





### Annual Congress on

# Medicinal Chemistry, Pharmacology & toxicology

July 30-31, 2018 Amsterdam, Netherlands

Medchem & Toxicology 2018

# **DAY 1** July 30, 2018

### Sessions

Medicinal Chemistry | Organic Chemistry | Immuno toxicology | Novel Targer drugs to the treatment of cancer | Drug discouvery and development | Reproductive and Developmental Toxicology | Food and Nutritional Toxicology | Environmental Toxicology | Pharmaceutical Sciences

Session Chair Alexander Terent'ev N.D. Zelinsky Institute of Organic Chemistry RAS, Russia Session Co-Chair Rocky Costello R.C. Costello & Assoc. Inc., USA

Session Introduction

Synthesis and evaluation of anisomelic acid like compounds for the treatment of HPV-mediated carcinomas
Yury Brusentsev, Abo Akademi University, Finland
Antibiotic peptides and antimicrobial secondary metabolites from endophytes of seaweeds
Chanda V. Berde-Parulekar, Gogate Jogalekar College, University Of Mumbai, India
Pesticide residues in Indian food and agricultural products
Madhura Mukadam, Gogate Jogalekar College, University Of Mumbai, India
Bioremediation of textile dye wastewater by using microbial isolates from dye effluents
Vikrant Berde, Gogate Jogalekar College, University Of Mumbai, India
Application of beta-cyclodextrins: from formulation to orphan drug
Miklos Vecsernyes, University of Debrecen, Hungary
A quasi-steady-state approximation to the basic target-cell-limited viral dynamics model with a non-cytopathic effect
Richard Cangelosi, Gonzaga University, Spokane, Washington, USA





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Yury Brusentsev et al., J Org Inorg Chem 2018, Volume 4 DOI: 10.21767/2472-1123-C3-008

## SYNTHESIS AND EVALUATION OF ANISOMELIC ACID LIKE COMPOUNDS FOR THE TREATMENT OF HPV-MEDIATED CARCINOMAS

Rajendran Senthilkumar<sup>1</sup>, Yury Brusentsev<sup>2</sup>, Preethy Paul<sup>1</sup>, Fang Cheng<sup>1</sup>, Maria Sippola-Thiele<sup>1</sup>, Patrik Eklund<sup>2</sup> and John E Eriksson<sup>1</sup>

<sup>1</sup>Turku Centre of Biotechnology, Finland <sup>2</sup>Abo Akademi University, Finland

uman papillomavirus (HPV) infection is now a well-established cause of different types of cancer including but not limited to cervical cancer. There are currently no specific treatments for patients with HPV-driven cancers. One common denominator of the HPV genotypes is the E6 and E7 proteins, which are mainly responsible for malignant and non-malignant phenotypes. Hence, they represent valuable targets for therapeutic intervention in HPV-driven cancers. We have already successfully shown a natural diterpenoid, anisomelic acid (AA) down-regulates E6 and E7 oncoproteins, leading to efficient inhibition of cell growth and induction of apoptosis. During the optimization of AA synthesis, we have identified few small molecules, which preferentially targets the HPV E6 and E7 proteins similar to AA mode of action, but, more efficient than AA in inducing apoptosis in cervical cancer cells. Furthermore, these 'HIT' molecules also showed specificity in killing HPV positive cells with different genotypes compared with human primary skin fibroblast cells. Indeed, cancer xenograft models in nude mice demonstrated proof of principle, where a decrease in tumour size was observed in HPV-driven tumours treated with our HIT compound(s).

#### Biography

Yury Brusentsev obtained his Master's degree in Chemistry from Moscow State University in 2003. He worked as a Researcher in R&D (drug development) for Pharmaceutical industry until 2009 and moved back to academia and received his PhD in 2017, the group of Patrik Eklund at Abo Akademi University. Now he is carrying out chemistry part of the drug discovery projects (drug design and synthesis of drug candidates) as a Postdoc researcher. His research interests are in Medicinal Chemistry, Advanced Organic Synthesis and Organometallic Chemistry.

