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POSTERS

CURRENT STATUS OF TRIGLYCERIDE STANDARDIZATION IN KOREA, AN EXPERIENCE FROM NATIONAL LIPID STANDARDIZATION PROGRAM FROM 2016 TO 2017

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Accurate and precise measurements of triglycerides (TG) are crucial in cardiovascular disease risk management. We examined standardized data to clarify the performance of routine TG methods in Korea through National Lipid Standardization Program from 2016 to 2017. Three samples were sent to the laboratory for each cycle, twice a year. The participating laboratories were required to repeat the sample measurements three times a day for two days. Total glycerides were measured in Korean Centers for Disease Control (CDC) by isotope dilution mass spectrometry, a method designed by CDC in the United States. The target values of triglyceride were determined by subtracting the free glycerol value measured by ReCCS (Reference Material Institute for Clinical Chemistry Standards) in Japan. We calculated the total coefficient of variance (CV), the percent bias, and the total error for each sample. Two routine methods were largely used by laboratories; The one is enzymatic method without glycerol blanking (nonblanking group) and the other is the with glycerol blanking (blanking group). The mean values of blanking group were consistently lower than those of nonblanking group. Regardless of the method of measurement, the imprecisions of most laboratories showed less than 2%, which qualified to the NCEP (National Cholesterol Education Program) criteria. However, in relation to bias, in about 1/4 of the laboratories, the bias was found to exceed the 5% NCEP criteria and appeared to be more prominent in the group using specific reagents. There was no significant difference between the two groups in terms of accuracy, but negative bias was more pronounced in nonblanking group than in blanking group. Because of outperformed precision, few laboratories had total error greater than 15%. In conclusion, the precision of triglycerides was found to be satisfactory in most laboratories in Korea but the accuracy still needs improvements.

BIOGRAPHY

Gye Cheol Kwon has completed his PhD in 1993 from Chungnam National University, South Korea. Currently he is the director/professor of Chugnam National University Hospital, vice president of Korean External Quality Assessment Scheme and will be the chairman of the Korean Society for Laboratory Medicine from 2019. His research interest is in mass spectrometry, triglyceride and pre-analytical issues in the laboratory.

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DRIED URINE SWABS AS A TOOL FOR MONITORING METABOLITE EXCRETION BY UPLC–MSMS

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We tested a large set (n=181) of dried urine samples spotted on regular cosmetic cotton swabs for quantitative UPLC–MSMS analysis of various metabolites. The agreement of measurements between conventional 24h urines and dried urine spots made from them in situ was evaluated by Passing–Bablok regression and Bland–Altman analysis after creatinine correction. There was full agreement in qualitative results making dried urine spots a simple method for urine sample collection, suitable for metabolomics profiling and for screening of compliance in clinical trials. The dried urine samples were stable for at least 9 months. This allows samples to be stored at room temperature and analysed later, thereby making logistics much easier in human studies. Quantitative analysis exposed certain limitations of dried urine spots. Results were underestimated in the range from 11–23% in case of tartaric acid, indoxyl sulfate, pyroglutamyl proline and DHEAS. However, full agreement was found in case of the alcohol intake related metabolites, ethyl sulfate and ethyl glucuronide. Partial overestimation ranging from 10–20% was observed in case of cresol sulfate. As a secondary objective, we examined variance of individual total daily creatinine excretion, which was found to be maximally 16%. This finding suggests that the individual creatinine correction factor calculated as an average individual value factor could be used in long–term clinical trials for correction of measurements in dried urine spots, provided that muscle mass is unchanged and the level of analytical offset is acceptable for the research purpose.

BIOGRAPHY

Rastislav Monošík has been a post–doc at the University of Copenhagen since 2015. He received his master's degree in food engineering and PhD in food biosensors from Slovak University of Technology. He was awarded FAPESP fellowship in 2013 to work at the University of São Paulo on microfluidic devices. His current focus as Marie–Curie fellow is on developing an objective tool for assessment of recent dietary intakes using multiplex UPLC–MSMS analysis of validated food intake biomarkers and improving the tool by a novel sampling technique (dried urine spots) and addition of promising food biomarkers following their validation.

