EuroSciCon

DAY 1

Scientific Tracks & Abstracts

6th Edition of International Conference and Exhibition on

Organic Chemistry

August 16-17, 2018 | Dublin, Ireland

DAY 1

August 16, 2018

Sessions

Computational Advances in Organic Chemistry | New Developments in Organic Chemistry | Medicinal and Bioorganic Chemistry | Physical Organic Chemistry | Organocatalysis and New Strategies | Organic Synthesis and Technologies | Organic Materials & Supramolecular Chemistry | Nanoparticles in Organic Chemistry

Session Chair
Elena R Milaeva
Lomonosov Moscow State University, Russia

Session Co-Chair
Alexander O Terentev
Russian Academy of Sciences, Russia

Session Introduction

Title: Organic and organometallic derivatives of α-tocopherol mimetics as promising antioxidants with dual functionality

Elena R Milaeva, Lomonosov Moscow State University, Russia

Title: Oxidative cross-coupling with C-O bond formation

Alexander O Terentev, N D Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, Russia

Title: Alginate and carrageenan-nanocellulose composite beads for efficient removal of metal cations

Korany A Ali, National Research Centre, Egypt

Title: DNA repair enzymes inhibition as a promising approach to new anti-cancer drugs

Konstantin Volcho, Novosibirsk State University, Russia

Title: Selected pesticides as acetylcholine esterase inhibitors: Theoretical and experimental studies

Biljana B Arsic, University of Nis, Republic of Serbia

Title: The synthesis of 3-amino-1-hetarylfluorene derivatives and their unprecedented side products

Ergin Yalcin, Gazi University, Turkey

Title: Nanocatalysis by sustainable advanced materials

Mian Gul Sayed, Institute of Chemical Sciences University of Swat KP, Pakistan

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Elena R Milaeva, J Org Inorg Chem 2018, Volume 4
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ORGANIC AND ORGANOMETALLIC DERIVATIVES OF α-TOCOPHEROL MIMETICS AS PROMISING ANTIOXIDANTS WITH DUAL FUNCTIONALITY

Elena R Milaeva
Lomonosov Moscow State University, Russia

The presentation will focus on a novel approach to construction of physiologically active organic and organometallic compounds based on computer-aided design, new synthetic approaches and extensive biological screenings. This study is focused on the design of hybrid compounds possessing 2,6-dialkylphenol group with dual modes of action – prooxidative activity and antioxidative activity. The presence of metal atom allows extensive modification including coordination to the targeted specific groups to control and tune toxicity-activity profiles. The synthesis and biological activity will be discussed. The anti/prooxidant activity has been studied *in vitro*, *ex vivo*, *in vivo* experiments.

Biography

Elena R Milaeva pursued PhD at the A N Nesmeyanov Institute of Organo-element Compounds of Russian Academy of Sciences in 1980. She is currently a Professor of organic chemistry, head of the department of medicinal chemistry & fine organic synthesis at Lomonosov Moscow State University respectively. Her research interests include: organic chemistry, medicinal chemistry, organometallic chemistry.

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Alexander O Terent'ev et al., J Org Inorg Chem 2018, Volume 4
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OXIDATIVE CROSS-COUPLING WITH C-O BOND FORMATION

Alexander O Terentev, Alexander S Budnikov, Stanislav A Paveliev and **Oleg V Bityukov**

N D Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Russia

Oxidative cross-dehydrogenative coupling methodology lies in the modern trend of organic chemistry. It eliminates necessity for installation of additional functional groups and affords direct coupling in one stage (via selective C-H activation) with limited amount of wastes, high atom- and step- economy. Oxidative cross-dehydrogenative C-C coupling were studied in detail; the C-N, C-P, and C-O cross-coupling reactions are less well developed. It is difficult to achieve high selectivity in the cross-dehydrogenative C-O coupling because the starting compounds are prone to side oxidation and fragmentation reactions giving, for example, alcohols and carbonyl compounds. This gives rise to a problem of searching for oxidizing agents and reaction conditions suitable for the cross-coupling of different types of substrates. We discovered oxidative cross C-O coupling of 1,3-dicarbonyl compounds, their heteroanalogs and heterocycles with peroxides, oximes and hydroxyamides. The best result obtained with the use of the widely available copper, iron, manganese or lanthanide salts as catalysts or oxidants.

