EuroSciCon

DAY 1

Scientific Tracks & Abstracts

8th Edition of International Conference on

Chemistry Education and Research

August 27-28, 2018 | Zurich, Switzerland

DAY 1

April 26, 2018

Sessions

Fundamentals of Chemistry Education | Biochemistry | Physical Chemistry | Advanced Organic & Inorganic Chemistry | Chemicals & Materials Science | Natural Product Chemistry | Pharma Chemistry | Future Scope of Chemistry

Session Chair
Kazue Tazaki
Kahokugata Lake Institute, Japan

Session Co-Chair
Vaishnavi Parikh
Genus Lifesciences, USA

Session Introduction

Title: **Efficacy of topical drug delivery and significance of semisolid bases**

Vaishnavi Parikh, Long Island University, USA

Title: **Misconception in chemistry textbooks and teachers as users: Case study on the concepts of quantum numbers and electronic configurations**

Kristian Handoyo Sugiyarto, Yogyakarta State University, Indonesia

Title: **Agronanochemical for Ganoderma fungal disease management**

Mohd Zobir Hussein, Institute of Advanced Technology UPM, Malaysia

Title: **Dimensional Tailoring of hybrid perovskites for efficient and stable solar cells**

Mohammad Khaja Nazeeruddin, Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, Ecole polytechnique fédérale de Lausanne (EPFL), CH-1951 Sion, Switzerland

Title: **The importance of chemistry education**

Rowshonara Khanam, Essential Drugs Ltd., Bangladesh

Title: **A hierarchical supercycle from carbon atom to synthetic chemists via artificial intelligent robots for future chemistry in universe**

Linghai Xie, Nanjing University of Posts & Telecommunications, China

Title: **Assessment of chemistry teachers stoichiometry pedagogical content knowledge and its implication chemistry students achievement in stoichiometry**

Nathaniel Ayodeji Omilani, Federal College of Education Abeokuta, Nigeria

Title: **Mesoporous materials in master courses**

Elena Aznar, Centro de Investigación Biomédica en Red de Bioingeniería Biomateriales y Nanomedicina, Spain

Title: **Biochemical properties of ALS and TEL effects on (P)RR induced processes in patients with diabetic neuropathies**

Anna Sh Archvadze, Tbilisi State Medical University, Georgia

Title: **Organic chemistry: Theory, reactivity, mechanisms in modern synthesis**

Pierre Vogel, Ecole Polytechnique Federale de Lausanne, Switzerland

Title: **Molecular dynamics simulations of oxygen species in a native skin membrane of interest for plasma medicine**

Dharmendra Kumar Yadav, Gachon University of Medicine and Science, South Korea

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EFFICACY OF TOPICAL DRUG DELIVERY AND SIGNIFICANCE OF SEMISOLID BASES

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[2]Genus Lifesciences, USA

Topical formulations are commercially avaiable in several dosage forms such as creams, gels, ointments, foam etc. Optimization of drug content in the dosage form is a critical quality attribue to balance the therapeutic activity of the drug molecule and localized toxicity. This study was therefore designed to screen various formulations for *in vitro* release of hydroquinone as a model drug from topical bases including diiferent non inonic and anionic gel based formulation in addition to the emulsion based cream formulation with and without different penetration enhancers and compared to cmmercially available product. Vertical Franz diffusion cell based on principle of equilibrium microdialysis, cellulose membrane and donated human skin membrane were utilized to evaluate release form different semisolid formulations. To estimate the drug release patterns, *in vitro* release data were treated to determine physicochemical parameters, such as steady state flux, diffusion coefficient, permeability coefficient and partition coefficient. The results led to development of a formulation that provided higher release of drug at half the concentration of the marketed product. It was also demonstrated that in case of topical formulations, not the concentration of the drug in the formulation but the nature of the base and layer of formulation in contact with the skin surface presents the drug release.

Biography

Vaishnavi Parikh has completed her PhD in Pharmaceutics from Philadelphia College of Pharmacy, University of Sciences. She has more than eight years of experience working as a Formulation Scientist in the pharmaceutical industry and currently works as a Manager of product development at Genus Lifesciences Inc. She has published several papers in reputed journals; presented at several international conferences; has been serving as a reviewer on six reputed journals and also an editor for the journal, *Insight-Automatic Control*.

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MISCONCEPTION IN CHEMISTRY TEXTBOOKS AND TEACHERS AS USERS: CASE STUDY ON THE CONCEPTS OF QUANTUM NUMBERS AND ELECTRONIC CONFIGURATIONS