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NATURALLY OCCURRING EXUDATES GUMS AS ECOFRIENDLY INHIBITORS FOR MILD STEEL CORROSION IN ACIDIC MEDIUM

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The corrosion inhibition potentials of gum exudates from *Daniella oliveri* (DO) and *Commiphora africana* (CA) for the corrosion of mild steel in H_2SO_4 have been studied using weight loss and thermometric methods at 303 and 333K. Results show that the exudates gums actually reduced the rates of corrosion of mild steel. Increase in the concentrations of the exudates gums increased their percentage inhibition efficiencies. Corrosion rate was found to increase with increase in temperature in the presence and absence of the gum exudates, though the corrosion rate was slower in the presence of the exudates gums. Both DO and CA exudates gums were found to obey Temkin and Langmuir adsorption models at all concentrations and temperatures studied. Physical adsorption mechanism was proposed from the adsorption parameters. Kinetic and thermodynamic parameters revealed that the adsorption process is spontaneous, exothermic and no significant difference was found between the inhibition efficiencies of DO and CA.

BIOGRAPHY

Onukwube N Dickson has completed his MSc. from Michael Okpara University of Agriculture, Umudike and also currently undertaking a Doctoral Degree program from the same University. He is a staff of Abia State Polytechnic, Aba, where he has held so many posts including;- Member, Abia State Polytechnic Think Tank committee, Member Local Organizing Committee (LOC) of the Quarter 3 National Executive Council (NEC) meeting of Academic Staff Union of Polytechnics (ASUP), Examination Officer, Chemistry Department . He has published many papers in reputable journals.

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ANALYTICAL CHARACTERISTICS OF NANO-ELECTROSPRAY OPERATED UNDER SUPER-ATMOSPHERIC PRESSURE

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High-pressure nanoelectrospray ionization (nanoESI) source is a recently developed technique in which the electrospray ionization is generated inside an enclosed chamber with gas pressure higher than the atmospheric pressure. In this paper, the performance of nanoESI under different gas pressures, emitter position, ion inlet temperature, additive for desalination are presented. Under a pressure of 2 bars, the nanoESI is almost eased from the electrical discharge problem, and that offers a wider tuning window for the emitter potential to produces a higher and more stable ion signal. With optimized ion inlet temperature, the high-pressure operation facilitates the generation of ion species of higher charge-state from the highly aqueous solution, and produced less sodium adducts. A preparation method for the high-throughput analysis of raw biological samples using disposable plastic nanoESI emitter could be described.
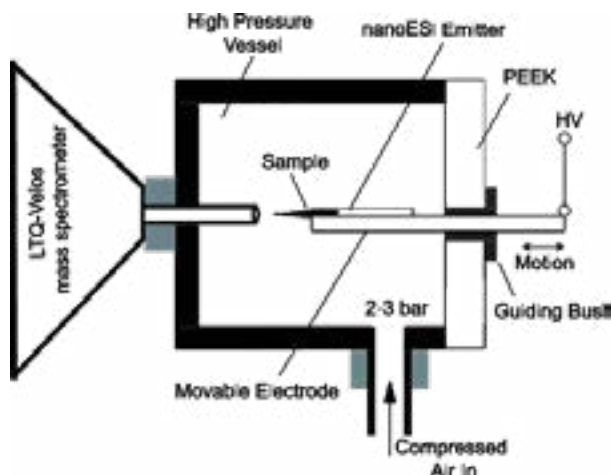
High pressure nESI ion source

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ACCEPTED ABSTRACTS

TWO ARE BETTER THAN ONE: WHY TO CONSIDER ESI AND MALDI

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For mass spectrometry-based proteomic analyses, matrix-assisted laser desorption/ionization (MALDI) and electrospray ionization (ESI) are the commonly used ionization techniques. Investigations performed on very large datasets with more than 72000 peptides showed the complementary character of the two methods not only regarding the identified peptides but also with respect to their amino acid composition, hydrophobicity, charge-related parameters and post-translational modifications. Focusing on phosphopeptides enriched by Fe-IMAC chromatography, considerable orthogonality between the two analytical workflows were identified. For instance, laser-based ionization allowed for the identification of an unexpectedly high number and percentage of phosphotyrosine sites. Furthermore, MALDI-TOF MS/MS clearly favored the identification of motif signatures for acidic residue directed kinases. In summary, the investigation of large-scale datasets using both LC-ESI-MS and off-line LC coupled to MALDI-MS allows for the generation of a complete dataset of peptides and post-translational modifications.

