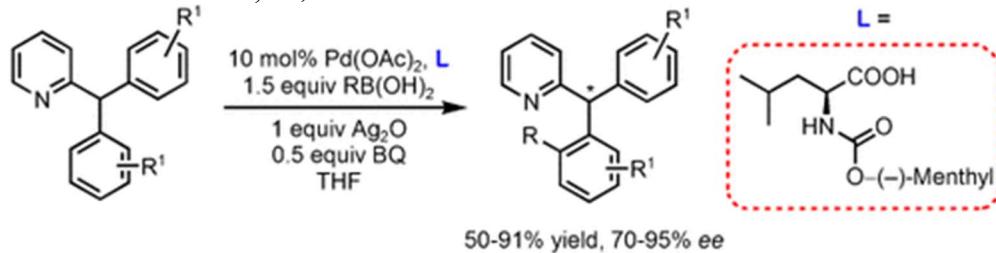
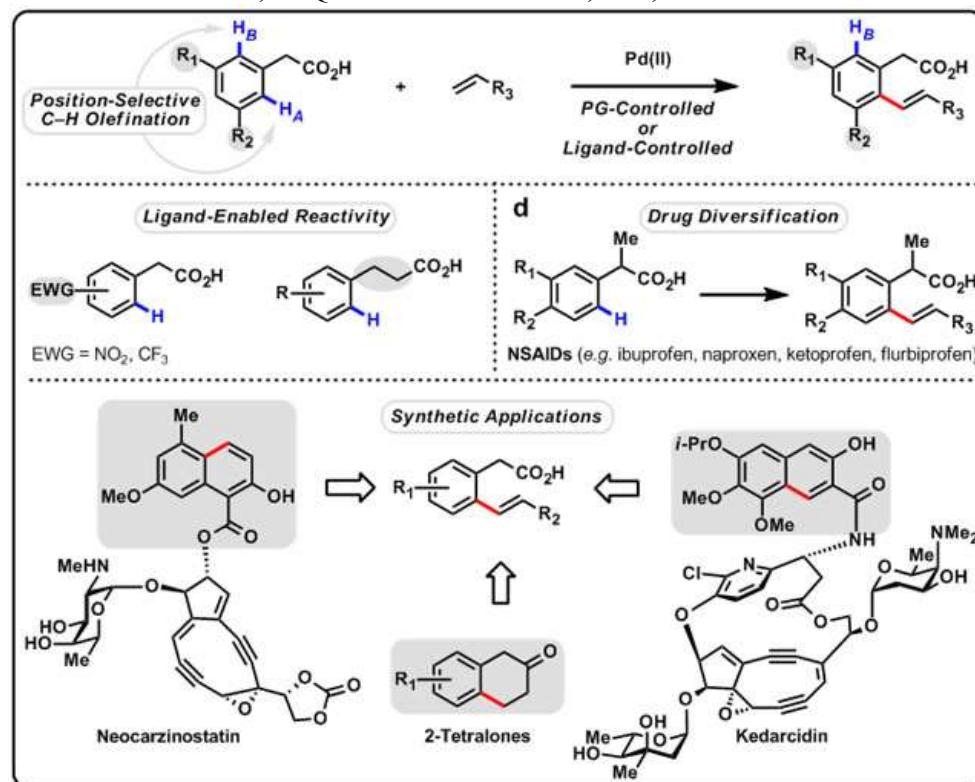


# Yu Group

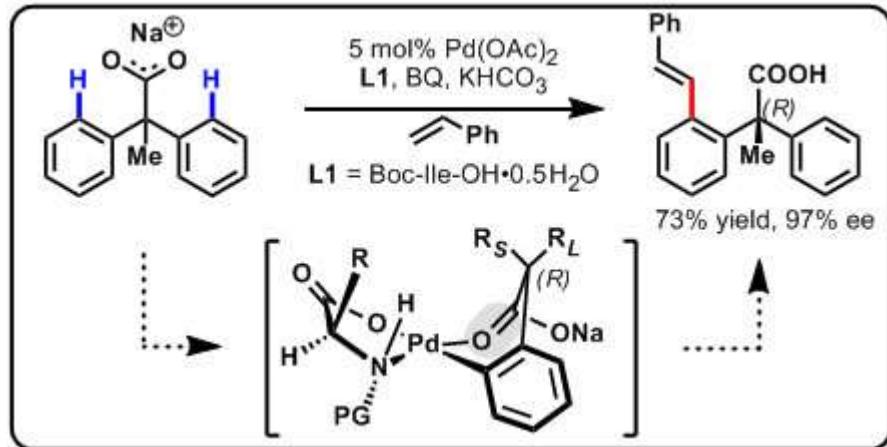
1. “Pd<sup>II</sup>-Catalyzed Enantioselective Activation of C(sp<sup>2</sup>)–H and C(sp<sup>3</sup>)–H Bonds Using Monoprotected Amino Acids as Chiral Ligands” Yu, J.-Q. et al. *Angew. Chem. Int. Ed.* **2008**, *47*, 4882.



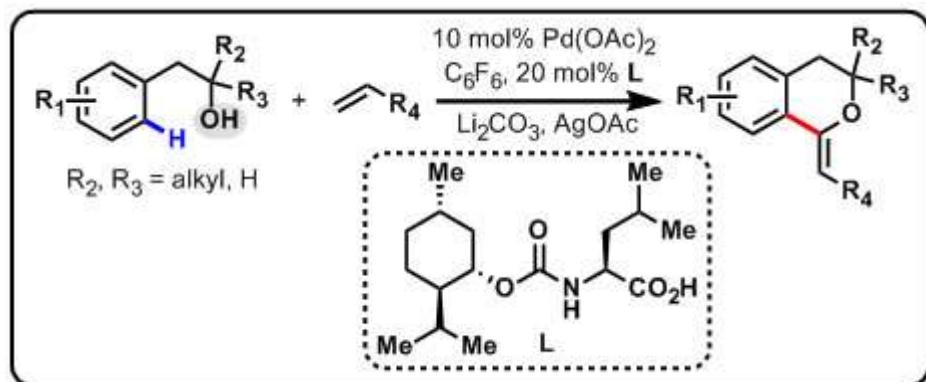
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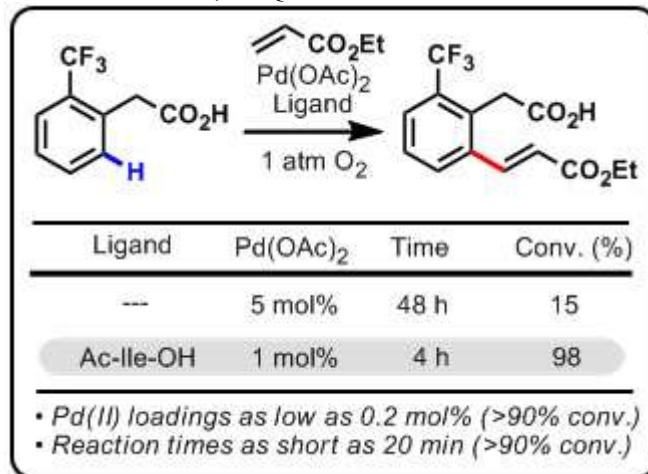
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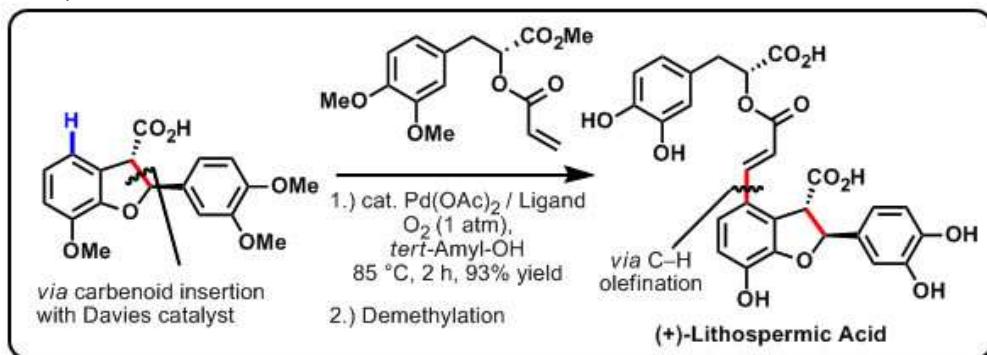


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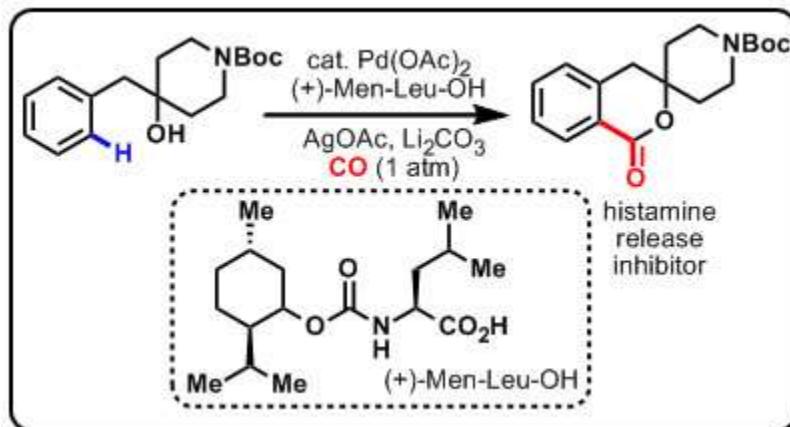


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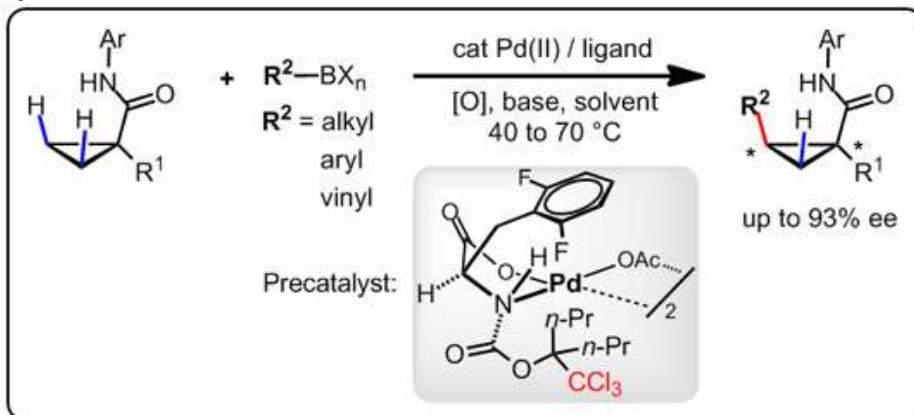


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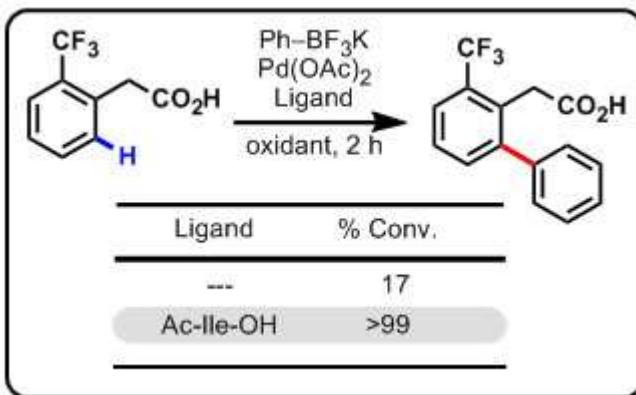


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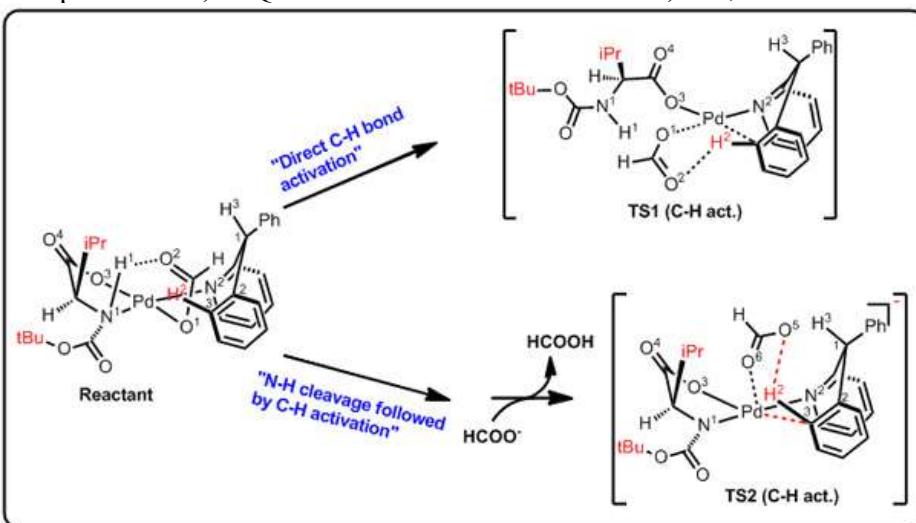
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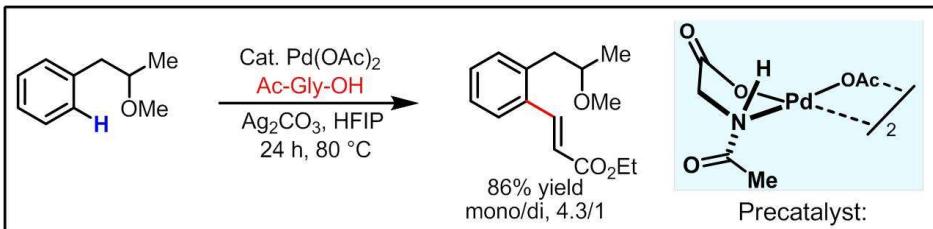
10. "Ligand-Accelerated Cross-Coupling of C(sp<sup>2</sup>)–H Bonds with Arylboron Reagents" Yu, J.-Q. *et al.* *J. Am. Chem. Soc.* **2011**, *133*, 18183.



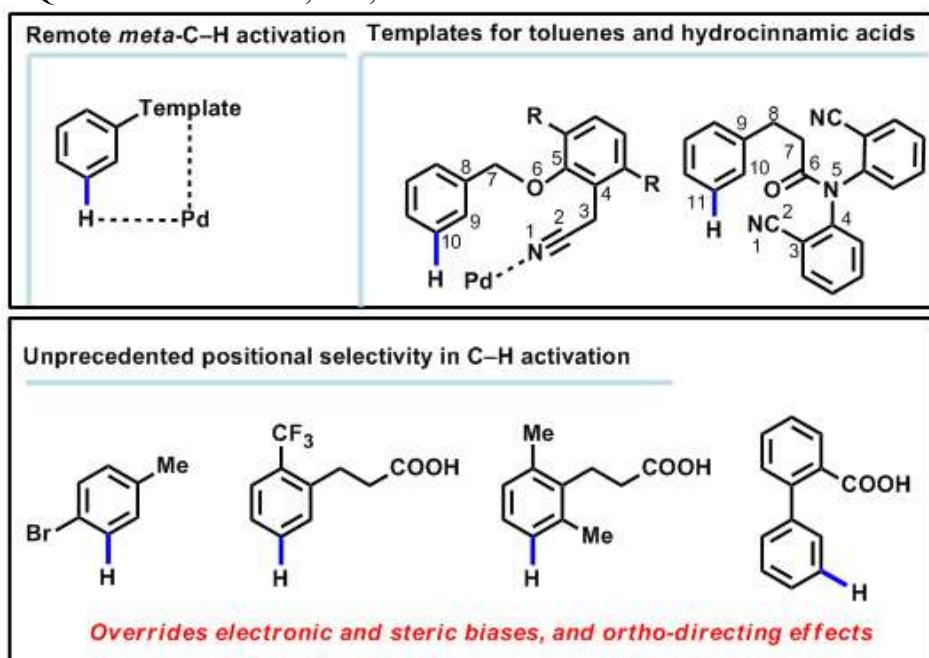
11. "Key Mechanistic Features of Enantioselective C–H Bond Activation Reactions Catalyzed by [(Chiral Mono-N-Protected Amino Acid)-Pd(II)] Complexes" Yu, J.-Q. *et al.* *J. Am. Chem. Soc.* **2012**, *134*, 1690.



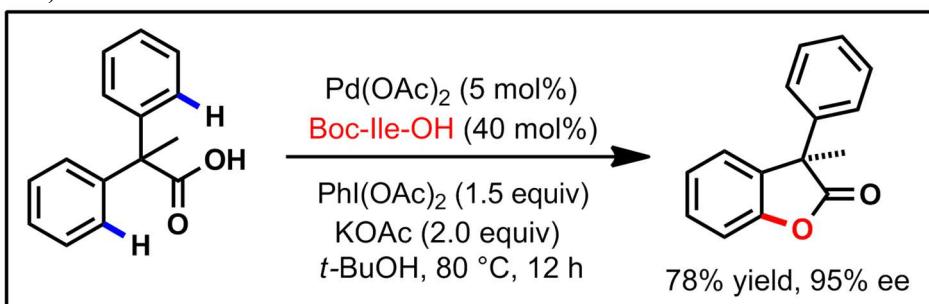
12. "Ether-Directed ortho-C–H Olefination with a Palladium(II)/Monoprotected Amino Acid Catalyst" Yu, J.-Q. *et al.* *Angew. Chem., Int. Ed.* **2012**, *52*, 1247.



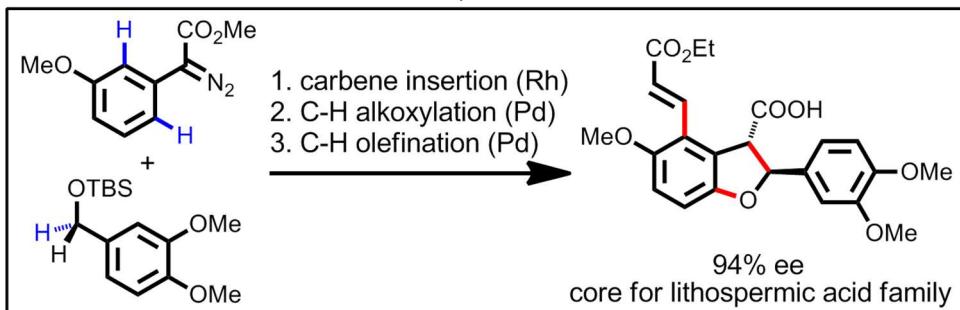
13. "Activation of Remote meta-C–H Bond Assisted by an End-on Template" Yu, J.-Q. *et al.* *Nature* **2012**, *486*, 518.



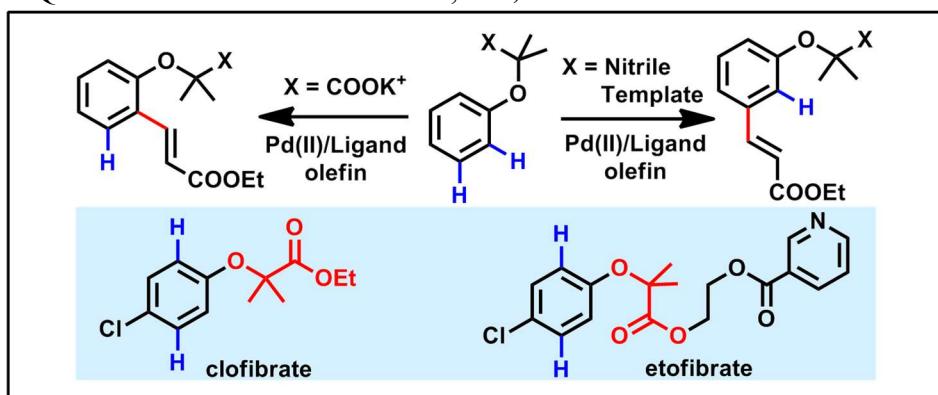
14. "Pd(II)-Catalyzed Enantioselective C–H Activation/C–O Bond Formation: Synthesis of Chiral Benzofuranones" Yu, J.-Q. *et al.* *J. Am. Chem. Soc.* **2013**, *135*, 1236.



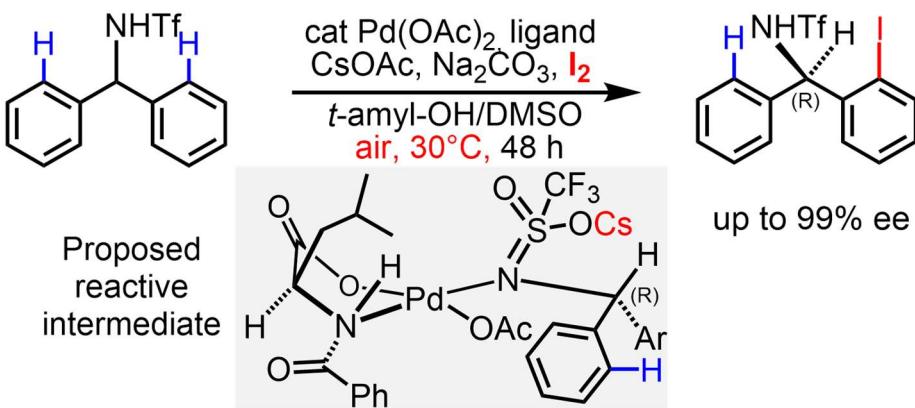
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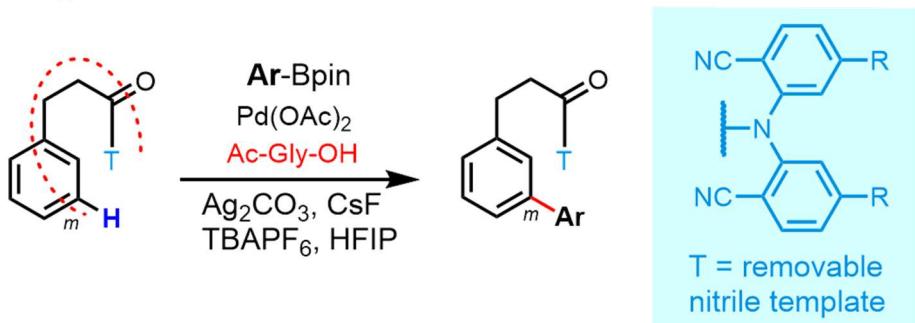
16. "Pd(II)-Catalyzed ortho- or meta-C–H Olefination of Phenol Derivatives" Yu, J.-Q. *et al.* *J. Am. Chem. Soc.* **2013**, *135*, 7567.



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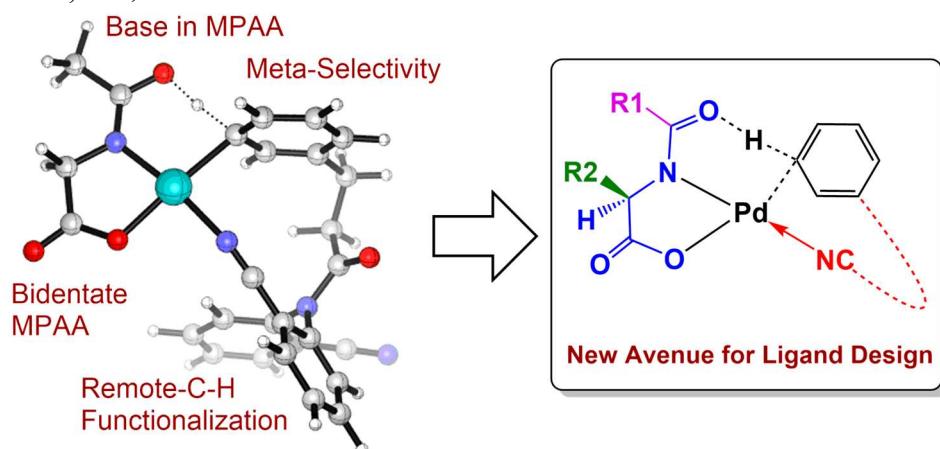


18. "Cross-Coupling of Remote meta-C–H Bonds Directed by a U-Shaped Template" Yu, J.-Q. *et al.* *J. Am. Chem. Soc.* **2013**, *135*, 18056.

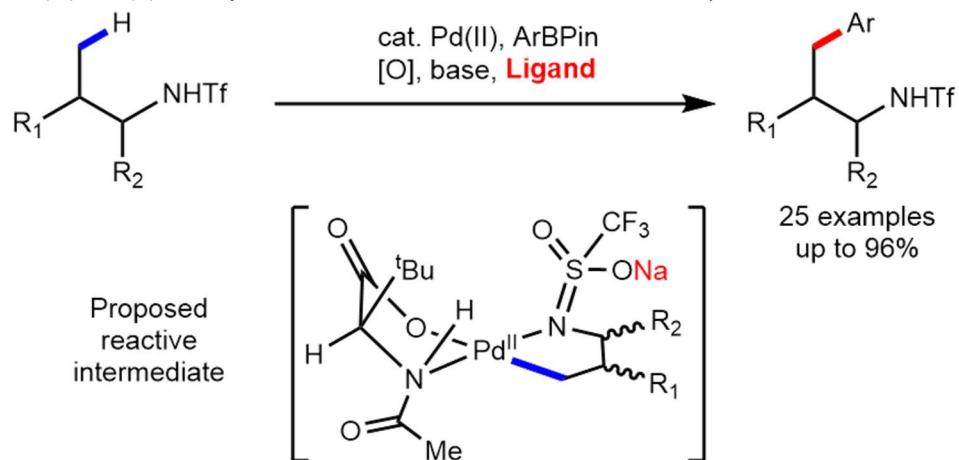


19. "Role of N-Acyl Amino Acid Ligands on Pd(II)-Catalyzed Remote C–H Activation of Tethered Arenes" Yu, J.-Q.; Wu, Y.-D. *et al.* *J. Am. Chem. Soc.*

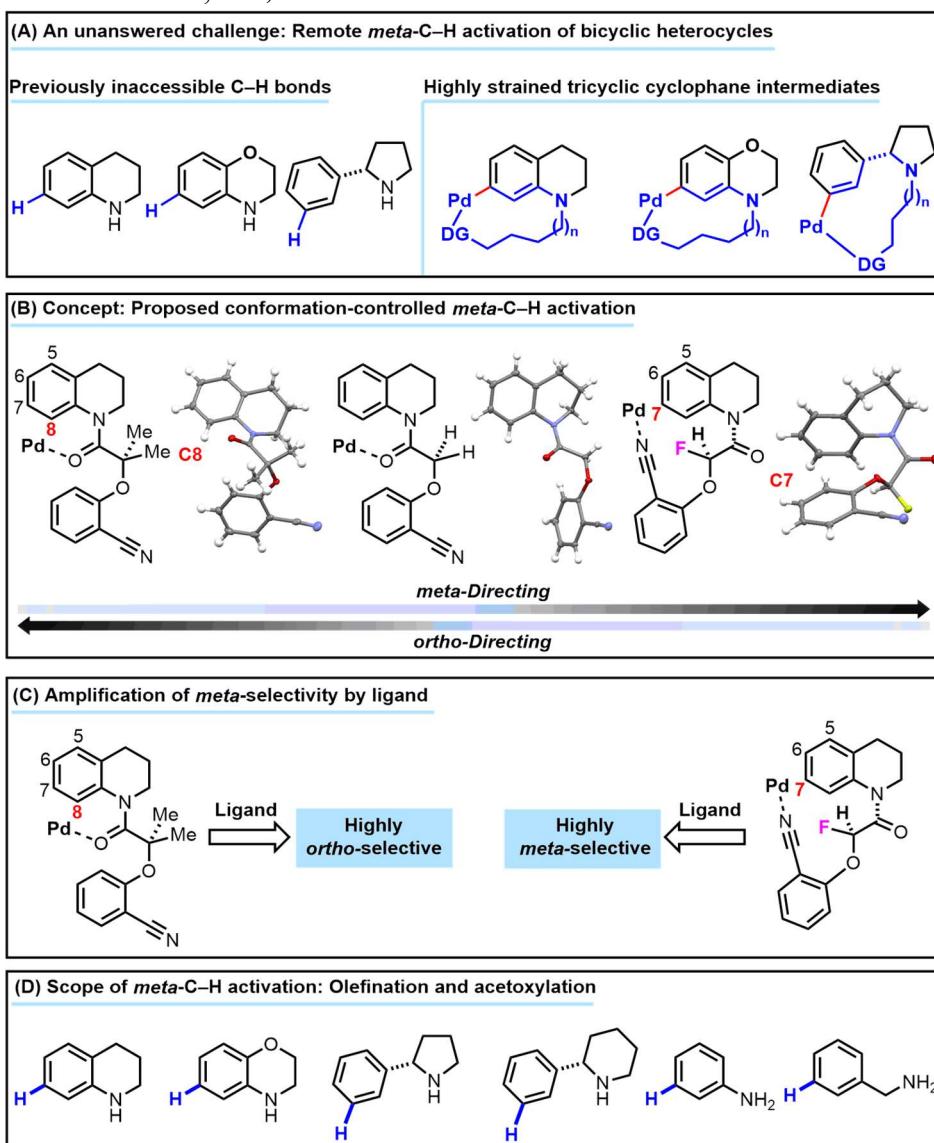
2014, 136, 894.