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Chemistry textbooks for senior high school commonly used by chemistry teachers as well as students have been reviewed on the concepts of quantum numbers and electronic configurations. A number of six textbooks and thirty teachers from fifteen senior high schools were taken as samples. Typically common misconceptions were found on the authors as well as the teachers. For quantum number ℓ=1, the ordering of $m\ell$: -1, 0, +1 is wrongly associated with alphabetic ordering of p orbitals: p_x, p_y, p_z, within five of the six textbooks; while the other one mistakenly stated that it is immpossible to know the relationship beween the two, and thus cartesian-axes labels are just arbitrarily. In accordance to Hund's rule, five of the six books stated that the unpaired electrons are always to be (m_s) of +½ (spin-up,), while the rest stated that it might also be (ms) of -½ ( ). In writing electronic configurations of elements for all textbooks it is always governed with aufbau principle due to increasing ($n+\ell$) of Madelung. In the case of (3)*d* block, [Ar] $4s^{(1-2)}$ $3d^{(1-10)}$ electronic configurations were favored in all textbooks, though four of them stated that [Ar] $3d^{(1-10)}$ $4s^{(1-2)}$ were also allowed. Thus, an odd statement appears that electronic configuration could be written in two ways. Three textbooks introduced the terms of the last and the n^{th} electron to be associated with the corresponding quantum numbers, and this leads to serious further misconceptions. No statement was found that the ordering of ($n+\ell$) pattern is actually only true for the first twenty elements. Similar misconceptions were also observed for teachers. Only seven teachers stated that the unpaired electrons can be either (m_s) +½ or (m_s) -½, however, all teachers always take (m_s) +½ as the correct answer. Nine teachers stated that the energy of 3d orbitals is lower than that of 4*s*, but the electronic configurations of transition elements were written as [Ar] $4s^{(1-2)}$ $3d^{(1-10)}$. Thus, eventhough some teachers seems to have different idea with the textbooks, they are inconsistent. It might be suggested that the chemistry textbooks must be revised to the correct concept by introducing the solution of Schrödinger equation and the correct order of energy of orbitals as observed by photoelectron spectroscopy.

Biography

Kristian Handoyo Sugiyarto gained his Drs. degree from Yogyakarta State University (UNY), Indonesia in 1978; while appointed to the academic staff of UNY (1979), he undertook MSc program in 1984-1987, and then continued to the PhD program in 1989-1992, both at the Department of Inorganic Chemistry, the School of Chemistry, UNSW, Australia, under the supervision of Prof. H A Goodwin. He then undertook a three-six-month Post-Doctoral research, again with Prof. H A Goodwin, 1995-1997. He has more than 20 international publications dealing with spin-crossover in iron(II) and some education were published in various international journal Scopus indexed, while more than 15 articles publised in local-national journals. He also undertook another six-month research in structural study by EXAFS analysis with Prof. Makoto Kurihara at Shizuoka University and with Prof. Saito A at Tokyo Gakugei University, 2002-2003. He also undertook a four-month academic recharging program for doing palladium complex with Prof. Stephen B Colbran at the School of Chemistry, UNSW, Australia, 2009-2010. He has also presented in several international conferences in Paris, Rome, UPSI Malaysia, and Bangkok, Thailand.

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AGRONANOCHEMICAL FOR *GANODERMA* FUNGAL DISEASE MANAGEMENT

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[2]Institute of Bioscience Universiti Putra Malaysia, Malaysia
[3]Malaysian Palm Oil Board, Malaysia

Oil palm is currently the world's main vegetable oil crop due to its high productivity and long life span. However, the yearly harvest was significantly reduced, due to the basal stem rot (BSR) disease which is caused by a fungus, *Ganoderma boninense*. In 2010, the incidence of BSR disease was estimated to be about 3.7% with estimated affected areas of around 60,000 hectares. Losses due to *Ganoderma* disease is estimated to be about USD 0.5 billion. For the control of Ganoderma, integrated sanitation, biological and chemical controls were suggested. In the later, fungicides such as hexaconazole and dazomet were found effective to eradicate *Ganoderma* inoculum within infected stumps, therefore reducing the spread of Ganoderma. The chemical control can be further improved via nanotechnology platform through fungicide nanodelivery system (FUNADS), which is expected to prolonging the productive life of the infected palm, reducing the frequency of applying time by controlled release approach and to reduce the toxicity by enclosed it in biodegradable and toxic-free materials. In this work, two fungicides; hexaconazole and dazomet as the guests were encapsulated into nanomaterials as the hosts (chitosan and layered double hydroxides) for the formation of various FUNADSs using the host-guest supramolecular chemistry approach. The chemical structure of the synthesized nanofungicides was evaluated using x-ray diffraction (XRD), electron microscopy, dynamic light scattering (DLS), Fourier transform infrared spectroscopy (FTIR), and thermogravimetric (TGA/DTG) analyses. The DLS and high resolution transmission electron microscopy (HRTEM) show the FUNADs can be synthesised using various host and guest combinations, and can be turned into the nanoparticles by adjusting the synthesis parameters. *In vitro* fungicide release from the FUNADs shows a sustained release manner. Furthermore, *in vitro* anti-fungal studies of the FUNADs against *G. boninense* shows better inhibition and lower EC_{50} value compared to their counterparts, the bare fungicides.

Biography

Mohd Zobir Hussein has completed his PhD in Physical Chemistry at the University of Reading, UK and Postdoctoral studies from Pennsylvania State University, USA, University of Southampton, UK, Victoria University of Wellington, New Zealand and University of Western Australia. He has worked as Professor of Chemistry at University Putra Malaysia (UPM). He has published more than 300 papers in reputed journals and 6 patents and has been serving as a research fellow at the Institute of Advanced Technology, UPM.

