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Pd-Catalyzed Divergent C(sp^2)−H Activation/Cycloimidoylation of 2-Isocyano-2,3-diarylpropanoates

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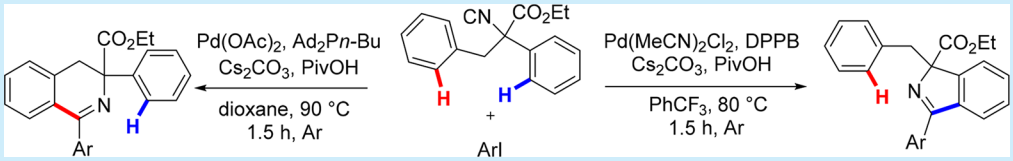
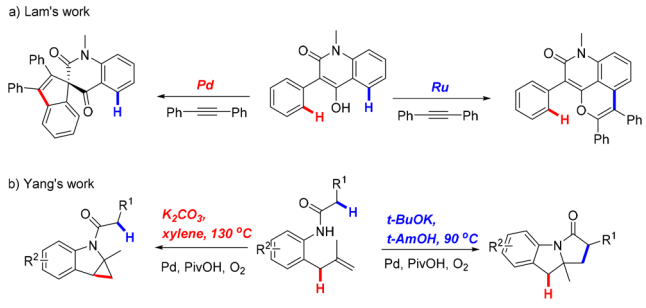
Supporting Information



ABSTRACT: A Pd-catalyzed site-selective C(sp^2)−H activation/cycloimidoylation of 2-isocyano-2,3-diarylpropanoates to construct diverse cyclic imine products has been developed. Six-membered 3,4-dihydroisoquinolines containing a C3 quaternary carbon center were generated dominantly by using bulky Ad_2Pn-Bu as a ligand, while five-membered 1,1-disubstituted 1*H*-isoindoles were formed preferentially in the presence of bidentate phosphine ligand DPPB. The selectivity for 1*H*-isoindole formation was enhanced by using steric hindered aryl iodides. DFT calculations suggested that the experimentally observed ligand-controlled selectivity was a result of *trans* effect.

During the past decade, transition-metal-catalyzed direct functionalization of inert C−H bonds has proven to be an atom- and step-economic strategy in constructing new chemical bonds.[1] Chiral ligand-controlled enantioselective C−H activation,[2] directing group-assisted regioselective functionalization of long distance *meta*- or *para*-C(sp^2)−H bonds over *ortho* ones,[3] and reactions via selective cleavage of less reactive C(sp^3)−H bonds are major challenging topics in the area of C−H activation.[4] Continuous achievements in these topics empower a C−H functionalization reaction as a practical and routine tool in total synthesis of natural products, as well as in late-stage modification of drug molecules.[5] However, divergent C−H functionalization reactions at different sites in the same substrate, controlled merely by catalyst, ligand, or other reaction conditions, are relatively undervalued.[6] In 2013, during the study of copper(II)-mediated aerobic C−H oxidation of *N*-(8-quinolinyl)benzamide, Stahl and coauthors discovered that directed methoxylation or chlorination of the benzamide group and nondirected chlorination of the quinoline motif were realized selectively under basic and acidic conditions, respectively.[7] Site-selective C−H functionalization of indole and thiophene could be finely tuned by concise selection of catalyst and solvent.[8] In addition to site-selective C−H modification of a parent scaffold, diverse frameworks could be constructed by cyclization reactions via activation of different C−H bonds. In 2013, Lam reported a novel C−H oxidative annulation of 2-aryl cyclic 1,3-dicarbonyl compounds with alkynes.[9] When palladium-*N*-heterocyclic carbene complex was used as the precatalyst, alkyne insertion between the 2-aryl C−H bond and the acidic α-C(sp^3)−H took place to provide spiroindenes exclusively. In contrast, when a ruthenium catalyst was applied, the oxidative annulation occurred between the oxygen of the directing group and the aromatic C−H on the main framework to produce benzopyrans selectively (Scheme 1a). In 2015, an elegant work by Yang demonstrated that the intermediate of amino-palladation of unsaturated anilide could activate the benzylic C−H or the amide α-C−H selectively, affording the corresponding three- and five-membered ring fused indolines under two optimized conditions (Scheme 1b).[10]

