



World Congress on
**Mass Spectrometry
&
Analytical Techniques**

September 19-20, 2018 Singapore

Special Session
Day 1

World Congress on

MASS SPECTROMETRY AND ANALYTICAL TECHNIQUES

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Kung Tien Liu

Everlight Chemical Industrial Corporation, Taiwan

Elucidation of unknown pharmaceutical degradation products: Structures and pathways

Algorithm for the elucidation of several unknown degradation products shown in the stability studies of Active Pharmaceutical Ingredients (APIs) and drug products, including structures and degradation pathways has been proposed. Collision Activated Dissociation (CID) fragments of APIs and their related intermediates, received using high-performance Liquid Chromatography-tandem Mass Spectrometry (LC-MS/MS) were achieved firstly. Accordingly, Multiple Reaction Monitoring (MRM) ion pairs and fragmentation pathways can be developed secondly. Meanwhile, considering the feasibility of secondary degradation products, core chemical structures that might occur in common in the degradation products were deduced. MRM ion pairs together with related biotransformation scanning (i.e. oxidation (+O, +2O), dehydration (-H₂O, -(H₂O)₂), carbon dioxide removal and HOAc removal) and Information-Dependent Acquisition (IDA) in the target HPLC retention regions were evaluated and compared thoroughly. Finally, unknown degradation products needed to be verified by the stability test samples. Countermeasures, such as pattern of stable isotopic peaks, kinetics studies and interference factors existed in reagents, manufacturing process raw materials and environment such as plasticizer and catalysts were investigated. Unexpected products and interaction between excipients were also identified.

Biography

Kung Tien Liu has completed his PhD from Department of Chemistry, National Taiwan University, Taiwan and has worked in Institute of Nuclear Energy Research (INER) more than 29 years. He also concentrates his major activities on the GxP related compliance issues for the development and applications of pharmaceuticals. Currently, he is the Deputy Director of Administration Office, Pharmaceutical B U, Everlight Chemical Industrial Co. (ECIC). He has been published more than 40 papers, patents and book chapters.

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HS-GCMS-SIM mode method template for identification of varieties of anionic, cationic and neutral surfactants as SIM-fingerprint-ID**Chong Mun Hwa and James Wedgebrow**
Synthomer Plc, Malaysia

Surfactants play an important role in reducing surface tension, as it enables the control interfacial tension between liquids or solid-liquids. The application has been increasing worldwide and safety concern regarding the long term exposure to surfactant has been long discussed. Hence, the identification of surfactants in final products is crucial. The new method has been developing in Head-Space Gas Chromatography Selected Ion Monitoring mode (HS-GCMS-SIM mode) allowed the collection of surfactants as SIM-fingerprint-ID. The advantage of the method is it applies to broad range surfactants containing different chemistries. In addition, the analyses incorporate green chromatographic technique which reduces environmental impact/pollution with simple sample preparations. This database allows direct identification of the types of surfactants without derivatization, fast analysis time and ability of low concentration tracing.

Biography

Chong Mun Hwa has completed her PhD from University Teknologi Malaysia and has more than 7 years of experience in analytical field. She is currently the Senior Analytical Chemist of Synthomer, an aqueous polymer organization. She has published paper in Microporous and Mesoporous Materials journal, a co-author for the book chapter membrane-based solid phase extraction (UTM), had 1 patent for method of extracting chemicals (nitrosamines) in water (PI 2014-003377).

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Metabolic analysis and transcriptomic response of *Escherichia coli* O157:H7 treated with electrolyzed water and mild heat**Hongshun Yang**