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DIMENSIONAL TAILORING OF HYBRID PEROVSKITES FOR EFFICIENT AND STABLE SOLAR CELLS

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Organic-inorganic lead halide perovskites have shown impressive power conversion efficiency (PCE) in a range of solar cell architectures.1-2 Despite the multiple ionic compositions that have been reported so far, the presence of organic constituents is an essential element in all the high efficiency formulations, with the methylammonium (MA) and formamidinium (FA) cations being the sole realistic options available to date. In this study, we demonstrate a novel three-dimensional (3D) perovskite with improved material stability as a result of the incorporation of an alternative organic cation, guanidinium, into the MAPbI3 crystal structure.3 The new MA1-xGuaxPbI3 perovskite shows enhanced thermal stability and intrinsically new structural and optoelectronic properties. This allows for stable and high-power conversion efficiencies over 20%, a fundamental step within the perovskite field

Biography

Dr. Md. K. Nazeeruddin received M.Sc. and Ph. D. in inorganic chemistry from Osmania University, Hyderabad, India. He joined as a Lecturer in Deccan College of Engineering and Technology, Osmania University in 1986, and subsequently, moved to Central Salt and Marine Chemicals Research Institute, Bhavnagar, as a Research Associate. He was awarded the Government of India s fellowship in 1987 for study abroad. In 2014, EPFL awarded him the title of Professor. His current research at EPFL focuses on Dye Sensitized Solar Cells, Perovskite Solar Cells, CO2 reduction, Hydrogen production, and Light-emitting diodes. He has published more than 509 peer-reviewed papers, ten book chapters, and he is inventor/co-inventor of over 50 patents. The high impact of his work has been recognized by invitations to speak at over 130 international conferences, and has been nominated to the OLLA International Scientific Advisory Board. He appeared in the ISI listing of most cited chemists, and has more than 49'000 citations with an h-index of 105. He is teaching "Functional Materials" course at EPFL, and Korea University; directing, and managing several industrial, national, and European Union projects. He was awarded EPFL Excellence prize in 1998 and 2006, Brazilian FAPESP Fellowship in 1999, Japanese Government Science & Technology Agency Fellowship, in 1998, Government of India National Fellowship in 1987-1988. Recently he has been appointed as World Class University (WCU) professor by the Korea University, Jochiwon, Korea (http://dses.korea.ac.kr/eng/sub01_06_2.htm), Adjunct Professor by the King Abdulaziz University, Jeddah, Saudi Arabia and Eminent Professor in Brunei.

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THE IMPORTANCE OF CHEMISTRY EDUCATION

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Chemistry education plays an important role in enhancing the quality of teaching, research and development as well as ensuring that students are equipped with good knowledge to produce intensive good and services to mean human needs for food, health care products and other materials aimed at improving the quality of life. Many studies and educational policy paper present a gloomy picture with respect to the learning of chemistry especially at the secondary education particularly in chemistry is unpopular among many students. The claim infers that students are in sufficient interested in chemistry learning. one of the reasons mentioned quiet frequently in that learners do not perceive chemistry and chemistry education as relevant both of themselves and for the society in which they live. Current educational policy suggests that chemistry teachers must make chemistry education "more relevant" in order to better motivate their students and interest them in chemistry studies. This book focuses on the relevance of chemistry education. It was inspired by a recently suggested definition and model of the relevance of science education in its adjustment to the teaching and learning of chemistry. In this context provide some insights regarding the Process by which the teachers perception of "Chemical literacy" developed and the way actual school practice influences teachers perception of "chemical literacy". As a pharmaceutical professionals, i think that there are many natural sources of chemistry like cassava and potato around of us. Students of Research and Develop department of schools and colleges are using those material by applying extraction method to get starch like maize starch from cassava and potato. This is how one can fulfill her or his demand of carbohydrate in food chart. However, commercially in large volume by supplying available as raw materials (starch can use to produce medicine of pharmaceutical variety latest drugs. As a result, many students will be encourage & sufficient interest to study & apply in chemistry learning and chemistry will be most popular among themselves. So, chemistry teaching in education & of its advancement, application every significant task is very important for our society.

Biography

Rowshonara Khanam has completed BSc Hon's & MSc in Chemistry from Eden Girls College of National University. Now I am working in a pharmaceutical Essential Drugs company limited as a chemist till now.

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A HIERARCHICAL SUPERCYCLE FROM CARBON ATOM TO SYNTHETIC CHEMISTS VIA ARTIFICAL INTELLIGENT ROBOTS FOR FUTURE CHEMISTRY IN UNIVERSE

