



International Conference on

MASS SPECTROMETRY AND PROTEOMICS

June 25-27, 2018 | Dublin, Ireland

DAY 1

Scientific Tracks & Abstracts

Day 1

SESSIONS

June 25, 2018

Application of Mass Spectrometry | Fundamental of Mass Spectrometry | Recent
Advancement in Mass Spectrometry | Proteomics

Session Introduction

Session Chair

Kihyung Song

Korea National University
of Education, South Korea

Title: Study of the interaction of active compounds with 3D printed chitosan/hyaluronic acid scaffolds in cell culture medium: a mass spectrometry approach

Lisa Elviri, University of Parma, Italy

Title: Development of new environmental high-voltage transmission electron microscope equipped with quadrupole mass spectrometer for observing catalytic reactions

Muto S, Nagoya University, Japan

Title: Theoretical Mass Spectrometry of Sexual Hormones

Kihyung Song, Korea National University of Education, South Korea

Title: Mass spectrometry in the workflow of personalized cancer treatment: Evaluation of protein expression, PTMs and activity

Serhiy Souchelnyskiy, Qatar University, Qatar

Title: SET reduction by miR-199b-5p attenuates Trichloroethylene-induced hepatocyte apoptosis

Xiaohu Ren, Shenzhen Center for Disease Control and Prevention, China

Title: Identification of protein targets in cerebral endothelial cells for brain arteriovenous malformation (AVMs) molecular therapies

Margaret Simonian, University of California Los Angeles (UCLA), USA

Title: Gas chromatographic-mass spectrometric determination of o-phthalic acid esters in low alcohol wines coupled with emulsion liquid-phase microextraction preconcentration

Krylov V A, N. I. Lobachevskii Nizhny Novgorod State University, Russia

Mass Spectrometry Congress 2018

STUDY OF THE INTERACTION OF ACTIVE COMPOUNDS WITH 3D PRINTED CHITOSAN/HYALURONIC ACID SCAFFOLDS IN CELL CULTURE MEDIUM: A MASS SPECTROMETRY APPROACH

Lisa Elviri, Ragaiolo M, Bergonzi C, Bianchera A and Bettini R
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One of the purposes of tissue engineering is that of developing synthetic or naturally-derived biological substitutes (scaffolds) capable to help injured tissues to heal properly. Polymeric materials are often selected as promising candidates for scaffolding thanks to their high surface-to-volume ratio, their structural similarity to the matrix and in function of their final biomedical purpose. Furthermore, 3D biomaterial manufacturing strategies show an extraordinary driving force for the development of innovative therapies in the tissue engineering field. Here, the behavior of 3D printed chitosan (CH) or CH/hyaluronic acid-based scaffolds was explored in terms of mechanical, morphological properties, and adsorbing properties of low molecular weight molecules and proteins contained in Dulbecco's modified medium High Glucose (DMEM) and bovine fetal serum (FBS), as a function of the gelation process. Scaffolds were made by a home-made 3D cryo-printing process from formulations with different concentrations of chitosan and chitosan and hyaluronic acid, gelled in 1.5 M potassium hydroxide, 1.5 M sodium carbonate or 28% w / v ammonia vapors. The water content of the scaffolds together with their mechanical strength and SEM morphological analyzes were evaluated. Finally, absorption tests were performed in order to qualitatively and qualitatively evaluate which substances the scaffold absorbs from the fetal bovine serum and the medium DMEM High Glucose. The analysis conducted by triple quadrupole and high resolution Orbitrap mass spectrometry, revealed that the scaffolds are able to absorb biological molecules present in medium and serum, and electrostatic interactions are the main driving forces. Furthermore, molecules presenting an aromatic ring or a sulfur group exhibited a preferred interaction pathway with the CH/HA scaffolds. The results as a function of the scaffold properties were presented and discussed.

BIOGRAPHY

Lisa Elviri has completed her PhD in 2001 from Parma University, IT. She is associate professor of analytical chemistry at the Food and Drug Department of the University of Parma. She work mainly on sample preparation, liquid chromatography, mass spectrometry based techniques, 3D printing and biomaterial for regenerative medicine. She has over 90 publications that have been cited over 2100 times, and her publication H-index is 26. She is the founder and president of M3datek Srl an innovative start-up dedicated to the 3D printing of biomaterial-based medical devices for regenerative medicine.