Scheme 1. Divergent C−H Functionalization/Cyclization



In recent years, applying functionalized isocyanide in C−H cycloimidoylation for the synthesis of heterocycles has gained ever-increasing interest.[11] In 2012, Takemoto reported a seminal work involving imidoylation and benzylic C(sp^3)−H activation to construct an indole skeleton (Scheme 2a).[12] Later on, our group used 2-isocyano-1,1′-biphenyls and tryptophan-derived

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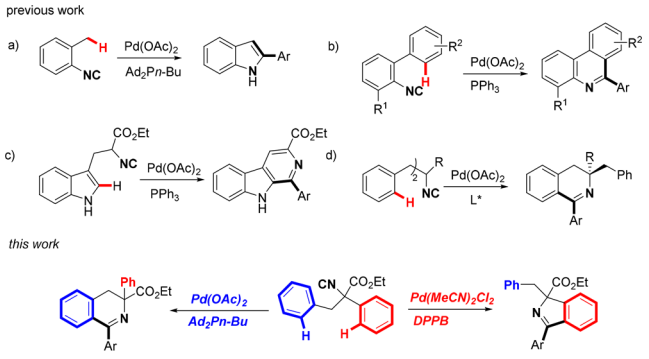
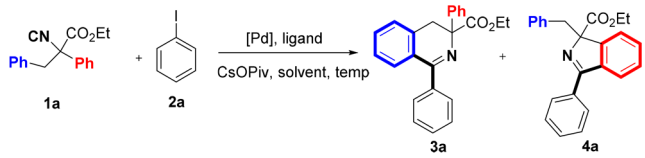
Scheme 2. C−H Activation/Cycloimidoylation



isocyanides for the preparation of phenanthridine and β-carboline derivatives through palladium-catalyzed C(sp^2)−H activation and imidoylative cyclization (Scheme 2b,c).[13] Recently, the first example of enantioselective C(sp^2)−H imidoylation was realized through desymmetrizing C(sp^2)−H activation of dibenzyl isocyanoacetates for the synthesis of 3,4-dihydroisoquinolines containing C3 quaternary stereogenic centers (Scheme 2d).[14] However, discriminating two types of C−H bonds in the same substrate to form different frameworks after cycloimidoylation is unprecedented. In this Letter, 2-isocyano-2,3-diarylpropanoates, which contain two different *ortho*-C(sp^2)−H bonds located 4 and 5 chemical bonds away from the isocyano group, are studied as a special class of functionalized isocyanides. Site-selective C(sp^2)−H activation/cycloimidoylation is realized by concise selection of ligands and reaction conditions, leading to six-membered 3,4-dihydroisoquinolines and five-membered 1,1-disubstituted 1*H*-isoindoles from the common starting material (Scheme 2).

The site-selective C(sp^2)−H cycloimidoylation of ethyl 2-isocyano-2,3-diphenylpropanoate **1a** was studied under palladium catalysis with phenyl iodide **2a**. The selection of phosphine ligand was first investigated in the presence of $Pd(OAc)_2$ as a precatalyst and CsOPiv in toluene, as shown in Table 1. When the common ligand PPh_3 was used, two cyclization products **3a** and **4a**, derived from respective activation of benzylic and phenylic C−H bond, were obtained in 76% total yield favoring the six-membered 3,4-dihydroisoquinoline **3a** (**3a**/**4a** = 2.0:1, entry 1, Table 1). However, neither **3a** nor **4a** could be efficiently produced when changing the ligand to P(*t*-Bu)$_3$ (entry 2). It was intriguing that when a more bulky ligand Ad_2Pn-Bu was applied the efficiency for the cyclization was regained (74%) with improved selectivity (**3a**/**4a** = 3.6:1, entry 3). To our delight, the selectivity was reversed in the presence of bidentate ligand DPPB, and five-membered 1,1-disubstituted 1*H*-isoindole **4a** was isolated as the major product (**3a**/**4a** = 1:5.4, entry 4). Extensive screening of other mono- and bidentate ligands could not improve the selectivity under otherwise identical conditions (see the Supporting Information (SI) for details). Next, the reaction conditions for the $Pd(OAc)_2/Ad_2Pn$-Bu catalytic system were finely tuned. The formation of **4a** was suppressed, and **3a** was produced in 60% yield at elevated temperature (90 °C). Further optimization revealed that the combination of Cs_2CO_3 and PivOH was superior to CsOPiv (entry 6). Satisfyingly, **3a** could be generated as the sole product in 83% yield by changing the solvent to dioxane and reducing the addition rate of **1a** to the reaction mixture (entry 7). However, to maximize the selectivity for formation of **4a**, palladium source, solvent, and other conditions were optimized with the ligand DPPB fixed. Finally,