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## ANTIBIOTIC PEPTIDES AND ANTIMICROBIAL SECONDARY METABOLITES FROM ENDOPHYTES OF SEAWEEDS

### Chanda V. Berde-Parulekar<sup>1</sup> and Upendra Lele<sup>2</sup>

<sup>1</sup>Assistant Professor,Gogate Jogalekar College, Ratnagiri, Maharashtra. India. <sup>2</sup>M.Sc Microbiology student, Gogate Jogalekar College, Ratnagiri, Maharashtra, India.

ndophytic bacteria are the bacteria which reside in symbiotic association Linside the cell. They have been shown to produce the same metabolites as that of seaweeds from which they are isolated. They also show many unusual but useful characteristics like production of vitamins, growth hormones for seaweeds, some host defence chemicals and metabolites. These endophytes can be isolated from the seaweeds and can be analyzed for their different activities in-vitro using different methods. Marine macroalgae are known to carry diverse bacterial communities which interact with their hosts in both harmful and beneficial ways. Algae hosts provide the bacteria with a rich source of carbon in the form of carbohydrate polysaccharides such as fucoidan, agar and alginate, which the bacteria enzymatically degrade. Thus, the major objective of the present study was to isolate, identify and characterize endophyte bacterial communities of different seaweed species Antibiotic peptides are one of the most important secondary metabolites produced by bacteria. These peptides are potent, broad spectrum antibiotics which demonstrate potential as novel thearapeutic agents. Due to vast array of resistivity against antibiotics shown by microorganisms; thus need of antimicrobial agent has come on the market last 30 years. The solution to this problem is peptide antibiotics. Peptide antibiotics have direct activity on the cell-wall of microorganisms causing disruption of cell membrane. Endophytic bacterial isolates were identified to species level by 16S rRNA gene sequence homology analysis and encompassed Gram-negative and Gram positive bacterial taxa. All bacterial isolates were screened for antimicrobial activity against the pathogenic test strains. This study provides the first account of the diversity and composition of bacterial populations of endophytes and demonstrates the ability of these bacteria to produce antimicrobial compounds. Despite recent advances in metagenomics, this study highlights the fact that traditional culturing technologies remain available tool for the discovery of novel bioactive compounds of bacterial origin.

**Keywords**— Sea-weeds, endophytic bacteria, antibiotic peptides, antimicrobial activity, protein purification, 16S rRNA sequence homology.

#### Biography

Dr. Chanda V. Berde Parulekar has completed her PhD at the age of 28 years from Microbiology Department of Goa University, Goa, India following 2 years of postdoctoral studies from the same department. She is involved in teaching and research in the field of Biotechnology for the past 12 years. She has 30 research publications in reputed journals, 2 book publications, 2 chapters in books in the pipeline and is an Editorial board member of JPABS. She has guided 62 M.Sc. research projects in Biotechnology and Microbiology. She has also attended more than 15 conferences, national and international. She is on the Board of Directors of Society for Environment, Biodiversity and Conservation, India.

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Madhura Mukadam, J Org Inorg Chem 2018, Volume 4 DOI: 10.21767/2472-1123-C3-008

## **PESTICIDE RESIDUES IN INDIAN FOOD AND AGRICULTURAL PRODUCTS**

### Madhura Mukadam

Gogate Jogalekar College, University Of Mumbai, India

he article aims to present an overview of various aspects of pesticide residues including their accumulation in food products, impact on human health, and the preventive measures to counter their toxic effects. Pesticides are considered a vital component of modern farming, playing a major role in maintaining high agricultural productivity. These are widely used in agriculture mainly to increase crop yields to cater huge supply of food products for increasing world population as well as to protect crops from pests and control insect-borne diseases. In the recent past, pesticide related issues have been extensively highlighted in the media including research journals and attracted wider debate and sharp focus among the interested groups in India. Indiscriminate and excessive application of synthetic pesticides damaged not only the environment and agriculture but also has entered into the food chain thereby affecting health and development. Pesticide residues are present in all agro-ecosystems, but the real risk to human health is through exposure to residues in primary and derived agricultural products. Accumulated pesticide residues in food products have been associated with a broad variety of human health hazards, ranging from short-term impacts such as headaches and nausea, to chronic impacts, such as various cancers, birth defects, infertility, and endocrine disruption. There is an urgent need to develop comprehensive intervention measures to reduce the potential health risk to consumers. The impact of pesticide residues can be minimized by taking certain measures such as the rational use of pesticides, promoting organic farming, exploit natural and bio pesticides, and proper implementation and amendment of pesticiderelated laws. It is also essential to improve the monitoring and surveillance programs and research on the topic, as well as training of health professionals to identify and report the cases of pesticide poisoning.

