HCS/HN/FST/BMI 7600: Metabolomics, Principles and Practice
Spring 2020, 3 credits

Meeting dates and location: Monday/Wednesday, 12:40-1:35pm (lecture), Wednesday 1:45-3:45pm (lab). Both lecture and lab are held in Kottman Hall 451 (Columbus) and Williams 123 (Wooster).

Course format: in person lecture and laboratory. For students stationed at OARDC: lectures and laboratories will be videolinked to Wooster, though we recommend for 2-3 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:
Chengyu Gao, 266 Parker, gao.807@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.

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 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 primary literature on metabolomics.
5. 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.

| Week | Week of | Topics, Assignments, Deadlines, Events | Instructor responsible |
|---|---|---|---|
| 1 | 1/6/2020 | Introduction: 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 |
| 2 | 1/13/2020 | Introduction continued:<br>Online materials and resources for metabolomics research<br>Metabolomics journal club activity #1 (instructor led) | Cooperstone |
| 3 | 1/20/2020 | Study design and sample collection | Cooperstone |
| 4 | 1/27/2020 | LC-MS sample preparation, data acquisition, pre-processing, compound identification<br>**Due**: assessment on introduction/online materials/study design & sample collection. | Kopec |
| 5 | 2/3/2020 | LC-MS sample preparation, data acquisition, pre-processing, compound identification | Kopec |
| 6 | 2/10/2020 | LC-MS sample preparation, data acquisition, pre-processing, compound identification. Special consideration for GC-MS<br>Metabolomics journal club activity #2 (student led) | Kopec, Gao |
| 7 | 2/17/2020 | NMR sample preparation, data acquisition, pre-processing, compound identification | Hatzakis |
| 8 | 2/24/2020 | NMR sample preparation, data acquisition, pre-processing, compound identification<br>**Due**: assessment on LC-MS sample preparation, data acquisition pre-processing, compound identification. | Hatzakis |
| 9 | 3/2/2020 | NMR sample preparation, data acquisition, pre-processing, compound identification<br>Metabolomics journal club activity #3 (student led) | Hatzakis |
| 10 | 3/9/2020 | Spring break (no classes) | |

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|---|---|---|---|
| 11 | 3/16/2020 | Data analysis<br>**Due**: assessment on NMR sample preparation, data acquisition pre-processing, compound identification. | Klein |
| 12 | 3/23/2020 | Data analysis | Klein |
| 13 | 3/30/2020 | Data analysis<br>Metabolomics journal club activity #4 (student led) | Klein |
| 14 | 4/6/2020 | Targeted analysis, quantification and validation<br>**Due**: assessment on Data analysis | Cooperstone |
| 15 | 4/13/2020 | Concluding topics | All |

Final: Tuesday, April 28, 2020 from 12-1:45pm (Kottman 451, our class meeting location)

Evaluations:

| Assignment | Due date | Percentage of grade |
|---|---|---|
| Take home assessment after each module: | | 40% |
| ○ Intro/study design/sample preparation | 1/29/2020 | 10% |
| ○ LCMS | 2/26/2020 | 10% |
| ○ NMR | 3/18/2020 | 10% |
| ○ Data analysis: | 4/8/2020 | 10% |
| Cumulative final (during finals week) | 4/28/2020 | 25% |
| • Journal club presentation and participation | | 20% |
| ○ Intro/study design/sample preparation | 1/15/2020 | |
| ○ LCMS | 2/12/2020 | |
| ○ NMR | 3/4/2020 | |
| ○ Data analysis | 4/1/2020 | |
| Design your own metabolomics experiment | 4/17/2020 | 15% |

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+).

| Percentage | Grade | Percentage | Grade |
|---|---|---|---|
| 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. In week 2, there 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 in weeks 6 (MS), 9 (NMR) and 13 (data analysis), each selected to focus on a particular technology or approach. Students will be graded based on their presentation to the class, and their participation in the other journal club activities.

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.

University policies:

**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 http://studentconduct.osu.edu/.

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

**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.