITATIVE ANALYSIS					
SERVICE	INFORMATION	SAMPLE NUMBER	INTERNAL RATES*	EXTERNAL ACADEMIC*	INDUSTRY RATES*
MRM/SRM Assay Development & Analysis	Method development for targeted quantitation of proteins, peptides or small molecules, LC-MS/MS data acquisition, data analysis and reporting	1-5	\$180 per sample	\$240 per Sample	\$300 per sample
		6+	\$130 per sample	\$190 per sample	\$250 per sample
Label Free Quantitation using LC-MS/MS Analysis in Triplicate	Trypsin digestion, clean-up, nanoLC-MS/MS data acquisition, database search and reporting, in triplicate	1-5	\$540 per sample	\$720 per sample	\$900 per sample
		6+	\$390 per sample	\$570 per sample	\$750 per sample
New Method Development	\$2000				
New Method Development & Validation	\$4000				
Protein Quantitation using Stable Isotope Labelling	PoA				
PTM Characterisation	PoA				

*All prices listed are ex. GST. Prices include UniSA Levies where applicable. Formal quotes are available upon request. Please negotiate a discount if there are more than 50 samples.

Repairs due to instrument damage resulting from operation without due care and attention will be charged to the users' organisation

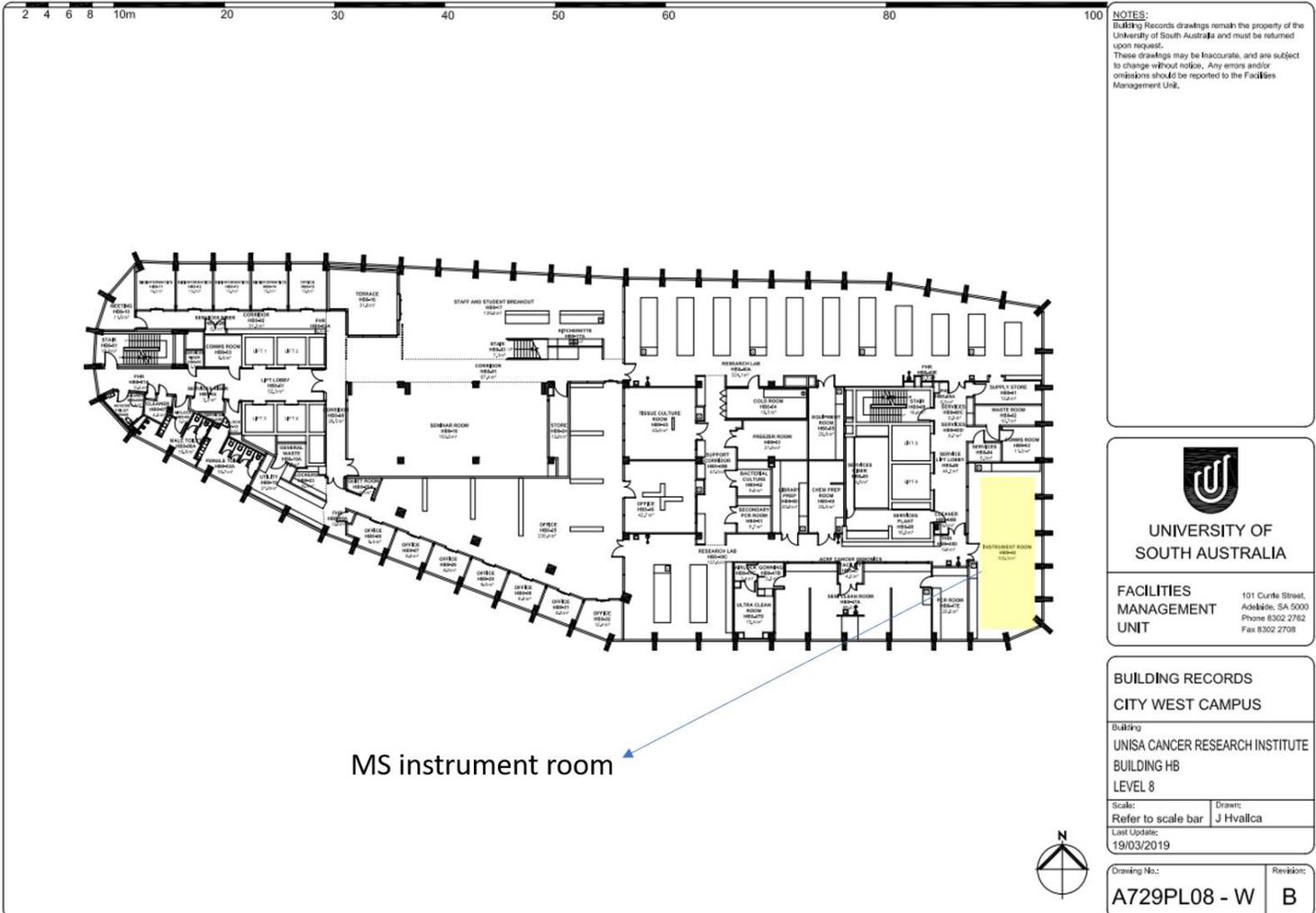


12.3 Mawson Lakes Campus Map





12.4 HB Building Level 8 Layout



12.5 Staff Contacts

UniSA Node Director of MSP

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If you have any enquiries, and do not know who to contact, the best place to start is the MSP email msp.bioplatforms@unisa.edu.au.