THE ATHENS INSTITUTE FOR EDUCATION AND RESEARCH

Abstract Book:

5th Annual International Conference on **Chemistry**

17-20 July 2017, Athens, Greece

Edited by
Gregory T. Papanikos

2017

Abstracts

5th Annual International Conference on Chemistry

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(In Alphabetical Order by Author's Family name)

Preface

This book includes the abstracts of all the papers presented at the *5th Annual International Conference on Chemistry, 17-20 July 2017*, organized by the Athens Institute for Education and Research (ATINER).

In total 16 papers were submitted by 20 presenters, coming from 12 different countries (Brazil, Egypt, France, Germany, Hungary, India, Iraq, Morocco, South Africa, Turkey, UK and USA). The conference was organized into 10 sessions that included a variety of topic areas such as nanomaterials, medicinal chemistry, and more. A full conference program can be found before the relevant abstracts. In accordance with ATINER's Publication Policy, the papers presented during this conference will be considered for inclusion in one of ATINER's many publications.

The purpose of this abstract book is to provide members of ATINER and other academics around the world with a resource through which to discover colleagues and additional research relevant to their own work. This purpose is in congruence with the overall mission of the association. ATINER was established in 1995 as an independent academic organization with the mission to become a forum where academics and researchers from all over the world could meet to exchange ideas on their research and consider the future developments of their fields of study.

It is our hope that through ATINER's conferences and publications, Athens will become a place where academics and researchers from all over the world regularly meet to discuss the developments of their discipline and present their work. Since 1995, ATINER has organized more than 400 international conferences and has published nearly 200 books. Academically, the institute is organized into seven research divisions and 37 research units. Each research unit organizes at least one annual conference and undertakes various small and large research projects.

For each of these events, the involvement of multiple parties is crucial. I would like to thank all the participants, the members of the organizing and academic committees, and most importantly the administration staff of ATINER for putting this conference and its subsequent publications together. Specific individuals are listed on the following page.

Gregory T. Papanikos
President

5th Annual International Conference on Chemistry
17-20 July 2017, Athens, Greece
Organizing and Academic Committee

All ATINER's conferences are organized by the Academic Committee (https://www.atiner.gr/academic-committee) of the association.

This conference has been organized with the additional assistance of the following academics, who contributed by chairing the conference sessions and/or by reviewing the submitted abstracts and papers:

1. Gregory T. Papanikos, President, ATINER.
2. Ellene Tratras Contis, Professor of Chemistry, Eastern Michigan University, USA.
3. Thomas J. J. Mueller, Professor, University of Dusseldorf, Germany.
4. Alaide Braga de Oliveira, Emeritus Professor, Federal University of Minas Gerais – UFMG, Brazil.
5. Kamal Kumar, Research Group Leader, Max Planck Institute of Molecular Physiology, Germany.
6. Nikos Mourtos, Head, Mechanical Engineering Unit, ATINER & Professor, San Jose State University, USA.
7. Bala Maheswaran, Academic Member, ATINER & Professor, Northeastern University, USA.
8. Robert Moonsamy Gengan, Associate Professor, Durban University of Technology, South Africa.
9. Santhi Sambamoorthy, Associate Professor, Bharathidasan University, India.
10. Jasim Salman, Deputy Dean and Assistant Professor, Al-Nisour University College, Iraq.
11. Vassilis Skianis, Research Fellow, ATINER.
12. Olga Gkounta, Researcher, ATINER.
13. Hannah Howard, Research Assistant, ATINER.

FINAL CONFERENCE PROGRAM
5th Annual International Conference on Chemistry,
17-20 July 2017, Athens, Greece
PROGRAM
Conference Venue: Titania Hotel, 52 Panepistimiou Avenue, Athens, Greece

C O N F E R E N C E P R O G R A M

Monday 17 July 2017

08:00-09:00 Registration and Refreshments

09:00-09:30 (Room B-10th Floor) Welcome and Opening Address

Gregory T. Papanikos, President, ATINER.

09:30-11:00 Session I (Room D-10th Floor): Medicinal Chemistry & Synthesis

Chair: Olga Gounta, Researcher, ATINER.

1. Kamal Kumar, Research Group Leader, Max Planck Institute of Molecular Physiology, Germany. Nature Inspired Synthesis Targeting "Common" and "Diverse" Scaffolds.
2. Milan Antonijevic, Principal Lecturer, University of Greenwich, UK, Ovidiu Novac, University of Greenwich, UK & Beatriz Sanchon-Lopez, University of Greenwich, UK. Assessment of Skin Occlusion Performance of Two Commercially available Emollient Gels.
3. Sanaa Sabour Alaoui, Assistant Professor, Sultan Moulay Slimane University, Morocco & Latifa Bouissane, Assistant Professor, Sultan Moulay Slimane University, Morocco. TWEAK New Therapeutic Target for Inflammatory Skin Diseases.

11:00-12:30 Session II (Room D-10th Floor): Synthesis and Nanomaterials I

Chair: Alaide Braga de Oliveira, Emeritus Professor, Federal University de Minas Gerais – UFMG, Brazil.

1. Thomas J. J. Mueller, Professor, Makromolekulare Chemie der Universität Düsseldorf, Germany, Alissa C. Götzinger, Makromolekulare Chemie der Universität Düsseldorf, Germany & Melanie Denissen, Makromolekulare Chemie der Universität Düsseldorf, Germany. Consecutive Multicomponent Syntheses of Pyrazoles – Diversity-oriented Approach to Blue Emitters and Emission Solvatochromic Dyes.
2. Robert Moonsamy Gengan, Associate Professor, Durban University of Technology, South Africa & Murugesan Arul, Durban University of Technology, South Africa. Preparation and Characterisation of a Boron Nitride Fused Sulfonic Acid Catalyst for the Synthesis of new Active Acridine Derivatives.
3. Marwa El-Hussieny Awad Mohamed, Researcher, National Research Centre, Egypt, Mansoura A. Abd-El-Maksoud, Researcher, National Research Centre, Egypt, Soher S. Maigali, Professor, National Research Centre, Egypt & Fouad M. Soliman, Professor, National Research Centre, Egypt. Reaction of Active and Stabilized Phosphours Ylides with Pyridine-diethanone and Oxopropanenitrile.

