

## Recent Advances in the Methodology for Environmental and Food Matrix Analysis - a report on the 5th National Conference on Environmental Mass Spectrometry



***This meeting, held on March 24th at the University of Chester, was an environmental mass spectrometry special interest group (EMSSIG) series event forming a part of the BMSS SIG meetings.***

***The main theme focussed on 'Recent Advances in the Methodology for Environmental and Food Matrix Analysis' and was linked to the Food and Nutrition SIG coordinated by Dr Simon Hird, thereby forming part of a conference week, during which three meetings were organised by Professor Chris Smith, which highlighted Nanotechnology and Food, and, Food Science and Technology.***

***In keeping with a trend in previous environmental sessions, now generalised at the BMSS annual meetings, several presentations highlighted the applications of mass spectrometry in highly topical areas. The meeting had an international flavour with presenters and delegates from Europe and the Middle East.***

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The oral and poster presentations were chosen specifically to reflect and balance the interests and activities of the mass spectrometry community interested in environmental & food analysis and the commercial and service organisations that meet these needs.

Since the last meeting in 2008 the pressure on Analysts to monitor ever-increasing numbers of compounds which are suspected (or convicted) of causing health problems to humans and wildlife is increasing. Some of the compounds that were of academic interest in terms of methodology design are now subject to legislation in terms of specific maximum levels which may be tolerated never more so than in the Food and Flavours sector. New emerging environmentally pollutants (EEP) originate from a variety of sources thus making the task for the analyst more difficult. The practitioners, in tandem with the Instrument manufacturers have risen to meet the challenge and this meeting gave a fascinating overview of where we currently are and, having a vested interest in our environment and the food chain, in seeing progress on all fronts.

Over 50 delegates (some of whom are shown in *Figure 1*) attended the meeting. To complement the Plenary and Session oral presentations by eminent scientists, 11 companies formed a trade show, which ran through the day to give an overview of commercially available products and solutions.



*Figure 1. Attending Delegates*

To open the meeting, the plenary lecture was given by Dr Enrico Davoli, Mario Negri, Milan, Italy whose talk was entitled 'A Review of Advanced MS Techniques in environmental studies: advantages and current limitations'.

Dr Davoli started by outlining the fact that in the last years the overall trends in analytical techniques for environmental analysis have been oriented towards high performance instrumentation capable of higher sensitivity and specificity. Mass spectrometry is one of the most important techniques for environmental analysis and the development of multistage and hybrid mass spectrometers (MS) increased the potential for highly complex environmental samples, but trace and ultra-trace analysis of environmental samples always pose difficulties due to sample complexity.

He further outlined the point that advanced techniques in environmental, pharmaceutical, forensic and other analytical fields are routinely used with multistage MS, mainly coupled to liquid chromatography, for targeted analysis. The use of triple quadrupoles coupled with HPLC, a very well established technique still brings new data about the environment, like pharmaceuticals and drug of abuse presence in surface water. As the MS complexity increases, specificity increases, bringing more and more sensitivity.

Sample preparation, always an extremely delicate step, can be reduced more and more, down to almost zero, for specific applications, such as food contamination. The orbitrap is a new mass analyser, which has been commercially available since 2005. The main feature of this mass analyser is the high resolution, and a relatively simple instrument operation and maintenance. The orbitrap offers large space charge capacity, high mass accuracy (1-5 ppm) and dynamic range greater than  $10^3$  thus allowing not only sample preparation reduction, but also chromatography, even for environmental samples. Data was presented for direct identification of drugs of abuse in surface water.

As mass spectrometry is the only technique capable of compounds identification at trace levels, it is fundamental to have available software systems as an aid in data mining. Still outstanding, for everyday needs however, is a lack of automated data interpretation for high resolution and tandem instrumentation.

Part of the problem is a lack of instrumentation software for data mining and part is a lack of standardised libraries for the new, high-end spectrometers. Advanced, new mass spectrometric techniques do not necessarily need large and complex instrumentation. Small benchtop quadrupoles, with chemometric approach, can be useful in new and emerging fields such as environmental odour pollution. Ultra small MS are emerging in the field of environmental monitoring, as distributed instrumentation, to continuously monitor different areas simultaneously.

Examples in more detail and postulated solutions were shown throughout the thought provoking and extremely interesting lecture.

Following the Plenary lecture, highly topical areas of interest were discussed in oral presentations some of which were preceded by Keynote lectures.

**Session I** concentrated upon 'Environmental Analysis' and was chaired by Graham Bonwick from the University of Chester.

The Keynote speaker was David Wood, Scientific Analysis Laboratories, Manchester who talked on the subject of 'MS Techniques for environmental analysis: a view from a commercial analytical laboratory'.

