RECENT ADVANCES IN BIOLOGY, BIOPHYSICS, BIOENGINEERING AND COMPUTATIONAL CHEMISTRY

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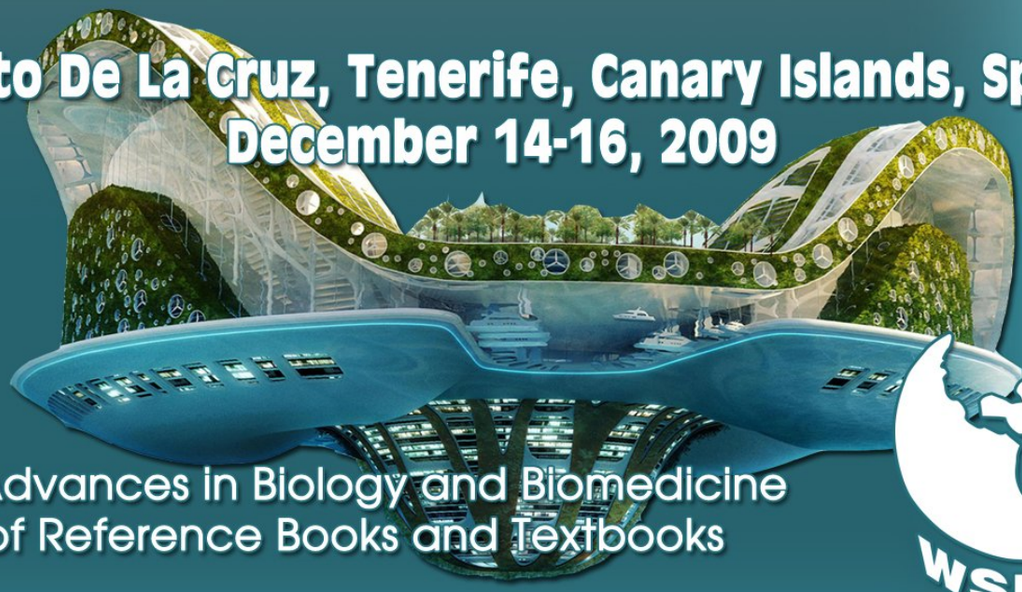
Proceedings of the 3rd WSEAS International Conference on
COMPUTATIONAL CHEMISTRY (COMPUCHEM '09)

**Puerto De La Cruz, Tenerife, Canary Islands, Spain,
December 14-16, 2009**



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Preface

This year the 5th WSEAS International Conference on CELLULAR and MOLECULAR BIOLOGY, BIOPHYSICS and BIOENGINEERING (BIO'09) and the 3rd WSEAS International Conference on COMPUTATIONAL CHEMISTRY (COMPUCHEM'09) were held at Puerto De La Cruz, Tenerife, Canary Islands, Spain, December 14-16, 2009. The conferences remain faithful to their original idea of providing a platform to discuss biology of cell, metabolism, molecular biology, neural modeling, biophysics, biochemistry, computer biology, genetics, theoretical chemistry, computational material science, numerical analysis for chemical engineering and chemistry, computational intelligence tools for chemistry and chemical engineering, computational molecular science and nanoscience, mathematical molecular medicine, chemical fluid mechanics, environmental chemical engineering etc. with participants from all over the world, both from academia and from industry.

Their success is reflected in the papers received, with participants coming from several countries, allowing a real multinational multicultural exchange of experiences and ideas.

The accepted papers of these conferences are published in this Book that will be indexed by ISI. Please, check it: www.worldses.org/indexes as well as in the CD-ROM Proceedings. They will be also available in the E-Library of the WSEAS. The best papers will be also promoted in many Journals for further evaluation.

Conferences such as these can only succeed as a team effort, so the Editors want to thank the International Scientific Committee and the Reviewers for their excellent work in reviewing the papers as well as their invaluable input and advice.

The Editors

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Plenary Lecture 1

Nanoparticles for the Transport of Antiretroviral Drugs across the Blood-Brain Barrier: A Potential Therapy for the Acquired Immunodeficiency Syndrome

Professor Yung-Chih Kuo
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Abstract: Transport of antiretroviral agents into the central nervous system is an important issue because human immunodeficiency viruses (HIV) have been found to reside and replicate themselves in the brain parenchyma. This yields a complicated treatment for the acquired immunodeficiency syndrome. Recently, novel nanoparticles (NPs) have been developed for carrying anti-HIV drugs across the blood-brain barrier (BBB). In this presentation, the anti-HIV drugs incorporated with NPs to circumvent the BBB included zidovudine, lamivudine, stavudine, didanosine, delavirdine, and saquinavir. These pharmaceuticals were loaded on the surfaces of polymeric NPs or entrapped in the matrix of solid lipid nanoparticles (SLNs). Polybutylcyanoacrylate, methylmethacrylate-co-sulfopropylmethacrylate, and poly(lactide-co-glycolide) were among the typical polymeric NPs, and various kinds of SLNs with lipid core of tripalmitin, cacao butter, docosanoic acid, stearic acid, and Compritol ATO 888 were also discussed. On the surfaces of the drug carriers, bioactive molecules including polysorbate 80, sorbitan monolaurate, phospatidylcholine, cholesteryl hemisuccinate, taurocholate, stearylamine, dioctadecyldimethyl ammonium bromide, heparin, L-arginine, and transferrin were applied to stabilization or modification. Effects of cold storage, pH value, synthesis duration, stirring speed, lyophilization, and composition on the drug delivery system, and physicochemical characteristics including particle size and shape, molecular weight, zeta potential, mobility, drug distribution, loading and entrapment efficiency, and release kinetics were shown. In addition, confluent monolayer of brain-microvascular endothelial cells (BMECs) from both bovine and human and an in vivo rat model were employed to the evaluation of permeability across the BBB. Presence of the medium chemicals including alcohol and glutamic acid was also considered. It was generally observed that cytotoxicity and transendothelial electrical resistance of BMECs cocultured with NPs were in reasonable range, and dramatic increase in the permeability of NPs-mediated system could be obtained. Moreover, impacts of the exposure to electromagnetic field (EMF) including power, wave type, frequency, modulation or depth of amplitude modulation, and modulation or deviation of frequency modulations were demonstrated. Finally, the evidence of vesicular endocytosis of drug-containing NPs by clathrin-coated endosome and the expression of tight junction and P-glycoprotein on the plasma membranes of BMECs were presented.