Table 1. Optimization of the Reaction Conditions[a]



entry	[Pd]/L	solvent	*t* (°C)	total yield (%)[b]	**3a**/**4a**
1	$Pd(OAc)_2$/L1	PhMe	80	76	2.0/1
2	$Pd(OAc)_2$/L2	PhMe	80	trace	
3	$Pd(OAc)_2$/L3	PhMe	80	74	3.6/1
4	$Pd(OAc)_2$/L4	PhMe	80	77	1/5.4
5	$Pd(OAc)_2$/L3	PhMe	90	60	>50/1
6[c]	$Pd(OAc)_2$/L3	PhMe	90	70	>50/1
7[c,d]	**$Pd(OAc)_2$/L3**	**dioxane**	**90**	**83(80)**[e]	**>50/1**
8[f]	$Pd(OAc)_2$/L4	PhMe	80	25	1/3.2
9[c]	$Pd(OAc)_2$/L4	$PhCF_3$	80	81	1/6.4
10[c]	$Pd(MeCN)_2Cl_2$/L4	$PhCF_3$	80	89	1/5.4
11[c,d]	**$Pd(MeCN)_2Cl_2$/L4**	**$PhCF_3$**	**80**	**95(93)**[e]	**1/5.8**

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), [Pd] (0.01 mmol, 10 mol %), ligand (0.02 mmol, 20 mol %), CsOPiv (0.12 mmol), in solvent (1 mL), in Ar. A solution of **1a** in solvent (1 mL) was added via a syringe pump within 1 h. [b]NMR yield with 1-iodo-4-methoxybenzene as an internal standard. [c]Cs_2CO_3 (0.12 mmol), PivOH (0.06 mmol). [d]**1a** was added within 1.5 h. [e]Isolated yield in parentheses. [f]Cs_2CO_3 (0.12 mmol). L1 = PPh_3, L2 = P(*t*-Bu)$_3$, L3 = Ad_2Pn-Bu, L4 = DPPB (1,4-bis(diphenylphosphanyl)butane).

the ratio of **3a**/**4a** reached 1:5.8 in a total yield of 95% when the reaction was catalyzed by $Pd(MeCN)_2Cl_2$ in $PhCF_3$ as the solvent (entry 11).

Having established the optimized reaction conditions for selective synthesis of **3a**, the scope and limitation for both aryl iodide and functionalized isocyanide was investigated (Scheme 3). Aryl iodides bearing electron-donating or -withdrawing substituents at the *para*- or *meta*-position afforded the desired products in good to excellent yields (**3a**−**3i**, 71−85%), and the possible five-membered side products **4** were not detected in all of the cases. Disubstitued iodobenzene, such as 1,2-dichloro-4-iodobenzene and 1-iodo-3,5-dimethylbenzene, also worked well in this reaction, leading to the corresponding products in good yields (**3k**, 81%; **3l**, 71%). However, when 1-iodo-2-methylbenzene was tested in the reaction, the selectivity dropped dramatically to provide **3j** and **4b** in 24% and 30% yields, respectively. The results indicate that the steric hindrance on aryl iodide favored the formation of 1*H*-isoindole derivative **4**. Heteroaromatic iodides were also tested, and the corresponding pyridine- and thiophene-substituted 3,4-dihydroisoquinolines **3m** and **3n** were formed exclusively, although diminished yield was observed for **3m** (60%). Next, isocyanides **1** substituted with a range of functional groups on the *para*-position of the benzyl ring were studied. Both electron-withdrawing ester, halide, and electron-donating methyl were well-tolerated, leading to the desired products in moderate yields and excellent selectivity (**3o**−**3r**, 69−74%). When chloride located at the *meta*-position, activation of either neighboring C(sp^2)−H bond took place, delivering a mixture of **3s** and its isomer **3s′** in 87% yield. It was worthy of noting that, when the chloride substituent was on the *ortho* position, 1*H*-isoindole **4c** was also generated in 10% yield, together with 44% yield of the desired product **3t**. The result indicated that the steric hindrance on the benzyl group also had significant influence on the selectivity. 2-Isocyano-2,3-diary-

