

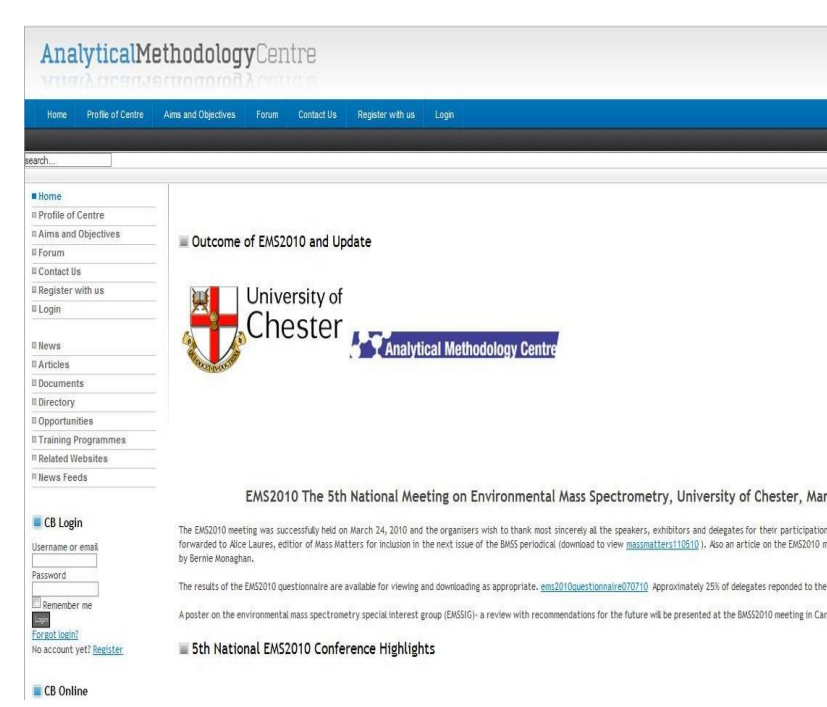
A Brief History of Environmental Mass Spectrometry, 1997 – 2017

Embracing EMSSIG and EFASIG (The BMSS)

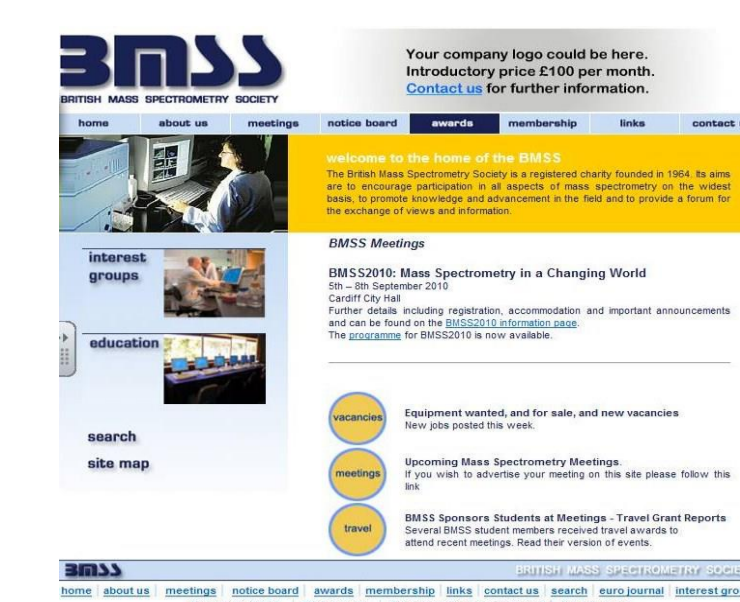
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EFASIG



1. Background

The first meeting on Environmental Mass Spectrometry (EMS) organised by a member of the BMSS was held at Salford in 1997. EMSSIG as a special interest group of the BMSS has been in existence since about 2002-3 and was set up to compensate for the discontinuation of a parallel half session devoted to EMS at the annual meetings of the BMSS and, furthermore, more recently the general MS session which replaced the EMS session. One day meetings entitled 2nd to 5th National Meeting on Environmental Mass Spectrometry, organised by EMSSIG in collaboration with the University of Chester, have been held biannually since 2004 and in 2010 the meeting combined the interests of the EMS and F/N SIGs (Simon Hird). In addition, this meeting formed a part of the conference week, March 22 to 26, 2010, which covered also Nanotechnology & Food and Food Science & Technology, which was coordinated by Prof Chris Smith at Chester.

