Coalesce Research Group

International Webinar on

MASS SPECTROMETRY & ANALYTICAL TECHNIQUES

August 05-06, 2021 | 11:00-18:00 (British Time)

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Scientific Program

International Webinar on

Mass Spectrometry & Analytical Techniques

Thursday
August 05, 2021

Day 1 - August 05, 2021 - British Summer Time (BST)	
11:00 - 11:10	Introduction
Oral Presentations	
11:10 - 11:35	A new, simple, efficient and robust multi-residue method based on pressurized-liquid extraction of agricultural soils to analyze pesticides by liquid chromatography coupled with a high-resolution quadrupole time-of-flight mass spectrometer **Giovanni Caria,** INRAE - LAS, France
11:35 - 12:00	Determination of 87Sr/86Sr isotopic ratio in olive oil by means of Multicollector-ICP MS **Emna Nasr,** IPREM and INRAP, France
12:00 - 12:25	Hyphenation of planar chromatography with mass spectrometry to identify bioactive saponins in complex plant extract **K. Nafti,** University of Toulouse and University of Tunis EL MANAR, Tunisia
12:25 - 12:50	Analysis of selected mycotoxins in maize from North-West, South Africa, using High performance liquid chromatography (HPLC) and other analytical techniques. **Theodora Ekwomadu,** Northwest University, South Africa
Lunch (12:50 - 13:30)	
Oral Presentations	
13:30 - 13:55	Accelerator mass spectrometry:state of the art and the fields of application **Doru Pacesila,** IFIN-HH, Romania
13:55 - 14:20	Quantification of benzothiazoles, benzotriazoles and benzosulfonamides in airborne particulate matter coupling microwave-assisted extraction with solid-phase microextraction gas chromatography tandem-mass spectrometry **Attilio Naccarato,** CNR-Institute of Atmospheric Pollution Research, Division of Rende, Italy
14:20 - 14:45	Investigation on Co(II), Cu(II), Mn(II), Ni(II) and Zn(II) azodye complexes derived 4[(E)-(4 Chlorophenyl) diazenyl]-3-methyl-1-phenyl-1H pyrazol-5-ol:Spectral Characterization and Electrochemical Determination of Dopamine and their Biological Applications **Malathesh Pari,** Kuvempu University, India
14:45 - 15:10	Chemical Reactors with Exothermic Reactions on the Plug Flow and Study it by New Approach Strategy ASM **M.R.Akbari,** University of Tehran, Iran
15:10 - 15:35	Tandem mass spectrometry approaches to know enzymatic enzyme activity **Manoj Kumawat,** ICMR-NIREH Bhopal, India
15:35 - 16:00	Mechanisms of manifestations of drought effect in plants revealed through proteomics studies **Vijay Kumar Dalal,** Deemed University, India
16:00 - 16:25	How electrospray tandem mass spectrometry (ESI-MS/MS) changed the fate of fecal steroid metabolites measurement in free-ranging Taiwanese pangolin (Manis pentadactyla pentadactyla) **Bharti Arora,** Wildlife Biology Researcher, India
Video Presentation	
16:25 -16:40	Pesticides in intensively agricultural vegetables and fruits in Akkar (Lebanon) **Wissam Sahyoun,** University of Lille, France
End of Day 1 Sessions	

Day-1
Oral Presentations

A NEW, SIMPLE, EFFICIENT AND ROBUST MULTI-RESIDUE METHOD BASED ON PRESSURIZED-LIQUID EXTRACTION OF AGRICULTURAL SOILS TO ANALYZE PESTICIDES BY LIQUID CHROMATOGRAPHY COUPLED WITH A HIGH-RESOLUTION QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETER

Giovanni CARIA
INRAE - LAS, France

Abstract

Background: The latest generation of liquid chromatograph coupled to high-resolution quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) now competes with quadrupole tandem spectrometers (LC-MS-MS) in terms of sensitivity and speed. In addition, it is possible to obtain additional information retrospectively on the organic composition of the analyzed soil. Due to the exponential increase of the storage capacities of computer hard drives and the speed of electronic processing of computer data, it is all the more possible to recover all of the data generated during the analysis of a soil extract.

Objective: The LC-QTOF-MS currently has an essential and primordial advantage; which is the entire transmission of the ions produced in the ionization source towards the mass spectrometer. This original feature opens the way to a probable full exploration of the organic composition of the soils.

Methods: A new method for the analysis of pesticides in agricultural soils by using liquid chromatography coupled with a high-resolution quadrupole time-of-flight mass spectrometer (LC-QTOF-MS) has been developed.

Results: Twenty-four pesticides including herbicides, insecticides or fungicides have been studied. The linearity of the external calibration of the pesticides obtained from levels of concentration ranging from 0.010 to 400 µg/L gives satisfactory results with the correlation coefficients higher than 0.99. The quantification limits of the equipment range from 0.010 to 1.250 µg/L and correspond to the lowest standard in the calibration range for which the residual deviation is less than 60%. An experimental design has been used to optimize the parameters of pressurized-liquid extraction (PLE) of pesticides in soils. The optimized conditions have been found by using methanol as extraction solvent at a temperature of 80°C, a pressure of 150 Bars and 2 extraction cycles of 5 minutes. The mean recoveries of pesticides (Mean) are higher than 72% with a relative standard deviation (RSD) less than 21%. These results demonstrate the good efficiency of PLE for the extraction of pesticides in agricultural soils of different nature. The LC-QTOF-MS is a sensitive, linear and robust instrument for the quantification of pesticides in unpurified soils extracts by external calibration. This analytical tool is not subjected to matrix effects of soil extracts.