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A failure of the quick knowledge transfer of one-pot protocols of a spirofluorene, SFX, to graduate inspired me deep thinking 12 years ago. A mutually four-element principle were described as the matter-energy-information-consciousness (MEIC) = whole cycle that can be also transformed into converse CIEM expression such as motivation-literature-experience-paper = knowledge or principle-design-engineering-innovation = technology as well as attention-blueprint-execute-existance = being by means of a self-similar self-analysis of mine at background of NJUPT. As a result, I am aware of Daoism and realized the coming era of consciousness after the update intelligence of machine that will completely change the role of chemists in society and universe. In order to keep up with the times, firstly, a hierarchical supercycle from carbon atom to synthetic chemists via artifical intelligent robots have been described that inspired students in the field of chemistry for the integration of knowledge at various area. Secondly, we offer a PhD course (PhDC) with 12 nodes that tell graduates how to discover the knowledge via the process of life-language-philosophy-science for transferring their attention from hot points of social society to research projects of chemistry area. Thirdly, a training course of operation under the logic decision with a feature of de-principle has been set up for the practice of experiment, characterization, simulation computing as well as the visualization of science data. Finally, center for molecular systems& organic devices (CMSOD) focus on researching one kind of molecular systems and organic devices for robots that play the similar roles of DNA and cells in bio-life. Up to date, it took last ten-year to discover the fluorenoid nano-gridarenes that is a giant family of hierarchical molecular worlds, including various monogrids, multigrids, oligogrids and polygrids as well as smart grids by cloning the objects at macroscopically human-scale world. Prospectively, self-similar four-element MEIC whole theory would make molecular intelligence possible that probably change the belief of human being.

Biography

Linghai Xie has completed his PhD in Macromolecular Chemistry by Fudan University (2006) and visiting researcher studies from Nanyang Technology University (2013). He has worked as professor of Organic Nanochemistry at Nanjing University of Posts and Telecommunications (NJUPT). He has published more than 180 papers in reputed journals and has been serving as a director of the Center for Molecular Systems & Organic Devices (CMSOD) at the Institute of Advanced Materials (IAM).

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ASSESSMENT OF CHEMISTRY TEACHERS STOICHIOMETRY PEDAGOGICAL CONTENT KNOWLEDGE AND ITS IMPLICATION CHEMISTRY STUDENTS ACHIEVEMENT IN STOICHIOMETRY

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Understanding stoichiometry is fundamental to chemistry learning just like basic mathematical operation is to mathematics. Students with difficulty in stoichiometry will be unable to solve many problems in various chemistry topics. Unfortunately, chemistry students have difficulty in stoichiometry globally. This problem cannot be solved without a thorough analysis and assessment of chemistry teachers' stoichiometry pedagogical content knowledge (CTSPCK) among other things. This cannot be underscored because of the central role teacher's play in the development of students' understanding of stoichiometry. To this end, this study carried out an assessment of stoichiometry pedagogical content knowledge (SPCK) of chemistry teachers. The components of SPCK measured in this study were: knowledge of instructional strategy in stoichiometry (KISS), knowledge of stoichiometry (KS), and the knowledge of students' understanding in stoichiometry (KSUS). The study further examined the influence of the level of CTSPCK on their students' achievement in stochiometry. The study adopted an expo-facto approach to survey, the sample comprised of 19 chemistry teachers selected from senior secondary schools Ijebu-Ode Local Government Area of Ogun State and their students (512). The instruments for data collection were: topic specific pedagogical content knowledge for stoichiometry questionnaire and students' knowledge of stoichiometry test. The result revealed that the mean score in KS components of CTSPCK was very good (x=6.05). On the other hand, mean score in the two other essential components of CTSPCK: (KISS; x =3.17) and (KSUS; x =1.21) were very poor. Based on the total score of teachers' SPCK, they were categorised as: novice (16), basic (2), developing (1) and experts (0). The study also found out that the level of CTSPCK has a significant influence on students achievement in stoichiometry ($F_{(2,518)}$=47.11; p<0.05). The main recommendation is an urgent effort to develop CTSPCK most especially KISS and KSUS components.

Biography

Nathaniel Ayodeji Omilani has completed his PhD in Science Education from the University of Ibadan, Ibadan, Oyo State, Nigeria. He currently holds an adjunct position in the Department of Science Mathematics and Technology Education in the same university. He has supervised many undergraduate and graduate students in the area of chemistry education and elementary science education. He has also taught courses preparing preservice chemistry and elementary science teachers both at the Department of Integrated Science, Federal College of Education, Osiele, Abeokuta and University of Ibadan. He has published 12 papers in reputed journals and has also read more than 9 papers in national and international conferences. His areas of interest and expertise in science/chemistry education are conceptual change and misconceptions in chemistry, integration of information communication and technology to science and chemistry, development of science teachers' pedagogical content knowledge and science curriculum (secondary and primary). He is also vast in data analysis in education research and instrumentation.

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MESOPOROUS MATERIALS IN MASTER COURSES

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Mesoporous materials are defined as porous materials with pores in the range of 2-100 nm. One of the most important class of mesoporous materials are MCM-41 silica-based materials due to their fascinating properties such as high homogeneous porosity, inertness, thermal stability, the presence of tunable pore sizes, homogeneous pore distribution and the possibility to easily functionalise the external (or internal) surface. These materials can be easily prepared with tailor-made pores of around 2 – 10 nm and show a very large specific surface area (up to 1200 m2/g), thus having a large load capacity. Additionally, their active functionalization to obtain advanced materials is a timely topic of research that could be very motivating and useful for future researchers and postgraduated students. Anchoring organic molecules, biomolecules, or supramolecules onto MCM-41 scaffoldings with different chemical natures, sizes, and shapes promotes the development of smart nanodevices that can be applied in certain scientific and technological fields such as catalysis, chemical remediation, drug delivery or sensing. For example, one attractive approach is to enhance their functionality using supramolecular concepts. It is possible to incorporate in their external surface functional groups or capping ensembles able to open or close at will for advanced controlled-release applications. These systems are constructed for finely tuning the delivery of chemical or biochemical species from voids of porous supports to a solution in response to predefined stimuli. Such gated materials are composed mainly of two subunits: (i) the porous inorganic support in which a cargo is loaded and (ii) certain molecular or supramolecular entities, generally grafted onto the external surface, which can control mass transport from pores. On the basis of this concept, a large number of imaginative examples have been developed. Their study and the preparation of simple systems could be very significant and appreciated by master students.