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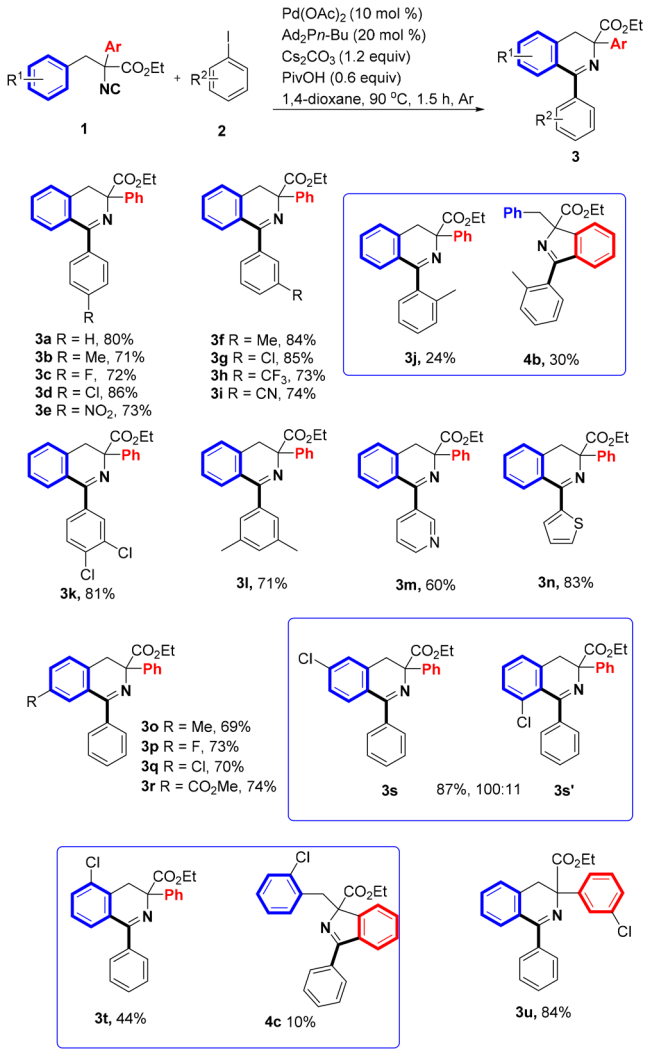
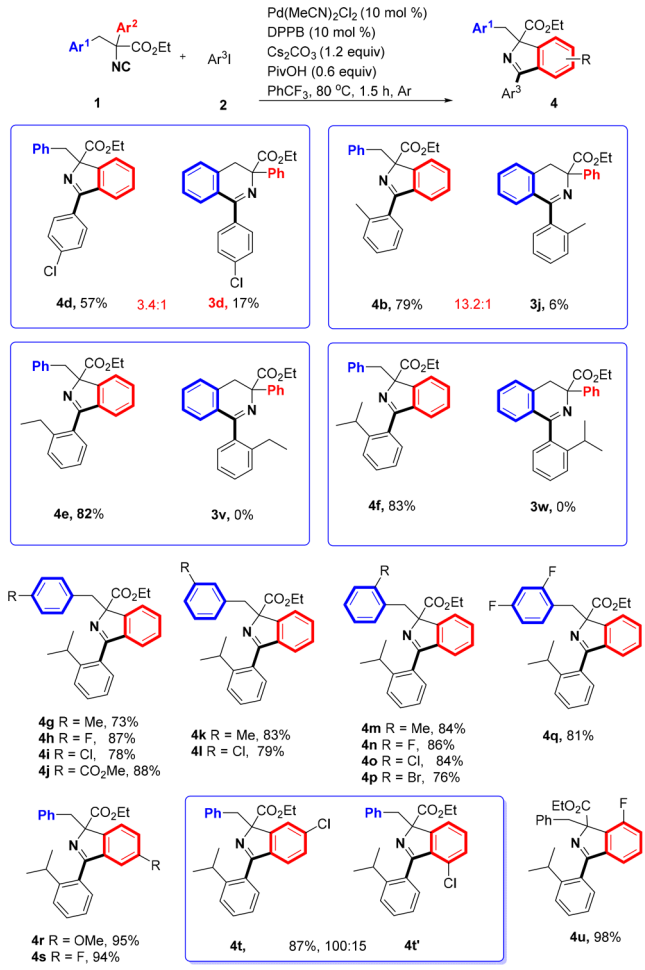
Scheme 3. Substrate Scope for Selective Synthesis of 3[a]



