

BiophysTO Lunchtime Seminar Series

Dr. Andre K. Yudin

Department of Chemistry University of Toronto Date Thursday, April 18 2019 12:00 – 1:00 pm Location McLennan Physical Laboratories Room MP606 60 St. George Street

Pizza and refreshments will be provided

Dominant rotors

This lecture will describe my lab's emerging interest in non-equilibrium systems. I will use macrocycles as a way to showcase functionally rich molecules that suffer from a poor understanding of conformational preferences. The emerging evidence suggests that a "butterfly effect" operates in large rings. It describes situations where a small change at a given position of a macrocycle results in disproportional consequences at distal position(s). Until recently, the available data has not translated into what matters most – a metric that describes the response of a given system to perturbation. To tackle this issue, we have implemented the concept of the dominant rotor, which corresponds to the bond that has the highest barrier to rotation. This simple approach has allowed us to evaluate response factors in a wide range of rings and led to the creation of two-well systems with controlled conformational behavior. To reach our objectives, we are designing amino acids and other building blocks that offer varying degrees of control over rotors. The most exciting outcome of this work is our capability to detect, study, and isolate conformational isomers in the 1-10 kcal/mol energy range. Our work underscores that operations away from equilibrium offer a fascinating possibility to control complex molecules.

Host: Dr. Walid A. Houry