12:30-14:00 Session III (Room D-10th Floor): Natural Products Chemistry

Chair: Thomas J. J. Mueller, Professor, Makromolekulare Chemie der Universität Düsseldorf, Germany.

1. Jasim Salman, Deputy Dean and Assistant Professor, Al-Nisour University College, Iraq. Optimization Study of Preparation Twigs Tamarisk Trees Activated Carbon for Removal of Pesticides.
2. Samira Boulbaroud, Assistant Professor, Sultan Moulay Slimane University, Morocco, Latifa Didou, PhD Student, Ibn Tofail University, Morocco, Fatima-Zahra Azzaoui, Assistant Professor, Hassan II University, Morocco & Ahmed Omar Ahami, Professor, Ibn Tofail University, Morocco. *Rosmarinus Officinalis L*. Leaf Extract Improves Memory Impairment Induced by Tropane Alkaloids Extracted from *Datura Stramonium.*

14:00-15:00 Lunch

15:00-16:30 Session IV (Room C-10th Floor): Special Topics in Sciences I

Chair: Robert Moonsamy Gengan, Associate Professor, Durban University of Technology, South Africa.

1. Daniel Schertzer, Professor, Ecole des Ponts ParisTech, France & Ioulia Tchiguirinskaia, Ecole des Ponts ParisTech, France. Spatial Chaos, Multifractal Vector Fields and Stochastic Clifford Algebra.
2. Isai Urasa, Professor, Hampton University, USA. Citizen Science in the Context of Indigenous Knowledge.

16:30-18:30 Session V (Room B-10th Floor): *A Symposium on The Future Developments and Prospects of Engineering and Science Education & Research in a Global World I*

Chair: Nikos Mourtos, Head, Mechanical Engineering Research Unit, ATINER & Professor, San Jose State University, USA.

1. Bala Maheswaran, Professor, Northeastern University, USA. Engineering Education via Innovations and Inventions (E2 via I2).
2. Itzhak Orion, Head of the Nuclear Engineering, Ben-Gurion University of the Negev, Israel. Nuclear Science Research and Education in Israel.
3. Jin He, Professor, Peking University, Shenzhen SOC Key Laboratory, China. New teaching technique and method function in the engineering and science education and research.
4. Haiduke Sarafian, Professor, The Pennsylvania State University, USA. The Research Aspect of College Education.
5. Thomas J. J. Mueller, Professor, Makromolekulare Chemie der Universität Düsseldorf, Germany. Life Science – Society.

For details on the discussion please click here.

21:00-23:00 The Pragmatic Symposium of the Conference as Organized in Ancient Athens with Dialogues, Food, Wine, Music and Dancing but fine tuned to Synchronous Ethics

Tuesday 18 July 2017

07:30-10:30 Session VI: An Educational Urban Walk in Modern and Ancient Athens

Chair: Gregory Katsas, Vice President of Academic Affairs, ATINER & Associate Professor, The American College of Greece-Deree College, Greece.

Group Discussion on Ancient and Modern Athens.
Visit to the Most Important Historical and Cultural Monuments of the City (be prepared to walk and talk as in the ancient peripatetic school of Aristotle)

11:00-12:30 Session VII (Room D-10th Floor): A Panel on New Potent Bioactive Azole Derivatives Containing Pharmacophore Groups

Chair: Kamal Kumar, Research Group Leader, Max Planck Institute of Molecular Physiology, Germany.

1. Alaide Braga de Oliveira, Emeritus Professor, Federal University de Minas Gerais – UFMG, Brazil, Tatiane F. Borgati, Federal University de Minas Gerais – UFMG, Brazil, Juliana S. Oliveira, Federal University de Minas Gerais – UFMG, Brazil, Maria Fernanda A. do Nascimento, Federal University de Minas Gerais – UFMG, Brazil, Guilherme R. Pereira, Pontifícia Universidade Católica de Minas Gerais, PUC Minas, Departamento de Física e Química, Instituto de Ciências Exatas e Informática / ICEI, Brazil, Geraldo Célio Brandão, Faculdade de Farmácia, UFOP, Brazil Antimalarial Activity of Natural Products-*1,2,3*-Triazole Derivatives and Molecular Docking Studies.
2. Tuba Yildirim, Associate Professor, Amasya University, Turkey, Elif Senkuytu, Gebze Technical University, Turkey, Yildiz Uludag, The Scientific and Technological Research Council of Turkey (TUBITAK), Turkey & Gönül Yenilmez Ciftci, Professor, Gebze

Technical University, Turkey. First Fluorenylidene Double Bridged Paraben Substituted Cyclotriphosphazene Compounds and DNA Interaction Analysis.

12:30-14:00 Session VIII (Room D-10th Floor): Synthesis and Nanomaterials II

Chair: Santhi Sambamoorthy, Associate Professor, Bharathidasan University, India.

1. Marta Palko, Lecturer, Institute of Pharmaceutical Chemistry, Hungary & Ferenc Fulop, Professor, University of Szeged, Hungary. Synthesis of Novel N-Heterocyclic Compounds Containing 1,2,3-Triazole Ring System via Domino-, "Click" and Retro Diels-Alder (RDA) Reactions.
2. Balint Lorinczi, MSc Student, University of Szeged, Hungary, Istvan Szatmari, Associate Professor, Institute of Pharmaceutical Chemistry, Hungary & Ferenc Fulop, Professor, University of Szeged, Hungary. Synthesis of Functionalized Kynurenic Acid Derivatives.

14:00-15:00 Lunch

15:00-16:30 Session IX (Room C-10th Floor): Special Topics in Sciences II

Chair: Jasim Salman, Deputy Dean and Assistant Professor, Al-Nisour University College, Iraq.

