METABOLOMICS DETECTION AND ANALYSIS
(HORT 579; 2 Credits)
Spring 2016

***Instructor*:** Dr. Adam Heuberger
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Term/Location: 6-week term (Feb 13- Mar 31)
MW, 1 – 5 PM (lecture and computer lab)
218 Shepardson

***Office Hours*:** By appointment

Course Description: A survey of experimental designs and workflows to generate, computationally process and analyze metabolite data. The course will cover methods to detect small molecules and proteins using mass spectrometry, and cover processing and interpretation of chemical data for metabolomics and proteomics studies. Course format includes lecture, computer lab, literature review, and student presentations.

Prerequisite: Graduate standing or permission of instructor. This class is designed to include non-majors with graduate standing. BS degree that includes coursework in biology and chemistry is preferred. An understanding of basic biology, biochemistry and statistics is recommended, but not required for this course. Prior coursework/knowledge in molecular biology and/or informatics will be beneficial for this course.

Objectives: Upon completion of this course, the students will be able to:

1. Apply specific content knowledge and vocabulary in the major areas encompassed by detection and analysis of metabolites.
2. Analyze and explain the mechanisms through which mass spectrometry techniques are used to detect metabolites.
3. Analyze and interpret chemoinformatics and statistics used to generate quantitative information in a metabolite experiment.
4. Evaluate and critique scientific literature that include metabolite detection and analysis.
5. Synthesize scientific literature and develop hypotheses and experimental designs in the field of metabolomics.
6. Develop and demonstrate critical thinking, analytical, written and oral communication skills by leading a class discussion.
7. Perform computational analysis of mass spectrometry datasets and interpret the data.

The course will involve lecture, scientific paper readings and computer labs. Students are expected to read the papers for each lecture and for class discussion.

Required/Recommended Knowledge Base: An understanding of basic biology, biochemistry and statistics is recommended, but not required for this course. Prior coursework/knowledge in molecular biology and/or informatics will be beneficial for this course. Students can bring custom data sets for use in the computer lab.

Readings: Readings will be provided on Canvas. Assigned journal articles will be mandatory reading and all other readings posted will be supplementary.

Grading: Students will be evaluated based on: class participation and quizzes (10%), exams (2 at 20% each), final exam (experimental design/proposal) (20%), manuscript worksheets (10%), and lab activities (20%).

Score	**Grade**
90-100	A
80-89	B
70-79	C
60-69	D
< 60	F

Class participation: Class participation will be evaluated by attendance, preparation for classroom discussions and activities, and handing in lab activities and worksheets on their due date.

Assignments: All students will…

1. Synthesize course material through exams and lab worksheets
2. Interpret research papers published in a top rated, peer reviewed journal (impact factor >3)
3. Provide constructive feedback on student presentations
4. Design hypothetical experiments in metabolomics and communicate results

Experimental design activities: Each student will work in a group to develop an experimental design to answer a fundamental question in the field of metabolomics. The question will be provided by the instructor, and each student will design an experiment that includes methods, materials, and data analysis procedures. The student will present the question and experiment to the class, and the class will participate to refine the experimental design as needed. **A write up of the experimental design activity will be the course final exam.**

Paper discussions: The instructor will be responsible for leading the paper discussions. A research paper will be provided to the class in advance and students are expected to have read the paper in preparation for class discussion. Students will fill out a worksheet that summarizes the main points of the paper and prepare questions for discussion.

Relevant text:

Lindon, John C., Jeremy K. Nicholson, and Elaine Holmes, eds. *The handbook of metabonomics and metabolomics*. Elsevier, 2011.

Weckwerth, Wolfram, and Günter Kahl, eds. *The handbook of plant metabolomics*. John Wiley & Sons, 2013.

Schedule (6-weeks):
*Readings are **required** for each lecture

DATE	ACTIVITY	MOD	TOPICS	Reading*
Mon 2/13	Lecture 1 Computer tutorial Lecture 2 Computer Lab	M1 M1 M2 M1, M2	Course overview; metabolomics and mass spectrometry chemical structures, using chemical databases GC-MS detection and analysis of volatiles and non-volatiles Begin Lab 1	Dett. (I – III/D) Dett. (V/C) Dett. (VIII/A-B) Dett. (IX)
Wed 2/15	Paper discussion Computer tutorial Computer lab	M2 M2 M1, M2	GC-MS metabolomics GC-MS **Lab 1** (structures) and **Lab 2** (GC-MS detection)	Cuadros 2016 Mastrangelo 2.4-2.7
Mon 2/20	Lecture 3, 4 Computer tutorial Computer lab	M3, M4 M3 M3	LC-TOF-MS, high resolution MS LC-TOF-MS metabolomics and annotations Begin Lab 3 (LC-MS detection)	Dett. (V/B) Dett. (VIII/C)
Wed 2/22	Paper discussion Computer tutorial Computer lab	M3 M4 M3, M4	LC-MS metabolomics absolute quantitation **Lab 3** (LC-MS metabolomics) and **Lab 4** (absolute quantitation)	
Mon 2/27	Lecture 5 Computer tutorial Review Computer lab	M5 M5	Data processing for analysis of multiple samples; Statistics Data processing using XCMS Exam 1 **Lab:** make-up time/work with custom data	Dett. *et al.* (VII)
Wed 3/1	**EXAM 1** Paper discussion Computer lab	 M5 M5	*content:* M1-M4 Data processing/metabolite ID **Lab 5:** Data processing/XCMS	
Mon 3/6	Lecture Computer tutorial Lecture Computer lab	M6 M6 M6 M6	Statistics used in metabolomics Statistics Data visualization Begin Lab 6 (statistics)	
Wed 3/8	Paper discussion Computer lab	M6 M6	Statistics **Lab 6** (statistics part 1) and **Lab 7** (statistics part 2)	
Mon 3/20	Lecture Paper discussion Computer lab Review	M7 M7 M7	Proteomics Proteomics **Lab 8 (**proteomics) Exam 2	
Wed 3/22	**EXAM 2** Tour Computer lab		*Content M5-M7* Proteomics and Metabolomics Facility; ICP-MS Make up labs/custom data; Experimental design activity	
Mon 3/27 Wed 3/29	Lecture Computer lab Presentations	M8	Other platforms/applications (MALDI, Biotyping, IM, ICP) Experimental design activity preparation Experimental design activities	