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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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