

HCS/HN/FST/BMI 7600: Metabolomics, Principles and Practice
Spring 2022, 3 credits

Meeting dates and location: Monday/Wednesday, 12:40-1:35pm (lecture), Wednesday 1:45-3:45pm (lab). Lectures will be held in person in Kottman 451.

Zoom links: Zoom links are only for students who have previously gotten approvals to attend virtually.

Mondays: Meeting ID: 950 7851 3178, Password: 043844

<https://osu.zoom.us/j/95078513178?pwd=eHRTTBLL0VzOGM4OWRqRWZITXBqQT09&from=addon>

Wednesdays: Meeting ID: 924 8206 9737, Password: 978948

<https://osu.zoom.us/j/92482069737?pwd=THp2cFEzZURVMUdjnBNc2xTLzNWUT09&from=addon>

Course format: in person lecture and laboratory. For students stationed at OARDC: lectures and laboratories will be Zoom-linked to Wooster, though we recommend for 2 labs that Wooster students travel to the Columbus campus for hands-on, wet lab experiences. The dates of these labs will be determined prior to the start of the course.

Instructors:

Jessica Cooperstone, Ph.D., Horticulture and Crop Science, 348 Howlett Hall
cooperstone.1@osu.edu

Rachel Kopec, Ph.D., Human Nutrition, 262G Campbell Hall
kopec.4@osu.edu

Emmanuel Hatzakis, Ph.D., Food Science & Technology, 233 Parker
chatzakis.1@osu.edu

Matthias Klein, Ph.D., Food Science & Technology, 313 Parker
klein.663@osu.edu

Teaching assistant:

Ziqi Li, li.11396@osu.edu

Office hours (for all instructors and TA): by appointment

Pre-requisites: Approval of instructor. Because of the interdisciplinary nature of this course, we understand students will have different backgrounds and we encourage you to discuss with the instructors your suitability for this course. However students will gain the most from the course if they understand the basics of univariate and multivariate statistical techniques, as well as the basics of spectroscopy. The instructors can suggest remedial reading material for those for whom this will be helpful.

The “LC-MS” and “Data analysis” modules of this class will use the [R](https://www.r-project.org/) environment (<https://www.r-project.org/>) and we recommend you use [RStudio](#). If you have no experience with R, please take the R Basics module of this [free online course](#) before the LC-MS portion of the course.

Textbooks/readings: no textbook required, readings as assigned

Course description: This course aims to introduce students to the principles and practice of metabolomics. Metabolomics is the study of the totality of small molecules existing within a system. We will focus here on the application of metabolomics to plant, food, nutrition and health-related research, although the concepts are applicable to other disciplines. Each part of the metabolomics workflow will be covered, with hands-on experience in sample preparation, data collection, data processing and analysis, modeling, contextualization, and validation. The course will also contain a journal-club component.

Goals: Students will learn the foundations of metabolomics and each part of the workflow from experimental design to data acquisition to data analysis. After completing the course, students will comprehend the strengths and pitfalls of the technology, understand the nomenclature and various experimental approaches, and have hands-on experience in analysis. In addition, they should be able to design multidisciplinary metabolomics studies and critically evaluate publications in the field. Overall, the course will prepare those who intend to directly apply these techniques to plant, food and nutrition-based research, and will give them confidence to interact with other scientists conducting metabolomics experiments.

Course objectives:

Students will have the ability to:

1. Recall and describe the fundamental principles of metabolomics, as applicable to any discipline.
2. Discuss each part of the metabolomics workflow including sample preparation, data acquisition, data processing, data analysis, data interpretation/contextualization.
3. Complete each part of the metabolomics workflow, including preparing samples, acquiring data, processing data, analyzing data, data interpretation/contextualization.
4. Read, interpret, review and present general primary literature on metabolomics.
5. Develop a thorough understanding of nutritional metabolomics as applied to plants, animals, and/or humans. Understand the types of nutrition-based research questions that can be asked via metabolomics, strengths and limitations of this approach, utility of multi-omic integration in elucidating novel pathways of metabolism, determining pathway flux, and assessing host-microbiome interactions.
6. Design a metabolomics experiment that is relevant and appropriate to their own research field/area of study.

Students will meet these course objectives through lecture, hands-on experience (laboratory), take-home assessments, presentation activities and designing their own metabolomics experiment.

Course schedule: Assignments are due at 11:59 pm on the day of the last meeting time of the week. Assignments may be moved to be due later than indicated below, but will not be moved to be due earlier.

