

Poster Presentation

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Protein Crystallization Controlled by Special Adhesion Molecules

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Protein precipitates from solution with decreasing amount of free water molecules available for protein hydration (water evaporation, binding water on precipitant molecules, etc.). However, a uniform stacking of protein molecules on the surface of a growing crystal requires an absolute dominance of a single protein-protein adhesion mode. Existence of any “mutually incompatible protein-protein adhesion mode” in the same crystal leads to stacking faults, leading to low quality crystals, or to a crystallization failure. As proteins possessing large molecular surface have usually more adhesion modes, we need substances that are able to modify kinetics of protein-protein adhesion in different adhesion modes. It can be done by “Protein Surface Active Molecules” (PSAM) [1] binding selectively and temporarily the protein surface. The PSAM are used either to block some adhesion modes, or to form crosslinks built-in permanently into the growing crystals. Thus, a combination of more “successful additives” in solution can act positively in synergy but also can lead to a complete failure depending on the specificity of the protein-adhesion properties. The theory of PSAM describes protein crystallization as a regular deposition of short-life-time protein-PSAM complexes and stresses a role of “sticking molecules” exhibiting highly specific adhesion to different protein surface patches active in the crystallization process. The concept of crystallization of “protein adducts” falling apart during their stacking into the crystal lattice may be more complicated for imagination but it provides explanations of many enigmatic crystallization phenomena, provides better control over the crystal quality and over preparation of different crystal forms. Proper choice of the PSAM active in formation of temporary protein-PSAM adducts eliminates deposition of protein molecules on the growing crystal surface in “incompatible protein-protein adhesion modes” and it is decisive for a success of protein crystallization in many cases. The use of PSAM allows to: increase the number of crystallizable proteins, minimize probability of stacking faults, grow more polymorphs showing the same protein molecule in different environments, select the polymorph ensuring the highest accuracy of structure determination. The work is supported by BIOCEV CZ.1.05/1.1.00/02.0109 from ERDF, MSMT projects EE2.3.30.0029, LG14009, CSF P302/11/0855.

[1] Hašek, J. (2006) *Z. Kristallogr.* 23, 613-619; Hašek, J. (2011) *J. Synchr. Radiation* 18, 50-52; Hašek, J. et al (2011) *Z. Kristallogr.* 28, 475-480.

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