

A study of urea-dependent denaturation of β -lactoglobulin by principal component analysis and two-dimensional correlation spectroscopy.

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Streszczenie

The water-urea- β -lactoglobulin interaction was studied by means of principal component analysis (PCA) and two-dimensional correlation spectroscopy applied to the urea concentration-dependent FTIR spectra of aqueous urea-protein solutions. The two $\nu(\text{C=O})$ and $\nu_{\text{as}}(\text{CN})$ bands coming from urea's absorbance, instead of the amide bands arising from protein, were employed in the analysis. To get a precise view of the changes induced by the urea concentration-controlled unfolding process, the absorbance variations developed in the ternary water-urea-protein system were compared with those observed in a binary water-urea system [Y.M. Jung et al., *J. Phys. Chem. B* **2004**, 108, 13008]. The comparative studies enabled to detect apparent differences between the absorbance changes caused solely by urea's concentration increase and by the urea-dependent unfolding process. Urea's ability to unfold protein was discussed in context of the indirect and the direct mechanism depending on urea's concentration. It was shown that both mechanisms are relevant, that is, the indirect for solutions below 3 M and the direct for solutions above 3 M concentration. The character of the mechanism is strictly correlated with the association level of urea molecule

Adres publiczny

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<https://www.acs.org/content/acs/en.html>