Week	Day	Topics, Assignments, Deadlines, Events	Instructor responsible
1	1/10/2022	<u>Introduction</u> : What is metabolomics? What kinds of questions can it help answer? Expectations of metabolomics vs. reality. Overview of the metabolomics workflow. Overview of mass spectrometry and NMR.	Cooperstone
	1/12/2022	<u>Introduction continued</u>	Cooperstone
2	1/17/2022	No class (MLK Jr. Day)	
	1/19/2022	<u>Introduction continued:</u> <u>Online materials and resources for metabolomics research</u>	Cooperstone
3	1/24/2022	<u>Study design and sample collection</u>	Cooperstone
	1/26/2022	<u>Study design and sample collection</u> Metabolomics journal club activity #1 (instructor led)	Cooperstone
4	1/31/2022	<u>LC-MS data acquisition</u>	Kopec
	2/2/2022	<u>LC-MS data acquisition</u> Due: assessment on introduction/online materials/study design & sample collection.	Kopec
5	2/7/2022	<u>LC-MS sample preparation and analysis (utilizing a nutrition-based sample set for lecture and hands-on lab activities)</u>	Kopec
	2/9/2022	<u>LC-MS compound identification, pathways enrichment</u> <u>LC-MS Lab day #1</u>	Kopec
6	2/14/2022	<u>Special considerations for GC-MS/VOC analysis</u>	guest lecture by Chris Zhu
	2/16/2022	<u>LC-MS compound identification, pathways enrichment</u> <u>LC-MS Lab day #2</u>	Kopec
7	2/21/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u> Metabolomics journal club activity #2 (LCMS, student-led)	Kopec/ Hatzakis
	2/23/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u> Due: assessment on LC-MS sample preparation, data acquisition pre-processing, compound identification.	Hatzakis
8	2/27/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u>	Hatzakis

	3/2/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u>	Hatzakis
9	3/7/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u>	Hatzakis
	3/9/2022	<u>NMR sample preparation, data acquisition, pre-processing, compound identification</u> Metabolomics journal club activity #3 (NMR, student led)	Hatzakis
10	3/14/2022	Spring break (no class)	
	3/16/2022	Spring break (no class)	
11	3/21/2022	<u>Data analysis</u>	Klein
	3/23/2022	<u>Data analysis</u>	Klein
12	3/28/2022	<u>Data analysis</u> Due: assessment on NMR sample preparation, data acquisition pre-processing, compound identification	Klein
	3/30/2022	<u>Data analysis</u>	Klein
13	4/4/2022	<u>Data analysis</u>	Klein
	4/6/2022	<u>Data analysis</u>	Klein
14	4/11/2022	Metabolomics journal club activity #4 (data analysis, student led)	Klein
	4/13/2022	<u>Targeted analysis, quantification and validation, continued</u> Due: assessment on data analysis	Cooperstone
15	4/18/2022	<u>Concluding topics:</u> Pathway analysis, network analysis, multi-omic integration	Cooperstone
	4/20/2022	Nutrition-based Metabolomics Applications: <ul style="list-style-type: none"> - nutrition-centric study design concerns - elucidating biomarkers of dietary intakes novel plant/food based metabolite identification <ul style="list-style-type: none"> - xenobiotic metabolism 	Kopec
16	4/25/2022	Nutrition-based Metabolomics Applications: <ul style="list-style-type: none"> - isotope labeling experiments of the TCA cycle - multi-omic integration, including gene x diet effects on metabolome and gut microbiome-host interactions - nutrition-relevant pathways analysis Nutrition focused metabolomics journal club activity #5 (instructor led)	Kopec

Final: Capstone assignment (take home) will be comprehensive and ask questions which probe knowledge gained from all course modules (i.e. Introduction, LC/GC-MS metabolomics, NMR, Data

analysis, targeted analyses, nutrition-based metabolomics applications and considerations). Due May 2, 2022

Evaluations: assignments are due by 11:59pm, and are to be submitted through Carmen.

Assignment	Due date	Percentage of grade
Take home assessment after each module:		40%
○ Intro/study design/sample preparation	2/2/2022	10%
○ LC-MS	2/23/2022	10%
○ NMR	3/23/2022	10%
○ Data analysis	4/13/2022	10%
Journal club presentation and participation		20%
○ Intro/study design/sample preparation (Instructor led)	1/26/2022	
○ LC-MS (Student led)	2/21/2022	
○ NMR (Student led)	3/9/2022	
○ Data analysis (Student led)	4/6/2022	
○ Metabolomics applications (Instructor led)	4/25/2022	
Design your own metabolomics experiment	4/25/2022	15%
Capstone assignment as a final (take home)	5/2/2022	25%

Grading Scale: The standard grading scale is below. Grades can be adjusted upward but will not be adjusted downward (e.g., an 88 can become an A- but an 81 will not become a C+).

