Three-Dimensional Molecular Modeling of Bovine Caseins: α_{s1}-Casein

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ABSTRACT

Structures derived from X-ray crystallography are extremely important in elucidating functional relationships for many proteins. However, the caseins of bovine milk are one class of noncrystallizable proteins. The complete primary and partial secondary structures of these proteins are known, but homologous proteins of known crystallographic structure cannot be found. Therefore, sequence-based predictions of secondary structure were made and adjusted to conform with global secondary structures determined by Raman spectroscopy. With this information, a three-dimensional structure for α_{s1}-casein was constructed using molecular modeling programs. The predicted structure of α_{s1}-casein contains a hydrophobic and a hydrophilic domain, which are connected by a segment of α-helix. This unrefined structure shows good agreement with global biochemical and chemical information concerning α_{s1}-caseins A, B, and C.

(Key words: casein structure, protein functionality, milk proteins)

tains eight to nine phosphate groups and has physical properties distinct from those of β- and κ-caseins. It has been theorized by some that α_{s1}-casein forms the framework for the casein micelle because it does not exhibit highly temperature-dependent interactions (8, 20). The combination of X-ray crystallography and molecular biology has contributed greatly to our understanding of the mechanisms of action of globular proteins. Although the techniques of molecular biology are now being applied to α_{s1}-casein, crystallographic structures will probably not be realized. This paper deals with three-dimensional molecular modeling for α_{s1}-casein. It is hoped that this model will represent a new starting point in the examination and exploration of casein structure and function.