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Posters

– 7. Protein translocation, assembly, and folding –

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Structural analysis of proteins forming the bacterial ribosome tunnel

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Ribosomes are ribonucleoprotein particles responsible for synthesis of a nascent chain, during which is messenger ribonucleic acid translated into amino acids. They play a crucial role in all three domains of life. The nascent chain leaves the ribosome through an exit tunnel located within the large ribosomal subunit. Plentiful interactions can be found between the nascent peptide and the tunnel walls, as an illustration, with the narrowest part formed by extended loops of two ribosomal proteins named uL4 and uL22. In addition, uL4 and uL22 also have globular parts at the surface of the ribosome. The proteins can through the globular parts interact with other proteins associated with the ribosomes.
It is not fully clear what roles play the two domains of the ribosomal proteins contributing to the tunnel walls and why the proteins evolved into their shapes. We address these questions by analyzing a set of experimental ribosome structures found in the Protein Data Bank. Root-mean-square fluctuation analysis reveals the flexible and the rigid sections, e.g. some of the most flexible amino acids of uL22 were at the tip of the loop intervening the tunnel. Principal component analysis of Cartesian coordinates suggests that some elements are structurally correlated. Sequence alignment complements the analyses as it offers an insight into conserved sections of the proteins and whether the critical ones are included. Observations from these analyses contribute to our understanding of ribosome function and regulation.

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The structure of human serum albumin upon interaction with catechin and metal ions

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Human serum albumin (HSA) is the prevailing protein in the blood plasma. Its natural function as a universal low-molecular compounds carrier as well as a promising ability to serve as a base for drug delivery systems rivet researcher's attention. Understanding the HSA structure upon its interaction with metal ions and bioactive molecules is necessary for biomedical applications. Catechin is one of the plant polyphenols displaying antioxidant activity and using in the development of new therapeutic forms and nanoparticle synthesis. This work is devoted to studying alteration in HSA structure in solutions containing mono- and divalent cations and catechin by the methods of UV absorbance, fluorescent and FTIR spectroscopy, spectrophotometrical melting, and diffusion layer potential measure.
The net charge of HSA at neutral pH in water solution is negative (−15e). In the presence of alkaline and alkaline-earth metal ions albumin's globule is more stable, than in water, and its charge tends to zero, whereas in the presence of transition metal ions strong protein aggregation is observed and assembled particles are positively charged. Catechin stabilizes tertiary and secondary structures of HSA but does not prevent its aggregation caused by transition metal ions.
A part of this work was performed at the Centre for Optical and Laser Materials Research (COLMR) in Research park of St.Petersburg State University.

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Effect of Hofmeister cations on α-lactalbumin amyloid fibrillization

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Amyloid fibrils have been formed *in vitro* from disease-associated as well as disease-unrelated proteins and peptides. α-lactalbumin (α-LA) is a suitable model protein for amyloid aggregation study due to its ability to form a molten globular state. Using a multi-technique approach, we have compared the effect of a variety of cations from the Hofmeister series (NH_4^+, Cs^+, K^+, Na^+, Mg^{2+}, Ca^{2+}) in the modality of chloride salts at two different concentrations on the amyloid formation of Ca^{2+}-depleted α-LA. The kinetics, the content of β-structure and amyloid fibril morphology have been studied using ThT and Trp fluorescence, FTIR spectroscopy and AFM microscopy. We found out, that the effect of cations on kinetic parameters of α-LA amyloid formation and morphology of α-LA fibrils is strongly correlated to salts concentration and their position in the Hofmeister series. The obtained results might contribute to a better understanding of the processes of amyloid self-assembly of globular proteins. This work was supported by the grants VEGA 2/0176/21, APVV-18-0284, and the MIUR grant (PRIN 20173L7W8K).

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The role of salt-bridge stability in the initial steps of insulin fibrillation

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We have studied how structural and sequence similarity of insulin variants from human (HI), bovine (BI), and glargine (GI) influence their thermal stability and aggregation propensity. We investigated the structural features and kinetics of fibrillation to shed light on the role of B-chain C-ter dynamics and salt-bridge stability in the initial steps of insulin fibrillation. Kinetic analysis showed that GI fibrillation is slower than BI and HI. AFM imaging confirmed the longer lag phase of GI fibrillation. After 42 h, BI and HI formed fibrillar species; but, only globular oligomers of GI were observed. These data point to GI's higher stability due to two additional Arg residues, Arg31B and Arg32B. NMR experiment showed atomic contacts and residue-specific interactions, particularly the salt-bridge and H-bond formed among C-ter residues Arg31B, Lys29B and Glu4 in GI. We propose that enhanced stability of native GI by strengthening salt bridge can retard tertiary collapse, a crucial event for oligomerization. The fluctuation of the B-chain C-ter residues plays a key role in the growth phase of insulin fibrillation.