Quantitative Modeling Tools for Prediction in Synthesis and Catalysis

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When faced with unfamiliar reaction space, synthetic chemists typically apply the reported conditions (reagents, catalyst, solvent, and additives) of a successful reaction to a desired, closely related reaction using a new substrate type. Unfortunately, this approach often fails owing to subtle differences in reaction requirements. Consequently, an important goal in synthetic chemistry is the ability to transfer chemical observations from one reaction to another. Therefore, we have aimed to develop a program that assists the rapid analysis of the general interactions that impart asymmetric induction allowing the quantitative transfer of this stereochemical information to new reaction components and mechanisms. This talk will outline how we have developed this approach that combines organic synthesis, quantum chemistry, and statistical modeling to predict and interpret reaction outcomes. Ultimately, these techniques enable models to be generated from one set of reactions and be deployed to predict another, streamlining reaction and catalyst development.