National University of Singapore, Singapore

Metabolite levels and gene expression in bacteria offer significant insights into the response of bacteria to disinfection intervention. The purpose of this study was to explore the possible mechanisms underlying the metabolic and transcriptomic changes of *Escherichia coli* O157:H7 in the response to Electrolyzed Water (EW) and mild heat treatments. The oxidant-sensitive probe 2', 7-Dichlorodihydrofluorescein Diacetate (H₂DCFDA) was used to assess the intracellular reactive oxidative species. The metabolomic changes were investigated by UPLC-QToF-MS coupled with multivariate analysis. EW (4 mg/L free available chlorine) combined with heat treatment at 50 °C resulted in 2.31 log CFU/mL reductions of *E. coli* O157:H7. The fluorescence intensity of EW at 50 °C showed the greatest and was 10 times greater than the control group. The decreased ribose-5-phosphate level strongly indicated affected nucleotide biosynthesis, which was consistent with nucleotide level in the *E. coli* O157:H7 cells in response to EW and heat treatments. A 50 fold increase in heat shock regulatory gene *rpoH* expression was found in 50 °C group and combined treatment group compared to the control group, while for EW group the gene expression remained unchanged. However, when treated with EW at 50 °C almost all the gene expressions (except *rpoH*) were dampened with about 0.024-, 0.286- fold decrease for *udk* (encoding uridine kinase) and *gadA* (encoding glutamate decarboxylase alpha), respectively, as compared to control group. The results demonstrate a synergistic effect of EW and heat treatment on inactivating *E. coli* O157:H7.

Biography

Hongshun Yang has completed his PhD from the University of Minnesota and Postdoctoral studies from University of Maryland College Park. He has published more than 90 papers in reputed journals and has been serving as an Editorial Board Member of LWT-Food Science and Technology.

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A stable acetylcholinesterase biosensor based on Au nanorod@SiO₂ core-shell nanoparticle doped chitosan-TiO₂ hydrogel for detecting organophosphate pesticides**Hui-Fang Cui, Ting-Ting Zhang and Wen-Wen Wu**
Zhengzhou University, China

In our previous work, we have developed a highly stable electrochemical acetylcholinesterase (AChE) biosensor for detecting Organophosphorus Pesticides (OPs) with a detection limit of 29 nM, simply by adsorption of AChE on Chitosan (CS) film modified CS-TiO₂ hydrogel immobilization matrix (denoted as CS/TiO₂-CS), which was transformed from colloidal solution to hydrogel *in situ* immediately after being cast on graphene film modified glassy carbon electrode. In this work, Au nano-rod (AuNR)@SiO₂ core-shell nanoparticles were synthesized and doped into the CS-TiO₂ hydrogel by directly mixing the nanoparticles with the colloidal solution before the hydrogel formation. The doping of AuNR@SiO₂ was found being homogeneous and significantly improving the electro-conductivity of the immobilization matrix. In contrast, the aggregation of naked AuNRs in the colloidal solution was observed. The mesoporous SiO₂ shell could not only protect the Au nanorods from aggregation and also allow the permeation of the enzyme substrate and product through the Au nanorod@SiO₂ nanoparticles. The catalytic activity of the AChE immobilized CS/AuNR@SiO₂@TiO₂-CS to acetylthiocholine is significantly higher than that missing the AuNR@SiO₂ in the matrix. The detection linear range of the biosensor to fenthion, a model OP compound, is from 18 nM to 22.6 μM, with detection limit of 10 nM and a total detection time of about 25 min. The biosensor is very reproducibly and stable both in detection and in storage and can accurately detect the fenthion levels in cabbage juice samples, providing a promisingly practical OPs biosensor with high reliability, simplicity, sensitivity and rapidness.

Biography

Hui-Fang Cui has been a Professor in School of Life Sciences, Zhengzhou University, China since 2007. She was recently appointed as Distinguished Professor by Zhengzhou University. She has received her PhD degree from Department of Biological Sciences, National University of Singapore in 2006 and worked as a Postdoctoral Research Fellow at Department of Biological Sciences, National University of Singapore from 2007 to 2008 and at School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore from 2006 to 2007. She has published more than 30 papers in reputed journals. Her research interests are biosensors, biotechnology and nanotechnology.

