Penn State Metabolomics Facility Policies and Procedures

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1. Policy Statement – The Penn State Metabolomics Facility housed in the Huck Institutes of the Life Sciences offers nominal and accurate mass spectrometry of synthetic compounds, and biomolecules (such as SPMs, lipids, metabolites, oligosaccharides, and oligonucleotides). Our main goal is to provide high quality data to researchers at Penn State and World-wide. Our focus is on identifying and quantifying small molecules (<1kDa) present in a wide variety of sample types including animal biofluids and tissues, bacteria, fungi, and plants. The facility offers both full-services and self-services for sample preparation, identification, and quantitation by liquid chromatography-mass spectrometry (LC-MS, LC-MS/MS, LC-MS^n) and gas chromatography-mass spectrometry as well as data analysis and interpretation.

2. Reason for Policy and Procedures – This document has been prepared as a reference for users to outline our facility's guidelines and expectations. We ask that all users review this document to ensure awareness and compliance with the rules and regulations being agreed to as part of using the Penn State Metabolomics Facility.

3. Publication Acknowledgement – All work performed in any of the Huck Institutes of the Life Sciences' shared facilities should be acknowledged in scholarly reports, presentations, posters, papers, and all other publications. Proper acknowledgment provides a visible measure of the impact of the Huck Institutes' shared facilities and is essential for our continued funding.

Include an acknowledgment any time the Metabolomics Facility provides services that support your research. If a staff member has made significant intellectual contribution (e.g. method development) beyond the routine sample analysis, please consider co-authorship.

Please always notify the Metabolomics Core Facility when acknowledgement is made.

Mandatory Minimum – Independent use of the Metabolomics Core Facility

"The co-authors would like to acknowledge the Huck Institutes' Metabolomics Core Facility (RRID:SCR_023864) for use of the [instrument name]"

Example 1 - Independent use of the Metabolomics Core Facility and guidance from staff "The co-authors would like to acknowledge the Huck Institues' Metabolomics Core Facility (RRID:SCR_023864) for use of the [instrument name] and [person's name] for helpful discussions on sample preparation."

Example 2 - Routine data collected by the Metabolomics Core Facility personnel (data interpreted by the user)

"The co-authors would like to acknowledge the Huck Instutites' Metabolomics Core Facility (RRID:SCR_023864) for use of the [instrument name] and [person's name] for collecting the data shown in Figure Y."

NIH and NSF Grant Attribution

Language for how our facilities may be described in grant proposals to both the National Institutes of Health and the National Science Foundation can be found:

https://www.huck.psu.edu/resources/faculty/working-at-the-huck/huck-facilities

4. Use of the Metabolomics Facility – The purpose of the facility is to offer nominal and accurate mass spectrometry of synthetic compounds, and biomolecules (such as SPMs, lipids, metabolites, oligosaccharides, and oligonucleotides). Our main goal is to identify and quantify small molecules (<1kDa) present in a wide variety of sample types including animal biofluids and tissues, bacteria, fungi, and plants.

The facility's full services include sample preparation, identification, and quantitation by liquid chromatography-mass spectrometry (LC-MS, LC-MS/MS, LC-MS^n) and gas chromatography-mass spectrometry as well as data analysis and interpretation. Additionally, self-service is available to anyone, with priority given to PSU users, who have received training from facility staff.

5. User Categories

Internal Users – Users belonging to one of Penn State's campuses.

Academic Users – Users outside of Penn State belonging to an academic institution, including an institution of higher education like a college or university, a public laboratory or department, and any not-for-profit group, such as hospitals.

External Users – Users belonging to a private sector, for profit company or entity where the intended goal of the research is to advance a profit seeking venture.

