



Agenda

de.NBI Computational Metabolomics face2face Hackathon 2021

metaRbolomics and more

Date: 22.-24.11.2021
Location: [Leucorea Wittenberg](#)
Room: SR

Live Agenda (this document): <https://bit.ly/3BCWjqt>

Participant folder: <https://bit.ly/3v4J0wM>

Participant notes: <https://bit.ly/3BKoUdv>

Information: [ELIXIR Germany Code of Conduct](#)

Twitter: [#metaRbolomics](#) (and maybe [#bioconductor](#), [@denbiOffice](#), [@IPB_Halle](#), ...)

2021-11-21 Sunday	
After 16:00	Arrival for people arriving on Sunday Most rooms will be available only after 16:00, and access to keys via a code will only be available for a few participants we have to name in advance.
	Self-organised and self-paid meetup in a nice bar in the City

2021-11-22 Monday	
7:30-9:00	Breakfast in Cafeteria Leucorea
10:00-11:15	Rest of Organisers arriving
11:30-13:30	Individual Break-out groups on city and/or science.
	Lunch in Cafeteria Leucorea
14:00	Welcome and workshop overview (Audimax)
	Metabolite Profiling
15:30-15:45	Coffee/tea, Pre-ordering Dinner
15:45	Metabolite Identification
18:00	Participant flash talks 1.

	<ol style="list-style-type: none"> 2. Michelle Tamara Berger: Non-targeted analysis of peptide glycation products from tandem mass spectra 3. Liesa Salzer: Why we need a R package with effective mobility transformation for CE-MS in Metabolomics 4. Helge Hecht: Potential Encodings of Mass Spectra for ML Applications 5. Michele Stravs: MSNovelist - de novo structure prediction from MS2 spectra. (Note: this is not specifically R-related. I can talk on R stuff / AnnotationFlow if desired.)
19:00	Dinner at Brauhaus (alcoholic beverages self-paid) Visit to Christmas market

	2021-11-23 Tuesday	
7:30-9:00	Breakfast in Cafeteria Leucorea	
9:00	Recap of last day	
9:15	Focus machine learning in metaRbolomics	
11:00-11:30	Coffee/tea	
11:00	TBA	
12:00-13:00	Lunch in Cafeteria Leucorea	
13:00	Group Picture and optional Walk in fresh air	
15.30-15:45	Coffee/tea	
15:45	Graph and Networks	
16:00		
17:45	Participant flash talks <ol style="list-style-type: none"> 6. Katyeny Manuela da Silva: Data filtering for untargeted metabolomics data in R 7. ... 	
19:00	Dinner at Wittenburger (alcoholic beverages self-paid)	
21:00	Library session:	

	2021-11-24 Wednesday	
7:30-9:00	Breakfast in Cafeteria Leucorea, Checkout, Pay alcoholic drinks in Cafeteria! Return name tags, last chance to get lunch card	
9:00	Recap of last day	
9:10	Participant flash talks: 8. ...	
9:15	TBA	TBA
10:30	Coffee/tea	
11:00	TBA	TBA

	Please fill-in this de.NBI event evaluation survey (single page, 14 questions)
12:00-13:00	Lunch
13:00	<p>Wrap-up. Upcoming events, upcoming possibilities.</p> <ul style="list-style-type: none"> ● BioC ? BioC Europe ? ● ELIXIR ? ● Metabolomics2022 Valencia, Spain June 19-23, 2022 ● https://CompMS.org/ mailing list <ul style="list-style-type: none"> ○ http://metabolomics-forum.com ○
13:50	<p>End of official programme.</p> <p>Seminar rooms will be available until 16:00.</p>