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Electroanalytical methods of energy storage and conversion**M V Reddy**

National University of Singapore, Singapore

Recent year's energy, water and health care are one of the important areas research carried out by worldwide researchers. Among all energy storage, Lithium Ion Batteries (LIBs) are extensively used in the present-day portable electronic devices and high-power applications like back-up power supplies and electric/hybrid electric vehicles. The commercial LIBs consist of layer-type lithium cobalt oxide, spinel LiMn_2O_4 or LiFePO_4 as the cathode and graphite or $\text{Li}_4\text{Ti}_5\text{O}_{12}$ as the anode material and a non-aqueous Li- ion conducting solution or immobilized gel-polymer are used as an electrolyte. LIBs need to satisfy several additional criteria, such as safety, toxicity, low cost and long cycle life. To understand reaction mechanisms advanced analytical techniques are needed. In my presentation, I will summarize our group studies on functional materials synthesis by molten salt synthesis, graphenothermal reduction and other facile chemical methods on various oxides, nitride materials and novel metal organic frame work cathode materials will be discussed. The functional materials characterized by various analytical techniques such as Rietveld refinement X-ray diffraction, X-ray absorption fine structure, X-ray photoelectron spectroscopy, SEM, TEM, density and BET surface area methods and cyclic voltammetry, galvanostatic cycling and electrochemical impedance spectroscopy techniques. I will discuss the advantages of morphology, nano/submicron size, matrix elements on capacity values and average charge-discharge voltages and its electrochemical performances and reaction mechanisms.

Biography

M V Reddy has pursued his PhD in Materials Science from ICMCB-CNRS, University of Bordeaux, France. For the last 15 years, he has been working on the materials for Li-ion battery materials (cathodes, anodes, super capacitors and solid electrolytes) including novel methods of synthesis, characterization and has experience in electro analytical techniques. He has published around 167 papers in various international journals. He is serving as an Editorial Advisory Board Member in Materials Research Bulletin and several open access journals. He also won Outstanding Science Mentorship award from Ministry of Education, Singapore and Inspiring Research Mentor award from NUSHS.

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A comprehensive study of a new versatile device based liquid phase micro extraction for stopped-flow and double-flow conditions in a single step**Maria Ramos Payan and Garcia Gonzalez**
University of Seville, Spain

A new geometry for a versatile microfluidic-chip device based liquid phase micro extraction was developed to enhance the preconcentration in microfluidic chips and to enable double-flow and stopped-flow working modes. The microchip device was combined with a HPLC procedure for the simultaneous determination of two different families as model analytes, which were parabens and Non-Steroidal Anti-Inflammatories (NSAIDs). The new miniaturized microchip proposed in this work allows not only the possibility of working in double-flow conditions, but also under stagnant conditions (stopped-flow) (SF- μ LPME). The sample (pH 1.5) was delivered to the SF- μ LPME at $20 \mu\text{L min}^{-1}$ while keeping the acceptor phase (pH 11.75) under stagnant conditions for 20 minutes. The highest enrichment factors (between 16 and 47) were obtained under stopped-flow conditions at $20 \mu\text{L min}^{-1}$ (sample flow rate) after 20 minutes of extraction whereas the extraction efficiencies were within the range of 27-81% for all compounds. The procedure provided very low detection limits between 0.7 and $8.5 \mu\text{g L}^{-1}$ with a sample volume consumption of $400 \mu\text{L}$. Parabens and NSAIDs have successfully been extracted from urine samples with excellent clean up and recoveries over 90% for all compounds. In parallel, the new device was also tested under double-flow conditions, obtaining good but lower enrichment factors (between 9 and 20) and higher extraction efficiencies (between 45 and 95) after 7 minutes of extraction, consuming a volume sample of $140 \mu\text{L}$. The versatile device offered very high extraction efficiencies and good enrichment factor for double-flow and stopped-flow conditions, respectively. In addition, this new miniaturized SF- μ LPME device significantly reduces the costs compared to the existing analytical techniques for sample preparation since this microchip requires few microliters of sample and reagents and it is reusable.

Biography

Maria Ramos Payan has pursued her PhD from University of Seville, Spain and Postdoctoral studies from University of Copenhagen, Denmark, University of North Carolina, USA and Microelectronic National Center of Barcelona, Spain. She is the Leader of the microfluidic research line. She has published more than 30 papers in reputed journals and has been serving as an Editorial Board Member of *repute*.