[a]Reaction conditions: **1** (0.1 mmol), **2** (0.12 mmol), $Pd(OAc)_2$ (0.01 mmol, 10 mol %), Ad_2Pn-Bu (0.02 mmol, 20 mol %), Cs_2CO_3 (0.12 mmol), PivOH (0.06 mmol) in 1,4-dioxane (1 mL) at 90 °C, in Ar. A solution of **1** in 1,4-dioxane (1 mL) was added via a syringe pump within 1.5 h.

Scheme 4. Substrate Scope for Selective Synthesis of 4[a]



[a]Reaction conditions: **1a** (0.1 mmol), **2** (0.12 mmol), $Pd(MeCN)_2Cl_2$ (0.01 mmol, 10 mol %), DPPB (0.01 mmol, 10 mol %), Cs_2CO_3 (0.12 mmol), PivOH (0.06 mmol) in $PhCF_3$, at 80 °C under Ar. A solution of **1a** in $PhCF_3$ (1 mL) was added via a syringe pump within 1.5 h.

lpropanoate containing *meta*-Cl on the phenyl group was also studied, and **3u** was isolated in 84% yield as the sole product.

Next, the generality for selective formation of 1*H*-isoindole **4** was examined (Scheme 4). Compared with iodobenzene (entry 11, Table 1), 1-chloro-4-iodobenzene generated both products with diminished yield and selectivity (74% yield in total, **4d**/**3c** = 3.4:1) under the same reaction conditions. However, when the reaction between **1a** and 1-iodo-2-methylbenzene was performed again under the $Pd(MeCN)_2Cl_2$/DPPB catalytic system in $PhCF_3$, the ratio of **4b**/**3j** jumped to 13.2:1 from 1.3:1, suggesting the significant influence of bidentate ligand on the outcome of selectivity. Surprisingly, when increasing the size of the *ortho* substituent from methyl to ethyl on iodobenzene, only the 1*H*-isoindole product **4e** (82% yield) was obtained, which was also the case using even sterically demanding 1-iodo-2-isopropylbenzene as an electrophile (**4f**, 83% yield); also the preparation of **4f** can be scaled up to 1 mmol with even higher yield (91%). Those results indicated that steric hindrance of both phosphine ligand and aryl iodide had synergistic influence on the selective formation of five-membered 1*H*-isoindole. Following this observation, the scope of functionalized isocyanide was explored using 1-iodo-2-isopropylbenzene as the coupling partner (Scheme 4). A variety of functional groups including Me, F, Cl Br, and CO_2Me on different positions of the benzyl moiety were compatible with reaction conditions, affording the corresponding products **4g**−**4q** in 73−88% yields with excellent selectivity. 2-Isocyano-2,3-diarylpropanoates bearing substituents on the 2-aryl ring, such as MeO, F, and Cl, underwent the site-specific C(sp^2)−H cycloimidoylation reaction smoothly to give 1,1-disubstituted 1*H*-isoindoles **4r**−**4u** exclusively in excellent yields (87−98%).

