

Here is a selection of the latest papers by BMSS members:-

Trace ^{56}Fe , $^{63/65}\text{Cu}$ and ^{64}Zn metal analysis in whole blood by SEC-HPLC-ICPMS

Griffin L, Cox M, Duckett CJ.

Chromatography Today Aug/Sept online edition 2016

The presence of ^{56}Fe , $^{63/65}\text{Cu}$ and ^{64}Zn in blood utilising dried blood spot sampling (DBS) technology was investigated. Extracted blood was analysed by SEC-HPLC for protein separation and SEC-HPLC-ICP-MS for metal. Proteins were found to be haemoglobin, myoglobin and transferrin; Metal determination saw correlated peaks of ^{56}Fe , $^{63/65}\text{Cu}$. However, ^{64}Zn peaks were much weaker and could therefore only be tentatively identified.

Coupling and optimisation of online nuclear magnetic resonance spectroscopy and mass spectrometry for process monitoring to cover the broad range of process concentration

Blanazs A, Bristow, TW, Coombes, SR, Corry T, Nunn, M, Ray AD.

Magn Reson Chem. 2016

Real-time online monitoring of chemical processes was carried out by coupling a mass spectrometer with an online reaction monitoring NMR. ^1H NMR was ideal for quantitation of high level components, whereas MS showed a

greater capability for detecting those at low level. This combination allows both qualitative and quantitative analysis of reaction components over the full process range.

LC-MS/MS application for urine free pyridinoline and free deoxypyridinoline: Urine markers of collagen and bone degradation

Tang JCY et al.

Clin. Mass Spectrom 2016

Pyridinoline (PYD) and

Deoxypyridinoline (DPD) are

markers used to evaluate bone

turnover status in patients and

monitor response to anti-resorptive

treatment. The paper describes a

LC-MS/MS method to quantify PYD

and DPD in urine. fDPD/Cr and fPYD/

Cr were elevated in patients with

metabolic bone disease. fDPD:fPYD

ratio can assist in the diagnosis of

type VI Ehlers-Danlos Syndrome

(EDS).

NAD acts as an integral regulator of multiple defense layers

Pétriacq P, Ton J, Patrit O, Tcherkez G, Gakière, G.

Plant Physiol 2016; 172, 1-15

This paper describes how the redox cofactor nicotinamide adenine

dinucleotide (NAD) can stimulate plant immunity by modulating oxidative stress and the hormonal balance. Extensive multivariate analysis of untargeted metabolic profiles obtained by UPLC-qTOF-MS shows that NAD itself mimics treatment with defence elicitors such as chitin.

Advances in LC: bioanalytical method transfer

Wright P, Wright A.

Bioanalysis 2016; 8 (17): 1837-1844 (2016)

There are three main reasons

for transferring from an existing

bioanalytical assay to an alternative

chromatographic method: speed,

cost and sensitivity. In this article,

chromatographic approaches are

considered in terms of what they

can offer the bioanalysts to improve

these three factors.

Analysis of chlorinated hydrocarbons in gas phase using portable membrane inlet mass spectrometry

Giannoukos S, Brkić, B, Taylor S.

Analytical Methods 2016; 8: 6607-6615

On-site chemical analysis of compounds that contribute (directly

or indirectly) towards ambient air pollution is a topic of great concern worldwide. This paper demonstrates proof of principle for trace detection (low ppb) and on-line monitoring of volatile chlorinated hydrocarbons in the gaseous phase using portable membrane inlet mass spectrometry (MIMS). MIMS response in periodic and dynamic processes was also successfully investigated.

Chemical Sniffing Instrumentation for Security Applications

Giannoukos S, Brkić B, Taylor S,

Marshall A, Verbeck GF.

Chemical Reviews 2016; 116(14): 8146-8172

This review investigates artificial

front end chemical sensors

approaches for border security

applications. It presents an overview

of existing available technologies

and instrumentation for threat

detection and monitoring. It

considers their functional and

operational principles. The

chemistries of interest focus on

threat compounds (drugs, explosives

and chemical warfare agents) and on

"human chemical signatures" with

biochemical relevance.