1. Santhi Sambamoorthy, Associate Professor, Bharathidasan University, India & Amala Subbiah, Lecturer, Bharathidasan University, India. Highly Selective and Sensitive Dual Channel Schiff Base Chemosensors for the Detection of Al(III), Fe(III) & Cu(II).
2. Latifa Bouissane, Assistant Professor, Sultan Moulay Slimane University, Morocco & Issam Forsal, Assistant Professor, Sultan Moulay Slimane University, Morocco. Novel Polysubstituted Indazoles Derivatives as Potential Antitumor Agents: Growth Inhibition and Apoptosis Induction.

16:30-18:30 Session X (Room B-10th Floor): *A Symposium on The Future Developments and Prospects of Engineering and Science Education & Research in a Global World II*

Chair: Bala Maheswaran, Professor, Northeastern University, USA.

1. Nikos Mourtos, Professor, San Jose State University, USA. Teaching & Learning Engineering in the 21st Century: Challenges and Opportunities.
2. Lluis Jofre, Professor, Universitat Politecnica de Catalunya (UPC), Spain. Catalonia Engineering and Science Educations and Research trends in the European Context.
3. Dong-Wook Jerng, Professor, Chung-Ang University, South Korea. Some Thoughts for Future Direction of Engineering/Science Education with Insights from a K-POP Story of BTS.
4. Isai Urasa, Professor, Hampton University, USA. International Higher Education: A Vehicle for Global Cooperation and Development in Science and Engineering.
5. Santhi Sambamoorthy, Associate Professor, Bharathidasan University, India. Creative and inimitable role played by Indian universities in science, engineering and research in a global world.
6. Ethel Petrou, Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA. Emerging trends in New York State Community Colleges-SUNY.

For details on the discussion please click here.

21:00- 22:30 Dinner

Wednesday 19 July 2017
Educational Island Tour or Mycenae and Epidaurus Visit

Thursday 20 July 2017
Delphi Visit

Sanaa Sabour Alaoui
Assistant Professor, Sultan Moulay Slimane University, Morocco
&
Latifa Bouissane
Assistant Professor, Sultan Moulay Slimane University, Morocco

TWEAK New Therapeutic Target for Inflammatory Skin Diseases

TWEAK, APRIL and BAFF are ligands of the TNF superfamily. Most of the time, they bind to specific receptors of the TNFR superfamily. TWEAK, biologically active in soluble form, it bind with high affinity to its specific receptor FN14. TWEAK can induce apoptosis of keratinocytes, despite the fact that its receptor, FN14, does not have a death domain in its intracellular part.

We studied the expression, the effect and signaling pathways of these two systems TWEAK/FN14 in normal skin and pathological.

In this study, we demonstrated for the first time, the mechanism by which TWEAK and its receptor FN14 induce apoptosis of keratinocytes. We show for the first time, this apoptosis is caspase and cathepsinB independent. It is due to the translocation of AIF from mitochondria to the nucleus. In addition to its apoptotic action, we described a new role for TWEAK in phase G2/M cell cycle arrest leading to the death of keratinocytes. This suggests that TWEAK plays a multiple effects on human keratinocytes. Finally, we note that the TWEAK/FN14 are normally expressed in the basal layer of the epidermis of normal skin and are overexpressed in the case of a benign (psoriasis) and malignant (squamous cell carcinoma) skin disease.

Our data suggest that the couple TWEAK/FN14 could be target, marker or useful tool in the therapy of skin disease (inflammatory, tumoral).

Milan Antonijevic
Principal Lecturer, University of Greenwich, UK
Ovidiu Novac
University of Greenwich, UK
&
Beatriz Sanchon-Lopez
University of Greenwich, UK

Assessment of Skin Occlusion Performance of Two Commercially available Emollient Gels

Introduction: Emollient therapy is the mainstay for treating dry skin conditions such as atopic eczema and psoriasis.[1] Healthcare professionals (HCPs) recommend emollient products based primarily on patient preference and cost.[2] Emollients work mechanically, mainly by forming an occlusive layer on/in the surface of the skin that traps in physiological moisture, plumping up cells, improving the natural barrier property and reducing penetration of allergens and irritants. Objective sub-clinical assessment of skin barrier function has traditionally been performed *in vivo* by measuring trans-epidermal water loss (TEWL) and/or epidermal hydration. Because clinical trials of this sort are both costly and time consuming, very limited information exists on the comparative effectiveness of different emollients and National Institute for Health and Clinical Excellence (NICE) has called for more research in this area.[3,4] Consequently, the aim of this study was to compare the occlusion capabilities of two commercially available emollient gel formulations, which appear to be therapeutically interchangeable, using a novel approach for measuring skin occlusion gravimetrically.

Materials and Methods: Occlusion was measured by reduction in cumulative evaporative weight loss from *ex vivo* human skin samples during 48 hours following single applications of two marketed emollients, DBG and IMG. Highly occlusive Vaseline™ (petroleum jelly) was used as a positive control.

1.5 cm x 1.5 cm full thickness human skin samples, obtained from one skin donor, were mounted in standard Franz Diffusion Cells and secured with Parafilm® and stainless steel clips. The receptor chambers of the diffusion cells were then filled with Phosphate Buffered Saline solution (PBS, pH=7.4) to bathe the undersides of the skin samples. Four assemblies were prepared for each product/control and then the formulations were applied and spread over the skin surface with a glass rod to achieve an applied dose of approximately 2 mg/cm^2

surface area of skin. The assemblies were weighed at baseline (T_0), and again after 5h, 24h and 48h.

The film-forming characteristics of the two hydrogel formulations were also compared by spreading them in a thin layer on the surface of glass petri dishes and observing their appearance over 24 hours.

Results: Occlusivity of the DBG hydrogel formulation was comparable to the positive control and substantially better than IMG, losing less than half as much weight over 48 hours. The film forming characteristics of the gels were also very different. Whereas DBG maintained a smooth, uniform film over 24 hours, the IMG formulation separated, leaking a clear liquid (subsequently determined to be isopropyl myristate, one of the key occlusive ingredients in the formulation). These performance differences are notable because the two hydrogels, DBG and IMG, appear to have similar compositions.