The ligand effect on the selectivity of the reaction was thoroughly investigated computationally.[15] The free energy barrier of the benzylic C−H cleavage (9.8 kcal/mol) is lower than that of the phenylic C−H cleavage (12.1 kcal/mol) with the sterically bulky Ad_2Pn-Bu ligand (Scheme 5). However, the energy barrier of benzylic C−H cleavage was determined to be 27.2 kcal/mol, which is 2.8 kcal/mol higher than that of phenylic C−H cleavage for the bidentate phosphine ligand DPPB. The steric influence of the bulky ligand Ad_2Pn-Bu makes one of the phosphine ligands dissociate automatically and thus enforces a coordinatively unsaturated palladium center in the C−H

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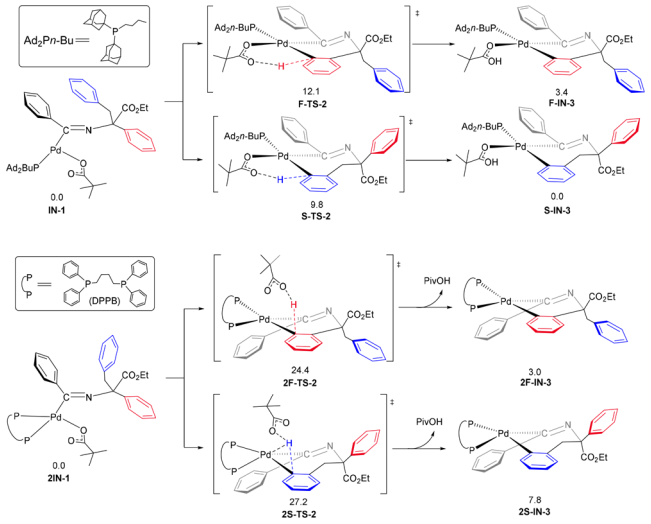
Scheme 5. Calculated C−H Cleavage Steps with Ad_2Pn-Bu and DPPB Ligands[a]



[a]All values are free energies in kcal/mol.

cleavage process. The η^2-coordination of the DPPB to the palladium center greatly lowers the ring strain of six-membered palladacycle and makes phenylic C−H bond activation favorable due to the strong *trans* effect of the phosphine ligand.

In summary, we had successfully developed an efficient and practical strategy for selective synthesis of two cyclic imine products from the same starting material by Pd-catalyzed C(sp^2)−H activation/cycloimidoylation. The selective synthesis of six-membered 3,4-dihydroisoquinolines was achieved by using bulky Ad_2Pn-Bu as a ligand, while the formation of five-membered 1*H*-isoindole products was determined by bidentate phosphine ligand DPPB, and the selectivity was enhanced by the steric hindrance of iodobenzene. DFT calculations agreed with the experimental observation in which the ligand-controlled selectivity was a result of the *trans* effect. This study provides the first example of ligand-controlled divergent C(sp^2)−H activation/cycloimidoylation of functionalized isocyanide with excellent selectivity.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.orglett.8b00346.

General experimental procedure and characterization data of the compounds (PDF)

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Notes

The authors declare no competing financial interest.

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■ REFERENCES

(1) Selected reviews: (a) Godula, K.; Sames, D. *Science* **2006**, *312*, 67. (b) Park, Y. J.; Park, J.-W.; Jun, C.-H. *Acc. Chem. Res.* **2008**, *41*, 222. (c) Chen, X.; Engle, K. M.; Wang, D.-H.; Yu, J.-Q. *Angew. Chem., Int. Ed.* **2009**, *48*, 5094. (d) Wencel-Delord, J.; Dröge, T.; Liu, F.; Glorius, F. *Chem. Soc. Rev.* **2011**, *40*, 4740. (e) Cho, S. H.; Kim, J. Y.; Kwak, J.; Chang, S. *Chem. Soc. Rev.* **2011**, *40*, 5068. (f) Kuhl, N.; Hopkinson, M. N.; Wencel-Delord, J.; Glorius, F. *Angew. Chem., Int. Ed.* **2012**, *51*, 10236.

