Molecular Dynamics Simulation of A2G80 Peptide Derived from Laminin α2 Chain

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Laminins, contained in basement membrane, have many functions such as cell adhesion, migration and wound healing [1]. A2G80 peptide (VQLRNGFPYFSY), derived from laminin α2 chain, was experimentally found to bind specifically to α-dystroglycan [2]. We perform molecular dynamics simulation of A2G80 peptide to study the conformation of the peptide. We found that A2G80 peptide shows stable conformation in water with β sheet structure or random coil structure like β structure. From the simulation of alanine-substituted peptides, we found that Tyr^9 is an important amino acid residue for determining the structure of A2G80. We compare the structures of A2G80 and Y9 peptide (Tyr^9 is substituted by Ala) and analyze the free energy landscape of the peptides.

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