Biography

Giovanni CARIA is a research engineer since 1993 from INRAE (French National Institute of research for agriculture, food and environment) responsible for organic pollutants analysis and method development. I prepare my PhD in my laboratory on the method development of organic compounds analysis in agricultural soils using pressurized-liquid extraction and a LC-QTOF-MS apparatus. I participate to international European and French standardization. I have an expertise about method development and validation. I developed the analysis of pesticides, polychlorobiphenyls, polycyclic-aromatic hydrocarbons and Dioxins in soils and obtained an accreditation.

DETERMINATION OF 87SR/86SR ISOTOPIC RATIO IN OLIVE OIL BY MEANS OF MULTICOLLECTOR-ICP MS

Emna Nasr
IPREM and INRAP, France

Abstract

Background: Olive oil is a key component of Mediterranean food diet. It is also largely consumed in the whole world (2,970,000 metric tons have been globally consumed 2019/2020 according to International Olive Council: IOC) and increasingly produced (World production of olive oil from IOC member countries has tripled in the last 60 years). Consequently, olive oil attracts fraudulent practices. It is now one of the most adulterated foods. False declaration of geographical origin is among the most prevalent forms of olive oil fraud and also the most hard to detect. The analysis of isotopes of Strontium isotopes allows foolproof geographic tracing since this isotopic signature initially characterize geological formations. Its determination in olive oil hasn't been largely developed because of the complexity of the matrix.

Objective: Development of reliable analytical method for Strontium separation from olive oil and precise determination of $^{87}Sr/^{86}Sr$ isotopic ratio

Methods: 10 olive oil samples were used for analytical development and NIST SRM 2387 (peanut butter) for method validation and quality control. Ultrasound assisted extraction of olive oil was optimally employed as sample preparation technique prior to Sr isotopic analysis. After Sr column purification, $^{87}Sr/^{86}Sr$ isotopic ratio was measured with high precision using Multicollector-ICP MS.

Results: $^{87}Sr/^{86}Sr$ isotopic ratio was successfully determined in olive oil samples with high precision. Recoveries were calculated at each step of analytical process. Obtained extraction recoveries were higher than 60% and Sr column separation recoveries were greater than 80%. $^{87}Sr/^{86}Sr$ isotopic ratio was measured in NIST 2387 after microwave assisted digestion and ultrasound assisted extraction for comparison and was equal to 0.709093 ± 0.000026 (n=8) and 0.709062 ± 0.000038 (n=6) respectively.

Conclusion: $^{87}Sr/^{86}Sr$ isotopic ratio can be determined with high precision in olive oil. The crucial step is to apply adequate pretreatments for Sr release from organic matrix. This analytical approach can be applied for olive oil geographical authentication studies.

Biography

Emna Nasr is a young scientist. After graduation from the school of engineering INSAT, Tunisia in Industrial Chemistry, she continued her studies as a doctoral student in joint supervision between IPREM/UPPA in France and INRAP/UTM in Tunisia, specializing in analytical chemistry. In order to protect from fraud Tunisian olive oil, recognized for its quality and widely exported, she has chosen to work on the geographical authentication of olive oil. This project is partially funded by the Eiffel Excellence Scholarship (Campus France) and the University of Tunis El Manar and also supported by the European TunTwin project. Likewise, as part of this project, Emna is involved in its coordination and currently occupies the post of Research Engineer at UPPA in parallel with her doctoral studies which will be achieved at the end of 2021.

HYPHENATION OF PLANAR CHROMATOGRAPHY WITH MASS SPECTROMETRY TO IDENTIFY BIOACTIVE SAPONINS IN COMPLEX PLANT EXTRACT

K. Nafti

University of Toulouse and University of Tunis EL MANAR, Tunisia

Abstract

Background: Saponins are widely distributed in the plant kingdom and possess a wide range of pharmacological properties. In recent years, advances in research on Astragalus species have been made due to their saponin content. Medicinal plants are the main source for the preparation and extraction of various modern drugs and pharmaceuticals like saponins.

The complexity of saponin chemistry maybe considered as a gap for many scientists and researchers to understand the relationship between the chemical structure and its medical or pharmaceutical behavior.

Astragalus species contain both cycloartane and oleanane saponins based on soyasapogenol B as the aglycone.

Objective: To isolate and identify saponins of interest in *Astragalus Hamosus*.

Method: To quantitatively recover saponins in *A. hamosus,* preliminary phytochemical screening was done, performing distinct solvent extraction pathways, and HPTLC/UV-vis studies were first carried out, to highlight the presence of saponins in the butanol extracts. A complex elution system based on three successive and progressive polarity solvents mix according to the method of Pedro et al[5] made it possible.

Results: HPTLC separative method performed the purification of each extract and achieve the separation and isolation of the polar saponins at RFs comprised between 0 to 0.4. The non-polar extracted co-analytes are retarded at higher RFs, in particular the triterpenoid aglycones at RF 0,68. To complete the previous results obtained with HPTLC/UV-vis, a direct HPTLC-MS hyphenation was further done to identify the spots of interest.

