Schedule for PhD course **"Introduction to nutritional metabolomics"**

28. of June to 2. of July 2021

Date/Time	Subject	Lecturer	Lecture room
Monday ***Theme: Introduction to basic concepts in LC-MS metabolomics research***			
9:00--9:30	Outline of the course and introduction of participants	*LOD*	A2-71.02
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*	
13:30--14:00	LC-MS based metabolomics Subject 1: Samples and sample preparation in metabolomics	*GLB*	
14:00--14:10	*Break*		
14:10--15:50	LC-MS based metabolomics Subject 2: Liquid chromatography and mass spectrometry principles Subject 3: LC-MS technologies for targeted and untargeted metabolomics	*GLB*	
15:50--16:00	*Break*		
16:00--16:30	LC-MS lab tour	*GLB*	
16:30--18:30	*Optional: Software installation troubleshooting, group-forming and tutorial*	*JS, TH, NP*	

Date/Time	Subject	Lecturer	Lecture room
Tuesday	***Theme: Metabolomics data preprocesing, normalization and annotation***		
9:00--9:30	Data preprocesssing in metabolomics: Basic concepts in preprocessing (e.g. feature detection, alignment, gap filling)	*JS*	A2-71.02
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, NP)*	
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 *Exercise: Hands on LC-MS data preprocessing (XCMS)*	*JS, TH, NP, HMR*	
	Lunch will be provided		
13:00--13:50	*Exercise: Hands on LC-MS data preprocessing (XCMS)*	*JS, TH, NP, HMR*	
	Break		
14:00--15:00	Introduction to normalization and transformations	*JS*	
	Break		
15:10-17:00	*Exercise: Continued exercise*	*JS, TH, NP*	
18:00--21:30	Dinner party		TBD

Wednesday ***Theme: Metabolomics data analysis***			
8:30--9:10	Data Analysis I: Univariate Methods	*MAR*	A2-71.02
	Break		
9:20--10:05	*Exercise: Hands on univariate analysis using R*	*MAR, JS, TH, NP*	
	Break		
10:15--11:15	Data Analysis II: Multivariate Approach - PCA	*MAR*	
	Break		
11:20--12:00	*Exercise: Hands on PCA using R*	*MAR, JS, TH, NP*	
	Lunch will be provided		
13:00--13:20	*Exercise: Hands on PCA using R*	*MAR, JS, TH, NP*	
	Break		
13:30--14:30	Data Analysis III: Multivariate Approach - PLSDA	*MAR*	
	Break		
14:40-17:00	*Exercise: Hands on PLSDA using R*	*MAR, JS, TH, NP*	
17:00-19:30	*Optional time with teachers available*	*JS, TH, NP*	

Date/Time	Subject	Lecturer	Lecture room
Thursday ***Theme: Metabolite identification***			
9:00--9:50	Metabolite Identification (Molecular formula, Interpretation of MS and MS/MS spectra, compound databases)	*GLB*	A2-71.02
	Break		
10:00--12:00	*Exercise: Fragmentation, adducts, annotation*	*GLB, JS*	
	Lunch will be provided		
13:00--13:40	Compound and spectral databases, in-silico prediction, levels of identification	*GLB*	
13:40--14:00	*Exercise: Fragmentation, adducts, annotation*	*GLB, JS*	
	Break		
14:10--15:30	*Exercise: Fragmentation, adducts, annotation*	*GLB, JS*	
15:30--17:00	*Exercise: Hands on - Identification of markers of food intake*	*GLB, JS*	
17:00--19:30	*Optional time with teachers available*	*GLB, JS*	

Friday ***Theme: Project work and presentation of results***			
8:30--11:30	Students presentations	*LOD, JS, GLB, HMR*	A2-71.02
11:30--12:00	Course Evaluation	*LOD, JS*	

Lecturers

LOD : Lars Ove Dragsted
JS: Jan Stanstrup
HMR: Henrik Munch Roager
GLB: Giorgia La Barbera
TH: Tu Hu
NP: Nicola Procházková
MAR: Morten Arendt Rasmussen