Molecular Dynamics Simulation of Coarse Grained Model of IPMDH Proteins

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Making nano-fibers with proteins [1] is an interesting and challenging field. We have tried to construct nano-fibers of proteins by introducing mutations on the amino acids while retaining the native structure of the proteins. In our previous studies of molecular dynamics simulation of all-atom model, we have found that IPMDH (3-isopropylmalate dehydrogenase) is a good candidate for a building unit of constructing nano-fibers because of the high stability of IPMDH [2, 3]. In this study, we have performed molecular dynamics simulation of coarse-grained model of IPMDH proteins. We have introduced mutations on the surface of IPMDH and found that the mutated IPMDHs are likely to make larger clusters than the wild type IPMDH.

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