Abstract Submitted
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Steered molecular dynamics simulations of a bacterial type IV pilus reveal characteristics of an experimentally-observed, force-induced conformational transition JOSEPH BAKER, Department of Physics, University of Arizona, NICOLAS BIAIS, Department of Biological Sciences, Columbia University, FLORENCE TAMA, Department of Chemistry and Biochemistry, University of Arizona — Type IV pili (T4P) are long, filamentous structures that emanate from the cellular surface of many infectious bacteria. They are built from a 158 amino acid long subunit called pilin. T4P can grow to many micrometers in length, and can withstand large tension forces. During the infection process, pili attach themselves to host cells, and therefore naturally find themselves under tension. We investigated the response of a T4 pilus to a pulling force using the method of steered molecular dynamics (SMD) simulation. Our simulations expose to the external environment an amino acid sequence initially hidden in the native filament, in agreement with experimental data. Therefore, our simulations might be probing the initial stage of the transition to a force-induced conformation of the T4 pilus. Additional exposed amino acid sequences that might be useful targets for drugs designed to mitigate bacterial infection were also predicted.

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