

Summaries of all articles

N.N. Kudryavtsev

Introductory article of the rector

I.B. Petrov

Mathematical modeling in medicine and biology by medium mechanics models

In this paper, we discuss numerical modeling in medicine and biology by using medium mechanics models and calculation methods for solving the corresponding equation systems in partial derivatives. This research direction at present is one of the most urgent and complex problems in modern science. The point is that modern medicine in common is an experimental science with large experience. But a through investigation of these processes and the prediction of their behaviour require full mathematical modeling.

Keywords: mathematical modeling, medicine, biology, medium mechanics models.

N.V. Voitenko, E.P. Kostyuk, P.G. Kostyuk

Pain syndromes and intracellular calcium signaling

Within the last period, more and more attention has been given to disorders of calcium homeostasis. These disorders at least accompany many types of neuropathic and inflammatory pain, and it cannot be ruled out that they are one of the reasons for the development of many pain-accompanied pathologies. The importance of understanding the ways by which the brain can alter pain processing stimulates the increasing number of investigations focused on events in the first relays in pain pathways: dorsal root ganglia and spinal dorsal horn neurons. Modern concepts of the pathways of pain information transmission are presented in the review. A few aspects of possible involvement at calcium signaling in neurons in the development of pain syndromes are discussed.

Keywords: pain syndrome, calcium homeostasis, dorsal root ganglia, spinal dorsal horn neurons.

D.M. Avtonomov, I.A. Agron, A.S. Kononikhin, E.N. Nikolaev

Creation of the database of accurate mass and time tags for a qualitative and quantitative approach in research of the proteome of human urine using isotope tagging

The urgent problem of modern biology and medicine (their physical methods of research) is to develop procedures for quick and precise human liquids, including their protein composition. Such liquids as blood, urine, eyewater have already been investigated on the subject of protein composition. The basic procedures now are rather slow and badly realized in terms of high-throughput quantitative analysis. Therefore, we propose the method for a fast and high-throughput analysis based on the ideology of accurate mass and time tag and isotope tagging.

Keywords: biology, medicine, human liquids, protein composition, accurate mass and time tag, isotope tagging, proteom, urine.

D.E. Vitkina, E.I. Shkolnikov, I.V. Petrova, V.I. Lebedeva, V.V. Volkov

The research of palladium-loaded polypropylene porous hollow fiber membranes by the dynamic desorption porometry method

The removal of dissolved oxygen from water is one of the most important technological problems during the water preparation for many fields of industry and engineering (boiler waters, microelectronics, food, oil and gas industries). The present promising approach to the water purification is the catalytic removal of dissolved oxygen from water by hydrogen over Pd catalyst. In the present work, Pd-loaded porous hollow fiber membranes with palladium integrated onto the external surface side of fibers are prepared and tested. The dynamic desorption porometry method was used for investigating the porous structure of catalytic hollow fiber membranes during their preparation. Membrane special structural changes in the palladium content of more than 1% were revealed. The concentration of dissolved oxygen in water was reduced to $7 \mu\text{g/l}$ by catalytic reaction.

Keywords: water purification, fiber membranes, porous structure, catalytic reaction, oxygen, palladium.

G.N. Vladimirov, A.S. Kononikhin, E.N. Ilina, V.M. Govorun, E.N. Nikolaev

Accurate mass measurements of polymerase chain reaction products as a genotyping approach

This paper is devoted to the study of a genotyping approach based on the accurate mass measurement. Different polymerase chain reaction (PCR) purification methods were examined. The purifying and desalting method for PCR product for analysis by electrospray ionization mass spectrometry and the determination of the deoxyribonucleic acid (DNA) base composition from mass spectrometrically measured accurate molecular masses was shown.

Keywords: purification methods, genotyping approach, mass measurement, polymerase chain reaction, determination of deoxyribonucleic acid.