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DEVELOPMENT OF NEW ENVIRONMENTAL HIGH-VOLTAGE TRANSMISSION ELECTRON MICROSCOPE EQUIPPED WITH QUADRUPOLE MASS SPECTROMETER FOR OBSERVING CATALYTIC REACTIONS

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In this paper, we introduce the new high-voltage electron microscopy-quadrupole mass spectrometer (HVEM-QMS) system and demonstrate redox reactions where the product gas species are unambiguously detected, associated with the expected structural changes, as follows: (i) CO_2 as a result of carbon nanotube (CNT) combustion by a Pd nano-particle catalyst in O_2 atmosphere was detected when a mixture of a CNT bundle and Pd fine particles was heated in ~ 10 Pa of O_2 gas. The Pd particles started to move around in CNTs $> \sim 200^\circ\text{C}$, and it appeared that the Pd particles decomposed the CNTs, because carbon atoms contacting Pd particles surface were burned to CO_2 , when QMS of m/Z 44 was detected; a good correlation was obtained between the TEM image and Q-Mass spectra, without a significant delay of the CO_2 detection onset with respect to the start of the Pd particles motion. (ii) Reduction of Rd_2O_3 nano-particles in vacuum: Rd_2O_3 nano-particles supported on ZrO_2 substrate were heated in vacuum, which was reduced to metal at temperatures $> \sim 200^\circ\text{C}$. Interestingly QMS detected no oxygen even during the transformation of Rd_2O_3 to metallic Rh. Instead species of m/Z 44 (in the form of CO_2) were unambiguously detected. This suggests that the emitted oxygen atoms were so chemically active in the atomic form as to instantly react with the surrounding carbon-origin contaminations, forming CO_2 . Further demonstrations will be presented.

BIOGRAPHY

Muto S has completed his PhD at the age of 28 years from Osaka University, Japan. He is the professor of Institute of Materials and Systems for Sustainability, Nagoya University, Japan and the director of High-Voltage Electron Microscopy Laboratory of Nagoya University. He has over 200 publications that have been cited over 2500 times, and his publication H-index is 27. His main interest is to visualize physical/chemical properties of various functional materials at nanometer scale, using transmission electron microscopy/spectroscopy techniques.

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Note:

THEORETICAL MASS SPECTROMETRY OF SEXUAL HORMONES

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Theoretical mass spectrometry of ESI-MS/MS can be obtained by classical trajectory simulations of collision-induced dissociation of protonated cation or deprotonated anion with Ar atom. This method can record the atomic coordinates of the system as a function of time by solving classical mechanics with forces calculated on the fly from quantum chemistry program. The potential between ion and Ar atom is given by analytical form of Buckingham potential. The coordinates of atoms can be visualized and analyzed to determine the structures and formation mechanisms of the fragment ions. The theoretical mass spectrometry of testosterone, boldenone, and estradiol will be presented with animations.

BIOGRAPHY

Kihyung Song has completed his PhD at the age of 31 years from Texas Tech University, USA. Since 1989, he has been a Professor of Department of Chemistry at Korea National University of Education. He is the chairman of the department now. He has published more than 110 papers in reputed journals including Science. His research gate index is 38.75.

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MASS SPECTROMETRY IN THE WORKFLOW OF PERSONALIZED CANCER TREATMENT: EVALUATION OF PROTEIN EXPRESSION, PTMS AND ACTIVITY

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High sensitivity has firmly established mass spectrometry as the method of choice for identification and analysis of proteins. Clinical challenge of personalification of anti-cancer treatment requires analysis of small quantities of proteins. There are more than 300 PTMs which affect functions of proteins, and mass spectrometry is so far the most efficient in their identification. All anti-cancer drugs act on or via proteins. Therefore, proteome analysis is essential for efficient diagnostic and selection of treatment. In my presentation, I will show examples of how we use mass spectrometry in our efforts of personalization of cancer treatment. Expression proteomics, with detection and identification of targets for potential anti-cancer treatment, is one of the examples. Another example is mass spectrometry imaging in combination with magnetic resonance imaging, to monitor responsiveness of cancer cells to treatment. Study of breast and renal cancer cells will be presented as examples. Unbiased detection of >30 PTMs in the same proteins from cancer vs normal cells will also be discussed in the context of tumorigenesis. Have mass spectrometry reached its limits? With a resolution of >0.0001 Da, an impact may have such phenomena as mass vs energy transformation. Isotope distribution in samples is another technical issue which may influence results. These technical aspects will also be discussed.