Conclusions: These results show marked differences in occlusion performance between marketed emollients, and even between formulations which, superficially, may appear to be similar. This is something that HCPs should be aware of when recommending these products.

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Latifa Bouissane
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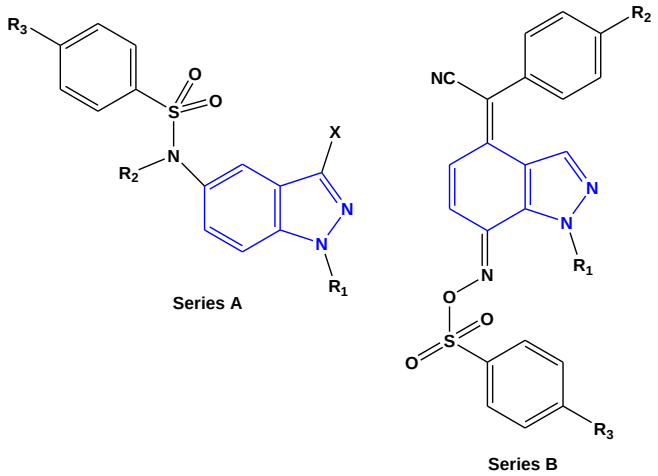
&
Issam Forsal
Assistant Professor, Sultan Moulay Slimane University, Morocco

Novel Polysubstituted Indazoles Derivatives as Potential Antitumor Agents: Growth Inhibition and Apoptosis Induction

Cancer is the second mortal disease with irregular cellular proliferation and metastasis after cardiovascular and cerebrovascular disease in the world. All cancer types cause a fifth of all cancer-related deaths [1] and are usually diagnosed in advanced stages [2]. The great cancer incidence worldwide increases the search for new, safer and efficient anticancer agents, aiming the prevention or the cure of this illness. Indazole core is the best skeleton to develop anticancer agents. It is recognized to be a highly effective pharmacophore in medicinal chemistry as well as being the core of important nitrogen-containing heterocycles that show a broad range of biological activities [3-6].

Trying to develop potent and selective anticancer agents, a series of novel polysubstituted indazoles (scheme) were synthesized and evaluated for their *in vitro* antiproliferative and apoptotic activities against two selected human cancer cell lines (A2780 and A549). Several compounds showed interesting antiproliferative activity with IC_{50} ranging from 0.64 to 21 μM on both cell lines. The most active indazoles were then tested in different pharmacological dilution conditions, adding three new cell lines (HGC-27, MDA-MB-231 and T47D) as targets, thus confirming their antiproliferative activity. Furthermore, these selected compounds were able to trigger apoptosis to a significant extent and to cause a block of cells in the S phase of the cell cycle, with a concomitant decrease of cells in the G2/M and/or G0/G1 phases and the generation of hypodiploid peaks.



Scheme

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Rosmarinus Officinalis L. Leaf Extract Improves Memory Impairment Induced by Tropane Alkaloids Extracted from *Datura Stramonium*

There have been long-established research trends into new neuroprotective drugs from natural product. *Datura stramonium (D. stramonium)* was investigated as a local source of tropane alkaloids which contain a methylated nitrogen atom (N-CH3) and include the anti-cholinergic drugs atropine, and scopolamine. The infusion of their leaves extract is taken orally for the treatment of asthma and sinus infections, and stripped bark are applied externally to treat swellings, burns and ulcers. The alkaloid extract of this plant taken orally can also induce impairment of the behavior affecting negatively the nervous system especially the memory. In the aim to improve the failure memory induced by alkaloids, we assessed to study the effects of subchronic administration of flavonoid extracts at 50 mg/kg from Rosmarinus officinalis L. on cognitive responses of rats linked with acetylcholinesterase (AchE) activity and acetylcholine (Ach) levels in the hippocampus, prefrontal cortex and cerebellum. Rosmarinus officinalis L. Our results showed that Rosmarinus officinalis L extract inhibited the AChE activity and enhanced the Ach levels in hippocampus, cerebellum and improved long-term memory evaluated by the recognition memory test suggesting that their flavonoid extracts can be a valuable candidate for the prevention and treatment of dementia.

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Geraldo Célio Brandão
Faculdade de Farmácia, UFOP, Brazil

Antimalarial Activity of Natural Products-*1,2,3*-Triazole Derivatives and Molecular Docking Studies

Malaria remains a serious endemic disease in 91 countries where high morbidity and mortality rates are registered. WHO estimated that 212 million cases and 429,000 deaths occurred globally, in 2015; most of the deaths were of children under 5 years, in Africa. The protozoans *Plasmodium falciparum* and *P. vivax* are the mainly parasites responsible for this disease; the first one being most virulent is responsible for 99% of deaths. Resistance of parasites to available antimalarial drugs and of vectors to insecticides used to prevent mosquitoes (*Anopheles* spp) vectors biting are great barriers to progress towards the WHO global goals of improving malaria-fighting tools that includes new vector control interventions, improved diagnostics and more effective medicines [1]. Among available medicines, the most notorious are quinine and artemisinin, both of them derived from plant remedies used to treat malaria. Ethnopharmacologically guided research is a valid approach in the quest of antimalarials and has yielded many lead molecules that represent templates or scaffolds for the synthesis of potentially active new chemical entities.

We are exploring this avenue starting with bioactive and abundant natural products such as lapachol, a prenylnaphthoquinone found mainly in Southamerican Bignoniaceae, and kaurenoic acid, a sesquiterpene widely occurring in different botanical families. Total synthesis of lapachol related naphthoquinones and *1,2,3*-triazole derivatives of lapachol and kaurenoic acid, *in vitro* antimalarial activity against chloroquine resistant *P. falciparum* W2 strain and molecular docking studies will be reported as a follow up to our first publication in this theme [2].