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FAST ANALYSIS BY AMBIENT MASS SPECTROMETRY COUPLED DIRECTLY TO MICROEXTRACTION

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The determination of trace residues and contaminants in complicated matrix often requires extensive sample preparation prior to instrumental analysis. Usually, sample preparation is the bottleneck in a whole analytical procedure, and minimized preparation steps are highly desired to reduce both time and sources of error. On the other hand, most analytical methods rely on the separation by liquid chromatography (LC) or gas chromatography (GC), which make the entire method complicated and time-consuming. Ambient mass spectrometry (AMS), in which the ionization takes place in open air under ambient conditions, is frequently used for the rapid determination or screening of analytes without the need of chromatography separation in some cases. In this presentation, we report our research to combine effective microextraction with AMS for high throughput analysis of targeted compounds in complex samples, including rapid screening for synthetic antidiabetic drug adulteration in herbal dietary supplements, rapid analysis of multiple phytohormones in fruit juice, fast analysis of triazine herbicides in environmental samples and four Sudan dyes in food samples.

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FACTORIAL DESIGN FOR METHOD DEVELOPMENT AIMING AT THE DETERMINATION OF CD AND PB IN CARROT AS ACIDIC SLURRY BY GF AAS FOR COMPLIANCE WITH INTERNATIONAL FOOD LEGISLATIONS

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Determining inorganic contaminants in vegetables by atomic spectrometry techniques remains as an analytical challenge. Considering Pb determination in vegetables by GF AAS, for instance, a severe sensitivity barrier is found when microwave oven (MW) is employed for sample digestion because of the sample mass restriction, which makes the analysis impracticable when intending compliance with international food regulations. Beyond the mass limitation, such classical approaches for sample digestion (block digester included) mandate employment of large volumes of acids, which are not environmentally friendly and are highly destructive to the spectrometers' parts, like graphite tube in GF AAS, which will them force large digest's dilution, leading to incompatibility with the low levels allowed for such compounds in international food legislations. Furthermore, an analytical method for official control of elements must be as simple as possible, reliable, present high sample throughput and a limit of quantification less than one fifth of the maximum level for the element, according to EC. The objective of this work was to develop a method for cadmium and lead determination in carrot by GF AAS aiming at compliance with international food regulations. Acidic slurry approach was investigated for Cd and Pb determination in dried carrots by GF AAS. A 2^2 factorial design was employed (for factors sample mass and HNO_3 volume), which provided recoveries of about 80% for both analytes for most of the combinations. The optimum experimental conditions for acidic slurry, compromising Cd and Pb responses following Pareto charts evaluation, were 200 mg of dried carrot plus 1 ml of HNO3, submitted to 2 hours of ultrasound bath, and sample final volume of 5 ml. Acidic slurries of carrots has showed simplicity and high efficiency, without the need of a complex sample preparation procedure or instrumentation.

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ABUSE DRUGS BY GAS CHROMATOGRAPHY MASS SPECTRUM

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Background: Drugs of abuse are any drug or substance which if taken by any route (oral-snuffing-injection) will lead to mood change, psychological disturbance and can affect brain functions and level of perception. The aim of this work is to evaluate the usefulness of using urine immunoassay kits for detection of some drugs of abuse, and study the correlation between the results obtained by EMIT and GC / MS techniques.