Brief Biography of the Speaker:
Dr. Yung-Chih Kuo is a professor at the Department of Chemical Engineering, National Chung Cheng University. His research interests are related to biomaterials, drug delivery system, tissue engineering, blood-brain barrier, nervous regeneration, cancer therapy, biophysics, and colloid and interface science. In these fields, he has authored or coauthored over 100 reviewed journal papers, abstracts, book chapters, and technical reports. He is an honor member of Phi Tau Phi Society and an active life member of Biochemical Engineering Society of Taiwan and Taiwan Institute of Chemical Engineers. He was often invited as a manuscript reviewer for over 20 journals and an external reviewer for academic awards, research grants, faculty recruitments and promotions, and hosting international symposium subsidy.

Plenary Lecture 2

Creation of Electromagnetic Structure-Creating Spaces to Improve the Growth of Some Types of Cells and Albumins

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Chief of biophysical department
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Abstract: There are given some constructions of bio-field simulators for creating the electromagnetic structure-creating spaces and improving the growth of some types of cells and albumins.
There are given investigations of such illnesses: outer covering wounds, anaemia, ligamentous disruption, neurology and diabetes mellitus, - with the help of different types of bio-field simulators..

Brief Biography of the Speaker:
Dr. Vladyslav Vlastopulo is a scientifically-commercial director of biophysical department on creating of new biomedical methods and devices, bio-field simulators in "Research Laboratories VVL", Odessa, Ukraine, and professor of cathedra of ways and methods of struggling with marine corrosion and biological fouling in Odessa Marine University. His research interests are related to biomedical, tribologycal, biotribologycal and mechanical engineering and also biophysics, bio-field simulators, computer fragmentary treatment of diseases demanding the operations, drug abuse patients, obesity patients, the using in video, audio products for creating attracted bioenergetic advertisement, creation of joints on basis of hydrodynamical lubricant theory. He has more than 120 papers, abstracts, book chapters and technical reports in biomedical, tribologycal, biotribologycal and mechanical engineering, and 50 of them are inventions of Soviet Union, Russian Federation and Ukraine. He is a member of more than 20 international conferences on mechanical, biomedical, tribologycal engineering.

Plenary Lecture 3

A New Way of Natural Oligopeptide Primary Structure Elucidation

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Abstract: For more than a century, natural oligopeptides have attracted scientific attention as important biochemical regulators. Since that time, thousands natural oligopeptide regulators have been described, and now ~600 new natural oligopeptides emerge annually, out of a literature of >70 000 publications each year on oligopeptide chemistry and biology according to PubMed database. Their primary structure is determined either directly or by translation from nucleotide sequences. Both these ways are experimental and laborous. But there are a lot of unrecognized protein sequences in different public databases which can contain unknown oligopeptide structures. Thereupon we have carried out a theoretical structure–function analysis of known uncharacterized protein amino acid residue sequences in order to identify new oligopeptide primary structures. As an example, grape (Vitis vinifera) proteins were chosen. A special computer analysis was developed for such analysis. The data of GenBank and SwissProt databases containing primary structures of unrecognized grape proteins, EROP-Moscow database containing information on structure and functions of plant regulatory oligopeptides and specially created computer programs for the comparison of GenBank or SwissProt information with EROP-Moscow data were used. This method permitted to reveal new potentially active regulatory oligopeptide sequences after alignment procedure. It was been found 21 grape protein structure sites homologues to known regulatory oligopeptides elucidated from other plant species. Their similarity with other plant oligopeptide primary structures was from 54.4 to 95.7%. They can be characterized as putative antimicrobial oligopeptides and rapid alkalinization factors. The problem of existence of these oligopeptide structures in grape is discussed. It has been proposed that rapid alkalinization factors can also possess antimicrobial activity. This way of oligopeptide structure elucidation can be extended to oligopeptide structures of any functional class.

Brief Biography of the Speaker:
Alexander A.Zamyatnin is scientist general of A.N.Bach Institute of Biochemistry, Russian Academy of Sciences, Moscow, Russian Federation and associated investigator of Santa Maria Technical University, Valparaiso, Chile. His area of expertise is endogenous oligopeptides (neuropeptides, hormones, toxins, antimicrobial), protein thermodynamics, structure-function relationship, ligand-receptor interaction, biosensors, computer biochemistry and biophysics, biological data bases, and drug design. He authored or co-authored over 200 scientific papers published in reviewed journals or presented at international conferences. He is the author of unique EROP-Moscow oligopeptide database (http://erop.inbi.ras.ru/; A.A.Zamyatnin et al. Nucleic Acids Research, 34, Database Issue, pp. D261-D266, 2006). He is a member of the European Peptide Society (from 1995).

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