6. Full-Service Information

A. Sample Submission

i. Submission Request – Users interested in submitting samples are asked to contact the facility Director, Ashley Shay (aes5254@psu.edu), prior to submitting samples to discuss the project to determine the best protocol to use for their desired outcome. Users are required to fill out the online request form on the Core's website. Internal users submitting samples that require an IBC protocol (for example, human blood, bodily fluid, tissues, cells, viruses, parasites, bacteria, etc.) are required to first be approved by ORP before the facility can proceed. Publications and previously used methods are encouraged to attach. Samples should not be physically sent to our facility until we have reviewed your submission information and approved your request.

ii. Submission Approval – Upon receipt of a request form, we will review the submission to ensure we have all the information needed to process the samples. Once approved, users will receive an email requesting them to deliver their samples at an agreed upon date and time. If the project was not discussed prior to submission, the samples will not be accepted.

iii. Sample Preparation for Submission – Samples must be submitted in the agreed upon format during discussions with the facility Director. For samples submitted for standard metabolomics protocols, metabolomics sample prep guidelines are provided. If extra time is required for us to process the samples because the guidelines were not followed, an extra cost will be applied.

iv. Sample Labeling – Samples should be submitted with clear legible labeling and a key with the following information: tube number, sample name (or abbreviated), amount per sample. Use permanent marker and not stickers or labels.

v. Shipping Samples – Users must receive sample submission approval prior to shipping samples to the facility. Any samples received prior to approval will be stored but will not

be processed until approval is complete. Once approved, users will be instructed to ship their samples and to provide the tracking # and estimated delivery date.

Users should ship using a sturdy container and appropriate packaging, including dry ice if needed. Users should ship using the fastest delivery method available to ensure samples get to our facility without damage or thawing. If samples are received damaged, thawed, or otherwise compromised, a staff member will contact you, but we are not to be held responsible. A staff member will notify you upon receipt of your samples.

Shipping Address:

The Pennsylvania State University
432 Science Drive
101 Huck Life Sciences Bldg
University Park PA 16802
ATTN: Ashley Shay

vi. Dropping Off Samples – Users must receive sample submission approval prior to dropping off samples. Any samples received prior to approval will be stored but will not be processed until approval is complete. Once approved, users will be instructed to bring their samples to the facility at an agreed upon date and time. If you attempt to drop off samples without confirming the date and time you may have to wait for assistance or return at another time. Users can either leave their containers with us or request the containers to be returned.

B. Customized or Collaborative Project – Users wishing to have a customized project or collaborative project should set up a consultation by emailing the facility Director, Ashley Shay (aes5254@psu.edu). The consultation, either in person or remotely, is to determine what outcome the user is looking for and whether our facility can help advance their research goals. Once a plan is in place, the user will be given a quote outlining cost. Upon agreement to the quote, the user will be asked to complete an online request form available on the Core's website. Letters of support for grant proposals are available upon request.

C. Sample Storage – Upon receipt, samples will be stored at the appropriate temperature. All samples received on dry ice will be stored at -80°C. If samples require unique storage conditions, please clarify in the "Other special instructions" section of the online request form. For information on length of storage of samples after processing is complete, please see section Sample Return or Disposal.

D. Cancellation Process – Users can cancel their sample submission request at any time without charge prior to shipping or dropping off samples. Once samples are received at our facility, users may request a cancellation, but there may be a charge depending on whether processing of the samples has already started. If we have received samples but have not begun processing, we will either dispose of the samples or return the samples using a customer provided pre-paid shipping label or by the user picking up the samples directly from the lab.

E. Sample Hold Requests – Users may request that their project be put on hold after samples have been received but not processed. We will hold samples for up to 6 months. After that time, we will dispose of the samples.

F. Sample Processing Time – The processing time for samples is dependent on service requested, the number of samples submitted, preparation methodology, and samples already in the queue. A customized project, requiring standard gathering, method development, troubleshooting, etc. will take a longer period to complete. Similarly, a project with a very large number of samples will require additional time.

G. Data Reporting – Staff members will send out the analyzed data to users at the email provided. If the user has any questions regarding data, we can assist by email. If any reprocessing is required because information was not provided during the submission, then an additional charge will be added. If instrument data files are required, they need to be requested. Access to the facility's cloud storage will be provided. Instrument data files will be available through the cloud storage for two weeks. Users are expected to archive data/instrument data files upon receipt.

H. Data Archiving – The instrument raw data files are saved to the facility's cloud storage for up to 5 years. After 5 years, the files will be deleted if necessary. Instrument raw data files will not be stored on instrument computers. Users are expected to archive analyzed data files and instrument raw data files upon receipt.

I. Sample Return or Disposal – Upon receipt of the analyzed data/instrument data files, users have up to 6 months to request remaining sample material be returned. To request samples be returned, users should provide us with access to a prepaid shipping label or arrange a date to pick-up their samples from the facility. Samples will continue to be stored in a stable environment, most often a -80 freezer. After 6 months, samples may be disposed of by staff if necessary. Some services require the use of all sample material, in which case nothing will be available to return.