<u>Percentage</u>	<u>Grade</u>	<u>Percentage</u>	<u>Grade</u>
93-100	A	73-76.9	C
90-92.9	A-	70-72.9	C-
87-89.9	B+	67-69.9	D+
83-86.9	B	60-66.9	D
80-82.9	B-	<60	E
77-79.9	C+		

Metabolomics journal club presentations:

One objective of this course is to give students experience in reading primary literature in the metabolomics field. There will be 5 journal club sessions. The first session will be an instructor led journal club style discussion about a primary piece of metabolomics literature. Students will be broken up into 3 groups, and there will then be 3, student led journal club discussions on MS, NMR and data analysis, each selected to focus on a particular technology or approach. A final journal club activity will be presented on metabolomics applications by the instructors.

We will have a Carmen discussion page for each journal club activity (for a total of 5). Student must submit information regarding strengths and weaknesses of each paper prior to presentation during class. We expect all students to actively participate in journal club discussion, and this participation will contribute towards your grade. The schedule for journal club activities is found under Course Schedule and Evaluations.

Design your own metabolomics experiment (2-3 single spaced pages):

The goal of this assignment is for you to think about how you can apply metabolomics to your thesis or dissertation research. This does not need to be an experiment you are actually planning to do.

Assignment should have the following sections:

Background: Background necessary to understand the purpose of the experiment.

Objective: what are you aiming to do? What is the goal of this experiment?

Hypothesis: what do you expect to see in your experiment?

Methods: discuss extraction approach, instrumental platform, data analysis strategy. This is the crux of the assignment and should be where the majority of your time is spent.

Limitations of this study design: what are the limitations of your design? What will this experiment not tell you?

When you refer to published research, you should cite it (the formatting of the citations does not matter, please just be consistent).

Course policies:

Attendance policy: We expect you to attend class as it will be critical to your learning this material, though we will not take attendance. Any class material you miss will be your responsibility to learn. If there are extenuating circumstances that cause you to miss class, please alert the appropriate faculty member for further discussion. If you would like to request to attend class virtually (e.g., you are sick, other unforeseen circumstances), please contact your instructors to discuss and obtain permission.

Late policy: We expect you to turn assignments in on time. However, we are reasonable and we want to see you master the material in this class. If there are extenuating circumstances that prevent you from turning in an assignment on time, please connect with the assigning faculty member as soon as possible after such a situation arises for further discussion. Unexcused late assignments will be docked 10% of total possible points per day late.

Course communication: Our primary mode of communication with class will be during class time, by email, and through Carmen. For graded assignments, you can expect feedback within 7 days, and you can generally expect replies to emails within 24-48 hours.

Plagiarism: all written assignments will be run through a plagiarism checker through Carmen. The results of this software are visible before assignments are turned in. Though the instructors understand the percent plagiarism score is not perfect, we do expect each student to conduct their own work, and not copy from published sources. Plagiarism will not be tolerated in this course. For any questions about plagiarism, please contact one of the instructors.

University Policies:

Course technology

All course materials are distributed via Carmen <http://carmen.osu.edu>, and grades can be viewed there. All course lectures and office hours will occur via Carmen Zoom <https://osu.zoom.us/>.

For help with your password, university e-mail, [Carmen](#), Zoom, or any other technology issues, questions, or requests, contact the OSU IT Service Desk. Standard support hours are available at [OCIO Help Hours](#), and support for urgent issues is available 24x7.

- **Self-Service and Chat support**: (<http://ocio.osu.edu/selfservice>)
- **Phone**: 614-688-HELP (4357)
- **Email**: 8help@osu.edu

- **TDD:** 614-688-8743

Baseline technical skills for online courses

- Basic computer and web-browsing skills
- Navigating Carmen: for questions about specific functionality, see the [Canvas Student Guide](#).
- CarmenZoom virtual meetings (go.osu.edu/zoom-meetings)

Technology skills necessary for this specific course

- Zoom text, audio, and video chat
- Recording a slide presentation with audio narration
- Recording, editing, and uploading video

Required equipment

- Computer: current Mac (OS X) or PC (Windows 7+) with high-speed internet connection
- Webcam: built-in or external webcam, fully installed and tested
- Microphone: built-in laptop or tablet mic or external microphone
- Other: a mobile device (smartphone or tablet) to use for BuckeyePass authentication

Required software

- [Microsoft Office 365](#): All Ohio State students are now eligible for free Microsoft Office 365 ProPlus through [Microsoft's Student Advantage program](#). Full instructions for downloading and installation is found at <https://ocio.osu.edu/kb04733>.