References

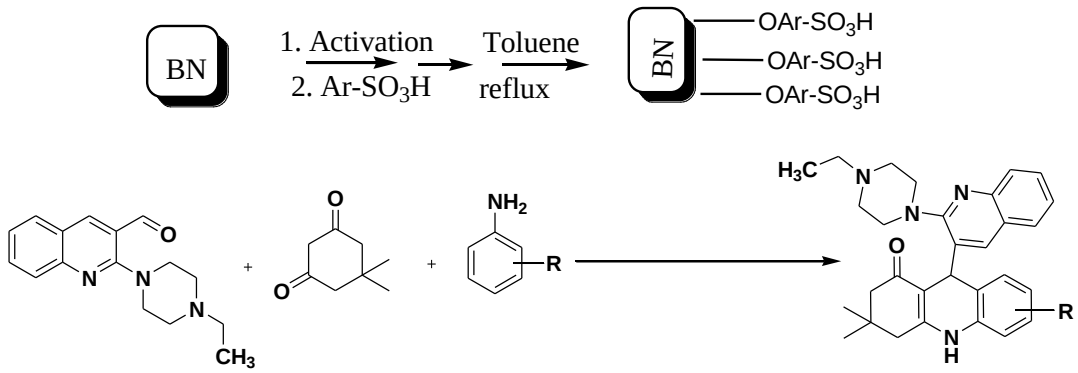
[1] World Malaria Report 2016. Geneva: World Health Organization; 2016.

[2]G.R. Pereira et al. European Journal of Medicinal Chemistry 73 (2014) 295-309.

Robert Moonsamy Gengan
Associate Professor, Durban University of Technology, South Africa
&
Murugesan Arul
Durban University of Technology, South Africa

Preparation and Characterisation of a Boron Nitride Fused Sulfonic Acid Catalyst for the Synthesis of new Active Acridine Derivatives

Two-dimensional nanomaterials are receiving much interest in the development of new heterogeneous catalysts. Among them, boron nitride has shown good potential because of its high elastic modulus, high melting-point and excellent thermal conductivity and as ideal reaction exchange material for the preparation of new organic molecules1. In this study, a novel heterogeneous acid catalyst was synthesised by treatment of activated boron nitride with a benzene sulfonic acid derivative via. a simple eco-friendly methodology. The preparation and characterization of this new nano-material will be discussed: their excellent physical, chemical and morphological properties were elucidated using FT-IR, XRD, TEM, SEM and Raman spectroscopy techniques. The catalytic activity will be described for the synthesis of some biologically active novel acridines. The recovery, recyclability and solvent effects will also be elaborated during this presentation.



Kamal Kumar
Research Group Leader, Max Planck Institute of Molecular Physiology, Germany

Nature Inspired Synthesis Targeting "Common" and "Diverse" Scaffolds

Molecular complexity and diversity represented by structures of natural products has always been a source of inspiration for organic and medicinal chemists. De novo construction of natural products often fails to provide adequate numbers and amounts of their analogues and derivatives for screening purposes. In the absence of feasible synthetic access to structurally diverse and complex molecules, modern probe and drug-discovery research has in a way been pushed to employ a significant number of accessible synthetic chemical libraries in biological screenings, despite their unimpressive returns in the last two decades. Nature – the chemist, in fact has more to offer to help design synthetic strategies to expand the biologically relevant chemical space that needs to be explored in biological screenings. In this talk, our efforts to concisely build structurally diverse molecular frameworks amenable to compound collection synthesis, in particular, by means of cascade reactions shall be presented. The emerging trends in this direction as well as the challenges that lie ahead for organic chemists will also be discussed.

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Balint Lorinczi
MSc Student, University of Szeged, Hungary
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&
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Professor, University of Szeged, Hungary

Synthesis of Functionalized Kynurenic Acid Derivatives

KYNA (4-hydroxyquinoline-2-carboxylic acid), is an endogenous product of the tryptophan (TRP) metabolism, a pathway known to be responsible for the production of nicotinamide adenine dinucleotide (NAD^+) and NAD phosphate ($NADP^+$).[1] Since KYNA is a neuroprotective agent able to prevent neuronal loss following excitotoxic, ischemia-induced and infectious neuronal injuries, there has recently been increasing interest in the synthesis and pharmacological studies of KYNA derivatives.[2] The substitution of the KYNA skeleton at positions 5-8 were achieved by starting from the corresponding aniline via modified Conrad-Limpach method. The hydroxy group at position 4 was transformed to ethers, or amines, while the carboxylic function at position 2, was mostly modified into the corresponding esters or amides.[3]

By the extention of the modified Conrad-Limpach method, the synthesis of kynurenic acid derivatives that contain additional hydroxy groups at positions 5-8 (**3a-d**) has been achieved. The synthesized dihydroxyquinoline-2-carboxylic acids have been transformed to new amides that contain *N*,*N*-dimethylethyl (**4a-d**), or pyrrolidylethyl (**5a-d**) groups as cationic side-chain. In case of xanturenic acid (**3d**), during the esterification protocol, the ether formation of a hydroxyl group has been assumed. This unexpected transformation has been proved to take place at position 4, leading to **6a,b**. By this latter selective ether formation the controlled substitution of the kynurenic skeleton can be prognostized.

