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International Conference on

ANALYTICAL CHEMISTRY

November 21-22, 2018 | Madrid, Spain

DAY 1

Scientific Tracks & Abstracts

Day 1

SESSIONS

November 21, 2018

Mass Spectrometry | X-Beam Spectrometry | Chromatography | Clinical Science Examination

Session Introduction

Session Chair

Gorgaslidze N
TSMU Iovel
Kutateladze Institute of
Pharmacochemistry, Georgia

Title: **Theoretical mass spectrometry**
Kihyung Song, National University of Education, Korea

Title: **A review of a relationship between coeliac disease and obesity: Not just failure to thrive**
Chelsea Spackman, Middlesex University, UK

Title: **The effect of gravitational waves and dark matter in daily life**
Edward H Jimenez, Central University of Ecuador, Ecuador

Title: **Study of the lipids from the fruits of *Corylus avellana L.*, growing in Georgia**
Gorgaslidze N, TSMU Iovel Kutateladze Institute of Pharmacochemistry, Georgia

Title: **The Lorentz transformation and the transverse Doppler effect**
Robert J Buenker, Bergische Universität Wuppertal, Germany

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Kihyung Song, J Chem Tech App 2018, Volume 2

THEORETICAL MASS SPECTROMETRY

Kihyung Song
National University of Education, Korea

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 have been a professor of department of chemistry at Korea National University of Education. He has published more than 110 papers in reputed journals including Science. His h index is 33.

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Chelsea Spackman, J Chem Tech App 2018, Volume 2

A REVIEW OF A RELATIONSHIP BETWEEN COELIAC DISEASE AND OBESITY: NOT JUST FAILURE TO THRIVE

Chelsea Spackman
Middlesex University, UK

The primary objective of this publication was to provide a systematic review of the literature on the relationship between CD and obesity. Further, the reviewer had the purpose of conducting an investigation on this correlation, ranging from paediatrics to adults, in specific areas such as the mechanism of the two conditions and the nutritional interventions. The mechanism review involved finding any pathogenic and pathophysiological link between the two conditions and investigating the possible association in clinical evidence and manifestations and of the symptoms. As a result, the present research was designed to establish a paper that can effectively inform not only the public but health care providers, concerning the importance of proper and time-sensitive diagnosis.

In order to achieve these objectives, the researcher conducted desk-based research, which involved a comprehensive review of numerous journal articles drawn from various publishers. The search strategy involved the use of both internal and external secondary sources of information. Moreover, the search strategy also considered the mechanistic pathology, functional physiology, and human intervention.

The key findings indicated that CD and overweight/obesity present together, and that this should be taken into account both in diagnosis by medical professionals, and in the design of nutritional interventions as a GFD diet is associated with weight gain, and this is probably a result of poor GFD protocols that rely on replacement foods rather than a healthy, individualised diet.

Conclusively, it was important to establish a link between obesity and CD based on the clinical implications of the findings, as well as the general health care field; where the present paper points out the proper diagnosis of both conditions, whether the symptoms are atypical or not. Hence, it was important to provide a precise nutritional intervention for future patients, which may involve an introduction of a GFD before diagnosis, and strict follow-up and education for the patients on the importance of this intervention.

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BIOGRAPHY

Chelsea Spackman completed her MSc at Middlesex University in the UK. She has been published once, and continues working on new research and articles, whilst seeing clients and maintaining her own business in Toronto, Canada.

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Edward H Jimenez et al., J Chem Tech App 2018, Volume 2

THE EFFECT OF GRAVITATIONAL WAVES AND DARK MATTER IN DAILY LIFE

Edward H Jimenez[1], Nicolas Recalde[2] and Esteban Jimenez Ch[3]
[1]Central University of Ecuador, Ecuador
[2]South Carolina University, USA
[3]Paul Sabatier University, France

Dark matter interacts with baryonic matter through gravitational force and weak force. There are reasons to believe it does not interact directly with the strong nuclear force. Moreover, if dark matter is hidden in the nuclear surface, then it can be detected through a variation of the effective K-edge cross section. On the contrary, if it is hidden inside the nuclear core, then it must produce a variation of the nuclear viscosity. The Femtoscope and low-energy x-ray spectroscopy allow us to measure the K-edge resonance and, at the same time, the absence or not of dark matter.

