ABSTRACTS

HYDRATION AND STABILITY OF NUCLEIC ACIDS WITH DIFFERENT AT- AND GC - COMPOSITION IN CONDENSED STATE

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In the suggested review the results of the investigation of influence of water on structure and stability of nucleic acids (NA) are generalized on the basis of literature dates and our method of studies of peculiarity hydration of NA with different nucleotide composition in the system NA - water with variable water content. An analysis showed that contribution of the water molecules in total energy of stabilization of helical structure of nucleic acids is up to 70-75% and contribution of H-bonds of Watson-Crick pairs in this energy does not exceed 25%. These results allowed to bring out effect of other factors except influence of water on formation and stabilization of DNA hydration shell.

THERMODYNAMICS OF HELIX-TO-COIL TRANSITION IN DUPLEX AND TRIPLEX COMPLEXES OF OLIGOADENILATE WITH OLIGOTHYMIDYLATE. INFLUENCE OF COVALENTLY ATTACHED DYE

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Helix-to-coil transitions in oligonucleotide $(dA)_{15}$ complexes with $(dT)_{10}$ and $(dT)_{12}$ as well as with intercalating phenazine dye attached covalently, have been thermodynamically analyzed. At molar strand ratios 1:1 and 1:2 and $\mu = 0.1$ and 1 thermodynamic transition parameters ΔH, ΔS and ΔG and equilibrium constants were calculated for duplex and triplex structures by using the «two state» model and the modified «staggering zipper» model. Declination of experimental dependencies from the «two state» model was found for duplexes containing phenazine attached. This effect is interpreted as a result of the effect of the impurity triplex state. It was stated by the help of model «staggering zipper» calculations that terminal group of the complexes are in a partially disordered state the degree of which increases with temperature. It is shown that strengthening of both complex types by the dye attached may be taken into account by multiplication of the complex binding constant by the attachment constant of the dye in the complementary structure.

PARAMETER DISTRIBUTED MODEL OF THE CONFORMATIONAL TRANSITIONS INDUCED WITH CHANGE OF RELATIVE HUMIDITY IN THE NUCLEIC ACID SAMPLES

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The parameter distributed model, which describes the conformational transitions induced with change of the sample relative humidity, is presented in the paper. Tree main nucleic acid conformational states are presumed in the model. The numerical calculations have been performed for evolution of the perturbations of the initially homogeneous biopolymer conformational state.

ENERGETIC AND DYNAMIC PROPERTIES OF WATER IN HYDRATE SHELL OF DNA

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A new approach to studying dynamic properties of water molecules bound to biopolymer matrices has been proposed. It is based on measuring dehydration energy of biopolymer-water systems at various levels of relative humidity with using the differential scanning microcalorimetry method. Correlation between the dehydration energy and nucleotide composition of a native DNA has been found. Some characteristics of dynamic mobility of the water molecules in the hydration shells of biopolymers studied have been calculated with using experimental data. Also, systems containing dinucleotides ApA, TpT, UpU and water clusters of various sizes (20, 40 and 200 water molecules) have been studied by Monte Carlo computer simulation. Results of this simulation correlate with appropriate calorimetric data.

QUANTUM-MECHANICAL STUDY OF NUCLEIC ACIDE BASE CATIONS

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With the aim to study spectroscopic properties of nucleic acid base cations electronic-excited states (EES) energy

calculations of four guanine cations, three adenine cations and its dications were performed by using of two versions of CNDO/S method. Results of these calculations were compared with experimental ones for cation forms of such bases to be studied formerly. This comparison shows enough good agreement between experimental EES energies and calculated ones. The calculations predict positions of the first UV absorption bands for adenine, guanine and cytosine cation forms which experimental results are absent till present time. These calculations, in particular, predict a blue shift of cytosine 07H cation UV absorption spectrum relatively neutral form spectrum. A red shift of N3H-, 01 OH- and N7H enol guanine cations, adenine N3H and N7H cations UV absorption spectrum is predicted, also.