The 2012 meeting was held at the Manchester Food Research centre, following Chris Smith's move to Manchester Metropolitan University. Three meetings organised in 2014, 2015 and 2017 have been held at BAT R & D, Southampton, hosted by Dr. Chris Wright, with the SIG undergoing a name change in 2015 to EFASIG to embrace food analysis in addition to environmental analysis (Christine Eckers initiative).

In 2014, a meeting, EMSSIGatWWEM2014, was arranged as a satellite of the WWEM Conference and Exhibitions at Telford following an invitation from David Hellyer and Marcus Pattison, which was repeated as EFASIGatWWEM2016.

This poster highlights the EMS meetings, 1997 to 2017, a review of the topics, the breadth of coverage with reference to the plenary, keynote and oral presentations. A summary is given of the interest in EMS from the MS community, commercial and academic organisations at large. Attention is also paid to the feasibility of on-line forum type or virtual meetings, one of which was attempted in 2009.

2. Analysis of meeting events

The ten meetings have been organised in the period from 2004 to 2017 and have involved a range of plenary & keynote lectures and 20 minute oral presentations with a small input from poster presentations. Additionally, exhibiting by commercial organisations has been encouraged and been well-supported by Mass Spectrometry and Chromatography instrumentation and related service organisations. The general format of the meetings has been largely conventional and except for 2006 the meetings were of one day duration in line with the conditions under which SIGs operate. In several of the meetings there has been an attempt to vary the format with the introduction of a forum, discussion and workshop type activities (2012).

The focus in 2015 was on presentations given by young researchers and early career scientists ably supported by experienced practitioners.

The topics of the plenary lectures have been also varied and several speakers have been invited from areas other than EMS but having an international standing. Keynotes have been featured to front each session to highlight particular aspects of EMS.

i. Plenary lectures

Following the invitation of international speakers to the EMS sessions, previously, in the annual meetings, the trend was continued in EMSSIG meetings in 2008 and 2010. Previously in 2004 and 2006 only keynote presentations were featured with speakers being UK based. The topics covered are summarised below:

- Novel strategies for the identification and determination of pharmaceuticals, illicit drugs and their degradation products in the environment by LC hybrid tandem MS systems (Q TRAP and Q TOF) (Damia Barcelo, Spain, 2008)
- A Review of Advanced MS Techniques in environmental studies: advantages and current limitations (Enrico Davoli, Italy, 2010)

ii. Keynote lectures

Keynote presentations (30 min.) have fronted each session usually involving 2 or 3 speakers from the UK & Europe in fields relating to the themes of the respective sessions. In 2010 because of the joint SIG event with Food & Nutrition the keynote for this session was appropriate to topics in the subsequent 20 min orals presented. However, Food Analysis did feature in a short session in EMS2006. Environmental analysis featured prominently in the 2012 and 2014 meetings with some aspects of food analysis, which was included in an official capacity from 2015 when the SIGs were merged (EFASIG). A summary of the topics covered is presented in Table 1.

Table 1. Summary of Keynote Presentations in EMS meetings to 2017

1997 Aspects of EMS, Speakers included David Games, Keith Hall and Jerry Hart

1998 – 2002, Half Sessions at BMSS Annual Meeting, including Keynotes from Ed Houghton, HFL, & Susan Richardson, EPA, Aspen, GA, USA

2004 Keynotes 1.Trace Analysis. David Anderson, Corus Trace organics in the Steel Industry
2. Assay & Residue Techniques Simon Hudson, Horseracing Forensic Lab. MS and Immunology in Horse Racing Forensics
3. Atmospheric Pollution/monitoring Bob Kalin, QU, Belfast Degradation of CS2 in the Environment

iv. ATTENDANCE

Attendance at meetings has varied with a peak of around 70 delegates in 2008 rising steadily from 2004 through 2006. However, disappointingly the attendance in 2010 was considerably down in spite of the fact that the meeting was one of three meetings alongside Nanotechnology & Food and Food Science & Technology in a conference week organised by Prof Chris Smith at the University of Chester. Subsequent meetings have varied in attendance from 35 to 65.