BIOGRAPHY

Serhiy Souchelnytskyi graduated from Lviv State University (1985) and obtained PhD degree at the Institute of Biochemistry (1992) in Lviv, Ukraine. He worked at the Institute of Biochemistry (Ukraine), INSERM U244 (France), Ludwig Institute for Cancer Research (Uppsala, Sweden), Karolinska Institutet and Karolinska University Hospital (Stockholm, Sweden), before joining Qatar University in 2015. He is involved in commercialization of research by developing diagnostic and personalization of cancer treatment. He has 125 publications, including 5 patents. He is involved in editorial works as an Editor and a member of Editorial boards, works frequently for granting agencies as an expert, and has received awards in the area of proteomics and cancer biology. Current projects are in development of personalized cancer medicine. Proteomics, systems biology and cancer signaling biology are used for individualized profiling of patients, their diagnostic and selection of the most efficient treatment.

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SET REDUCTION BY MIR-199B-5P ATTENUATES TRICHLOROETHYLENE- INDUCED HEPATOCYTE APOPTOSIS

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Jianjun Liu**

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Trichloroethylene (TCE) is a commonly used industrial solvent and widespread environmental pollutant, exposure to which can cause severe liver damage. Previously we have observed in a model of TCE-induced apoptosis of cultured human hepatocytes (L-02 cell line) that SET (a protein encoded by the SET gene in humans) is abnormally elevated which acts as a key mediator of the induction of apoptosis, however, the potential molecular mechanisms modulating SET in that model remain unclear. In this study, through a screening of various databases six microRNAs were predicted to potentially regulate SET. Subsequent experiment indicated that three (miR-199b, miR-21, and miR-23a) of them were decreased in TCE-treated L-02 cells. Further analysis using a dual luciferase reporter assay and miR-199b-5p knockdown/overexpression in L-02 cells revealed that only miR-199b-5p could suppress SET, through direct binding to its 3'-UTR. Functional studies indicated that miR-199b-5p attenuated TCE-induced apoptosis of L-02 cells through the inhibition of SET. In summary, the present study suggests that in TCE-induced cytotoxicity in cultured hepatocytes miR-199b-5p may down-regulate SET, thus further attenuating the toxic response to TCE.

BIOGRAPHY

Xiaohu Ren has completed his PhD in 2015 from Southern Medical University, and now, he is post-doctor of Key Laboratory of Modern Toxicology of Shenzhen. His major research interests include molecular mechanisms of environmental chemical-induced liver injury, proteomic profiling of potential biomarkers for the diagnosis of environmental chemical exposure. He has published more than 20 research papers. Additionally, in the past few years, he has received over six grants, such as Science and Technology Plan Projects of Guangdong, National Science Foundation for Young Scholars of China, National Science Foundation of China, and so on.

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IDENTIFICATION OF PROTEIN TARGETS IN CEREBRAL ENDOTHELIAL CELLS FOR BRAIN ARTERIOVENOUS MALFORMATION (AVMs) MOLECULAR THERAPIES

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Macquarie University Sydney, Australia

To develop a new molecular targeted treatment for brain (AVMs), identification of membrane proteins that are localised on the AVM endothelium is crucial. Current treatment methods are surgery and radiosurgery. However, complete occlusion post radiosurgery are achieved within 3 years, while patient remain at risk of haemorrhage. This study aims to identify potential protein targets in AVM endothelial cells that discriminate these vessels from normal vessels; these proteins targets will be investigated for the molecular therapy of brain AVMs to promote rapid thrombosis after radiosurgery. We employed *in vitro* and *in vivo* biotinylation that we developed, and mass spectrometry to detect cell surface-exposed proteins in cultures of murine cerebral endothelial cells (bEnd.3) and the rat model of AVM. Two forms of mass spectrometry were applied (iTRAQ-MS and MS^E) to identify and quantify membrane protein expression at various time-points following irradiation which simulates a radiosurgical treatment approach. Immunocytochemistry was used to confirm the expression of selected membrane proteins. ProteinPilot V4.0 software was used to analyse the iTRAQ-MS data and the MS_E data was analysed using ProteinLynx Global Server (PLGS) version 2.5 software.

