

Three-Dimensional Molecular Modeling of Bovine Caseins: A Refined, Energy-Minimized κ -Casein Structure

T. F. Kumosinski¹, E. M. Brown¹, and H. M. Farrell Jr.¹

¹ US Department of Agriculture, Eastern Regional Research Center, Agricultural Research Service, Philadelphia, PA

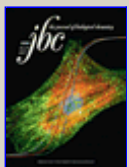
A refined three-dimensional molecular model of κ -casein has been produced using energy minimization techniques and a Kollman force field on a previously reported predicted three-dimensional structure. This initial model was constructed via molecular modeling techniques from sequence-based secondary structural prediction algorithms. Both the initial and refined structures agreed with global secondary structure analysis from vibration spectroscopy. The refined structure contained many of the features of the initial model, including two sets of antiparallel β sheet structures containing predominantly hydrophobic side chains, which could form interaction sites with α_{s1} -casein. Two types of energy-minimized dimer and tetramer models are presented: 1) using Cys as potential intermolecular disulfide binding sites and 2) using the two sheets as possible hydrophobic self-association sites, without Cys interactions. All structures yielded good stabilization energies and are in agreement with chemical, biochemical, and physical chemical results obtained for κ -casein.

Key Words: casein structure • protein functionality • milk proteins

Submitted on September 30, 1992

Accepted on March 22, 1993

This article has been cited by other articles:



JBC Online

HOME

H. Ecroyd, T. Koudelka, D. C. Thorn, D. M. Williams, G. Devlin, P. Hoffmann, and J. A. Carver

Dissociation from the Oligomeric State Is the Rate-limiting Step in Fibril Formation by κ -Casein

J. Biol. Chem., April 4, 2008; 283(14): 9012 - 9022.

[\[Abstract\]](#) [\[Full Text\]](#) [\[PDF\]](#)

This Article

- ▶ [Full Text \(PDF\)](#)
- ▶ [Alert me when this article is cited](#)
- ▶ [Alert me if a correction is posted](#)

Services

- ▶ [Similar articles in this journal](#)
- ▶ [Similar articles in PubMed](#)
- ▶ [Alert me to new issues of the journal](#)
- ▶ [Download to citation manager](#)
- ▶ [Get Permissions](#)

Citing Articles

- ▶ [Citing Articles via HighWire](#)
- ▶ [Citing Articles via Google Scholar](#)

Google Scholar

- ▶ [Articles by Kumosinski, T. F.](#)
- ▶ [Articles by Farrell, H. M.](#)
- ▶ [Search for Related Content](#)

PubMed

- ▶ [PubMed Citation](#)
- ▶ [Articles by Kumosinski, T. F.](#)
- ▶ [Articles by Farrell, H. M., Jr.](#)



Journal of Dairy Science

[▶ HOME](#)

R. W. Lencki

Evidence for Fibril-Like Structure in Bovine Casein Micelles

J Dairy Sci, January 1, 2007; 90(1): 75 - 89.

[\[Abstract\]](#) [\[Full Text\]](#) [\[PDF\]](#)



Journal of Dairy Science

[▶ HOME](#)

E. L. Malin, E. M. Brown, E. D. Wickham, and H. M. Farrell Jr.

Contributions of Terminal Peptides to the Associative Behavior of {alpha}s1-Casein

J Dairy Sci, July 1, 2005; 88(7): 2318 - 2328.

[\[Abstract\]](#) [\[Full Text\]](#) [\[PDF\]](#)



Journal of Dairy Science

[▶ HOME](#)

H. M. Farrell Jr., R. Jimenez-Flores, G. T. Bleck, E. M. Brown, J. E. Butler, L. K. Creamer, C. L. Hicks, C. M. Hollar, K. F. Ng-Kwai-Hang, and H. E. Swaisgood

Nomenclature of the Proteins of Cows' Milk--Sixth Revision

J Dairy Sci, June 1, 2004; 87(6): 1641 - 1674.

[\[Abstract\]](#) [\[Full Text\]](#) [\[PDF\]](#)

[HOME](#) [HELP](#) [FEEDBACK](#) [SUBSCRIPTIONS](#) [ARCHIVE](#) [SEARCH](#) [TABLE OF CONTENTS](#)

[Copyright © 1993 by the American Dairy Science Association ®.](#)