Molecular Dynamics Simulation of Prion Protein

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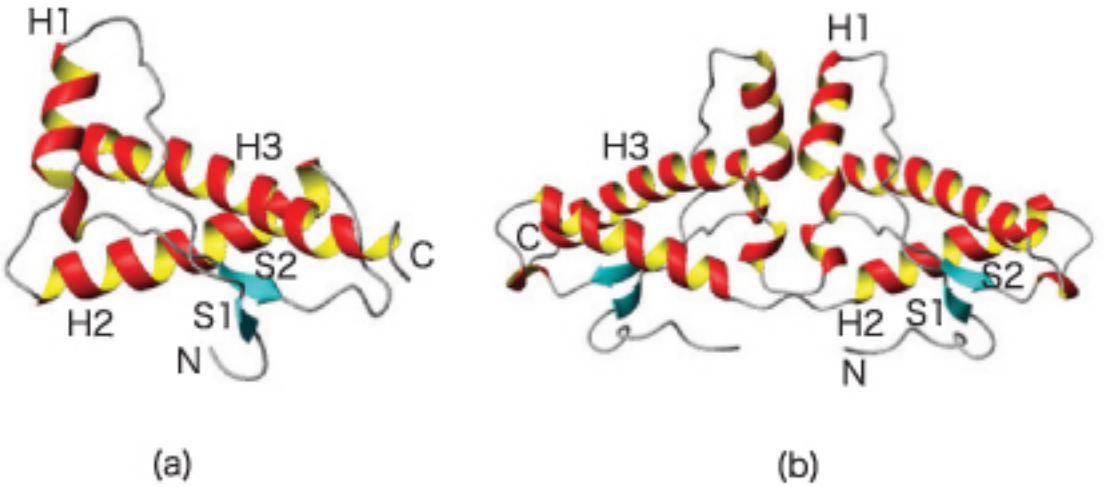
A central theme in prion protein research is the detection of the process that underlies the conformational transition from the normal cellular form (PrP^{C}) to its pathogenic isoform, PrP^{Sc}. Although the three-dimensional structures of monomeric and dimeric human prion protein (HuPrP) have been revealed by NMR spectroscopy and X-ray crystallography, the process underlying the conformational change from PrP^{C} to PrP^{Sc} and the dynamics and functions of PrP^{C} remain unknown. The dimeric form is thought to play an important role in the conformational transition. In this study, we performed molecular dynamics (MD) simulations on monomeric and dimeric HuPrP to investigate the differences in the properties of the monomer and the dimer from the perspective of dynamic and structural behaviors.



Schematic ribbon diagram of HuPrPc. (a) monomer, (b) dimer