Table 1 continued

2006 Keynotes: Multi-Component Environmental Analysis Using MRM Protocols. Dr. J. Upton, Varian Ltd, Mass spectrometry and the evaluation of food ; Dr. Chris Wright, Safety & Environmental Assurance Centre, Unilever Ltd ; Novel Applications of MALDI-TOF: Recent advances in the profiling of microorganism Vic Parr, SAL, Ltd.

2008 Plenary: Professor Damia Barcelo, IIQAB-CSIC, Department of Environmental Chemistry,Barcelo 'Novel strategies for the identification an determination of pharmaceuticals, illicit drugs and their degradation products in the environment by LC hybrid tandem MS systems (Q TRAP and Q TOF) Keynotes:Recent Advances in Analysis in the Water Industry, Dr Rakesh Kanda, STL Accreditation in Environmental Analysis - MCERTS and Beyond Ms Deborah Hudson, UKAS

2010 Plenary: A Review of Advanced MS Techniques in environmental studies: advantages and current limitations:Dr Enrico Davoli, Head of Mass Spectrometry, Capo Laboratorio Spettrometria di Massa Istituto di Ricerche Farmacologiche "Mario Negri", Milan Keynotes 'MS Techniques for environmental analysis: a view from a commercial analytical laboratory', David Wood, Scientific Analysis Laboratories ; 'Allergen detection, quantitation and confirmation in Nuts, Cereals, Milk etc. by LC/MS/MS' Dr Bert Popping, Eurofins, UK

2012 An Interactive Workshop for Improving Productivity in Environmental & Food Screening using LC- MS and GC-MS.

Session 1. Regulatory & Analytical Considerations ; Session 2. A. Software Considerations, What is available. B. What is required (Investigative Laboratories) ; Session 3. A. Contract Analysis Laboratories -Recent Advances in capability ; B. What is on offer (Instrument/Service Providers)

• 2014 Recent Advances in Chromatography-Mass Spectrometric Techniques to Environmental & Food Matrix Analysis.

Keynotes: Marc Suter, EAWAG, Switzerland, Mass Spectrometry in Ecotoxicology ; Steve Rowland, University of Plymouth, GCxGC-MS of supercomplex mixtures of organic pollutants: a hump no more!"

2014 at WWEM, Focus on Aspects of the applications of chromatography-mass spectrometry to environmental water analysis (in keeping with remit from WaterWasteEnvironmentalManagement, WWEM)

2015 Young Scientists and Early Career Researchers (8 presenters), from Universities of Keele, Liege, MMU, Portsmouth (2), KCL with representatives from BAT & FERA and experienced practitioners

2016 at WWEM Focus on Comprehensive Chromatography Mass Spectrometry

• Keynote: Peter Tranchida, Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, Polo Annunziata, Università degli Studi di Messina, GCxGC/MS and LCxLC/MS for the Analysis of Environmental and Food Matrices.

2017 Advances in the Innovations of the applications of chromatography-mass spectrometry.

Keynotes: Isolation, characterisation, environmental occurrence and toxicity of polar fractions from crude oils Steve Rowland, University of Plymouth

Real time analysis and multi-dimensional separations: Geochemical and medical applications Michael Wilde, University of Leicester

v. Support from GC/LC/MS Instrumentation, Service and Accessory Organisations

The meetings have been admirably supported by commercial organisations who have exhibited a range of instruments and products important to the utilisation & applications of Chromatography Mass Spectrometry in Environmental Analysis. Not only have these organisation taken part as exhibitors they have strongly supported the scientific programme as presenters without which the meetings would have been more difficult to hold.

Anton Parr Ltd., AB SCIEX Ltd., Advanstar, Agilent Technologies Biotage AB, Bruker Daltonics Ltd., Buchi, Crawford Scientific, Cyonics Ltd., Domnick Hunter Group, Genevac, Grace (Alltech) Associates, Greyhound Chromatography & Allied Chemicals, Hidden Analytical Ltd., Impspx, Ionic MSV, Kinesis, Kore Technology Ltd., Leco UK Ltd., LGC, NEPAF, Phenomenex, Promochem, Presearch Ltd., QMX Ltd., SAI Ltd., SGE Europe Ltd., Shimadzu Ltd., SPEC Certiprep, Taylor Francis, Thames Restec Ltd., Thermo Fisher, Varian Ltd., Waters Corporation

iii. Oral presentations

Oral presentations of 20 min duration featured in all the topic areas fronted by the Keynotes, the themes for which with session designation are listed in Table 1. To cover the topics presented in depth is not possible here, however Table 2 summarises the areas featured with presenter affiliations