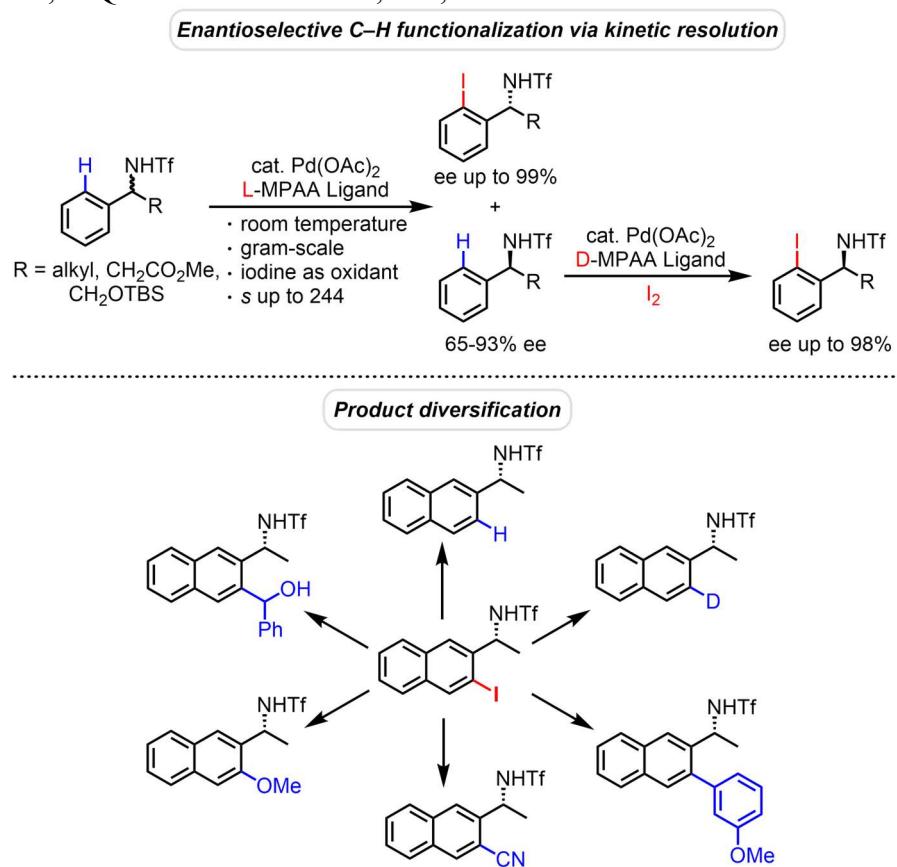
20. "Ligand-enabled cross-coupling of C(sp<sup>3</sup>)–H bonds with arylboron reagents via Pd(II)/Pd(0) catalysis" Yu, J.-Q. et al. *Nature Chemistry* 2014, 6, 146.



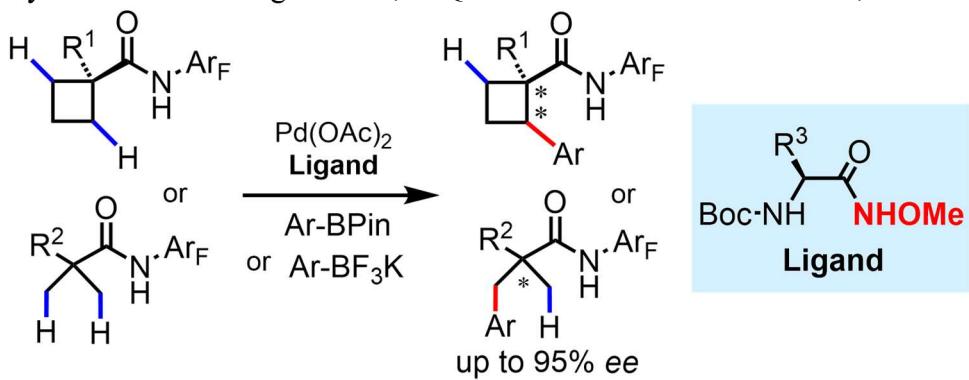
21. "Conformation-Induced Remote meta-C–H Activation of Amines" Yu, J.-Q. et al. *Nature* 2014, 507, 215.



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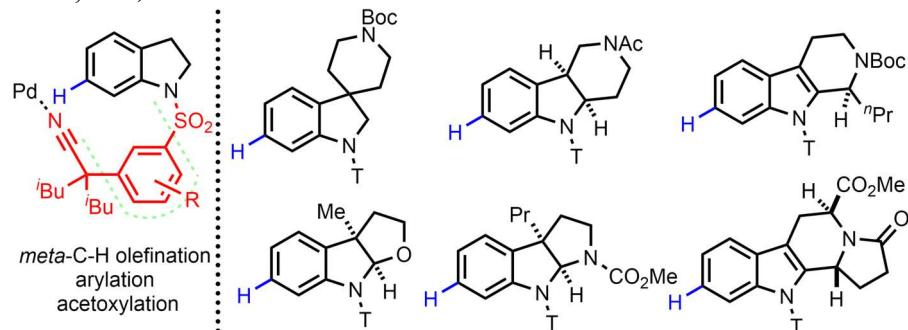


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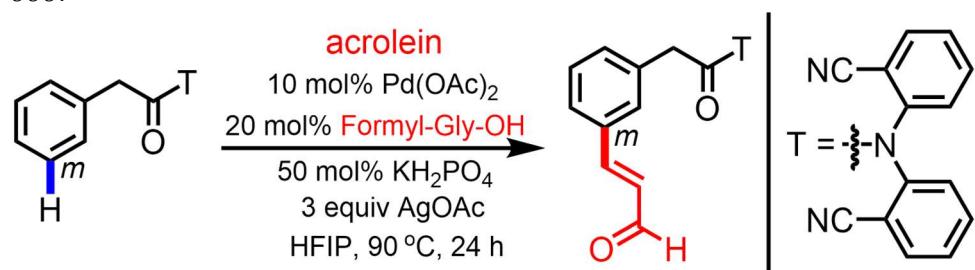


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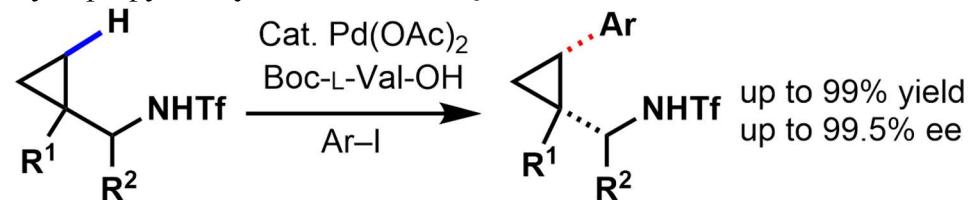
2014, 136, 10807.



25. "Remote meta-C–H Olefination of Phenylacetic Acids Directed by a Versatile U-Shaped Template" Yu, J.-Q. et al. *Angew. Chem. Int. Ed.* **2015**, 54, 888.



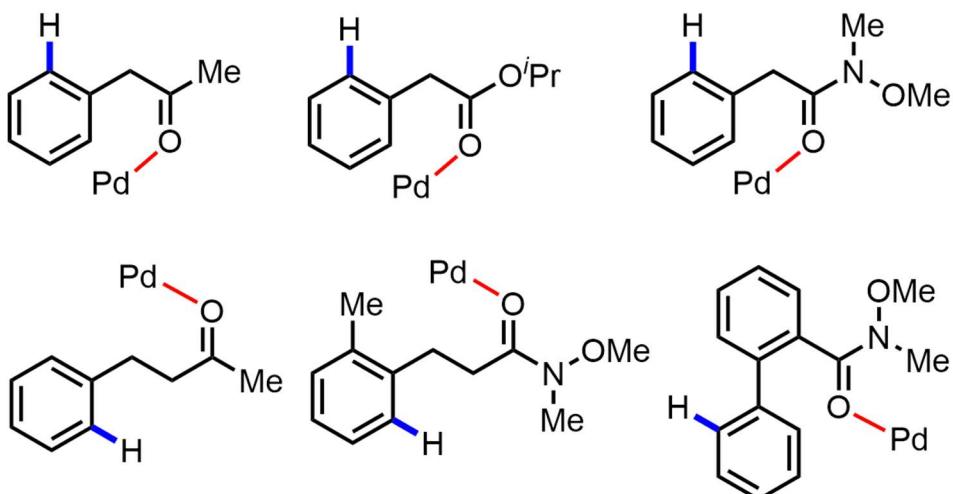
26. "Palladium(II)-Catalyzed Highly Enantioselective C–H Arylation of Cyclopropylmethylamines" Yu, J.-Q. et al. *J. Am. Chem. Soc.* **2015**, 137, 2042.



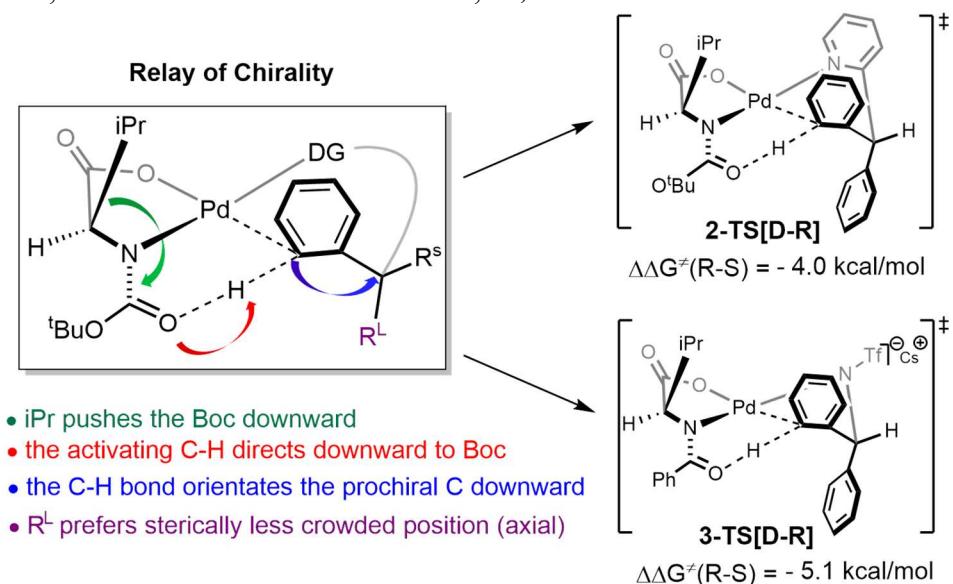
First example of enantioselective  
C–H arylation via Pd(II)/Pd(IV) catalysis

27. "Pd(II)-Catalyzed C–H Functionalizations Directed by Distal Weakly Coordinating Functional Groups" Yu, J.-Q. et al. *J. Am. Chem. Soc.* **2015**, 137,

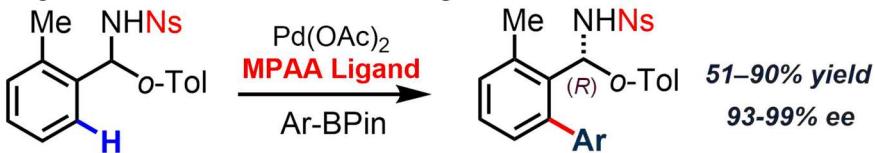
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28. "Ligand-Accelerated ortho-C–H Olefination of Phenylacetic Acids" Yu, J.-Q. *et al. Org. Synth.* **2015**, 92, 58.
29. "A Combined IM-MS/DFT Study on Pd(MPAA)-Catalyzed Enantioselective C–H Activation: Relay of Chirality through a Rigid Framework" Yu, J.-Q.; Wu, W.-D. *et al. Chem. Eur. J.* **2015**, 21, 11180.

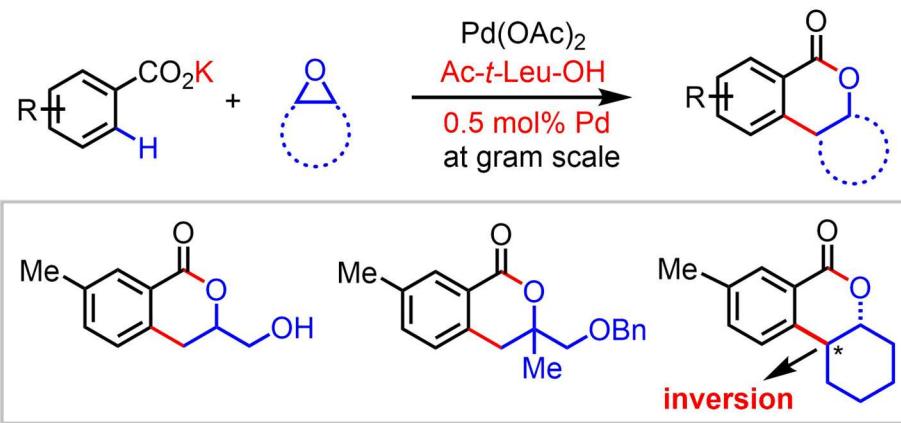


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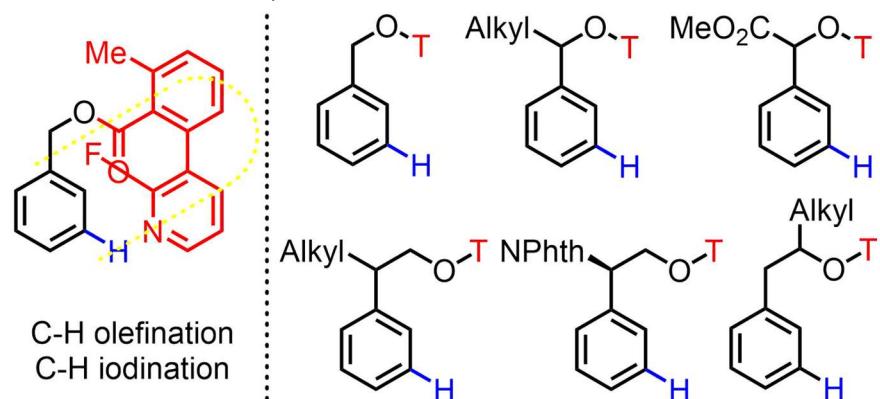


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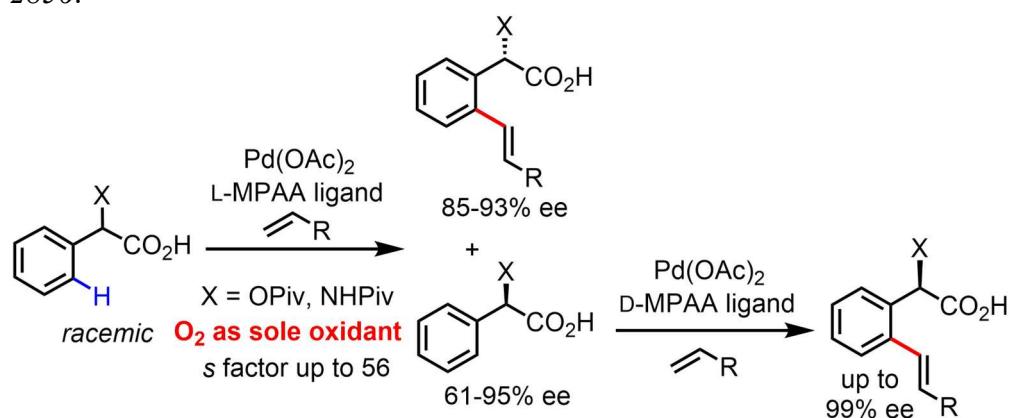
10950.



32. "Remote Meta-C–H Activation Using a Pyridine-Based Template: Achieving Site-Selectivity via the Recognition of Distance and Geometry" Yu, J.-Q. *et al.* *ACS Cent. Sci.* **2015**, *1*, 394.



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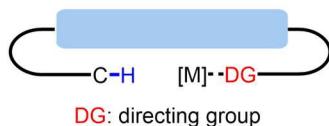


34. "Functionalization of C(sp<sup>3</sup>)–H bonds using a transient directing group" Yu, J.-Q. et al. *Science* **2016**, *351*, 252.

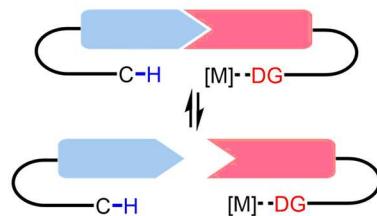
**A**

Two Strategies for Directed C–H Activation

pre-installed directing groups



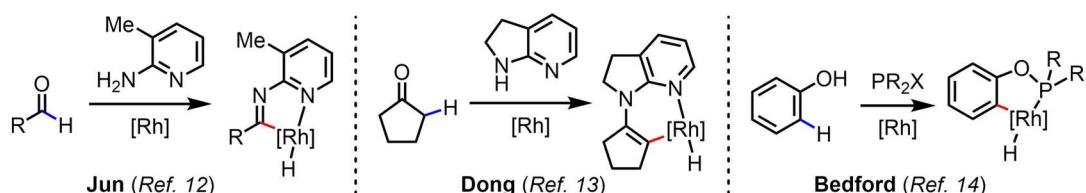
transient directing groups



Disadvantage: requires installation and removal of the directing group

**B**

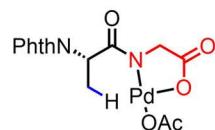
Pioneering Examples of Reversibly Linked Directing Groups



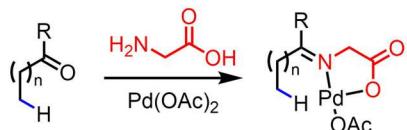
**C**

C(sp<sup>3</sup>)–H Arylation Using Amino Acid as Transient Directing Group

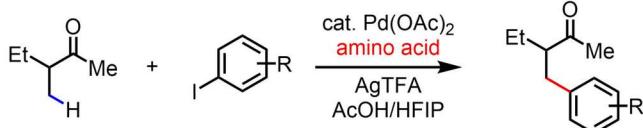
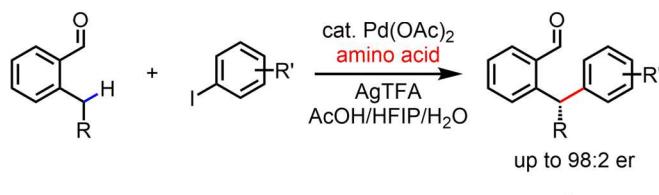
C(sp<sup>3</sup>)–H Activation of Peptides



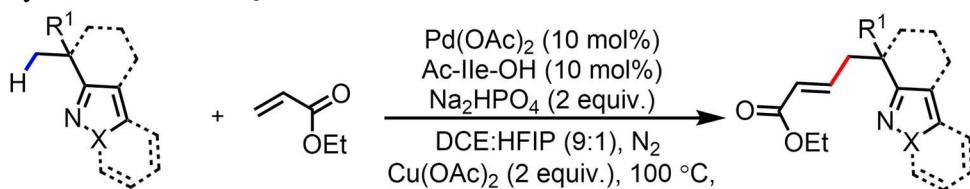
Design of Transient Amino Acid Directing Group



This Work

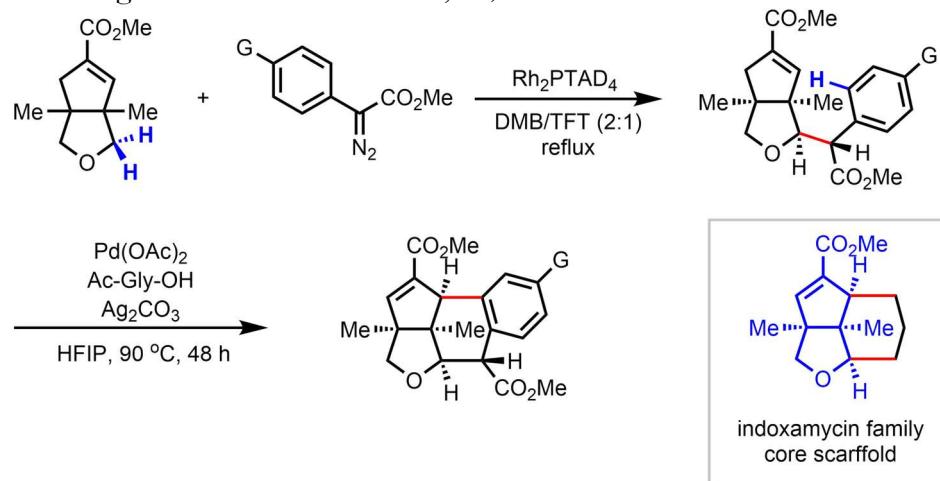


35. "Ligand-Promoted C(sp<sup>3</sup>)–H Olefination en Route to Multi-functionalized Pyrazoles" Yu, J.-Q. et al. *Chem. Eur. J.* **2016**, *22*, 7059.

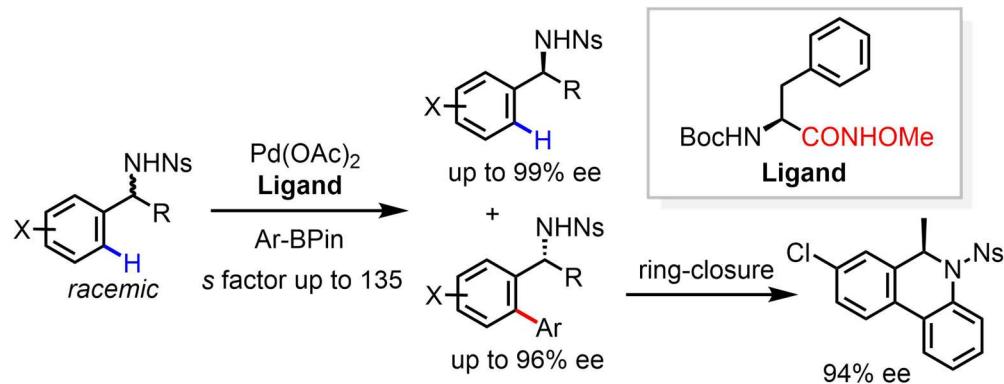


36. "Rapid Construction of a Benzo-Fused Indoxamycin Core Enabled by Site-Selective C–H Functionalizations" Yu, J.-Q.; Davies, H. M. L.; Sorensen, E. J.

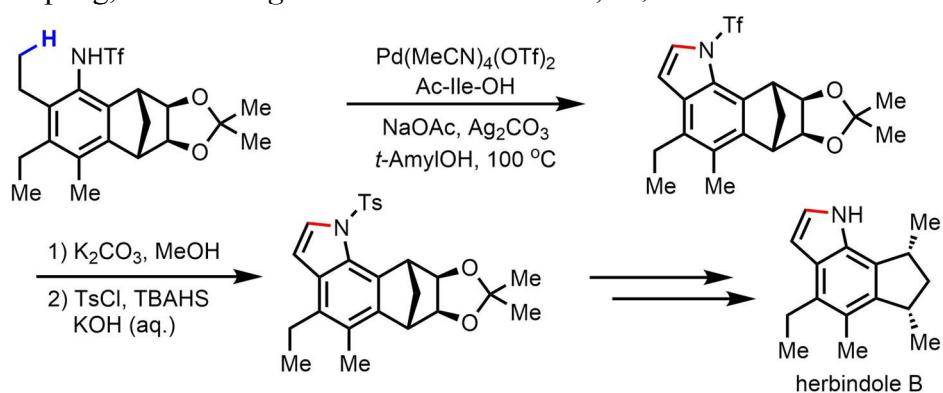
*et al. Angew. Chem. Int. Ed.* **2016**, *55*, 8270.



37. "Kinetic Resolution of Benzylamines via Palladium(II)-Catalyzed C–H Cross-Coupling" Yu, J.-Q. *et al. J. Am. Chem. Soc.* **2016**, *138*, 7796.

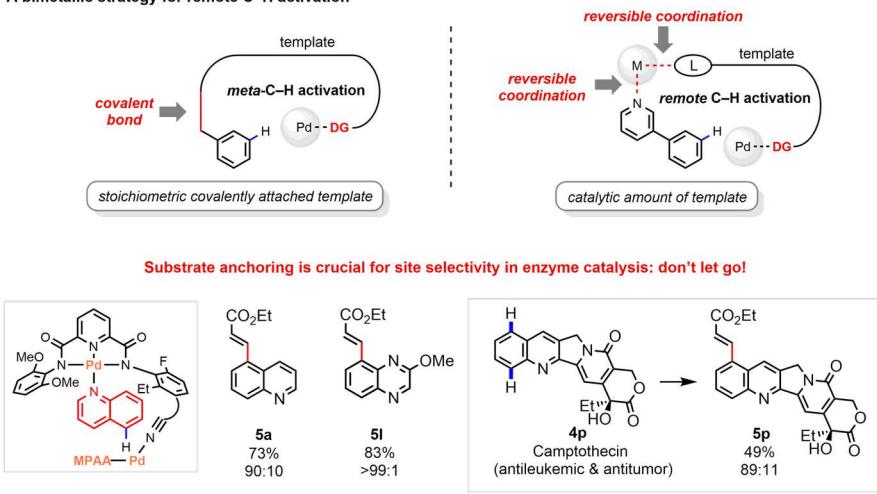


38. "Application of a Palladium-Catalyzed C–H Functionalization/Indolization Method to Syntheses of cis-Trikentrin A and Herbindole B" Yu, J.-Q.; Sarpong, R. *et al. Angew. Chem. Int. Ed.* **2016**, *55*, 11824.

