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

6 to 10 July 2020

Date/Time	Subject	Lecturer	Lecture room
6 July Monday	***Theme: Introduction to basic concepts in LC-MS metabolomics research***		
9:00--9:30	Outline of the course and introduction of participants	*LOD*	
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	*GLB*	
	Lunch will be provided		
13:00--13:30	Experimental design	*LOD*	
	Break		A001 + A009
13:40--14:00	Navigating freely-available software tools for metabolomics analysis	*JS*	
	Break		
14:10--16:10	LC-MS based metabolomics Subject 1 : Samples and sample preperation in metabolomics (*GLB*) Subject 2 : Liquid chromatography and mass spectrometry principles (*CDG*) Subject 3: LC-MS technologies for targeted and untargeted metabolomics (*CDG*)	*CDG, GLB*	
16:20--17:00	LC-MS lab tour	*CDG, GLB*	
17:30--19:30	*Optional: Software installation troubleshooting, group-forming and tutorial*	*JS, CP, MX*	
Date/Time	Subject	Lecturer	Lecture room
7 July 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*	
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, CP, 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 *Exercise: Hands on LC-MS data preprocessing (XCMS)*	*JS, CP, MX, HMR*	A001 + A009
	Lunch will be provided		
13:00--13:50	*Exercise: Hands on LC-MS data preprocessing (XCMS)*	*JS, CP, MX, HMR*	
	Break		
14:00--15:00	Introduction to Normalization and transformations	*CP*	
	Break		
15:10-17:00	*Exercise: Hands on data normalization and annotation*	*JS, CP, MX*	
18:00--21:30	Dinner party		TBD
8 July Wednesday	***Theme: Metabolomics data analysis***		
8:30--9:10	Data Analysis I: Univariate Methods	*JS*	
	Break		
9:20--10:05	*Exercise: Hands on univariate analysis using R*	*JS, CP, MX*	
	Break		
10:15--11:15	Data Analysis II: Multivariate Approach - PCA	*CP*	
	Break		
11:20--12:00	*Exercise: Hands on PCA using R*	*JS, CP, MX, HMR*	A001 + A009
	Lunch will be provided		
13:00--13:20	*Exercise: Hands on PCA using R*	*JS, CP, MX, HMR*	
	Break		
13:30--14:30	Data Analysis III: Multivariate Approach - PLSDA	*CP*	
	Break		
14:40-17:00	*Exercise: Hands on PLSDA using R*	*JS, CP, MX, HMR*	
17:30-19:30	*Optional Tutorial*	*JS, CP, MX*	
Date/Time	Subject	Lecturer	Lecture room
9 July Thursday	***Theme: Metabolite identification***		
9:00--9:50	Metabolite Identification (Molecular formula, Interpretation of MS and MS/MS spectra, compound databases)	*GLB*	

	Break		
10:00--12:00	*Exercise: Fragmentation, adducts, annotation*	*GLB, JS, CDG*	
	Lunch will be provided		
13:00--14:00	Compound and spectral databases, in-silico prediction, levels of identification	*GLB*	A001 + A009
	Break		
14:10--15:20	*Exercise: Fragmentation, adducts, annotation*	*GLB, JS, CDG*	
	Break		
15:30--17:00	*Exercise: Hands on - Identification of markers of food intake*	*GLB, JS, CDG*	
17:30--19:30	*Optional Tutorial*	*GLB, JS, CDG*	
10 July Friday	***Theme: Project work and presentation of results***		
8:30--11:30	Students presentations	*LOD, JS, CDG, HMR, GLB,*	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
GLB : Giorgia La Barbera
CP : Ceyda Pekmez
MX : Muyao Xi