Carmen Access

You will need to use [BuckeyePass](#) multi-factor authentication to access your courses in Carmen. To ensure that you are able to connect to Carmen at all times, it is recommended that you take the following steps:

- Register multiple devices in case something happens to your primary device. Visit the [BuckeyePass - Adding a Device](#) help article for step-by-step instructions.
- Request passcodes to keep as a backup authentication option. When you see the Duo login screen on your computer, click "Enter a Passcode" and then click the "Text me new codes" button that appears. This will text you ten passcodes good for 365 days that can each be used once.
- Download the [Duo Mobile application](#) to all of your registered devices for the ability to generate one-time codes in the event that you lose cell, data, or Wi-Fi service.

If none of these options will meet the needs of your situation, you can contact the IT Service Desk at 614-688-4357 (HELP) and the IT support staff will work out a solution with you.

Academic Misconduct: It is the responsibility of the Committee on Academic Misconduct to investigate or establish procedures for the investigation of all reported cases of student academic misconduct. The term "academic misconduct" includes all forms of student academic misconduct wherever committed; illustrated by, but not limited to, cases of plagiarism and dishonest practices in connection with examinations. Instructors shall report all instances of alleged academic misconduct to the committee (Faculty Rule 3335-5-487). For additional information, see the Code of Student Conduct at [Student Life http://studentconduct.osu.edu](http://studentconduct.osu.edu).

Ohio State's academic integrity policy

Academic integrity is essential to maintaining an environment that fosters excellence in teaching, research, and other educational and scholarly activities. Thus, The Ohio State University and the Committee on Academic Misconduct (COAM) expect that all students have read and understand the

University's *Code of Student Conduct*, and that all students will complete all academic and scholarly assignments with fairness and honesty. Students must recognize that failure to follow the rules and guidelines established in the University's *Code of Student Conduct* and this syllabus may constitute "Academic Misconduct."

The Ohio State University's *Code of Student Conduct* (Section 3335-23-04) defines academic misconduct as: "Any activity that tends to compromise the academic integrity of the University, or subvert the educational process." Examples of academic misconduct include (but are not limited to) plagiarism, collusion (unauthorized collaboration), copying the work of another student, and possession of unauthorized materials during an examination. Ignorance of the University's *Code of Student Conduct* is never considered an "excuse" for academic misconduct, so I recommend that you review the *Code of Student Conduct* and, specifically, the sections dealing with academic misconduct.

If we suspect that a student has committed academic misconduct in this course, we are obligated by University Rules to report my suspicions to the Committee on Academic Misconduct. If COAM determines that you have violated the University's *Code of Student Conduct* (i.e., committed academic misconduct), the sanctions for the misconduct could include a failing grade in this course and suspension or dismissal from the University.

If you have any questions about the above policy or what constitutes academic misconduct in this course, please contact me.

Other sources of information on academic misconduct (integrity) to which you can refer include:

- The Committee on Academic Misconduct web pages ([COAM Home](#))
- *Ten Suggestions for Preserving Academic Integrity* ([Ten Suggestions](#))
- *Eight Cardinal Rules of Academic Integrity* (www.northwestern.edu/uacc/8cards.htm)

If you have any questions about the above policy or what constitutes academic misconduct in this course, please reach out to your instructor.

Copyright disclaimer: The materials used in connection with this course may be subject to copyright protection and are only for the use of students officially enrolled in the course for the educational purposes associated with the course. Copyright law must be considered before copying, retaining, or disseminating materials outside of the course. Intellectual Property (covered by copyright) includes Course materials (Text, Audio, Video, Multimedia, Sims, Apps, etc.), and Student Generated materials

Disability Services: The University strives to make all learning experiences as accessible as possible. If you anticipate or experience academic barriers based on your disability (including mental health, chronic or temporary medical conditions), please let me know immediately so that we can privately discuss options. To establish reasonable accommodations, I may request that you register with Student Life Disability Services. After registration, make arrangements with me as soon as possible to discuss your accommodations so that they may be implemented

in a timely fashion. SLDS contact information: slds@osu.edu; 614-292-3307; slds.osu.edu; 098 Baker Hall, 113 W. 12th Avenue.

