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Interaction enthalpies of solid bovine pancreatic α-chymotrypsin with organic solvents: comparison with FTIR-spectroscopic data

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Abstract

Calorimetric heat effects and integral absorbance changes observed in the FTIR spectra were measured at immersing solid bovine pancreatic α-chymotrypsin in organic solvents and water at 298 K. Enthalpy changes upon the immersion of the enzyme in different media are in a good linear correlation with the corresponding IR-absorbance changes. Based on calorimetric and FTIR data, all the solvents were divided into two groups. The first group of solvents includes carbon tetrachloride, benzene, nitromethane, acetonitrile, 1,4-dioxane, *n*-butanol, *n*-propanol and pyridine in which no significant heat evolution and structural changes were found at the solid enzyme immersion. Second group of the solvents includes dimethyl sulfoxide, methanol, ethanol, and water. Immersion into these media, results in the solid protein swelling and involves significant exothermic heat evolution and structural changes in the protein. Dividing of different media in these two groups is in a qualitative correlation with the solvent hydrophilicity which is defined as partial excess molar Gibbs free energy of water at infinite dilution in a given solvent. The first group of solvents includes liquids with hydrophilicity exceeding 2.7 kJ/mol. The hydrophilicity of the second group solvents is <2.3 kJ/mol. Hydrogen bond donating ability of the solvents assists in the protein swelling. Hydrogen bonding between protein and solvent is assumed to be a main factor controlling the swelling of solid protein preparation in the solvents at room temperature.

Keywords: Bovine pancreatic α-chymotrypsin; Organic solvent; Interactions enthalpies; Isothermal immersion calorimetry; FTIR-spectroscopy

1. Introduction

It has been firmly established that solid proteins immersed in organic solvents with low water contents demonstrate some remarkable properties: catalysis of the reactions not feasible in aqueous media [1,2], greatly enhanced thermostability [3,4] and molecular bioimprinting [5,6]. This powerful biotechnological potential of proteins in organic media depends strongly on the nature of organic solvent. However, ''there is still inadequate knowledge about protein–solvent interactions. This is definitely a rate-limiting step in the further growth of this area'' [7].

To understand the effects of organic media on properties and catalytic activity of proteins, we should elucidate the state of protein macromolecules subjected to such extraordinary conditions. This aim may be achieved by studying the relationships between the thermodynamic and structural parameters of formation

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