

Schedule for PhD course “Introduction to nutritional metabolomics”

17 to 21 August 2020

Date/Time	Subject	Lecturer	Lecture room
17 August Monday <i>Theme: Introduction to basic concepts in LC-MS metabolomics research</i>			
9:00--9:30	Outline of the course and introduction of participants	LOD	A001 + A009
9:30--10:05	Perspectives and goals of metabolomics	HMR	
	Break		
10:15--10:50	Metabolomics in Nutrition	HMR	
	Break		
11:00--12:00	Overview of the metabolomics pipeline From sample to data interpretation	LOD	
	Lunch will be provided		
13:00--13:30	Experimental design	LOD	
	Break		
13:40--14:00	Navigating freely-available software tools for metabolomics analysis	NVM	
	Break		
	LC-MS based metabolomics		
14:10--16:10	Subject 1 : Samples and sample preparation in metabolomics (GDG) Subject 2 : Liquid chromatography and mass spectrometry principles (CDG) Subject 3: LC-MS technologies for targeted and untargeted metabolomics (CDG)	CDG	
16:20--17:00	LC-MS lab tour	CDG	
17:30--19:30	<i>Optional: Software installation troubleshooting, group-forming and tutorial</i>	JS, MX	
Date/Time	Subject	Lecturer	Lecture room
18 August Tuesday <i>Theme: Metabolomics data preprocessing, normalization and annotation</i>			
9:00--9:30	Data preprocessing in metabolomics: Basic concepts in preprocessing (e.g. feature detection, alignment, gap filling)	JS	
9:30--9:40	Conversion of raw data	JS	
9:40--10:00	A brief introduction to R: Basic syntax, working in Rstudio	JS	
	Break		
10:10--10:40	A brief introduction to R: We import data together, modify it, and export	JS, TH, MX	
10:40--11:30	XCMS walk-through and CAMERA annotation	JS	

11:30--12:00	Presentation of exercise LC-MS dataset: Extraction of food intake markers <i>Exercise: Hands on LC-MS data preprocessing (XCMS)</i>	JS, TH, MX, HMR	A001 + A009
	Lunch will be provided		
13:00--13:50	<i>Exercise: Hands on LC-MS data preprocessing (XCMS)</i> Break	JS, TH, MX, HMR	TBD
14:00--15:00	Introduction to Normalization and transformations Break	NVM	
15:10-17:00	<i>Exercise: Hands on data normalization and annotation</i>	JS, TH, MX	
18:00--21:30	Dinner party		
19 August Wednesday Theme: Metabolomics data analysis			
8:30--9:10	Data Analysis I: Univariate Methods Break	JS	A001 + A009
9:20--10:05	<i>Exercise: Hands on univariate analysis using R</i> Break	JS, CP, TH, MX	
10:15--11:15	Data Analysis II: Multivariate Approach - PCA Break	CP	
11:20--12:00	<i>Exercise: Hands on PCA using R</i>	JS, CP, TH, MX, HMR	
	Lunch will be provided		
13:00--13:20	<i>Exercise: Hands on PCA using R</i> Break	JS, CP, TH, MX, HMR	
13:30--14:30	Data Analysis III: Multivariate Approach - PLSDA Break	CP	
14:40-17:00	<i>Exercise: Hands on PLSDA using R</i>	JS, CP, TH, MX, HMR	
17:30-19:30	<i>Optional time with teachers available</i>	JS, CP, TH, MX	
Date/Time	Subject	Lecturer	Lecture room
20 August Thursday Theme: Metabolite identification			
9:00--9:50	Metabolite Identification (Molecular formula, Interpretation of MS and MS/MS spectra, compound databases)	JS	

10:00--12:00	Break <i>Exercise: Fragmentation, adducts, annotation</i>	JS, CDG, XZ	A001 + A009
	Lunch will be provided		
13:00--14:00	Compound and spectral databases, in-silico prediction, levels of identification	JS	
	Break		
14:10--15:20	<i>Exercise: Fragmentation, adducts, annotation</i>	JS, CDG, XZ	
	Break		
15:30--17:00	<i>Exercise: Hands on - Identification of markers of food intake</i>	JS, CDG, XZ	
17:30--19:30	<i>Optional time with teachers available</i>	JS, CDG, XZ	
21 August Friday <i>Theme: Project work and presentation of results</i>			
8:30--11:30	Students presentations	LOD, JS, CDG, HMR, MX	A001 + A009
11:30--12:00	Course Evaluation	LOD, JS	

Lecturers

LOD : Lars Ove Dragsted

JS: Jan Stanstrup

CDG : Cristian De Gobba

HMR: Henrik Munch Roager

CP : Ceyda Pekmez

MX : Muyao Xi

TH: Tu Hu

XZ : Xiaomin Zhou

NVM : Natalia Vazquez Manjarrez