Conclusion: The results highlighted the presence of AZUKISAPONIN V, at Rf 0,2.

Subsequently, work is underway to understand the relationship between saponin structure and the biological effects such as antibacterial, antioxidant and moreover anti-Alzheimer activity by the Ellman tests. A direct coupling between HPTLC and the Ellman test is study.

Biography

Khouloud NAFTI is enrolled in the 3rd year of a PhD thesis in supramolecular chemistry at University of Toulouse and University of Tunis EL MANAR. She did five years in biology, genetic specialty at the Faculty of Sciences of Tunis. During these years she mastered several molecular genetics techniques such as DNA extraction, PCR, Southern Blot and cloning. These competences in biology are now enriched thanks to her thesis in chemistry where she performs in analytical chemistry area. Indeed, her thesis subject relates to the evaluation of the anti-acethylcholinesterase activity of saponins identified from astragalus hamosus.

ANALYSIS OF SELECTED MYCOTOXINS IN MAIZE FROM NORTH-WEST, SOUTH AFRICA, USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC) AND OTHER ANALYTICAL TECHNIQUES.

Theodora Ekwomadu

Northwest University, South Africa

Abstract

Background: Contamination of foods by mycotoxins has been linked to various health and economic implications to both man and animals

Objectives: To evaluate the incidence of mycotoxins contaminating commercial and small-scale maize in North-west and to evaluate potential health risks for consumers based on South African and international regulations. Also to ascertain the sensitivity/specificity of HPLC over other analytical methods used.

Methods: A total of 100 maize samples were randomly collected from commercial and small-scale farmers across the North-west, South Africa. Mycotoxin analysis was done using Immuno-affinity column for extraction and clean-up, Thin Layer Chromatography (TLC), HPLC and Enzyme Linked Immunosorbent Assay (ELISA) for quantification.

Results: Results obtained revealed that fumonisinB1 was the most contaminant mycotoxin in the small-scale and commercial samples with incident rate of 100% and 98.6% respectively. Aflatoxins (AFs) contamination in samples occurred at incidences of 26.7% in small-scale samples and 25.0% in commercial samples. The levels of AFs were varied between 0.080-9.34 µg/kg and 0.32-8.60 µg/kg in small scale and commercial samples respectively, though still within the EU acceptable limits of 10 µg/kg (Total aflatoxin). Furthermore, ochratoxin A has high incident rate of 97.8% and 93.0% and ranged from 3.60-19.44 µg/kg and 1.60-9.89 µg/kg respectively in small-scale and commercial maize samples while ZEA occurred in 50% and 55% of small-scale and commercial samples respectively.

Conclusion: Results demonstrate that maize especially those from small-scale farmers may contribute to dietary exposure to mycotoxins. Farmers and consumers should be alerted to the dangers of mycotoxins contamination in maize with resultant health risks. Also, HPLC method was more specific for mycotoxin detection than ELISA. The HPLC results were lower than the percentages recorded using the ELISA which confirmed the sensitivity of the HPLC over ELISA. This could be attributed to cross-reactivity with related substances resulting in overestimation in ELISA.

Biography

Theodora Ekwomadu is conducting research under the food security and safety niche area of North-West University, South Africa. Her research focus is on mycotoxins, especially *Fusarium* free and masked mycotoxins in South Africa; risk assessment with regards to food safety and public health.

ACCELERATOR MASS SPECTROMETRY: STATE OF THE ART AND THE FIELDS OF APPLICATION

Doru Pacesila
IFIN-HH, Romania

Abstract

Accelerator Mass Spectrometry (AMS) is a high sensitivity elemental analysis technique that has been imposed over the last 4 decades. Currently, due to its unmatched performance in determining stable or long half-life isotope concentrations and at a very low concentration in nature, AMS technique is used in many applications from various fields. These include: archeology (using 14C, 10Be, 26A, 36Cl, 129I isotopes, biomedical sciences (14C, 26A, 41Ca), astrophysics (14C, 10Be, 36Cl, 41Ca, 129I, 244Pu), geology (10Be, 26A, 36Cl) etc.. In the last years, the interest for applications using actinide series isotopes has increased, for example 231Pa, 236U, 237Np, 239,240Pu. In this presentation I will talk about the importance of this method and its fields of application.

QUANTIFICATION OF BENZOTHIAZOLES, BENZOTRIAZOLES AND BENZOSULFONAMIDES IN AIRBORNE PARTICULATE MATTER COUPLING MICROWAVE-ASSISTED EXTRACTION WITH SOLID-PHASE MICROEXTRACTION GAS CHROMATOGRAPHY TANDEM-MASS SPECTROMETRY.

Attilio Naccarato

CNR-Institute of Atmospheric Pollution Research, Italy

Abstract

Background: Traditional extraction methods are still widely used in official methods of analysis for solid matrices. These approaches are expensive, time-consuming, and environmentally unfriendly. For several years now, major efforts have been made to develop alternative, high-throughput analytical methods for the extraction of pollutants from solids following the basic requirements of Green Analytical Chemistry. Benzothiazoles (BTHs), benzotriazoles (BTRs), and benzenesulfonamides (BSAs) are chemicals used in several industrial and household applications. Despite these compounds are emerging pollutants, there is still a lack of information about their presence in outdoor air samples.

