

# $\alpha$ -helix propensities of homo-oligomers in aqueous solution studied by multicanonical simulations

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Helix-coil transitions of peptide and protein systems provide important insight into protein folding problem. In a previous work, thermodynamics of helix-coil transitions of homo-oligomers in gas phase were studied by multicanonical algorithms.<sup>1)</sup> Homo-oligomers of length 10 were considered for three characteristic amino acids, alanine (helix former), valine (helix indifferent), and glycine (helix breaker). It was shown that the obtained helix propagation parameters  $s$  of the Zimm-Bragg model for the three amino acids were in remarkable agreement with the experimental values.<sup>1)</sup>

In this poster, we present the results of our study of helix-coil transitions in amino-acid homo-oligomers in aqueous solution by multicanonical algorithm. The solvation term is based on the solvent-accessible surface area and the parameters of Ooi *et al.*<sup>2)</sup> were used. We calculate average values of total potential energy, its component terms, helicity, and specific heat as a function of temperature. The results of homo-oligomers

in aqueous solution are compared with those in gas phase. Zimm-Bragg  $s$  and  $\sigma$  parameters are also obtained as a function of temperature. The results for homo-oligomers and alanine rich peptides are compared with the implications of the experimental results. The present results are based on Refs. 3 and 4.

## References

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