



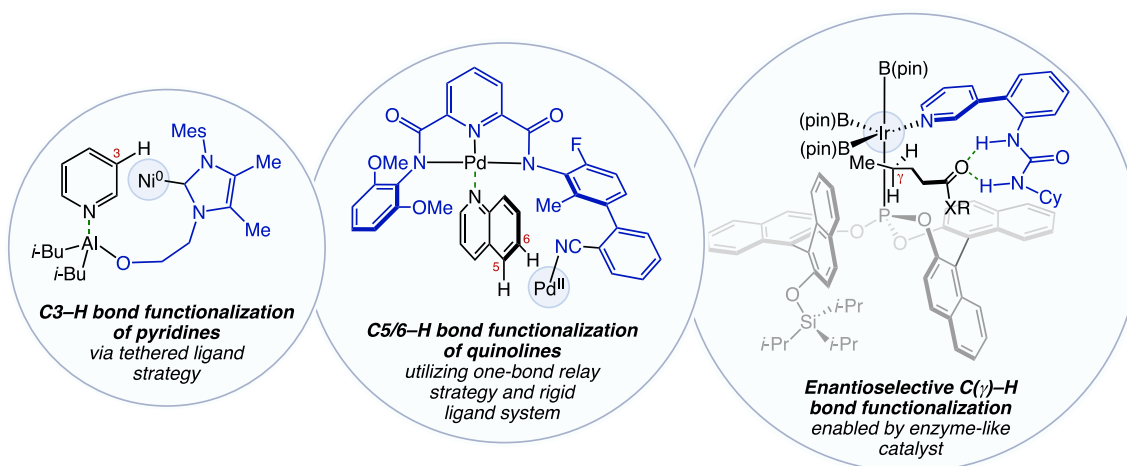
# Harnessing Bifunctional Ligands for Regioselective C–H Bond Functionalization

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**Abstract:** The diversification of organic molecules is fundamental to the discovery of new compounds with desirable properties.<sup>1</sup> A common means to achieve structural diversification is through functional group interconversion, in which a functional group is transformed using a suitable set of reagents. The selectivity of these interconversions is dictated by the unique chemical properties of each functional group and the reactivity of the reagents used for the transformation. An emerging strategy for the diversification of organic molecules is in the functionalization of unactivated C–H bonds, or those that are traditionally inert. The ability to selectively cleave and transform unreactive C–H bonds can be transformative in the ability to derivatize late-stage chemical structures. Although significant advances have been made in this area, achieving site-selectivity remains a major challenge, especially at remote positions or in cases where multiple electronically or sterically comparable C–H bonds are present.

This seminar will highlight recent advances in C–H bond functionalization that harness non-covalently bound directing groups that guide regioselectivity.<sup>1</sup> First, a tethered ligand strategy will be described, which enables the C3–H bond functionalization of pyridine derivatives.<sup>1</sup> Next, a rigid template method will be discussed, which facilitates the remote functionalization of previously inaccessible C5–H and C6–H bonds of quinoline derivatives.<sup>1</sup> Additive effects will be covered, as well as computational studies of the mechanism for this transformation. Lastly, an enzyme-like Ir catalyst will be described, which promotes the enantioselective C( $\gamma$ )–H borylation of aliphatic acid derivatives via several substrate–ligand and ligand–ligand interactions.<sup>1</sup> Key design elements and origins of selectivity will be explored throughout this seminar, as well as an outlook on future directions.



**Monday, February 28, 2022 | 3:00 p.m.**  
**1240B Kinsey Pavilion & Zoom**