Objective: In this presentation, I am going to present a new eco-friendly method for the quantification of BTHs, BTRs, and BSAs in airborne particulate matter (PM10).

Methods: The extraction of fourteen analytes from PM10 was accomplished by microwave-assisted extraction (MAE) using an environmentally friendly mixture of water and ethanol. Solid-phase microextraction (SPME) was used to analyze the target compounds from the MAE extract by gas chromatography-tandem mass spectrometry (GC-MS/MS). The best working conditions for MAE and SPME were examined multivariately by experimental design techniques. The target compounds were quantified in selected reaction monitoring acquisition mode.

Results: The proposed method was carefully validated, and the achieved results were satisfactory in terms of linearity, lower limit of quantification (picograms per cubic meter), intra- and inter-day accuracy (81–118% and 82–114%, respectively), and precision (repeatability and reproducibility in the range 2.3–17% and 7.4–19%, respectively).

Conclusion: The application in a real monitoring campaign showed that the developed protocol is a valuable and eco-friendly alternative to the methods proposed so far. Each MAE run of 22 min, allows for the preparation of up to 15 samples that can be analyzed directly by SPME without additional clean up or pre-concentration steps, thus achieving an important improvement in sample throughput when compared to the literature findings.

Biography

Attilio Naccarato is a researcher at the Institute of Atmospheric Pollution Research (CNR-IIA) and holds the position of Adjunct Professor at the University of Calabria. He is involved in National and European projects aimed at the monitoring of persistent and emerging pollutants including mercury in the environmental compartments. Besides, his research activity focuses on method development for the analysis of pollutants in environmental, food, and clinical matrices using different analytical strategies such as microextraction approaches, mass spectrometry-based techniques, and multivariate optimization. He also serves as an Associate Editor on the editorial board of Chemical Papers (Springer), Frontiers in Analytical Science, and Separations (MDPI).

INVESTIGATION ON CO(II), CU(II), MN(II), NI(II) AND ZN(II) AZODYE COMPLEXES DERIVED 4[(E)-(4 CHLOROPHENYL) DIAZENYL]-3-METHYL-1-PHENYL-1H PYRAZOL-5-OL: SPECTRAL CHARACTERIZATION AND ELECTROCHEMICAL DETERMINATION OF DOPAMINE AND THEIR BIOLOGICAL APPLICATIONS.

Malathesh Pari

Kuvempu University, India

Abstract

Transition metal complexes of Co(II), Cu(II), Mn(II), Ni(II), and Zn(II) with azodyes of novel heterocyclic pyrazole derived from 3-methyl-1-phenylpyrazole and diazonium salt of chloroaniline have been synthesized and characterized based on elemental analysis, mass, IR, H 1 NMR, magnetic and thermogravimetric studies and cyclicvoltametry. The synthesized Cobalt (II) complex derived from 4[(E)-(4 Chlorophenyl) diazenyl]-3-methyl-1 -phenyl-1H pyrazol-5-ol modified glassycarbon electrode (Co(II) CMPP-GCE) 0.5 µL of this homogenius suspension was coated on glassy carbon electrode (GCE). Compared to both the bare GCE and Co(II)CMPP-GCE, the modified Co(II)CMPP-GCE enahanced the positive peak current (ipa) of dopamine by about five times. Linear plots of the dopamine were constructed using the standard addition method using cyclicvoltammogram (CV) techniques under the aquaitic conditions. While the linear range was determined as 0.5–10.0 µm/L in pH 7.0 PBS the limit of detection (LOD) and sensitivity and linear reggrision eqeation is 0.166 µmol/L and 0.624 µAµM-1 , Y = 0.624x+0.3609 respectively. Subsequently, CV studies were carried out to elucidate the electrochemical behavior and electrode mechanism of the DA. Finally, using modified Co(II)CMPP-GCE, the developed CV method was applied with low relative error for recovery of DA in dopamine hydrochloride solution. The ligand and its complexes have been screened for their antimicrobial activity against different bacterial and fungal strains. Along with this antioxidant studies has also been evaluated where it was found that metal complexes were more active than the ligand.

CHEMICAL REACTORS WITH EXOTHERMIC REACTIONS ON THE PLUG FLOW AND STUDY IT BY NEW APPROACH STRATEGY ASM.

M.R.Akbari
University of Tehran, Iran

Abstract

In this paper, our aims are accuracy, capabilities and power at solving set of the complex non-linear differential at the reaction chemical. As all experts know most of engineering actual systems behavior in practical are nonlinear process and analytical scrutiny these nonlinear problems are difficult or sometimes impossible.

Our purpose is to enhance the ability of solving the mentioned nonlinear differential equations at chemical engineering and similar issues with a simple and innovative approach which entitled ''Akbari-Sara's Method'' or ''ASM''.

Introduction and theatrical formulation

In this literature, we have set nonlinear differential equations governing of kinetic the plug reactor to chemical reaction that can be investigated and resolved response and the actual reactions at reactors for scientists and engineers is very important, because they know the real answer for analysis and design of reactors against chemical reactions are important and highly sensitive in of executive tasks are created. Other methods compared to ASM do not have this ability to gain the solution of the presented problem in high precision and accuracy so nonlinear differential equations such as the presented problem in this case study should be solved by utilizing new approaches like AGM, Akbari Ganji Method. In recent years, analytical methods in solving nonlinear differential equations have been presented and created by Mohammadreza Akbari, these methods are called *AKLM* (Akbari Kalantri Leila Method in August 2020) , *ASM* (Akbari Sara's Method in August 2019) and *AYM* (Akbari Yasna's Method in April 2020) , *MR.AM* (MohammadReza Akbari Method in November 2020) and *IAM* (Integral Akbari Method in November February 2021). .