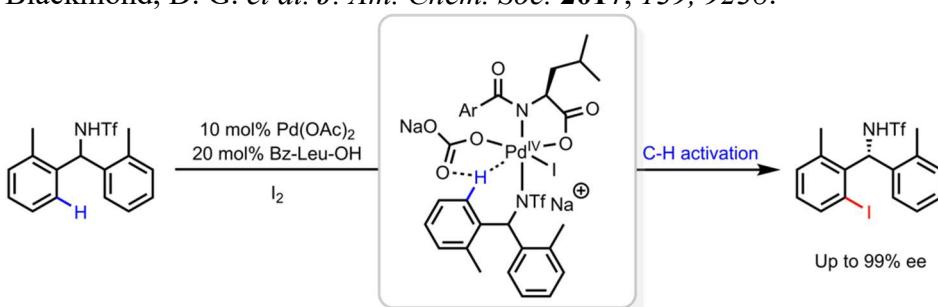


39. "Remote site-selective C–H activation directed by a catalytic bifunctional template" Yu, J.-Q. *et al. Nature* **2017**, *543*, 538.

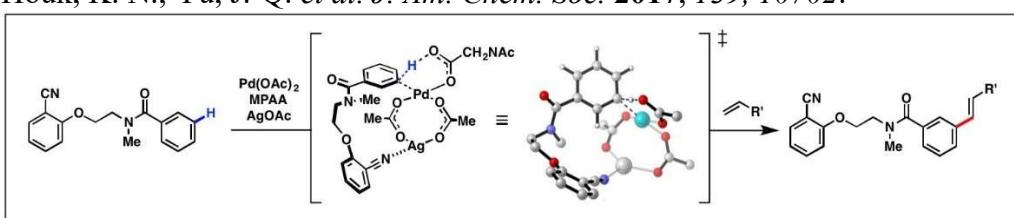
A bimetallic strategy for remote C–H activation



40. "A Role for Pd(IV) in Catalytic Enantioselective C–H Functionalization with Monoprotected Amino Acid Ligands under Mild Conditions" Yu, J.-Q.; Blackmond, D. G. *et al. J. Am. Chem. Soc.* **2017**, *139*, 9238.



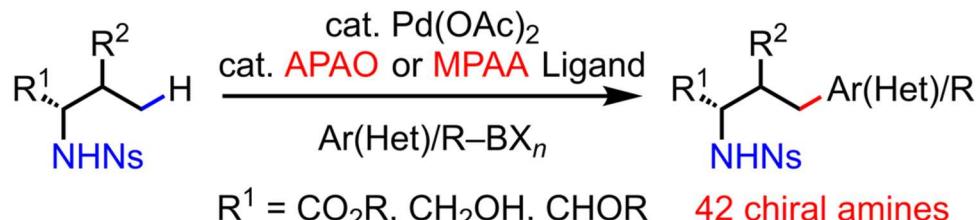
41. "Experimental and Computational Development of a Conformationally Flexible Template for the Meta-C–H Functionalization of Benzoic Acids" Houk, K. N.; Yu, J.-Q. *et al. J. Am. Chem. Soc.* **2017**, *139*, 10702.



42. "Enantioselectivity Model for Pd-Catalyzed C–H Functionalization Mediated by the Mono-N-protected Amino Acid (MPAA) Family of Ligands" Yu, J.-Q.; Musaev, D. G. *et al. ACS Catal.*, **2017**, *7*, 4344.

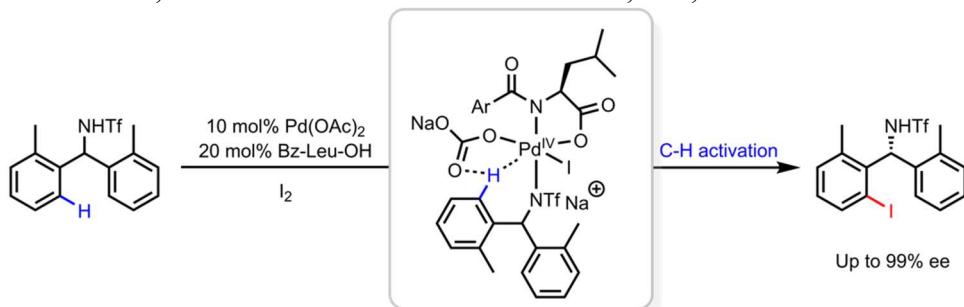
43. "Ligand-Enabled Gamma-C(sp<sup>3</sup>)–H Cross-Coupling of Nosyl-Protected Amines with Aryl- and Alkylboron Reagents" Yu, J.-Q. *et al. ACS Catal.* **2017**,

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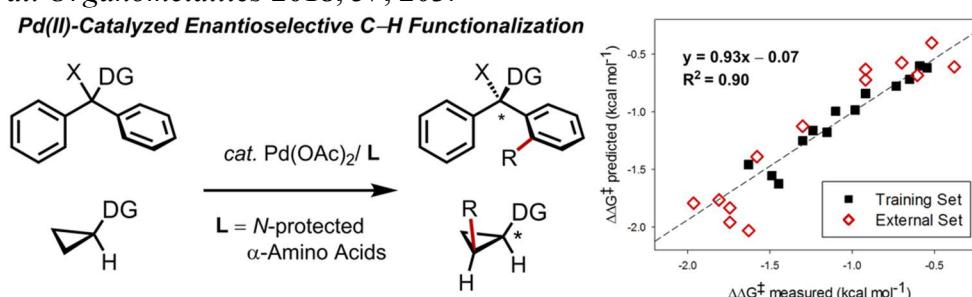


- A common protecting group as directing group
- First example of  $C(sp^3)$ -H cross-coupling of amines with alkylboron reagents

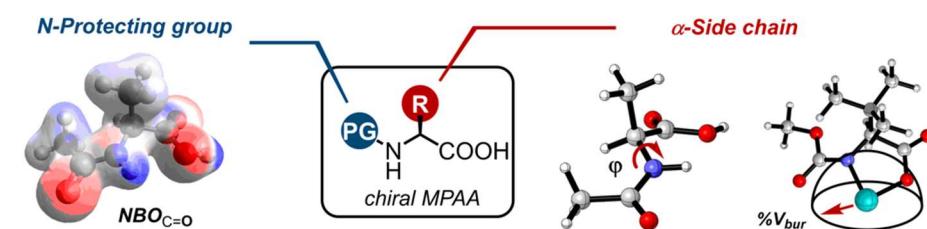
44. "Dynamic Ligand Exchange as a Mechanistic Probe in Pd-Catalyzed Enantioselective C–H Functionalization Reactions Using Monoprotected Amino Acid Ligands" Yu, J.-Q.; Blackmond, D. G. *et al. J. Am. Chem. Soc.* **2017**, *139*, 18500.
45. "A Role for Pd(IV) in Catalytic Enantioselective C-H Functionalization with Monoprotected Amino Acid Ligands under Mild Conditions" Yu, J.-Q.; Blackmond, D. G. *et al. J. Am. Chem. Soc.* **2017**, *139*, 9238.



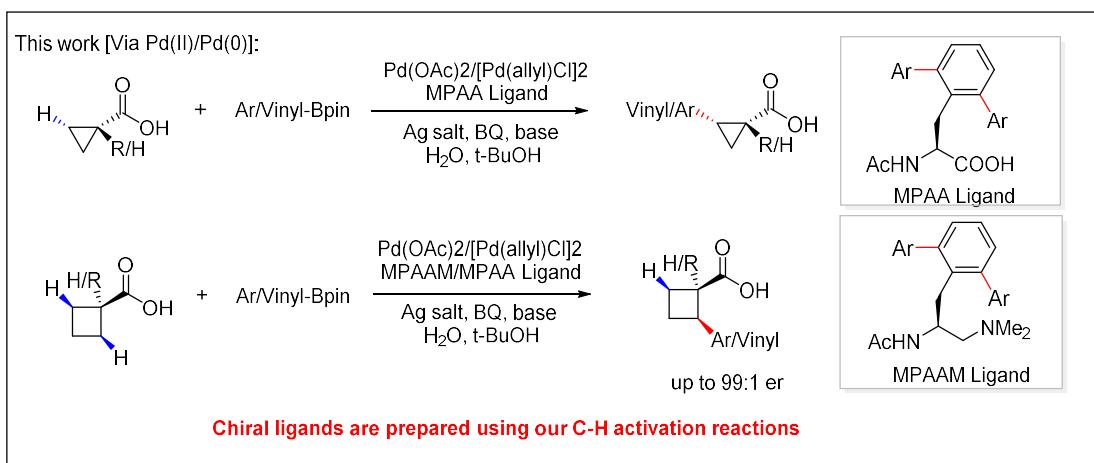
46. "Quantifying Structural Effects of Amino Acid Ligands in Pd(II)-Catalyzed Enantioselective C–H Functionalization Reactions" Yu, J.-Q.; Sigman, M. S. *et al. Organometallics* **2018**, *37*, 203.



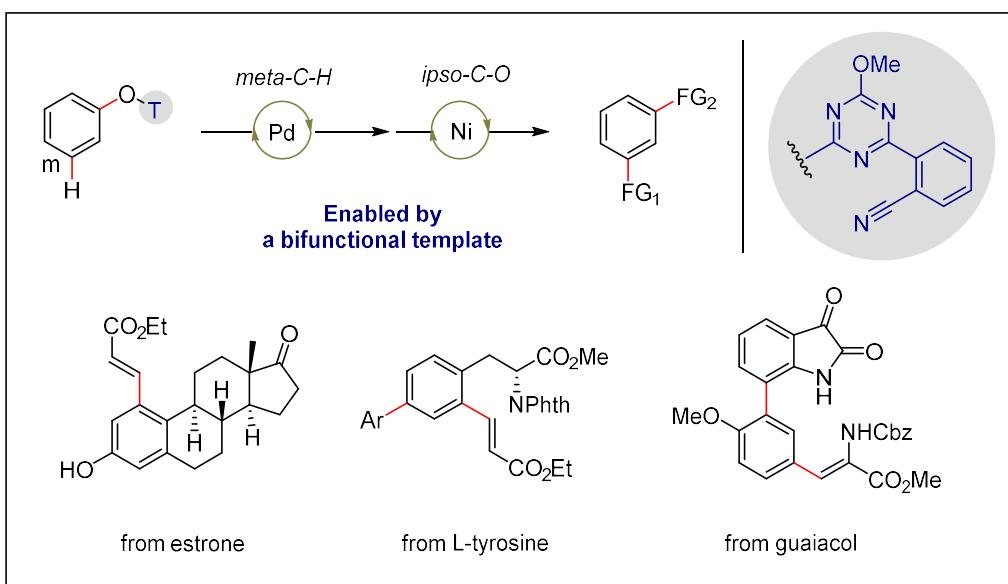
*multivariate analysis unravels the structural effects on the enantioselectivity*



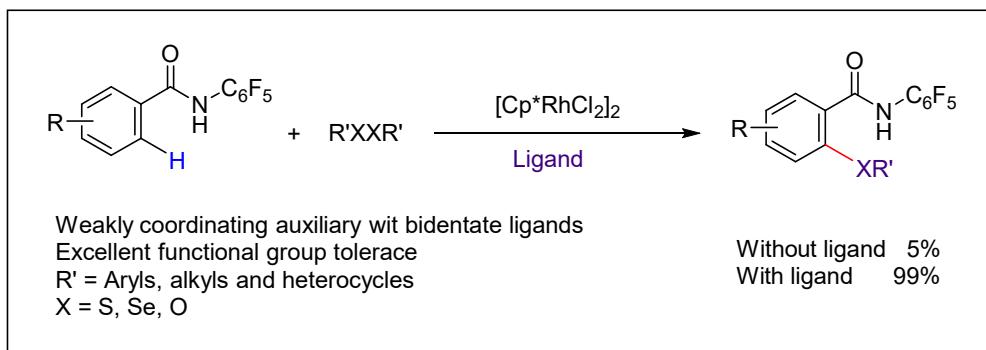
47. “Pd(II)-Catalyzed Enantioselective C(sp<sup>3</sup>)–H Activation/Cross-Coupling Reactions of Free Carboxylic Acids.” Yu, J.-Q. et al. *Angew. Chem. Int. Ed.* **2019**, *58*, 2134.



48. “Sequential Functionalization of meta-C–H and ipso-C–O Bonds of Phenols” Xie, S.; Jin, Z.; Yu, J.-Q. et al. *J. Am. Chem. Soc.* **2019**, *141*, 1903.

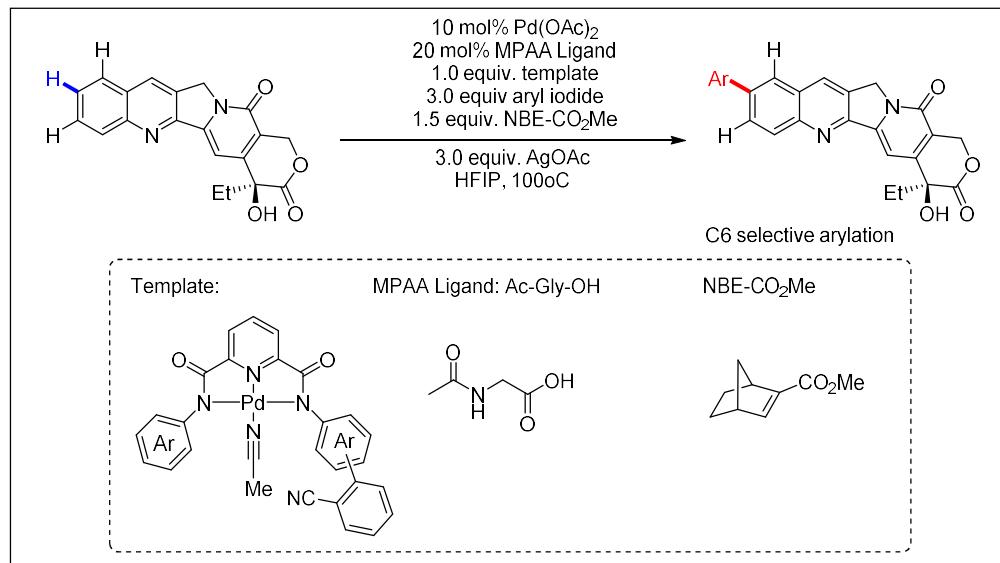


49. "Ligand-Promoted Rh(III)-Catalyzed Thiolation of Benzamides with a Broad Disulfide Scope" Sun, W.Y.; Yu, J.-Q.; Lu, Y. *Angew. Chem. Int. Ed.* **2019**, *58*, 9099.



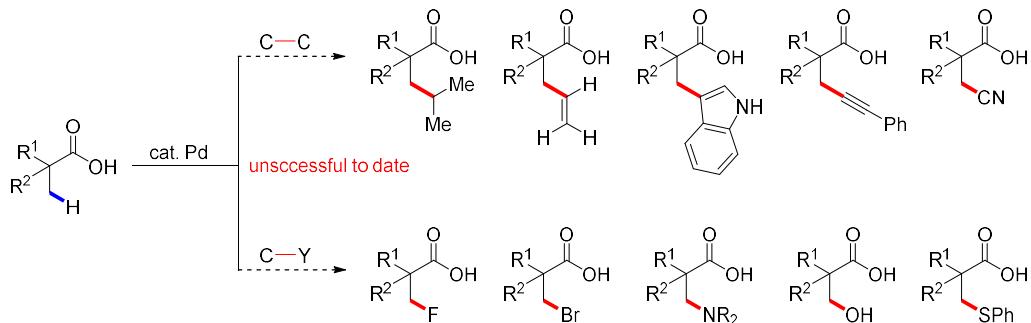
50. "Differentiation and functionalization of remote C-H bonds in adjacent positions"

Yu, J.-Q. et al. *Nature Chemistry* **2020**, *12*, 399.

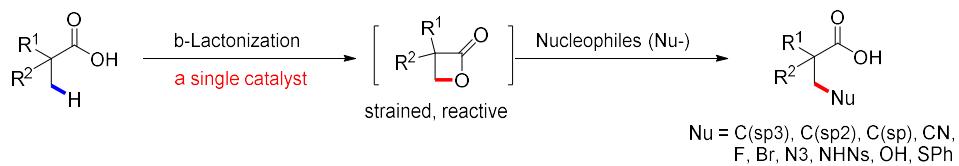


51. "Lactonization as a general route to  $\beta$ -C(sp<sup>3</sup>)-H functionalization" Yu, J.-Q. et al. *Nature*. 2019, 577, 656.

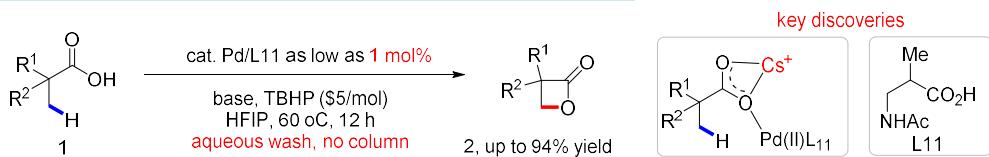
**A Limitations in  $\beta$ -C(sp<sup>3</sup>)-H functionalization of free carboxylic acids**



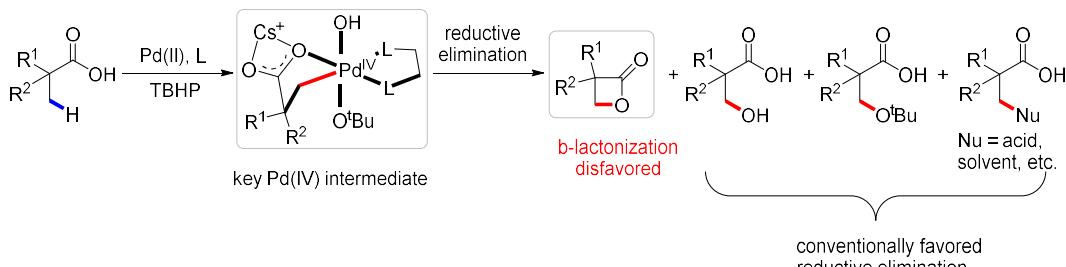
**B One-for-all strategy:  $\beta$ -Lactone as a stepping stone for a myriad of transformations**



**C Ligand-enabled  $\beta$ -C(sp<sup>3</sup>)-H lactonization: practical and scalable**

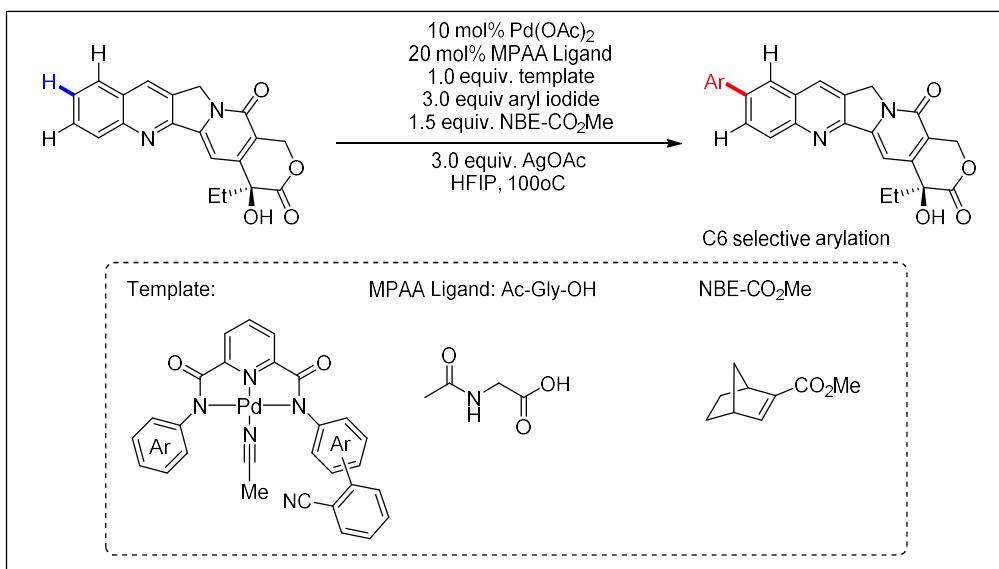


**D Challenges: multiple reductive elimination pathways of Pd(IV) centers**

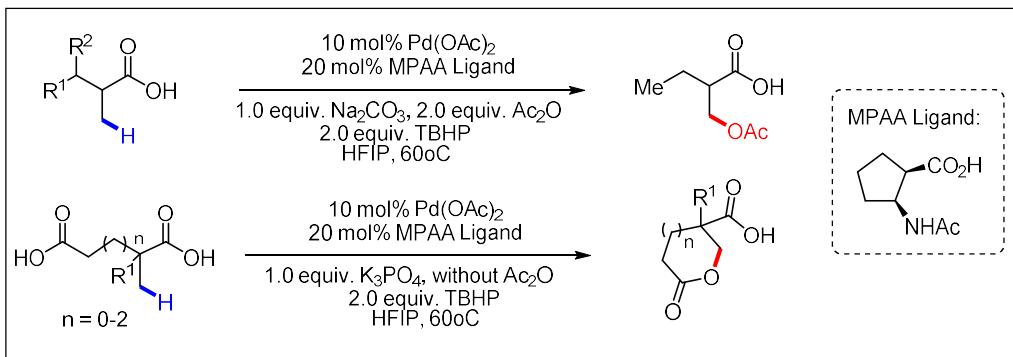


52. "Differentiation and functionalization of remote C-H bonds in adjacent positions"

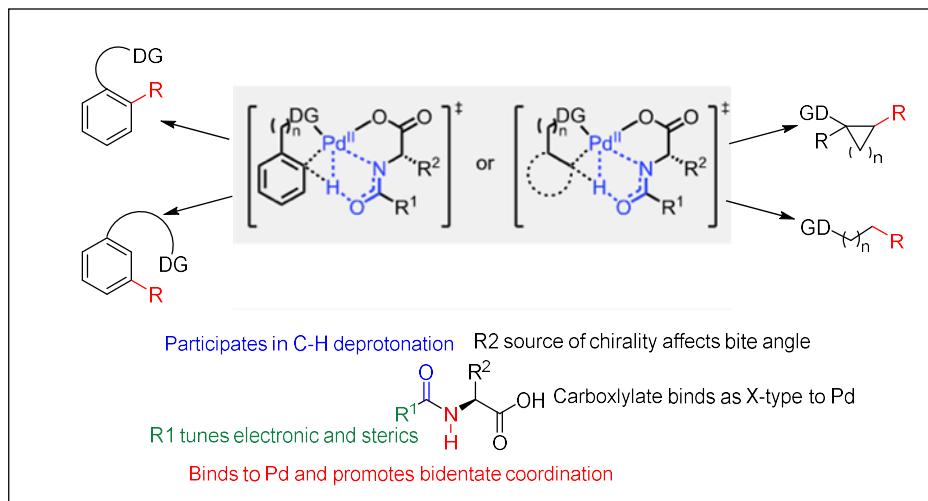
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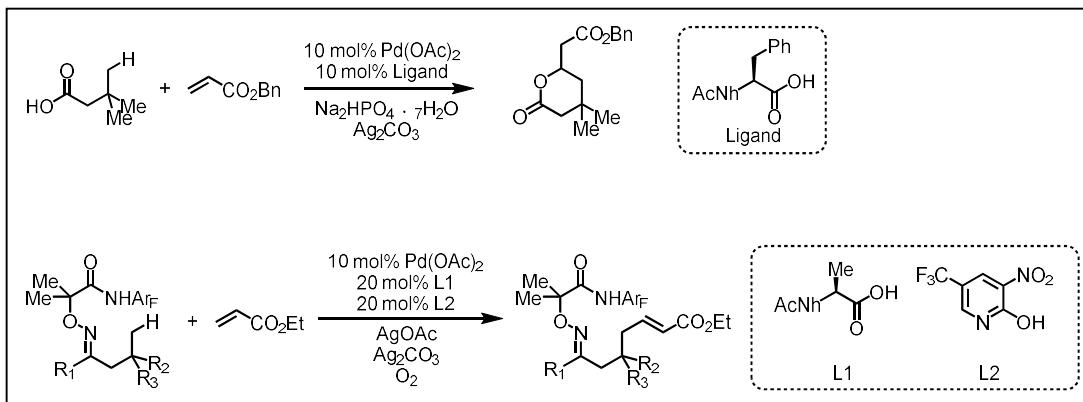
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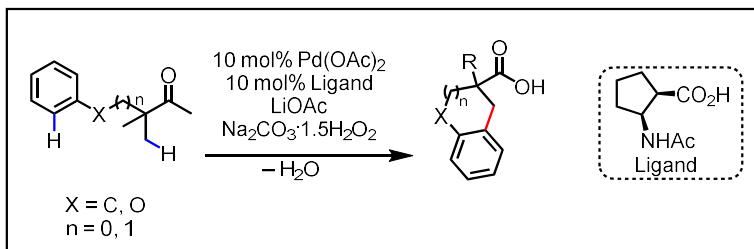
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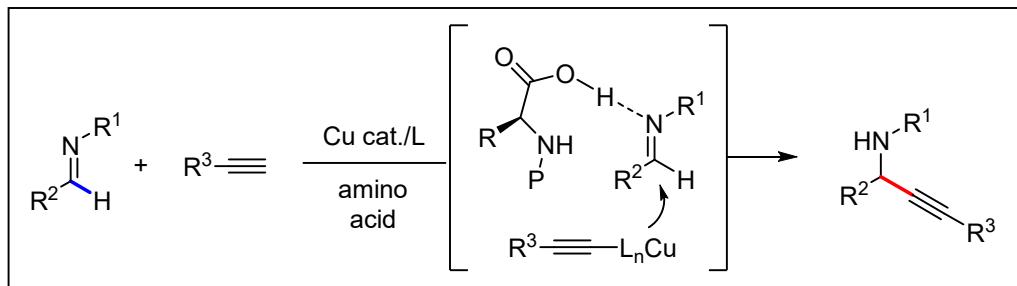


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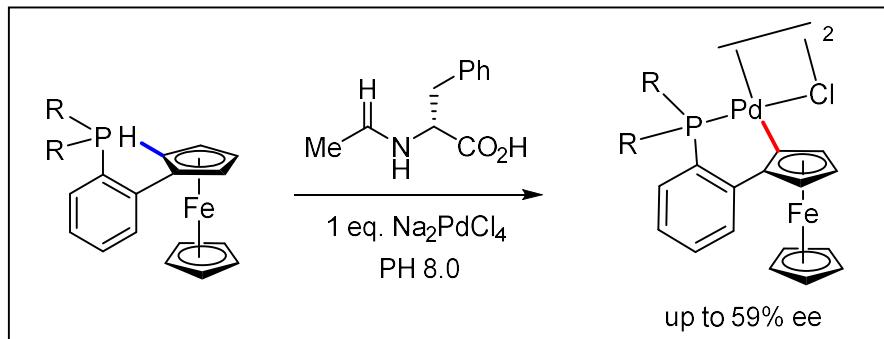