#### Biography

Madhura Mukadam has completed her PhD from University of Mumbai. She is working as an Associate Professor in Department of Zoology, Gogate Jogalekar College, Ratnagiri. She has published more than 30 papers in reputed journals and has been serving as an Editorial Board Member of repute.

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# BIOREMEDIATION OF TEXTILE DYE WASTEWATER BY USING MICROBIAL ISOLATES FROM DYE EFFLUENTS

### Chanda V Berde Parulekar<sup>1</sup>, Sagar P Salvi<sup>1</sup> and Vikrant B Berde<sup>2</sup>

<sup>1</sup>Gogate Jogalekar College, Ratnagiri, Maharashtra, India <sup>2</sup>Arts, Commerce and Science College, Lanja, Maharashtra, India

Residual dyes, auxiliaries and chemicals are often left in the process water and discharged with the wastewater. Therefore the wash off from the dye house invariably contains large amount of residual dye. The three major chromophores of various commercial dyes are Azo, Antraquinone and Indigo. These effluents are discharged to sewers from where they enter into the Municipal wastewater treatment plants. In the dye-manufacturing units, there is considerable debate on the level of environmental hazard produced by coloured effluents. Nonetheless, although the problem of colour could be argued as only aesthetic, it is accepted that the problem has to be rectified. Thus, the mounting pressure on the industry to treat the dye house effluents have led to a host of new and old technologies competing to provide cost effective solution to the problem of residual colour imparted by dyes. For the present work, textile effluent and sludge was used for isolation of dye decolorizes. Total 21 isolates were selected on the basis of their Gram reaction and colony characteristics. Both types of organisms, Gram positive and Gram negative were found present with dominant being the Gram negative species. Then five potential bacterial and four fungal isolates was selected on the basis of their dye decolorizing ability of four dyes, basic fuchsin, blue, yellow, and orange. The complexity of the dye led to variable percentage of decolorization of different dyes by the same organism. Bioremediation of environmental pollutants relies on the pollutant degrading capabilities of naturally occurring microbes. Employing static treatment was successful in not only decolorization of dyes but extensive degradation of the dyes was achieved. This result was supported by sharp reduction in toxicity of degradation metabolites on the germination and early seedling growth in wheat and green gram and the bacterial toxicity, when compared with original dye compound.

#### Biography

Chanda V Berde Parulekar has completed her PhD from Microbiology Department of Goa University, Goa, India following 2 years of Postdoctoral studies from the same department. She is involved in teaching and research in the field of Biotechnology for the past 12 years. She has 30 research publications in reputed journals, 2 book publications, 2 chapters in books in the pipeline and is an Editorial Board Member of *JPABS*. She has guided 62 MSc research projects in Biotechnology and Microbiology. She has also attended more than 15 conferences, national and international. She is on the Board of Directors of Society for Environment, Biodiversity and Conservation, India.

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Miklos Vecsernyes et al., J Org Inorg Chem 2018, Volume 4 DOI: 10.21767/2472-1123-C3-008

## APPLICATION OF BETA-CYCLODEXTRINS: FROM FORMULATION TO ORPHAN DRUG Miklos Vecsernyes<sup>1</sup>, Ferenc Fenyvesi<sup>1</sup>, Judit Varadi<sup>1</sup> and Ildiko Bacskay<sup>1</sup>

