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Hydration of Three-Piece K Peptide Fragments Studied by Means of Fourier Transform Infrared Spectroscopy

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Abstract : Background: The hallmark of neurodegenerative diseases, including Alzheimer's and Parkinson's diseases, is an aggregation of the abnormal forms of peptides and proteins. Water is essential to functioning biomolecules, and it is one of the key factors influencing protein folding and misfolding. However, the hydration studies of proteins are complicated due to the complexity of protein systems. The use of model compounds can facilitate the interpretation of results involving larger systems. Objectives: The goal of the research was to characterize the properties of the hydration water surrounding the two three-residue K peptide fragments INS (Isoleucine - Asparagine - Serine) and NSR (Asparagine - Serine - Arginine). Methods: Fourier-transform infrared spectra of aqueous solutions of the tripeptides were recorded on Nicolet 8700 spectrometer (Thermo Electron Co.) Measurements were carried out at 25°C for varying molality of solute. To remove oscillation couplings from water spectra and, consequently, obtain narrow O-D semi-heavy water bands (HDO), the isotopic dilution method of HDO in H_2O was used. The difference spectra method allowed us to isolate the tripeptide-affected HDO spectrum. Results: The structural and energetic properties of water affected by the tripeptides were compared to the properties of pure water. The shift of the values of the gravity center of bands (related to the mean energy of water hydrogen bonds) towards lower values with respect to the ones corresponding to pure water suggests that the energy of hydrogen bonds between water molecules surrounding tripeptides is higher than in pure water. A comparison of the values of the mean oxygen-oxygen distances in water affected by tripeptides and pure water indicates that water-water hydrogen bonds are shorter in the presence of these tripeptides. The analysis of differences in oxygen-oxygen distance distributions between the tripeptide-affected water and pure water indicates that around the tripeptides, the contribution of water molecules with the mean energy of hydrogen bonds decreases, and simultaneously the contribution of strong hydrogen bonds increases. Conclusions: It was found that hydrogen bonds between water molecules in the hydration sphere of tripeptides are shorter and stronger than in pure water. It means that in the presence of the tested tripeptides, the structure of water is strengthened compared to pure water. Moreover, it has been shown that in the vicinity of the Asparagine - Serine - Arginine, water forms stronger and shorter hydrogen bonds. Acknowledgments: This work was funded by the National Science Centre, Poland (grant 2017/26/D/NZ1/00497).
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