

ABSTRACTS

EFFECT OF Mg^{2+} ON DOUBLE AND TRIPLE HELIX FORMATIONS BETWEEN POLY(dA) AND POLY(dT)

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The Mg^{2+} ion effect on conformational transitions in double- and triple-helical structures formed by poly(dA) with poly(dT) has been studied in 10 mM cacodylate buffer, pH 7, containing 0.1 M Na^+ . The investigations were carried out by the method of thermal denaturation using UV absorbance and Rayleigh light scattering detections of melting transitions. Temperatures of helix-to-coil transition of poly(dA)-poly(dT) and triplex-to-duplex of poly(dA)-2poly(dT) increase linearly with $\log[Mg^{2+}]$ and more quickly in the last case that results in the superposition of these transitions at $[Mg^{2+}] \geq 15$ mM. At $[Mg^{2+}] \geq 20$ mM during the melting of the both structures aggregation was observed, which arised, according to Bloomfield and co-workers, due to formation of cross-links by Mg^{2+} ions bridges between partially unplaited polymer strands and disappeared after the end of melting. It is established that at the presence of 0.1 M NaCl magnesium ions do not induce the partial formation of the triplex structure in poly(dA)-poly(dT) (disproportionation) as is postulated by other authors in some papers.

KEY WORDS: polynucleotides, double and triple helices, magnesium ion, helix-to-coil transitions, Rayleigh scattering

INFLUENCE OF HYDRATTON ON THE TAUTOMERISM OF NUCLEIC ACID BASES: COMPUTER SIMULATION BY MONTE CARLO METHOD

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An extensive computer simulation of nucleic acid bases hydration and their main tautomeric forms is performed by the Monte Carlo method. It is shown that the lactam form of guanine and amino form of cytosine in water cluster are energetically more preferable than their lactim form and imino form respectively. The greater stability of the usual tautomeric forms of these bases in water cluster as compared with their rare tautomeric forms entirely due to energetically more favourable interaction of water molecules with each other. At the same time it is detected that the imino form of adenine and lactim forms of thymine and uracil are more stable than the corresponding amino form and lactam form. This fact is determined by more favourable interaction of the base rare forms with a water.

KEYWORDS: nucleotide bases, tautomerism, hydration, Monte Carlo method, computer simulation

HYDRATION OF THE VARIOUS STRUCTURAL FORMS OF POLYRIBOCYTIDILIC ACID AND ITS COMPONENTS BY A MONTE CARLO METHOD.**2. THE INFLUENCE OF PROTONATION ON HYDRATION OF CYTOSINE ASSOCIATES.**

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The processes of association neutral and protonated on N3-site cytosine in water and influence of protonation on cytosine associates interaction with aqueous environment have been studied by Monte Carlo method. The structural and energetic characteristics of hydrogen-bonded pair of neutral (C) and protonated (C⁺) cytosine (HB-pair) and stacked-dimers of both cytosine forms with 200 water molecules have been received. It was shown, that the formation of HB-pair in water is energetically unfavourable, but in vacuum such HB-pair is stable. The formation of stacked-dimers C-C and C⁺-C⁺ in water is energetically preferable. The preference of stacked-dimer C-C in water is connected with the energetic preference of the dimer-water interaction and with the favourable change in water structure around monomers during their association. The energetic preference of C⁺-C⁺ stacked-dimer formation in water is determined by the strong water-dimer interaction and formation of water bridges between cytosines stabilized such associate. The hydration schemes of the three associates have been determined.

KEYWORDS: cytosine associates, protonation, hydration, a Monte Carlo method

VIBRATIONAL ANALYSIS OF THE WATSON-CRICK BASE PAIR ADENINE-URACIL. AN AB-INITIO QUANTUM-CHEMICAL STUDY.