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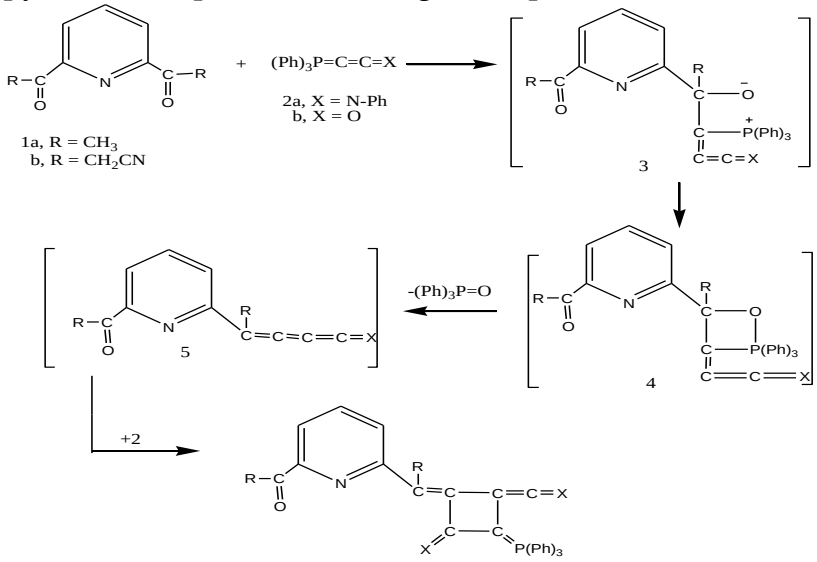
Reaction of Active and Stabilized Phosphours Ylides with Pyridine-diethanone and Oxopropanenitrile

It is well known that pyridine derivatives are widely used in medicine and agriculture as anticancer drugs[1], antihypertension medications, antiviral, herbicides, and pesticides. Herein we report on the synthesis and biological investigation of pyridine, phosphanylidene, cyclobutanes.[2-4] Therefore, a comparative study on the reactions of the active nucleophilic and stabilzied phosphonium ylide with pyridine-2,6-diethanone (**1a**) or pyridine-2,6-bis-oxopropanenitrile (**1b**) have been investigated. The reaction of the active (N-phenyliminovinylidene)- (**2a**) (oxovinylidene) triphenylphosphorane (**2b**) with compounds **1a** and **1b** afforded the corresponding phosphanylidene pyridine cyclobutanes (**6a-d**) along with triphenylphosphane oxide. Formation of the cyclobutane, **6a-d** occurs by the [2+2]-cycloaddition of the carbonyl group in **1** to the ylidic C-P bond of **2** to give the oxaphosphetane **4**, through the dipolar intermediate **3**. Expulsion of triphenylphosphane oxide, afforded the unstable ketene **5**, which is followed immediately by [2+2]-cycloaddition to a second molecule of **2** giving the four-membered ring phosphoranylidene, cyclobutane **6**. On the other hand, the reaction of the stabilized the phosphonium ylides namely, methoxycarbonyl- (**7a**), ethoxycarbonyl-(**7b**), acetyl-(**7c**), benzoyl methylenetriphenylphosphorane (**7d**) with the pyridine derivatives **1a** and **1b** in hot toluene afforded the corresponding olefins **11a-h**. In this case the ylide carbon atom adds to the carbonyl group to give the intermediate betaines **8**. In the second step a four member ring **9** is formed, which is decomposed into an olefin **10** and triphenylphosphane oxide. Compound **10** react with another molecule of the phosphorane to give the final products **11a-h**.

The structure of the new products was assigned according to consistent analytical and spectroscopic data (IR, ^{1}H-, ^{13}C-, ^{31}P-NMR and

MS). The new compounds will be evaluated as anticancer agents. So by simple methods we could prepare carbocyclic phosphours and olefinic pyridine compounds of biological importance.



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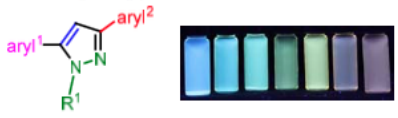
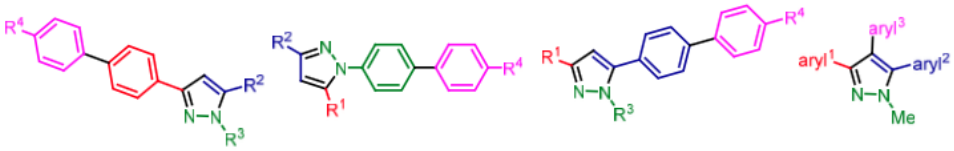
Consecutive Multicomponent Syntheses of Pyrazoles – Diversity-oriented Approach to Blue Emitters and Emission Solvatochromic Dyes

Pyrazoles are important UV absorbers(1) and due to their photophysical properties they have received considerable attention as optical brighteners in detergents(2), and highly selective fluorescence sensors(3). They often display blue emission and large Stokes shifts, which makes them suitable in OLED applications(4) and in dye-sensitized solar cells(5).

As part of our program to develop diversity-oriented syntheses of functional chromophores(6) we have disclosed approaches to substituted pyrazoles based upon consecutive multicomponent reactions based upon sequentially catalyzed processes(7). The substance libraries obtained by this approach allow comprehensive structure-fluorescence correlations and, eventually, the optimization of the fluorescence quantum yields. Furthermore, emission solvatochromic donor-acceptor pyrazole libraries can be efficiently generated.



Consecutive Four-Component Synthesis of Emission Solvatochromic Pyrazoles



Consecutive Four-Component Syntheses of Efficient Blue Emissive Pyrazoles

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Synthesis of Novel N-Heterocyclic Compounds Containing 1,2,3-Triazole Ring System via Domino-, "Click" and Retro Diels-Alder (RDA) Reactions

Isoindoloquinazolines are important heterocyclic ring systems that occur as a core structure in a variety of naturally occurring alkaloids and synthetic compounds. Several isoindoloquinazoline derivatives have a range of biological activity. 1,2,3-Triazoles are known as a promising class of *N*-heterocycles, they have exhibited cytotoxic, anti-HIV-1, acetylcholinesterase inhibitory, and antituberculosis activities.[1,2] These two ring containing heterocyclic compounds create a number of new possibilities of use, and therefore develop a simple and efficient synthesis can be particularly useful.[3] Herein, in continuation of our work on the synthesis of novel *N*-heterocycles[4], we report the synthesis of new racemic and enantiomeric *diendo*- and *diexo*-□-aminonorbornene *N*-propynyl amides **2a,b** and the results of their domino ring-closure reactions with 2-formylbenzoic acid followed by "click" and RDA reaction of the synthesized heterocycles.

