Two-dimensional ^{1}H-NMR and CD structural analysis in a micellar medium of a bovine α_{S1}-casein fragment having benzodiazepine-like properties

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(Received 25 April/18 July 1997) – EJB 97 0595/3

The conformation of the benzodiazepine-like decapeptide, YLGYLEQLLR, corresponding to residues 91–100 of bovine α_{S1}-casein, has been examined in SDS micelles using CD, two-dimensional ^{1}H-NMR and restrained molecular-dynamics simulation. Evidence is presented that the decapeptide adopts a rigid structure in water/SDS micellar medium, but not in water or dimethylsulfoxide. The three-dimensional structure, consistent with the proton-proton distances obtained from the quantitative analysis of the two-dimensional NOEs, was generated by restrained energy minimization and molecular-dynamics simulation. In water/SDS micellar medium, YLGYLEQLLR adopts an amphipathic helicoid structure with distinct hydrophobic and hydrophilic faces. The relative disposition of the tyrosine aromatic rings was compared with that of the aromatic rings in the benzodiazepines.

Keywords: α_{S1}-casein; benzodiazepine-like peptide; NMR; molecular dynamics; circular dichroism.