Sangwook Wu et al., J Proteomics Bioinform 2017, 10:8(Suppl)
DOI: 10.4172/0974-276X-C1-0100

Study on the conformational transition between the alternative and collapsed form of prethrombin-2: Targeted molecular dynamics and free energy sampling

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The alternative and collapsed forms of prethrombin-2 are revealed by X-ray crystallogrphy. We analyzed the conformational transition from the alternative to the collapsed form employing targeted molecular dynamics simulation and 2-dimensional free energy landscape using WHAM method. Some hydrophobic residues (W60d, W148, W215, and F227) show a significant difference between the two conformations in the conformational transition process. We show that the four hydrophobic residues undergo concerted movement from dimer to trimer transition *via* tetramer state in the conformational change from the alternative to the collapsed form. Also, we reveal that the concerted movement of the four hydrophobic residues is controlled by movement of specific loop regions behind. In this study, we discuss the difference between the transition path generated by the targeted Mplease let m eD simulation and the transition path with minimum Boltzmann weighting on the two-dimensional free energy surface (FES).

Biography

Sangwook Wu received his B.A. degree in Biochemistry from Yonsei University (Korea) in 1990. After working as a Scientist at Samsung Display Devices (1995-1999), he obtained his Ph.D. in theoretical condensed matter physics from Iowa State University (1999-2005). He joined the computational biophysics lab at UNC-Chapel Hill (Dr. Lee Pedersen) as postdoctoral research associate (2005-2014). From 2014 to the present, he has been a faculty member at Pukyong National University in Korea. His research interests are in the areas of computational dynamics of biological macromolecules.

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