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Global Discovery Chemistry

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Through collaboration with the Jensen group at MIT, the chemical technologies group has been exploring the use of a self-optimizing reactor (SOR) with the ability to simultaneously optimize discrete and continuous variables in a minimal number of experiments. The current research project seeks to incorporate catalyst parameterization models into the algorithms of the SOR, thereby allowing a more profound understanding of chemical transformations and the ability to extrapolate to new reactivity and catalyst space. Thus, the project seeks to develop a new paradigm in reaction optimization and discovery.

Our proposal builds on collaboration with the laboratory of Professor Matthew Sigman (*J. Am. Chem. Soc.* 2017, 10613) to parameterize and synthesize ligands for cross coupling reactions. We are looking to expand this approach to Ni-catalyzed cross coupling reactions. The renaissance in sp²-sp³ and sp³-sp³ Ni-catalyzed cross coupling has brought a wave of new synthetic disconnections to medicinal chemists. This explosion of new reactivity space offers a great opportunity to design and screen for new catalysts. The specific goals of this project are to design and enumerate a virtual set of ligands that covers a range of steric and electronic space. The virtual space will be used to define ligand parameters that can be incorporated into the SOR, and subsequently synthesized and tested. Similar to Pd catalysis in the late 90s, discovery of more active and robust catalysts for Ni catalyzed chemistry will help usher in a new age cross coupling chemistry.

Selected Publications

Allosteric inhibition of SHP2 phosphatase inhibits cancers driven by receptor tyrosine kinases.

Chen YN, LaMarche MJ, Chan HM, Fekkes P, Garcia-Fortanet J, Acker MG, Antonakos B, Chen CH, Chen Z, Cooke VG, Dobson JR, Deng Z, Fei F, Firestone B, Fodor M, Fridrich C, Gao H, Grunenfelder D, Hao HX, Jacob J, Ho S, Hsiao K, Kang ZB, Karki R, Kato M, Larrow J, La Bonte LR, Lenoir F, Liu G, Liu S, Majumdar D, Meyer MJ, Palermo M, Perez L, Pu M, Price E, Quinn C, Shakya S, Shultz MD, Slisz J, Venkatesan K, Wang P, Warmuth M, Williams S, Yang G, Yuan J, Zhang JH, Zhu P, Ramsey T, Keen NJ, Sellers WR, Stams

T, Fortin PD.

Nature. 2016 Jul 7;535(7610):148-52.

Enantioselective Construction of Vicinal Stereogenic Quaternary Centers by Dialkylation: Practical Total Synthesis of (+)- and meso-Chimonanthine.

Overman LE, Larrow JF, Stearns BA, Vance JM.

Angew Chem Int Ed Engl. 2000 Jan;39(1):213-215.

Asymmetric catalysis with water: efficient kinetic resolution of terminal epoxides by means of catalytic hydrolysis.

Tokunaga M, Larrow JF, Kakiuchi F, Jacobsen EN.

Science. 1997 Aug 15;277(5328):936-8.

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