Describe problem and mathematical Formulation

We consider a well-mixed continuous stirred tank reactor fig (1) with the reaction and set of nonlinear differential equations. Parameters F (the flow rate), c_0 (the initial molar concentration) , T_0(the initial temperature),Q (the rate of heat input to the reactor), V(the volume of the reactor), E, ΔH, k_0 (the pre-exponential constant reaction), c_p and ρ denote the heat capacity and density of the fluid in the reactor.

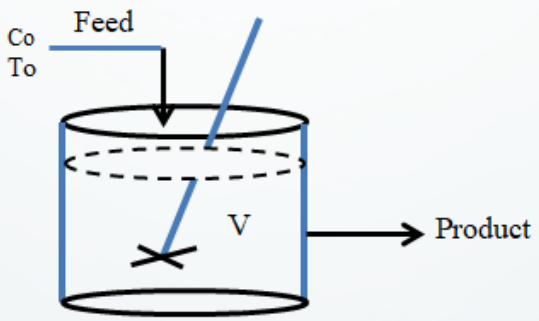

Fig.1. The schematic diagram of the physical model.

$$A \rightarrow B \quad , \quad r_A = ko \exp\left(-\frac{E}{RT}\right) c_A \quad ; \quad IC: \; c(0) = co \quad , \quad T(0) = To$$

Set of nonlinear differential equations as follows:

$$V \frac{\mathrm{d}}{\mathrm{d}t} C_A(t) = F\left[C_{A0} - C_A(t)\right] - ko\, Exp\left(-\frac{E}{R\,T(t)}\right) V C_A(t)$$

$$V \frac{\mathrm{d}}{\mathrm{d}t} T_A(t) = F\left[T_{A0} - T_A(t)\right] + ko\left(\frac{-\Delta H}{\rho\, cp}\right) Exp\left(-\frac{E}{R\,T(t)}\right) V C_A(t) + \frac{Q}{\rho\, cp}$$

The solution of the mentioned problem by ASM will be obtained as follows:

$$c(t) := \frac{\Gamma}{\psi} - \frac{To^2 \Delta^2}{\psi} Exp\left(\frac{-\psi\, t}{\Delta\, To^2}\right) \quad ; \quad T(t) := \frac{\Gamma 1}{\psi 1} - \frac{\Delta 1^2\, To^2}{\psi 1} Exp\left(-\frac{\psi 1\, t}{\Delta 1\, To^2}\right)$$

The following new variables are introduced as:

$$\psi = To^2\, co\, \eta\, ko\, e^{-\frac{2\varepsilon}{To}} - co^2 \eta^2 \varepsilon\, e^{-\frac{2\varepsilon}{To}} + 2\, To^2 \beta\, co\, \eta\, e^{-\frac{\varepsilon}{To}} + To\, \beta\, co\, \eta\, \varepsilon\, e^{-\frac{\varepsilon}{To}}$$

$$- To^2\, \alpha 1\, \eta\, e^{-\frac{\varepsilon}{To}} - \alpha 2\, co\, \eta\, \varepsilon\, e^{-\frac{\varepsilon}{To}} - To^3 \beta^2 + To^2\, \alpha 2\, \beta$$

$$\psi 1 = -To^2\, co\, ko^2 e^{-\frac{2\varepsilon}{To}} + co^2\, \eta\, ko\, \varepsilon\, e^{-\frac{2\varepsilon}{To}} - 2\, To^2\, \beta\, co\, ko\, e^{-\frac{\varepsilon}{To}} - To\, \beta\, co\, ko\, \varepsilon\, e^{-\frac{\varepsilon}{To}}$$

$$+ To^2\, \alpha 1\, ko\, e^{-\frac{\varepsilon}{To}} + \alpha 2\, co\, ko\, \varepsilon\, e^{-\frac{\varepsilon}{To}} - To^2 \beta^2\, co + To^2\, \alpha 1\, \beta$$

$$\Gamma 1 = co^3\, \eta\, ko\, \varepsilon\, e^{-\frac{2\varepsilon}{To}} - To\, \beta\, co^2\, ko\, \varepsilon\, e^{-\frac{\varepsilon}{To}} - To^2\, \alpha 1\, co\, ko\, e^{-\frac{\varepsilon}{To}} + \alpha 2\, co^2\, ko\, \varepsilon\, e^{-\frac{\varepsilon}{To}}$$

$$- To^2\, \alpha 1\, \beta\, co + To^2\, \alpha 1^2 \quad ; \quad \Delta 1 = ko\, co\, e^{-\frac{\varepsilon}{To}} + \beta\, co - \alpha 1$$

By selecting the physical values at below:

$$V := 20\,(L); R := 8.314\,\frac{J}{mol.K}; co := 0.6\frac{mol}{L}; To := 310\,K; \Delta H := -4.78 \cdot 10^4 \frac{J}{mol}; ko := 7.20$$

$$\cdot 10^{-2} \min^{-1}; E := 83.1\frac{J}{mol}; cp := 0.539\,\frac{J}{g.K}; \rho := 1000\frac{g}{L}; F := 2\frac{L}{\min}; Q := 100\frac{L}{\min}$$

