Workflow4Experimenters 2023

Overview

Processing, statistical analysis, and **annotation** of **metabolomics data** is a complex task for **experimenters** since it involves many steps and requires a good knowledge of both the **methodology** and **software** tools. The <u>Workflow4metabolomics.org</u> (W4M) online infrastructure provides a user-friendly and high-performance environment with advanced computational modules for building, running, and sharing **complete workflows for LC-MS, GC-MS, FIA and NMR analysis**. Such features are of major values for teaching computational metabolomics to experimenters, and previous courses using W4M since 2014 have been very successful.

For this new session, format changes:

- From 06 to 10/03: theoretical sessions in videoconference from 10am to 12pm

- From 20 to 24/03: practical sessions with the 1st hour of each day dedicated to short reminders and participant questions (following the theoretical session).

Pre-Registration: form (deadline 31/12/2022)

Goals: During this course, participants will learn how to use the W4M infrastructure to analyze **their own dataset**. Online sessions will be dedicated to **methodology and tools**. Face-to-face sessions will be devoted to **tutoring**. For these practical sessions, the participants will work on their own data (prerequisite for the training is to have a data set).

Date:

- from March, Monday 6 to Friday 10 2023: 10-12 am (Paris hour): theoretical sessions
- from March, Monday 20 (lunch time) to Friday 24 (lunch time) 2023: practical sessions

Costs: 1200€ for academic and **2500 € for private institution** (to cover expenses for trainers, organization, materials and meals)

Including: Lunch, coffee break, pedagogic support and the Thursday social event Not included: travel expenses, accommodation and 3 diners (Monday, Tuesday, Wednesday)

Target audience: LC-MS, GC-MS, NMR, FIA-MS and DI-MS experimenters (e.g. biologists, chemists).

Materials: Participants will use their laptop to perform the analysis on their W4M account. All presentations, reference datasets and workflows will be available online.

Invited speaker: Helge Hecht (Masaryk University, République Tchèque)

Tutors: Each participant will be paired with a duo of tutors (preprocessing / statistics experts) who will help him/her preparing data and assist him/her during each analysis step.

Location: Institute of Complex Systems, Paris (France)

Language: English

Number of attendees: 25 max.

Sponsors: <u>ELIXIR</u>, French Bioinformatics Institute (<u>IFB</u>), French Infrastructure for Metabolomics and Fluxomics (<u>MetaboHUB</u>), Francophone Network for Metabolomics and Fluxomics (<u>RFMF</u>)

Program

W	Webinars											
Start		MONDAY 6th March TUESDAY 7th March			WEDNESDAY 8th March	THURSDAY 9th March		FRIDAY 10th March				
	09:00											
09:00												
09:30	10:00											
10:00	10:30	Galaxy session : initiation and data	[MS] Data Preprocessing M. Pétéra / Y. Guitton	[NMR] Data Preprocessing C Canlet / M. Tremblay-Franco	Statistical analysis M. Pétéra / M. Tremblay- Franco	[MS] Annotation Y. Guitton / R. Weber	[NMR] Annotation C. Canlet	Parallel sessions				
10:30	11:00											
11:00	11:30											
	12:00		Signal Drift and Batch-Effect Correction - M. Pétéra									
12:00	12:30											
12:30	14:00											
14:00	14:30											
	15:00											
	15:30											
	16:00 16:30											
	16:30											
	17:30											
	18:00											
	18:30											
18:30	19:00											
19:00	19:30											
19:30	20:00											
20:00	20:30											

Practicals

Start	End	MONDAY 20th March	TUESDAY 21th March		WEDNESDAY 22th March	THURSDAY 23th March		FRIDAY 24th March
08:30	09:00		[MS] Data	[NMR] Data	Statistical analysis	[MS] Annotation	[NMR] 1D and 2D	Parallel sessions
09:00	09:30		Preprocessing	Preprocessing		MS and MSMS	Annotation	
09:30	10:00		Tutoring	Tutoring	Tutoring	Tutoring	Tutoring	
10:00	10:30							
10:30	11:00		Break		Break	Break		Break
11:00	11:30		Tutoring	Tutoring	Tutoring	Tutoring	Tutoring	Week debrief and Survey
	12:00		-	ch-Effect Correction				
12:00	12:30		Tuto	oring				
12:30	14:00		Buffet lunch		Buffet lunch	Buffet lunch		Lunch boxes
		lunch						
	14:30	round table	Tutoring		Tutoring	Tutoring	Tutoring	
	15:00	-						
	15:30	Tutoring						
	16:00							
	16:30	Break	Break		Break	Break		
	17:00	Tutoring	Tuto	oring	Tutoring	Tutoring	Tutoring	
	17:30							
_	18:00							
	18:30 19:00							
18:30	19:00							
19:00	19:30							
19:30	20:00					20h00 - Social ev	ent : Gala dinner	
20:00	20:30							

Scientific committee

Université Libre de Bruxelles : Cédric Delporte, Florence Souard

ELIXIR-France (IFB) : Gildas Le Corguillé

MetaboHUB : Marie Tremblay-Franco, Mélanie Pétéra, Cécile Canlet, Binta Diemé, Franck Giacomoni, Yann Guitton and the W4M coreteam

IRBA (Institut de Recherche Biomédicale des Armées) : Céline Dalle

For any requests, please contact the team: contact * AT * workflow4metabolomics.org



See you soon in Paris !