Title: Developing Data-Driven Physical Organic Analysis Tools for Reaction Optimization and Interrogation

Matthew S. Sigman[*]

Department of Chemistry, University of Utah, Salt Lake City, UT (USA)

Chemists are often guided by intuition when predicting the how and where an organic molecule will react. This is based on wisdom and a fundamental understanding of reactivity. However, while this method facilitates the majority of reaction development in organic and related chemical fields, the reality is that we rely significantly on optimizing reactions and structures for a desired outcome and/or function. While a routine process, optimization protocols can cause a considerable investment of time and do not always provide an adequate solution. Therefore, we have aimed to develop a program that assists the rapid analysis of structure function relationships to reveal not only better systems, but also the underlying reasons for improved performance of substrates, catalysts, or other functional materials. The lecture will outline how we have put into practice a method that combines the foundational promise of traditional physical organic chemistry with modern "big data" analysis tools to ultimately precisely predict and understand the performance of new reaction components and energy materials.