Biography

Dr Elena Aznar is researcher of the Biomedical Research Center Network (CIBER) in the area of Bioengineering, Biomaterials and Nanomedicine at Instituto de Reconocimiento Molecular y Desarrollo Tecnológico in Universitat Politècnica de Valencia. She is co-author of 57 publications (h-index of 26), has participated in 22 projects and holds 2 patent. Her research interests involve the development of new funtional porous materials. Specially, she works on the developement of gated materials for sensing and drug delivery applications in the biomedical area.

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BIOCHEMICAL PROPERTIES OF ALS AND TEL EFFECTS ON (P) RR INDUCED PROCESSES IN PATIENTS WITH DIABETIC NEUROPATHIES

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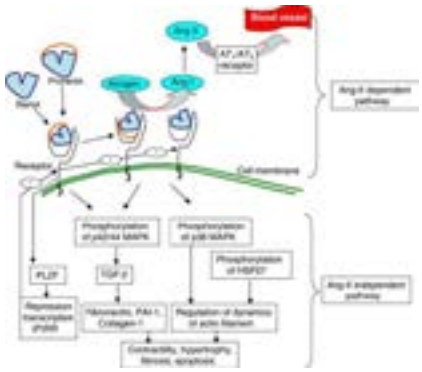
Background: Diabetes mellitus (DM) is the most common cause of diabetic neuropathy (DN). In 2014 the WHO estimated an overall prevalence of 422 million (8.5%). The incidence of diabetic neuropathy approaches 50% in most diabetic populations; its treatment still remains unresolved. The optimal therapy involves: blood glucose level control, anticonvulsants, antidepressants and opioid administration, though it does not change pathogenic pattern. It has been identified that tumor necrosis factor alpha (TNFα) and renin-angiotensin aldosterone system (RAAS) play a significant role in Type I and Type II diabetes development. The discovery of (pro) renin receptor, (P)RR, has made the renin–angiotensin system (RAS) more multifaceted. After binding to the receptor, renin/prorenin carry out their functions either in angiotensin-II-dependent or - independent pathways that may facilitate the generation of angiotensin-I or activation of second messenger, respectively. The data collected in the present-day indicate the essential pathogenic role of TNFα and RAAS in the development of T2DM and diabetic neuropathy (DNP) through the activation of Ag II or/and transcription factor MAPK and NFκB an important factors in the control of cell proliferation, differentiation, and apoptosis. In our study we study aliskiren efficacy, that indirectly inhibit the binding of renin to prorenin/renin receptor (P)RR by changing the local conformation of renin. On the other hand, this renin inhibitor significantly decreases the mRNA expression of (P)RR in the kidney cortex of diabetic hypertensive Ren2 rats.

Methodology & Theoretical Orientation: The study population consists of 30 individuals diagnosed with diabetes mellitus (DM) complicated with DNP. The enrolled subjects are divided into two main groups: group I to take aliskiren and group II with the same pathology, proceeding with the treatment without aliskiren but given telmisartan (ARB), for certainty of aliskiren efficacy. At the start of the trial and on completion of the six weeks period TNFa level and C-peptide (for T2DM) will be determined.

Findings: Aliskiren improves conditions of T2DM patients with DNP. Namely, the symptoms of neuropathy are reduced, the blood TNFa level is reduced and C-peptide level is increased.

Conclusion & Significance: Our results confirm hypothesis that TNFα and RAAS may play a substantial role in the development and progression of T2DM as well as in pathogenesis of DPN. Aliskiren has modulatory impact on TNFα, as well as on renin/prorenin both pathways. So, we have results for clinical and pharmacological analysis of aliskiren application in diabetic neuropathy.



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2. A H M Nurun Nabi and Fumiaki Auzuki (2010) Biochemical properties of renin and prorenin binding to the (pro)renin receptor. Hypertension Research 33:91-97.
3. A Sadeghpour, M Rappolt, D Ntountaniotis, et al. (2015) Comparative study of interactions of aliskiren and AT1 receptor antagonists with lipid bilayers. BBA 1848(4):984-994.

4. A H M N Nabi, Kazal B Biswas, Akio Ebihara et al. (2013) Renin angiotensin system in the contex of renin, prorenin, and the (pro)renin receptor. Reviews in Agricultural Science 1:43-60.
5. K B Biswas, A H M Nurun Nabi, F Suzuki, et al. (2010) Aliskiren binds to renin and prorenin bound to (pro) renin receptor *in vitro*. Hypertens Res. 33(10):1053-9.

