Supporting information:

Direct Access to Isoindolinone Derivatives by Palladium-Catalyzed C-H Activation and Isocyanide Insertion by Using Molecular Oxygen as the Sole Oxidant

Dongqi Wang, a† Sheng Cai, a† Rong Ben, a† Yang Zhou, a Xingwei Li, a and Jing Zhao, ab Wei Wei, a* and Yong Qian, a*

a Institute of Chemistry and Biomedical Sciences, State Key Laboratory of Pharmaceutical Biotechnology, School of Life Sciences, Nanjing University, Nanjing 210093, China.
b Shenzhen Key Lab of Nano-Micro Material Research, School of Chemical Biology and Biotechnology, Peking University Shenzhen Graduate School, Shenzhen 518055, China.
c Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China.
† These authors contributed equally to this work.
Fax: +86 0755 2603 3174
E-mail: yongqian@nju.edu.cn; weiwei@nju.edu.cn
**I Kinetic Isotope Effect**

**Intermolecular Kinetic Isotope Effect**

A mixture of 1a-d5 (51.6 mg, 0.33 mmol), 1a (50 mg, 0.33 mmol), Pd(OAc)$_2$ (7.5 mg, 0.03 mmol), Cs$_2$CO$_3$ (161.8 mg, 0.49 mmol) and tert-butylisonitrile (37.5 µl, 0.33 mmol) in toluene 2ml was stirred at 90 °C for 1 h under O$_2$ atmosphere. The reaction was cooled to room temperature and then the solvent was evaporated to dryness in vacuo. The residual was separated on a silica gel column to get the product (yield: 61%). $^1$H NMR (400 MHz, CDCl$_3$) δ 8.26 (d, $J = 7.2$ Hz, 1H), 7.77 (d, $J = 6.7$ Hz, 1H), 7.71 – 7.39 (m, 2H), 4.07 (s, 3H), 1.76 (s, 9H).

The intermolecular KIE was determined by $^1$H NMR: $K_{H}/K_{D}=2.2$
NMR Spectra
NOESY Spectra of 3aa