When *diendo*- and *diexo*-*N*-propynyl amides **2a,b** were reacted with 2-formylbenzoic acid using microwave irradiation, a pentacyclic isoindolo[2,1-*a*]quinazolines **3a,b** were obtained diastereoselectively, which were then converted by "click" reaction of the terminal acetylene

group. The "click" reaction was carried out in the presence of a catalytic amount of copper (II) sulfate and sodium ascorbate with "in situ" prepared organic azide, and the expected 4-substituted 1,4-triazoles **4a,b** were formed. When subjected to a microwave-mediated RDA reaction, the pentacycles **3a,b** and **4a,b** provided tricyclic pyrimido[2,1-*a*]isoindoles **5** and **6** through loss of cyclopentadiene.

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Optimization Study of Preparation Twigs Tamarisk Trees Activated Carbon for Removal of Pesticides

Mesoporous activated carbon prepared from twigs tamarisk trees (TOT) using physiochemical activation (potassium hydroxide treatment and carbon dioxide gasification). Central composite design (CCD), two factor interaction (2FI) and quadratic models were employed to correlate the activated carbon preparation variables. The effects of the activation temperature, activation time and chemical impregnation ratios on the carbon yield, bentazon, carbofuran and 2,4-dichlorophenoxyacetic acid (2,4-D) removal were investigated. From the analysis of variance (ANOVA), the most influential factor on each experimental design response was identified. The optimum conditions for preparing activated carbon from twigs tamarisk trees were found to be activation temperature of 700.0 C, activation time of 1.00 h and chemical impregnation ratio of 2.0 The carbon yield was found to be 17.0% while the removal of bentazon, carbofuran and 2,4-D were found to be 84.0, 95.0 and 94.7%, respectively.

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Highly Selective and Sensitive Dual Channel Schiff Base Chemosensors for the Detection of Al(III), Fe(III) & Cu(II)

Chemosensor may be defined as a device which can convert a chemical signal into an electrical signal indicative of the presence of an analyte. Though many Schiff bases which find application as chemosensors are in the literature, schiff bases which are highly cost effective as well as of inimitable quality are not only limited in number but also much saught after.

The element aluminium is intertwined with our day to day activities. The proliferation of aluminium in human bodies retards numerous enzyme activities, thereby hampering iron metabolism coupled with severe damage to central nervous system. Aluminium absorption also causes alzheimer and parkinson's diseases. Besides, aluminium affects the life of aquatic animals by causing osmoregulatory failure in them.

Iron plays a vital role in human as well as animal health. However high levels of accumulation of Fe^{3+} ends up with many metabolic disorders, certain type of cancers and malfunction of organs like heart and liver.

Copper is essential for the growth and development of many organs like heart, brain and also bones. It plays a vital role in iron absorption as well as synthesis of various proteins and enzymes. It increases immunity and paralyzes free radicals that cause considerable damage to the cells.

The present report focuses on the study of cation sensing properties of two Schiff base receptors formed by the facile condensation of 2,4-dihydroxy acetophenone first with toluidine and then with anisidine and characterized by IR,UV, ^{1}H NMR and Mass spectral studies. Both the Schiff bases were grown into single crystals from 1:1 ethanol acetonitrile medium by slow evaporation technique and found to belong to monoclinic type with space group $P2_1/c$. Hirshfeld surface analysis based on DFT method with 3-21G as basis set was used to calculate various intermolecular interactions. Fingerprint plots were made to find out the percentage of different types of interactions and pie chart was also portrayed.

Cation recognizing profile of the two receptors was explored by UV-visible and fluorescence spectroscopy methods. Receptor 1 was ascertained to detect Al^{3+} ions and receptor 2 had a response for Fe^{3+} & Cu^{2+} ions , both over a panel of several other similar metal ions.

Absorption Studies

To evaluate the sensing ability, receptors 1 & 2 were made to interact with two equivalents of various metal ions such as Na^{+}, Mg^{2+}, Ca^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, $Fe^{3+,}$ Cu^{2+}, Zn^{2+}, Sr^{2+}, Cd^{2+}, Ba^{2+}, Hg^{2+}, Pb^{2+} & Al^{3+} . While receptor 1 had a successful interaction with Al^{3+} ions , receptor 2 had the same with Fe^{3+} & Cu^{2+} ions. These interactions were evidenced by the emergence of a new peak at 303nm in the absorption spectrum of receptor 1 and at 365nm & 461nm in the case of receptor 2. The synergistic ability was further corroborated by incremental titrations. These changes in the absorption behaviour of the receptors may be imputed to the formation of complexes between the receptors and the metal ions, thus paving the way for LMCT transitions.

Binding Constant and Stoichiometry

Binding constant of receptor 1 with Al^{3+} was determined to be $11.17x10^{3}$ and that of receptor 2 with Fe^{3+} & Cu^{2+} were $1.43x10^{2}$ and $1.65x10^{2}$ respectively.

Job's plot analysis hinted a 2 : 1 stoichiometry for complex formation between the receptors and metal ions.

Fluorescence Studies

As done in absorption studies, the two receptors were examined for fluorescence sensing properties with different metal cations. An enormous enhancement of fluorescence intensity of about 117 fold with a substantial blue shift to an extent of 50nm was caused during the trapping of Al^{3+} ion by receptor 1; whereas a bathochromic shift of 60nm & 50nm was the result of sensing of Fe^{3+} and Cu^{2+} ions by receptor 2. A very small amount of quenching was also observed with receptor 2. The fluorescence enhancement may be ascribed to the formation of rigid complex chelate system indicating the presence of CHEF effect and the quenching may be probably due to electron or energy transfer process between the metal ion and receptor 2.