The solution is rewritten as follows:

$$c(t) := 332.7146555 - 22.71465617\, e^{-0.1745968863\, t}$$

$$T(t) := 0.3447209382 + 0.2552790620\, e^{-0.1747717806\, t}$$

Comparing the achieved solutions by Numerical Method and ASM (Akbari Sara's Method)

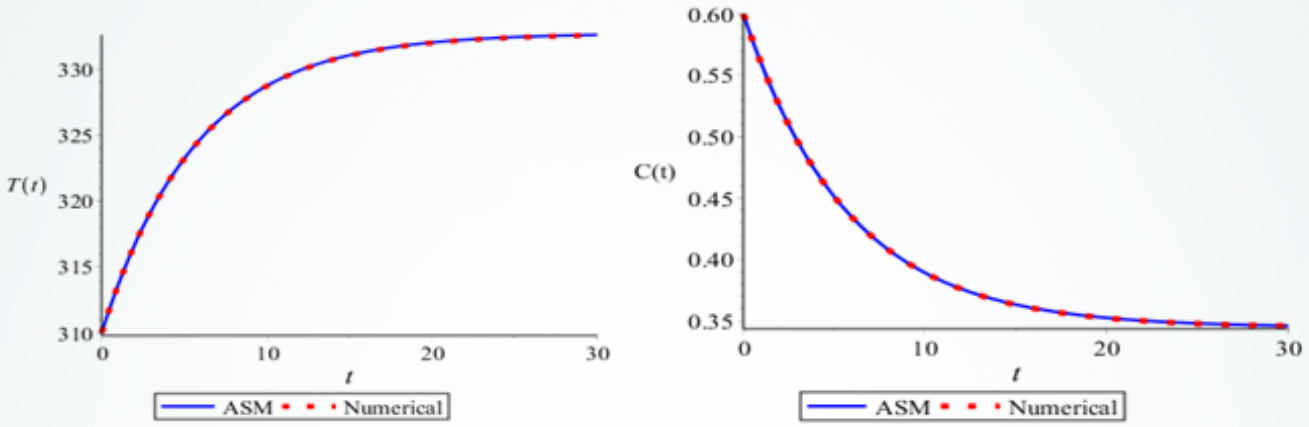

Fig2. A comparison between ASM and Numerical solution for concentration and temperature.

Conclusion: In this article, we introduce a innovation method (by M.R.Akbar) in the field of engineering and basic sciences for analytical solution of nonlinear differential equations in the Exothermic Chemical Reactor on the plug flow and so due to the chemical reaction for the concentration as well as the heat generated, we are encountered one complicated set of nonlinear differential equations have been introduced in chemical reaction for plug flow and analyzed completely by Akbari-Sara's Method (*ASM*), and also the obtained results have been compared with Numerical Method(Runge-Kutte 4^{th}).A modern method (ASM) for solving all kinds of complicate nonlinear differential equations in the engineer field and basic science which can be PDEs and ODEs has been presented. This methods are newly created and they can have high power in analytical solution of all kinds of industrial and practical problems in engineering fields and basic sciences for complicated nonlinear differential equations.

TANDEM MASS SPECTROMETRY APPROACHES TO KNOW ENZYMATIC ENZYME ACTIVITY.

Manoj Kumawat
ICMR-NIREH Bhopal, India

Abstract

Background: Mass Spectrometry (MS) technology is advancing at a rapid pace, mass resolution, and sensitivity, as well as improved ion separation, detection and dissociation technologies. The powerful mass-spectrometry-based technologies now offer unprecedented insights into the composition, structure, function and control of the proteome, shedding light on complex biological processes and phenotypes.

Objective: We described current MS approaches in protein characterization, including a bottomup method for protein identification and quantitative proteomics

Methods: We used Thermo LTQ Orbitrap XL mass spectrometer in our present study. Bottomup method is a widely followed proteomic approach, wherein proteins are investigated through proteolytic peptides. Lysozyme protein was subjected to proteolysis by trypsin, and then the resulting tryptic peptides are subjected to liquid chromatography coupled to mass spectrometric characterization (LC-MS).

Results: We detected tryptic two peptides SSGTSYPDVLK (m/z 1153.58) and SGIQVR (m/z 659.39) results from auto-proteolysis of trypsin. The sequences of these two peptides were confirmed by LC-ESI-MS/MS spectra.

Conclusion: This data suggests a good example of enzymatic mis-cleavage.

Biography

My background includes six years of professional research experience; including My current role as an Post-Doctoral Fellowship by ICMR fund project "Identification of novel drug-resistant genes in multi-drug resistant (MDR) from clinical isolated Salmonella Typhimurium by random mutagenesis." under the supervision of Dr Manoj Kumar at National Institute for Research in Environmental Health, Bhopal. I am also member of technical specification team (HRMS, IPMS, and GCMS/MS etc.). Also handle the LC- MS/MS, GC-MS and IP-OES instruments at central instrumental facility at ICMR-NIREH Bhopal.

MECHANISMS OF MANIFESTATIONS OF DROUGHT EFFECT IN PLANTS REVEALED THROUGH PROTEOMICS STUDIES.