*A.A. Gorenberg, A.N. Kostrov, O.M. Sarkisov, V.A. Nadtochenko,
V.V. Nikandrov*

Catalytic reactions on the surface of mesoporous titanium dioxide films with immobilized hydrogenase

A titanium dioxide electrode modified with immobilized hydrogenase from purple bacterium *Thiocapsa roseopersicina* produces voltammogram with both cathodic and anodic catalytic currents in either a methylviologen containing buffer or containing no electron carrier buffer saturated with H_2 . It was shown that the reaction of direct electron transfer from solid state — semiconductor TiO_2 to the active catalytic center of hydrogenase from purple bacterium *Thiocapsa roseopersicina* occurs. It was determined that the exchange current amounts to $78 \mu A/sm^2$ when MV^{2+} is used as an electron carrier.

Keywords: catalytic reactions, mesoporous films, titanium dioxide, immobilized hydrogenase, semiconductor TiO_2 , methylviologen MV^{2+} .

P.P. Grigal, N.I. Khorseva

Ten-fingers chaotic tapping: fingers motor activity age differences

We invented a new method for finger motorics computer diagnostics — ten-finger chaotic tapping (it is covered by patent of the Russian Federation N 2314743, filing date 11.04.2006). This paper describes its validity and reliability. Using this method, we analyzed age differences in finger motor activity for children from 5 to 14 years old and adults. For example, we for the first time evaluated age differences for rigidity and synkinesis.

Keywords: finger motoric, computer diagnostic, ten-finger chaotic tapping. testing, age differences.

*A.D. Zalessky, A.I. Shushin, I.V. Reshetov, V.A. Derzhavin, V.V. Buchanov,
O.M. Sarkisov*

Optical laser manipulator using femtosecond pulses

We developed the setup for manipulating (i.e. displacements, stretching, rotations, etc.) nano- and microscopic objects by means of «optical trapping». Operation factors, which determine the applicability of femtosecond pulses for manipulating these objects, are analyzed in detail. With the use of the setup developed, the possibility of manipulations with femtosecond pulses such as the displacement and orientation of single cells, is demonstrated experimentally. It is also shown that this setup can be applied to destructing cancer cells and the excision of fragments from the agglomerate of cancer cells resulting from chemical bounds rupture caused by the multiphoton absorption of femtosecond light pulses.

Keywords: optical laser, manipulating, femtosecond pulses, «optical trapping», nano- and microscopic objects, displacement and orientation of single cell, multiphoton absorption.

*A.V. Kaminina, V.S. Shalgunov, T.D. Volkova, D.O. Koroev, M.B. Oboznaya,
N.I. Medvinskaya, A.N. Samokhin, N.V. Bobkova, O.M. Volpina*

An approach to the immunotherapy of Alzheimer's disease using induction antibodies to the $\alpha 7$ -subunit of the acetylcholine receptor

The main possibility to use immunization with the fragments of the $\alpha 7$ -subunit of the acetylcholine receptor for the memory improvement of mice with Alzheimer's disease was investigated. It was shown that immunization with protein-carrier conjugates of the fragments of the $\alpha 7$ -subunit improved the spatial memory of mice in the experimental model of Alzheimer's disease, led to the production of antibodies, permeating blood-brain barrier, and resulted in a decrease of β -amyloid level in the mice brain. It was revealed that immunization with fragment 173-193 of the acetylcholine receptor $\alpha 7$ -subunit without conjugation with the protein carrier had a protective effect on the memory of mice in the model of Alzheimer's disease. Peptide 173-193 seems to be a promising candidate for the design of synthetic vaccine against Alzheimer's disease.

Keywords: Alzheimer's disease, immunization, memory improvement, fragments of the $\alpha 7$ -subunit of the acetylcholine receptor, β -amyloid level, synthetic vaccine.

