



Extracting Rates and Activation Free Energies from Single Molecule Force Spectroscopy



Olga K. Dudko, Ph.D.
Mathematical & Statistical Computing
Laboratory
Division of Computational Bioscience
Center for Information Technology
National Institutes of Health

Thursday, March 15, 2007

4:00 PM (refreshments)

33-105 Center for the Health Sciences

ABSTRACT:

Single-molecule force spectroscopy using atomic force microscopes, laser optical tweezers, etc. has the potential to provide unprecedented insights into the structure, dynamics, interactions, and mechanical properties of individual molecules. However, the theory used to extract the kinetics of molecular transitions from single-molecule force experiments remains highly contentious. We present a unified framework for extracting kinetic information from single molecule pulling experiments at constant force or constant pulling speed. Our procedure, based on Kramers theory of diffusive barrier crossing, provides estimates of not only the intrinsic rate coefficient and the location of the transition state, as in the widely used phenomenological approach based on Bell's formula, but also the free energy of activation. A quantitative relation between the data collected in two types of measurements - at constant force and constant force-ramp speed - is established. We consider the uniqueness of the extracted kinetic information and suggest guidelines to avoid over-interpretation of experiments. We demonstrate the efficiency of our theory by analyzing nanopore unzipping measurements of individual DNA hairpin molecules under voltage.

Host: Dr. Tom Chou, tomchou@ucla.edu

BIO
MATH
SEMINAR