BIOGRAPHY

Margaret Simonian has PhD in Advanced Medicine and MPhil in Biological Sciences from Macquarie University- Australia. She works as a Researcher at UCLA David Geffen School of Medicine, and previously as a Senior Research Fellow at LA-Biomedical Research Institute at Harbor-UCLA, and at Macquarie University. Her research interests focuses on utilizing Proteomics and Molecular Biology in biomarker discovery and drug development of diseases, such as brain arteriovenous malformations (AVMs), brain tumors , aneurysms and multiple sclerosis. Her research on brain AVMs was the first to utilise proteomics to identify protein targets of AVM molecular and vascular therapies post radiosurgery. She presented her research in many international conferences and published in many peer reviewed journals. She is also a reviewer for the Journal of Proteomics, Journal of Arthritis & Research Therapy and Journal of European Proteomics. An Associate Editor for the Journal of Applied Biotechnology and Bioengineering, and Editorial Board Member for Journal of Data Mining in Genomics & Proteomics, and Journal of Science publications, as well as an Organizing Committee Member for the International Conference on Precision Medicine 2017.

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Note:

GAS CHROMATOGRAPHIC-MASS SPECTROMETRIC DETERMINATION OF O-PHTHALIC ACID ESTERS IN LOW ALCOHOL WINES COUPLED WITH EMULSION LIQUID-PHASE MICROEXTRACTION PRECONCENTRATION

Krylov V A

N. I. Lobachevskii Nizhny Novgorod State University, Russia

Esters of o-phthalic acid are very dangerous for human health. In this study the high sensitive gas chromatographic-mass spectrometric determination of phthalates in low alcoholic beverages (champagne, red and white wine) coupled ultrasound-assisted emulsification-microextraction was developed. The sources of possible systematic errors were investigated: Leaking of o-phthalates from chromatographic septum; contamination of phthalate in solvents; influence of macro components of wines (sugar, alcohol, anthocyanins); the hydrolysis of o-phthalates and others. For the first time it is shown that the impact of these factors can lead to an overestimation or underestimation of the actual concentration of impurities by 1-2 orders of magnitude. The methods of accounting or elimination of systematic errors are proposed. Purification of solvents by Rayleigh distillation method allows to obtain samples with impurity content lower than $(1-4) \cdot 10^{-3} \text{ mgL}^{-1}$. Containers for sampling and storage of samples to be analyzed should be made of borosilicate glass or quartz. The content of o-phthalates in wines was $0.03 - 1 \text{ mgL}^{-1}$. The limits of detection of esters of o-phthalic acid are at the level of $10^{-6} - 10^{-5} \text{ mgL}^{-1}$ and are highly competitive with the best world results. The relative expanded uncertainty of the determination of toxicants is at the level of 13- 30%.

BIOGRAPHY

Krylov V A, Doctor of Chemistry, Professor, Head of the Division of Analytical Chemistry of the Nizhny Novgorod State University. The main direction of scientific research of professor Krylov is the development of the theory and applications of chromatography for the analysis of high purity substances, environmental objects and development of methods of the microextraction. The attained detection limits for molecular impurities constitute 10^{-6} to 10^{-11} wt % and hit a record low. He is the author of more than 200 scientific papers, including reviews on the analytical chemistry of high purity volatile substances, air and liquid-liquid microextraction preconcentration.

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Note:



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DAY 2

Scientific Tracks & Abstracts

Day 2

SESSIONS

June 26, 2018

Application of Mass Spectrometry | Ionization Techniques
Chromatography | HPLC

Session Introduction

Session Chair

Jianjun Liu

Shenzhen Center for
Disease Control and
Prevention, China

Title: **GC-C-IRMS and 1H-NMR characterization of synthetic bis(methylthio)methane in truffle flavorings**

Monica Bononi, University of Milan, Italy

Title: **Automation of sample preparation for mass spectrometry in biomedical projects**

Nazariy Souchelnytskyi, Qatar University, Qatar

Title: **Down-regulation of p53 by SET contributes to TCE-induced DNA damage through inhibition of H3K79 di-methylation**