EXPERIMENTAL AND THEORETICAL STUDY OF INTERMOLECULAR INTERACTIONS IN THE RECOGNITION COMPLEX OF METHYLURACILE AND ACRYLAMIDE

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Structural and energetical parameters of the intermolecular interactions in the model recognition complex between the 1-methyluracyl and side chains of the aminoacids Asparagyine and Glutamine were determined. Enthalpy value of the complex formation, measured by the method of temperature dependent field ionization mass spec-trometry is equal to (-40,6±4,2) kJ/mole and it is in a good agreement with the values of interaction energy in two most favourable dimer configurations, calculated by MP2 and DFT methods.

IR-SPECTROSCOPIC STUDY OF Cu^{2+} ION INTERACTION WITH DNA IN AQUEOUS SOLUTIONS CONTAINING ADDITIONS OF 1,2-PROPANEDIOL AND GLYCEROL

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The present work studied the Cu^{2+} ion interaction with DNA in aqueous solutions containing low (up to 20 v %) additions of glycerol or 1,2-propanediol at 29 and 45^{0}C by IR-spectroscopy. Cu^{2+} ions were shown to induce the DNA transition into compact form in aqueous and water-glycerol (propanediol) solutions both at 29 and at 45^{0}C. This process is of high positive cooperativity. 1,2-propanediol added to the DNA aqueous solution increases cooperativity of the DNA transition into compact state and decreases the Cu^{2+} ions concentration required to induce DNA compactisation. The 1,2-propanediol effect increases monotonously with the rise of its volume concentration (in the concentration range 0-20 v %) at 29 and 45^{0}C. In contrast to propanediol, the glycerol effect on DNA compactisation is of non-monotonous character: small (4 v %) glycerol additions to DNA aqueous solution decrease cooperativity of the DNA transition into compact state at 29^{0}C. Comparison of effects of small additions of 1,2-propanediol and glycerol for which dielectric permeability of solution changes practically the same, on the Cu^{2+}-induced DNA condensation, permits the conclusion that the DNA condensation induced by the Cu^{2+} ions depends not only on dielectric permeability but on the structure of the solution formed.

TERMOTROPIC CHANGES OF FIBRINOGEN CONFORMATION

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The information concerning the structural changes of fibrinogen molecule at temperatures from 4 to 52°C has been obtained by means of UV-spectroscopy and dielectric-spectroscopy methods. Besides the known conformational transition II (at about 10°C), under physiological conditions conformational transition at 18-22°C has been observed in fibrinogen. This transition might be connected with structural transition in D-domain of fibrinogen and accompanied by an increase in tryptophanyl accessibility to the solvent. Revealed conformational transition, probably, determines the character of the temperature dependence of blood platelet aggregation.

PHYSICO-MATHEMATICAL MODEL OF BIOMACROMOLECULE CONFIGURATION FLUCTUATION IN A VISCOSITY MEDIUM.

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In this work the physico-mathematical model allowing to compute the probability of fluctuative alteration of configuration of long linear macromolecular and to take into account the influence of medium viscosity, in which the macromolecules are suspended, has been developed.

THE PHYSICO-MATHEMATICAL MODEL OF HYPOTONIC HEMOLYSIS OF HUMAN ERYTHROCYTES BEHAVIOURE. I. SWELLING STAGE.

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In this work the physico-mathematical model of hypotonic hemolysis of human erythrocytes has been developed. It describes the kinetics of this phenomenon under cells plunging into hypertonic water solution of electrically neutral permeable substance during the swelling of cell to critical volume.

USING OF DSM FLUORESCENCE SPECTRA INHOMOGENEOUS BROADENING ANALYSIS FOR INVESTIGATION OF MODEL AND NATURAL MEMBRANES STRUCTURAL CHANGES

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Modification of inhomogeneous broadening parameters analysis method in reference to fluorescent probe DSM was developed. Possibilities of the method using for investigation of model and biological membranes structural changes under influence of proteins, ionizing radiation and low temperatures were studied. It was shown that DSM spectra analysis allows receiving of information about character of probe microenvironment polarity under different conditions.