Table 2. Summary of Oral Presentations in EMS meetings, 2004 to 2017

Year Session number & theme	Presenter Affiliation	Abbreviated Topic
2004 IA. Trace Analysis	Sheffield Hallam U ; Waters Corp Manchester U	• Isocyanates by MALDI ; • Screening of Dioxins etc. by GC TSO ; • Natural and Anthropogenic Halocarbons in the Environment
IB Instrumentation	SAL Cyonics Varian	• New method of Quantitation for GC/MS • Portable Bench Top MS for Environmental • Tandem MS in the Environmental Laboratory
II. Assay and Residue Techniques	Environment Agency Applied Biosystems CSL	• Pharmaceuticals and Pesticide Residues by LC/MS/MS • Pesticides and Metabolites by HPLC/MS/MS • Multi-residue Screening of Pesticides by LC-MS/MS
III. Atmospheric Pollution/monitoring	Kings College Queen's U, Belfast	• Airborne Particulate Matter in London • Isotopic Analysis of atmospheric gases & methyl halides
2006 I. Environmental Analysis	Sheffield Hallam U CSL Hall Analytical	• Study of Dermal Absorption of Isocyanates by MALDI • How Multi-purpose is Multi-residue pesticide analysis • The Supelco Dioxin Prep System – Florisil Version
II. Environmental Analysis	Waters Corp. York U Kings College	• Multi-residue Analysis Blacklist Priority Pollutants in Water • Analysis of Oxidised Organics in Aerosols GC ² TOF-MS • Sorption of PAHs to soils using Thermal Techniques & MS
III. Food Analysis	CSL Bruker Daltonics	• Determination of Brominated Flame Retardants in Foods • Toward Total Sample Screening&Retrospective Analysis
2008 I. Methodology for Environmental Analysis	Varian Unilever LGC	• Rapid Screening using Intelligent Data Systems • Challenges in the Analysis of Volatile Siloxanes • High Accuracy Mass Determination of Malachite Green
II. Environmental Analysis Protocols	Applied Biosystems EHS (Northern Ireland) Thermo Fisher, Bremen	• Trace Contaminants in Potable Waters by LC/MS/MS • Organophosphorous Pesticides & Organonitrogen Herbicides by GC/Ion Trap MS • Multi-component Target Compound GC/MS Analysis
III. Accreditation & Discussion Forum	Forum led by Applied Biosystems with 3 topics and A Discussion of MCERTS and Its Merits & Disadvantages	
2010 1. Environmental	CNRS, France ALMSCO Int Applied Biosystems	• Multilab residue routine analysis of pesticides in pollens • Detection & ID of trace analytes: advanced software/new GC-TOF • Quantitation & Confirmation of targets in Environmental Waters
II. Food & Nutrition	CSL Applied Biosystems FERA	• LC-UV-MS-TOF of Glucosinolates • High Throughput Screening of Pesticides • Results of FAPAS pesticide Efficiency Testing
III. Selected Topics	Imperial College	Limitations of MS for Mass Range of Polydisperse Samples
2012 Regulatory & Analytical Considerations	Environment Agency BAT FERA	• The Water Framework Directory • Analytical challenges for the chemical assessment of foods • Nanomaterials & the chemical safety of food
Software considerations: what is available?	ACDLabs ALMSCO	• Using software for automation • Target compound identification software
What is required?	FERA Flemish Environ. Agency CSols	• Proficiency Testing/LEAP scheme specific to the water industry • Monitoring work under WFD and the instrumentation used • Maintaining Optimal Quality of Analysis Using The Right Laboratory Informatics Tools and Processes
Contract Analysis Laboratories	SAL	• MS Techniques in Environmental Analysis – A view from a commercial laboratory
What is on offer? (Instrument/Service Providers)	Agilent ThermoFisher	• Workflows for effective screening strategies by LC and GCM • Advances in MS technology for higher selectivity in complex matrices by GC/MS/MS
2014 Data systems / instruments for EA	ACDLabs Thermofisher	• "Where have I seen this before? Building mass spectral databases without human effort • Recent advances on the use of Orbitrap Mass Analyser associated to Environmental Analysis