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Vibrational spectra of the Watson-Crick base pair adenine-uracil were calculated for the first time using the DFT/B3LYP/6-31++G** level of theory with the accounting for the electron correlation. The complete analysis of the vibrational spectra of the base pair was carried out and the force fields of the monomers and dimer were determined. The spectral manifestations of the H-bonding in the base pair adenine-uracil were summarized. The interaction energies of the base pair were calculated at the MP2 and DFT levels of theory with the accounting for the basis set superposition error correction and zero-point vibration energy correction. They are -47.8 and -6.0 kJ/mol, respectively. The calculated energies are found to be in good agreement with the experimental data.

KEY WORDS: adenine-uracil, quantum-chemical ab-initio calculations, vibrational spectra, molecular parameters.

RELAXATION AND SPECTROSCOPIC MANIFESTATIONS OF HYDRATION OF POLYRIBOCYTYDYLIC ACID

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Hydration and structure state of polyribocytidylic acid (poly(rC)) have been studied in solutions and humid films. The role of water in forming different structures of poly(rC) was elucidated. In solutions, the hydration values of single-strand (pH 4.5), double-strand (pH 7.8) and disordered (pH 3.3) forms of poly(rC) were determined with a differential EHF-dielectrometer using the measurements of dielectric permittivity at wavelength 7.6 mm. In humid films, distribution of water molecules on the hydration sites for these structures has been found with IR spectroscopy. Hydration models of the single and double-strand structures of poly(rC) were developed using X-ray and these data.

KEY WORDS: polycytidylic acid, hydration, infrared spectra, millimeter region, structural transitions

INTERACTION OF Ni²⁺ IONS WITH HOMOPOLYNUCLEOTIDES CONTAINING ADENINE AND URACIL AND THEIR MONOMERS

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Interactions of Ni²⁺ ions with AMP, UMP, single-chain poly A, poly U, double-chain poly A-poly U and three-chain poly A:2 poly U have been studied by the method of differential UV spectroscopy. The coil → helix transition observed in polynucleotides is due to the Ni²⁺ ion binding to oxygen atoms of phosphate groups. The nickel coordination to bases takes place only in the case of single AMPs and single-chain poly A. The formation of a chelate N7-Ni²⁺-(PO₄)⁻ induces melting of this polymer. Melted parts form compact particles with the effective radius ~100 Å.

KEY WORDS: UV spectroscopy, homopolynucleotides, metal ions

INFLUENCE OF HYDRATION ON TAUTOMERISM OF 6-THIOGUANINE.

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The theoretical calculation of complexes of 6-thioguanine thiol and thion tautomers was performed by means of B3LYP and HF methods. The greater stability of complex having included the thion tautomer by 17.6 kJ/mol and 8.1 kJ/mol correspondingly was shown. It accords with experimental data that 6-thioguanine exists in water mainly in the shape of thion tautomer, although it exists in gas phase as thiol tautomer.

KEY WORDS: 6-thioguanine, tautomerism, quantum-mechanical calculations

THE FRIZZING REGIME EFFECT ON THE INTERACTION BETWEEN FIBRINOGEN AND DSM FLUORESCENCE PROBE

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The interaction between fibrinogen and DSM fluorescence probe in protein solutions frizzed with different rates up to -8 °C and -196 °C has been studied by using the fluorescence spectroscopy method. Two types of probe binding centers have been detected on the fibrinogen molecule. These centers have distinct parameter values of fluorescence spectra. It has been shown, that greater conformational damages take place under slow cooling conditions than under fast ones.

KEY WORDS: fibrinogen, conformation, fluorescence spectroscopy, probe, binding, frizzling, cooling rate

PROPERTIES OF A SOLUTION OF GLYCINE IN AN INTERVAL OF TEMPERATURES 20-70 °C ON DATA OF MICROWAVE DIELECTROMETRY AND VISCOSIMETRY

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The changes of viscosity and relaxation times of 20 % of a glycine solution in the interval of temperatures 20-70 °C are studied. The technique of measurement of viscosity is described. Data on static permittivity and relaxation times calculated according to Debye model, taking into account average relaxation times in the solution, are presented. The deviations of values calculated from ones measured by alternative methods are discussed. A possible mechanism of change of dielectric parameters in the range of temperatures considered is offered.