Recent Publications

1. **A O Terentev et al. (2014) Iminoxyl radical based strategy for intermolecular C-O bond formation: cross dehydrogenative coupling of 1,3 dicarbonyl compounds with oximes. Adv. Synth. Catal. 356(10):2266-2280.**
2. **I B Krylov, V A Vil' and A O Terent'ev (2015) Cross-dehydrogenative coupling for the intermolecular C-O bond formation. Beilstein J. Org. Chem. 11(2015):92-146.**
3. **I B Krylov et al. (2017) Selective cross-dehydrogenative C–O coupling of N-hydroxy compounds with pyrazolones: introduction of the diacetyliminoxyl radical into the practice of organic synthesis Org. Chem. Front. 4(10):1947-1957.**

Biography

Alexander O Terentev pursued PhD Degree (2000); DSc Degree (2009). He worked as a Professor at the D Mendeleev University of Chemical Technology of Russia (2011). He became the head of laboratory at N D Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences (2014), head of laboratory in All Russian Research Institute of Phytopathology (2016). He has published 3 chapters of books, 100 research papers, and 30 patents. His research interests include: organic chemistry, medicinal and agricultural chemistry and chemical technology.

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ALGINATE AND CARRAGEENAN-NANOCELLULOSE COMPOSITE BEADS FOR EFFICIENT REMOVAL OF METAL CATIONS

Korany A Ali and **Samir Kamel**
National Research Centre, Egypt

Different modified bio-polymeric matrices of carrageenan and alginate with cellulosic nonmaterial were prepared in the form of beads. The nanocellulosic materials were prepared from dissolved bagasse pulp and include cellulose nanocrystals (CNC), cellulose nanofibers (CNF) and tricarboxy cellulose nanofibers (TPC-CNFs). The prepared bio-polymeric matrixes were characterized by transmission electron microscopy (TEM), FT-IR (Fourier transform infrared spectroscopy), X-ray diffraction (XRD) and scanning electron microscope (SEM). The capabilities of the modified bio-polymeric matrices beads to chelate several metal cations were evaluated and showed high removal efficiency towards removing Ca^{2+}, Mg^{2+}, Fe^{2+}, Pb^{2+}, Cu^{2+} metal cations.

Biography

Korany A Ali is working as an Associate Professor at National Research Centre, Egypt.

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DNA REPAIR ENZYMES INHIBITION AS A PROMISING APPROACH TO NEW ANTI-CANCER DRUGS

Konstantin Volcho[1,2]

[1]N N Vorozhtsov Novosibirsk Institute of Organic Chemistry RAS, Russia
[2]Novosibirsk State University, Russia

The cytotoxic effects of chemotherapy and radiation that are clinically used to treat malignances are directly related to their propensity to generate DNA damage. The capacity of cancer cells to recognize DNA damage and initiate DNA repair is a key mechanism for therapeutic resistance to chemotherapy. Therefore, the targeting of DNA repair enzymes can be used as a strategy to potentiate the cytotoxicity of the currently available DNA damaging agents towards cancer cells. PARP1 (poly ADP ribose polymerase 1, the enzyme involved in DNA repair) inhibitors such as Olaparib, Rucaparib and Niraparib are in clinical use already. New and very promising target for antitumor therapy is tyrosyl-DNA phosphodiesterase 1 (Tdp1). It plays a key role in the removal of DNA damage resulting from inhibition of topoisomerase 1 (Topo1) with camptothecin and its clinical derivatives irinotecan and topotecan. Furthermore, Tdp1 is known to be capable of removing the DNA damage induced by other anticancer drugs commonly used in clinical practice. To date, a number of Tdp1 inhibitors of various types including dual Tdp1/Topo1 inhibitors are known. A set of very potent Tdp1 inhibitors was found by us among natural products derivatives. We designed new inhibitors using targeted modifications of terpenoids, coumarins, usnic acid and other types of natural products. Moreover, we found that benzopentathiepine derivatives are very effective inhibitors of Tdp1. Important that the ability of the inhibitors used in non-toxic concentration to enhance the cytotoxicity of camptothecin and topotecan, the established topoisomerase 1 poison, was demonstrated. Thus, we discovered of new original Tdp1 inhibitors, effectively inhibiting DNA repair in tumor cells for use as the components of complex anticancer drugs.