(2) (a) Kim, J. H.; Daniliuc, S.; Glorius, F. *ACS Catal.* **2016**, *6*, 7652. (b) Smalley, A. P.; Cuthbertson, J. D.; Gaunt, M. J. *J. Am. Chem. Soc.* **2017**, *139*, 1412. (c) Chen, X.; Yang, S.; Li, H.; Wang, B.; Song, G. *ACS Catal.* **2017**, *7*, 2392. (d) He, J.; Shao, Q.; Wu, Q.; Yu, J.-Q. *J. Am. Chem. Soc.* **2017**, *139*, 3344. (e) Li, S.-X.; Ma, Y.-N.; Yang, S.-D. *Org. Lett.* **2017**, *19*, 1842. (f) Plata, R. E.; Hill, D. E.; Haines, B. E.; Yu, J.-Q.; Blackmond, D. G. *J. Am. Chem. Soc.* **2017**, *139*, 9238. (g) Lin, Y.; Ma, W.-Y.; Sun, Q.-Y.; Cui, Y.-M.; Xu, L.-W. *Synlett* **2017**, *28*, 1432. (h) Loup, J.; Zell, D.; Oliveira, J. C. A.; Keil, H.; Stalke, D.; Ackermann, L. *Angew. Chem., Int. Ed.* **2017**, *56*, 14197. (i) Jang, Y.-S.; Dieckmann, M.; Cramer, N. *Angew. Chem., Int. Ed.* **2017**, *56*, 15088.

(3) (a) Luo, J.; Preciado, S.; Larrosa, I. *J. Am. Chem. Soc.* **2014**, *136*, 4109. (b) Kuninobu, Y.; Ida, H.; Nishi, M.; Kanai, M. *Nat. Chem.* **2015**, *7*, 712. (c) Yang, G.; Butt, N.; Zhang, W. *Chin. J. Catal.* **2016**, *37*, 98. (d) Bisht, R.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2016**, *138*, 84. (e) Davis, H. J.; Mihai, M. T.; Phipps, R. J. *J. Am. Chem. Soc.* **2016**, *138*, 12759. (f) Bisht, R.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2016**, *138*, 84. (g) Hoque, M. E.; Bisht, R.; Haldar, C.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2017**, *139*, 7745. (h) Fang, L.; Saint-Denis, T. G.; Houk, K. N.; Yu, J.-Q. *J. Am. Chem. Soc.* **2017**, *139*, 10702. (i) Zhang, Z.; Tanaka, K.; Yu, J.-Q. *Nature* **2017**, *543*, 538.

(4) Selected reviews: (a) Campos, K. R. *Chem. Soc. Rev.* **2007**, *36*, 1069. (b) Baudoin, O. *Chem. Soc. Rev.* **2011**, *40*, 4902. (c) Qiu, G.; Wu, J. *Org. Chem. Front.* **2015**, *2*, 169. (d) Baudoin, O. *Acc. Chem. Res.* **2017**, *50*, 1114.

(5) (a) Gutekunst, W. R.; Baran, P. S. *Chem. Soc. Rev.* **2011**, *40*, 1976. (b) Pitts, A. K.; O'Hara, F.; Snell, R. H.; Gaunt, M. J. *Angew. Chem., Int. Ed.* **2015**, *54*, 5451. (c) Hui, C.; Xu, J. *Tetrahedron Lett.* **2016**, *57*, 2692. (d) Mahajan, P. S.; Humne, V. T.; Tanpure, S. D.; Mhaske, S. B. *Org. Lett.* **2016**, *18*, 3450. (e) Reddy, M. C.; Jeganmohan, M. *Chem. Sci.* **2017**, *8*, 4130. (f) Zhang, Z.; Wang, J.; Li, J.; Yang, F.; Li, A.; Zhang, W.-D. *J. Am. Chem. Soc.* **2017**, *139*, 5558. (g) Lv, J.; Wang, B.; Yuan, K.; Wang, Y.; Jia, Y. *Org. Lett.* **2017**, *19*, 3664. (h) Chen, D. Y.-K.; Youn, S. W. *Chem. - Eur. J.* **2012**, *18*, 9452. (i) He, J.; Hamann, L. G.; Davies, H. M. L.; Beckwith, R. E.J. *Nat. Commun.* **2015**, *6*, 5943. (j) Kong, X.; Zhang, H.; Cao, C.; Shi, Y. *Bioorg. Med. Chem.* **2016**, *24*, 1376. (k) Jeon, M.; Mishra, N. K.; Kim, H. S.; Kim, I. S. *J. Org. Chem.* **2016**, *81*, 9878. (l) Moore, T. O.; Paradowski, M.; Ward, S. E. *Org. Biomol. Chem.* **2016**, *14*, 3307. (m) Jardim, G. A.M.; Silva, T. L.; Bower, J. F.; Júnior, E. N. da S *Eur. J. Med. Chem.* **2017**, *136*, 406. (n) Kim, S.; Chakrasali, P.; Han, S. B.; Kim, I. S. *J. Org. Chem.* **2017**, *82*, 7555. (o) Liu, T.; Qiao, J. X.; Poss, M. A.; Yu, J.-Q. *Angew. Chem., Int. Ed.* **2017**, *56*, 10924.