## Other Groups

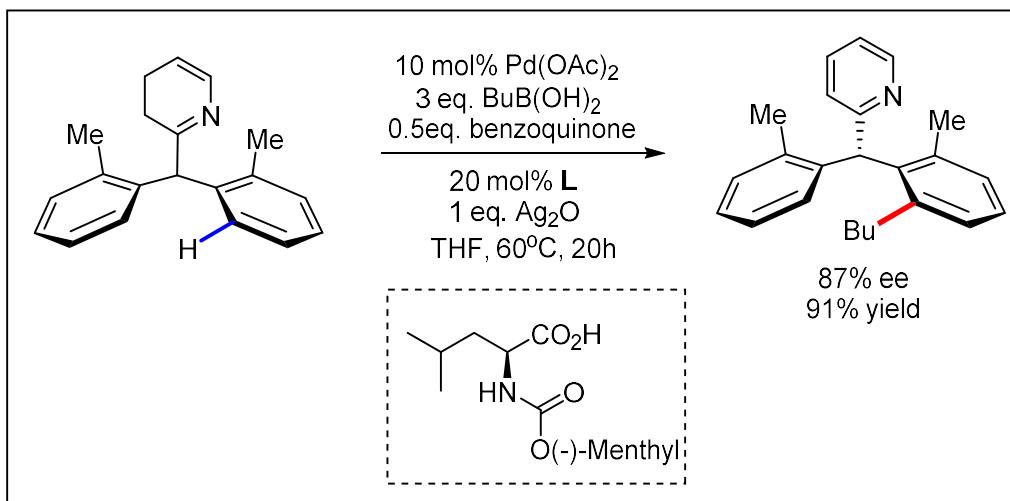
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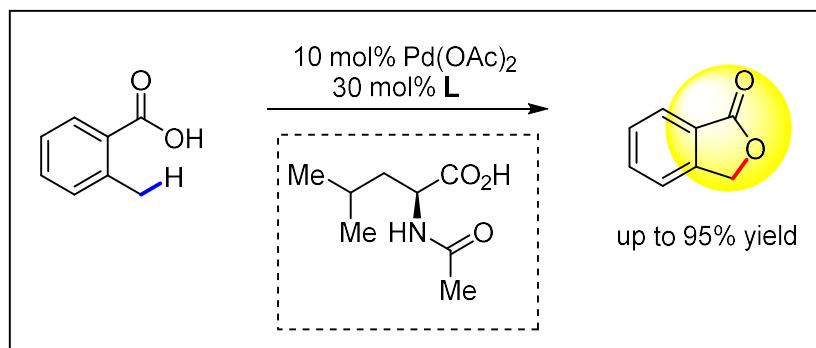
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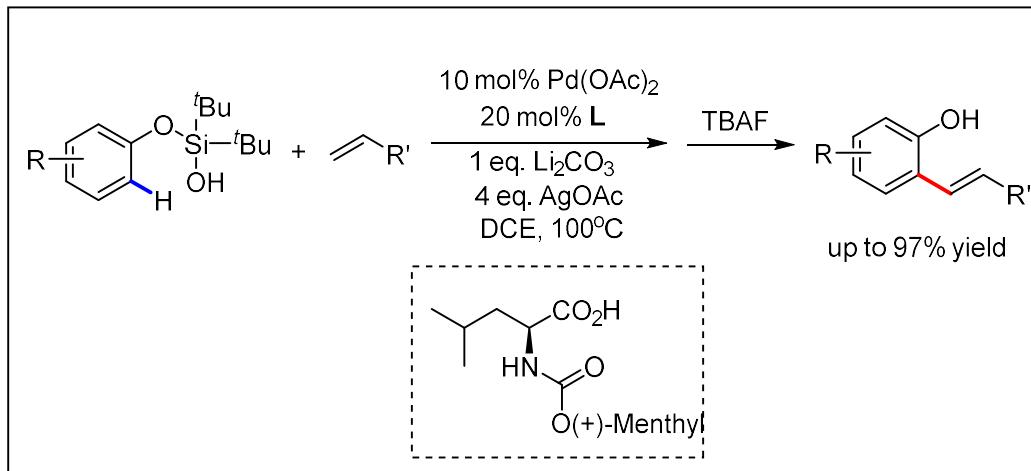
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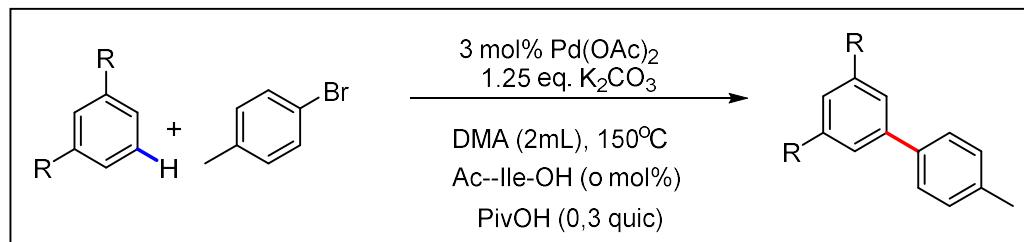
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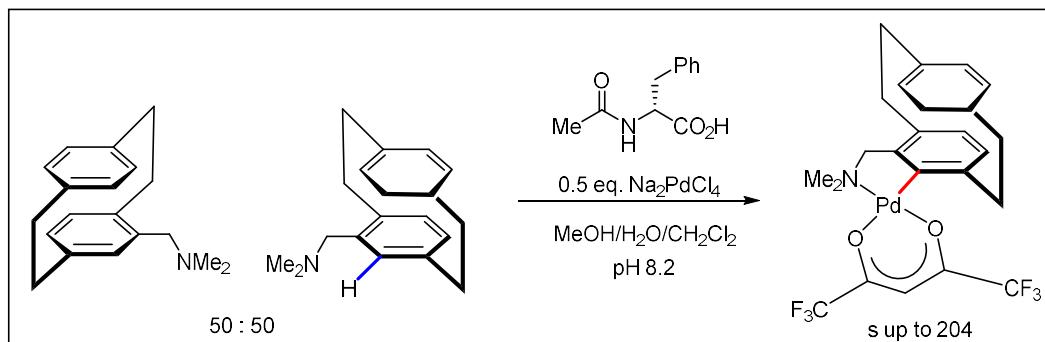
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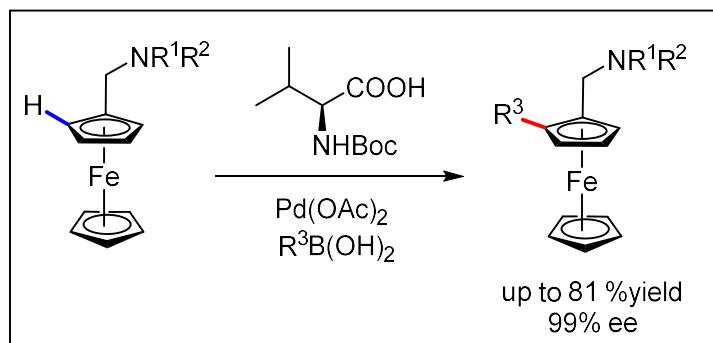
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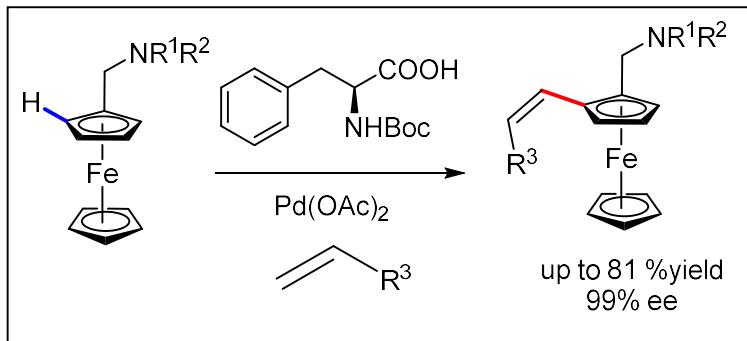
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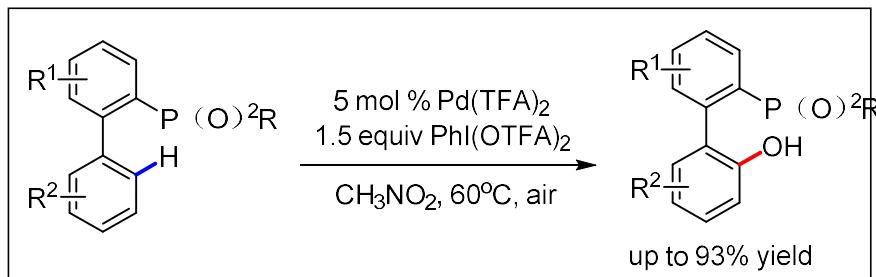
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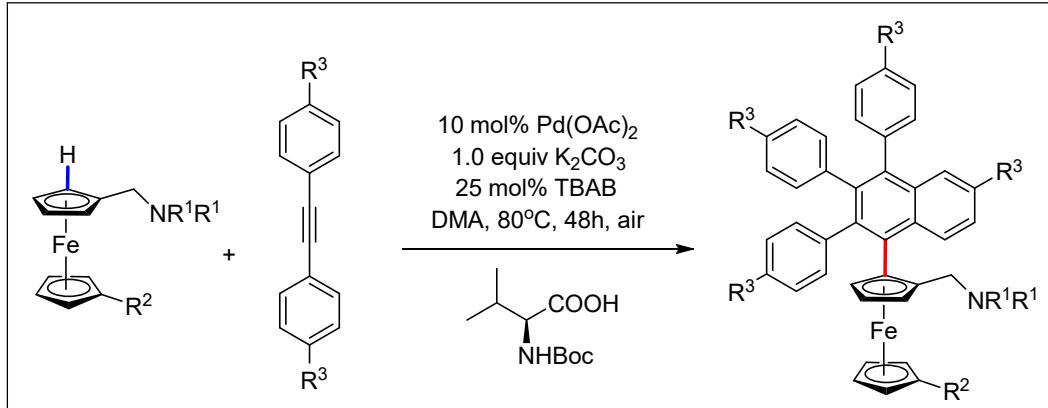
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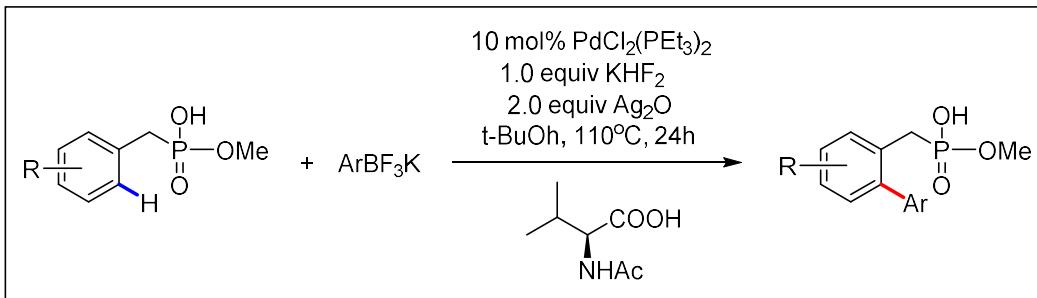
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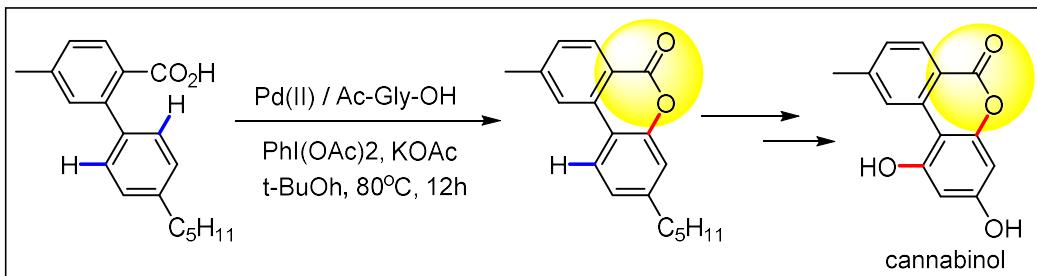
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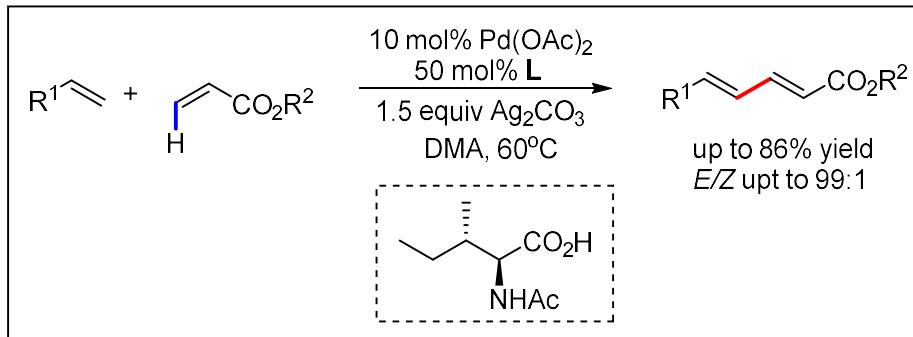
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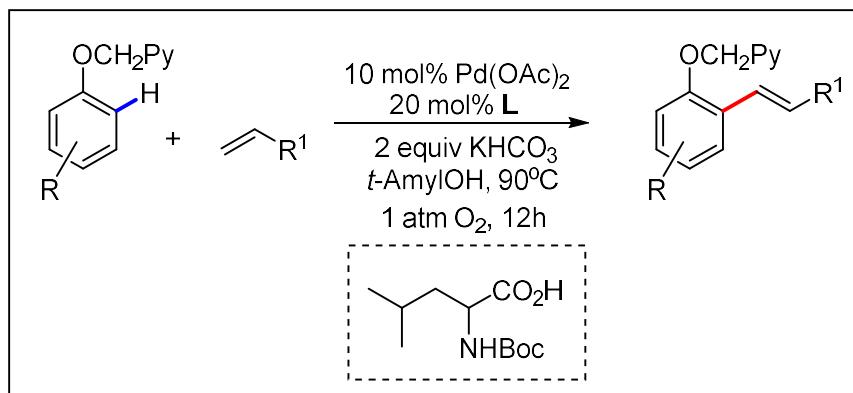
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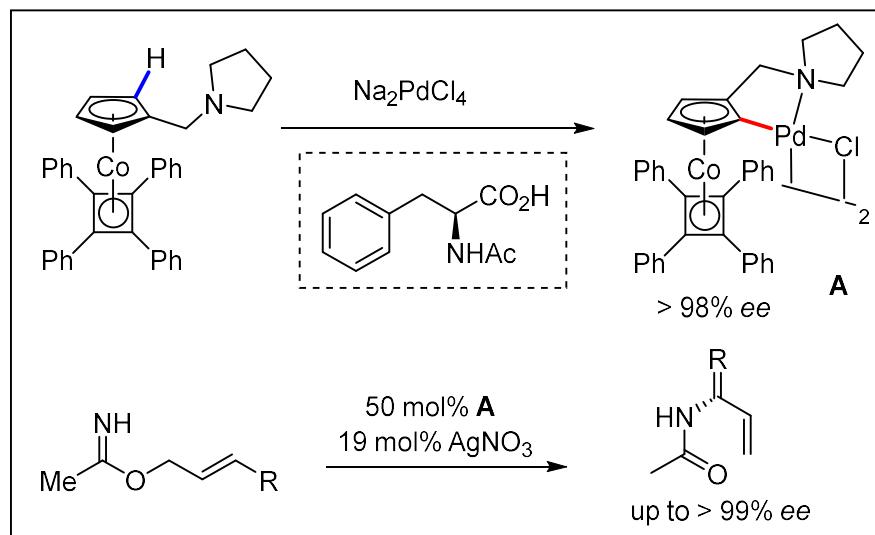
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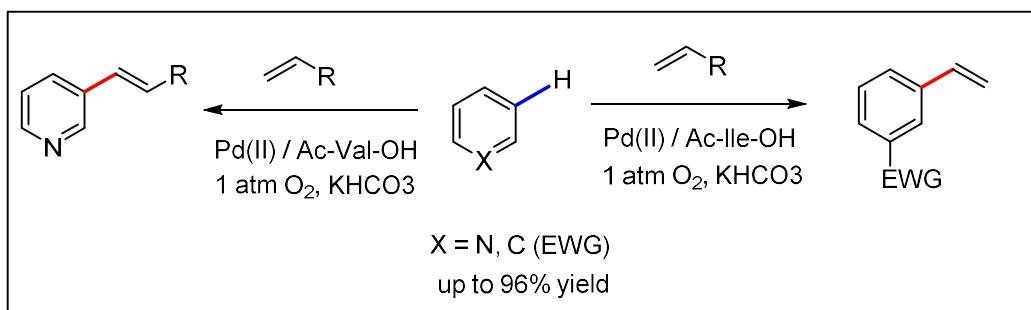
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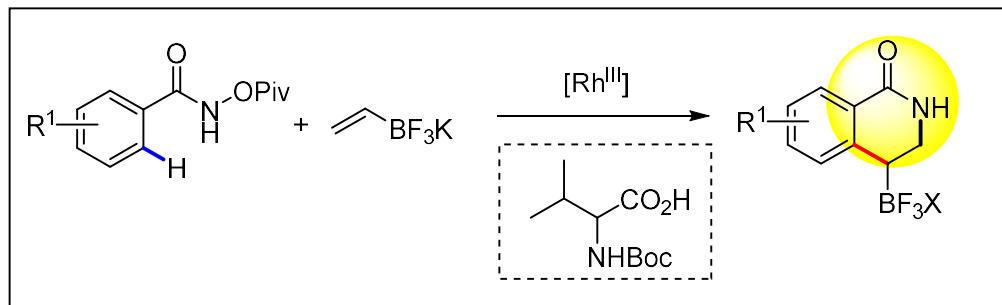
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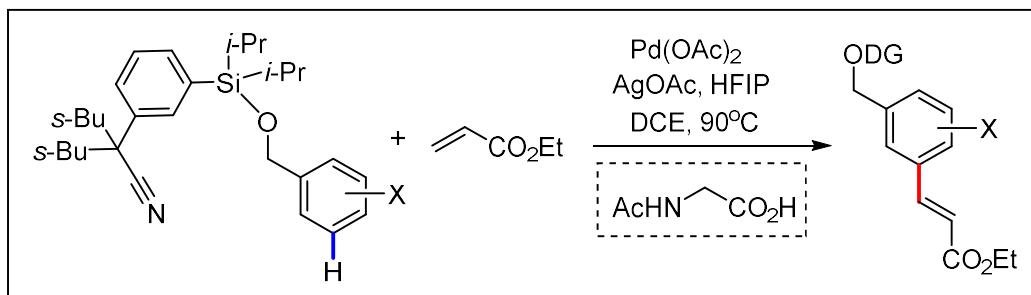
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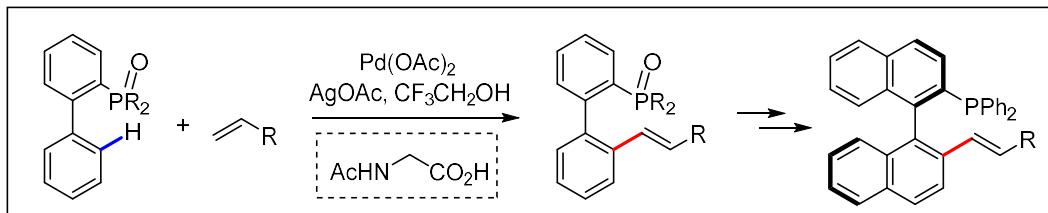
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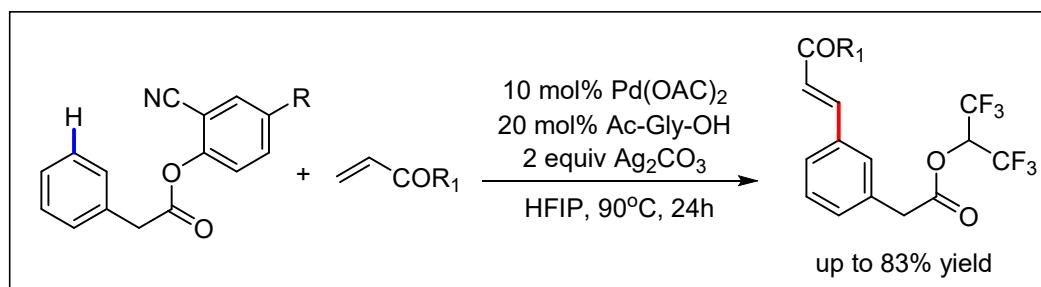
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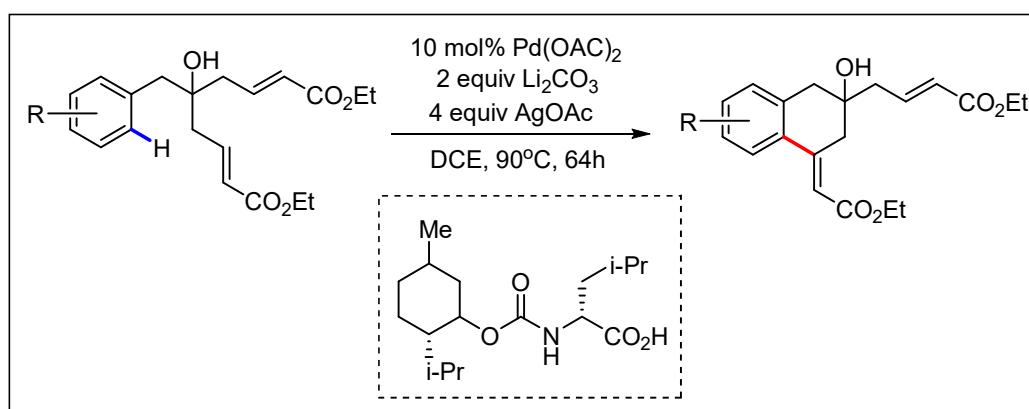
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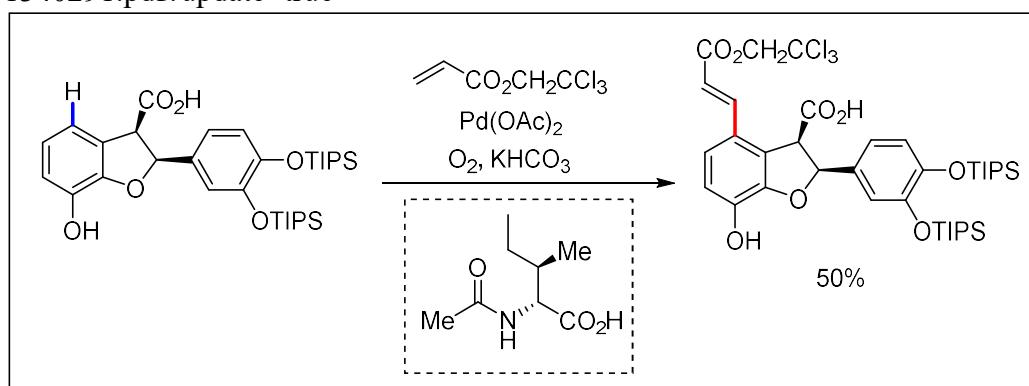
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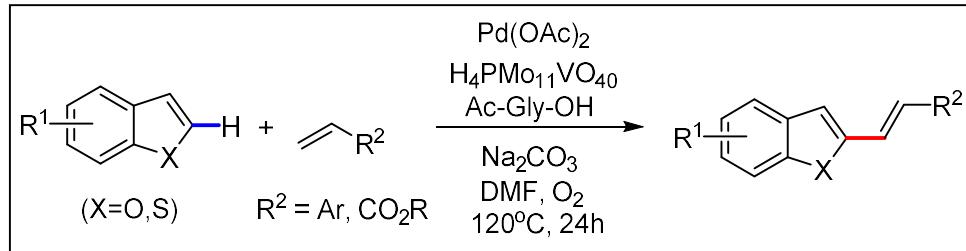
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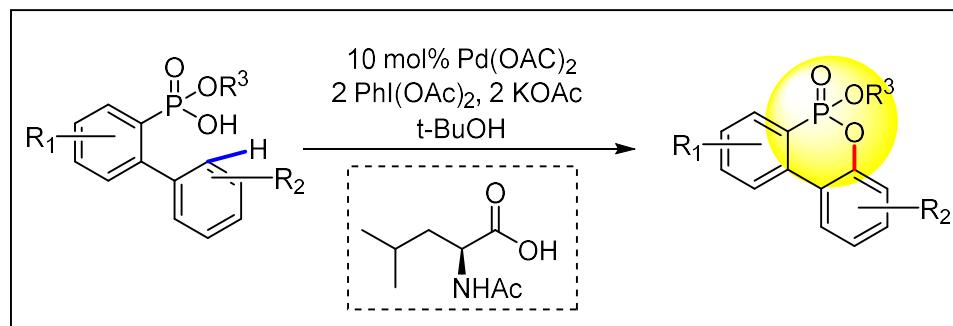
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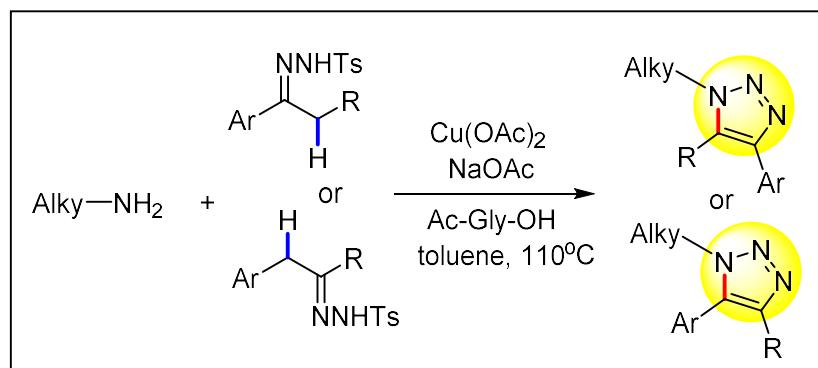
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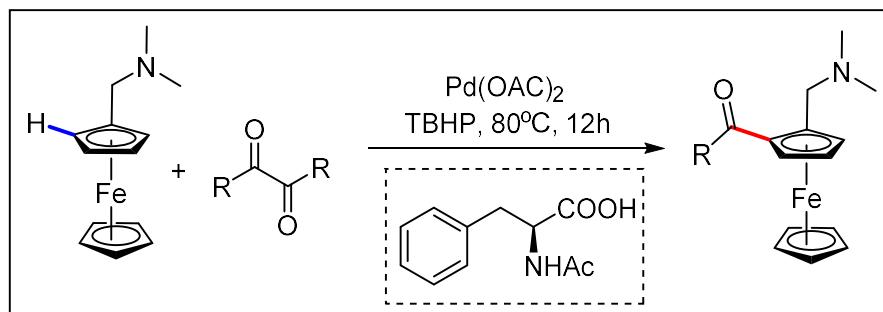
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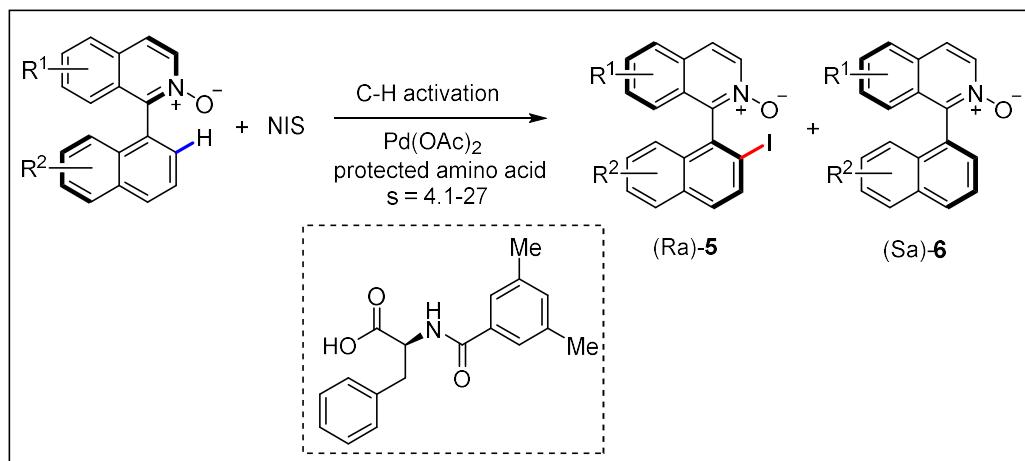
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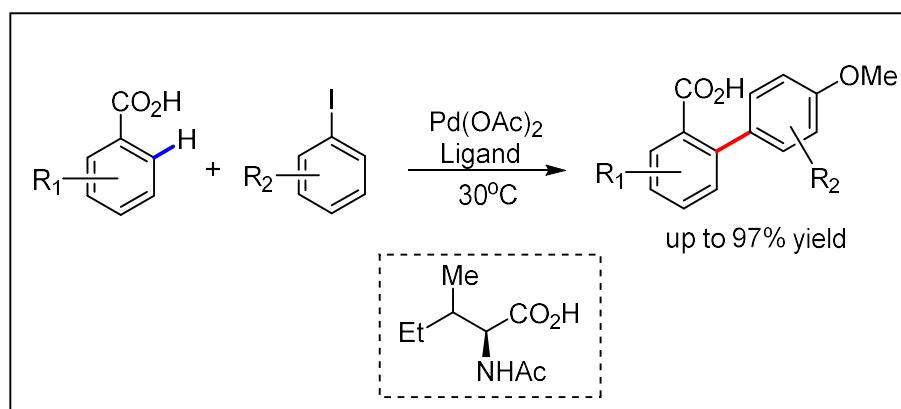
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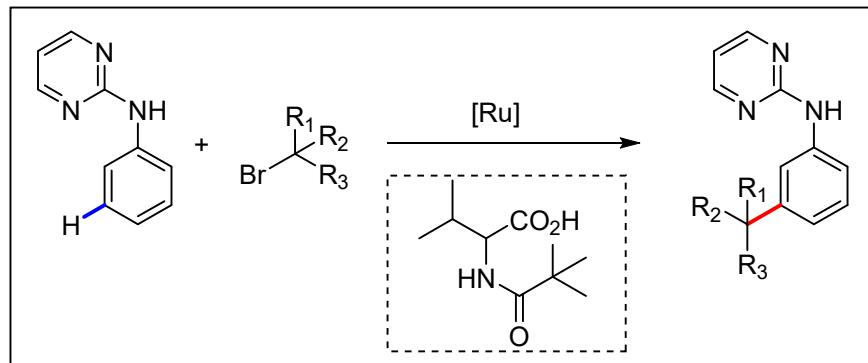
