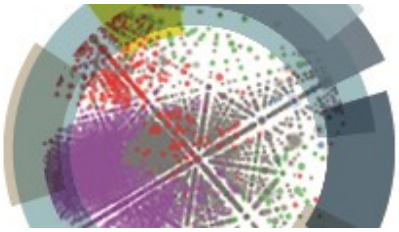
Challenges in analysis of complex natural mixtures

Faraday Discussion



13–15 May 2019
Edinburgh, UK

Monday 13 May

11:30	Registration, Tea and Coffee	
12:00	Lunch	
12:45	**Welcome and Introductions** Professor Dušan Uhrín, *Chair of Scientific Committee*	
12:55	**Outline of Discussion Format** Suzanne Howson and Ella Wren, *Royal Society of Chemistry Publishing Editors*	
13:00	**Introductory Lecture** (Session Chair: Dušan Uhrín) Philippe Schmitt-Kopplin *Helmholtz Zentrum München, Germany*	
	Session 1: Dealing with Complexity (Session Chairs: Mark Barrow, Ruth Godfrey)	
14:00	**Combating selective ionization in the high resolution mass spectral characterization of complex mixtures** Ryan P. Rodgers *Future Fuels Institute, USA*	Paper 24965
14:05	**Complexity of dissolved organic matter in the molecular size dimension: insights from coupled size exclusion chromatography - mass spectrometry** Jeffrey Hawkes *Uppsala University, Sweden*	Paper 25476
14:10	Discussion	
15:00	Afternoon tea	
15:30	**Perspectives on the future of multi-dimensional platforms** Peter J. Schoenmakers *Universiteit van Amsterdam, The Netherlands*	Paper 24966
15:35	**Collection and identification of an unknown component from Eugenia uniflora essential oil exploiting a multidimensional preparative three-GC system employing apolar, mid-polar and ionic liquid stationary phases** Danilo Sciarrone *University of Messina, Italy*	Paper 25708
15:40	**On the benefits of using multivariate analysis in mass spectrometric studies of combustion-generated aerosols** Dumitru Duca *University of Lille, France*	Paper 25360
15:45	Discussion	
17:00	Lightning presentations (by invitation of the scientific committee)	
17:30	Poster Session and Wine Reception	
19:00	Close of session	

Tuesday 14 May

	Session 2: High Resolution Techniques (Session Chairs: Don Jones and Mathias Nilsson)	
09:00	**Online supercritical fluid extraction mass spectrometry (SFE-LC-FTMS) for sensitive characterization of soil organic matter** Ljiljana Paša-Tolić *Pacific Northwest National Laboratory, USA*	Paper 24967
09:05	**Structural investigation of coal humic substances by selective isotopic exchange and high-resolution mass spectrometry** Alexander Zherebker *Skolkovo Institute of Science and Technology*	Paper 25345
09:10	**Reduced dimensionality hyphenated NMR experiments for the structure determination of compounds in mixtures** Nicholle Bell *University of Edinburgh, UK*	Paper 25253
09:15	Discussion	
10:30	Morning Tea	
11:00	**Unraveling the complexity of complex mixtures by combining high-resolution pharmacological, analytical and spectroscopic techniques: antidiabetic constituents in Chinese medicinal plants** Dan Stærk *University of Copenhagen, Denmark*	Paper 24968
11:05	**Characterising polar compounds using supercritical fluid chromatography–nuclear magnetic resonance spectroscopy (SFC–NMR)** Fleur van Zelst *Radboud University, The Netherlands*	Paper 25147
11:10	**Polar mixture analysis by NMR under spin diffusion conditions in viscous sucrose solution and agarose gel** Pedro Lameiras *CNRS, France*	Paper 25479
11:15	Discussion	
12:30	Lunch	
	Session 3: Data Mining and Visualisation (Session Chairs: Timothy Ebbels and Mark Barrow)	
13:30	**Joint and unique multiblock analysis of biological data – multiomics malaria study** Johan Trygg *Umeå University, Sweden*	Paper 24969
13:35	**Deciphering complex metabolite mixtures by unsupervised and supervised substructure discovery and semi-automated annotation from MS/MS spectra** Justin van der Hooft *Wageningen University, The Netherlands*	Paper 25113
13:40	**Multivariate analysis applied to complex biological medicines** Tim Rudd *National Institute for Biological Standards and Control, UK*	Paper 25354
13:45	Discussion	
15:00	Afternoon tea	
15:30	**Resolving complex hierarchies in chemical mixtures: how chemometrics may serve in understanding the immune system** Jeroen Jansen *Radboud University, The Netherlands*	Paper 24970
15:35	**An integrated approach for mixture analysis using MS and NMR techniques** Ricardo Moreira Borges	Paper 25296

	Federal University of Rio de Janeiro, (UFRJ), Brazil	
15:40	Discussion	
16:30	Close of sessions	
18:30	Pre-Dinner Drinks – South Hall Dining Room	
19:00	Conference Dinner – South Hall Dining Room	

Wednesday 15 May

	Session 4: Future Challenges and New Approaches (Session Chairs: Mathias Nilsson and Dusan Uhrin)	
09:00	**Focusing on "the important" through targeted NMR experiments: An example of selective 13C-12C bond detection in complex mixtures** Ronald Soong *University of Toronto, Canada*	Paper 24971
09:05	**Application of novel solid phase extraction-NMR protocols for metabolic profiling of human urine** Dan McGill *Imperial College London, UK*	Paper 24973
09:10	**Structural analysis of heavy oil fractions after hydrodenitrogenation by high-resolution tandem mass spectrometry and ion mobility spectrometry** Carlos Afonso *University of Rouen-Normandy, France*	Paper 25432
09:15	**Understanding structural complexity of dissolved organic matter: isomeric diversity** Francisco Fernandez-Lima *Florida International University, USA*	Paper 25487
09:20	Discussion	
11:00	Morning Tea	
11:30	**Automatised pharmacophoric deconvolution of plant extracts – application to Cinchona bark crude extract** Marc-André Delsuc *Université de Strasbourg, France*	Paper 24972
11:35	**Challenges in the decomposition of 2D NMR spectra of mixtures of small molecules** Caroline Chaux, *Aix Marseille University, France*	Paper 25311
11:40	**Systems biology approach to elucidation of contaminants biodegradation in complex samples- integration of high-resolution analytical and molecular tools** Caroline Gauchotte-Lindsay *University of Glasgow, UK*	Paper 25480
11:45	Discussion	
13:00	**Concluding Remarks Lecture** (Session Chair: Dušan Uhrín) Roy Goodacre *University of Liverpool, UK*	
13.40	**Acknowledgements**	
13.45	**Close of meeting and Lunch**	

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.