Chemical & Physical Sciences
UNIVERSITY OF TORONTO
MISSISSAUGA

**COLLOQUIUM**
**TUESDAY, SEPTEMBER 15, 2015**
**12:00 NOON – 1:00 PM**
**IB250**

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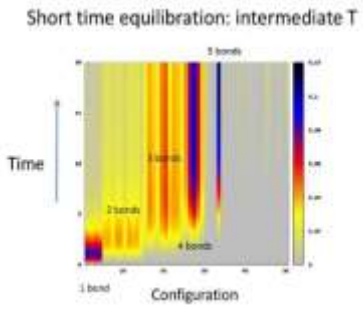
## Exploring the connection between thermodynamics and folding dynamics in simple model proteins





A simple model of a protein is introduced to facilitate the exploration of the connection between the morphology of the free energy surface of the protein and its folding dynamics. A microscopic theory for the dynamics of the system is developed that reduces to a Markovian model of the kinetics under well-defined conditions. Microscopic expressions for the rate constants that appear in the Markov state model are analyzed and expressed in terms of a temperature-dependent linear combination of escape rates that themselves are independent of temperature. A simple model of a helical-folding protein is constructed and its smooth free energy morphology is characterized. The dynamics of the system are analyzed within the Markov state model and it is demonstrated that for short chains, the relaxation is primarily single-exponential and becomes independent of temperature in the low-temperature regime. The profile is more complicated for longer chains, where multi-exponential relaxation behavior is seen at intermediate temperatures followed by a low temperature regime in which the folding becomes rapid and single exponential. It is demonstrated that the behavior of the equilibration profile as the temperature is lowered can be understood in terms of the number of relaxation modes or "folding pathways" that contribute to the evolution of the state populations.