KEY WORDS: glycine, relaxation time, permittivity, aqueous solutions.

HIGH CONDUCTANCE CALCIUM-DEPENDENT POTASSIUM CHANNELS IN THE MEMBRANE OF GUINEA PIG TAENIA COLI

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High conductance calcium-dependent potassium (K(Ca)) channels in isolated membrane fragments from guinea pig taenia coli smooth muscle cells (SMCs) have been studied using "outside-out" and "inside-out" patch-clamp recording techniques. Currents carried via these channels were studied with the "whole cell" patch-clamp technique also. It was shown that charybdotoxin-sensitive K(Ca) channels are presented widely in these cells. They have a high conductance - 125 ± 24 pS at $[K^+]/[K^+]_0 = 23$. In addition to Ca^{2+} -dependence, these channels were voltage-dependent also, but have no a voltage-dependent inactivation. Fast inactivation of these K(Ca) is dependent only on sub-membrane intracellular Ca^{2+} concentration ($[Ca^{2+}]_i$). Time course of the decay of current carried via high conductance K(Ca) channels was found to follow closely the rate of Ca^{2+} current inactivation. It was suggested that the main source of Ca^{2+} , needed for the activation of high conductance K(Ca) channels, is entrance of Ca^{2+} ions into the cell via L-type Ca^{2+} channels.

KEY WORDS: smooth muscle cells, membrane, K(Ca) channels, conductance, $[Ca^{2+}]_i$, charybdotoxin, voltage-dependence, inactivation

THE INVESTIGATION OF PERMEABILITY OF CYTOPLASMATIC MEMBRANES FOR WATER AND ENERGY OF ACTIVATION OF WATER TRANSPORT THROUGH CELL MEMBRANE

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The method of studying of cytoplasmatic membrane permeability for water was described. The given method allows one to calculate the coefficient of mammalian ova and embryo cytoplasm membrane permeability for water on basis measurement of cell volume changes in time in solutions of different composition and temperature by using of physic and mathematical model and Kedem-Katchalsky equations. And also the energy of activation of water transport through cell membranes was determined.

KEY WORDS: osmotic reaction, cytoplasmatic membrane permeability, cell volume, energy of activation.

NUMERIC MODELLING OF THE PROCESS OF CRYOPROTECTANT REMOVAL FROM A CELLULAR SUSPENSION

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The resistance of frozen-thawed cells to posthypertonic lysis during the process of their single washing-out from a cryoprotectant has been investigated by means of the method of numeric modelling using the transmembrane mass transfer equation. It has been shown, that the dilution values of thawed cellular suspension by means of washing-out solution and the concentration of non-penetrating substances in cells in it affect the strongest effect on the result of this procedure.

KEY WORDS: numeric modelling, cryoprotectant, posthypertonic cryohemolysis.

ON POSSIBLE SCENARIO OF SPACE AND TIME EVOLUTION OF SELF-ORGANIZATION IN BIOLOGICAL MEDIA

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The results of the stationary diffraction theory, the spectral theory of open systems and the theory of Mors' critical knots of dispersion equation of boundary self-organizing biomedica permit one to determine the analytic dispersion laws and build on their basis the nonlinear evolution equation to describe local space and time processes of continuous biomolecule media. On the simplest examples of nonlinear equation solutions for flat media interfaces it has been demonstrated the variety of dynamical phenomena appearing when macromolecule self-organization occurs.

KEY WORDS: diffraction, dispersion, catastrophe, interface, self-organization, chirality

THE ROLE OF CELL MOTILITY IN THE OVERGROWTH OF METASTATIC CELLS IN A HETEROGENEOUS TUMOUR

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The mathematical model of the growth kinetics of a heterogeneous tumour consisting of two cell subpopulations: fast-growing and non-motile subpopulation and slow-growing but motile one, - has been created to study the metastatic cell dominance phenomenon. The results obtained showed that the migrating capacity of the cells (as an inherent cellular characteristic) can result in the growth advantage of these cells in a heterogeneous tumour.

