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THE COMBINATION OF CHEMOMETRICS AND 2D NIR CORRELATION SPECTROSCOPY IN THE ANALYSIS OF DENATURATION PROCESS

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Despite extensive theoretical and experimental studies the structure of the protein-solvent interface is subject of many controversy. Understanding the processes that occur in aqueous solution requires understanding of the solvent influence on the structure of protein.

The aim of this study is to investigate the applicability of NIR methods in the study of hydration phenomena in protein solutions. Temperature-induced changes in NIR spectra of -lactoglobulin (BLG) in aqueous solutions have been investigated by means of two-dimensional correlation spectroscopy (2DCOS) and principal component analysis (PCA). With the temperature increase the balance of forces between the BLG's interaction with itself and the BLG's interaction with its environment is disrupted leading to BLG unfolding.

Significant differences of 2D signals and distinct discrepancies of loading on PC1 and PC2 were observed as a result of temperature increase. In the native folded conformation of BLG, most of the nonpolar amino acids are hidden in the centre of the structure, out of contact with water molecules, while charged groups are outside, in the contact with water. The polar groups promote low density Ih-type structure in the water outside this first hydration shell. When BLG unfolds it assumes a more extended configuration on which the previously buried nonpolar groups are exposed to water and promote the higher density II-type structure outside its first shell. Detailed assignments of bands attributed to the bulk water, different states of the hydrated water and the changed conformation of BLG are proposed.