Ligand-Controlled Chemodivergent Suzuki Cross Coupling using Palladium-N-Heterocyclic Carbene Catalysts

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The successful synthesis of complicated organic molecules such as pharmaceuticals, agrochemicals, and organic materials requires an extensive toolbox of synthetic strategies for constructing carbon-carbon bonds. Problems can arise, however, when a molecule contains multiple functional groups that are reactive toward the same transformations. For example, both arylbhalides and aryltriflates can undergo palladium-catalyzed Suzuki cross-coupling in the presence of arylboronic acids. Control of selectivity between these two electrophilic sites using different Pd-phosphine catalysts has been described previously, but the scope of such methodology is severely limited. In this presentation, we describe the discovery of an orthogonal pair of Pd-N-heterocyclic carbene (Pd-NHC) catalysts for chemodivergent cross-coupling of aryl chlorides and aryl triflates with phenylboronic acids and demonstrate the synthetic utility of these catalysts with diverse boronic acids and substrates. The mild conditions used in these reactions allows for high functional group tolerance with respect to both substrates and boronic acids. We additionally present experimental and computational evidence that the origin of selectivity using Pd-NHC catalysts is dissimilar to the mechanism of selectivity control using Pd-phosphine catalysts.