KEY WORDS: mathematical model, cell motility, heterogeneous tumour, metastatic cells

MODELING OF CELL RECEPTIVE FIELDS OF VISUAL ANALYZER**R.V. Lyakhovetsky, T.P. Palatniy, T.V. Korobko, V.R. Lyakhoetsky, V.L. Zyma***Taras Shevchenko Kyiv University, 64, Volodymyrska str., Kyiv, 01033, Ukraine*

The creation of precise maps of receptive fields (RF), by the method of mathematical modeling has been investigated. We have shown that in electrical field of double syncytium (photoreceptors - horizontal cells), under the influence of dot stimulus springs up a delve, which have form of difference of gaussians. This allows presuming photoreceptor's RF and sets demands for "retina chip". Precise maps of circular and rectangular RF have been designed, which are the base for description of the properties of RF of complex cells and hypercolumn, including the possibility to normalize the dimensions of input signals.

KEY WORDS: cells of visual analyzer, models of receptive fields, elements of neurocomputer

STUDY OF RADIATION-INDUCED ALTERATIONS IN OXIDOREDUCTASE ACTIVITY IN THE PRESENCE OF MEMBRANOTROPIC AGENTS**A.V. Finashin, V.N. Tkachenko, V.V. Tovstiyak***Kharkov National University, 61077, Kharkov, Svobody sq. 4, e-mail: tovstiyak@pem.kharkov.ua*

The activity of microsomal oxidoreductases has been studied under the influence of radiation in the doses 10^2 - 10^4 Gy. The activity of both enzymes has been found to decrease upon irradiation in the dose 10^4 Gy. It has been shown that radiation-induced effects do not depend on the protein's concentration range 0.2-0.23 mg/ml. Oxidoreductase radiative inactivation has been found not to correlate with the lipidperoxidation. The peculiarities of the action of compounds, modifying the membrane structural state (triton X-100, glutaraldehyde, butanol) on the oxidoreductase radioresistivity have been established.

KEY WORDS: microsomal oxidoreductases, irradiation, modification of enzyme radioresistivity.

PROLONGED CHRONIC IRRADIATION EFFECTS ON DNA STRUCTURE IN THE CHERNOBYL ZONE**S.V. Kornilova***B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine.**47 Lenin Ave., 310164, Kharkov, Ukraine, e-mail: kornilova@ilt.kharkov.ua*

Properties of DNA from animals exposed to prolonged irradiation in the Chernobyl APS zone were studied by methods of viscometry, thermal denaturation, IR spectroscopy and electrophoresis. In DNA preparations from liver and spleen an abnormal number of low molecular DNA was revealed, that increases in following generations of animals as well as with their ages. This effect is especially pronounced in DNA from liver. It is shown that the low molecular DNA is riched in GC-pairs and consists of four fraction, namely: 1) ~500 nucleotide pairs (n.p.), 2) ~1500-2000 (n.p.), 3) ~4000-5000 n.p. and 4) an admixture with ~20000 n.p. It was found too that DNA preparations from tissues of experimental animals contain ferrum, zinc, selenium and other elements the contents of which are by dozen times higher than those of control preparations. Cu added into food of animals living currently in the zone intensifies the radiation influence. Model experiments on the combined effect of irradiation and Cu ions on DNA from blood lymphocytes revealed synergism of their effect. Zinc has a lesser influence on DNA physico-chemical properties than copper ions have. Experimental results on properties of DNA from regenerated liver cells after hepatectomy in animals exposed to prolonged irradiation evidence the increase of latent damages of DNA under irradiation, that manifests itself as low molecular DNA fractions the number of which reaches 65%. A model of DNA damages under the action of low doses of ionizing irradiation and Mt^{2+} ions was proposed.