Biography

Konstantin Volcho pursued his PhD in 1997 from Novosibirsk State University, Russia. Since then he has been working in the department of medicinal chemistry at Novosibirsk Institute of Organic Chemistry (Russia). He is a Professor of Russian Academy of Sciences. His research interests include development of novel treatments against nervous system disorders, antivirals and anticancer agents, usually based on natural products derivatization. He has published about 150 papers in reputed journals. He is an inventor in more than 35 issued patents. Three compounds found with his participation are currently in preclinical studies as anti-parkinsonian, analgesic and antidepressant agents.

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Biljana B Arsić et al., J Org Inorg Chem 2018, Volume 4
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SELECTED PESTICIDES AS ACETYLCHOLINE ESTERASE INHIBITORS: THEORETICAL AND EXPERIMENTAL STUDIES

Biljana B Arsić[1,2], Milan Mladenović[3], Nevena Stanković[3], Nezrina Mihović[3], Rino Ragno[4,5] Andrew Regan[2], Jelena Milićević[6], Tatjana M Trtić Petrović[6] and **Ružica Micić[7]**

[1]University of Niš, Republic of Serbia
[2]The University of Manchester, UK
[3]University of Kragujevac, Republic of Serbia
[4]Sapienza University of Rome, Italy
[5]Alchemical Dynamics, Italy
[6]Vinča Institute of Nuclear Sciences, University of Belgrade, Republic of Serbia
[7]University of Priština, Republic of Serbia

Ligand-based or structure-based *in silico* methods, as well as *in vitro* methods were used for the evaluation of the inhibition of *Mus musculus* and *Homo sapiens* acetylcholinesterase by commercially available selected pesticides. Crystal structures of simazine, monocrotophos, dimethoate, and acetamiprid were used for the unconstrained conformational search with various force fields (FFs) implemented in Monte Carlo/Multiple Minimum (MC/MM) approach. Unconstrained conformational searches were applied in the determination of intersynaptic pre-bound conformations of other commonly used pesticides (atrazine, propazine, carbofuran, carbaryl, tebufenozide, imidacloprid, diuron, monuron, and linuron). Moreover, energies of global minima, calculated with the best performing FFs, were compared with selected pesticides toxicities against *Mus musculus*. For the majority of pesticides, low energies of global minima in pre-bound states correlate with high toxicity. The targeted pesticides are acetylcholinesterase (AChE) inhibitors, so structure-based (SB) studies, in the form of molecular docking and molecular dynamics (MD) on either *Mus musculus* AChE (mAChE) or *Homo sapiens* AChE (hAChE), were performed to predict their pharmacology. The mechanistic pathways were established, and additionally confirmed by QM DFT mechanistic studies, which can be further used in the discovery of novel pesticides with desirable lower toxicity against humans. We paid special attention to the mechanism of hAChE inhibition by atrazine, propazine, and simazine. The QM DFT (quantum mechanics – density functional theory) mechanistic studies implied that atrazine, propazine, and simazine could be considered as reversible hAChE inhibitors, administered in high concentrations, and confirmed by concentration-dependent kinetic studies of hAChE inhibition.

