Metabolomics in Toxicology

Course Programme

Day	Time	Session	
	08:45 – 09:00	Registration	
	09:00 – 09:15	**Lecture: Introduction to Metabolomics in Toxicology at the BMTC** *Dr Andrew Southam*	
	09:15 – 09:35	**Lecture: Introduction to Metabolomics** *Dr Andrew Southam*	
	09:35 – 10:15	**Lecture: Experimental Design for Toxicology Research** *Dr Martin Jones*	
	10:15 – 10:45	**Lecture: Sample Preparation in Metabolomics** *Dr Andrew Southam*	
	10:45 – 11:00	Break	
	11:00 – 12:00	**Lecture: Introduction to LC and HRMS/MS** *Dr Martin Jones*	
Day 1	12:00 – 12:40	Lunch	
	12:40 – 12:50	Transition to Laboratories	
	12:50 – 14:50	**Lab Session: Group 1** *Dr Andrew Southam* Biphasic sample prep, reconstitution of pre-prepared samples and loading into LC system.	**Lab Session: Group 2** *Dr Martin Jones* UHPLC-MS setup and calibration, configuring LC system and priming solvents.
	14:50 – 15:05	Break	
	15:05 – 17:30	**Lab Session: Group 1** *Dr Martin Jones* UHPLC-MS setup and calibration, configuring LC system and priming solvents.	**Lab Session: Group 2** *Dr Andrew Southam* Biphasic sample prep, reconstitution of pre-prepared samples and loading into LC system.

Day 2	09:00 – 10:00	**Lab Session: Group 1** *Dr Andrew Southam* (U)HPLC-HRMS method configuration on QE+ (HILIC)	**Lab Session: Group 2** *Dr Martin Jones* (U)HPLC-HRMS method configuration on ID-X (lipids*)*
	10:00 – 10:30	**Lab Session: Group 1** *Dr Martin Jones* (U)HPLC-HRMS method configuration on ID-X (lipids)	**Lab Session: Group 2** *Dr Andrew Southam* (U)HPLC-HRMS method configuration on QE+ (HILIC)
	10:30 – 10:50	Break	
	10:50 – 11:15	**Workshop: Sequence Set-Up in Excel** *Dr Ralf Weber / Dr Martin Jones*	
	11:15 – 12:15	**Lecture: Introduction to Full-Scan Metabolomics Data Processing** *Dr Ralf Weber / Dr Martin Jones*	
	12:15 – 13:00	Lunch	
	13:00 – 14:30	**Workshop: Full-Scan Metabolomics Data Processing** *Dr Ralf Weber / Dr Martin Jones*	
	14:30 – 15:00	Break	
	15:00 – 16:15	**Lecture: Univariate and Multivariate Statistics** *Dr Gavin Lloyd*	
	16:15 – 17:30	**Workshop: Univariate and Multivariate Statistics** *Dr Gavin Lloyd*	

Day 3	09:00 - 09:40	**Lecture: Overview of Instrumentation and Their Potential in Metabolite Identification** *Dr Martin Jones*
	09:40 – 10:40	**Lab Session: HRMS/MS Method Setup** *Dr Martin Jones (Group 1) / Dr Andrew Southam (Group 2)*
	10:40 – 11:00	Break
	11:00 – 12:00	**Lab Session: HRMS/MS Method Setup** *Dr Andrew Southam (Group 1) / Dr Martin Jones (Group 2)*
	12:00 – 12:40	Lunch
	12:40 – 13:40	**Lecture: Metabolite Annotation and Identification** *Dr Ralf Weber / Dr Martin Jones*
	13:40 – 14:25	**Lecture: Introduction to Processing, Filtering and Annotating Fragmentation Data** *Dr Ralf Weber / Dr Martin Jones*

14:25 – 14:45	Break
14:45 – 15:45	**Workshop: Metabolite Identification with Compound Discoverer / mzCloud** *Dr Ralf Weber, Dr Martin Jones, Dr Andrew Southam*
15:45 – 16:15	**Q&A: Tips and Tricks from the Experts**