

## Possible Mechanism of Non-Monotone Behavior of Helix–Coil Transition Temperature in Two-Component Solvent

Sh. A. Tonoyan, A. V. Asatryan\*, D. L. Hayrapetyan,  
Y. Sh. Mamasakhlisov, and V. F. Morozov

*Yerevan State University, Yerevan, Armenia*

\**asarevik@gmail.com*

Received September 25, 2015

**Abstract**—Within the frameworks of generalized model of polypeptide chain (GMPC) the concentrational behavior of helix–coil transition temperature of biopolymer in two-component solvent was observed on the simplest models. It is shown that if the solvent and the ligand interact with the biopolymer at different binding sites, and even if both components influence the helical state in the same way, the model allows one to obtain the non-monotone character of the melting temperature behavior of biopolymer depending on the ligand concentration. It is shown that changes in the regime of helical state stability is not always related with the competition of stabilizing and destabilizing interactions of blend components but can be the result of the cumulative effect of both components.

**DOI:** 10.3103/S1068337216010151

**Keywords:** helix–coil transition, polypeptide chain, biopolymer

### 1. INTRODUCTION

The biological cell is a complex medium filled with the various chemicals of low and high molecular compounds in the aqueous surroundings. For this reason, the study of biological macromolecules, such as proteins and nucleic acids, as a rule, is carried out in the presence of other chemical compounds in the aqueous solution [1, 2]. As is well-known, *in vivo* the polymers exhibit the biological activity also in the complex aqueous saline environment. The aqueous solutions of biological macromolecules are the complex systems. They are difficult to investigate experimentally; their numerical studies require huge resources but their purely theoretical research almost impossible. However, the study of such systems is necessary to understand the biological processes. In this regard, it is important to develop the simplest models of interaction between the biopolymer–water solution that will solve the existing problems, at least partially.

In the complex aqueous solution, there are many mechanisms for interaction with the molecules of solution the biological macromolecules. Water can both compete with the repeating units of biopolymers to form the hydrogen bonds, as well as do not compete and be bounded with the repeating units changing the pattern of intramolecular interactions. Similarly, the others low molecular weight substances, the ligands, dissolved in water, can interact. Almost all biological phenomena are related to the interaction of macromolecules with the ligands. In our previous publications [3–6], we considered the various models that take into account the various interactions of the biopolymer–ligand–solvent. The result is a number of interesting effects, which influence the various mechanisms of interaction on such parameters, as the