University of Debrecen, Hungary

Beta-cyclodextrins are widely used excipients in pharmaceuticals and foods. Nowadays extensive research is focused on the cyclodextrinbased therapy of cholesterol-releated disorders such as neurodegenerative and cardiovascular diseases. The conventional application of cyclodextrins is the solubility and absorption enhancement of poorly soluble drugs by the formation of host-gust complexes. On the other hand cyclodextrins can interact with natural cell membrane components like cholesterol or phospholipids. At high concentration it causes membrane damage and cell death, which is responsible for their cytotoxicity. A new renaissance started in the research and application of cyclodextrins a few years ago. The number of novel derivatives are increasing and new applications has been appeared especially in the field of cell biology and drug delivery. Recently it was discovered, that cyclodextrins are internalized into different cell types by endocytosis at non-toxic concentrations and this phenomenon opens new perspectives in the application of cyclodextrins. Hydroxypropyl beta cyclodextrin (HPBCD) and sulfobutyl ether sodium formulation excpient (SBEBCD) derivatives are safe and considered to be non-toxic. Therefore, they appeared in parenteral applications and recently HPBCD was approved as an orphan drug in the treatment of a cholesterol storage disorder, Niemann-Pick Disease Type C.

#### Biography

Miklos Vecsernyes has completed his degree of Pharmacy in 1982 and his PhD at 1997 from Albert Szent-Gyorgyi Medical School, Szeged, Hungary. He is the Director of Department of Pharmaceutical Technology, and the Dean of Faculty of Pharmacy, University of Debrecen. He has published more than 100 papers in reputed journals and has been serving as Rreviewer of several journals. His scientific interest is focused on Biopharmacy, Neuroendocrinology, Absorption and Bioavailability of Drugs and Pharmaceutical Excipients, especially Cyclodextrins.

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## A QUASI-STEADY-STATE APPROXIMATION TO THE BASIC TARGET-CELL-LIMITED VIRAL DYNAMICS MODEL WITH A NON-CYTOPATHIC EFFECT

### **Richard Cangelosi<sup>1</sup>, Elissa Schwartz<sup>2</sup> and David Wollkind<sup>2</sup>**

<sup>1</sup>Gonzaga University, Spokane, Washington, USA <sup>2</sup>Washington State University, Pullman, Washington, USA

Analysis of previously published target-cell limited viral dynamic models for pathogens such as HIV, hepatitis, and influenza generally rely on standard techniques from dynamical systems theory or numerical simulation. We use a quasi-steady-state approximation to derive an analytic solution for the model with a non-cytopathic effect, that is, when the death rates of uninfected and infected cells are equal. The analytic solution provides time evolution values for all three compartments of uninfected cells, infected cells, and virus. Results are compared with numerical simulation using clinical data for equine infectious anemia virus (EIAV), a retrovirus closely related to HIV, and the utility of the analytic solution is discussed.

#### Biography

Richard Cangelosi has earned a PhD in Mathematics from Washington State University in 2014. His research interests include Modelling Nonlinear Phenomena with Application to Biology and Ecology, Models for Biological Pattern Formation, Delay Equations, Perturbation Theory, Chaos Theory and the Fractal Geometry of Strange Attractors. He is currently a Faculty Member at Gonzaga University.

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### Sessions

Advances in Pharmacological Research | Pharmaceutical Chemistry | Nanomedicine and Nano-biotechnology | Medicinal and Bioorganic Chemistry | Organic Chemistry | Novel Targer drugs to the treatment of cancer | Drug Design and Drug Development

Session Chair Konstantin Volcho Russian Academy of Science, Russia Session Co-Chair Thomas Sanderson INRS-Institut Armand-Frappier, Canada

Session Introduction

Title:	Blocking metastatic properties of head and neck cancer by multifunctional nanoparticle-based saracatinib
	Yong Teng, Dental College of Georgia, Augusta University, Augusta, GA, USA
Title:	The centers of premeltons signal the beginning and ends of genes
	Henry M. Sobell, University of Rochester, USA
Title:	Retrosynthetic software for practicing chemists: Novel and efficient in silico
	Lindsey Rickershauser, Cheminformatics Technologies division, MilliporeSigma, USA
Title:	Eating Away Your Cancer
	Xu Chen, University of the Rockies, USA
Title:	Metal modified heterogeneous catalysts for synthesis of pharmaceutical components: reaction mechanism and catalyst evaluation
	Narendra Kumar, Abo Akademi University, Turku/Åbo, Finland
Title:	Metal-based Nanoparticles and Heavy Metals on Spermatogenesis: Preclinical studies
	Maria de Lourdes Pereira, University Campus of Santiago, Portugal

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> Yong Teng et al., J Org Inorg Chem 2018, Volume 4 DOI: 10.21767/2472-1123-C3-008

