Conformation Analysis of Peptides Derived from Laminin Alpha 1-2 Chain Using Molecular Dynamics Simulation


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Laminin is one of the components of the basement membrane and, laminin has diverse biological activities [1-2], such as promotion of cell attachment, cell migration, tumor metastasis, neurite outgrowth and angiogenesis [2]. Previously, Suzuki et al. identified several functional peptides (EF1-EF5) derived from LG4 modules of laminin alpha 1-5 chains [3]. Previous results showed that biological activities of N-terminal and C-terminal truncated peptide of EF1 are enhanced by disulfide bond [3], and the importance of hairpin-like structure was suggested. By contrast, the EF2 does not have biological activity despite the homologous sequence of the EF1 [4]. Based on these results, the relationship between conformation and activity can be suggested. Thus, we perform conformation analysis of EF1 and EF2 using molecular dynamics simulations.

In this study, we perform simulated annealing and structure sampling with NPT ensemble (300K, 1bar). We obtain 150 samples of several peptides by simulated annealing. The EF1 peptides have hairpin-like structure, and the EF2 peptides have distorted structure as compared with the structure of EF1. Molecular dynamics simulation with NPT ensemble is performed for 500 ns. Though conformation of the EF1 after 500 ns maintains hairpin-like structure, the conformation of EF2 after 500 ns does not. These results show that hairpin-like structure is important for cell attachment activity of EF1. Thus, we suggest that the EF2 peptide does not have biological activity because of the fluctuation of structure.