[P20] Network analysis on the conformational change of c-Src tyrosine kinase by employing molecular dynamics simulation

Hyunjung Yoon, Pukyong National University

A non-receptor Src-family protein tyrosine kinases (SFKs) play a critical role in cell growth, differentiation, and various metabolism by controlling cell signal. The regulation of cell signaling by SFKs is mediated by the conformational activation/inactivation of the tyrosine kinases. We investigated the conformational change of c-Src, one of the member of SFKs, from the inactive form (PDB id: 2SRC) to the active form (PDB id: 1Y57) employing targeted molecular dynamics (TMD) simulation. In this study, we proposed the potential allosteric pathway for the conformational change of the c-Src tyrosine kinase based on network analysis.