



PDB was performed. Structural data set of protein structures (resolution 1.2 Å or better) was prepared and analyzed on the presence of tryptophan residues and their location. It is known, that tryptophan is most rare amino-acid in protein structures therefore it was not surprising that up to 25 % of protein structures from the set did not contain any tryptophan. The atoms of indole ring of about 20 % of analyzed tryptophans were completely buried. On the other side, the indole ring of 12 % of tryptophans was classified as “fully exposed” to the solvent. Further inspection of these “fully exposed”

tryptophans and crystal contacts mediated by their indole ring atoms led us to the conclusion, that tryptophan can be useful in protein crystallization. In spite of the possible negative influence of tryptophans with solvent accessible side chains on protein solubility, and maybe also other protein properties, we believe that tryptophans located on the protein surface might improve crystallizability of proteins and optimize crystal packing.

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SL7

BIOCHEMICAL AND STRUCTURAL CHARACTERIZATION OF NEW HALOALKANE DEHALOGENASE DBEA FROM *Bradyrhizobium elkani* USDA94

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A novel enzyme belonging to the family of haloalkane dehalogenases (EC 3.8.1.5) was isolated from *Bradyrhizobium elkani* USDA94. Haloalkane dehalogenases are important class of microbial enzymes with catalytic activity for detoxification of halogenated aliphatic compounds. DbeA protein is closely related to DbjA enzyme from *Bradyrhizobium japonicum* USDA110 (71% identity), but has different biochemical properties. DbeA is generally less active than DbjA and has a higher specificity towards brominated and iodinated compounds. Crystal structure of

novel haloalkane dehalogenase DbeA of *Bradyrhizobium elkani* USDA94 has been solved and refined using diffraction data to 2.2 Å resolution. Overall fold and topology of DbeA is very similar to related enzymes with known structure. Structural comparison discovered differences in active site tunnel, which can explain differential substrate specificities and inhibitor affinities.

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CRYSTALLIZATION OF HIGHER PLANT PHOTOSYSTEM II

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The aim of this work carried out in collaboration with Laboratorio de Estudios Cristalográficos, (Granada, Spain) is to crystallize higher plant photosystem II (PS II) for high resolution X-ray diffraction study and resolve the structure of mentioned protein supercomplex.

The combination of centrifugation (sucrose density) and chromatography techniques (ion exchange, gel filtration) for extraction and purification of the PSII complex from solubilized thylakoid membranes of the *Pisum sativum* L. chloroplasts are used. The complex activity throughout the isolation routine with optical spectroscopy and polarographic measurements of oxygen evolution rates are tested. All possible methods and approaches for crystal-

lization of both membrane and soluble proteins will be used to produce crystals of PSII in diffraction quality.

New protocol for hydroponics plant growth under controlled conditions has been already established. Nowadays the protocol for isolation of the PS II enriched thylakoid membranes is re-designed and implemented into testing. The screening for most suitable buffers and detergents that will sustain maximum PSII activity throughout the isolation routine will be performed. Later the crystallization trials of the PSII protein complex will be setting up.

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