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A portable chip for microextraction and subsequent optical detection in a single step. Determination of norfloxacin in water samples.**María Ramos Payán**

Department of Analytical Chemistry, University of Seville, 41012, Spain

In recent years, the miniaturization of new methodologies has become a dominant trend due to the advantages they present. On the one hand, microextraction techniques integrated into microfluidic devices on chip have been able to be connected online to instrumental techniques for direct analysis. The development of new detection devices using optical fibers allows measuring new compounds more quickly and requiring less sample volume. In this work, we present for the first time the coupling between two miniaturized systems: a microextraction microchip device based liquid phase microextraction and an optical detection device using optical fibers (fluorescence), allowing on-line determination in a single portable device using a very low sample volume. The first step was a clean-up sample treatment and the extraction of the analyte (norfloxacin), whereas the second step was the direct determination of norfloxacin using optical fibers. The microextraction procedure was carried out at optimal extraction conditions (dihexylether as organic solvent, pH 3 as sample solution, pH 12 as acceptor solution, and 1 μ L/min as flow rate for sample and acceptor solution). Finally, the device has been successfully applied to environmental samples.

Biography

María Ramos Payán has expertise in improving sample preparation techniques focused on microfluidic-chip devices as miniaturization. The novelty of her microfluidic devices offer more advantages than the existing methodologies. Maria has worked at different institutions (University of Seville, University of Huelva, University of Lund, University of Copenhagen, University of North Carolina, USA, Microelectronic National Center of Barcelona and Universitat Autònoma de Barcelona). Currently, she works at University of Seville with the aim of implementing optical detection into microfluidic devices for multiple different applications.

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Advances in ICP-MS: Clinical applications and human bio-monitoring**Ciprian Mihai Cirtiu**

National Institute of Public Health of Quebec, Canada

Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is now regarded as one of the most powerful analytical techniques for trace and ultra-trace analysis of elements. It finds applications in various fields and applies to different matrices like environmental (air and water quality check, waste water treatment plants), geochemical (soil), drugs and pharmaceuticals (quality control), food and beverages, petrochemical as well as biological matrices (clinical, occupational and environmental medicine, human bio-monitoring). ICP-MS coupled to separation techniques (chromatography) is proving an invaluable detection technique to characterize elemental species (toxicology, quantitative proteomics). A more recent way to use ICP-MS is in time-resolved mode, which allows analyzing nanoparticles in Single-Particle ICP-MS mode (SP-ICP-MS). At the Centre de Toxicologie du Québec, a branch of the Institut National de Santé Publique du Québec (INSPQ, Québec, Canada) we are aiming at developing ICP-MS-based analytical methods to assess trace and ultra-trace elements in biological matrices. The methods are developed and validated following general guidelines of ISO/IEC 17025. In the present work, an overview of various recent applications of ICP-MS methods will be given, with focus on clinical applications (screening, speciation, toxicology), bio-monitoring (health surveys) and preparation of proficiency testing materials as part of the quality assessment schemes organized by CTQ. Current research and development activities are directed towards the development of new technologies and methodologies for the analysis of emerging products in order to advance knowledge in terms of toxicology and human bio-monitoring.

Biography

Ciprian Mihai Cirtiu has completed his PhD in the Université de Sherbrooke (2007) on the development of functionalized materials for the electro-catalytic hydrogenation reaction. From 2007 to 2008, he has worked as Post-doctorate at UQAM on the fabrication and characterization of semi-conductive nanoparticles for electrochemical solar cell and olivine-type lithium-iron phosphate nanoparticles for Li-ion batteries. In 2008, he joined the group of Professor Audrey Morres in McGill University as Postdoctoral Fellow to work on the development of new hybrid materials for catalytic reactions as well as the synthesis, characterization and application of zero-valent iron nanoparticles for groundwater remediation. He has joined the "Centre de Toxicologie du Québec" at Institut National de Santé Publique de Québec in 2011 as Analytical Development Chemist. In January 2013 he was named Head of Trace Metals Division. His research activities are oriented towards the development of new technologies and methodologies for the analysis of emerging products (nanoparticles, metals, rare earths elements, etc.) in order to advance knowledge in terms of toxicology and human bio-monitoring. He has 23 articles in peer reviewed journals, 2 patents, 38 oral communications and 25 posters to his credit.