7. Self-Service Information

A. Use of Core Instruments – At the PSU Metabolomics Facility, we offer our frequent users the opportunity to access our facility instrumentation for self-service work and provide the opportunity to get training on state-of-the-art equipment. To become a self-service user, or to start a new project, a consultation meeting with the director is required to discuss the scope and feasibility of the intended project. The user will be expected to complete safety training and instrument training/familiarization with facility staff. Users will need to follow the approved method agreed to during training, and get any changes approved by a staff member. Users will be expected to book time on the instrument by contacting a staff member in advance to check on instrument availability. Upon completing work, users are required to log the number of hours of instrument usage and provide an internal order number for billing. Users will be respectful of facility space and will maintain order and cleanliness. Misuse of the facility or the equipment will lead to having access revoked.

B. New Users/New Projects:

1. For new projects, we require all users (new and approved) to set up a meeting with us to consult about the project, pricing, and method development.

2. Self-service users must be properly trained and approved by facility staff before being permitted to sign-up and operate the equipment.

a. Users may receive preliminary training from facility staff. The training session from facility staff can be used to setup the new method. Self-service users may not operate the instrument alone until they have passed a thorough check-off procedure with facility staff. Those failing to pass will require further training and a re-test.

A self-service user must be able to set-up the instrument alone and troubleshoot any problems related to the set-up (leaks or blockage) and software/method. For more advanced issues, users must contact facility staff.

C. Approved Self-Service Users:

1. Sign-up must be requested by email to aes5254@psu.edu

2. New Procedures: Notify facility staff **BEFORE** any new procedures (including new buffers, method, etc) are used on the instrument to have them approved first.

3. Hardware Changes: If your method necessitates changes being made to the standard LC-MS set-up, all hardware must be set back to the original starting configuration. We do, however, encourage minimal changes to the standard configuration given the expected multi-user environment. Facility staff will make the required hardware changes.

4. Waste Container Maintenance: Every time you use the instrument, please indicate on the waste tag attached to the waste container the compound names used if not already listed. If the bottle is close to being ¾ full before you start, please notify facility staff, or switch out the bottle for an empty bottle with a new chemical waste tag. Place the full waste container in the chemical waste pick-up container located beneath the sample preparation bench.

5. Report the total # of hours (including blanks, QCs, and standards) and the total number of hours for samples. The total # of hours for samples will be used for billing.

6. Please report any hardware problems/errors with the instrument to a facility staff member immediately.

7. Self-service users are responsible for backing up and storing their data and method files.

8. Do not hesitate to ask if you are unsure about something.

D. Instruments Available for Self-Service Use – Self-Service users who have been properly trained by staff may access the following mass spectrometers:

i. Thermo Orbitrap Fusion Lumos Tribrid

ii. Thermo Exactive Plus

iii. Thermo TSQ Quantis Plus

iv. Thermo Orbitrap Exploris 120

E. Reserving Time on Facility Instruments

i. Reservation Process – Contact a staff member to book time on an instrument in advance. Reservations are scheduled on a first-come first-serve basis and users are expected to only reserve times that they will need. The facility reserves the right to reschedule in cases where the instrument is down, or full-service projects are delayed and require more time on the instrument to be completed.

ii. Cancellation Process – Please give at least 48 hours' notice in case of cancellation.

iii. Need for Extended Hours – If a user underestimates the amount of time needed for their project, they should notify a staff member immediately. They may be allowed to extend their reservation time, although there is no guarantee.

F. Self-Service User Training

i. University Training

a. Users will have completed all required University trainings (blood borne pathogens, lab safety, etc) before proceeding to work in the facility.

ii. Instrument Training

a. Individual Training – Users may receive training from facility staff. During training by a staff member, assistance with method development based on information provided by users will be given. The time required for the individual training will depend on the user's background. If the user is already proficient with using the equipment, familiarization time and assessment will still be required.

b. Assessment and Competency – Users may not operate an instrument alone until facility staff are confident with the user's abilities to operate the instrument. A self-service user must be able to set up the instrument alone and troubleshoot any problems related to the set-up (leaks or blockage) and software/method. For more advanced issues, users must contact facility staff.

c. New Procedure or New Project – Users wishing to switch methods or start a new project must notify facility staff before making any changes (including new buffers, methods, etc.). Users may be able to implement changes or start a new project without additional training subject to the approval of the director. Other users may need to complete additional training with staff.

d. Data Analysis Training – Users can receive training in data analysis upon request.