D.V. Kulyamin, V.P. Dymnikov

The simulation of the quasi-biennial oscillations of the zonal wind in the equatorial stratosphere

The paper focuses on the simulation of the quasi-biennial oscillations (QBOs) of the zonal velocity in the equatorial stratosphere. A relative role of waves of different scales in the formation of the period of the oscillations of the zonal wind is studied by a coupled low-parameter model combining two mechanisms for excitation of the QBO: one through the interaction of planetary waves with the mean flow at critical levels and the other through gravity-wave obliteration. The conditions that are required to reproduce the QBO in general circulation models are discussed.

Keywords: quasi-biennial oscillations (QBOs), zonal wind, equatorial stratosphere, planetary waves, gravity-wave, general circulation.

Y.A. Mazur, N.Y. Oparina

Molecular modeling of stop-codon's recognition by eukaryotic release factor eRF1

Translation termination in eukaryotes involves the recognition of all three stop codons (UAA, UAG, UGA) by factor eRF1. It is known that the N-terminal domain of these factor is responsible for stop codon decoding, however the exact location of the binding site and the recognition mechanism remain unknown. In our work, we study the interaction of the 2-nd and 3-rd nucleotides of stop-codon with eRF1 N-terminal domain using molecular modelling approaches. Models of specific complexes of eRF1 N-terminal domain with dinucleotides AA, AG and GA were designed. It was shown that the binding of N-terminal domain of eRF1 with «nonspecific» dinucleotide GG is also possible with similar energies in comparison to «specific» dinucleotides AA, AG, GA. Nevertheless, the binding site for «specific» and «nonspecific» dinucleotides are different. It was demonstrated for the «specific» complexes that all ligand contacts with the Thr122, Ser123 and Tyr125 residues of eRF1. For these residues, the functional importance in stopcodon recognition was previously shown experimentally. The Virtual mutagenesis of these positions (Thr122, Ser 123 → Gln122, Phe123) allowed us to obtain the results compatible with experimental data.

Keywords: molecular modeling, stop-codon recognition, factor eRF1, dinucleotides, virtual mutagenesis.

D.M. Murashov

Automated cytological specimen image segmentation technique based on the active contour model

The problem of automated cell nuclei segmentation in cytological images for the automated diagnostics of hematological diseases is studied. A snake-based technique for detecting cell nuclei boundaries is proposed. Unlike the known active contour model techniques, the problem is formulated as the problem of nonlinear dynamic object stabilization. The active contour «capture range» is extended by the wave propagation model. For automated snake initialization, the procedure based on thresholding a channel in CIE Lab color space is used. Computing experiments show the efficiency of the proposed technique.

Keywords: automated cell nuclei segmentation, cytological images, automated diagnostics of hematological diseases, active contour model, computing experiments.

A.S. Petrushev

3D model of chemically active glow discharge in air

The 3D computing model of glow discharge in a parallel-plate configuration is presented. The model consists of equations for electron and ion continuity, Poisson's equation for the coupled with charged particles distributions electric field. The processes of collisional ionization, ion-electron recombination, electron heating, the vibrational excitation of quantum energy levels of molecule N_2 are taken into account. To describe the distribution of nitrogen molecules on excited vibrational levels the kinetic processes are included in the model: the excitation of vibrational levels by electron collisions, VV- and VT-relaxation, chemical kinetics. The finite-difference numerical simulation method used for solving governing kinetic equations is described in detail. The numerical simulation results are obtained for the two-dimensional DCD in molecular nitrogen at pressure 5 torr and Emf of power supply 2000 V. The predicted electronic temperature and the distribution of molecular nitrogen on excited vibration levels are analyzed.

Keywords: 3D computing model, glow discharge, ionization, ion-electron recombination, vibrational excitation, electron collisions, electronic temperature, excited vibration levels.

