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Hydrodynamic approach to compute reorientation times of NATA protein in different solutions: comparison with Molecular Dynamics and experiment YEVGEN MELIKHOV, Inst of Fundamental Technological Research, Polish Academy of Sciences, MARIA L. EKIEL-JEZEWSKA, Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland, GOURI S. JAS, KRZYSZTOF KUCZERA, The University of Kansas, Lawrence, Kansas, United States — Molecular Dynamics (MD) is usually applied to compute translational and rotational diffusion coefficients and the corresponding rotational correlation time for peptides, such as N-acetyl-tryptophan-amide (NATA). Besides viscosity effects, specific solute-solvent interactions are present and a continuous change of the shape of NATA molecule is observed. MD approach allows simplification of this process segregating the whole dynamics into very limited number of conformers with corresponding time population and therefore, allowing extraction of Brownian dynamics for a particular conformer from MD. Now, knowing the structure of a particular conformer, we propose to study self-diffusion using hydrodynamic bead model, where each atom is represented by a separate bead. Such analysis adds to a better understanding of a fluid-molecule interaction. In this paper, we present comparison of experimental and computational (MD and hydrodynamic bead model) studies of reorientational motions of NATA in water, urea, GdmCl and proline. We found that rotational correlation times of NATA molecule in these solutions are very similar in MD and hydrodynamic bead model, matching experiment, if interactions between a co-solvent and NATA and ther effect on the local solute dynamic are taken into account.

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