G. Laboratory Use Expectations

i. PPE – Staff and Self-Service users are expected to don appropriate PPE when using our facility. At a minimum, users should wear gloves and lab coats when working with samples and chemicals. Gloves will be provided by our facility. Self-Service users are expected to supply their own lab coat. Goggles are available upon request.

ii. Provided Space – Users will have access to lab bench space. Users are expected to keep their work within these spaces.

iii. Materials and Small Equipment Available – The core facility has the following materials and small equipment available for use gloves, pipets, pipet tips, 1.7 mL, 2.0 mL, 15mL, and 50mL tubes, vortex, sonicator, nitrogen gas evaporator, and speedvacs. These are available in case users need to prep some samples.

iv. Completion Tasks – (i.e. clean-up, disposal, etc.)

a. Clean Up – Users are expected to keep the facility and instruments clear and orderly. Items should be returned to their proper places once finished with them.

b. Hardware Changes – All hardware must be set back to the original starting configuration.

c. Waste Container Maintenance – When using the instrument, users should indicate the compound names used, if not already listed, on the tag located on the waste container. If the bottle is close to being ¾ full before you start, please notify a facility staff member, or switch out full bottle for an empty bottle with a new chemical waste tag. Place the full waste container in the chemical waste pick-up container located beneath the sample preparation bench.

d. Usage Reporting – Users must report the total # of hours (including blanks, QCs, and standards) and the total number of hours for samples. The total # of hours for samples will be used for billing.

e. File Backup and Storage – Users are responsible for backing up and storing their data and method files. For instrument computers that are not attached to the internet and do not have an anti-virus installed, users should either use a brand-new flash drive to get their files or ask a staff member to scan their flash drive for viruses prior to using it. Otherwise, files can be uploaded and shared via cloud storage.

H. Help or Error Requests During Instrument Use – Staff will be available to help during normal operating hours. If the issue is the result of instrument malfunction not resulting from user error, the user will not be responsible for the cost. If the issue is the result of a user error, the user will be responsible for the cost of replacement components if needed. Users should never hesitate to ask if they are unsure about something.

I. Instrument Damage – Users are responsible for any damages caused to the instrument because of their use and they will incur charges for parts and labor associated with the repair if necessary. Significant damage to the instrument because of negligence on the part of the user may result in loss of all self-service privileges.

J. Loss of Use – Users that are unable to abide by the above expectations outlined in the Self Service Users section of this document may lose self-service privileges. We ask that all users be respectful of staff, the facility, and our time so that we don't have to take such actions.

8. Payment for Service

A. User Fees – User fees are based on the fee schedule listed in iLab. Fees are tiered based on user type (internal, academic, or external). These fees are reassessed each year and any changes are effective for samples billed after July 1. Samples submitted for services listed on iLab are charged using a flat rate per hour. See below for more information on obtaining a quote.

Upon submitting samples, users agree to accept liability for all applicable service fees associated with their project. If an added step or different approach is required while processing the samples, we will notify the user in advance to agree with the change and the new cost. To avoid being charged extra for our standard services, we ask users to follow our guidelines outlining how we expect samples to be submitted and address any questions with us before submitting samples.

In the event that an experiment is unsuccessful for whatever reason, the determination whether to charge the use fee will be based on whether the outcome was caused by a staff member, instrument error, or by user error. In the case where it was the fault facility staff or instrument error users will not be charged. In the case where it was the fault of the user, such as improper pre-submission sample preparation, using wrong solvents, using wrong method, or submitting incorrect samples, etc the charges will still apply for all work completed.

B. Invoicing – Users will be invoiced through iLab at the beginning of the subsequent calendar month after work is completed.

C. Quotes – For customers wishing to request a quote, please email the facility Director, Ashley Shay (aes5254@psu.edu). Final price is subject to change based on services and time rendered. Quotes expire at the end of the fiscal year (June 30th).

I, _____ attest that I have read, understood, and agree to the policies

(Signature)

and procedures of the Penn State Metabolomics Core Facility.