Molecular Dynamics Simulation of Loop Region Peptides in Laminin Alpha Chain

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Peptides are important material and have been studied in relation to drug discovery and membrane permeability [1]. In this paper, we focus on the EF1 peptides, which are located on the loop region of the E and F strands of LG4 module and interact with α2β1 integrin [2] to be dependent on the conformation. We perform simulated annealing calculations [3] for EF1 and its derivative fixed conformation by cyclization (cycloEF1). We have found that both EF1 and cycloEF1 tend to form loop structure.

[1] S. Kawamoto, M. Takasu, T. Miyakawa, R. Morikawa, T. Oda, S. Futaki, H. Nagao, J. Chem. Phys. 134 (2011) 095103, 1-6.

[2] N. Suzuki, H. Nakatsuka, M. Mochizuki, N. Nishi, Y. Kadoya, A. Utani, S. Oishi, N. Fujii, K. Kleinman and M. Nomizu, J. Biol. Chem. 278 (2003) 45697-45705.

[3] K. Umezawa, J. Ikebe, M. Nomizu, H. Nakamura and J. Higo, Biopolymers 92 (2009) 124-131.