Jianjun Liu, Shenzhen Center for Disease Control and Prevention, China

Title: **Characterisation of luxury animal fibers and fur through LC-QTOF analysis**

Riccardo Dall'Anese, Buzzi Lab, Italy

Title: **HPLC-Fluorescence Method for the Enantioselective Analysis of Propranolol in Rat Serum Using Immobilized Polysaccharide-Based Chiral Stationary Phase**

Aymen k. Al- Suwailem, King Saud University, Saudi Arabia

Title: **The Role of Programmed Cell Death 'Apoptosis' in the Development of Inner Sulcus in the Cochlea**

Tarfa M Peter, Gombe State University, Nigeria

Title: **High throughput proteomic analysis using different OFFGel fractionation panels**

Sameh Magdeldin, Suez Canal University, Egypt

Title: **Journey of Mass Spectrometry**

Lokesh Kumar Gupta, TEVA API India Pvt. Limited, India

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GC-C-IRMS AND ¹H-NMR CHARACTERIZATION OF SYNTHETIC BIS(METHYL-THIO)METHANE IN TRUFFLE FLAVORINGS

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³University of Salento, Italy

Tuber magnatum (white truffle), *Tuber aestivum* (summer truffle), and *Tuber melanosporum* (black truffle) are the most well-known species belonging to the genus *Tuber* F.H. Several reports have considered the constituents responsible for the typical aroma and have also studied the quantitative and qualitative fluctuations of these compounds, depending upon truffle type and geographical origin [1-5]. The corresponding naturally-occurring identical compound, easily synthesized by the petroleum oil industry and supported in olive oil, is used as a flavoring agent for truffle flavored food products. Among the "white truffle-like" flavored foods, extra virgin olive oil, flavored with bis(methyl-thio)methane (BMTM), used as a seasoning occupies the most important position in the market. The largely distributed flavored seasoning offered an opportunity to characterize the synthetic BMTM by Isotope Ratio Mass Spectrometry (IRMS) and Proton Nuclear Magnetic Resonance (¹H-NMR) spectroscopy. Analysis by GC-C-IRMS of various samples of synthetic BMTM from different origins allowed the investigation of the global $\delta^{13}\text{C}$ values. Analysis by ¹H NMR of a synthetic standard and of a "white truffle-like" flavor consisting of synthetic BMTM as the principal component allowed the investigation of the isotopic distribution of ¹³C/¹²C ratio in two characteristic sites of this molecule. An easily produced extract using methanol-d₄ allowed the identification and the characterization of BMTM available in "white truffle-like" flavorings distributed on the specialized flavorings market as synthetic BMTM supported in olive oil. The data reported in this paper are the first GC-C-IRMS and ¹H NMR contributions to the characterization of synthetic BMTM available on the flavoring market and in "white truffle" flavors used to prepare the seasoning produced by dilution of BMTM in olive oil. Here, the behavior of 3D printed chitosan (CH) or CH/hyaluronic acid-based scaffolds was explored in terms of mechanical, morphological properties, and adsorbing properties of low molecular weight molecules and proteins contained in Dulbecco's modified medium High Glucose (DMEM) and bovine fetal serum (FBS), as a function of the gelation process. Scaffolds were made by a home-made 3D cryo-printing process from formulations with different concentrations of chitosan and chitosan and hyaluronic acid, gelled in 1.5 M potassium hydroxide, 1.5 M sodium

carbonate or 28% w / v ammonia vapors. The water content of the scaffolds together with their mechanical strength and SEM morphological analyzes were evaluated. Finally, absorption tests were performed in order to qualitatively and qualitatively evaluate which substances the scaffold absorbs from the fetal bovine serum and the medium DMEM High Glucose. The analysis conducted by triple quadrupole and high resolution Orbitrap mass spectrometry, revealed that the scaffolds are able to absorb biological molecules present in medium and serum, and electrostatic interactions are the main driving forces. Furthermore, molecules presenting an aromatic ring or a sulfur group exhibited a preferred interaction pathway with the CH/HA scaffolds. The results as a function of the scaffold properties were presented and discussed.