Aspects of Environmental and Food Analysis	Markes International Plant Biotech., GR&D Camb. University of Portsmouth Kings College London FERA Bruker Daltonics	• Select-eV: Increasing dimensionality in GCxGC-TOFMS of environmental contaminants • From masses to meanings – challenges and solutions in processing and visualising high precision mass spectrometry data sets • The identification of environmental pollutants in surface and well water samples using non-targeted QTOF based screening and data processing • Approaches to "unknown" screening in environmental water samples • What's in Your Food? LC-MS/MS Workflows & Tools to Identify and Screen for Known and Unknown Residues – with ease • Mass spectrometry profiling tools to verify the declared origin of timber • Applying Enhanced Confirmation Criteria for Multi-Residue Pesticide Screening Using of an Ultra-High Performance LC-QTOF system
2015 Introduction to the Young Scientists and Researchers Group	University of Liege University of Plymouth	• High Resolution Gas Chromatography coupled to Mass Spectrometry for the analysis of volatile organic compounds • Identification of petroleum acids by GCxGC-MS: A new method based on an old approach
Experienced Practitioners	University of Portsmouth BAT R & D Keele University University of Portsmouth Kings College London FERA	• Development of a diffusive gradient in thin-films (DGT) technique for organotin compounds in sediment pore-water • Thermal Desorption Gas Chromatography Time of Flight Mass Spectrometry for the analysis of aerosols. • The effect of ageing on the metabolic profile of meat • Use of the Chemcatcher® passive sampler for monitoring polar pesticides • The Use of Accurate Mass Ion Ratio in 'Semi-Targeted' Approaches for the Detection of Pharmaceuticals in the River Thames • Exposing the exposome: Metabolomics and environmental toxicology
2016 at WWEM Aspects of Comprehensive GC/LCMS	Water Resources Wales Waters Anatune Sepsolve LGC SAL UCL	• Identifying pollutants in unusual matrices by GCxGC-TOF MS: What can breast implants tell us about bio-accumulation • Rapid Evaporative Ionisation Mass Spectrometry (REIMS) for The Discrimination of Different Species of Meat and Fish • Real-time Analysis of United States EPA Method TO-14A Compounds Using SIFT-MS • Comprehensive insights into tobacco smoke using flow-modulated GCxGC-TOF MS • Multidimensional chromatography for the certification of environmental reference materials • The Application of GCxGC-FID to Environmental Hydrocarbon Analysis • Suspect screening of emerging contaminants using liquid chromatography-high resolution mass spectrometry and in-silico methods
Aspects of the applications of GC/LC MS	University of Leicester University of Birmingham	• Real-Time Mass Spectrometric Analysis of Hydrocarbons from Crushed Shales • Using refillable diffusion tubes for VOCs, SVOCs and oxygen-sensitive VOCs for calibration of PTR TOF MS
Discussion session	SCIEX Waters corporation University of Warwick Presenter Participation	• Screening and Quantitation of Emerging Environmental Pollutants in Drinking and Waste Water • Environmental Screening of Water Samples Utilising Ion Mobility Enabled High Resolution Mass Spectrometry • Analytical Methods for Profiling of Water from Athabasca Oil Sands • 1. Aspects of Analytical Method Validation. • 2. Increased Peak Capacity: Is it a question for conventional/comprehensive techniques
2017	Sepsolve LGC Advion/Univ. of Loughborough RSSL Agilent Technologies VUV Analytics University of Birmingham BAT R & D Anatune IMSPEX University of Glasgow	• Dual-channel GCxGC-FID for routine TPH Analysis • Government Chemist role in referee cases • The use and application of the Advion expression compact MS • Introduction to PTR-MS • Enhancing the Chromatography MassSpectrometry Experience • The analysis of food and beverages by GC-VUV • Robust Compositional Data Analysis • Vapeomics • SPE and Twister to enhance heptachlor and heptachlor epoxide (pgf) from water using GC-QTOF in NCI mode. • Applications of GC/IMS for food and environmental samples • Simplified pressurised liquid extraction of coal tar contamination samples for carbonand stable isotope analysis of PAHs

Chromatography MS- Analytical & Environmental Analysis (30) ; Universities (20) ; Industry (20) ; Utilities (10) ; Forensic Labs (10) ; Accreditation (10)