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Keywords: tubulin, chaperons, electron microscopy.

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Structures of a group II chaperonin.

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Thermosomes are group II chaperonins responsible for protein refolding in an ATP-dependent manner. Little was known regarding the conformational changes of thermosomes during their functional cycle due to lack of high-resolution structure ofin open state. We reported the first complete crystal structure of thermosome (rATcpnβ) in open state from *Acidianus tengchongensis*. There is a ~30° rotation of the apical and lid domains compared to the previous closed structure. Besides, the structure reveals a conspicuous hydrophobic patch in the lid domain and residues locating in this patch are conserved across species. Both the closed and open forms of rATcpnβ were also reconstructed by electron microscopy (EM). Structural fitting revealed the detailed conformational changes from open to closed state. Structural comparison as well as protease K digestion indicated only ATP binding without hydrolysis does not induce chamber closure of thermosome.

Besides, we have solved a lot of cryoEM structures of rATcpn in different assemblies and functional states with different conformations using data collected on Titan Krios. We discovered that the cooperativity between heterologous subunits is indispensable for the performance of complete chaperonin function and clarify the structural basis for the functional cooperativity.

Keywords: thermosome, crystallography, cryoEM

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The structure of the *in vivo* assembled CCT:G protein β1 subunit complex reveals a novel CCT substrate binding mechanism mediated by hydrophobic interactions

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The eukaryotic cytosolic chaperonin CCT/TriC plays a crucial role in the folding of a set of very important proteins [1]. The CCT substrate recognition mechanism has been found, in the case of the cytoskeletal proteins actin and tubulin, to be based on specific interactions involving charged and polar residues of both the chaperonin and the unfolded substrate. Here we show for the first time the three-dimensional reconstruction of the complex formed by CCT and the G protein β_1 subunit, isolated *in vivo* from insect cells. $G\beta_1$ represents the major class of CCT substrates, the WD40 repeat proteins that form β-propeller structures [2]. The electron microscopy analysis reveals that $G\beta_1$ interacts specifically with the apical domain of CCTβ. $G\beta_1$ binding experiments with several CCT chimeric proteins confirm the specific interaction with CCTβ and map $G\beta_1$ binding to a hydrophobic core of amino acids located in α-helix 9 and in the loop between β-strands 6 and 7, facing the chaperonin cavity. From these results, a model for the folding of $G\beta_1$ mediated by CCT and its co-chaperone PhLP1 is proposed.

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Self-assembly of copolymers containing a polypeptide block

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The self-assembly of PEGylated peptides containing a modified sequence from the amyloid β peptide, FFKLVFF, has been studied in aqueous solution [1]. PEG molar masses, PEG1k, PEG2k and PEG10k were used in the conjugates. It is shown that the three FFKLVFF-PEG hybrids form fibrils comprising a FFKLVFF core and a PEG corona. The β-sheet secondary structure of the peptide is retained in the FFKLVFF fibril core. At sufficiently high concentrations FFKLVFF-PEG1k and FFKLVFF-PEG2k form a nematic phase, while PEK10k-FFKLVFF exhibits a hexagonal columnar phase. Simultaneous small angle neutron scattering/shear flow experiments were performed to study the shear flow alignment of the nematic and hexagonal liquid crystal phases. On drying, PEG crystallization occurs without disruption of the FFKLVFF β sheet structure leading to characteristic peaks in the x-ray diffraction pattern and FTIR spectra. The stability of β-sheet structures was also studied in blends of FFKLVFF-PEG conjugates with poly(acrylic acid) (PAA). While PEG crystallization is only observed up to 25 % PAA content in the blends, the FFKLVFF β-sheet structure is retained up to 75% PAA in FFKLVFF-PEG/PAA blends.

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Ionic liquids (IL): structures model

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There are two opposite opinions on the structure of IL: on one