## BLOCKING METASTATIC PROPERTIES OF HEAD AND NECK CANCER BY MULTIFUNCTIONAL NANOPARTICLE-BASED SARACATINIB

## Yong Teng<sup>1,4,5</sup>, Liwei Lang<sup>1</sup>, Chloe Shay<sup>2</sup> and Xuli Wang<sup>3</sup>

<sup>1</sup>Dental College of Georgia, Augusta University, Augusta, GA, USA <sup>2</sup>Emory Children's Center, Emory University, Atlanta, GA, USA <sup>3</sup>University of Utah, Salt Lake City, UT, USA <sup>4</sup>Medical College of Georgia, Augusta University, Augusta, GA, USA <sup>5</sup>College of Allied Health, Augusta University, Augusta, GA, USA

he metastatic disease significantly decreases the survival rate of patients with head and neck squamous cell carcinoma (HNSCC). Src, a non-receptor tyrosine kinase, plays critical roles in tumor progression and metastasis. However, whether to effectively inhibit the function of Src in HNSCC remain elusive. We report, for the first time, blockade of Src kinase activity by saracatinib which effectively suppressed invasion and metastasis of HNSCC in preclinical animal models. Mechanistic assessment of the drug effects in HNSCC cells showed that saracatinib induced suppression of invasion/metastasis through downregulating the expression levels of Vimentin and Snail proteins and reversing Src-dependent epithelial-mesenchymal transition. In tests in mice, saracatinib was loaded into the novel multifunctional nanoparticles exhibited superior effects on suppression of HNSCC metastasis compared with free drug, which is mainly attributed to highly specific and efficient tumor-targeted drug delivery system. These findings and advances are of great importance to the development of Src-targeted nanomedicine as a novel treatment modality against HNSCC, especially for more extensive tumors.

#### Biography

Dr. Teng earned his Ph.D. from Sun Yat-sen University in 2007. He is an Assistant Professor in the Dept. of Oral Bio at AU. He has authored more than 70 articles and chapters in reputed journals and books and serves on the grant review panels of CDMRP-PCRP-Ad-CET, NYUAD, and NFSC. He has demonstrated an excellent commitment to serve the scientific community through numerous editorial and reviewing activities.

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Henry M Sobell, J Org Inorg Chem 2018, Volume 4 DOI: 10.21767/2472-1123-C3-008

## THE CENTERS OF PREMELTONS SIGNAL THE BEGINNING AND ENDS OF GENES Henry M Sobell

University of Rochester, USA

Premeltons are examples of emergent structures (i.e., structural solitons) that arise spontaneously in DNA due to the presence of nonlinear excitations in its structure. They are of two kinds: B-B (or A-A) premeltons form at specific DNA-regions to nucleate site-specific DNA melting. These are stationary and, being globally nontopological, undergo breather motions that allow drugs and dyes to intercalate into DNA. B-A (or A-B) premeltons, on the other hand, are mobile, and being globally topological, act as phaseboundaries transforming B-into A-DNA during the structural phase-transition. They are not expected to undergo breather-motions. A key feature of both types of premeltons is the presence of an intermediate structural-form in their central regions (proposed as being a transition-state intermediate in DNAmelting and in the B- to A- transition), which differs from either A- or B-DNA. Called beta-DNA, this is both metastable and hyperflexible, and contains an alternating sugar-puckering pattern along the polymer-backbone combined with the partial-unstacking (in its lower energy-forms) of every other base-pair. Beta-DNA is connected to either B- or to A- DNA on either side by boundaries possessing a gradation of nonlinear structural-change, these being called the kink and the antikink regions. The presence of premeltons in DNA leads to a unifying theory to understand much of DNA physical-chemistry and molecularbiology. In particular, premeltons are predicted to define the 5' and 3' ends of genes in naked-DNA and DNA in active-chromatin, this having important implications for understanding physical aspects of the initiation, elongation and termination of RNA-synthesis during transcription. For these and other reasons, the model will be of broader interest to the general audience working in these areas. The model explains a wide variety of data, and carries within it a number of experimental predictions - all readily testable - as will be described in my talk.