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Recent advances in sample preparation methods**Yingying Wen**

Hainan Medical University, China

Sample preparation is a crucial bottleneck in the whole analytical process. Moreover, samples such as environmental and biological samples are complex in which the concentration of the target analytes is very low. Sample preparation methods have aroused increasing interest in research on analytical the bioanalytical techniques field, as they have the key roles in obtaining high clean-up and enrichment efficiency in the analysis of trace targets presented in the complex matrices. Recently, except the traditional sample preparation methods (i.e. SPE and LLE), more and more new sample preparation methods are applied prior to chromatography, spectrometry and electrochemistry analysis, for example, Dispersive Liquid-Liquid Micro Extraction (DLLME), Salting-out Assisted Liquid-Liquid Extraction (SALLE), cloud point extraction (CPE), etc. In DLLME, an appropriate mixture of extraction and disperser solvents is rapidly injected into an aqueous sample by a syringe. The fine particle of extracting solvent that is dispersed into aqueous phase forms a cloudy solution and allows its interaction with the analytes. The analytes are extracted from the sample to the fine droplets of extraction solvents. After centrifugation, phase separation is achieved and the enriched analytes is analyzed by some instrumental methods. SALLE is based on the formation of a biphasic system of mutual miscibility of two liquids by addition of additives, i.e. salts and sucrose. Considering the organic solvents as extraction and protein precipitation agents, SALLE is an excellent alternative used for biological sample. CPE is based primarily on the hydrophobic interaction between solutes and surfactants. It has become an alternative to conventional solvent extraction due to several possible advantages such as low cost, environmental safety, high capacity to concentrate a wide variety of analytes of widely varying nature with high recoveries and high enrichment folds.

Biography

Yingying Wen has been graduated with a BA degree and PhD from Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences. Further, she had joined Hainan Medical University. Her research work focuses on sample preparation and chromatographic separation, including solid phase extraction and liquid phase extraction techniques, as well as chromatographic separation methods such as LC/MS and GC/MS. She is the author and co-author of more than 20 original research papers and several reviews.

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Validation of a tandem mass spectrometric method for direct analysis of free amino acids in riceG V V Liyanaarachchi¹, H P P S Somasiri¹, K R R Mahanama² and P A N Punyasiri²¹Industrial Technology Institute, Sri Lanka²University of Colombo, Sri Lanka

The role of Free Amino Acids (FAAs) in deciding the organoleptic characteristics of food has inspired growing concern in researching on FAA levels present in food. With this apparent relationship of FAAs to taste which are present in minute quantities, there is an increased demand for analytical methods sensitive in trace level detection. This study presents the validation results of the method developed for direct, un-derivatized analysis of FAAs in rice using Liquid Chromatography-tandem Mass Spectrometry (LC-MS/MS). Satisfactory chromatographic resolution of 20 FAAs was achieved using LC-MS/MS detection in Electrospray Ionization (ESI) mode. Selectivity of the method was assured considering the qualifier to quantifier ratio. The detection and quantification limits were in the range 0.4-1.0 mg/kg and 0.6-1.2 mg/kg respectively. Method had a wide linear range over 1.25-100 mg/kg range with regression coefficients greater than 0.999 obtained over seven calibration levels. Precision measured in terms of repeatability and reproducibility, expressed as percentage relative standard deviation (%RSD) was below 10% for all the amino acids analyzed. Recoveries obtained for samples fortified at three concentration levels covering the working range of the method were in the range of 80-110%. Measurement uncertainties of the studied analytes with the coverage factor ($k=2$), were below 14% and the method was found robust over other grains including corn, wheat, finger millet and black gram. The developed LC-MS/MS method is reproducible and accurate, allowing determination of un-derivatized FAAs in rice and comply with the international method validation guideline requirements available for trace level analysis.

Biography

G V V Liyanaarachchi has completed his PhD in Analytical Chemistry from the University of Colombo in Sri Lanka. He serves as a Consultant and as a Technical Expert for national and international committees and organizations and has won several awards in recognition of his work. He has over 22 publications/communications published in reputed journals together with two patents and currently serves as a Senior Deputy Director at the Chemical and Microbiological Laboratory of Industrial Technology Institute (ITI) of Sri Lanka.

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