This was then followed by three presentations on various aspects of harnessing the increasing power of Mass Spectrometry to solving some extremely pertinent analyses of major concern to environmentalists

Firstly we heard from Laure Wiest, Service Central d'Analyse, (S.C.A) du CNRS, Solaize, France who spoke on the topic of 'Multi-residue routine analysis of 57 pesticides by Gas Chromatography coupled with Time of Flight Mass Spectrometry in Honeybee's pollens'.

This was followed by Gareth Roberts, ALMSCO International, Llantrisant who talked about 'Detection and identification of trace target analytes using advanced automated software with a new GC-TOF mass spectrometer'.

Finally Dr Stephen Lock, AB SCIEX presented on 'Quantitation and Confirmation of Pesticides, Pharmaceuticals, and Personal Care Products in Environmental Water Samples'.

The Keynote speaker who started **Session II** on the topic of Food & Nutrition was Dr Bert Poppin, Eurofins, UK who spoke about 'Allergen detection, quantitation and confirmation in Nuts, Cereals, Milk by LC/MS/MS'.

Allergens have moved into the focus of consumers, food authorities and industry alike. Current analytical methods have several shortcomings. Analysis of allergens by LC-MS/MS offers a number of advantages but still have to overcome several hurdles. Dr Poppin's presentation gave a summary of activities and progress in this field.

The legal requirement for the quantification of allergens for food packaging is not consistent across North America and Europe. The USA legislators demand that eight groups be identified where as Canada is demanding ten in total yet in Europe this increases to 14 in total. In order to further muddy the waters the actual constituents of the allergen groups varies from geographic area to area.

While the regulatory framework in different countries is already complex enough and makes the choice for the allergic consumer already difficult, the analytical side has no less challenges. To determine allergens currently two main techniques are being used: one is ELISA which is an acronym for enzyme linked immuno sorbent assay, and PCR, the acronym or polymerase chain reaction. PCR is based on the detection of DNA. The technique is for this kind of analysis typically not qualitative but only qualitative. In addition detection levels in the low ppm range can only be achieved with allergens containing higher levels of DNA. That typically applies to plant-based allergens like nuts, soya and sesame but not to some animal-based products like egg or milk. In addition the presence of DNA may not necessarily indicate the presence of offending allergenic structures, meaning that the protein that triggers the allergic reaction may not be present while the DNA still is. However for regulatory purposes this is irrelevant as any detection of a component deriving from an allergenic product triggers labelling.

It can be said that none of the available techniques tackles all problems of allergen analyses.

Most recently, a new approach has been considered: the analysis of allergens using mass spectrometry methods. Some groups including Eurofins have already shown proof of principle, i.e. that the technique works to detect allergens. Initial studies in our laboratory involved the identification of appropriate precursor masses and transitions. Other groups have looked at heat stability of target peptides for LC-MS/MS analysis and identified several.

In addition, the European 6th Framework Project MoniQA has established a laboratory subgroup, which guides and drives the developments in this field. At a recent meeting in Ivrea, Italy, requirements for appropriate MS targets were discussed. Dr Poppin's presentation gave a summary of the different activities ongoing and highlighted recent progress in this area.

A series of presentations around the same Food and Nutrition theme then followed.

'LC-UV-MS-TOF profiling of glucosinolates'. Don Clarke, FERA, Sand Hutton, York

'High throughput screening for over 1000 pesticides in fruit and vegetable using a hybrid triple quadrupole – linear ion trap LC/MS/MS system', Dr Pamela Stoddart, AB SCIEX.

'Results of FAPAS pesticide residue proficiency testing - is mass spectrometry capturing everything?' Mark Sykes, FERA, Sand Hutton, York.

**Session III** then opened with a Keynote Lecture from Dr Alan Herod, Imperial College, London on 'Limitations of mass spectrometry for determining the mass range of polydisperse samples (such as coal liquids and petroleum asphaltenes)' Followed by an interactive discussion forum, which allowed Delegates to pose questions to presenters (oral and poster) to open up topics for discussion. Some interesting and thought provoking topics were raised.

All in all the meeting gave an opportunity for some in-depth discussions amongst practitioners of the art of running Mass Spectrometers to those whose need is more focussed on the application of the data produced and its relevance to the environment and dietary habits of the general public.

The meeting was organised by the Chester Centre for Science Communication and the University of Chester in conjunction with the Environmental Mass Spectrometry special interests group (EMSSIG) and formed part of the BMSS promoted meetings series. The local organising committee consisted of Dr Peter Baugh, Professor Graham Bonwick, Professor Chris Smith and Dr Simon Herd.

Following the meeting it was decided that there should be another meeting in 2012 although the exact format was yet to be decided but would incorporate feedback from the 2010 attendees.

More details can be obtained at [www.analyticalmethodologycentre.co.uk](http://www.analyticalmethodologycentre.co.uk) where several of the speaker's slides may be downloaded under the EMS2010 tab.