Biography

Anna Sh Archvadze has over 8 years' experience as a Medical Doctor. Over 15 years of experience as a Trainer/Teacher of Medical Sciences. Over 11 years of experience in health and social project/program development, execution, monitoring and completion and; Over 7 years of experience in International Project Management working for the World Bank Financed Heath projects, Over 5 years' experience in an assessment of training needs; design and elaboration of training programs, provision of trainings for emergency care medical staff and for health-care services providers, Over 10 years of experience in supervision of the contract performance with medical institutions, pharmaceutical firms, governmental and non-governmental organizations.

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ORGANIC CHEMISTRY: THEORY, REACTIVITY, MECHANISMS IN MODERN SYNTHESIS

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Modern synthesis including asymmetric synthesis, have made fantastic progress during the last 40 years, especially by developing and applying new catalytic reactions. This contributes to render modern technologies more and more sustainable. Synthetic chemists, biochemists and chemical engineers must be able to predict whether a given equilibrium under given conditions will be exergonic or not. For that, thermochemical calculations and statistical thermodynamics are extremely simple, accurate and valuable tools to answer this question. In the same time one needs to be able to predict the rate of the reactions that will lead to the above equilibrium. Knowledge of reaction mechanisms (how nature transforms matter) and theories of reactivity are the most useful tools to help the molecular scientists. The Vogel-Hook textbook has been written to help engineers of molecules to approach satisfying answers to the above questions and help scientists to understand the dynamics of molecules. It complements other textbooks of organic chemistry and physical organic chemistry. It also gives a lot of data the molecular scientists will find useful for the invention of new reactions and processes. It presents the most important concepts of the reactivity of organic and organometallic compounds. The book present 8 chapters that are: equilibria and thermochemistry; additivity rules for thermodynamic parameters and deviations; the rates of chemical reactions; molecular orbital theories; pericyclic reactions; organic photochemistry; catalytic reactions and; transition metal-catalyzed C-C bond forming reactions. A companion workbook gives the literature references and answers to problems.

Biography

Pierre Vogel, PhD degree from the University of Lausanne, 1969 (Prof. H. Prinzbach). After post-doctoral stays at Yale University, New Haven, USA (Prof. Martin Saunders) and at Syntex, Mexico-City (Prof. Pierre Crabbé) he return to Lausanne and become Full Professor of chemistry in 1977, first at the University of Lausanne, then (2001) at the EPFL. He has authored and co-authored more than 525 scientific publications and collected more than 12'100 citations.

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MOLECULAR DYNAMICS SIMULATIONS OF OXYGEN SPECIES IN A NATIVE SKIN MEMBRANE OF INTEREST FOR PLASMA MEDICINE

Dharmendra Kumar Yadav, Surendra Kumar, Saloni and **Mi-Hyun Kim**
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Computational modeling at the molecular or atomic scale can be very useful to obtain a better insight in plasma medicine. Different atomic scale modeling approaches can be used to study the direct interaction of plasma species with biomolecules or the consequences of these interactions for the biomolecules on a somewhat longer time scale. In this work, molecular dynamics simulations are employed to investigate the mechanisms of interactions between reactive oxygen plasma species (H_2O_2, HOO, HO and O_2) and native skin membrane from an atomistic point of view. The result of dynamic distribution study of reactive oxygen species, i.e. H_2O_2 and O_2 revealed that, these species interact with cholesterol, as one of the primary target in lipid-peroxidation of skin-lipid bilayer. Moreover, the permeability of reaction oxygen species, i.e. H_2O_2, HOO, HO, and O_2 along the skin-lipid bilayer is measured by free energy profile. The result of free energy profile shows that, these species in spite of high energy barrier easily travel throughout the membrane. Thereby, breeching the free energy barriers, these reactive oxygen species are able to permeate into the cells, accordingly inflicting oxidative stress, and might lead to apoptosis. Collectively, the insight acquired from simulations may help in better understanding of the oxidation stress at atomic level. Our simulation result provides fundamental insights into the mechanisms underlying the interactions between reactive oxygen plasma species and the skin-lipid bilayer at the atomic level.

Biography

Dharmendra Kumar Yadav has completed his PhD in Biological Science from CSIR-Central Institute of Medicinal and Aromatic Plants, Lucknow, India and Postdoctoral studies from Hanyang University Korea and University of Delhi, India. He has worked as Young Scientist at All India Institute of Medical Science Jodhpur, India. He has published more than 40 papers in reputed journals, 03 Book Chapter and US Patent. He is presently working as a Research Professor at Gachon University of Medicine and Science, Incheon city, Korea.