Requesting accommodations: If you would like to request academic accommodations based on the impact of a disability qualified under the Americans with Disabilities Act and Section 504 of the Rehabilitation Act of 1973, contact your instructor privately as soon as possible to discuss your specific needs. Discussions are confidential. In addition to contacting the instructor, please contact the Student Life Disability Services at [614-292-3307](tel:614-292-3307) or ods@osu.edu to register for services and/or to coordinate any accommodations you might need in your courses at The Ohio State University. Go to [Office of Student Life - Disability Services](#) for more information.

Accessibility of course technology: This online course requires use of Carmen (Ohio State's learning management system) and other online communication and multimedia tools. If you need additional services to use these technologies, please request accommodations with your instructor.

- [Carmen \(Canvas\) accessibility](#)
- Streaming audio and video
- Synchronous course tools
- [Definition OSU](#)
- [Overview of Accessibility at OSU](#)

Counseling and Consultation Services: As a student you may experience a range of issues that can cause barriers to learning, such as strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance or reduce a student's ability to participate in daily activities. The Ohio State University offers services to assist you with addressing these and other concerns you may be experiencing. If you or someone you know are suffering from any of the aforementioned conditions, you can learn more about the broad range of confidential mental health services available on campus via the Office of Student Life's Counseling and Consultation Service (CCS) by visiting ccs.osu.edu or calling 614-292-5766. CCS is located on the 4th Floor of the Younkin Success Center and 10th Floor of Lincoln Tower. You can reach an on call counselor when CCS is closed at 614-292-5766 and 24 hour emergency help is also available through the 24/7 National Suicide Prevention Hotline at 1-800-273-TALK or at suicidepreventionlifeline.org.

David Wirt, wirt.9@osu.edu, is the CFAES embedded mental health counselor. He is available for new consultations and to establish routine care. To schedule with David, please call 614-292-5766. Students should mention their affiliation with CFAES when setting up a phone screening.

Creating an environment free from harassment, discrimination, and sexual misconduct:

The Ohio State University is committed to building and maintaining a community to reflect diversity and to improve opportunities for all. All Buckeyes have the right to be free from harassment, discrimination, and sexual misconduct. Ohio State does not discriminate on the basis of age, ancestry, color, disability, ethnicity, gender, gender identity or expression, genetic information, HIV/AIDS status, military status, national origin, pregnancy (childbirth, false pregnancy, termination of pregnancy, or recovery therefrom), race, religion, sex, sexual orientation, or protected veteran status, or any other bases under the law, in its activities, academic programs, admission, and employment. Members of the university community also have the right to be free from all forms of sexual misconduct: sexual harassment, sexual assault, relationship violence, stalking, and sexual exploitation.

To report harassment, discrimination, sexual misconduct, or retaliation and/or seek confidential and non-confidential resources and supportive measures, contact the Office of Institutional Equity:

1. Online reporting form at equity.osu.edu,
2. Call 614-247-5838 or TTY 614-688-8605,
3. Or Email equity@osu.edu

The university is committed to stopping sexual misconduct, preventing its recurrence, eliminating any hostile environment, and remedying its discriminatory effects. All university employees have reporting responsibilities to the Office of Institutional Equity to ensure the university can take appropriate action:

- All university employees, except those exempted by legal privilege of confidentiality or expressly identified as a confidential reporter, have an obligation to report incidents of sexual assault immediately.
- The following employees have an obligation to report all other forms of sexual misconduct as soon as practicable but at most within five workdays of becoming aware of such information: 1. Any human resource professional (HRP); 2. Anyone who supervises faculty, staff, students, or volunteers; 3. Chair/director; and 4. Faculty member.

This course adheres to The Principles of Community adopted by the College of Food, Agricultural, and Environmental Sciences. These principles are located on the Carmen site for this course; and can also be found at <https://go.osu.edu/principlesofcommunity>. For additional information on Diversity, Equity, and Inclusion in CFAES, contact the CFAES Office for Diversity, Equity, and Inclusion (<https://equityandinclusion.cfaes.ohio-state.edu/>). If you have been a victim of or a witness to a bias incident, you can report it online and anonymously (if you choose) at <https://studentlife.osu.edu/bias/report-a-bias-incident.aspx>.