

Metabolomics LC/MS Data Processing and Statistical Analysis

Course Programme

Day	Time	Session
	09:00 – 09:15	Introduction
	09:15 – 09:45	Lecture: Course tools and software <i>Dr Gavin Lloyd</i>
	09:45 – 10:15	Workshop: Using structToolbox and RMarkdown <i>Dr Gavin Lloyd</i>
	10:15 – 10:30	Break
	10:30 – 11:00	Lecture: Raw LCMS data and conversion <i>Dr Ralf Weber / Dr Martin Jones</i>
	11:00 – 12:00	Workshop: Raw LCMS data and conversion <i>Dr Ralf Weber / Dr Martin Jones</i>
	12:00 – 12:30	Lunch
Day 1	12:30 – 13:00	Lecture: Peak detection and alignment <i>Dr Ralf Weber / Dr Martin Jones</i>
	13:00 – 13:55	Workshop: Generating peak tables with XCMS <i>Dr Ralf Weber / Dr Martin Jones</i>
	13:55 – 14:00	Break
	14:00 – 14:30	Lecture: Peak tables, meta data and more <i>Dr Gavin Lloyd</i>
	14:30 – 15:00	Workshop: Making data ready for analysis <i>Dr Gavin Lloyd</i>
	15:00 – 15:15	Break
	15:15 – 16:00	Lecture: QA/QC and multi-step signal filtering <i>Dr Gavin Lloyd</i>
	16:00 – 17:00	Workshop: QA/QC and multi-step signal filtering <i>Dr Gavin Lloyd</i>

Day 2	09:00 – 09:45	Lecture: Peak Matrix Processing <i>Dr Gavin Lloyd</i>
	09:45 – 10:30	Workshop: Peak Matrix Processing <i>Dr Gavin Lloyd</i>
	10:30 – 10:45	Break
	10:45 – 11:15	Lecture: Univariate statistics for comparing two groups <i>Dr Gavin Lloyd</i>
	11:15 – 12:00	Workshop: Analysing a two-group LCMS metabolomics study <i>Dr Gavin Lloyd</i>
	12:00 – 12:30	Lunch
	12:30 – 13:00	Lecture: Univariate statistics for more complex study designs <i>Dr Gavin Lloyd</i>
	13:00 – 13:55	Workshop: Analysing a multi-level study design using ANOVA <i>Dr Gavin Lloyd</i>
	13:55 – 14:00	Break
	14:00 – 14:45	Lecture: Exploratory multivariate analysis <i>Dr Gavin Lloyd</i>
	14:45 – 15:30	Workshop: Exploratory multivariate analysis of LCMS datasets <i>Dr Gavin Lloyd</i>
	15:30 – 15:45	Break
	15:45 – 16:15	Lecture: Supervised multivariate analysis <i>Dr Gavin Lloyd</i>
	16:15 – 17:00	Workshop: Supervised multivariate analysis of LCMS datasets <i>Dr Gavin Lloyd</i>

Day 3	09:00 – 09:45	Lecture: Metabolite feature annotation <i>Dr Gavin Lloyd</i>
	09:45 – 10:30	Workshop: Metabolite Mashing in R <i>Dr Gavin Lloyd</i>
	10:30 – 10:45	Break
	10:45 – 11:15	Lecture: Pathway Analysis <i>Dr Ralf Weber</i>
	11:15 – 12:00	Workshop: Pathway Analysis <i>Dr Gavin Lloyd</i>

12:00 – 12:30	Lunch
12:30 – 13:00	Lecture: Data processing and analysis project (part 1) <i>Dr Gavin Lloyd</i>
13:00 – 13:55	Workshop: Project Workshop <i>Dr Gavin Lloyd</i>
13:55 – 14:00	Break
14:00 – 14:15	Lecture: Data processing and analysis project (part 2) <i>Dr Gavin Lloyd</i>
14:15 – 15:15	Workshop: Project Workshop (cont.) <i>Dr Gavin Lloyd</i>
15:15 – 15:30	Break
15:30 – 16:00	Workshop: Project Workshop (cont.) <i>Dr Gavin Lloyd</i>
16:00 – 16:30	Lecture: Project Presentations <i>Dr Gavin Lloyd</i>
16:30 – 17:00	Q&A: Ask the Experts