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DAY 2

Scientific Tracks & Abstracts

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DAY 2

August 28, 2018

Sessions

Fundamentals of Chemistry Education | Biochemistry | Advanced Organic & Inorganic Chemistry | Chemicals & Materials Science | Chemical Engineering | Nuclear Chemistry | Pharma Chemistry | Future Scope of Chemistry

Session Chair
Mahesh Narayan
The University of Texas at El Paso, USA

Session Co-Chair
Linghai Xie
Nanjing University of Posts & Telecommunications, China

Session Introduction

Title: 20 years after the Nakhodka oil spill accident in the Sea of Japan

Kazue Tazaki, Kahokugata Lake Institute, Japan

Title: Structural study on powdered complex of $[Cu(phen)_3](CF_3COO)_2.2.4H_2O$

Kristian Handoyo Sugiyarto, Yogyakarta State University, Indonesia

Title: Rational design of new ligands as human adenosine receptor antagonists: Transition from tricyclic to bicyclic scaffold-based derivatives

Cheong Siew Lee, International Medical University, Malaysia

Title: Peer led team learning and the living workbook

Mahesh Narayan, The University of Texas at El Paso, USA

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20 YEARS AFTER THE NAKHODKA OIL SPILL ACCIDENT IN THE SEA OF JAPAN

Tazaki Kazue, Fukuyama Atsuko, Tazaki Fumie, Shintaku Yoshiaki, Sintaku Mutsuko, Katayama Kazuya, Nakamura Keiichi, Takehara Teruaki, Katsura Yoshihiro and **Shimada Keisuke**

Kahokugata Lake Institute, Japan

On January 2, 1997, the Nakhodka, a Russian tanker loaded with 19,000 kl of C-type heavy oil, was broken up into sections and submerged off Oki Island, Shimane Prefecture, Japan, which yielded serious environmental problems throughout the shores of Hokuriku district. We report the characterization of C-type heavy oil, 20 years after the Nakhodka oil spill accident, based on observations in the field on January 18 in 2017. We studied the microstructure, mineralogy, chemical composition, and radioactivity associated with the microorganisms in soils contaminated with C-type heavy oil with fishing net and rope, using a combination of microtechniques, analytical data. The fish gears that had buried in a beach show high concentration of Na, P, S, Cl, Sr, and Pb, which is predominantly indigenous to the spilled C-type heavy oil, whereas Na, Al, Si, P, S, Ca, Fe, and Sr are detected on the fin whale skeletons that has stored in a museum after being collected. X-ray powder diffraction (XRD) of the contaminated soils after 20 years showed consistent with paraffin, graphite and calcite. Many kinds of hydrocarbon-degrading bacteria, such as *Micrococcus bacillus* and filamentous fungus were found in oil-contaminated soils after 20 years in the coast of Wajima, Ishikawa Prefecture, Japan. To date, no report has described the results of electron microscopy observations and in this research; such observations are introduced, including the real-life occurrence of bioremediation by hydrocarbon-degrading bacteria, graphite, and paraffin wax. These observations could lead to simple methods of removing C-type heavy oil from the environment.

Biography

Tazaki Kazue has completed her PhD in Doctor of Science (Geology, Mineralogy), Tokyo Kyoiku University, Japan. She has worked as Post Doctorate Visiting Fellow at Geological Survey of Canada, ISPG in Calgary, Research Associate at McGill University in Montreal, and Senior Research Associate at The University of Western Ontario, London, Ontario, Canada. She has worked as Associate Professor, at Shimane University, and as Professor, at Kanazawa University, Japan. She was a Visiting Professor at Lac Hong University, in Vietnam and Visiting Professor at the University of Dodoma, Tanzania. She has published more than 500 papers of Environmental Sciences. She got many awards from the Geological Society of Japan, Natural Sciences and Engineering Research Council of Canada, Mineralogical Society of Japan, Clay Mineralogical Association of Japan, Ishikawa TV, the Earth Science Award of Chigaku Dantai Kenkyu-Kai, and the award of International Solopetitmist Society Contribution.

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STRUCTURAL STUDY ON POWDERED COMPLEX OF [CU(*PHEN*)$_3$] (CF$_3$COO)$_2$.2.4H$_2$O

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The blue powdered complex of hydrated tris-phenanthroline(II) trifluoroacetate has been isolated by interaction of the corresponding nitrate salt in aqueous solution and slightly excess of bipyridine in ethanol on the addition of an excess of saturated potassium triflate solution and reducing the solvent. The thermogravimetric analysis/differential thermal analysis (TGA/DTA) confirmed the loss of 4.983% mass of the complex corresponding to 2.4 H_2O (0.6% error), while atomic absorption spectroscopy (AAS) measurement showed the content of metal to be 6.24% corresponding to the theoretical value of 7.28% (14.28% error) in [Cu(*phen*)$_3$](CF$_3$COO)$_2$.2.4H$_2$O. Moreover, the analysis of conductance producing the charge ratio of cation by anion to be 2:1, clearly confirms the formula. The magnetic moment, eff, of this complex which was to be 1.95-1.99 BM, indicates that the complex is paramagnetic corresponding to an unpaired electron. UV-Vis spectrum of the complex reveals the only one absorption observed at about 677 nm (14770 cm^{-1}), being associated with the spin allowed transition, $^2E_g \rightarrow {}^2T_{2g}$. The extinction coefficient of 57.8 Lmol^{-1}cm^{-1} indicates the adoption of octahedral environment in this complex. The infrared spectrum shows absorptions of ligand group which is influenced by the metal-ligand interaction in this complex. The powder XRD analysis of this complex was refined by Rietica-Le Bail method and found to be fit as triclinic crystal system and space group of PI, with parameters of a=10.8985 Å, b=41.0532 Å, c=16.1082 Å, α=98.2720°, β=91.9544°, γ =82.4071°, V=7068.8295Å3, Z=1, *Rp*=1.83 and *Rwp*=5.70 *Rexp*=0.37. The goodness of the fitting, GOF=231.4, was also reflected by the derived Bragg R-Factor of 0.03.