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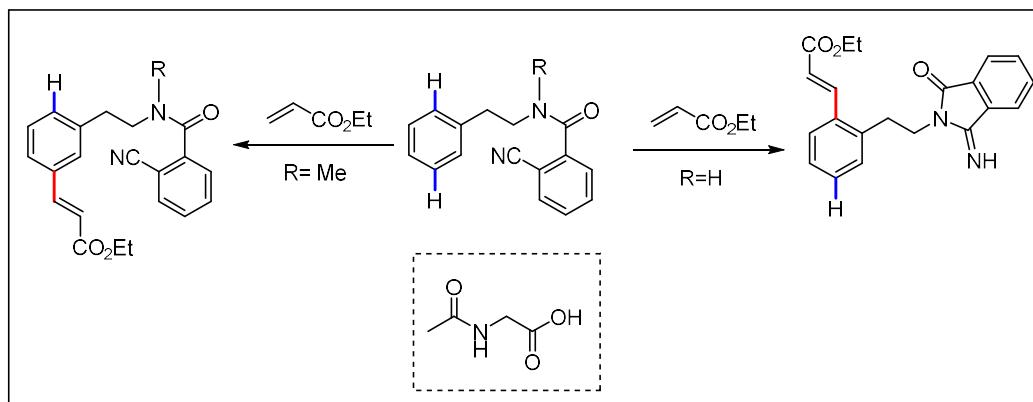
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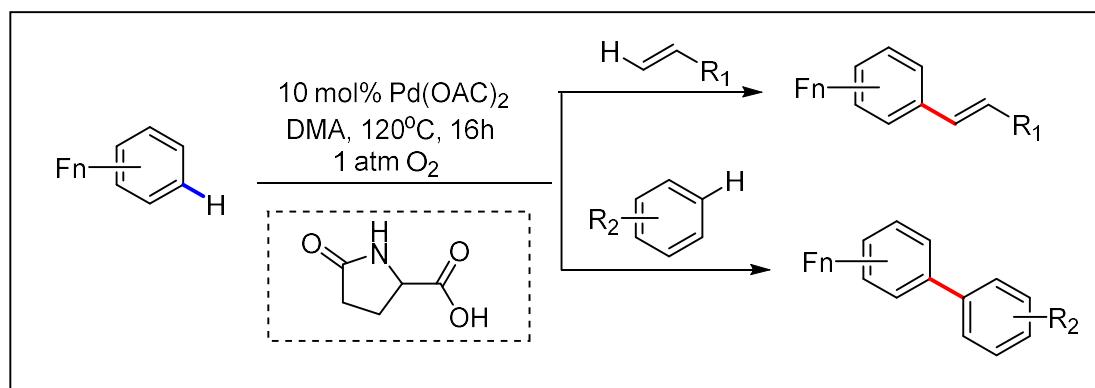
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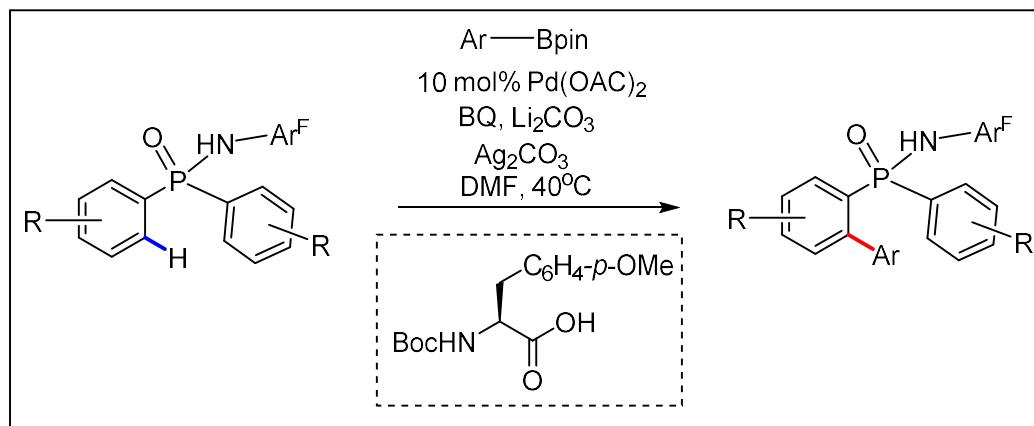
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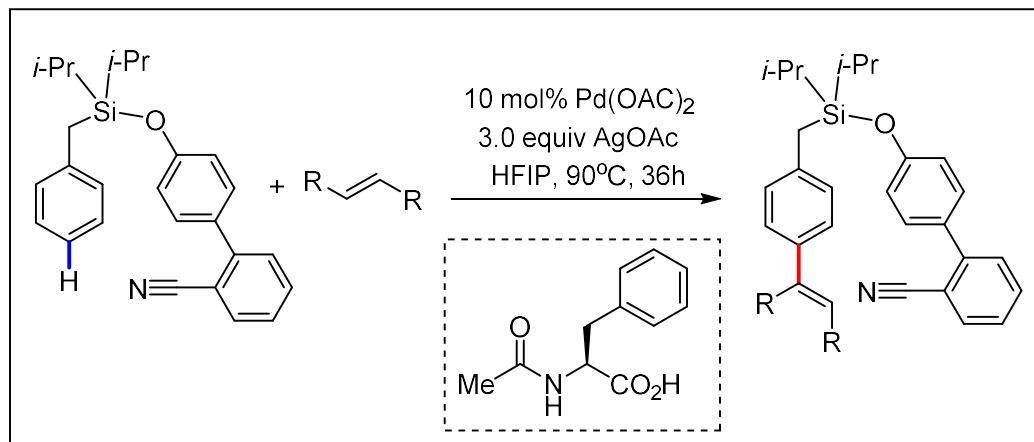
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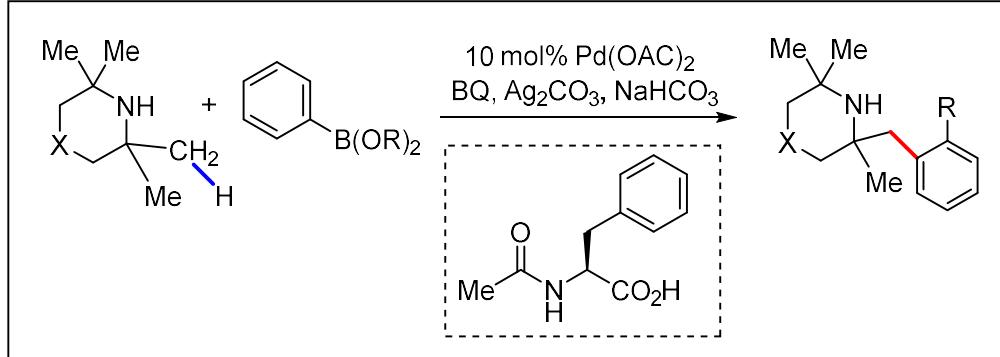
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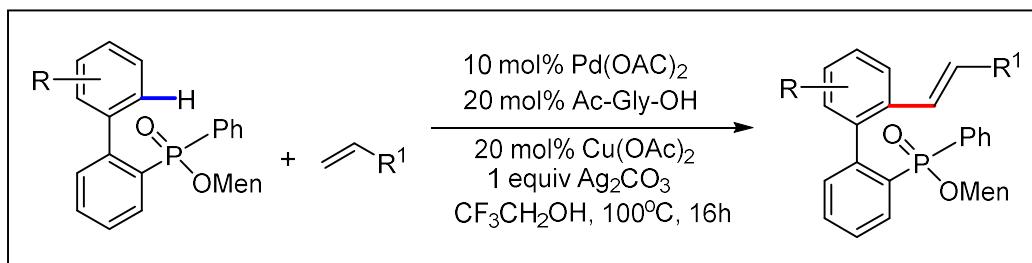
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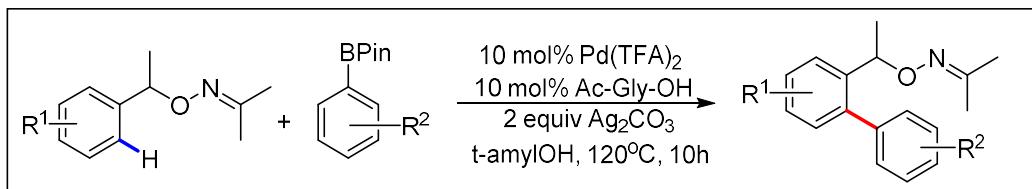
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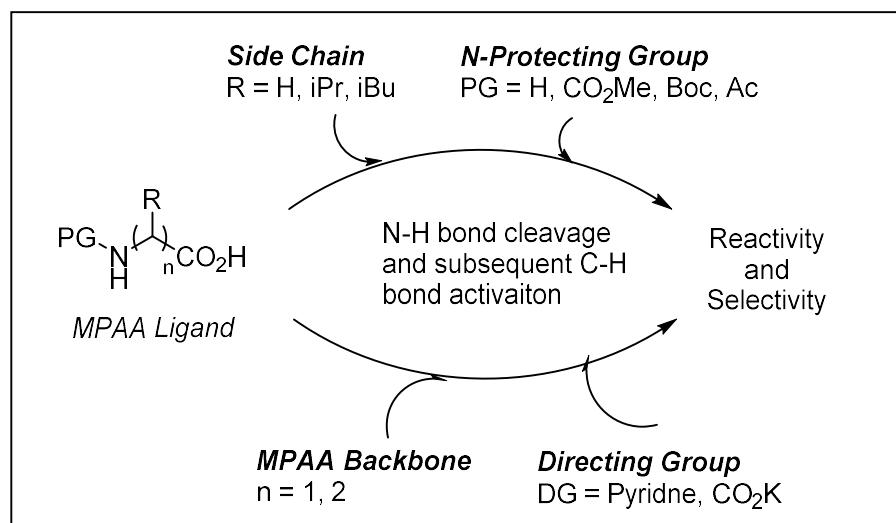
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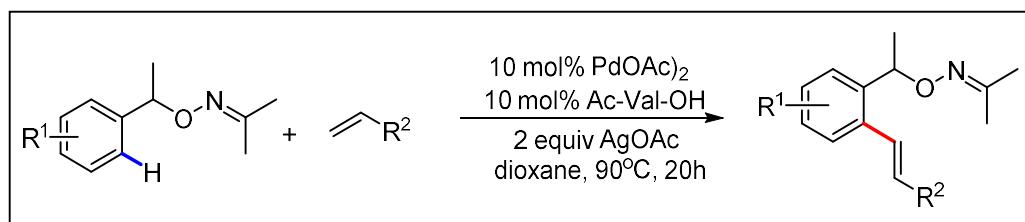
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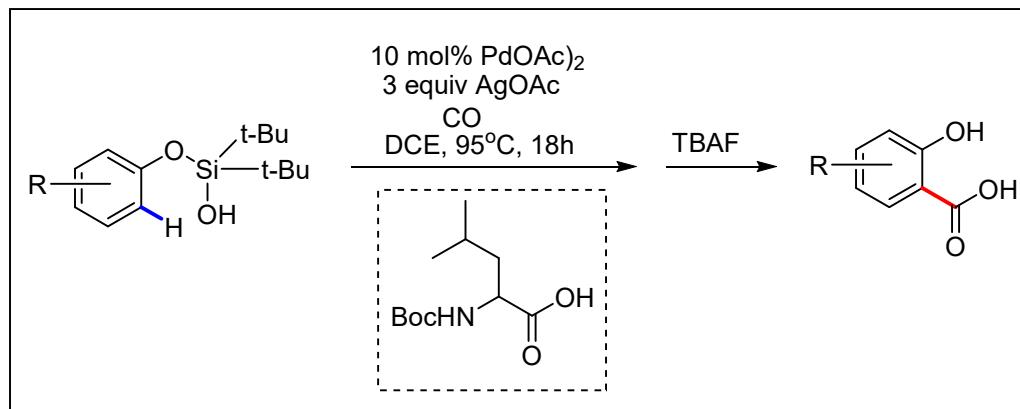
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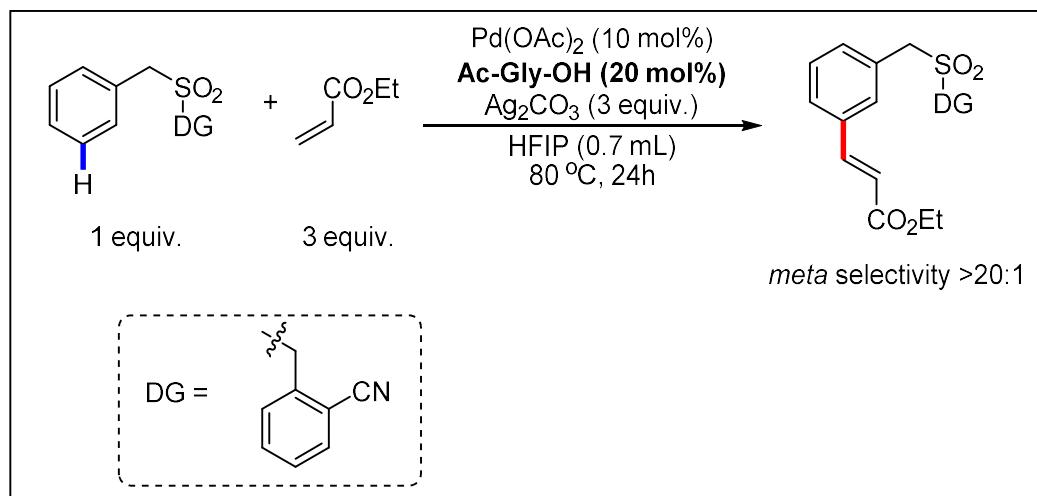
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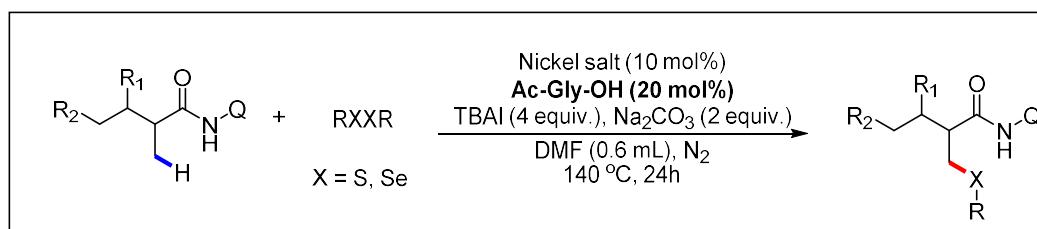
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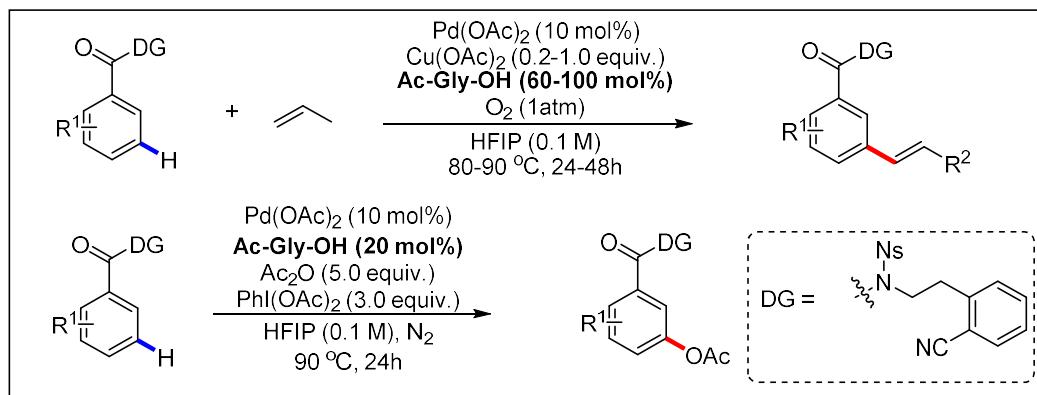
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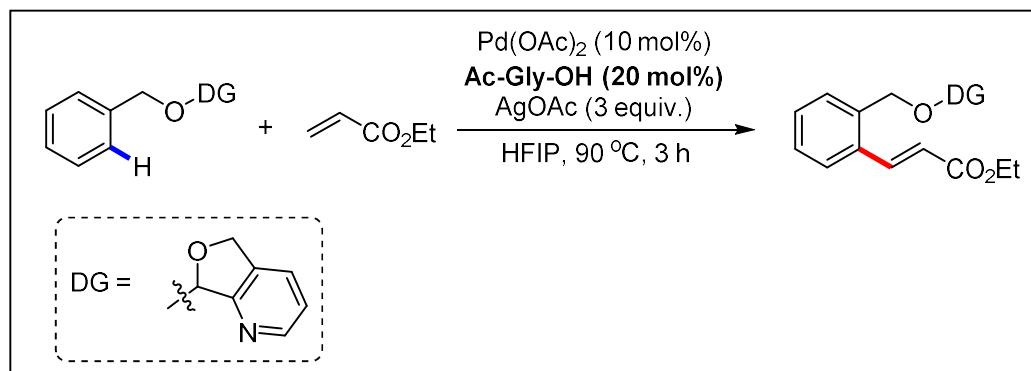
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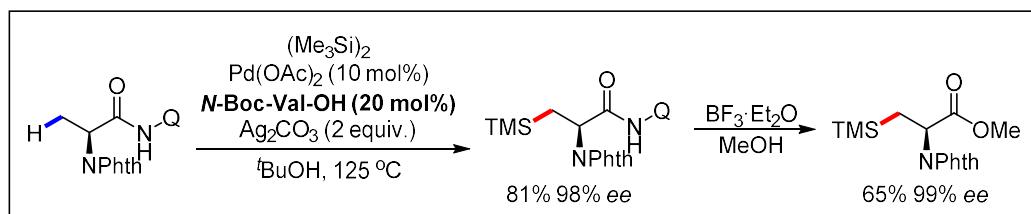
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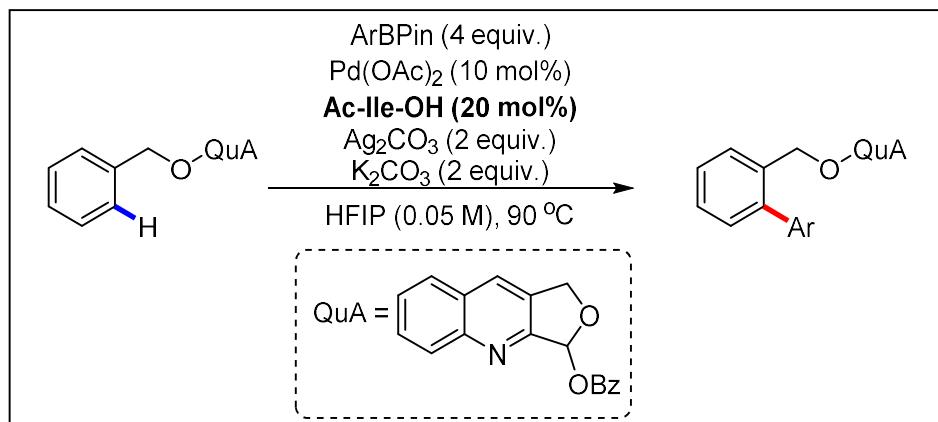
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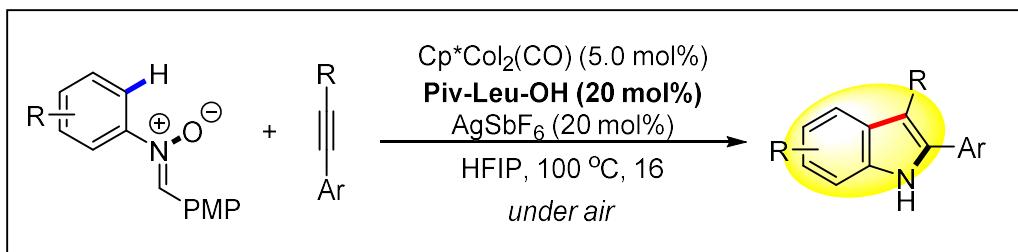
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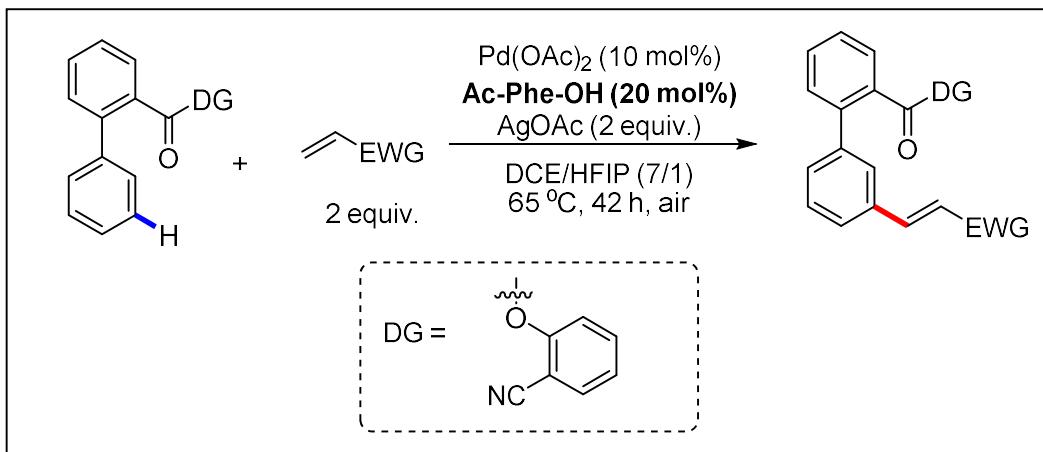
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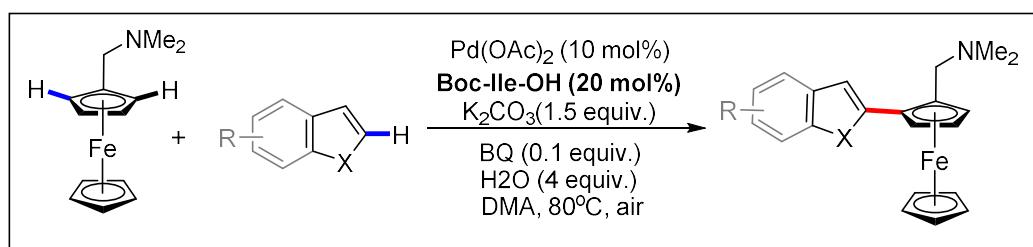
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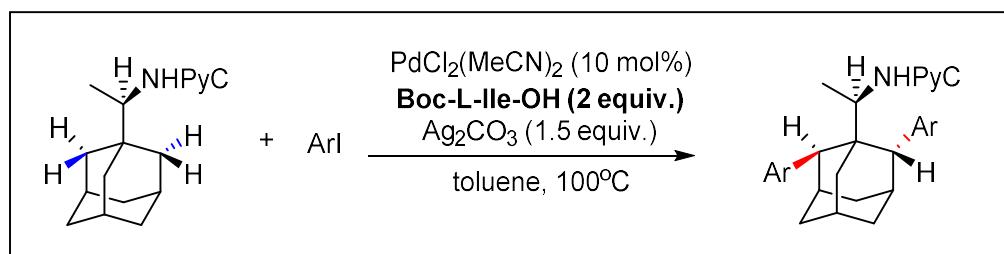
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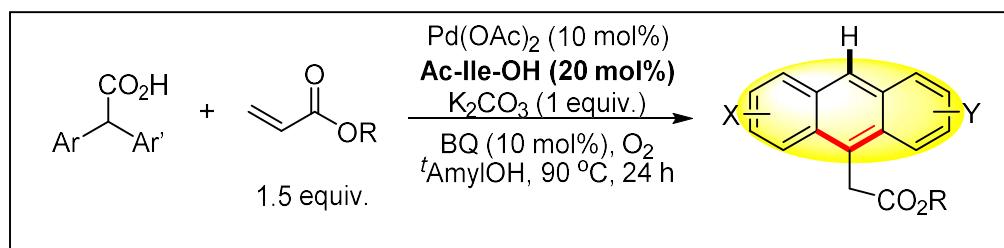
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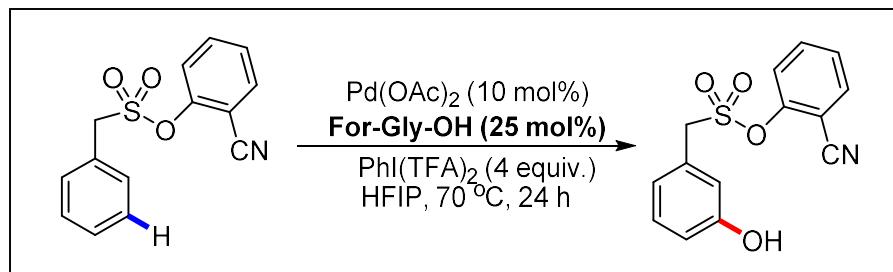
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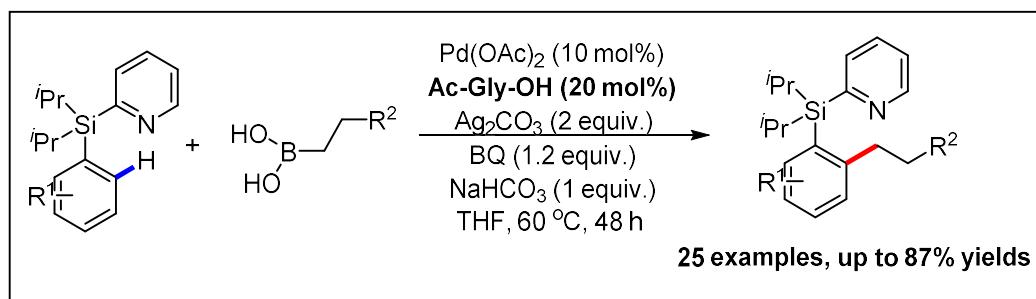
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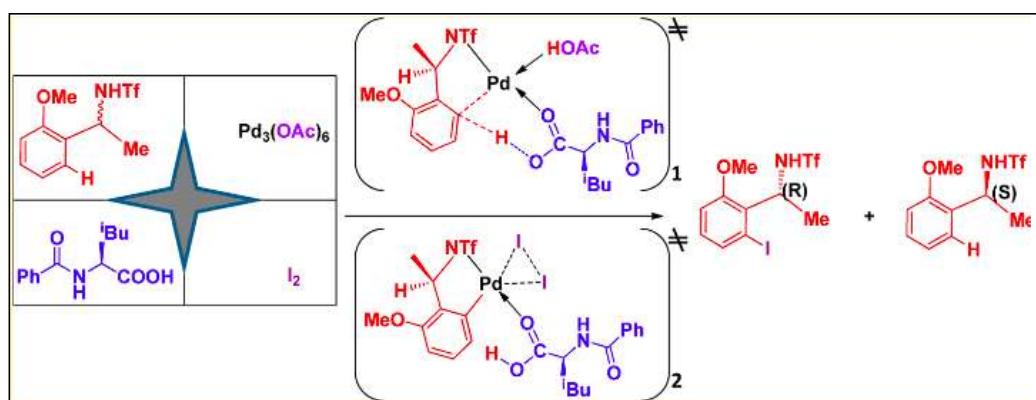
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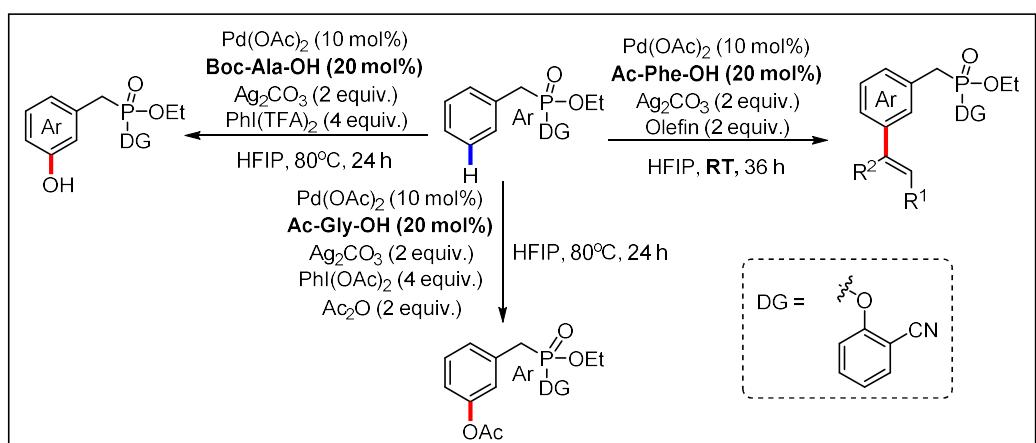
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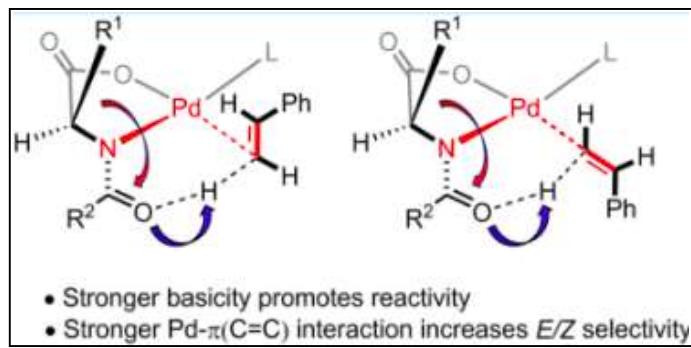
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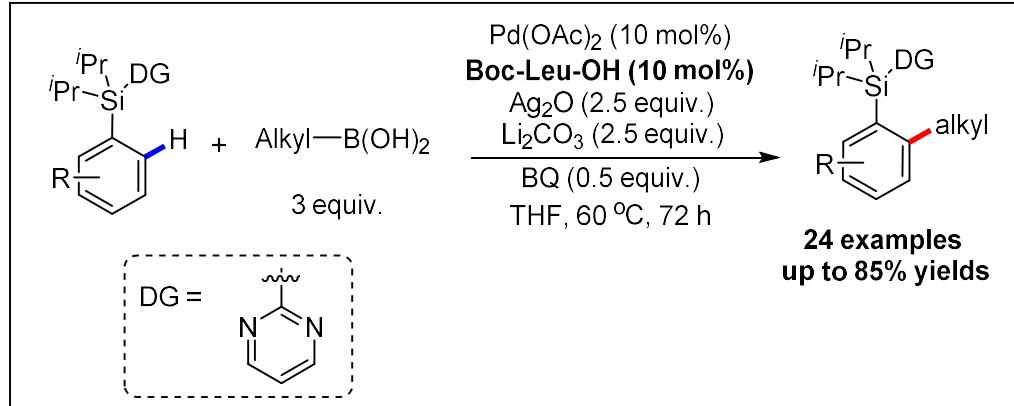


