

Head of Laboratory

Zuev Y.F., D. Sc. (Chemistry), professor, Honored Scientist Republic of Tatarstan Contact phone number

+7(843)2319036

Lab members

Stoikov I. I.– Leading Research Scientist в.н.с., D. Sc. (Chemistry), Professor (ivan.stoikov@m ail.ru
) Ermako
va E. A. – Senior Research Scientist, Cand. Sc. (Chemistry)

Zaharchenco N. L. – Research Scientist, Cand. Sc. (Biology)

Idiyatullin B. Z. – Senior Research Scientist, Cand. Sc. (Biology)

Makshakova O. N.– Research Scientist, Cand. Sc. (Biology)

Sitnitsky A. E.– Senior Research Scientist, Cand. Sc. (Physical and Mathematical Sciences)

Faizullin D. A. – Senior Research Scientist, Cand. Sc.

Khairutdinov B. I. – Senior Research Scientist, Cand. Sc.(Physical and Mathematical Sciences)

Konnova T. A. – Juniour Research Scientist, PhD., Cand. Sc. (Biology)

Bogdanova L. R. – Juniour Research Scientist, Cand. Sc. (Biology)

Valiullina J. A. – Juniour Research Scientist

Kurbanov R. H. – Research Engineer

Bakirova D. R. – Research Technician

Mukhamedova L. N. – Postgraduate Student

Interest area of research

Intramolecular recognition and intramolecular signal transmission in functional protein-ligand complexes

General results:

1. The enzyme enhanced model of rate- promting vibration was constructed. Assuming, that the source of vibration in this model is an oscillating electric field, produced by long lasting local oscillatory modes in protein secondary structure. The interaction force of RPV with reaction coordinate was estimated. It was shown, that reaction acceleration could reach to 7-8 degrees.

- 2. The application of Brownin dynamic method to diffusion- controlled protein interaction reactions (such as dimerization, enzyme inhibitor complexes formation) and enzyme- substrate complexes for electric field was developed.
- 3. The basic mechanisms of microenviroment (synthetic and natural microgeneous systems, based on amiphylic compounds) activity in catalysis of hydrolytic splitting of peptides and complex etheric bounds were established.
- 4. For the first time the structure of hydrate envelope and mechanism of its modification in the presence of aprotic organic solvents for polypeptides with various chemical modification of side group and various type of the secondary structure were shown. The role of weak hydrogen C H•••O and C H type bonds in stabilization of homopolypeptides, that are differ in amino acidic residues structure (polarity, length and reactivity of side group) in complexes and aprotic solvents was shown
- 5. The intromolecular signal transduction mechanism, consisting of correlated interaction changes of protein amino acids was determined. (By the example of carbohydrate-building proteins galectin 1 and galectin 2) The result was included in the list of priority achievements of RAS, 2010.
- 6. . It was established that the main factors of Candida rugosa s lipase activity in microheterogenius systems, based on amphophilic compounds, were enzyme alteration of the structure and the colloidal system state. The model of Candida rugosa lipase activity based on the micelle catalytic exchange effect that is substrate microsurrounding change and its availability to enzyme active center was proposed.
- 7. It was shown that secondary structure changes and the associative feachers of betta-casein in hydro-ethanol solution were determined by the solvent structure, which depends on its compositions and temperature. The secondary structures content and the size of betta-casein correlated with the concentration borders of different microgenenius structure existence in mixed solvent. Opposite to the relevant opinion about betta-casein spiralization under higher temperatures conditions, it was established that temperature rising increase disordered structure formation.
- 8. The protective activity aimed at the inhibition of the aggregation process and preservation of partial functional activity of the proteins such as alcohol dehydrogenase, catalase, immunoglobulin G was shown. It was demonstrated that chaperon- like activity of recombinant betta-caseins mainly depended on location of the injected cystein residue and the proteins structural state.
- 9. It was shown that on the tripcine-ingibitor complexation the amplitude of functionally important loops fluctuation is changing, providing energy redistribution between amino acid residues of protein polypeptide chain. The substrate reinforces the correlation between the motion of amino acid residues of active center and residues of substrate-binding pocket.