Materials & Methods: Drug toxicology tests are most commonly performed on urine, since most drugs and their breakdown products are excreted in the urine at higher concentration. A total number of 449 inhabitant urine samples were collected from patients admitted to emergency hospital, Mansoura University. 449 urine samples were analyzed by EMIT and GC / MS for benzodiazepine, barbiturate, opiate and cannabinoid.

Results: Revealed that urine immunoassay kit is useful for rapid preliminary screening of abuse drug. GC / MS results confirm that 245 samples (54.56 %) are positive of the total number of samples. These positive samples by GC / MS were as follows; benzodiazepines; 159 ((clonazepam, oxazepam, temazepam), barbiturates; 58 (thiobarbiturate, butabarbital, seconal) and opiates; 28 (methadone metabolite)).

Conclusions & Recommendations: GC / MS analysis must be done for accurate identification and confirmation of EMIT results. In addition, it is recommended as the most suitable technique for obtaining optimum analytical results.

Keywords; Urine samples, EMIT, GC/MS.

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MASS SPECTROMETRY AND PROTEOMICS APPLICATIONS

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Mass spectrometry (MS) is widely recognized as a powerful analytical tool for molecular research. MS is used by researchers around the globe to identify, quantify, and characterize biomolecules like proteins from any number of biological conditions or sample types. As instrumentation has advanced, and with the coupling of liquid chromatography (LC) for high throughput LC MS/MS, a proteomics experiment measuring hundreds to thousands of proteins/protein groups is now commonplace. While expert practitioners who best understand the operation of LC MS systems tend to have strong backgrounds in physics and engineering, consumers of proteomics data and technology are not exposed to the physio chemical principles underlying the information they seek. Since articles and reviews tend not to focus on bridging this divide, our goal here is to span this gap and translate MS ion physics into language intuitive to the general reader active in basic or applied biomedical research. Here, we visually describe what happens to ions as they enter and move around inside a mass spectrometer. We describe basic MS principles, including electric current, ion optics, ion traps, quadrupole mass filters, and Orbitrap FT analyzers.

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APPLICATION OF TWO DIMENSIONAL HIGH PERFORMANCE LIQUID CHROMATOGRAPHY–MASS SPECTROMETRY ON TESTING VITAMIN D

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The use of a particle beam interface (PBI) in LC–MS has faded because of its poor resolution and low sensitivity for many compounds. It also does not perform well in reversed-phase systems with a high percentage of water. This manuscript describes two-dimensional LC to overcome the problems of PBI, both in the identification of unknown samples and in the quantitative determination of metabolites of vitamin D in human plasma. For the identification of unknown components, the reversed-phase solvent in the first dimension was transferred to an isocratic normal solvent system in second dimension by column switching. Moreover, only the peaks of interest (components) in the first dimension were transferred into the second LC column for mass analysis. For the quantitative determination of the metabolite of vitamin D, the peak width of analyte in the second dimension was greatly narrowed, and interference was excluded such that high sensitivity and resolution resulted. The limit of quantification for the test metabolite of vitamin D in human plasma can reach 0.050 ng/ml with injection volume of 50 ml. A new instrumentation, Absiex LC-MS-MS is going to be employed in the new study of Vitamin D test.

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POTENTIAL USE OF BIOMARKERS IN CLINICAL PRACTICE: ALPHA DEFENSIN AND SYNOVIAL FLUID

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Alpha defensin in synovial regards potential biomarker for identification of periprosthetic joints infections (PJI). The only commercially available test is an in situ immunocromatographic device. Orthopedics use the device under their direct responsibility, either as part of pre surgery patient assessment or, intra operatively, to make treatment decisions according to the likelihood of infection. In this diagnostic path flow, the availability of a method not prone to interferences, with high sensitivity and specificity, can be of great help to clinicians. LC-MS methods are considered to meet needs in terms of analytical performance and are widely used to measure new biomarkers. The aim of our study was to implement a methods to accurately measure Alpha defensin in synovial fluids. Several issues had to be addressed: the synovial fluid matrix viscosity, the need of a standard Alpha defensin peptide and a valid Internal Standard (IS), the definition of analytical protocol and, finally, the method validation. As preliminary step the uniqueness of peptides derived from trypsin digestion of Alpha defensin was checked by liquid chromatography - time of flight mass spectrometry. Synovial fluids samples from primary knee arthroplasty were used as negative matrix; a synthetic matrix (simulant) was produced and measures of spiked samples were run in parallel. The quantitative analysis was performed with two different instruments (liquid chromatography with time of flight or triple quadrupole mass spectrometry, LC-QTOF or LC-MS/MS) and two different methods (negative matrix spike and simulant synovial fluid spike) by spike of different concentrations of synthetic marker peptide. The quantitative method was developed with dynamic range from 0.1 to 100 µg/ml.