We present two methods on the use of K-edge XANES spectroscopy for organic and inorganic compounds, one theoretical and one experimental. We can determine the absence or not of dark matter in the atomic nucleus, essentially in Phosphorus, Xenon, Thulium and Chromium. The algorithms are sufficiently manageable. This allows us to illustrate that our experimental arrangement is in agreement with underground laboratories providing direct detection experiments such as SNOLAB, Gran Sasso, Canfranc, Deep Underground Science and Engineering Laboratory and the China Jinping Underground Laboratory.

On the other hand, after processing the information of 12000 cancer patients, who have received doses of radiation with energies of the order of 6 MeV, we review all the treatment protocols before an irradiation. We have detected in a single file, recorded in radiography and digital information, where a part of the LINAC moved at a speed close to light in a vacuum, indicating a possible existence of gravitational waves. The coefficient $\Delta L / L = 0.00005$, is higher than the value measured on 2017 by Nobel Prize in physics, which is $\Delta L / L = 10^{-18}$.

BIOGRAPHY

Edward H Jimenez has a PhD in Applied Mathematics from the University of Saint Etienne in France, his Bachelor is in Nuclear Physics and his masters are in Game Theory and Artificial Intelligence. Currently, he is a professor at the Central University of Ecuador in the Faculty of Chemical Engineering, and has worked for 19 years in the oil industry in the area of catalysis and nanotechnology of Si / Al / P using x-ray spectroscopy. He has published more than 20 papers with referee and 6 books of high impact in Ecuador. Nicolas Recalde, has worked for 15 years in cancer radiotherapy at Georgetown University Medical Center and Inova Health System, USA. He was Chief Medical Physicist at Potomac Radiation Center in Virginia, USA. He is a diplomate of the American Board of Radiology and a member of the American Association of Physicists in Medicine.

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Gorgaslidze N et al., J Chem Tech App 2018, Volume 2

STUDY OF THE LIPIDS FROM THE FRUITS OF *CORYLUS AVELLANA L.*, GROWING IN GEORGIA

Gorgaslidze N, Kikalishvili B, Turabelidze D, Sulakvelidze Ts and **Malania M**
TSMU I. Kutateladze Institute of Pharmacochemistry, Georgia

Usual hazel-Coryllus avellana L. (Betulaceae) appropriates to high shrubby plant is widely spread in Georgia. Fruits of the hazel is rich in lipids and biologically active compounds: proteins, vitamins B, C, E, PP; paclitaxel, microelements. Lipids from them is used in medicine: as cholagogic, in time of atherosclerosis, rheumatism, skin, hypertonic diseases, in oncological practice, as medical-prophylactic means.

From the fruits of Usual hazel there was derived lipids in amount 60%. Using the TLC there were established substances of following classes: hydrocarbons, triacylglycerides, free fatty acids, sterines. There were determined some physical-chemical constants of the crude lipids: Acid number-2-3 mg KOH, iodine number I-100-108, index of refraction n-1,460, specific weight d-0,943. On the following stage of the investigation with the help of method high performance liquid chromatography-HPLC were identified ten fatty acids: dodecanic acid-0,10mg/%, tetradodecanic acid-0,10mg/%, hexadecanic acid-5,1 mg/%, octadecanic acid-1,65 mg/%, 9-octadetsenic acid-80,61 mg/%, 9,12-octadecadienic acid-14,28mg/%, 9,12,15-octadecatrienic acid-0,12mg/%, eicosanic acid-0,18mg/%, docosanic acid - 0,10mg/%, tetracosanic acid-0,11mg/%. In the sum of polar lipids there were revealed five phospholipids, lizophosphatidilcholin Rf-0,18, lizophosphatidilaethanolamin Rf-0, 37, phosphatidilchocholin Rf-0, 54, phosphatidilaethanolamine Rf-0, 66, N-acylphosphatidilaethanolamine Rf-0, 86. The sums neutral lipids obtained from the fruits of hazel consist unique ratio of saturated, unsaturated and polyunsaturated fatty acids. In the sum neutral lipids of hazel dominates 9-octadetsenic and 9,12,15-octadecatrienic acids. By the pharmacologically studies there was established that lipids from the fruits of hazel possess gastroprotectoric action.