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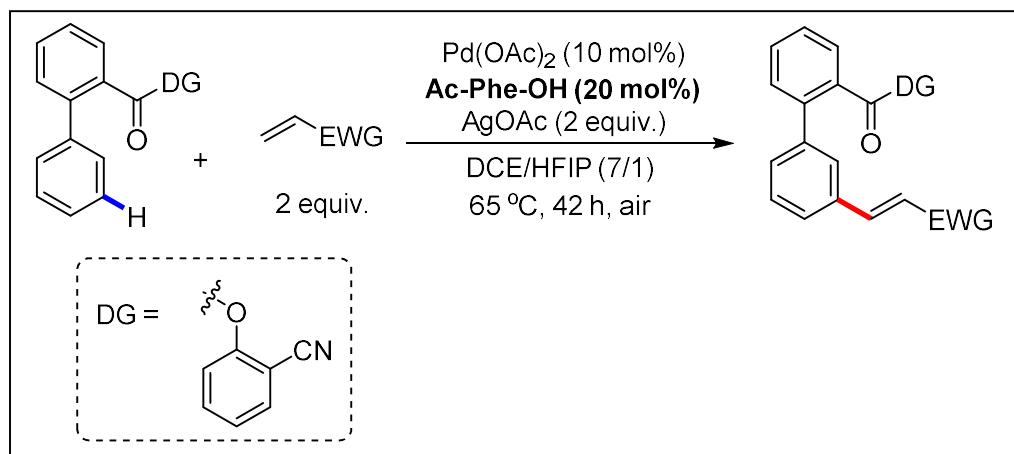
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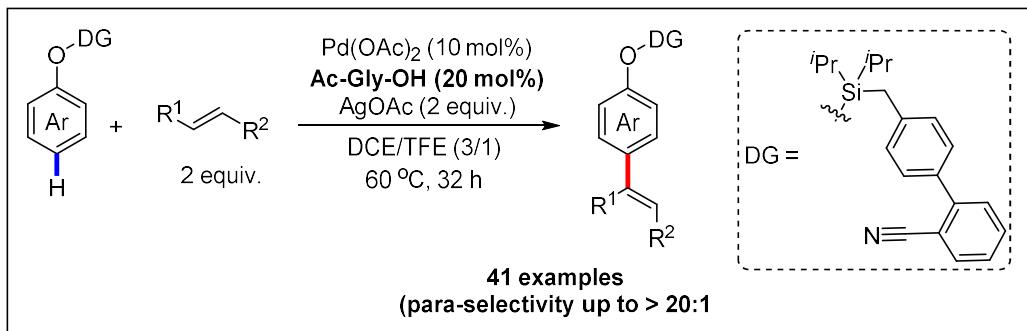
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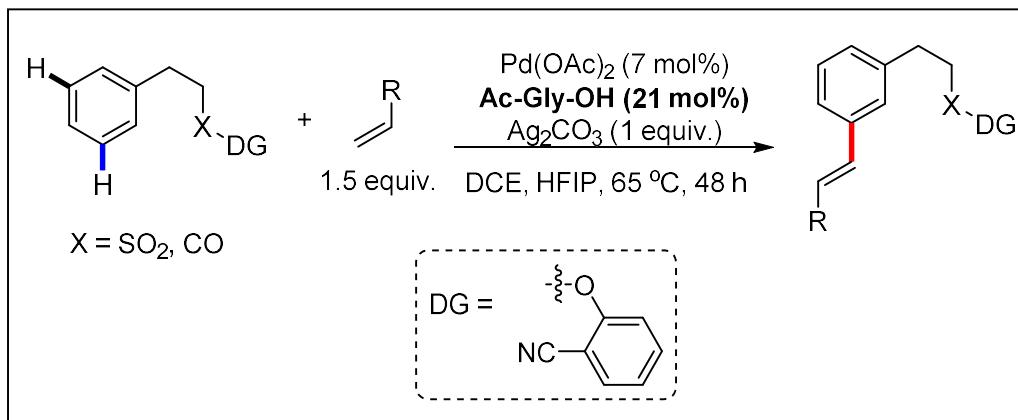
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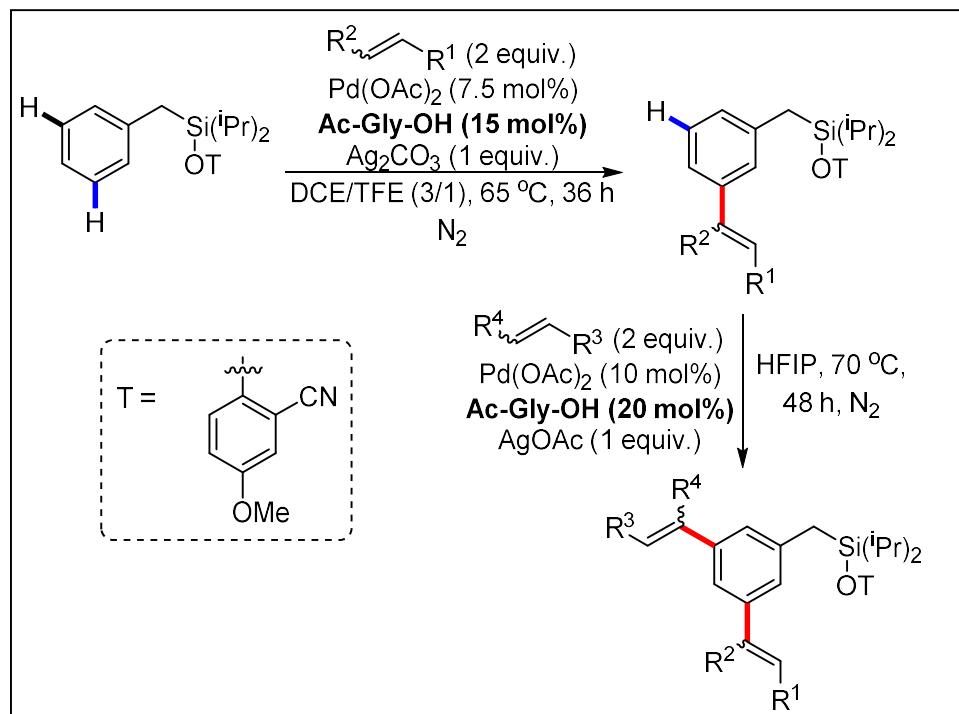
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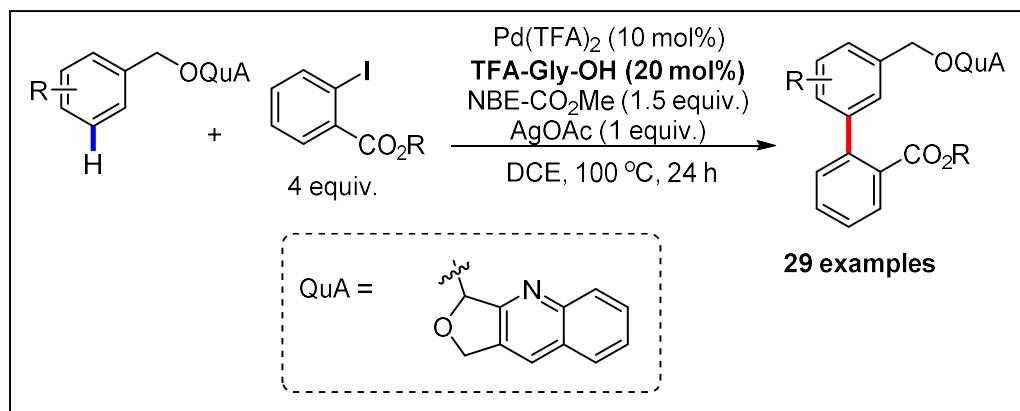


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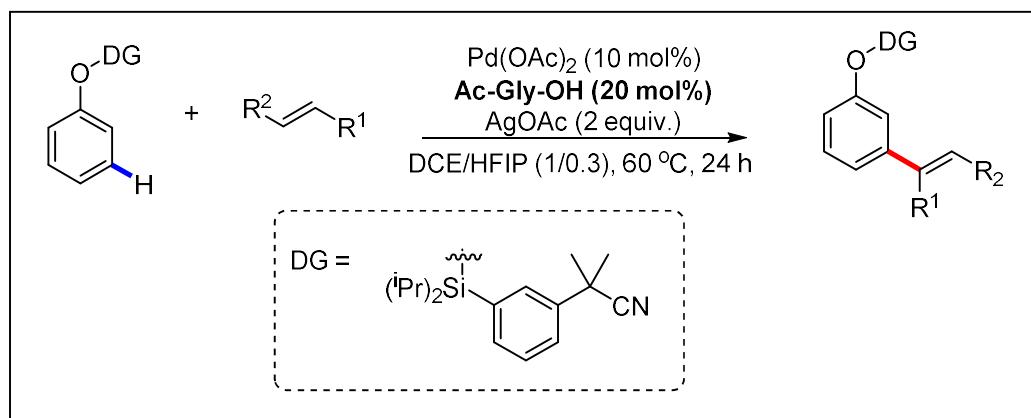
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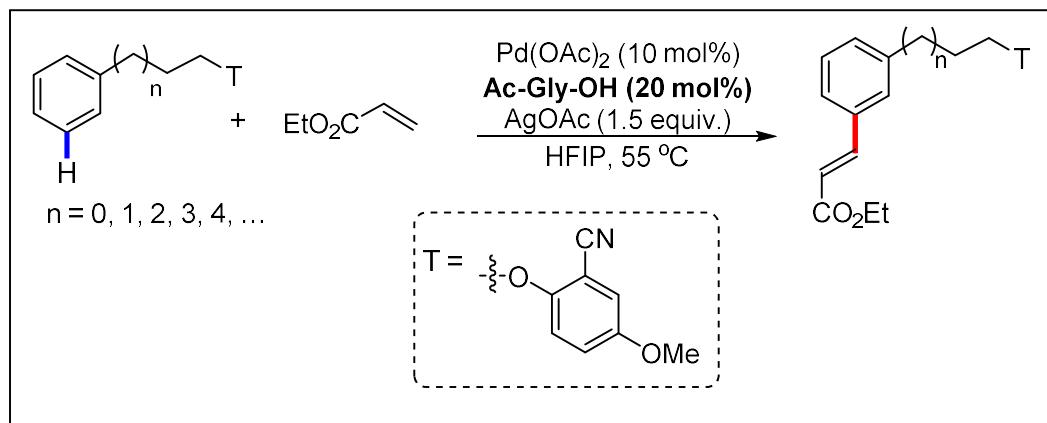


