

Modeling protein conformations in water: theory and experiment

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A brief overview of the Zimm-Bragg model for protein conformations in water and its main results are presented in the report. Estimated partition function provides access to the thermodynamics of the problem and results in expressions for the measurable quantities. The suggested theoretical formulas are fitted to the experimental data on protein conformations, obtained from circular dichroism and differential scanning calorimetry. The modification of the theory allows to extract values of hydrogen bonding energies in the range of 1-8 kJ/mol. A very good level of fit obtained proves the qualitatively correct model chosen and suggests a new and complementary way to post-process the data from classical experimental methods.