



**International Summer Sessions in Metabolomics**

time	instructor	room		
<b>Monday 26</b>				
9.00- 10.00	Dr. Oliver Fiehn	4202	Welcome , course overview, explaining the different parts, groups, time lines Metabolomics overview	
10.00- 10.05			break	
10.05- 11.35	Dr. Sean Adams	4202	<u>study designs</u> Human and animal cohort studies - study designs	
11.35- 11.40			break	
11.40- 13.10	Dr. Daniel Kliebenstein	4202	Plant studies - designs combining genotyping and physiology	
13.10- 14.10			lunch	
14.10- 15.30	Dr. Oliver Fiehn Mine Palazoglu (plant)	4202 1226	<u>lab work 1 - sample prep + data acquisition</u> Plant tissue sample prep group A	Plant "study design florigen" group C+D
	Dr. Ingrid Gennity (blood)	1226	Blood biocrates sample prep group B	
15.30- 15. 45			break	
15.45- 17.05	Dr. Oliver Fiehn Mine Palazoglu (plant)	4202 1226	Plant tissue sample prep group C Blood biocrates sample prep group D	Plant "study design florigen" group A+B
17.05- 17.20	Dr. Ingrid Gennity (blood)	1226	break	
17.20- 17.50	Dr Fiehn, Palazoglu,Dr Gennity	4202	discussion day 01	
<b>Tuesday 27</b>				
9.00- 10.30	Dr. Teresa Fan and Dr. Andrew Lane	Auditorium 4202	Stable isotope-resolved metabolomics for bench-to-bedside translational research discussion on fluxomics	
10.30- 10.40			break	
10.40- 11.40	Dr. Ralf Bogumil	4202	<u>sample preparation</u> Blood TARGET METABOLOMICS	
11.40- 12.40	Dr. John Newman	4202	Blood - lipid mediators	
12.40- 13.40			lunch	
13.40- 15.00	Dr. Ralf Bogumil Dr. Ingrid Gennity (blood)	4202 1226	<u>lab work 1 - sample prep + data acquisition</u> Blood biocrates sample prep group A	Biocrates data processing group C+D
	Mine Palazoglu (plant)	1226	Plant tissue group sample prep B	
15.00- 15.10	Dr. Ralf Bogumil	4202	break	
15.10- 16.30	Dr. Ingrid Gennity (blood) Mine Palazoglu (plant)	1226 1226	Blood biocrates sample prep group C Plant tissue sample prep group D	Biocrates data processing group A+B
16.30- 16. 40			break	
16.40-17.10	Palazoglu,Drs Gennity, Fiehn, Bogumil	4202	discussion day 02	

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<b>Wednesday 28</b>				
9.00- 10.00	Dr. John Newman	4202	Lipid mediators case studies	
10.00- 11.00	Dr. Nilesh Gaikwad	4202	Steroid Metabolome: case studies and methods	
11.00- 11.10			break	
11.10- 12.10	Dr. Carolyn Slupsky	4202	NMR based Metabolomics: case studies and methods	
12.10-13.10			lunch	
13.10- 14.40	Mimi Swe, Mine Palazoglu Dr. John Newman, Dr. Scott Stanley	1226	<u>Lab visit</u> Lab tours groups C+D	<b>GC-TOF MS data acquisition</b> Plant group A+B GCTOF MS
14.45- 14.50			break	
14.50- 16.20	Mimi Swe, Mine Palazoglu Dr. John Newman, Dr. Scott Stanley	1226	Lab tours groups A+B	Plant group C+D GCTOF MS
16.20- 16.30			break	
16.30-17.00	Fiehn, Palazoglu, Gennity	4202	discussion day 03	
<b>Thursday 29</b>				
9.00-10.00	Dr. Carlito Lebrilla	4202	Glycans QTOF	
10.00-11.00	Dr. Tomas Cajka	4202	Complex lipids QTOF	
11.00- 11.10			break	
11.10- 12.10	Dr. Douglas J. Rowland	4202	Imaging in drug metabolism and beyond	
12.1--13.10			lunch	
13.10-14.40	Dr. Bill Wikoff Dr. Tomas Cajka, Dr. Carlos Leon	4202 1226	Mass Spectrometry for Metabolomics group C+D	<b>LC-QTOF MS data acquisition</b> Plant group A+B QTOF MS
14.40-15.00			break	
15.00-16.30	Dr. Bill Wikoff Dr. Tomas Cajka, Dr. Carlos Leon	4202 1226	Mass Spectrometry for Metabolomics group A+B	Plant group C+D QTOF MS
16.30-16.45			break	
16.45-17.15	Drs Fiehn, Wikoff, Cajka, Leon	4202	discussion day 04	
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<b>Friday 30</b>				
8.30- 10.15	Dr. Nobuo Tanaka	4202	<u>Case studies:</u> Achieving higher performance in LC - a fundamental approach	
10.15- 10.30			break	
10.30-11.45	Dr. Carlos Leon/ Dr. Bill Wikoff	Comp Lab 2020	LC-MS Data Handling: Mass Hunter Qualitative Analysis	
11.45-13.00			lunch	
13.00-13.45	Dr. Tobias Kind	Comp Lab 2020	Lecture1: Handling molecules and mass spectra	
13.45-14.30	Dr. Tobias Kind	Comp Lab 2020	Lecture 2: Mass spectral databases and database search	
14.30-14.40			break	
14.40-15.25	Dr. Tobias Kind	Comp Lab 2020	Lecture 3: MS Tools and Concepts (mass accuracy, resolving power)	
15.25-16.25	Dr. Bill Wikoff	Comp Lab 2020	Avoiding Pitfalls in Metabolomics	
16.25-17.00	Drs Fiehn, Wikoff, Cajka, Kind	Comp Lab 2020	discussion and question week 1	