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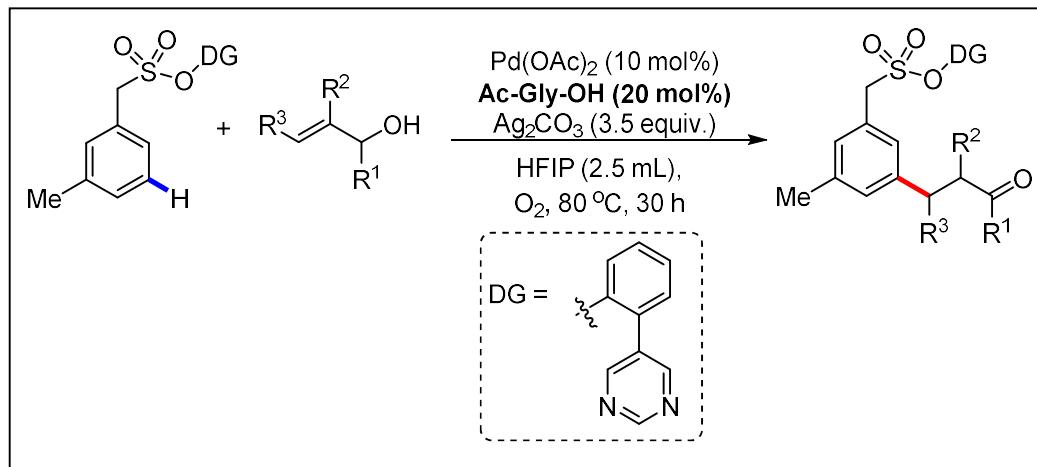
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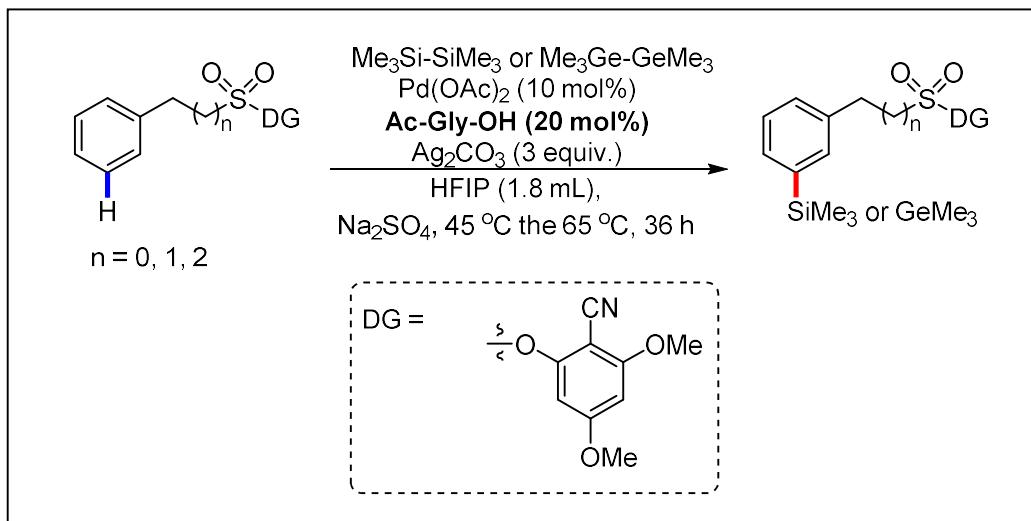
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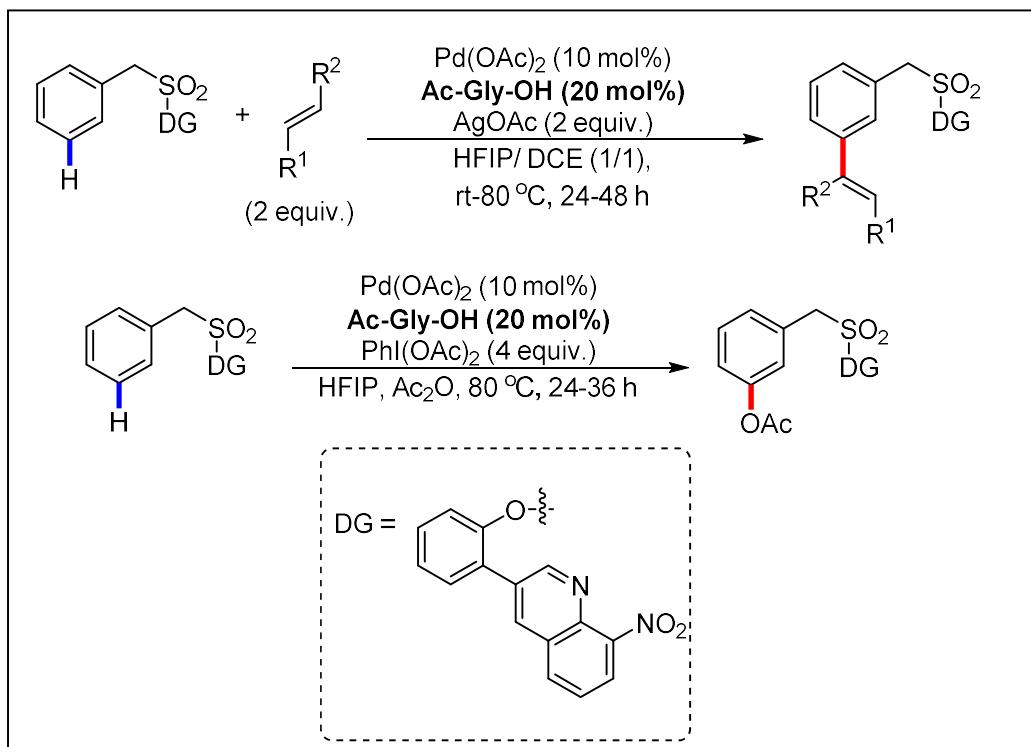
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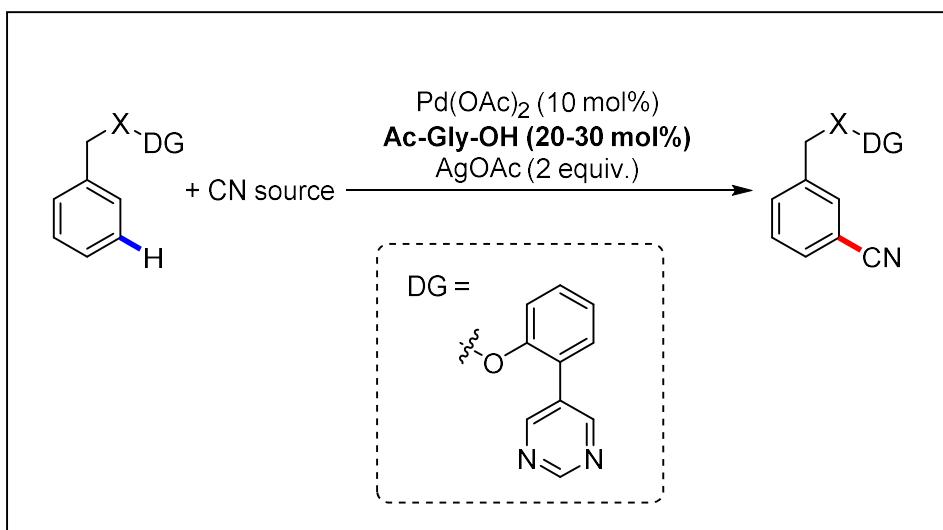
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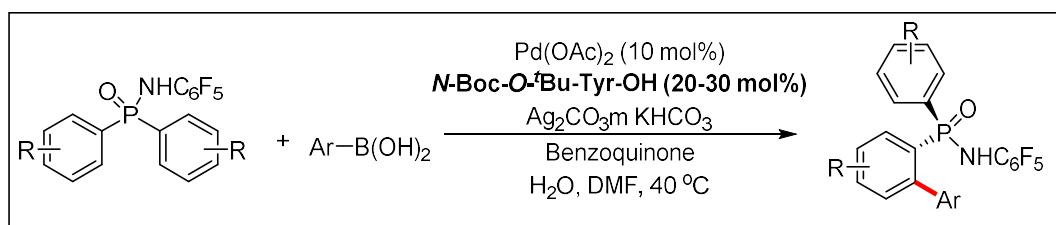
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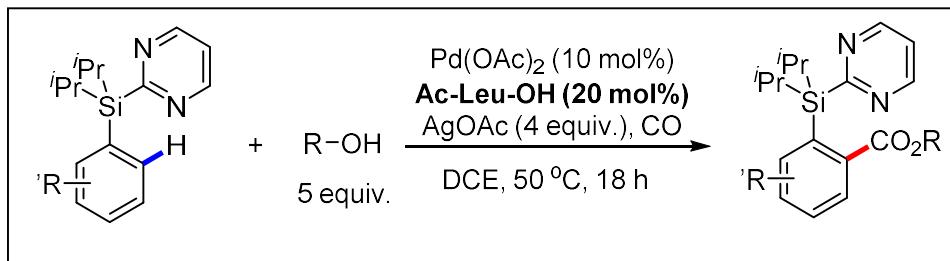
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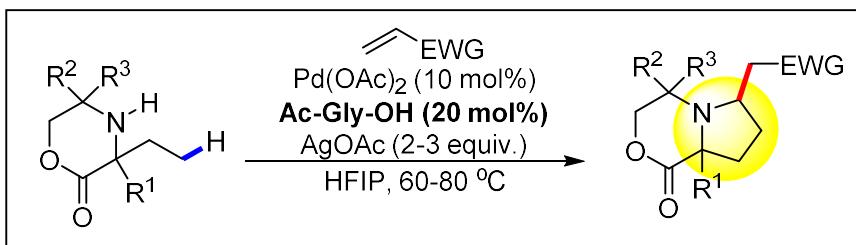
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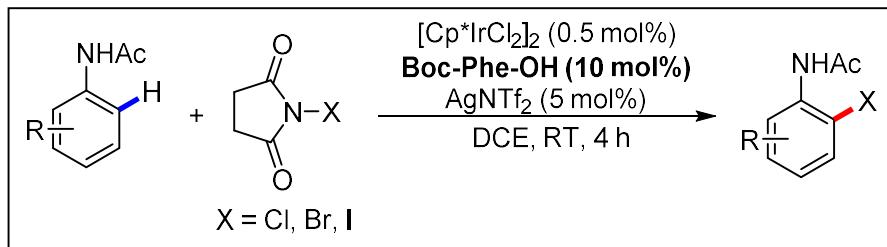
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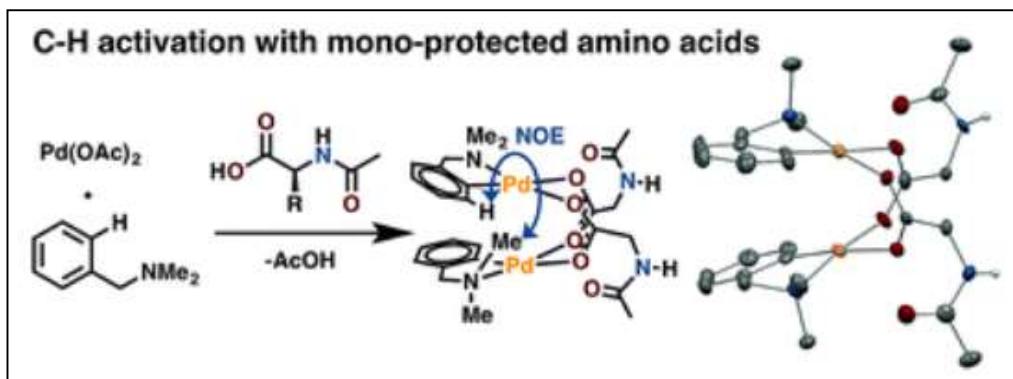
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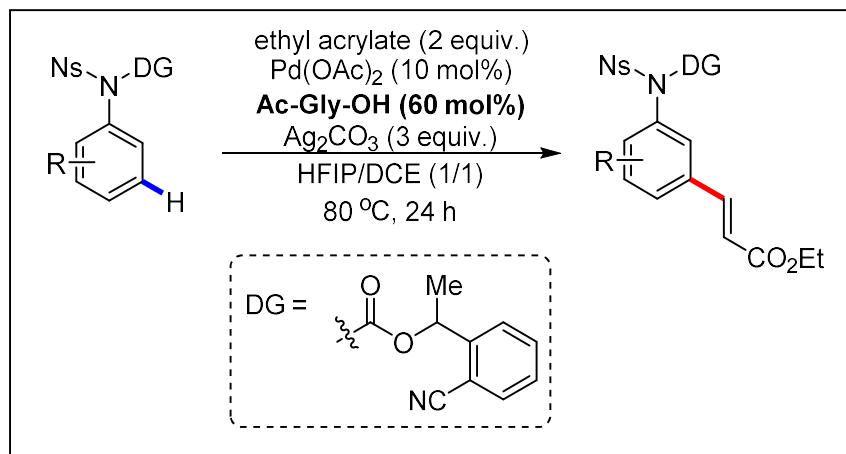
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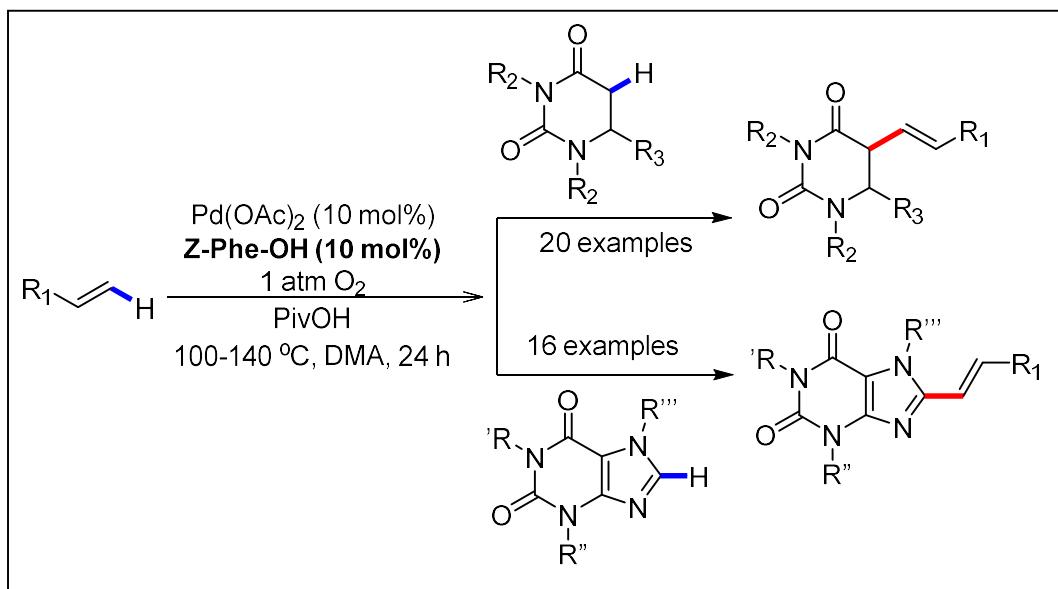
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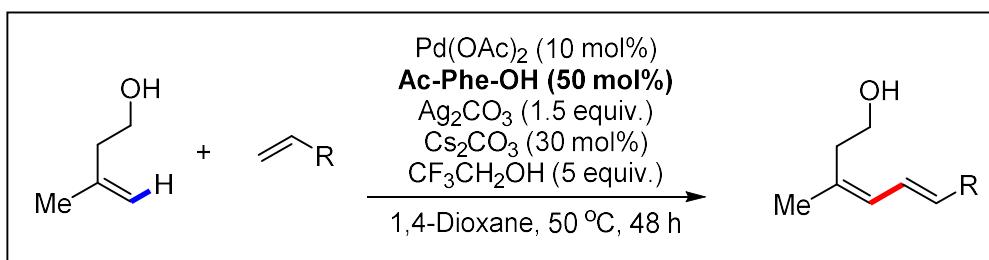
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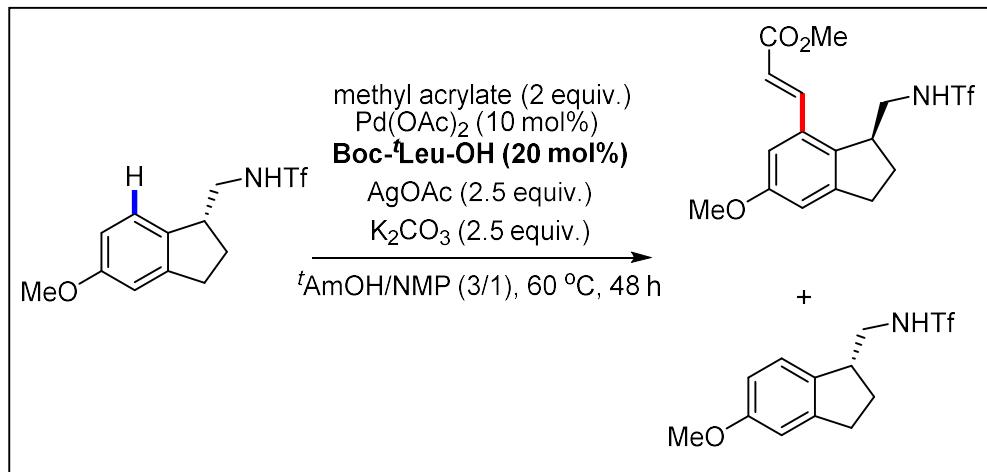
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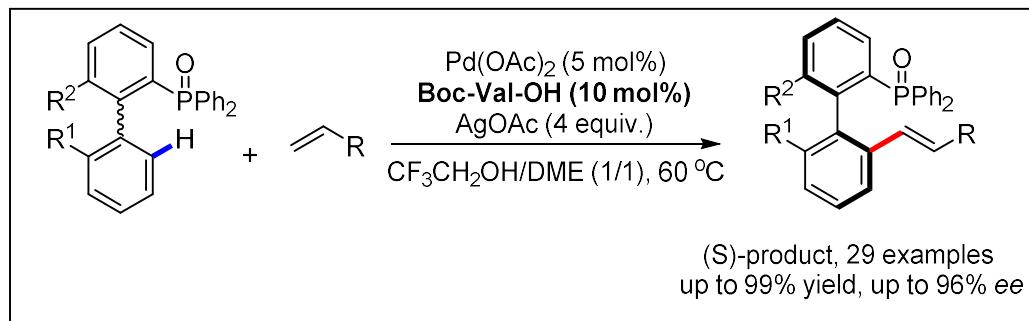
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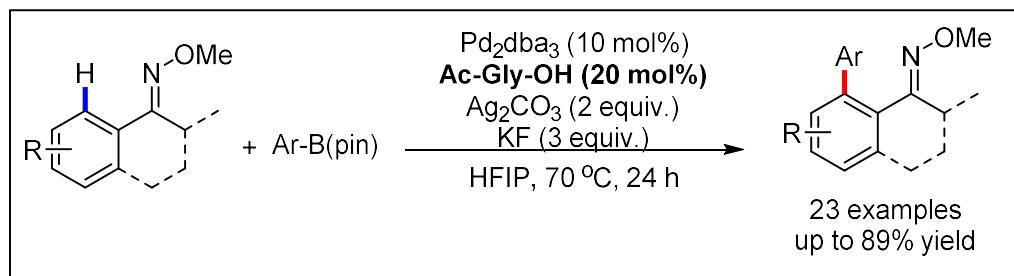
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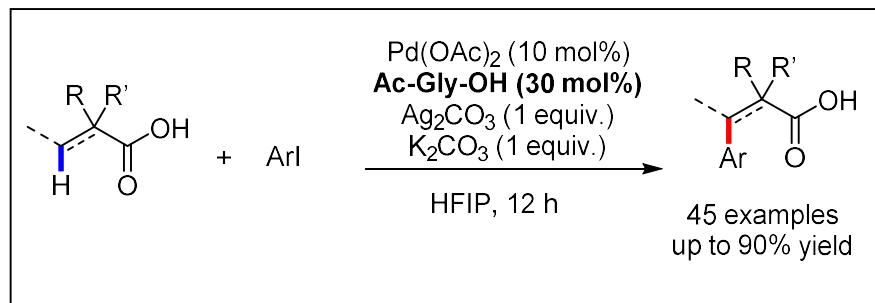
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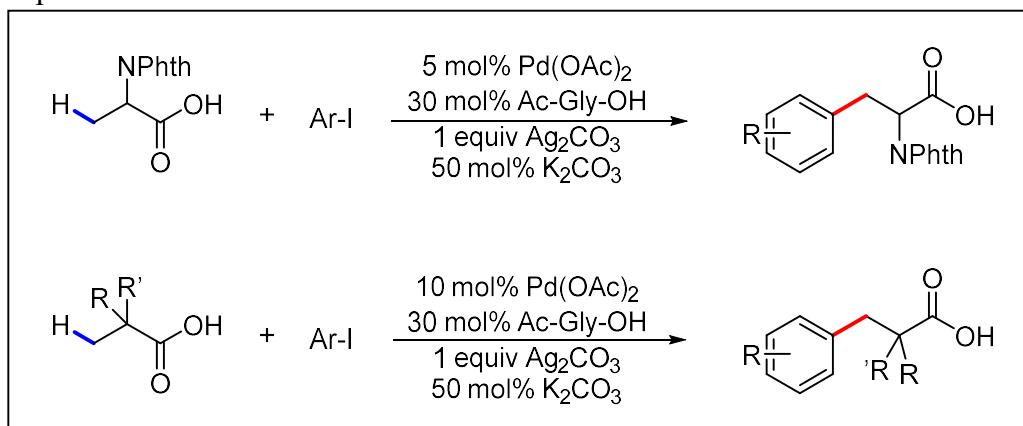
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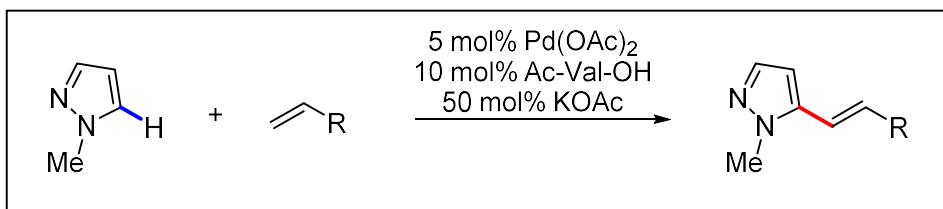
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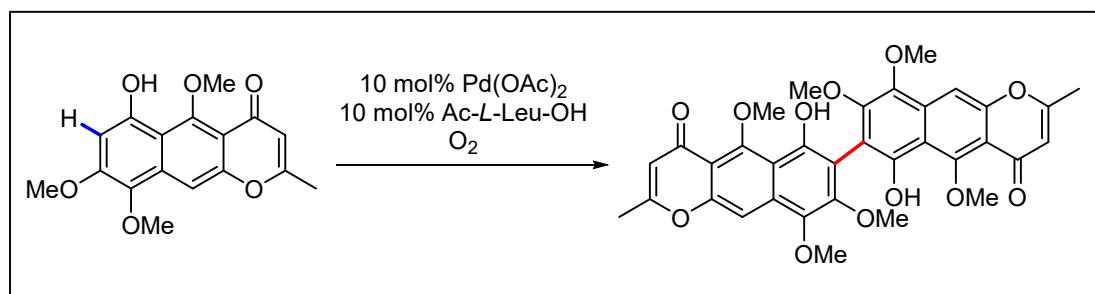
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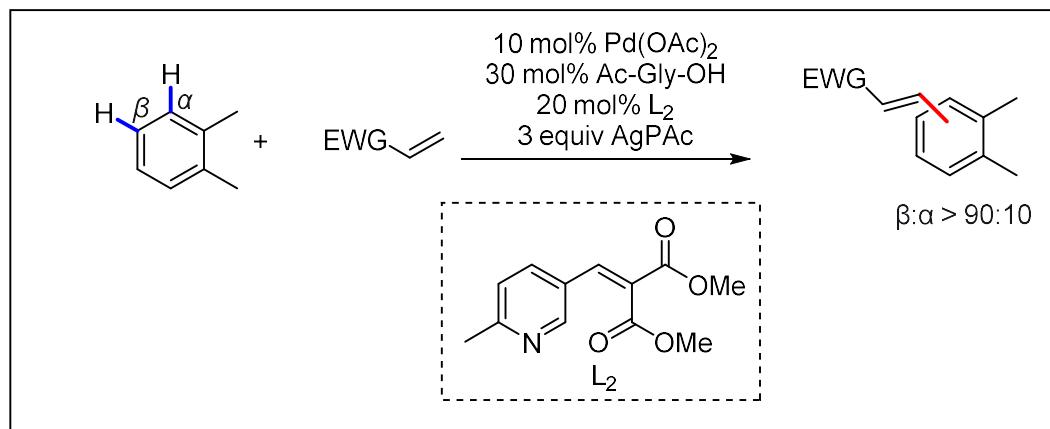
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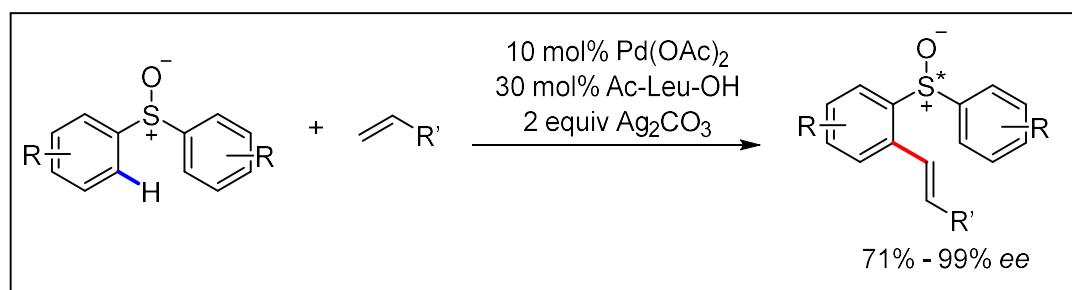
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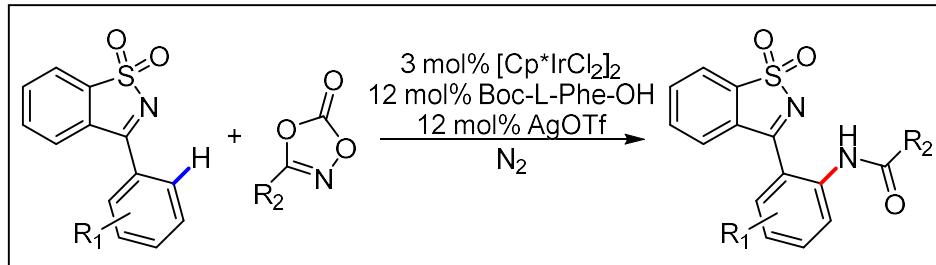
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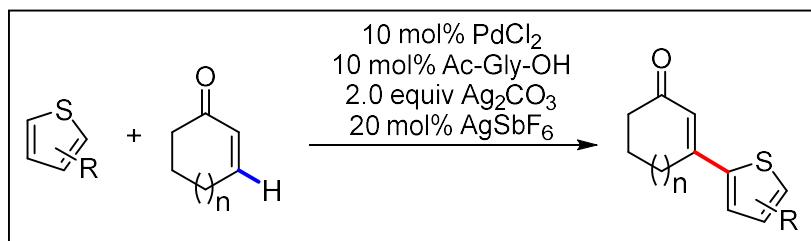
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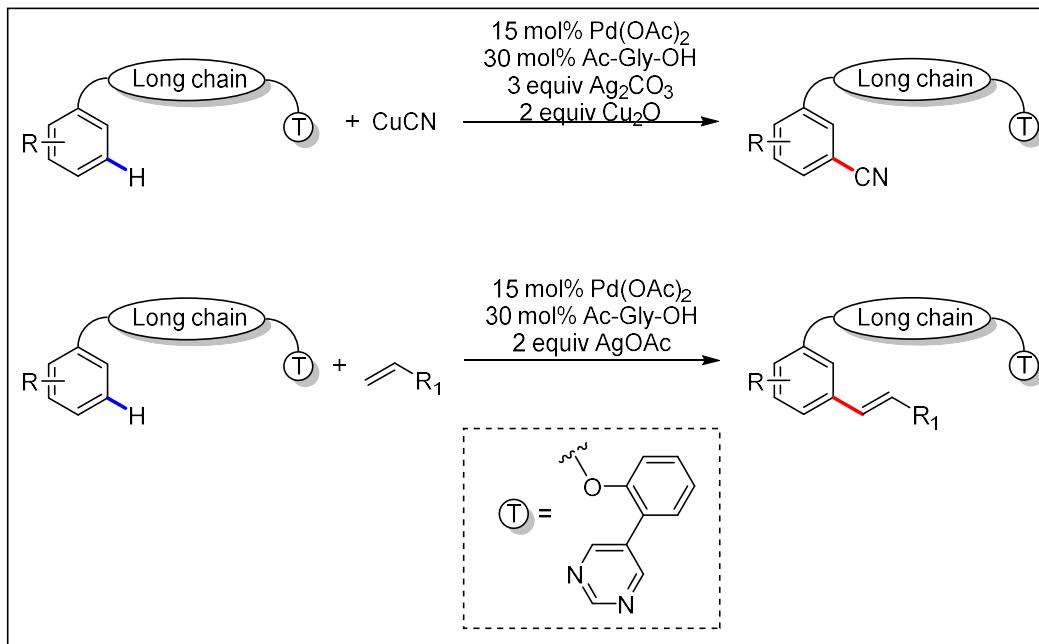
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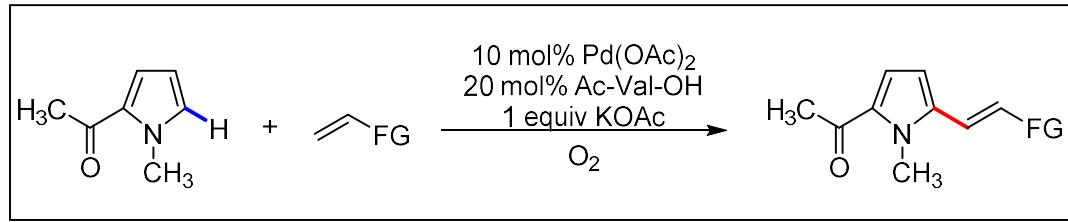
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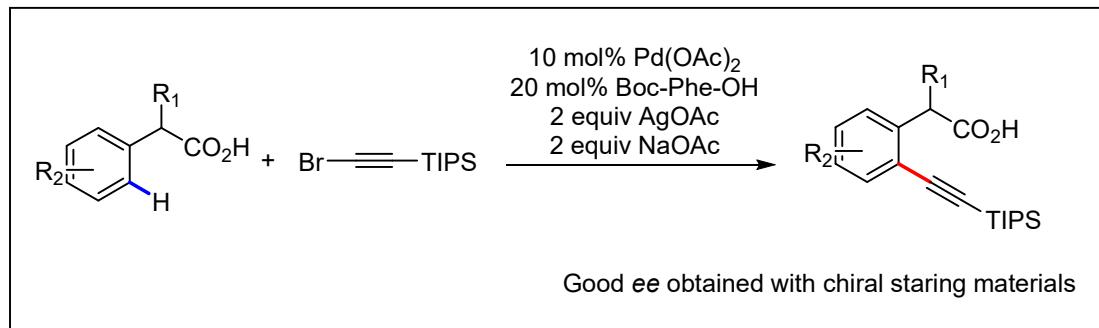
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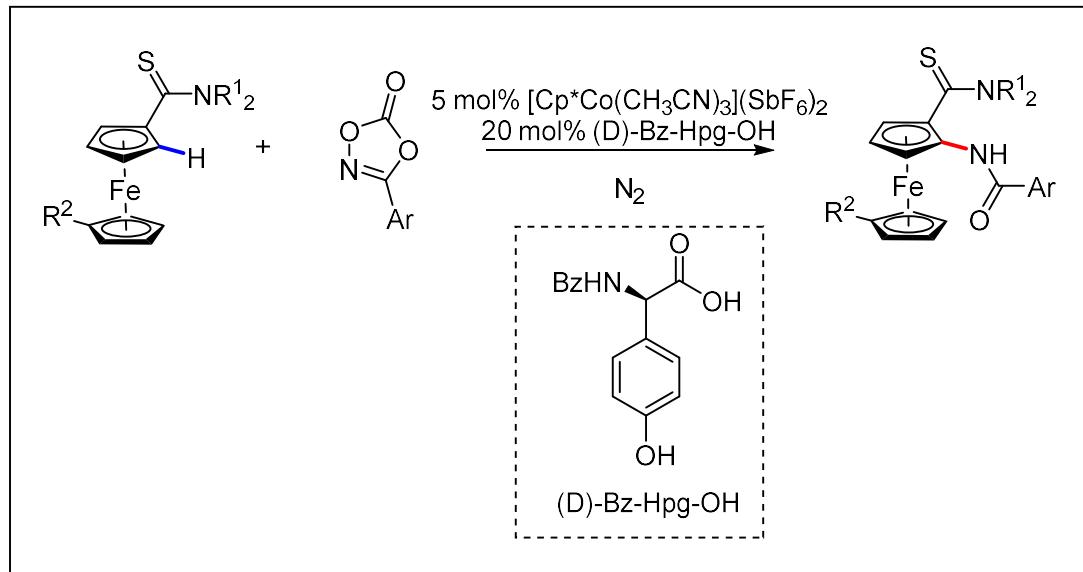
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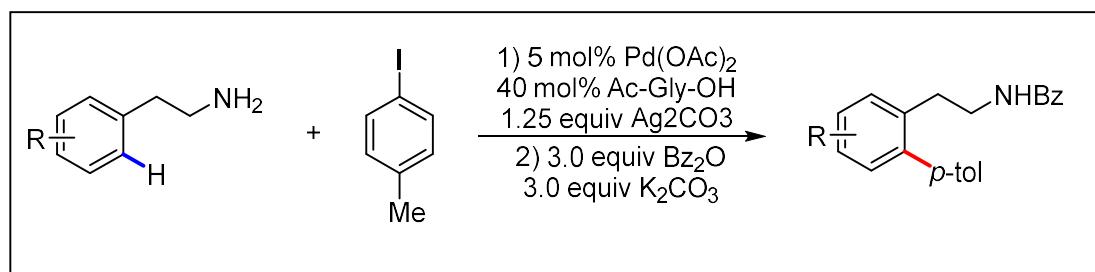
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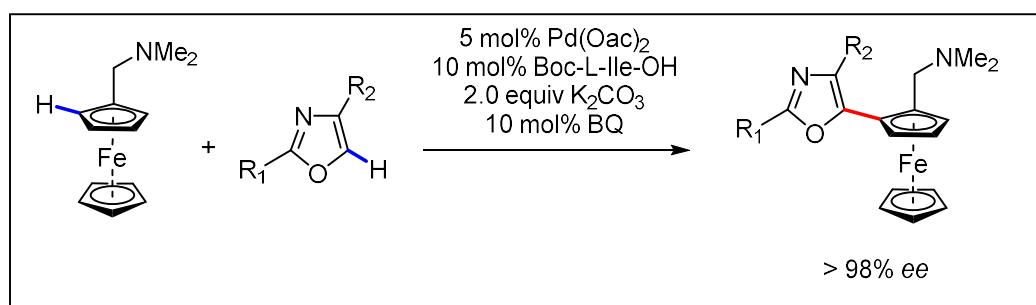