Biography

Kristian Handoyo Sugiyarto gained his Drs. degree from Yogyakarta State University (UNY), Indonesia in 1978; while appointed to the Academic Staff of UNY (1979), he undertook MSc program in 1984-1987, and then continued to the PhD program in 1989-1992, both at the Department of Inorganic Chemistry, the School of Chemistry, UNSW, Australia, under the supervision of Prof. H A Goodwin. He then undertook a three-six-month Postdoctoral Research, again with Prof. H A Goodwin, 1995-1997. More than 20 international publications dealing with spin-crossover in iron(II) and some education were published in various international journal Scopus indexed, while more than 15 articles published in local-national journals. He also undertook another six-month research in structural study by EXAFS analysis with Prof. Makoto Kurihara at Shizuoka University and with Prof. Saito A at Tokyo Gakugei University, 2002-2003. He also undertook a four-month Academic Recharging Program for doing palladium complex with Prof. Stephen B Colbran at the School of Chemistry, UNSW, Australia, 2009-2010. He has also presented in several international conference in Paris, Rome, UPSI Malaysia, Bangkok Thailand.

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RATIONAL DESIGN OF NEW LIGANDS AS HUMAN ADENOSINE RECEPTOR ANTAGONISTS: TRANSITION FROM TRICYCLIC TO BICYCLIC SCAFFOLD-BASED DERIVATIVES

Cheong Siew Lee[1], Pastorin Giorgiab[2], Spalluto Giampieroc[3] and **Klotz K-Nd[4]**

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There are four known subtypes of human adenosine receptors, classified as A1, A2A, A2B and A3 adenosine receptors. They regulate a large array of physiological and pathological functions in the human body. Ligands targeting these adenosine receptor subtypes have been reported to possess therapeutic potential in various diseases. Of note, antagonists of the adenosine receptor subtypes have been shown to be pharmacologically beneficial in modulating Alzheimer's disease, Parkinson's disease, inflammatory disorders and cancer. Over the past decades, medicinal chemists have strived to synthesize and characterize new derivatives as human adenosine receptor antagonists with biological activities of interest. In particular, our research group has been working on the rational design, structural optimization and characterization of new compounds acting as potent human A3 and A2A adenosine receptor antagonists. These compounds have displayed good binding affinities ranging from nanomolar to low micromolar. In this paper, structural modification of new derivatives based on tricyclic scaffold template, and subsequent transition to the design of new compounds with bicyclic scaffold will be discussed in details. In addition, molecular modeling studies, such as molecular docking and quantitative structure-activity relationship analysis performed in tandem to rationalize the binding affinity profiles obtained from the pharmacological studies will also be elaborated. In brief, the integration of medicinal chemistry, pharmacology and computational approaches employed has led to the identification of potent and selective human adenosine receptors antagonists.

Biography

Dr Cheong Siew Lee has obtained her degree in Pharmacy and PhD in Medicinal Chemistry from the National University of Singapore, Singapore. She has then undergone her postdoctoral training at the Institut für Pharmakologie, Universität Würzburg, Germany. Currently, she works as a lecturer at the Department of Pharmaceutical Chemistry, International Medical University, Malaysia. Her research interests revolve mainly around structural optimization of new ligands targeting adenosine receptors and dopamine receptors as well as application of computational approaches and pharmacological characterization in the drug design and discovery. Her research work has been published in various top international peer-reviewed journals and book chapters.

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PEER LED TEAM LEARNING AND THE LIVING WORKBOOK

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Since 2001, The University of Texas at El Paso (UTEP), originally through grants from the National Science Foundation (I-STAR:Integrative Science Success, Teaching, and Retention Program), has developed and enhanced the talent pool of undergraduate students in science and engineering from the Paso del Norte region of the United States by implementing and honing the concept of peer led team learning (PLTL). Students register for workshops that are co-requisite with lectures in certain introductory science and mathematics courses. These workshops are led by peer leaders, students who have successfully passed the course and are selected for this role. Research has shown that the peer leaders are best able to facilitate the understanding and further refinement of concepts for undergraduates in these gatekeeper courses as opposed to learning only in a lecture setting. These peer leaders are equipped with an eclectic repository of educational techniques which are constantly refined and expanded through participation in weekly meetings, summer training sessions, travel to educational conferences, and generation and transmission of educational materials. Over the course of UTEP's PLTL implementation, significant data have been gathered in terms of the impact that this program has had in improving several aspects of Science, Technology, Engineering and Mathematics (STEM) curricula and its absorption. UTEP was a founding campus in the formation of the Peer-Led Team-Learning International Society as well as the development of a funding mechanism via a living workbook which aid in sustaining the program. The concept and content of the workbooks will be also discussed in this presentation.

Biography

Mahesh Narayan has completed his PhD in Biophysics at The Ohio State University and pursued Postdoctoral studies at Cornell University. Currently, he is a Professor of Chemistry at The UTEP and serves on the Editorial Board of *PLOS One* and *Cell Biochemistry and Biophysics.* He has published extensively in the areas of protein folding, Parkinson's disease and pedagogical inroads in Chemistry.

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