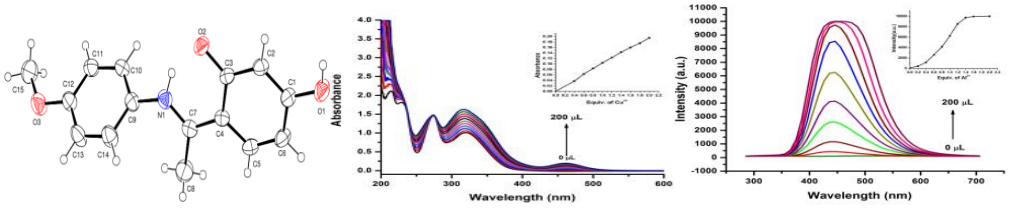
Selectivity and Reversibility

To ascertain the selectivity and reversibility of receptor 1 towards Al^{3+} and that of receptor 2 towards Fe^{3+} & Cu^{2+} ions in the midst of various competing ions, fluorescence behaviour of the receptors was scrutinized in the presence of all other metal ions taken for study.While we could notice no interference by competing species in receptor 2, we could understand that interference was induced by Fe , Mg and Pb in the case of receptor 1.

The reversibility of the receptors' sensing action was evaluated by EDTA titrations. Upon addition of two equivalents of EDTA to a solution of receptor 1 & Al^{3+}, receptor 2 & Fe^{3+} and receptor 2 & Cu^{2+} , absorption as well as emission patterns similar to that of a free receptor were procured, proving indubitably the reversible nature of the sensing function of receptors.

The detection limit of receptor 1 for Al^{3+} was 6.5318×10^{-9} M and limits of receptor 2 for Fe^{3+} & Cu^{2+} were 1.265×10^{-6}M & 4.086×10^{-6}M respectively.

It can be concluded that Schiff base receptors prepared from commonly available reagents could act as cost effective, selective, sensitive and reversible sensors for Al^{3+}, Fe^{3+} & Cu^{2+} ions over many other metal ions.



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Spatial Chaos, Multifractal Vector Fields and Stochastic Clifford Algebra

There have been numerous attempts to analyse and simulate chaotic systems whose spatial extension is of prime importance, such as turbulence, weather and climate. This was done at first with mono/uni-scaling approaches (e.g. structure functions, rescaled range or spectral analyses), however multifractal techniques are required to grasp the fundamental feature of intermittency, to track and simulate the scaling singularities of the underlying equations instead of relying on numerical, scale truncated simulations of these equations (e.g. Royer et al., 2008, Lovejoy and Schertzer, 2013 for climate).

Domains of multifractal fields can arbitrarily large, but on the contrary their codomains have been rather restricted to be 1D. This prevents to deal with the key question of complex component interactions and their non trivial symmetries. The latter are unfortunately indispensable to answer to challenging questions such as the climatology of (exo-) planets based on first principles (Pierrehumbert, 2013) or to fully address the question of the relevance of quasi-geostrophic turbulence and to define an effective, fractal dimension of the atmospheric motions (Schertzer et al., 2012).

Orthogonal rotations and mirror symmetries are used to generate a Clifford algebra of stable Levy generators of multifractal cascades with arbitrarily large codomains, e.g. large dimensional manifolds. These processes are endowed with universal statistical and robust algebraic properties, both defining the basic symmetries of the corresponding fields (Schertzer and Tchiguirinskaia, 2015).

In this presentation, we will emphasise respective role of the spherical and hyperbolic geometries depending on the signature of the quadratic form of the algebra. This should help to overcome current obstacles to the use of multifractal analysis and simulation at their full extent.

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Citizen Science in the Context of Indigenous Knowledge

The conduct of scientific work by members of the general public is broadly called "Citizen Science". The attention and popularity that this practice has gained in recent years stem from the realization of the vital role it can play in the acquisition of knowledge about the natural world. Modern technological advances have also played an important role in its proliferation. Citizen science has been practiced for years in a variety of forms. This presentation will discuss the practice of citizen science in the context of Indigenous Knowledge.

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First Fluorenylidene Double Bridged Paraben Substituted Cyclotriphosphazene Compounds and DNA Interaction Analysis

Background: Interaction between DNA and drugs are commonly studied for drug discovery and also pharmaceutical development processes. Cyclophosphazene compounds with anti-microbial and anti-tumor activity have been investigated in cancer cell lines. Moreover, they have also been analysed as anti-cancer agents in different studies whether to provide potential drug molecules or not (Patel et al., 2012; Çiftçi et al., 2016).

Methods: Firstly the reactions of hexachlorocyclotriphosphazene (trimer) (**1**) with 4,4′-(9-fluorenylidene) dianiline (**2**) were studied and polyaromaticfluorenylidene double bridgedcyclotriphosphazene compounds (**3**) were obtained. Then, the reaction of these compounds (**3)**with parabens: methyl 4-hydroxybenzoate, (**4**); ethyl 4-hydroxybenzoate, (**5**); propyl 4-hydroxybenzoate, (**6**); butyl 4-hydroxybenzoate (**7**), benzyl paraben (**8**) were performed, respectively. Fluorenylidene double bridged full paraben substituted cyclotriphosphazene compounds (**9-13**) were obtained. All products were fully characterisated by mass spectrometry, ^{31}P NMR and ^{1}H spectroscopy. Interactions between pUC18 plasmid DNA and fluorenylidene double bridgedparaben substituted cyclotriphosphazene compounds (**3**, **9-13**) were examined by DNA-binding activities with agarose gel electrophoresis technique.

Results: The native plasmid form of DNA is called covalently closed circular or supercoiled DNA (form I). When DNA strands are cut or damaged the single nicked open circular form (form II) or linearized DNA (form III) plasmid occurs. The effects of the compounds on DNA were examined by analyzing the existence of the Form I, II and III of DNA on agarose gel electrophoresis. We found that the lowest

concentration (7.81 uM) of compound 3 resulted in the breakage of DNA to create form III (linear). Moreover, all the doses of the compound 9 showed the creation of form III. Therefore, we concluded the interaction between the compound and the plasmid DNA. The electrophoresis lines clearly indicated difference in concentration depended on DNA effect of compound 13 from 15.63 to 125 µM, while no difference was observed between the control lines and the lowest compound concentration (7.81 µM) tested.

Conclusions: This study showed that these compounds affect the plasmid DNA, causing a noteworthy increase in form II and form III. From the synthesized products, compounds (**3**, **9-13**) had also shown DNA binding properties that show their potential drug molecules.

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