#### Biography

Henry M Sobell has completed his studies at Brooklyn Technical High School (1948-1952), Columbia College (1952-1956), and the University of Virginia, School of Medicine (1956-1960). Instead of practicing clinical medicine, he then went to the Massachusetts Institute of Technology (NIT) to join Professor Alexander Rich in the Department of Biology (1960-1965), where, as a Helen Hay Whitney Postdoctoral Fellow, he learned the technique of single crystal X-ray analysis. He then joined the Chemistry Department at the University of Rochester, having been subsequently jointly appointed to both the Chemistry and Molecular Biophysics departments (the latter at the University of Rochester School of Medicine and Dentistry), becoming a full tenured Professor in both departments (1965-1993). He is now retired and living in the Adirondacks in New York, USA.

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# RETROSYNTHETIC SOFTWARE FOR PRACTICING CHEMISTS: NOVEL AND EFFICIENT IN SILICO PATHWAY DESIGN VALIDATED AT THE BENCH

## Lindsey Rickershauser and Sarah L Trice

MilliporeSigma, Darmstadt, Germany

In a continuously evolving landscape of in silico chemical intelligence and n a continuousiy evolving randscape or in since machine learning, computer assisted synthetic planning has come to the forefront of discussion in the cheminformatics space. Herein, we describe an experiment in which Chematica, retrosynthetic design software, was used to plan synthetic pathways of eight structurally diverse bioactive and natural products. In each instance, the computer-planned routes were not only executed successfully in the laboratory, but also offered significant improvements over previous routes, circumvented patented routes and/or produced targets not synthesized previously. Chematica's unique approach to build their expert database of known reactions by hand coding each transformation has allowed this tool to become a bench chemist's ally by learning chemistry much like a chemist would themselves, and suggesting diverse pathways towards their targets, thus generating ideas and providing cost effective routes based on each user's unique needs. As a product of over 15 years of research, this unique tool is poised to not only get better with time, but also revolutionize the way chemists approach designing pathways to their complex targets.

#### Biography

Lindsey Hess Rickershauser is currently a Technical Application Scientist in the Cheminformatics Technologies division of MilliporeSigma, a business of Merck KGaA, Darmstadt, Germany. She got her PhD in Organic Chemistry in 2010, working under Professor Gary Posner at Johns Hopkins University. During her PhD work, her concentrations were on synthesizing analogs of vitamin D and artemisinin dimers for biological activity, and synthetic methodologies of enantioselective sigmatropic rearrangements. From then, she had a short venture at Chemical Abstracts Services in the cheminformatics space, after which, she joined Cerilliant Corporation (then a subsidiary of Sigma-Aldrich) as a Senior Scientist specializing in certified reference materials in the clinical, diagnostic & forensic industries. During her six-year tenure as a Senior Scientist, she specialized in stable label isotope incorporation to both pharmaceutical and illicit drugs and their metabolites (concentrating on D and <sup>13</sup>C incorporation). Later, she joined the Cheminformatics Technologies division where she has been actively part of launching the retrosynthetic design software acquired in 2017.

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# EATING AWAY YOUR CANCER

### Xu Chen and William Wargo

<sup>1</sup> Xu Chen (University of the Rockies) <sup>2</sup>William Wargo (University of the Rockies)

uring recent forty years, thyroid cancer rates had gone up constantly. Denerally, the best treatment for thyroid benign or malignant nodules is surgery, but surgery is very costly. Thyroid health affected mental health, while mental health affected suicide rate. During the recent 15 years, American suicide rate also went up. This paper was about how to eat, exercise, and improve mental health to better thyroid health and consequently improve mental health. As wealthy as America is, people are not eating right. Foods contain poisons to make them look appealing. Our drinking water is not helping either. For people with low economic class, they even have less choices than the rest of the world. To understand how to eat to survive thyroid cancer, this researcher went through more than five thousand threads/emails online longterm thyroid cancer survivors group. Among the survivors, this researcher picked out five typical cases who survived thyroid cancer from eight years to close to 50 years. From these five cases' discussion, this researcher tentatively summarized the best practices in diet, exercise, and improving mental health in improving thyroid health, and consequently keeping thyroid cancer in remission.

Keywords- Cancer, exercise, diet, thyroid.