BIOGRAPHY

Gorgaslidze N has completed her PhD at the age of 37 years from Saint-Petersburg State Chemical-Pharmaceutical Academy, Russia. She is a director of TSMU Iovel Kutateladze Institute of Pharmacochemistry and professor at the department of Social and Clinical Pharmacy at Tbilisi State Medical University. She has published more than 100 papers in reputed journals, the author of 4 books and 2 patens. She is a member of organizing committee of several international conferences and meetings. She has more 40 years of teaching experience at the Tbilisi State Medical University, Georgia. She is founder of the Georgian Pharmaceutical Association (President 2002-2005) and newspaper - "Pharmacy. She is member of scientist and young pharmacists of Georgia. Nana Gorgaslidze has long timework experience in the Ministry of Health, Labor and Social Affairs of Georgia in field of state control of quality medicinal and pharmaceutical products and other departments of the same ministry.

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THE LORENTZ TRANSFORMATION AND THE TRANSVERSE DOPPLER EFFECT

Robert J Buenker
Bergische Universität Wuppertal, Germany

According to the Δy=Δy' equation of the Lorentz transformation (LT) of the special theory of relativity (STR), the value of any distance interval measured on a moving object that is oriented transverse to the velocity of that object should be independent of its relative speed to the observer. It is known from experiments with the transverse Doppler effect, however, that the wavelength of light emitted from a moving source *increases uniformly in all directions* with its speed relative to the observer. When one combines the Δy=Δy' axiom from STR with the above experimental finding, the unavoidable conclusion is that the *in situ* value of the wavelength must also vary with the state of motion of the light source. Otherwise, it is impossible to explain how the laboratory observer could find that the wavelength of the light from the accelerated source changes even when it is measured in a direction which is transverse to its velocity relative to this source. Experimental measurements indicate that this is not the case, however: the *in situ* value of the wavelength of light from a given source is always the same, regardless of the latter's state of motion. The Relativity Principle (RP) on which STR is based also leads to this conclusion. The only way to reconcile theory with experiment under these circumstances is to *reject the Δy=Δy'* claim of STR. Instead, one must assume *that the lengths of objects increase upon acceleration in the same proportion as the rates of clocks slow down*, independent of their orientation to the direction of relative motion to the observer.

BIOGRAPHY

Robert J Buenker was working at Fachbereich C-Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Gaussstr. 20, D-42097 Wuppertal, Germany. Robert research interest includes Lorentz transformation, astrophysics, and relativity principle. Robert is an honorary author for Journal of Astrophysics and Aerospace Technology. Robert has authored of several research articles like GPS-Compatible Lorentz transformation that satisfies the relativity principle.

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DAY 2

Scientific Tracks & Abstracts

Day 2

SESSIONS

November 22, 2018

NMR Spectroscopy | Mass Spectrometry

Session Introduction

Session Chair

Viachaslau Barodka
Johns Hopkins University
USA

Title: **Application of mass spectrometry and NMR analytical techniques to the structural elucidation of phenolic compounds**

Nour Eddine ES-SAFI, Mohammed V University in Rabat, Morocco

Title: **Determination Atorvastatin pharmacokinetic parameters in rats by LC/MS-MS with traditional licorice beverage**

Wael Abu Dayyih, University of Petra, Jordan

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Nour Eddine ES-SAFI, J Chem Tech App 2018, Volume 2