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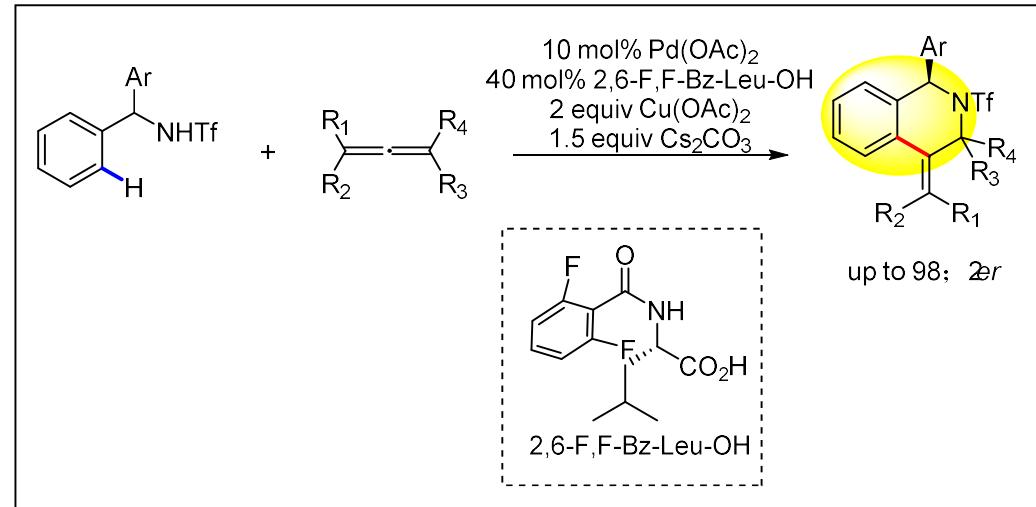
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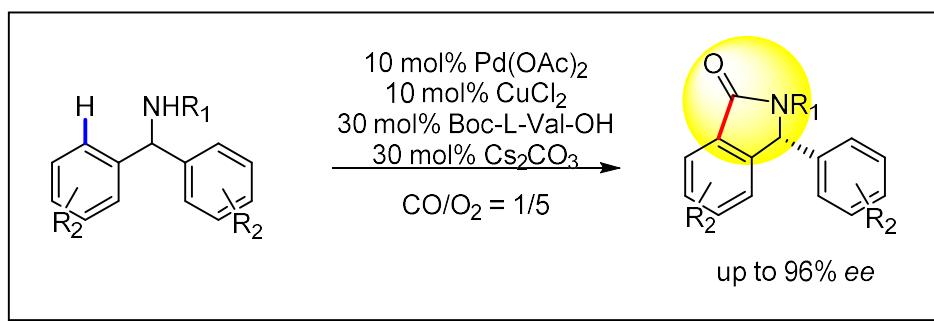
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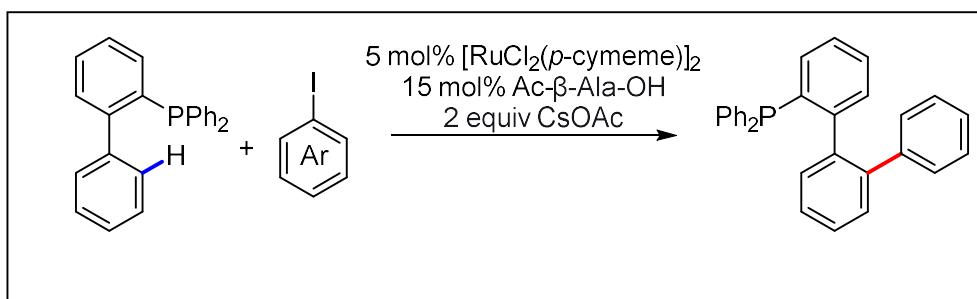


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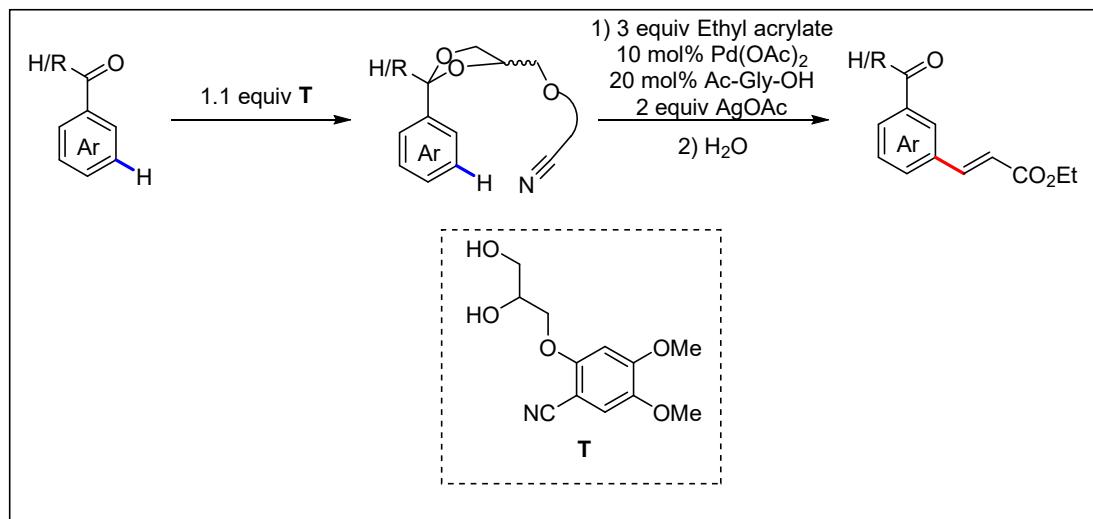
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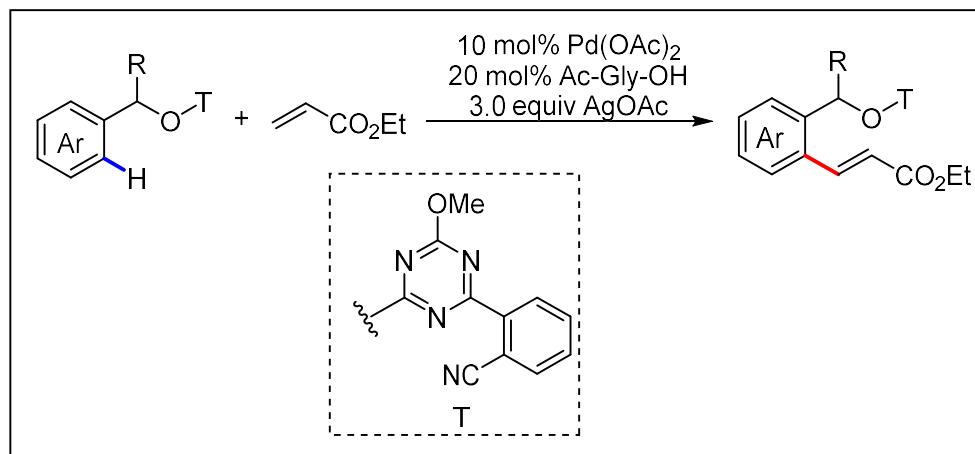
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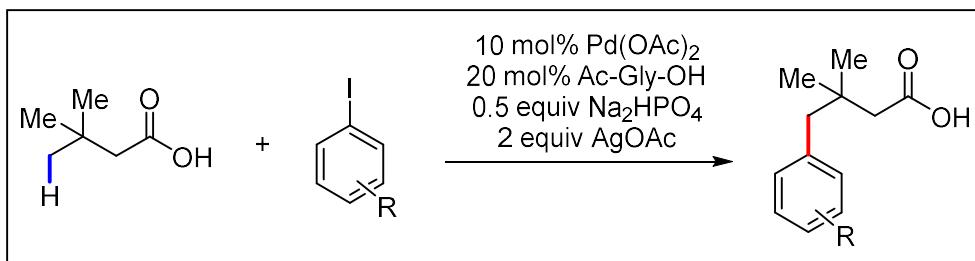
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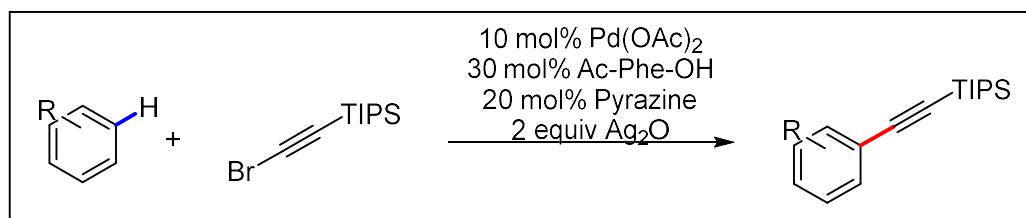
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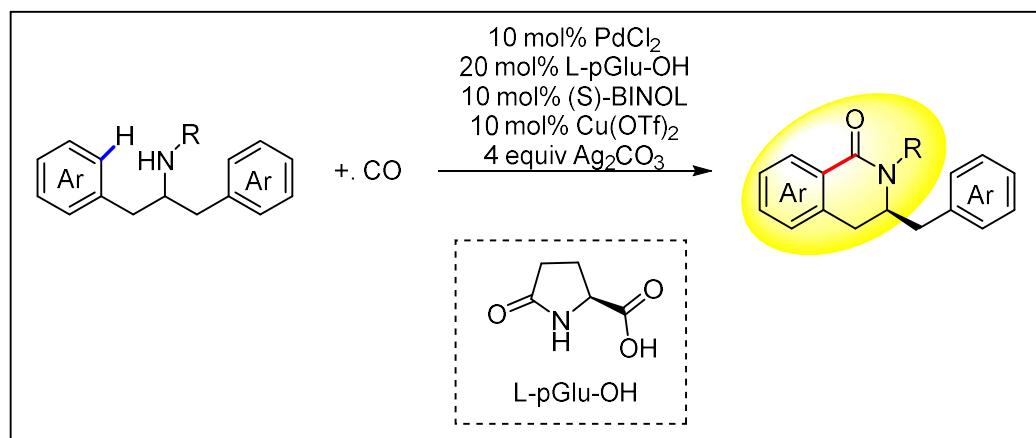
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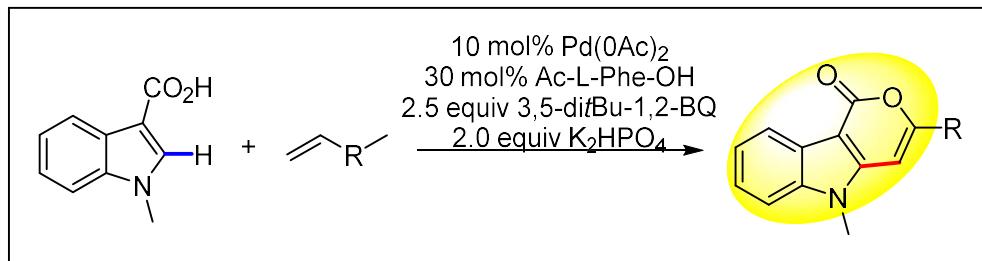
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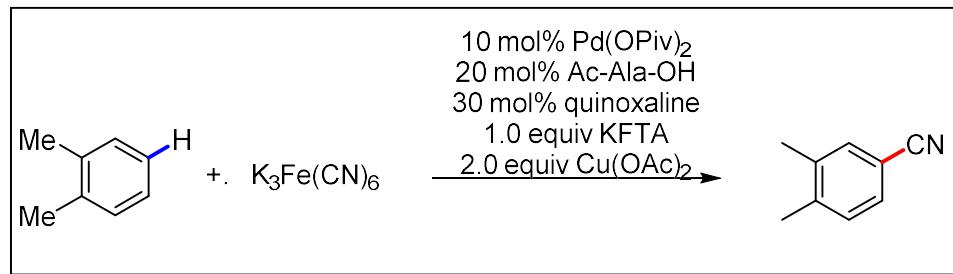
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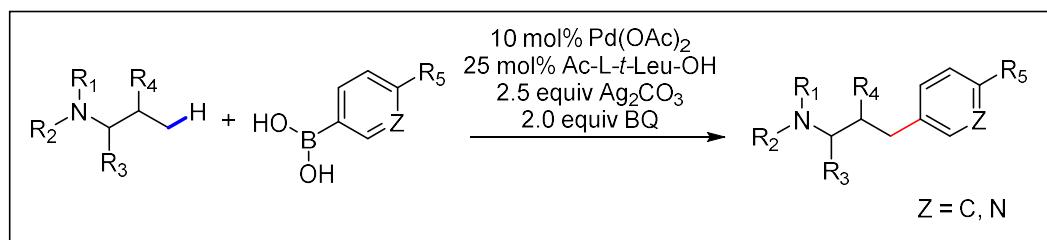
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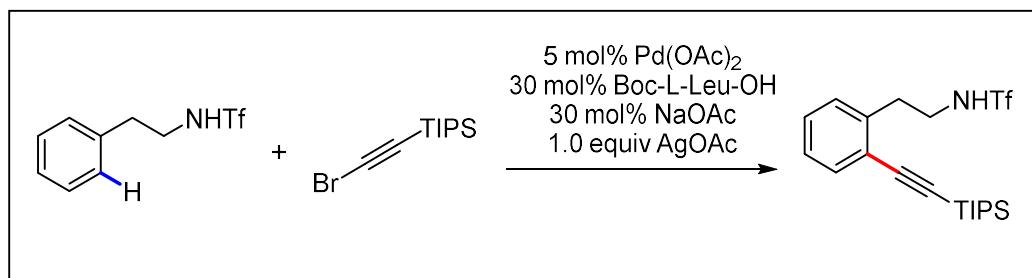


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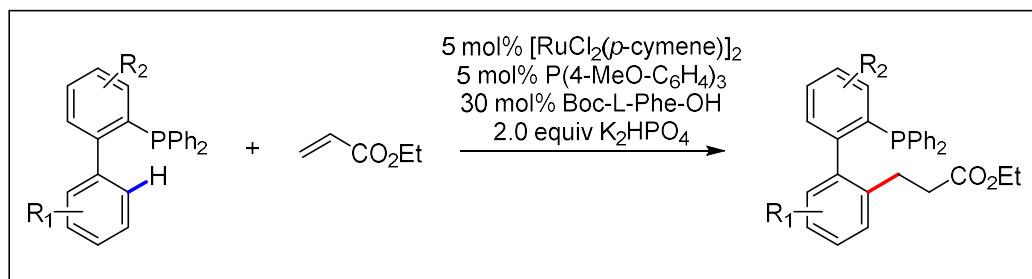
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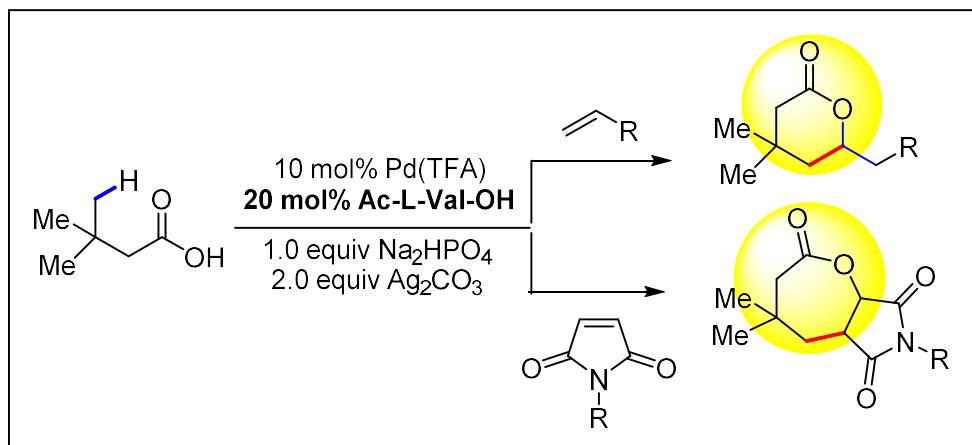
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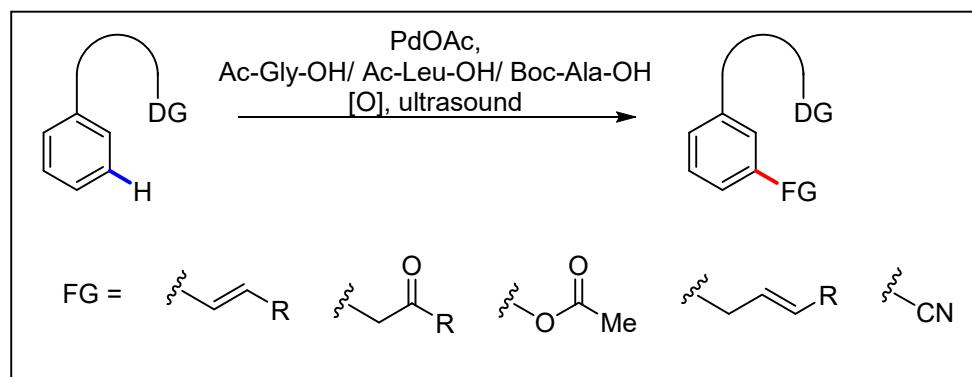


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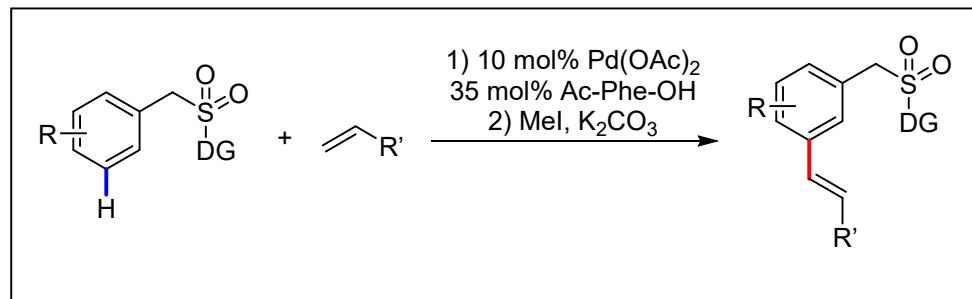
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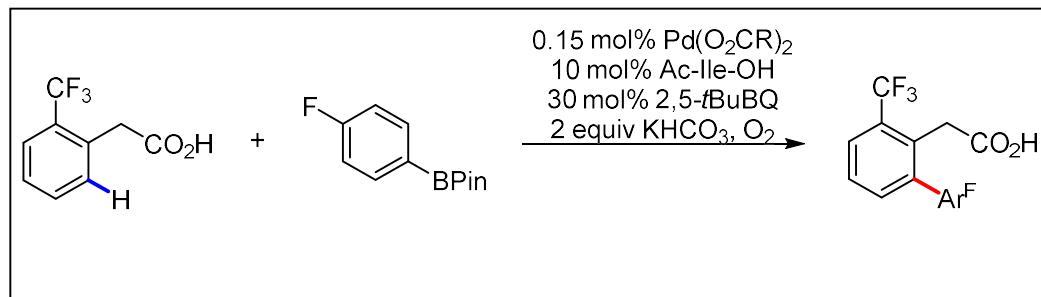
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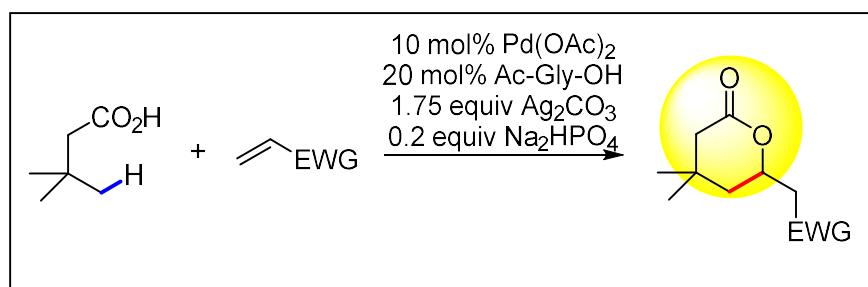
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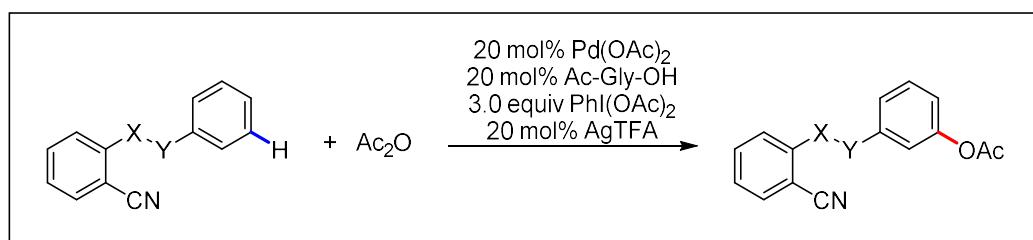
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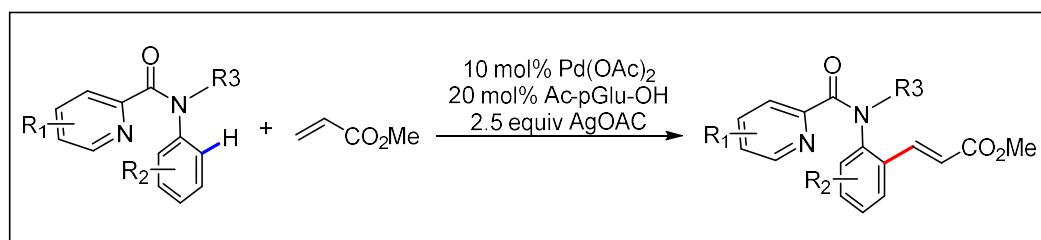
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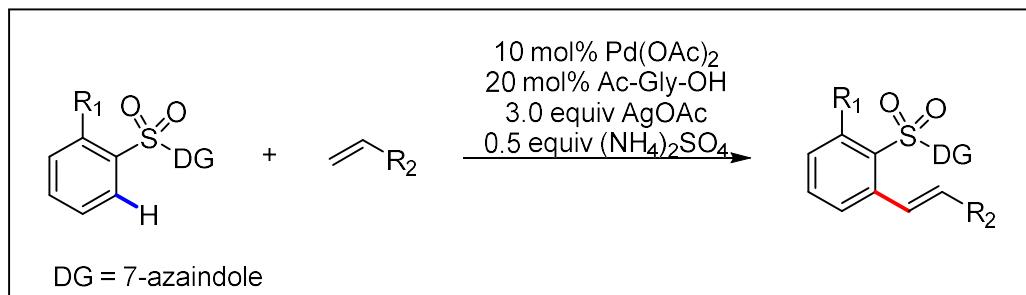
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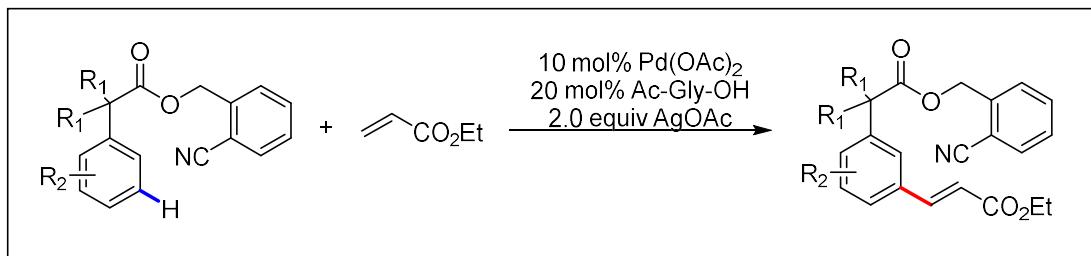
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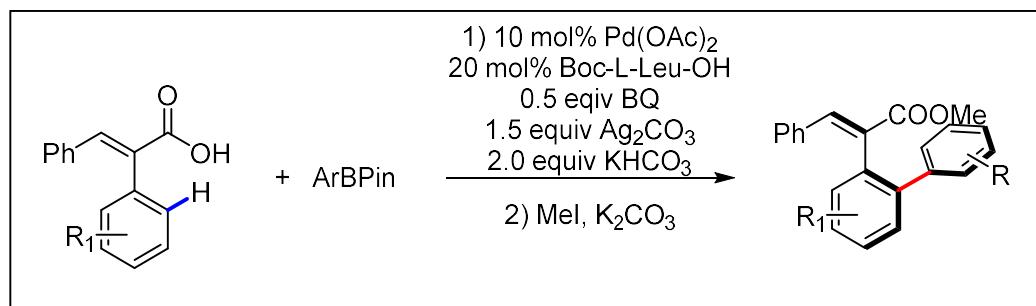
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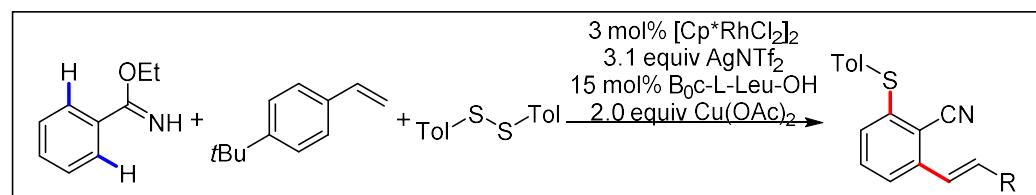
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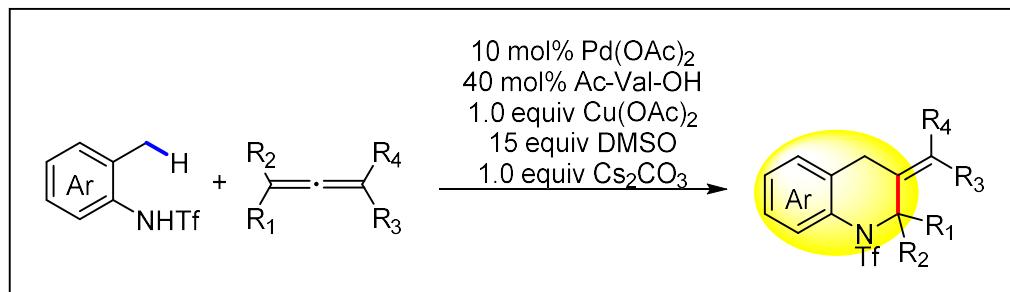
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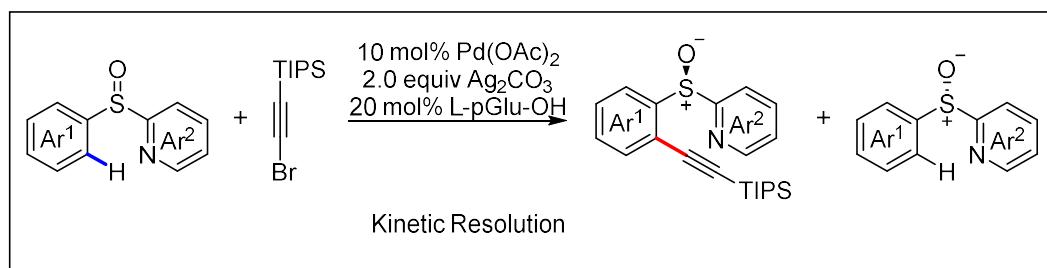
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