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AUTOMATION OF SAMPLE PREPARATION FOR MASS SPECTROMETRY IN BIOMEDICAL PROJECTS

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Analysis of separated full-length proteins may be more informative as compared to a shotgun peptidomics approach. However, automation of separation and identification of proteins is a serious challenge. When LC-MS/MS approach is well-automated, 2DE and MS/MS demands a lot of hands-on work. We will present our experience in development of automation for sample preparation for MALDI TOF mass spectrometry. Examples will show applications of the sample preparation robotics in studies of protein nitration, phosphorylation and expression in human cancer cells and breast tumor biopsies. Separation of proteins was performed by 2D gel electrophoresis, and for sample preparation were used liquid handling stations. By incorporation in the proteomics workflow of robotics stations, we enhanced capacity of sample preparation in at least 10 folds. Tecan and Genomics Solution robotics were used, and will be presented as examples of technical solutions.

BIOGRAPHY

Nazariy Souchelnytskyi studied at the Royal Institute of Technology (Stockholm), Uppsala University and Nakademin (all in Sweden). Mr. Nazariy Souchelnytskyi has been working as a proteomics core facility manager at the Ludwig Institute for Cancer Research (Uppsala, Sweden), Karolinska Institutet and Karolinska University Hospital (Stockholm, Sweden). Mr. Nazariy Souchelnytskyi is a Chief Technology Officer at Oranta CancerDiagnostic AB (Sweden). He has 9 publications in the application of proteomics and mass spectrometry in biomedical research.

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DOWN-REGULATION OF P⁵³ BY SET CONTRIBUTES TO TCE-INDUCED DNA DAMAGE THROUGH INHIBITION OF H3K79 DI-METHYLATION

Jianjun Liu, Xiaohu Ren, Zhihong Chen, Jiawen Ruan and Nuanyuan Iuo

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Trichloroethylene (TCE) is an occupational and environmental chemical that can cause severe hepatotoxicity. Previously we have observed in a model of TCE-induced apoptosis of cultured human hepatocytes (L-02 cell line) that SET (a protein encoded by the SET gene in humans) is abnormally elevated which acts as a key mediator in TCE-induced hepatic cytotoxicity, but the underlying mechanisms still remain elusive. In this study we found that TCE induced DNA damage in liver cells using comet assay. Additionally, SET related histone methylation were analyzed using the combination of triton-acid-urea polyacrylamide gel electrophoresis (TAU-SDS-PAGE) and LC-MS/MS. 22 SET-mediated abnormally altered histone methylation were identified and the H3K79 di-methylation (H3K79me₂), which was related with DNA damage and gene transcription, was validated by Western-blot analysis. We revealed that SET inhibited H3K79 di-methylation within the promoter region of p⁵³ under the treatment of TCE by using chromatin immunoprecipitation-quantitative PCR (CHIP-qPCR) analysis. Further inhibition of H3K79 specific methyltransferase DOT1L verified that SET-mediated decreasing H3K79 di-methylation caused down-regulation of p⁵³ and aggregated DNA damage. These findings indicate that SET aggregates TCE-induced DNA damage through partially blocking the repair process via dysregulation of p⁵³.

BIOGRAPHY

Jianjun Liu has completed her M.D. in 1989 from University of Xiangtan, and now, she is post-doctor supervisor of Southern Medical University. Her major research interests include proteomic analysis and biomarker screening of chemical pollutant-induced damage to human, safety assessment of nano-materials, development of testing techniques for food safety. She has published more than 70 research papers. Additionally, in the past five years, she has received over ten grants, such as National Science Foundation of China, the Guangdong Natural Science Foundation, Sanming Project of Medicine in Shenzhen, and so on.

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CHARACTERIZATION OF LUXURY ANIMAL FIBERS AND FUR THROUGH LC-QTOF ANALYSIS

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Luxury animal fibres have an important economic contribution for the textile sector because they are widely used in the production of clothing fabrics: considering the extensive use of these materials it is frequent to come across adulterations or counterfeiting of materials in order to take economic benefits from the marketing of textile products. Traditional methods of identification are based on a microscopic analysis (optical microscopy or SEM) exploiting the morphological characteristics of the cuticles structure of the fibres. The proposed [1] and developed method of analysis is based on an extraction of proteins which are present in the cytoskeletal structure of animal fibres and subsequent identification of marker peptides by liquid chromatography coupled with high resolution mass spectrometry (LC-QTOF). High-resolution mass spectrometry analysis makes it possible to identify with more precision the marker peptides of various animal species (e.g. cashmere, wool and yak) and to study specific markers for the identification of animals from furs, also guaranteeing an intra-species classification of the animal (e.g. different types of foxes). The high efficiency of this analytical technique and its objectivity makes it the best assistboth for the identification of animal fibers in forensic sector and for the systematic determination in the product sector.

