DETERMINATION OF THE STRUCTURE OF A FOLDING NUCLEUS IN BOVINE β-LACTOGLOBULIN USING UV FLUORESCENCE AND IR/UV DOUBLE RESONANCE SPECTROSCOPY IN THE GAS PHASE[a]

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The amino acids in the 19th through 23rd positions of bovine β-lactoglobulin, Trp-Tyr-Ser-Leu-Ala, have been identified as a folding nucleus[b], a region of the protein that folds first and may induce or facilitate the proper folding of the remainder of the protein. Thus, the intramolecular interactions in this region of the molecule are of particular interest. Reported here are the structures of Ac-Trp-Tyr-NH_2, Ac-Trp-Tyr-Ser-NH_2, and Ac-Trp-Tyr-Ser-Leu-NH_2 as determined by UV fluorescence and UV/IR double resonance spectroscopy. Shifts in the positions of N-H and O-H bands provide information about hydrogen bonds and π-electron interactions involving the peptide backbone and/or residues. Predicted structures are then compared with similar peptides and the lowest energy structures determined by *ab initio* calculations to further justify the assignment of the structure.

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[b]L. Ragona, M. Catalano, L. Zetta, R. Longhi, F. Fogolari, and H. Molinari. *Biochemistry* (2002), **41**, 2786-2796.