Biography

Biljana B Arsic pursued her PhD on the investigation of macrolide antibiotics as anti-bacterial and potential anti-malarial medicines at The University of Manchester, United Kingdom. She is a scientific associate in the department of mathematics, faculty of sciences and mathematics, University of Nis, Republic of Serbia. She has published 37 papers in peer-reviewed journals in english, two books in Serbian related to teaching, one chapter in the edited book in english, and attended numerous conferences and symposia. She worked as an associate editor, also was a member of the editorial board, and is currently reviewer for numerous journals in english.

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Ergin Yalcin, J Org Inorg Chem 2018, Volume 4
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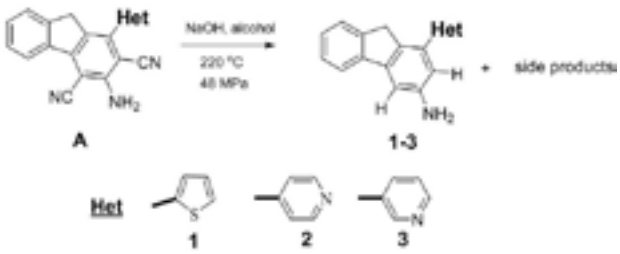
THE SYNTHESIS OF 3-AMINO-1-HETARYLFLUORENE DERIVATIVES AND THEIR UNPRECEDENTED SIDE PRODUCTS

Ergin Yalcin
Gazi University, Turkey

Aminofluorene and its derivatives have proved to be one of the most widely studied candidates among in cancer research. They have also found its applications as efficient ds-RNA fluorescent probe. Most common approach for the synthesis of aminofluorene is based on the hydrogenation of corresponding nitro/nitrile fluorenes as starting material. However, to the best of our knowledge, decyanization reaction has never been used to obtain 1-hetarylsubstituted-3-aminofluorene. Furthermore, the desired compounds are also difficult to afford through conventional protocols such Suzuki coupling, functionalizing of bromide substituted fluorene etc. The decyanization reaction provides not only the removal of cyano groups from the structure but also unprecedented side products because of harsh reaction conditions, such as the alkylated 1-hetaryl-3-aminofluorene derivatives. In this study, on a facile protocol to obtain 1-hetaryl-3-aminofluorene and its side products besides the catalytic reduction of various corresponding nitro-substituted fluorene compounds which are difficult to synthesize by other methods. Furthermore, a proposed mechanism has been outlined for the achieved novel type of aminofluorene products by means of XRD, Mass and NMR spectroscopy.



Recent Publications

1. Yalcin Ergin et al. (2017) Novel fluorene/fluorenone DNA and RNA binders as efficient non-toxic ds-RNA selective fluorescent probes. Tetrahedron. 74(5):535-543.

2. B Sahoo et al. (2017) Biomass-derived catalysts for selective hydrogenation of nitroarenes. ChemSusChem. 10(15):3035-3039.

3. Formenti Dario et al. (2017) Co-based heterogeneous catalysts from well-defined α-diimine complexes: discussing the role of nitrogen. Journal of Catalysis. 351:79-89.

Biography

Ergin Yalcin currently works at the Graduate School of Natural and Applied Sciences of Gazi University. His research interest focuses on the synthesis of novel ligands which may have interaction with biomolecules (G-Quadruplex DNA, ds-DNA, RNA etc.) that have a challenging task to identify biological important processes. He is also interested in: Ligand- DNA/RNA interaction, supramolecular chemistry and sensing of molecules.

