CaMKK1 (Ser100 in CaMKK2) functions as the primary 14-3-3 binding site. Furthermore, a second 14-3-3 binding motif located at the C-terminus containing phosphorylated Ser475 in CaMKK1 (Ser511 in CaMKK2) has also been suggested. Although the C-terminal 14-3-3 binding motif (sequence RSLpSAP) is a canonical "mode I" 14-3-3 binding site, the N-terminal motif (sequence RKLpSLQE) contains a Gln residue at the position +2 relative to the phosphorylated residue pSer. Bioinformatics survey of 14-3-3 binding sites revealed that Gln is seldom found at +2 because the Pro residue and, to a lesser extent, Ser, Gly and Asp also, are frequently found at this position. To elucidate the structural basis of interactions between 14-3-3 proteins and the 14-3-3 binding motifs of CaMKK, we solved the crystal structures of phosphopeptides containing both 14-3-3 binding motifs of CaMKK bound to 14-3-3. The structures showed that both phosphopeptides interact with the amphipathic groove of 14-3-3 similarly to other 14-3-3 complexes. Nevertheless, in the case of the N-terminal motif, the interaction between the side-chain of Gln at the position +2 relative to pSer and the phosphate group appears to abruptly change the direction of the polypeptide chain. This study was supported by the Czech Science Foundation (Projects 16-02739S) and the Initial Training Network, funded by the H2020 Marie Curie Actions of the European Commission under Grant Agreement 675179.

P.19-024-Wed
Structural bases of inactivation of methionine γ-lyase by suicide substrates

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Pyridoxal 5′-phosphate-dependent methionine γ-lyase (MGL; EC 4.4.1.11) catalyzes the γ-elimination reaction of L-methionine and the β-elimination of S-substituted L-cysteine analogues to produce alkyl mercaptans, ammonia and α-keto acids. The enzyme was identified in a number of pathogenic bacteria and primitive eukaryotes. It is absent in mammalians. Thus MGL might be considered as a target in pathogens. We demonstrated that the enzyme catalyzes the γ-elimination reaction of L-methionine and L-homocysteine sulfoxides and the β-elimination reaction of S-alk(en)yl-L-cysteine sulfoxides which are accompanied by an inactivation of the enzyme in both γ- and β-elimination reactions. Three SH-groups of MGL were found to be modified by thiosulfinates, the products of the γ- and β-elimination reactions of sulfoxides. Spatial structures of MGL inactivated in the reactions with L-methionine sulfoxide and S-ethyl-L-cysteine sulfoxide were solved at 1.46 A and 1.59 A. Three SH-groups of the enzyme, Cys4, Cys115 and Cys245 were found to be oxidized to S-alkyl-cysteines. Inactivation of MGL in the β-elimination reaction depends on a length of the thioalkyl groups at the active site residue Cys115. Thioethyl group "prevents" effective substrate binding, while thiomethyl does not. Inactivation of the enzyme in the γ-elimination reaction is mainly due to the oxidation of Cys115. Analysis of the structures revealed that the presence of either thiomethyl fragment or thioethyl fragment at Cys115 results to an inability of Tyr113 to be a general acid catalyst at the stage of methyl mercaptan elimination. Sulfoxides of S-alkyl (allyl)-L-cysteines, suicide substrates of the enzyme, may be potential antimicrobial agents in MGL-containing pathogens. The work was supported by the Russian Science Foundation (project No. 15-14-00009).

P.19-025-Mon
Effect of various additives on the processes of aggregation and dissociation of coat proteins of several helical plant viruses

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Factors determining the direction of aggregation and dissociation processes of the coat protein (CP) of several helical plant viruses have been studied. The ability of various additives (polyelectrolyte's, surfactants and same peptides) to prevent protein aggregation was analyzed. We have shown that the CP of *potyvirus* – Potato Virus A (PVA) – forms associates – clusters consisted of 30 subunits of CP's, that retain in water-salt solution with increased ionic strength and pH (pH 10.5, 0.5 M NaCl). To analyze a low-resolution structure of the protein in solution, we used a method of Small-Angle X-ray Scattering. It was shown that particles of CP PVA do not dissociate under the influence of 10 mM dextran sulfates (15, 100 kDa) but dissociate under the action of 5 mM sodium dodecyl sulfate (SDS). We observed formation complexes of "CP-SDS", consisting of 10–12 small particles joined together as "necklace and bead" complex. The similar effect of SDS is shown for serum albumins (BSA, HSA). Spectral methods show the preservation of secondary structure and loss of tertiary one of the complexes of CP PVA -SDS. The effect of additives on the process of aggregation was studied in the model of amorphous aggregation CP's of *potyvirus* PVA and *tobamovirus* TMV, induced by heating to 42C. We tested specially selected neuropeptides (5–7 aa) and immunomodulatory peptide (2–3 aa). The kinetics of aggregation was monitored by UV absorption at 320 nm by UV-2600 Spectrophotometer and Dynamic Light Scattering by Malvern ZetaSizer instrument. Among some tested peptides, several peptides were effective in suppressing aggregation; others accelerated this process. The possible mechanism and role of disordered segments of CP's plant viruses in the processes their aggregation and dissociation are discussed. The work was supported by the Russian Foundation for Basic Research (projects 18-04-00525) and by the Federal Agency of Scientific Organizations (Agreement N 007-Г3/Ч3363/26) in part of SAXS.

P.19-026-Tue
Structural studies of human superoxide dismutase (SOD1) with its metallochaperone

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The final stages of Cu-chaperone (hCCS) dependent maturation of human Superoxide dismutase (hSOD1), which involves the transfer of copper and disulfide oxidation, have not been fully elucidated. The difficulty is in obtaining human hSOD1-hCCS complexes that are stable over time for crystallisation and

FEBS Open Bio 8 (Suppl. S1) (2018) 107–496 DOI: 10.1002/2211-5463.12453