Centre for Research in Molecular Modeling
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Catalytic Enantioselective α-Tosyloxylation of Ketones: Mechanistic Aspects and Insights on Chiral Induction

The chemistry of iodine(III) is broad and there is a growing interest for the development of enantioselective methodologies mediated by these compounds. In this class, the α-tosyloxylation of ketone derivatives using iodine (III) is a particularly powerful one, as it yields α-tosyloxy ketones – versatile chiral synthons that enable rapid access to numerous α-chiral ketones through nucleophilic displacement. This type of reaction can be rendered catalytic and enantioselective by the use of chiral iodine(I)-based catalysts. In our effort for the development of novel chiral catalysts to efficiently conduct this transformation, we have discovered important electronic and steric effects on both the activity and selectivity of the catalysts. Evaluation of a wide array of catalysts has also enabled us to better understand the chiral induction process. Using a mix of computational and experimental chemistry, insights into the reaction mechanism have been unearthed.

Claude Legault pursued graduate studies as an NSERC and FQRNT scholar at Université de Montréal in the research group of Professor André B. Charette. In 2005, he obtained his Ph.D. degree for his work on the development of novel asymmetric methods for the synthesis of polysubstituted piperidines. In 2006, he joined the research group of Professor Kendall N. Houk at UCLA as an NSERC postdoctoral fellow. During this stay, he acquired an expertise in computational chemistry and used this tool to understand the selectivities obtained in various synthetic methods. In july 2008, he started his academic career as assistant Professor in the Department of Chemistry at Université de Sherbrooke. His research group focuses on the development of simple and efficient synthetic methodologies of broad applicability and the use of computational chemistry to facilitate this research process.