Vijay Kumar Dalal
Deemed University, India

Abstract

Drought is one of the main environmental factors limiting crop production. Drought prone areas are increasing worldwide with the climatic changes. Minimization of the increasing spread and effect of drought on crop production is one of the backbones to achieve UN sustainable development goals. Drought stress is manifested in the plants through several mechanisms. Proteomics have shed light on a number of those mechanisms which includes but not limited to photosynthesis, plant homeostasis, changes in transcription factor, perception of drought and relaying its signal, changes in antioxidant machinery, RNA synthesis and processing, translational machinery, secondary metabolites production, membrane integrity, hormonal regulation, cell shape or cytoskeleton, protein-protein interaction, retrotransposons, sulphur metabolism, alteration in protein conformational, hormonal changes and osmolyte production. How these processes are altered in plants as a result of drought and how drought resistance is developed in plants, will be discussed.

HOW ELECTROSPRAY TANDEM MASS SPECTROMETRY (ESI-MS/MS) CHANGED THE FATE OF FECAL STEROID METABOLITES MEASUREMENT IN FREE-RANGING TAIWANESE PANGOLIN (*MANIS PENTADACTYLA PENTADACTYLA*).

Bharti Arora
Wildlife Biology Researcher, India

Abstract

Electrospray ionization mass spectrometry (ESI-MS) has gained popularity in clinical laboratories for structural study or identification of metabolites in complex biological samples for quantitative measurements. Thus far, MS/MS has been used extensively to determine metabolites in different matrices such as urine and urine in a range of species. Additionally, MS/MS has been used for fecal steroid analyses to understand stress hormone metabolism in ruminants, steroid overuse in livestock, and measurement of gonadal and adrenal metabolites in primates. However, studies of fecal hormones in pangolin have not yet benefitted from this advantageous technique. Pangolins, the sole representative of order Pholidota, are certainly devoid of concrete endocrinological reports causing a major setback in the survival of this species in both wild and captivity.

Objective: We intend to identify and quantify reliably measurable steroids in the following adrenal and gonadal steroid metabolites: glucocorticoids, gestagens, estrogens, and androgens extracted from free-ranging Taiwanese pangolin (Manis pentadactyla pentadactyla) using electrospray tandem mass spectrometry (ESI-MS/MS).

Methods: ESI-MS/MS used 48 and 32 fecal samples procured from 22 males and 14 females pangolins, respectively. Radio-telemetry was employed to obtain the fecal samples from the burrows of radio-tagged pangolin individuals from 200-2017. The fecal samples were extracted with modification in extant established methods for gonadal and adrenal steroid extraction. After extraction, the samples were recombined in a suitable solvent for mass spectrometry analysis. The method was validated by calibration curves, the limit of detection (LOD), and the limit of quantification (LOQ). Finally, physiological validation was performed to evaluate gender-related differences in the species.

Results: The main gestagens detected in the Taiwanese female fecal samples belonged to the pregnane series (allopregnanolone and pregnanolone). The 5α configuration (allopregnanolone) had a higher median concentration in all the female fecal samples over other gestagens metabolites (progesterone, pregnanolone, 5α-pregnane-3,20-dione). The aromatic steroid estrogen yielded estrone (E1) and estradiol 17β (E2), where E2 levels were significantly higher than E1 in all fecal samples. The extensive breakdown of androgens in the male fecal samples revealed that the testosterone (T) and epiandrosterone (EpiA) are formed, and EpiA had a significantly higher median concentration in all the male fecal samples over a lower median concentration of T. The fecal samples of both males and females showed the presence of both cortisol and corticosterone. However, the median concentration of corticosterone was higher in both males and females over the lower median concentration of cortisol.

Conclusion: Some of the main adrenal and gonadal metabolites can be predicted by exploiting MS/MS, which can steer research to potentially assess the reproductive status of captive and free-ranging pangolin species. This method of fecal steroid metabolites identification and quantification can be successfully replicated in identifying metabolites in other endangered fauna.

Biography

Bharti Arora specializes in wildlife biology and the conservation of endangered fauna. Her scientific understanding targets both scientific and non-scientific audiences to simplify her work and knowledge, which the masses could understand. She is a budding researcher and has developed the technique to analyze metabolites in Taiwanese pangolin, a unique work never executed before due to the elusive nature of the species. Additionally, she has exclusively worked on the hormonal cycle of the charismatic species pangolin and wishes to continue to enlighten scientific audiences with missing knowledge gaps of the most trafficked mammal in the world.

Video Presentation

PESTICIDES IN INTENSIVELY AGRICULTURAL VEGETABLES AND FRUITS IN AKKAR (LEBANON)

Wissam Sahyoun
University of Lille, France

Abstract

Background: Akkar is the second agricultural city in Lebanon and have 80% of inhabitant of the country. The cultivated area represents one third of the total area of Akkar (80,000 hectars of agricultural land). Previous studies have indicated that organochlorine pesticides have been used to protect agricultural products and to increase yields. In addition, their residues have been detected at high levels in the groundwater of some villages of Akkar, which are the main source of drinking water for the inhabitants.

Objective: To identify and quantify pesticides in vegetables and fruits from intensive agriculture in Akkar.

