



Université de Montréal, Montréal, QC, Canada

THIRD INTERNATIONAL SYMPOSIUM
ON C-H ACTIVATION

May 30 – June 2, 2016

IL11 – The Functionalization of C–H Bonds

M. Christina White*

Department of Chemistry, University of Illinois Urbana-Champaign, 270 RAL, Box 58-5, 600 South Mathews Avenue, Urbana, IL 61801 (USA)

Email: mcwhite7@illinois.edu

Advances in achieving site-selectivity in small molecule catalyzed C–H oxidations without the use of directing groups will be discussed. The first approach is the development of small molecule catalysts that are sensitive to the inherent electronic, steric, and stereoelectronic differences between C–H bonds in complex molecule settings. A second, complimentary approach termed “trajectory restriction” uses minimal steric blocking elements incorporated into a small molecule catalyst to increase catalyst/substrate non-bonding interactions, while maintaining structural flexibility such that substrates of diverse topologies are accommodated. Using a combination of these approaches, unprecedented site-divergent diversification of complex bioactive molecules like artemisinin can now be easily achieved. To maximally benefit from these approaches, a user-friendly catalyst reactivity model that calculates and even predicts the major site of oxidation as well as the magnitude and direction of the site-selectivity in complex substrates as a function of catalyst has been developed and will be discussed.