KEY WORDS DNA, chronic irradiation, low molecular fractions, viscometry, IR-spectroscopy, metal ions

THE MOLECULAR MECHANISMS OF CONNECTIVE TISSUE VISKO-ELASTIC PROPERTIES FORMATION UNDER THE INFLUENCE OF EXOGENOUS MECHANICAL LOAD**A.E. Kuzmis, O.B. Garbuzenko, E.E. Persky, L.A. Utevskaia***V.N. Karazin Kharkov National University, Kharkov, 61077, Ukraine*

The investigation of the mechanical load influence on collagen concentration and synthesis intensity and visko-elastic properties of tail tendons, skin and aorta of different ages rats in vivo and in vitro has been done. Iminoacid and radioizotop analysis were used. The values of visko-elastic properties tissue were calculated by the corresponding graphs of stain-deformation. It was shown that mechanical load which influences on the organs leads to the changes connective tissue metabolism and finally to the formation of organs visko-elastic properties that are optimal to this influence.

KEY WORDS: mechanical load, visko-elastic properties, deformation, collagen, synthesis, age

SPECTROPHOTOMETRIC ANALYSIS OF MELTING CURVES OF DNA-BIOLOGICALLY ACTIVE NUCLEOSIDE MIXTURES AS A METHOD FOR DETECTION OF THE DNA DAMAGES**E.B. Kruglova, N.A. Gladkovskaya***Institute for Radiophysics and Electronics, NAS of Ukraine, 12 Acad. Proskura str., Kharkov, 61085, Ukraine*

Recently we have shown that DNA molecules extracted from epididymis of the Wistar male rats exposed to low doses of gamma radiation and the control DNA molecules interact with some of pyrimidine nucleosides (NUC) in different ways. Using UV-melting curves of the DNA-NUC mixtures for the model DNA samples we show that this differences are connected with the conformational

changes of the DNA helix. Model DNA samples were obtained by means of the partial denaturation of the calf thymus DNA in the salt-free aqueous solutions. The level of DNA damages of DNA molecules in such solutions depends on the DNA concentration. It was shown that such DNA damages lead to the changes in the melting curves of DNA-NUC mixtures which are similar to those for the DNA from irradiated tissues. It has been found also that the binding mechanisms of cytosine arabinoside (Ara-C) and 6-azacytosine (6AZC) with DNA molecules which have some modification in secondary structure are different.

KEY WORDS: salt-free DNA solutions, low radiation doses, UV melting curves, spectrophotometry, cytosine arabinoside, 6-azacytidine, the DNA damages

INFLUENCE OF X-IRRADIATION AND PROTECTOR, ALTAN, ON ERYTHROCYTE RESISTANCE

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The influence of x-irradiation and preparation altan on hemolysis by acid rat and human erythrocytes. The x-irradiation of 6 Gy dose causes the decrease of acid resistance of erythrocytes of both rat and oncology patients. It has been shown that altan therapy (perorally) performed before and after x-irradiation decreases the radiation effect on animal and human erythrocyte hemolysis sufficiently. Under such conditions the x-irradiation did not cause the change of ion (K^+ , Na^+ , Ca^{2+} , Mg^{2+}) ion concentrations both inside the erythrocytes and in blood plasma. Survival of altan-recipient rats was 2.5 times greater in 15-30 days after irradiation. The possible mechanism of altan radioprotection properties.

KEY WORDS: x-irradiation, erythrocytes, altan, hemolysis, acid resistance, cations, survival, radioprotectors

LOW-INTENSE MICROWAVE RADIATION INFLUENCING THE EFFECTIVE THICKNESS OF A NON-INTERMINGLED WATER LAYER ADJACENT TO A LIPID ERYTHROCYTE MEMBRANE

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Using an NMR technique, the thickness of a non-intermingled water layer adjacent to an erythrocyte membrane is determined. Half an hour low-intense microwave radiating is found to have decreased the effective thickness of the non-intermingled layer by 11 %. It is shown that this result cannot be account for only by thermal processes in a sample, arising under radiating.

KEY WORDS: erythrocyte, membrane, diffusion water exchange, non-intermingled liquid layer hear the membrane, electromagnetic microwaves

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