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- 1. Gabdrakhmanov D.R., Voronin M.A., Zakharova L.Ya., Konovalov A.I., Khaybullin R.N., Strobykina I.Yu., Kataev V.E., Faizullin D.A., Gogoleva N.E., Konnova T.A., Salnikov V.V. Zuev Yu.F. // Supramolecular design of biocompatible nanocontainers based on amphiphilic derivatives of a natural compound isosteviol // *Phys. Chem. Chem. Phys.*, 2013, 15: 16725—16735.
- 2. Ermakova E., Miller M.C., Nesmelova I.V., López-Merino L., Berbís M.A., Nesmelov Y., Tkachev Y.V., Lagartera L., Daragan V.A., André S., Cañada F.J., Jiménez-Barbero J., Solís D., Gabius H-J., Mayo K.H. // Lactose binding to human galectin-7 (p53-induced gene 1) induces long-range effects through the protein resulting in increased dimer stability and evidence for positive cooperativity // Glycobiology, 2013, 23: 508-523.
- 3. Makshakova O., Ermakova E. // Effect of organic molecules on hydrolysis of peptide bond: A DFT study // Chemical Physics, 2013, 415: 282–290.
- 4. D. Faizullin, N. Zakharchenko, Yu. Zuev, A. Puzenko, E. Levy, Yu. Feldman // Hydration of AMP and ATP Molecules in Aqueous Solution and Solid Films // Int. J. Mol. Sci. 2013, V.14, P. 22876-22890.
- 5. Litvinov, Faizullin D.A., Zuev Yu.F., Weisel J.W. // The a-helix to b-sheet transition in stretched and compressed hydrated fibrin clots // Biophysical Journal 2012. V.103. P. 1020 1027.
- 6. Ryazantseva I.N., Saakov V.S., Andreyeva I.N., Ogorodnikova T.I., Zuev Y.F. // Response of pigmented Serratia marcescens to the illumination. // Journal of Photochemistry and Photobiology B: Biology - 2012. V.106. P. 18-23.
- 7. Grigorev I.V., Korobeinikov V.A., Cheresiz S.V., Pokrovsky A.G., Zaharova L.Y., Voronin M.A., Lukashenko S.S., Konovalov A.I., Zuev Y.F. // Cation geminal surfactants as a new source plasmid DNA transportation into the cells // Doklady Akademii Nauk. Doklady Biochemistry and Biophysics 2012. T.445. P. 349–352.
- 8. A.E. Sitnitsky // Analytic treatment of nuclear spin—lattice relaxation for diffusion in a cone model // *Journal of Magnetic Resonance* 2011, V.213, P.58–68.
- 9. D.A. Faizullin, N.N. Vylegzhanina, O.I. Gnezdilov, V.V. Salnikov, A.V. Galukhin, I.I. Stoikov, I.S. Antipin, Yu. F. Zuev // Influence of nature of functional groups on interaction of tetrasubstituted at lower rim p-tert-butyl thiacalix[4]arenes in 1,3-alternate configuration with model lipid membranes // *Applied Magnetic Resonance* 2011, -V.40, P.231–243.
- 10. E. A. Ermakova, N. L. Zakhartchenko, Yu. F. Zuev // Brownian dynamics simulation of substrate motion near active site of enzyme entrapped inside reverse micelle // Euroupia n Biophysical Journal
- 2010, V.39, P.1335-1341.

- 11. A.E. Sitnitsky // Model for solvent viscosity effect on enzymatic reactions // *Chemical Physics* 2010, V.369, P.37–42.
- 12. I. V. Nesmelova, E. A. Ermakova, V. A. Daragan, M. Pang, M. Menéndez, L. Lagartera, D. Solís, L. G. Baum, K. H. Mayo // Lactose binding to galectin-1 modulates structural dynamics, increases conformational entropy, and occurs with apparent negative cooperativity // *Journal of Molecular Biology* 2010, V.397, P.1209-1230.
- 13. E.A. Ermakova, N.L. Zakhartchenko, Yu.F. Zuev // Effect of surface potential of reverse micelle on enzyme-substrate complex formation // Colloids and Surfaces A:

 Physiochemical and Engineering Aspects

 2008, V. 317, P.297-302.
- 14. E.A. Ermakova, N.L. Zakhartchenko, Yu.F. Zuev // Effect of surface potential of reverse micelle on enzyme-substrate complex formation / Colloids and Surfaces A: Physiochemical and Engineering Aspects
 , 2008 V. 317 P. 297-302.
- 15. Ermakova E. // Brownian dynamics simulation of the competitive reactions: Binase dimerization and the association of binase and barstar / Biophysical Chemistry, 2007 V. 130 P.26-31.
- 16. Zuev Yu.F., Vylegzhanina N.N., Zakhartchenko N.L. // Effects of protein solubilization on the structure of surfactant shell of reverse micelles / *Applied Magnetic Resonance*, 2003 V.25 P.29-42.
- 17. Zuev Yu.F., Mirgorodskaya A.B., Idiyatullin B.Z. // Structural properties of microheterogeneous surfactant-based catalytic systems. Multicomponent self-diffusion NMR Approach / Applied Magnetic Resonance, 2004 V.27 P.489-500.
- 18. Sitnitsky A.E. // Modeling the "glass" transition in proteins / Journal of Biomolecular Structure and Dynamics, 2002 V.19 P.595-605.
- 19. Л.Я. Захарова, Ф.Г. Валеева, Л.А.Кудрявцева, Ю.Ф.Зуев // Факторы, определяющие мицеллярный эффект в реакциях нуклеофильного замещения / *Ж* урнал Физической Химии , 2000, Т.74, № 11, C.2006-2010.
- 20. Feldman Yu., Kozlovich N., Nir I., Garti N., Archipov V., Idiatullin Z., Zuev Yu., Fedotov V. // Mechanism of transport of charge carriers in the sodium bis(2-ethylhexyl) sulfosuccinate—water—decane microemulsion near the percolation temperature threshold / *Journal of* Physical Chemistry , 1996 V.100 P.3745-3748.
- 21. Feldman Yu.D., Zuev Yu.F., Polygalov E.A., Fedotov V.D. // Time domain dielectric spectroscopy. A new effective tool for physical chemistry investigation / Colloid and

Polymer Science , 1992 – V. 270 - P. 768-780.