Methods: This work is focused on the optimization and application of QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) method for the extraction and purification and GC-MS/MS analysis for the quantification of pesticides in fruits and vegetables. For the GC-MS/MS analysis, the multiple reaction monitoring (MRM) mode have been optimized and used for better selectivity.

Results: The method offers satisfactory accuracy with the extraction yield ranging from 70 to 120% (with 2 matrices spiked with 3 concentration levels), good precision with the coefficients of variation RSD ≤ 6% and a good linearity in the range of concentration between 0.0001 and 10 µg/ml with the R 2>0.99.

Conclusion: The sample preparation technique using QuEChERS with citrate buffer and determination by gas chromatography coupled with tandem mass spectrometry for the analysis of multi-residue pesticides in tomatoes and cucumbers resulted in a fast, efficient and safe process with limited waste production. Another advantage of the method is related to the high recovery rates of the pesticides, 70- 120%, and the accuracy of the results, verified by the coefficients of variation of ≤20%. For application for the real samples, the most of pesticides selected were below the MRL or below of the limit of quantification (LOQ).

Biography

Wissam Sahyoun is currently in the 3rd year of PhD and works on the analysis of organic micropollutants including pesticides in fruits and vegetables. He has his expertise in the QuEChERS sample preparation technique and GC-MS/MS analysis. The QuEChERS is widely used for multi-class or multi-residue analysis of different types of pesticides, mainly in agriculture. This method has been commonly used for the determination of pesticide residues in various matrices. It is a fast, easy to use, inexpensive, efficient, robust and safe method. In addition, the application of this method, including acetate buffer (Lehotay, Maštovská and Lightfield, 2005) and citrate buffer (Anastassiades, Scherbaum, Taşdelen, and Štajnbaher, 2007) versions, allows for the extraction of acidic, basic and neutral compounds, giving accurate and fair results due to high analyte recovery.

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August	
2nd Online International Conference on Applied Microbiology and Beneficial Microbes	August 26-27, 2021
September	
2nd International Webinar on Dentistry and Dental Materials	September 02-03, 2021
Webinar on Nursing and Health Care	September 06-07, 2021
2nd International Webinar on Big Data Analytics & Data Science	September 06-07, 2021
3rd International Webinar on Material Science & Nanotechnology	September 16-17, 2021
2nd International Webinar on Addiction, Psychiatry and Mental Health	September 16-17, 2021
October	
3rd World Congress on Neuroscience and Brain Disorders	October 28-29, 2021
2nd International E-meeting on Biopolymers and Bioplastics	October 28-29, 2021
2nd International E-meeting on Renewable Energy and Sustainable Technologies	October 28-29, 2021
November	
5th International Webinar on 3D Printing & Additive Manufacturing	November 08-09, 2021
4th International Webinar on Materials Science & Engineering	November 08-09, 2021
2nd International Webinar on Graphene and Semiconductors	November 08-09, 2021
5th International Webinar on Nanotechnology & Nanomaterials	November 08-09, 2021
International Webinar on Diamond, Carbon and Advanced Energy Materials	November 08-09, 2021
International Webinar on Forensic Science	November 09-10, 2021
International Webinar on Herbal Medicine & Complimentary Alternative Healthcare	November 11-12, 2021
2nd International Webinar on Biocatalysis & Green Chemistry	November 11-12, 2021
4th International Webinar on Catalysis and Chemical Engineering	November 11-12, 2021
3rd International webinar on Chemistry and Applied Sciences	November 11-12, 2021
International Webinar on Functional Materials and Chemical Engineering	November 11-12, 2021
International Webinar on Organic and Inorganic Chemistry	November 11-12, 2021
5th International Webinar on Agriculture, Food science and Technology	November 11-12, 2021
4th International Webinar on Plant Science & Molecular Biology	November 11-12, 2021
3rd Online International Conference on Aquaculture and Fisheries	November 15-16, 2021

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3rd Online International Conference on Environmental Sustainability and Climate Change	November 15-16, 2021
3rd Online International Conference on Recycling and Waste Management	November 15-16, 2021
International Webinar on Biochemical and Environmental Engineering	November 15-16, 2021
International Webinar on Smart Grid & Green Energy Systems	November 15-16, 2021
2nd Webinar on Laser, Optics & Photonics	November 15-16, 2021
2nd International Webinar on Magnetism and Magnetic Materials	November 15-16, 2021
Online Global Summit on Infectious Diseases	November 17-18, 2021
International Webinar on Petroleum Engineering and Natural Gas	November 17-18, 2021
International Webinar on Oil and Gas Technology	November 17-18, 2021
International Webinar on Internal Medicine & Patient Care	November 17-18, 2021
International Webinar on Ceramics and Composite Materials	November 18-19, 2021
International Webinar on Glass Problems in Ceramics Engineering	November 18-19, 2021
International Webinar on Smart Materials	November 18-19, 2021
International Webinar on Applied Science & Engineering	November 18-19, 2021
International Webinar on Biomedical, Electronics & Devices	November 18-19, 2021
International Webinar on Biomaterials & Devices	November 18-19, 2021
2nd Online International Conference on Diabetes and Endocrinology	November 29-30, 2021
2nd Online International Conference on Nutrition and Nutraceuticals	November 29-30, 2021

BOOKMARK YOUR DATES

3rd International Webinar on

POLYMER SCIENCE & BIOMATERIALS

November 08 - 09, 2021

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