University of Wisconsin-Milwaukee

Dept. of Physics
COLLOQUIUM

Combining in vitro *and* in silico *Single-molecule Force Spectroscopy to Characterize Protein Mechanics*

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Friday, 19 October 2018

3:30 PM (coffee/cookies at 3:15 PM)

Lapham Hall – Room 160

Steered Molecular Dynamics (SMD) simulations have been used to depict the underlying molecular details of protein mechanics. At the molecular level, these behaviors are governed by mechanically active proteins. Such proteins can sense and respond to force by undergoing conformational changes or modulating their function in a variety of ways. Several diseases are linked to mutations in mechanically active proteins. SMD simulations were employed to assist molecular biologists in investigating how mutations associated to skeletal dysplasia, and mitral valve dysplasia change human filamins' structure and its mechanosensing. How do cellulosomal complexes become ultrastable when exposed to force, and what are the mechanics that make pathogenic bacteria adhere to their human hosts so viciously?

Our findings in both cellulosomes and adhesin studies have revealed that a precise steered molecular dynamics (SMD) protocol can nearly replace an experimental single molecule force spectroscopy approach.

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