(6) (a) Vanchura, B. A., II; Preshlock, S. M.; Roosen, P. C.; Singleton, D. A.; Smith, M. R., III *Chem. Commun.* **2010**, *46*, 7724. (b) Santhoshkumar, R.; Mannathan, S.; Cheng, C.-H. *J. Am. Chem. Soc.* **2015**, *137*, 16116. (c) Zhang, J.; Sha, S.-C.; Bellomo, A.; Tomson, N. C.; Walsh, P. J. *J. Am. Chem. Soc.* **2016**, *138*, 4260. (d) Ding, D.; Mou, T.; Feng, M.; Jiang, X. *J. Am. Chem. Soc.* **2016**, *138*, 5218. (e) Chen, X.; Zheng, G.; Li, Y.; Song, G.; Li, X. *Org. Lett.* **2017**, *19*, 6184.

(7) Suess, A. M.; Ertem, M. Z.; Cramer, C. J.; Stahl, S. S. *J. Am. Chem. Soc.* **2013**, *135*, 9797.

(8) (a) Grimster, N. P.; Gauntlett, C.; Godfrey, C. R. A.; Gaunt, M. J. *Angew. Chem., Int. Ed.* **2005**, *44*, 3125. (b) Phipps, R. J.; Grimster, N. P.; Gaunt, M. J. *J. Am. Chem. Soc.* **2008**, *130*, 8172. (c) Ueda, K.;

DOI: 10.1021/acs.orglett.8b00346
Org. Lett. XXXX, XXX, XXX−XXX

Yanagisawa, S.; Yamaguchi, J.; Itami, K. *Angew. Chem., Int. Ed.* **2010**, *49*, 8946. (d) Campbell, A. N.; Meyer, E. B.; Stahl, S. S. *Chem. Commun.* **2011**, *47*, 10257.
(9) Dooley, J. D.; Chidipudi, S. R.; Lam, H. W. *J. Am. Chem. Soc.* **2013**, *135*, 10829.
(10) Du, W.; Gu, Q.; Li, Z.; Yang, D. *J. Am. Chem. Soc.* **2015**, *137*, 1130.
(11) (a) Wang, J.; Luo, S.; Li, J.; Zhu, Q. *Org. Chem. Front.* **2014**, *1*, 1285. (b) Wang, J.; Luo, S.; Huang, J.; Mao, T.; Zhu, Q. *Chem. - Eur. J.* **2014**, *20*, 11220. (c) Xiong, Z.; Wang, J.; Wang, Y.; Luo, S.; Zhu, Q. *Org. Chem. Front.* **2017**, *4*, 1768. (d) Wang, J.; Tang, S.; Zhu, Q. *Org. Lett.* **2016**, *18*, 3074.
(12) Nanjo, T.; Tsukano, C.; Takemoto, Y. *Org. Lett.* **2012**, *14*, 4270.
(13) (a) Li, J.; He, Y.; Luo, S.; Lei, J.; Wang, J.; Xie, Z.; Zhu, Q. *J. Org. Chem.* **2015**, *80*, 2223. (b) Tang, S.; Wang, J.; Xiong, Z.; Xie, Z.; Li, D.; Huang, J.; Zhu, Q. *Org. Lett.* **2017**, *19*, 5577.
(14) Wang, J.; Gao, D.-W.; Huang, J.; Tang, S.; Xiong, Z.; Hu, H.; You, S.-L.; Zhu, Q. *ACS Catal.* **2017**, *7*, 3832.
(15) DFT calculations are detailed in the Supporting Information.

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