#### Biography

Xu Chen is not an academic guru. She did research about thyroid cancer due to personal reasons because thyroid problems are very common among women. Xu Chen is currently working on her Doctoral degree through University of the Rockies in Colorado, US. Currently, Xu does not have an academic job. She is an actor in Boston Tea Party, Boston, MA.

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## METAL MODIFIED HETEROGENEOUS CATALYSTS FOR SYNTHESIS OF PHARMACEUTICAL COMPONENTS: REACTION MECHANISM AND CATALYST EVALUATION

## Narendra Kumar<sup>1</sup>, Martina Stekrova<sup>1,2</sup>, Paivi Maki-Arvela<sup>1</sup>, Alexandra Torozova<sup>1</sup>, Konstantin P Volcho<sup>3</sup>, Nariman F Salakhutdniov<sup>3</sup> and Dmitry Yu Murzin<sup>1</sup>

<sup>1</sup>Abo Akademi University, Turku/Abo, Finland

<sup>2</sup>Department of Organic Technology, Institute of Chemical Technology, Prague, Czech Republic <sup>3</sup>Novosibirsk Institute of Organic, Russian Academy of Sciences, Novosibirsk, Russia

Efficient, pristine, high yield and cost effective synthesis of pharmaceutical components, drugs, vitamins and fragrances using metal modified heterogeneous catalysts are important from the academic and industrial point of view. The research results in this lecture will cover the opening of monoterpene epoxide to a potent anti-Parkinson compound over Fe- and Ce- modified beta zeolite and Si-MCM-41 mesoporous material. A novel reaction pathway for synthesis of (1R, 2R, 6S)-3-methyl-6-(prop-1-en-2-yl) cyclohex 3-ene-1, 2-diol with high selectivity using isomerization of verbenol oxide over metal modified heterogeneous catalyst will be presented. Furthermore, effect of acidity and texture of H-beta-25, H-beta-300 microporous-, H-MCM-48 mesoporous and hybrid microporous materials on the synthesis of paramenthanic diol exhibiting anti-Parkinson activity will be elaborated. The highest selectivity to desired product of diol was obtained over mild acidic H-Beta-300 catalyst. Influence of methods of metal modification and types of supports in the two step synthesis of presentation will be reaction mechanism, catalyst synthesis, characterization and evaluation of catalytic properties in liquid phase reactions. The in-depth physico-chemical characterization results of catalyst will be correlated with the catalytic activity and selectivity to the desired products. It is noteworthy to report that metal modified heterogeneous catalysts were possible to be regenerated and reuse for the reactions studied.

#### Biography

Narendra Kumar obtained his Doctor of Technology in Chemical Engineering from Abo Akademi University, Turku, Finland. He has been working at the Laboratory of Industrial Chemistry and Reaction Engineering, Abo Akademi University since 1990 to till present. His duties are research, education, teaching, supervision of PhD, MSc and BSc students. His research focuses on Heterogeneous catalysis, catalyst synthesis and characterization, petro-chemical reactions, fine chemicals, pharmaceuticals and speciality chemicals synthesis, environmental catalysis, catalytic reaction mechanism. He has given several plenary, keynote and invited lectures at international Conferences. He has over 250 peer reviewed articles in international journals in the field of heterogeneous catalysis, chemical engineering, fine chemicals, pharmaceuticals & speciality chemical synthesis and environmental catalysis. He has received several awards and his h-index is 31. He is a Member of the editorial board of the *Journal Waste and Biomass Valorization*.

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## METAL-BASED NANOPARTICLES AND HEAVY METALS ON SPERMATOGENESIS: Preclinical studies