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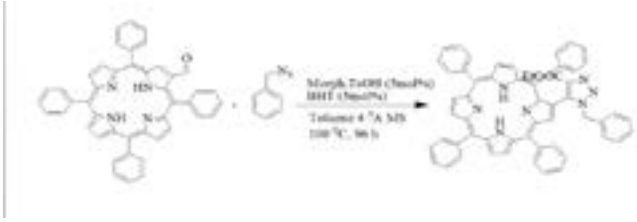
METAL FREE SYNTHESIS OF BETA-TRIAZOLE TETRA PHENYL PORPHYRINS AND RELATED COMPOUNDS

Mian Gul Sayed
University of Swat, Pakistan

The convergence of supramolecular chemistry and polymer science especially porphyrin chemistry offers many powerful approaches for building functional nanostructures with well-defined dynamic behavior. The efficient metal-free three-component reactions to synthesize 1,4,5-trisubstituted 1,2,3-porphyrin-triazoles from available materials, such as porphyrin-aldehydes, nitroalkanes, and organic azides, and also from porphyrin aldehydes, nitroalkanes, and porphyrin azides is described. The process is enabled by an organocatalyzed (morpholine:p-toluenesulfonicacid) Knoevenagel condensation of the formyl group with the nitro compound, which is followed by the 1,3-dipolar cycloaddition of the azide to the activated alkene. The reaction features an excellent substrate scope, and the products are obtained with good yield and regioselectivity. This methodology was used for the synthesis of fused triazole heterocycles from nitroporphyrin and organic azides.



Biography

Mian Gul Sayed completed his PhD from the University of Malakand, Dir Lower Khyber Pakhtunkhwa, Pakistan. He did his research in the department of chemistry Ku Leuven University at Belgium under the supervision of Professor Wim Dehaen. He is currently serving as an Assistant Professor at the Institute of Chemical Sciences of University of Swat, Khyber Pakhtunkhwa, Pakistan.

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DAY 2

Scientific Tracks & Abstracts

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DAY 2

August 17, 2018

Sessions

Organic Synthesis and Technologies | Organic Materials & Supramolecular Chemistry | Nanoparticles in Organic Chemistry

Session Chair
Shigeki Matsunaga
National Institute of Technology Nagaoka College, Japan

Session Co-Chair
Alexander Khenkin
Weizmann Institute of Science, Israel

Session Introduction

Title: **Stereocontrolled synthesis of chiral N- and O-heterocycles**

Don M Coltart, University of Houston, USA

Title: **Nanocatalysis by sustainable advanced materials**

Manoj B Gawande, Regional Centre of Advanced Technologies and Materials Palacky University, Czech Republic

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Don M Coltart, J Org Inorg Chem 2018, Volume 4
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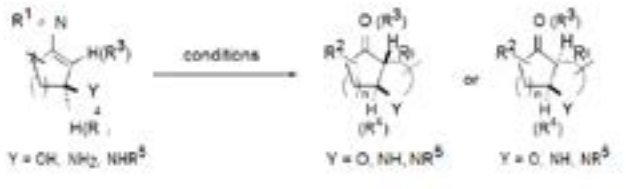
STEREOCONTROLLED SYNTHESIS OF CHIRAL N- AND O-HETEROCYCLES

Don M Coltart
University of Houston, USA

Greater than 80% of drugs and biologically active natural products are nitrogen- or oxygen-based, and many of these exist as nitrogen or oxygen heterocycles. While many such drugs and natural products are also chiral, relatively few contain chiral nitrogen/oxygen heterocycles, a limitation that is due in large part to a lack of effective and broadly applicable methods for their preparation. However, as drug development moves away from the use of unsaturated (flat), structurally simple achiral compounds and seeks out more stereochemically sophisticated chiral compounds having higher degrees of saturation, the need for methods for the synthesis of chiral nitrogen/oxygen heterocycles has become increasingly important. We have developed stereocontrolled synthetic approaches to a wide range of saturated and partially saturated chiral nitrogen/oxygen heterocycles through the use of two newly developed azoalkene-based moieties, the details of which are described herein.



