

Molecular Dynamics Study on an Adipokinetic Hormone Peptide in Aqueous Solution

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Lom-AKH-I is a member of the adipokinetic hormone/red pigment concentrating hormone (AKH/RPCH) family of peptides found in flying insects. A molecular dynamics simulation at room temperature (293 K) in water has been performed to survey the folding path of the Lom-AKH-I peptide in water and to establish the secondary structure of Lom-AKH-I. The obtained results indicate the presence of an undefined extended conformation.