### Maria de Lourdes Pereira

CICECO - Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal

ale reproductive function integrates delicate biological systems (tissues Mand gametes) strongly susceptible to a myriad of factors including man made engineered nanomaterials, heavy metals and metalloids. Metalbased nanoparticles (NPs) are broadly used in biomedical field especially as drug delivery systems, therapy in some pathologies namely cancer, and imaging. Furthermore, its application on assisted reproductive technologies is also emphasized. It is also worth noting for example, the benefits of nanoselenium in sperm motility in experimental models. However, strong evidences demonstrate the adverse impact of these nanosystems, and some metal compounds on reproductive hormonal axis, and spermatogenesis in animal models and man. Semen quality decay is largely referred at both occupational and environmental settings. This work critically analyses the up-to-date information of the influence of some metal-based nanoparticles (eg. Au-NPs, ZnO-NPs), metals (eg. lead, cadmium, and chromium) on male reproductive health. In addition, data from our preclinical studies will be focussed on genotoxicity trials, antioxidant biomarkers, histopathological, and ultrastructural tools. In addition semen analysis will be highlighted. Some discrepancies in the literature were reported among experimental studies due to different procedures in experimental design (dose, route of exposure, and duration). However, in general, the factors mentioned above affect male reproductive health, through oxidative stress which results in reversible and/ or irreversible changes in testosterone-producing cells, spermatogenesis, and sperm quality parameters. Heavy metals such as cadmium induce severe damage into the blood-testicular barrier, thus compromising fertility.

#### Biography

M L Pereira is an Associate Professor with Habilitation at Department of Medical Sciences, University of Aveiro, and Member of the Associate Laboratory CICECO-Aveiro Institute of Materials. She got her PhD in Biology (Animal Cytology) at the University of Aveiro. Her teaching activities include essentially Cytology and Histology, and Cell Biology. She was Director of the Master on Molecular and Cell Biology (2008-2018) at University of Aveiro. Her research has been focused on the adverse effects of heavy metals, nanoparticles, and pesticides on animal models, especially male reproductive function, combining histological, cell biology and ultrastructural approaches. She co-authored more than several papers in international journals, and has been serving as an Editorial Board Member of some journals, acting also as referee.

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## SUGAR MIMETICS TOWARD AN ANTI-CANCER THERAPEUTIC VACCINE Pierre Vogel and Loay Awad

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ancer-associated mucin glycoprotein MUC1 is characterized by the presence of altered carbohydrates such as Tn (-N-acetylgalactosamine), sTn (sialyl-1-6-Tn) and the Thomsen-Friedenreich (TF: -D-Galp-1-3 -D-GalNAcp) antigen (tumor associated carbohydrate antigens: TACAs) that are conjugated to proteins via O--galactosylation of serine or/and threonine. Patients immunized with synthetic TF conjugated with KLH (keyhole limpet hemocyanin) + QS21 adjuvant can generate IgM and IgG antibodies.1 Because the disaccharide TF is hydrolyzed rapidly in the body, strong immune response requires longer lived disaccharides. Fluororinated TACAs have been proposed which elicit IgG antibodies found to cross-react with native TF epitopes.2,3 We have found that the C-linked disaccharide analogue 1 (constructed applying Danishesky's method for the conjugation with KLH 4) + QS21 adjuvant induces a strong immune response in mice. Interestingly, much weaker immune response was observed with a stereoisomeric antigen constructed with the -C-galactoside analogue of TF disaccharide ( -D-Galp-1-CH2-3- -D-GalNAc-O-Ser).5 Several strategies and methods have been developed for the synthesis of C-linked disaccharides including disaccharide mimetics incorporating iminosugars C-linked to sugars and sugar mimetics such as conduritols and cyclitols. The latter work was motivated by the search for specific glycosidase and glycosyltransferase inhibitors that are potential drugs against cancers and other diseases.



#### Biography

P. Vogel was born in Cully (Switzerland) Oct. 23, 1944. In 1969, he did his Ph.D under supervision of Prof. H. Prinzbach at the Institute of Organic Chemistry, University of Lausanne. He spent two years at Yale University, New Haven, Connecticut, USA with Prof. Martin Saunders, Prof. J. A. Berson, K. A. Wiberg and P.v.R. Schleyer (Princeton University). He worked then as a Research chemist at Syntex S.A., in Mexico with Prof. PCrabbé before the return to the University of Lausanne in 1973. As of 1977 he became Professor of organic chemistry at the University of Lausanne. In 1991 he was Vice-Chairman of the Institute of organic Chemistry, University of Lausanne until 2001. He was also part-time grad.school teacher at the Universities of Rouen and Caen from 1991 to 1993 and Part-time professor at Ecole Polytechnique de Palaiseau from 1993-2000. Since 2001 he is Professor of organic chemistry at the EPFL.

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