Recent Publications

1. **Uteuliyev M M, Nguyen T T and Coltart D M (2015) Diastereoselective addition of Grignard reagents to α-epoxy N-sulfonyl hydrazones. Nature Chem. 7:1024-1027.**
2. **Hatcher J M, Kohler M C and Coltart D M (2011) Catalytic asymmetric addition of thiols to nitrosoalkenes leading to chiral non-racemic α-sulfenyl ketones. Org. Lett. 13(15):3810-3813.**
3. **Hatcher J M and Coltart D M (2010) Copper-(I) catalyzed addition of Grignard reagents to in situ-derived N-sulfonyl azoalkenes: an alkylation procedure applicable to the formation of up to three contiguous quaternary centers. J. Am. Chem. Soc. 132(13):4546-4547**

Biography

Don M Coltart obtained his Master's Degree from the University of Manitoba (Canada) under the supervision of Professor James L Charlton and then joined the research group of Professor Derrick L J Clive at the University of Alberta where he obtained his PhD. His Postdoctoral work was conducted at the Memorial Sloan-Kettering Cancer Center as Natural Sciences and Engineeering Research Council, Alberta Heritage Foundation for Medical Research, and CRI Scholar under the supervision of Professor Samuel J Danishefsky. He began his independent career at Duke University in 2004 and moved to the University of Houston in 2012 where he is an Associate Professor. His research interests include: the development of methods for asymmetric carbon–carbon bond formation, the application of those methods to the total synthesis of structurally complex biologically active natural products, and the study of those compounds in biological systems.

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NANOCATALYSIS BY SUSTAINABLE ADVANCED MATERIALS

Manoj B Gawande
Regional Centre of Advanced Technologies and Materials Palacky University, Czech Republic

Advanced nanocomposites have contributed to catalysis and are prime choice for the researchers in various important catalytic protocols and benign conversions. The nanocatalysts include magnetic-nanocomposites, carbon-based nanomaterials, core-shell (Pd@Pt) catalysts and morphology-dependent iron oxides. Sustainable nanotechnology improvements over the years have recommended significant and extraordinary series of progresses in the design of heterogeneous nanocatalysts. Notably, nanomaterials for catalysis can now be envisioned and organized with need for exact catalytic applications. Core-shell nanocomposites, morphology-dependent iron oxide and metal supported nanoparticles can be synthesized via more ecological paths with distinctive structure, morphology and composition. Our recent research activity on the practice of nanomaterials/ nanocatalyst and its catalytic applications will be highlighted.

Recent Publications

1. **Gawande M B et al. (2014) Microwave-assisted chemistry: synthetic applications for rapid assembly of nanomaterials and organics. Account of Chemical Research. 47(4):1338-1348.**
2. **Gawande M B, Branco P S and Varma R S (2013) Nano-magnetite (Fe3O4) as a support for recyclable catalysts in the development of sustainable methodologies. Chemical Society Reviews. 42(8):3371-3393.**
3. **Gawande M B et al. (2015) Core–shell nanoparticles: synthesis and applications in catalysis and electrocatalysis. Chemical Society Reviews. 44(21):7540-7590.**
4. **Goswami A et al. (2017) In Situ generation of Pd–Pt core–shell nanoparticles on reduced graphene oxide (Pd@Pt/rGO) using microwaves: applications in dehalogenation reactions and reduction of olefins. ACS Applied Material and Interfaces. 9(3):2815-2824.**

Biography

Manoj B Gawande pursued his PhD Degree in Chemistry in 2008 from the Institute of Chemical Technology, Matunga, Mumbai, India. After several research stints in Germany, South Korea, Portugal, Singapore, and England presently, he is working as an Associate Professor and Head of Nanocatalysis Group at RCPTM, Faculty of Science, Palacky University, Olomouc, Czech Republic. His research interests include: nanocatalysis and advanced nanomaterials and their applications. He is currently supervising several Doctoral students and Postdoctoral workers. He has published over 90 scientific publications, including reviews, patents, editorials, and articles. In 2017, he was admitted as a Fellow of Royal Society of Chemistry (RSC), UK.

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