SCHOOL OF NATURAL SCIENCES

SEMINAR SERIES

Complexity in Catalysis: Mechanisms, Noncovalent Interactions, and Natural Product Modifications

In pursuit of understanding the complex relationship between structure and function, classical and modern mechanistic studies were employed in several Pd-catalyzed enantioselective alkene functionalizations. First, classical experiments were performed to gain insight into the redox-relay Heck reaction. Next, to extend the redox-relay Heck reaction to a different alkene substrate class, modern structure-function relationships between ligand and substrate substituent effects and enantioselectivity were identified, which suggest attractive noncovalent interactions (NCIs) in the selectivity-determining step. Finally, structure-function relationships revealed mechanistic insight into the Pd-catalyzed 1,1-difunctionalization of alkenes, rendered enantioselective by using a chiral anion phase transfer strategy. These studies also suggest specific NCIs that are likely at play in the selectivity-determining step. In theme with exploring the role of NCIs in catalysis, a final project will be discussed. An aspartic acid/peracid catalytic cycle was applied to the oxidation of geldanamycin to access analogues of this promising anti-tumor agent. Depending on the peptide sequence appended to aspartic acid, different epoxide products result from site-selective oxidation. Current studies to understand the origins of peptide-derived selectivity and biological testing of these analogues are underway.

Monday, 12/16/19	**9:30am - 10:30am**	**COB 1, Rm. 265**	For more information, contact: Professor Christine Isborn at cisborn@ucmerced.edu

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Born and raised in South Texas, Margaret attended Trinity University in San Antonio, TX obtaining her B.S. in chemistry. She then pursued a Ph.D. in chemistry with Prof. Matthew Sigman at the University of Utah, where she studied the mechanisms of several enantioselective palladium-catalyzed reactions using classical and modern mechanistic tools. Margaret is now a postdoctoral fellow with Prof. Scott Miller at Yale University, where she is investigating peptide-catalyzed site selective oxidation of natural products.