BIOGRAPHY

Riccardo Dall'Anese completed in 2010 the Bachelor's Degree in Industrial Chemistry at University of Padua and completed in 2012 the Master Degree in Chemistry for Clinical, Forensic and Sport at University of Turin. From 2013 to 2015 wor as Analytical Technician at Buzzi Lab (Prato, Italy) and from 2015 up to now work as Analytical Lab Manager at Buzzi Lab (Prato, Italy).

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HPLC-FLUORESCENCE METHOD FOR THE ENANTIOSELECTIVE ANALYSIS OF PROPRANOLOL IN RAT SERUM USING IMMOBILIZED POLYSACCHARIDE-BASED CHIRAL STATIONARY PHASE

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Tstereoselective high-performance liquid chromatographic (HPLC) method was developed and validated to determine S-(-)- and R-(+)-propranolol in rat serum. Enantiomeric resolution was achieved on cellulose tris(3,5-dimethylphenylcarbamate) immobilized onto spherical porous silica chiral stationary phase (CSP) known as Chiralpak IB. A simple analytical method was validated using a mobile phase consisted of n-hexane-ethanol-triethylamine (95:5:0.4%, v/v/v) at a flow rate of 0.6 mL min⁻¹ and fluorescence detection set at excitation/emission wavelengths 290/375 nm. The calibration curves were linear over the range of 10–400 ng mL⁻¹ (R = 0.999) for each enantiomer with a detection limit of 3 ng mL⁻¹. The proposed method was validated in compliance with ICH guidelines in terms of linearity, accuracy, precision, limits of detection and quantitation, and other aspects of analytical validation. Actual quantification could be made for propranolol isomers in serum obtained from rats that had been intraperitoneally (i.p.) administered a single dose of the drug. The proposed method established in this study is simple and sensitive enough to be adopted in the fields of clinical and forensic toxicology. Molecular modeling studies including energy minimization and docking studies were first performed to illustrate the mechanism by which the active enantiomer binds to the β -adrenergic receptor and second to find a suitable interpretation of how both enantiomers are interacting with cellulose tris(3,5-dimethylphenylcarbamate) CSP during the process of resolution. The latter interaction was demonstrated by calculating the binding affinities and interaction distances between propranolol enantiomers and chiral selector. Chirality 00:000–000, 2014.

Key Words: propranolol; enantioselective; Chiralpak IB; HPLC-FD; molecular modeling.

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THE ROLE OF PROGRAMMED CELL DEATH 'APOPTOSIS' IN THE DEVELOPMENT OF INNER SULCUS IN THE COCHLEA

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Hearing loss is one of the most common chronic diseases that affect both young and old but it is most prevalent in old people. This condition is generally irreversible in humans and can be due to the loss of hair cells, which are unable to regenerate. However, recent evidence of some regenerative ability reported in a number of non-mammal vertebrates have given us hope that, in the future a solution may be discovered. Although several advances have been recorded in this field in recent times and there are still challenges ahead. This study tried to investigate the formation of the inner sulcus located in the cochlea, as it is thought that, the processes involved during the development of this important region are most likely due to apoptosis or another type of programmed cell death, although this has not yet been confirmed. Mouse expressing an EGFP (green fluorescent protein) reporter at the Tecta locus was used. Specimens were stained with phalloidin as a general cell stain of f-actin and this was combined with (Terminal deoxynucleotidyl transferase dUTP Nick End) TUNEL staining in order to observe whether dying cells are the result of programmed cell death. Very little TUNEL staining was observed in the developing sulcal region, although some were seen in the associated mesenchymal cells in the cochlea. In some of the sections, Blebbing as well as extrusion of some cells that are thought to be undergoing programmed cell death were evident during the formation of the sulcus. The formation of the sulcus occurs earlier in the basal region of the cochlea than in the apical part following the regression of the greater epithelial ridge (GER) cells. Counting of nuclei in the sulcal region during the formation suggest that cells are being lost. It is not easy to establish whether these cells that are being removed could be due to apoptosis or another type of programmed cell death.