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week 02

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<b>Monday 2</b>			
			<b><u>data processing - theory</u></b>
9.00- 10.00	Dr. Tobias Kind	4202	Lecture 4: GC-MS data handling (data alignment, deconvolution, DB search)
10.00-11.00	Dr. Tobias Kind	4202	Lecture 5: LC-MS data handling (data alignment, deconvolution, MS/MS)
11.00-11.15			break
11.15-12.15	Dr. Tobias Kind	4202	Lecture 6: Tools for mass spectral interpretation and simulation
12.15-13.30		4202	lunch and group picture
			<b><u>Lecture - Introduction to statistics, multivariate analysis and data visualization</u></b>
13.30-14.30	Dr. Dmitry Grapov	4202	Introduction to Multivariate Data Analysis and Visualization
14.30-15.30		4202	Clustering and Projection Pursuits
15.30-15.45			break
15.45-16.45	Dr. Dmitry Grapov	4202	Metabolomics data analysis case studies
16.45-17.00	Drs Kind, Grapov, Fiehn	4202	discussion
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<b>Tuesday 3</b>			
			<b><u>data processing - refresher + discussion</u></b>
			<b><u>computer lab - data processing &amp; compound ID theme 1</u></b>
9.00 - 9.15			
9.15- 10.15	Mine Palazoglu	Comp Lab 2020	GC-quadrupole MS raw data analysis (1) mass spectral deconvolution and AMDIS batch analysis
10.15- 11.15	Mine Palazoglu	Comp Lab 2020	GC-quadrupole MS raw data analysis (2) batch analysis with MassProfilerProfessional including recursive workflow
11.15- 11.30			break
11.30-12.30	Dr. Tobias Kind	Comp Lab 2020	NIST MS search for GC-MS (forward, reverse, hybrid, sequential search; retention time prediction; data import/export)
12.30-13.30			lunch
			<b><u>computer lab - data processing &amp; compound ID theme 2</u></b>
13.30-14.15	Dr. Oliver Fiehn	Comp Lab 2020	GC-TOF MS raw data analysis (1): mass spectral deconvolution, compound identification with retention indices
14.15-15.00	Dr. Oliver Fiehn	Comp Lab 2020	GC-TOF MS raw data analysis (2): generating target lists for profiling
15.00- 15.15			break
15.15-16.00	Dr. Oliver Fiehn	Comp Lab 2020	GC-TOF MS raw data analysis (3): the BinBase DB algorithm and using the BinBase data reports
16.00- 16.15			break
16.15-17.30	Dr. Tomas Cajka	Comp Lab 2020	GCxGC TOF MS raw data analysis: analysis of beer aroma
17.30-18.00			walking over campus to Mondavi Institute for Wine and Food Science
18.00-18.45	Dr. Charles Bamforth	Mondavi	<b>The science of beer brewing - tour</b>
19.00 -21.00	Dr. Charles Bamforth	Genome Center	Beer tasting <i>Genome Center</i>

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			<b>Wednesday 4</b>
9.00- 9.15			<b><u>data processing - refresher + discussion</u></b>
			<b><u>computer lab - data processing &amp; compound ID theme 1</u></b>
9.15- 10.15	Mark Siveria / Dr. Tobias Kind	Comp Lab 2020	MZmine
10.15-11.15	Dr. Tobias Kind	Comp Lab 2020	Compound Identification for LC-MS 1: (adducts, m/z-lookup, MS/MS fragment analysis, MSn library search)
11.15-11.30			break
11.30-12.30	Dr. Tobias Kind	Comp Lab 2020	Compound Identification for LC-MS 2: (retention time prediction, mass spectral trees, in-silico spectra)
12.30-13.30			lunch
			<b><u>data processing - BinBase ...</u></b>
			<b><u>computer lab - data processing &amp; compound ID theme 2</u></b>
13.30-14.30	Dr. Carlos Leon/ Brian DeFelice	Comp Lab 2020	LC-MS Data Processing: Untargeted Approach
14.30-15.30	Dr. Carlos Leon/ Brian DeFelice	Comp Lab 2020	LC-MS Data Processing: Mass Profiler Professional
15.30-15.45			break
15.45-16.45	Dr. Carlos Leon/ Brian DeFelice	Comp Lab 2020	LC-MS Data Processing: Targeted Approach
16.45-17.00		Comp Lab 2020	discussion
			<b>Thursday 5</b>
	Dr. Dmitry Grapov	Comp Lab 2020	<b><u>computer lab - Metabolomics Data Analysis</u></b>
9.15- 10.15		Comp Lab 2020	Univariate statistics and power analysis
10.15-11.15		Comp Lab 2020	Correlation and Cluster Analysis
11.15-11.30			break
11.30-12.30		Comp Lab 2020	Principal Components Analysis I
12.30-13.30			lunch
13.30-14.30		Comp Lab 2020	Principal Components Analysis II
14.30-15.30	Dr. Dmitry Grapov	Comp Lab 2020	Partial Least Squares I
15.30-15.45			break
15.45-16.45		Comp Lab 2020	Partial Least Squares II
16.45-17.00		Comp Lab 2020	discussion
19:00	622 Third Street, Davis		<b>Manna</b> (Korean Restaurant)
			<b>Good Bye dinner</b>
			<b>Friday 6</b>
9.15- 10.15	Dr. Dmitry Grapov	Comp Lab 2020	Introduction to biochemical databases
10.15-11.15		Comp Lab 2020	Network mapping I
11.15-11.30			break
11.30-12.30		Comp Lab 2020	Network mapping II
12.30-13.30			lunch
13.30- 14.30	Palazoglu, Drs Fiehn, Kind, Grapov	Comp Lab 2020	discussion and evaluation