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The Theoretical Structural Study of the Oscteocalcin (7-19), Biochemical Marker of Bone Metabolism

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Osteocalcin is a major noncollagenous matrix protein of bone and dentin. It is considered to take part in bone formation and remodeling. Osteocalcin is known as a biochemical marker of bone metabolism. Proline-rich segment 7-19 (H-Gly^{7}-Ala^{8}-Pro^{9}-Val^{10}-Pro^{11}-Tyr^{12}-Pro^{13}-Asp^{14}-Pro^{15}-Leu^{16}-Glu^{17}-Pro^{18}-Arg^{19}-OH) of the osteocalcin is used also for diagnostic medical treatment of some bone diseases the as a biochemical marker of the bone formation. The presence of proline residues in the sequence of this segment allowed us to suppose that this tridecapeptide in free state, is recognized by monoclonal antibody specific for this seqment at the physiology processes, may have a quite definite spatial structure or relatively restricted conformational properties. For this aim, we studied the conformational properties of the osteocalcin (7-19) by means of theoretical conformational analysis. Theoretical conformational study of this peptide segment was carried out basing on its fragmental analysis. Calculation indicated that all low-energy conformations of the tridecapeptide may be presented by means of three families conformers with identical backbone form of the N-terminal nonapeptide and different forms of C-terminal part. The lowest energy conformations of each of these families adopt the beta-sheet structures connected by two or three beta-turns. For all conformations of the first family are distinctive formation of beta-turn by residues 8-11, for conformations of second family – formation beta-turns by residues 8-11 and 12-15, and for conformations of third family – formation beta-turns by residues 8-11, 10-13, and 12-15. All geometrical and energetical parameters of optimal spatial structures of peptide were obtained in our investigation, and the distance between different functional groups were measured. Important specific interactions between residues, that are necessary for stabilization of low-energy conformations, also were determined. The solution of given structured problem for the proline-rich segment of osteocalcin gives concrete information on spatial organization of whole molecule and may help the understanding of the mechanism of action of osteocalcin in the process of mineralization.