Direct Analysis and Quantification of Metaldehyde in Water using Reactive Paper Spray Mass Spectrometry

Maher S, Jjunju FP, Damon DE, Gorton H, Maher YS, Syed SU, Heeren RM, Young IS, Taylor S, Badu-Tawiah AK.

Sci. Rep. 2016; 6: 35643

Metaldehyde is extensively used as a systemic molluscicide on a wide range crops. Contamination due to run-off, has led to increased concentration of the pesticide in surface waters. For the first time, rapid analysis (<~1 minute) of metaldehyde residues in water is demonstrated using reactive paper spray mass spectrometry. Residues were detectable in raw water samples without any pre-concentration/separation steps.

Human neutrophil kinetics: modeling of stable isotope labeling data supports short blood neutrophil half-lives

Lahoz-Beneytez J, Elemans M, Zhang Y, Ahmed R, Salam A, Block M, Niederalt C, Asquith B, Macallan D. Blood 2016; 127(26): 3431-8

Stable isotope tracers can be used to discriminate between different kinetic models in human physiological systems. In this paper re-analysis was undertaken of the in vivo kinetics of human neutrophils labelled with either deuterium-labelled water or glucose. Key phases in neutrophil life were identified, confirming their relatively-long post-

mitotic bone-marrow maturation phase (~6 days) and their short half-life in blood (~0.8 days).

Orthogonal Assessment of Biotherapeutic Glycosylation: A Case Study Correlating NGlycan Core Afucosylation of Herceptin with Mechanism of Action

Upton R, Bell L, Guy C, Caldwell P, Estdale S, Barran PE, Firth D Anal. Chem. 2016; 88(20): 10259-10265

Endo S and Endo S2 enzymes are combined with 'LC'-MS to enable the quantification of afucosylation in the monoclonal antibody Herceptin®, alongside a biosimilar candidate. Differences in afucosylation amongst the samples were correlated with mode of action by investigating the effect on receptor binding by SPR analysis and determining the in vitro activity in a cell based bioassay.

Tooth enamel oxygen "isoscapes" show a high degree of human mobility in prehistoric Britain

Pellegrini M, Pouncett J, Jay M2, Pearson MP, Richards MP. Sci. Rep. 2016; 6: 34986

Past human mobility is a topic of great interest in archaeology. Oxygen isotopes are often used to support these investigations, given the relationship between values in the environment and in body tissues. $\delta^{18}O$ values from archaeological

teeth were used to create a geostatistical model of variation for the British Isles, which helped assessing that British prehistoric folks were highly mobile already 4000 years ago.

Mapping the Complete Glycoproteome of Virion-derived HIV-1 gp120

Provides Insights into Broadly Neutralizing Antibody Binding

Panico M et al.

Sci Rep. 2016; 6:32956

A new publication in Nature Scientific Reports, involving a collaboration between Imperial College and Biopharmaspec's mass spectrometry and glycoproteomic experts, working in collaboration with expert virologists in the USA, describes a landmark study in the characterization of virion-derived Envelope Glycoprotein gp120 of the human immunodeficiency virus, HIV-1.

The Type B Flagellin of Hypervirulent Clostridium difficile is Modified with Novel Sulphonated Peptidylamido-Glycans

Bouche L et al.

J Biol Chem. 2016

The intestinal pathogen Clostridium difficile colonizes the gastrointestinal tract when the normal microbiota is disturbed after antibiotic treatment, causing C. difficile infection (CDI) in susceptible patients. This new discovery phase research describes the structural characterization of novel flagellar glycans from a number of hypervirulent strains of C. difficile.

Paper accepted?

Would you like to see your new paper highlighted in the next edition of Mass Matters? If so, please email BMSS publicity secretary, Patricia Wright (pwright@smithers.com) with the full citation and a very brief summary (less than 60 words). A selection of those received will be published.