

High-Resolution Mass Spectrometry – a promising tool for the identification of organic contaminants

PEAK Applied Course A34/22

Wednesday, November 16, 2022, Forum Chriesbach FC C20 and hybrid

Nr.	Time	Topic	Speaker
	ab 08.30	Registration	
	08.50 - 09.00	Welcome and Introduction	Juliane Hollender
		Presentation – Basics	
1	09.00 - 09.20	High resolution mass spectrometry (HRMS/MS) - <i>Terms, Definitions, Hardware</i>	Heinz Singer
2	09.20 – 09.40	Typical HRMS processing workflows - <i>Principles, Software</i>	Michele Stravs
		Presentation – Applications	
3	09.40 - 10.00	Target Screening by LC-HRMS/MS - <i>Case Study: Quantification of drugs in wastewater</i>	Stephan Baumgartner
4	10.00 - 10.20	Suspect Screening by LC-HRMS/MS - <i>Case Study: Identification of cyanotoxins in lake water</i>	Elisabeth Janssen
	10.20 – 10.45	Coffee Break	
		Presentation – Prioritization of non-targets features & Quality control	
5	10.45 - 11.10	Data-driven approaches for prioritization	Teofana Chonova
6	11.10 – 11.30	Prioritization for identification using data-driven effect prediction	Kasia Arturi
7	11.30 – 12.00	Quality control in non-target screening	Wolfgang Schulz
	12.00 – 13.00	Lunch	
		Software Demonstration and Exercises with own computer	
8	13.00 – 13.30	MS1 Data evaluation <i>e.g. homologue series detection with envihomolog, isotope pattern with enviPat</i>	Simon Mangold
9	13.30 – 14.15	Chemical and biological transformation products (TPs) selection, detection and identification <i>Prediction of TPs with e.g. Biotransformer/enviPath; TPs fragmentation search</i>	Corina Meyer, Tarek Manasfi
	14:15 - 14:45	Coffee Break	
10	14:45 – 16.45	Structure elucidation using MS2 data <i>MS/MS libraries search, in silico prediction with e.g. Sirius</i>	Michele Stravs
	16.45 – 17.00	Online course evaluation	
	17.00	Apéro; Lab tour as requested	