GROWTH KINETICS OF MULTICELLULAR TUMOR SPHEROIDS: ANALYSIS BY MATHEMATICAL MODELLING

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Effect of oxygen and glucose on the cellular heterogeneity and growth kinetics of multicellulat tumor spheroids has been analyzed by a mathematical model. The model takes into account the processes of cell division, death and transition from proliferation to rest in which oxygen and glucose are considered as nonspecific regulatory factors of cell viability. The model was used to analyze growth kinetics and cellular heterogeneity of EMT6/Ro murine mammary carcinoma cell spheroids growing under the standard conditions. The model gives a good representation of growth kinetics and oxygen distribution in spheroids and allows to study the proliferative heterogeneity of their cells. The comparison of model predictions with experimental data showed, that oxygen consumption rate per cell estimated theoretically more than 4 times lower as that measured experimentally.

APPLICATION OF QUASIPOLYNOMIALS IN STOCHASTIC SIMULATION OF PHARMACOKINETIC

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In the paper structural functional pharmacokinetic model was constructed. Methods of probable simulation was used. The new approach to the choice of analytical expression for the unimodal probability density function is offered. The domain of function is positives semiaxis and it has infinite zero and cipher zero . Model of system which consists of several consecutive blocks is examined. An entrance of each subsequent block is the previous block exit.

INFLUENCE OF γ -IRRADIATION ON STATE OF DNA ION - HYDRATION SHELL

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The effect of γ-radiation on the state of DNA hydration shell has been investigated. The changes of dielectric permittivity of DNA aqueous solutions irradiated at doses 19, 370, and 1650 Gy have been studied using the differential dielectrometric method. The DNA state was checked by conductance-measuring and electrophoresis methods. Some noticeable changes of DNA hydration at 370 and 1650 Gy have been found. It has been shown that the effects revealed are due to the breach of water backbone structure arising from double helix reconstructions which appear to be a result of radiation deoxyribosyl lesions and also to the appearance of DNA radiation-altered bases.

INFLUENCE OF γ-RADIATION ON STRUCTURAL STATE OF DNA IRRADIATED AT VARIOUS HUMIDITY LEVELS

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A study of γ-radiation influence on calf thymus NaDNA at various relative humidity levels has been carried out with using gel-electrophoresis and UV-spectroscopy techniques. It has been shown that irradiated DNA samples differ from check sample in molecular mass (fragment lengths) distribution due to partial fragmentation of DNA molecules, the fragmentation degree depending upon relative humidity of the sample during irradiation. The most destruction of DNA is observed at minimum (0%) and maximum (90%) relative humidity, and the least one - in the interval of 56-64% relative humidity. UV-spectroscopy data give evidence of that with increase of relative humidity of DNA samples irradiated with a certain dose shift of DNA melting temperature towards its increase is observed. It is concluded that main targets of γ-radiation influence on DNA are diesteric bonds between AT-pairs.

THE INFLUENCE OF IONIZING RADIATION ON THE Mg^{2+}-ATPase OF ERYTHROCYTE PLASMATIC MEMBRANE ACTIVITY

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The alteration of Mg^{2+}-ATPase activity under the comparison of ionizing radiation influence in small and large dose diapasons (from 4 10^{-3} to 10^{3} Gr) on the erythrocyte plasmatic membrane have been studied. The Michaelis' constant and maximum rate of enzymic reactions were determined. The data obtained during the experiment give us possibility to suppose, that under the dose equal 1 Gr the ionizing radiation effect is stipulated by action of water radiolysis products, and under the dose equal 10^{3} Gr - by combinative action of direct and indirect radiation influence.

THE ROLE OF THE LIPID AND THE PROTEIN IN RADIATION DEFEAT OF THE ERYTHROCYTE MEMBRANES

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The intensity processes of the lipid peroxidation, microtenacity of free and fixed of the lipid, polarization of membrane proteins under the influence of ionizing radiation in doses $10 \div 10^{3}$ Gr have been investigated. The interconnection between level of radiation defeat of membrane's lipid and conformation agility of membrane's protein have been established.

ON A POSSIBLE CAUSE OF OBSERVABLE "RESONANCE" EFFECTS OF MICROWAVE IRRADIATION ON BIOLOGICAL OBJECTS

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Physical mechanism is advanced for arising the response of biological objects to microwaves of nonthermal intensity. Swipping the frequency results in shifting the fine spatial pattern of the field along the path of propagation in near zone of the antenna. Therefore, the biological object fixed in this zone is affected by different amount of radiation when the frequency is being changed. In according with this, the dependencies of the response obtained in described conditions are not recommended to be called "resonance".