*M.L. Pridatchenko, I.A. Tarasova, C. Masselon, A.V. Gorshkov,
M.V. Gorshkov*

A universal approach to generation of databases of peptide accurate mass and time tags using critical chromatography of biomacromolecules

In this work the feasibility to generate unified and independent of the experimental separation parameters retention time scale for peptides measured using different instruments and separation protocols has been considered. Particularly, a concept of linear correlation between retention times of biomacromolecules has been proposed and verified experimentally. A range of separation parameters in which the linear correlation between measured retention times of peptides has been experimentally determined. Based on the observed functional correlation between retention times of peptides, a procedure for scaling of retention times into the unified normalized time scale has been proposed. The normalization procedure has been further experimentally tested for LC data obtained for complex proteolytic peptide mixtures. It was shown that the accuracy of normalized retention times in the new scale is about 1% that is compared with the accuracy of chromatography measurements. The proposed approach can be useful in generation of LC/MS databases of peptide markers of proteins in the «shotgun» proteomic studies.

Keywords: proteolytic peptide mixtures, functional correlation, retention time, LC/MS databases of peptide markers, critical chromatography of biomacromolecules.

A.V. Timofeev

«Abnormal» kinetic temperature and features of dynamics of dusty plasma

The analysis of the causes of the sharp increase in the average kinetic energy of dust particles in the plasma of low-pressure gas discharge is carried out. The analytical equations of motion of dust particles are resulted by consideration of dust system in plasma in terms of the theory of vibrations with the account of inconstancy of a charge of a dust particle. Basic possibility of occurrence of a parametrical resonance of fluctuations of dust particles is found out and conditions of its occurrence are estimated. It turned out that the condition of occurrence of a resonance is close to the conditions of laboratory experiments on dusty plasma.

Keywords: dusty plasma, plasma of low-pressure gas discharge, parametrical resonance, parametrical resonance, vibrations and fluctuations of dust particles.

*R.A. Tychko, N.Y. Oparina, O.L. Zinoveva, E.S. Kropotova, M.V. Zinoveva,
T.D. Mashkova, L.P. Ovchinnikov*

Quantitative estimation of YB-1 expression level change in non-small cell lung cancer.

Y-box binding proteins belong to a family of RNA/DNA- binding proteins involved in gene expression regulation, DNA reparation and recombination, mRNA stabilization and splicing. Mammalian Y-box proteins are shown to affect expression of genes which take part in tumour growth regulation. In this study, we evaluated mRNA content of YB-1 gene coding one of human Y-box proteins in non-small cell lung cancer by quantitative RT-PCR. YB-1 mRNA level was relatively high both in normal lung tissues and in adjacent to tumour tissues. Significant decrease in mRNA level was observed in 67% of tumours in comparison with in adjacent normal tissues. No considerable increase of YB-1 mRNA content was revealed in any NSCLC sample.

Keywords: RNA/DNA- binding proteins, DNA reparation and recombination, YB-1 gene coding.

V.G. Fedotov, A.V. Selkin, A.G. Bazhenova

Bragg reflection spectrum formation of photonic crystal structures

The Bragg reflection spectra of opal-like photonic crystals are studied. The dispersion relations for eigenmodes of the electromagnetic field in a photonic crystal for different directions of light incidence are calculated. It is shown that the Bragg diffraction of light from the crystal planes inclined to the surface leads to a significant modification of eigenmode energy spectra. The calculated eigenmode dispersion curves in the range within the photonic band gaps are compared to the experimental Bragg reflection spectra.

Keywords: bragg reflection spectrum, opal-like photonic crystals, eigenmode energy spectra, dispersion curves.

*V.V. Yants, N.V. Golovkin, V.Y. Terebinov, O.N. Kharybin, I.A. Popov,
E.N. Nikolaev*

Desorption Electrospray Ionization method application to drugs and biological samples analysis

The desorption electrospray Ionization (DESI) method was invented by Prof. R. Graham Cooks'group in 2004. DESI is an atmospheric ionization method which allows one to perform direct sample analysis without sample preparation. In this method, analyte ions are produced due to the interaction of charged droplets of solvent with the sample surface; these ions are transported to a mass spectrometer through the atmospheric interface. In this paper, the DESI possibilities for drugs and biological samples analysis are described.

Keywords: desorption electrospray Ionization, mass spectrometer, drugs and biological samples.