BIOGRAPHY

Tarfa M Peter has completed his MSc. from University of Maiduguri, Borno State, Nigeria. He is the Histology lecturer, in the Department Human Anatomy, Gombe State University. He has published more than 10 papers in reputed journals and is presently undergoing his Ph. D in Ahmadu Bello University Zaria.

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HIGH THROUGHPUT PROTEOMIC ANALYSIS USING DIFFERENT OFFGEL FRACTIONATION PANELS

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⁴Niigata University, Japan

OFFGEL fractionation of mouse kidney protein lysate and its tryptic peptide digest has been examined in this study for better understanding the differences between protein and peptide fractionation methods and attaining maximum recruitment of this modern methodology for in-depth proteomic analysis. With the same initial protein/peptide load for both fractionation methods, protein OFFGEL fractionation showed a preponderance in terms of protein identification, fractionation efficiency, and focusing resolution, while peptide OFFGEL was better in recovery, number of peptide matches, and protein coverage. This result suggests that the protein fractionation method is more suitable for shotgun analysis while peptide fractionation suits well quantitative peptide analysis [isobaric tags for relative and absolute quantitation (iTRAQ) or tandem mass tags (TMT)]. Taken together, utilization of the advantages of both fractionation approaches could be attained by coupling both methods to be applied on complex biological tissue. A typical result is shown in this article by identification of 8262 confident proteins of whole mouse kidney under stringent condition. We therefore consider OFFGEL fractionation as an effective and efficient addition to both label-free and quantitative label proteomics workflow.

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JOURNEY OF MASS SPECTROMETRY

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From decades spectrometry has been accepted as a key analytical tool for understanding and characterization of molecules in chemistry, the level of world-wide research activity in this field promises that these capabilities will continue to improve, rapidly. Over the period of time sensitivity of spectroscopy tools have been improved to work at micro level and in more depth, ultimately become a faster research tool; such tools now being used as process analytical tools (PAT) giving online understanding of characteristics of a molecule during research/development and in production. Same time their utilization has widen up by coupling these tools with liquid chromatography, and thermal measurement tools e.g. (LC-MS-MS, LC-NMR, DSC-FTIR.....etc.). Mass spectroscopy has achieved horizons from single quadrupole to triple quadrupole, MS-TOF & the Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) these have become a powerful and widespread analytical tool in life science and health sector. The dynamic mass range (1-300 kDa), high accuracy and sensitivity make it a superior method for analysis of all kinds of biomolecules including proteins, nucleic acids, metabolites and carbohydrates. Particularly in drug discovery, where compound identification and purity from synthesis and early pharmacokinetics are determined, MS has proved indispensable outcomes. Today, the MS practitioner can choose among a range of ionization techniques which have become robust and trustworthy on a variety of instruments with demonstrated capabilities. In combination with 2D-electrophoresis, MALDI-TOF-MS is particularly suitable for the identification of protein spots via mass fingerprint or micro sequencing. Same time MS-TOF is widely used in pharmaceutical word, TOF has improved the sensitivity by increasing the path length in TOF tube, so ion remain in path of light for longer time increasing sensitivity, on other side measurement tolls has been improved to see the mass number in several digits can differentiate molecules having closure mass and differentiating isotopes. Software calculates elemental formula, for which confirmation performed by comparing theoretical fragments to the obtained TOF-MS/MS of molecule. In this review I had evaluated and focused on advancement and updates in MS field, with respect to technology update & applications.

BIOGRAPHY

Lokesh Kumar Gupta has completed his PhD at the age of 25 years by researching in University of Delhi and Ch. CS University Meerut, India. He is an analytical research scientist and serving as Chief Manager of Analytical R&D team with TEVA India (a world leader in generic pharmaceuticals). Focusing on pharmaceutical-research, cGMP compliance aspects and conducting technical trainings to pharmaceutical scientists. He is participating and discussing his commended research in several national/international seminars/conferences. Apart from several awards and recognitions, Dr. Gupta had published 45 research articles in peer reviewed reputed journals of chemistry & spectroscopy and serving as an eminent referee for several journal of international repute.

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