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A BAYESIAN SOLUTION TO JOINTLY REMOVE THE BASELINE AND INCREASE THE RESOLUTION OF MASS SPECTROMETRY DATA

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There have been recent advances in different Mass spectrometry technics: Time-of-Flight (TOF), Matrix Assisted Laser Desorption/Ionization (MALDI), Orbitraps, Quadrupoles, Ion traps, Gas chromatography-mass spectrometry (GCIMS), Fourier Transform Ion Cyclotron Resonance (FT- ICR), etc. Each technic has his advantages and drawbacks. There is no all purpose perfect system. Data, signals and images coming out of these systems have many limitations: baseline, drift, noise, low resolution, limited dynamics, etc. We can always improve these data by further processing (post-processing) if we can model these imperfections either in deterministic or probabilistic ways. The main tools are inverse problems and the Bayesian inference frameworks. In this tutorial presentation, through the deconvolution example, first the basics of the Bayesian inference are presented. Then, a hierarchical prior model and a data generative model are assembled to handle both the background elimination and the resolution improvement. A few simulation examples show the difficulties and the improvements we can obtain.

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DIAGNOSTIC ACCURACY OF CANNABINOID TESTING BY LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY IN HUMAN HAIR

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Objective: To determine the diagnostic accuracy of Cannabinoids testing by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS) in human hair and to compare it with urine for detection of cannabis use in civil heavy vehicle drivers

Materials and Methods: This diagnostic accuracy(validation) study was carried out at Department of Forensic Medical Sciences Laboratory (FMSL), Forensic Toxicology Section, Armed Forces Institute of Pathology Rawalpindi, Pakistan. Hair and urine samples of about 151 civil heavy vehicle drivers were collected from various urban and rural areas of Punjab.

Result: Sampling technique was non-probability convenient. About 10 ml of urine volume was collected and stored at -20 °C. Hair strands, about the thickness of a pencil shaft, were collected from the posterior vertex of scalp.It was cut as close to the root as possible, and kept at room temperature till further analysis Separation of compounds was done on Agilent Poroshell 120 EC-C18 column (2.1 x 7.5mm.7 micron) and analyzed on a 6460 Triple Quadrapole LC-MS along with software Mass hunter ©. Results: Al the 151-male civil heavy vehicle drivers, who were included in the study, were categorized into three main groups. There were 69(71.5%) truck drivers,43(28.5 %) were 20-wheeler drivers, whereas bus drivers were 39(25. 8%).Mean age was 36±10.82 years. Subjects were stratified according to the age into four main groups: 20-25 y: 28(18.5%); 26-40 y: 73(48.3%), 41-60 y:47(31.1%) and >60 y:3(2%).

Conclusion: This study highlights the importance of hair as an alternative biological matrix due to its good diagnostic yield, easy non -invasive specimen collection and distinctive potential of analyte stability, as well as wider period of detection as compared to urine.

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QUADRUPLED ION TRAPS WITH SPHERICAL AND GEOMETRIES OPTIMIZATION

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Quadrupole ion traps with spherical as well as cylindrical geometries are designed and analyzed. For this purpose, an optimization is carried out in order to suppress the contribution of the electric octupole moment in the potentials inside the traps. As a validation, three stability regions computed for these optimized geometries are compared with those obtained for a quadrupole Paul trap, and excellent agreements are found. The spherical and cylindrical traps have some advantages in comparison with the hyperbolic Paul trap.

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