

SMS Workshop – Untargeted metabolomic data processing and analysis

“From raw data to peak tables and beyond”

November 5, 2019, Insel Spital Bern

Program

Date	Time	Session	Comment
5.11	10.00 -10.15	Course introduction Endre	<ul style="list-style-type: none">• Meet your lecturers and workshop mates• General goals of the course• Course program
	10.15-10.45	Introduction to data analysis in untargeted metabolomics Endre	<ul style="list-style-type: none">• General workflow• Challenges• Limitations
		Coffee break	
	11.00 -13.00	Hand on session 1 Data processing – Part I Endre, Sebastian	<ul style="list-style-type: none">• LC-MS data• xcms by cosmiq or MetaboAnalystR 2.0• Setting-up parameters• Work flow• Result output
	13.00 -14.00	Lunch	
	14.00 -15.30	Hand on session 2 Data processing – Part II Endre, Sebastian	<ul style="list-style-type: none">• DI, FI and IMS-MS data• xcms by cosmiq or MetaboAnalystR 2.0
		Coffee Break	
	16.00 -17.30	Hand on session 3 Metaboanalyst tools Stefan, Sebastian	<ul style="list-style-type: none">• Normalization• Transformation• m/z peaks to pathways (mummichog et al.)
	17.30 -17.45	Wrap-up All	Discussion, feedback