Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **1983** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

Escherichia coli's RfaH studied by all-atom Monte Carlo simulation (G)*

Wednesday 13 June 2018 14:00 (15 minutes)

RfaH is a compact two-domain multi-functional protein from the bacteria $Escherichia\ coli$ ($E.coli$). Its C-terminal domain (CTD) has been shown experimentally to be able to undergo a complete conformational change from an α-helix bundle to a β-barrel structure. The α-helix bundle to β-barrel fold switch accounts for the observed dual role of RfaH, whereby it regulates transcription as well as enhances translation. We employ all-atom Monte Carlo simulations to investigate the stabilities of the two structural forms of RfaH and the character of transition between them. Our simulations reveal that the stand-alone α-helix CTD is relatively unstable despite the stabilizing interactions with the N-terminal domain (NTD). Moreover, we observe the stability of the stand-alone β-barrel conformation to be always higher than the α-helix bundle structure. Thus, we conclude that the α-helix bundle to β-barrel fold switch of the CTD in RfaH is thermodynamically favoured in our model.

Author: Mr AINA, Adekunle (Memorial University of Newfoundland)

Co-author: WALLIN, Stefan (Memorial University of Newfoundland)

Presenter: Mr AINA, Adekunle (Memorial University of Newfoundland)

Session Classification: W3-4 Soft matter and molecular dynamic (DPMB/DCMMP) | Matière molle et dynamique moléculaire (DPMB/DPMCM))

Track Classification: Physics in Medicine and Biology / Physique en médecine et en biologie (DPMB-DPMB)