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Calculation of the proton chemical shifts as a tool to explain the peculiarities of 1H NMR spectra of protein in a compact denatured state

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Abstract

Using the protein crystal structure the chemical shift dispersions of binase α-CH protons were calculated for protein in native state and in a compact denatured one. The same models of internal fields with different adjusting parameters were used to describe data for protons disposed in regions of both regular and irregular secondary structures. It was shown that peculiarities of 1H NMR spectra, observed for compact denatured proteins, could be explained through fluctuations of hydrogen bonds network in conserved secondary structures.