Tensile-force-induced propeller-twist change of actin subunits in actin filament

***Yasuhiro Inoue[1], Tetsuya Fujii[2], Taiji Adachi[1]**

[1]Institute for Frontier Medical Sciences, Kyoto University, Japan.
[2]Department of Microengineering, Kyoto University, Japan.

*Corresponding author: inoue@frontier.kyoto-u.ac.jp

Actin filament (F-actin) plays a critical role in many cellular functions. Actin has two major domains that form a propeller twist in globular actin. Upon polymerization, these two major domains are untwisted and flattened. This structural transition stabilizes the F-actin structure and affects the affinity of molecules bound to actin subunits through steric hindrance. Because mechanical forces exerted on F-actin may change the subunit structure including the propeller twist, the force-induced propeller-twist change can be a molecular basis of mechanochemical coupling. In this study, we employed molecular dynamics (MD) simulations of F-actin to investigate the change in the propeller-twist angle of the actin subunits in F-actin induced by a tensile force. Our MD simulations revealed that the tensile force increased the propeller-twist angles of actin subunits positioned toward the plus end of F-actin and decreased these angles of subunits positioned toward the minus end.

Keywords: Actin filament, Actin subunit structure, Molecular dynamics simulation, Biomechanics