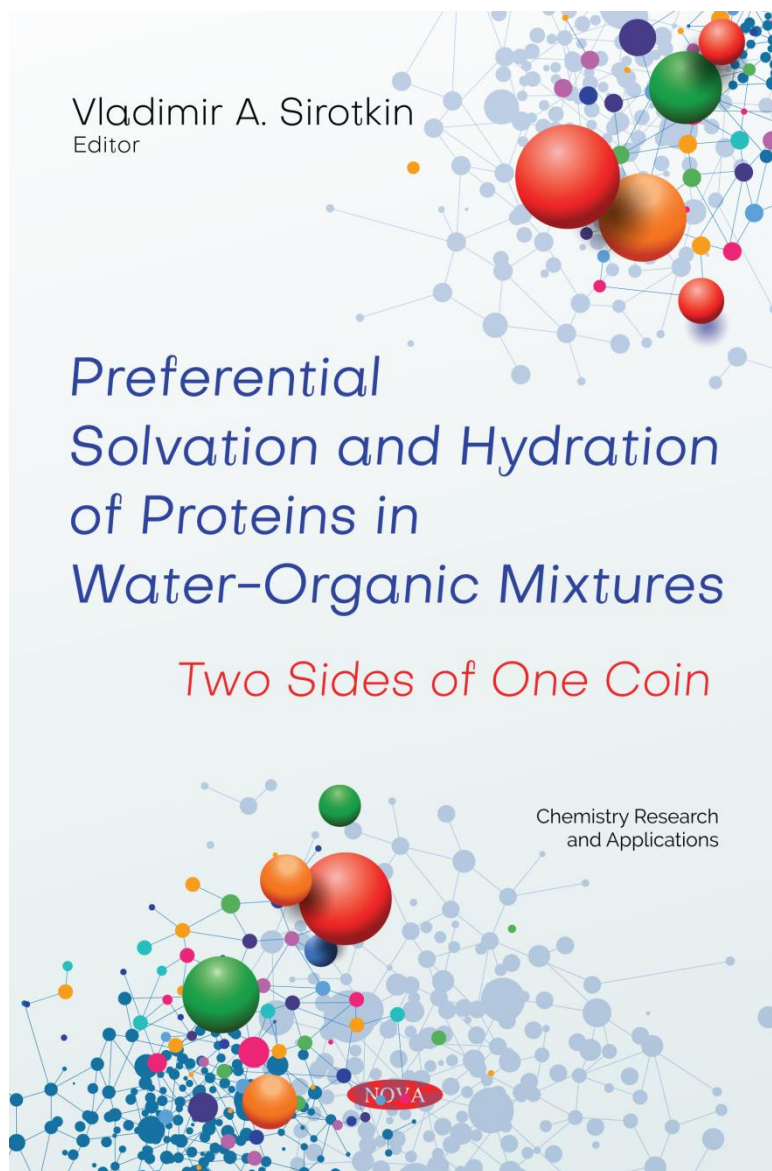


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*Chapter 3*

## **Preferential Hydration of $\alpha$ -Chymotrypsin IN ACETONITRILE: COMPARISON WITH FTIR SPECTROSCOPY**

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### **ABSTRACT**

The aim of this study is to monitor the preferential hydration of the protein macromolecules at low and high water content in water-organic mixtures. Our approach is based on the analysis of the absolute values of the water/organic solvent sorption. We applied this approach to estimate the protein stabilization/destabilization due to the preferential interactions of  $\alpha$ -chymotrypsin with water-acetonitrile mixtures. At high water content, proteins are preferentially hydrated. At the intermediate water content, the preferential interaction changed from preferential hydration to preferential binding of acetonitrile. From infrared spectra, changes in the structure of proteins were determined through an analysis of the structure of the amide I band. Acetonitrile augments the intensity of the  $1626\text{ cm}^{-1}$  band assigned to the intermolecular  $\beta$ -sheet aggregates. At low water content, the proteins are in a glassy (rigid) state. The H-bond accepting acetonitrile molecules are not effective in solvating the dehydrated protein molecules alone. Therefore, the acetonitrile molecules are preferentially excluded from the protein surface, resulting in the preferential hydration.

**Keywords:** preferential solvation, preferential hydration, protein, water, acetonitrile

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