APPLICATION OF MASS SPECTROMETRY AND NMR ANALYTICAL TECHNIQUES TO THE STRUCTURAL ELUCIDATION OF PHENOLIC COMPOUNDS

Nour Eddine ES-SAFI
Mohammed V University in Rabat, Morocco

Polyphenols are natural products involved in plants defense. They are recognized as one of the largest and most widespread class of plant constituents occurring throughout the plant kingdom and are also found in substantial levels in commonly consumed fruits, vegetables and beverages. Phenolic compounds form one of the main classes of secondary metabolites with a large range of structures, and contribute to the organoleptic and nutritional qualities of fruits and vegetables. Polyphenols have attracted considerable interest because of their ubiquitous occurrence within the plant kingdom and numerous important properties. They are receiving increasing attention as natural antioxidants and potential health promoting agents and their eventual health effects are attracting considerable interest in the international scientific community. Many epidemiological studies suggested that long term consumption of diets rich in plant polyphenols offer protection against development of several chronic pathologies. Most of the experimental results demonstrate that polyphenols have several biological activities. Phenolic compounds are also highly unstable compounds which undergo numerous enzymatic and chemical reactions during postharvest food storage and processing thus adding to the complexity of plant polyphenol composition. Among these compounds flavonoids (flavones, flavonols, anthocyanins, proanthocyanidins, ..) constitute one of the most ubiquitous groups of all plant phenolics. Owing to their importance in food organoleptic properties and in human health, a better understanding of their structures, their reactivity and chemical properties in addition to the mechanisms generating them appears essential to predict and control food quality. Therefore, a number of efforts have been made during the last decades to design versatile analytical techniques to explore their structural characterization. The aim of this lecture is to present an overview of our findings on polyphenols and their importance on human health. Results concerning their isolation, their structural elucidation through NMR and MS techniques, their hemisynthesis in addition to some of their biological properties will be given.

Note:

BIOGRAPHY

Nour Eddine ES-SAFI completed his PhD in organic chemistry in 1997 from Mohammed V University in Rabat, Morocco. He undertook postdoctoral studies and research at the French National Institute for Agricultural Research. He is currently working at the Ecole Normale Supérieure, Mohammed V University in Rabat as deputy director and a full professor. His research focuses on natural products, especially polyphenols, their structural elucidation, their antioxidant activity and their role in food technology and human health. He has published many research papers and he is reviewer for various international scientific journals. He is editorial board member of various scientific journals and is editor in chief of the *Green and Sustainable Chemistry* journal.

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DETERMINATION ATORVASTATIN PHARMACOKINETIC PARAMETERS IN RATS BY LC/MS-MS WITH TRADITIONAL LICORICE BEVERAGE

Wael Abu Dayyih and **Eyad Mallah**
University of Petra, Jordan

Atorvastatin is a synthetic second generation3-hydroxy-3- methyl-glutaryl-coenzyme (HMG-CoA) reductase inhibitor which lowers plasma cholesterol levels by inhibiting the HMG-CoA reductase that catalyzes the conversion of HMG-CoA to mevalonate, an early and rate-limiting step in cholesterol biosynthesis in the liver. Atorvastatin is metabolized in the body by cytochrome P450 3A4 enzyme system (abbreviated CYP3A4). Atorvastatin is widely used in many countries in the treatment of severe familial or non-familial hypercholesterolemia. The objective of this randomized controlled study was firstly, developing and validating a simple and simultaneous LC/MS method to quantify Atorvastatin in rat serum. Secondly, investigating the effects of Liquorice fresh beverage on the pharmacokinetics of Atorvastatin in serum rats. Atorvastatin was determined in rat's plasma using high resolution, sensitivity and validated Liquid Chromatography–Mass Spectrometry (LC-MS); The mobile phase was (75% methanol, 25% of 0.2% Formic acid in water), ACE 5 C8 Column (50 X 2.1 mm, 5µ), 1.0 ml/min flow rate, 5 microliters Auto-sampler injection volume, and Glimepiride as an internal standard. The analytical method was linear with acceptable recovery, precision and accuracy. A significant ($P<0.05$) effect of single dose of Liquorice after 2 hours from administration of Atorvastatin, and significant effect of repeated doses of Liquorice after 6 hours from administration of Atorvastatin. There was no significant effect ($P>0.05$) of single dose Liquorice juice on Atorvastatin C-max (29.847 ng/ml), and repeated doses of Liquorice the C-max was (40.113 ng/ml) which is also considered as a non- significant effect ($P>0.05$) We conclude that the effects of Liquorice beverage on Atorvastatin varies between single and repeated doses and this can be a result and could affect Atorvastatin pharmacokinetics.

Keywords: Licorice, Atorvastatin, LC/MS. Rat Plasma, Validation, Pharmacokinetic.

BIOGRAPHY

Wael Abu Dayyih is a PhD holder and currently with the Department of Pharmaceutical Medicinal Chemistry and Pharmacognosy, Faculty of Pharmacy and Medical Sciences-University of Petra, Jordan. His reseach interests include HPLC; Pioglitazone; Sucralose; Pharmacokinetic; Interaction.

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