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Methyl Ketone Oxime Esters as Nucleophilic Coupling Partners in Pd-Catalyzed C−H Alkylation and Application in the Synthesis of Isoquinolines

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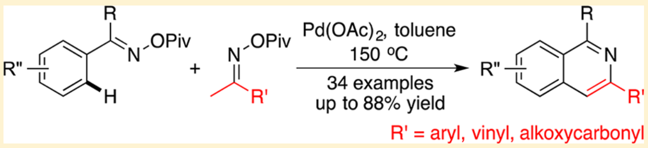
Supporting Information



ABSTRACT: Methyl ketone oxime esters have been found to be excellent coupling partners for $C(sp^2)-C(sp^3)$ bond formation via Pd-catalyzed aromatic C−H activation. This transformation forms the basis of an approach to regioselectively synthesize substituted isoquinolines via coupling with aryloxime esters. Our mechanistic studies suggested that the reaction proceeded through Pd(II)-catalyzed aromatic C−H activation, tautomerization, and a 1,3-shift of the palladacycle-ligated methyl ketone oxime ester to enable the C−C bond formation by reductive elimination, and intramolecular condensation of an imido-Pd(II) intermediate to form the heterocycle. The aryloxime group not only was used as a directing group for Pd-catalyzed aromatic C−H activation but also functioned as an internal oxidant to allow the reaction to be redox-neutral. Our study illuminated the scope and limitations of this C−H alkylation process, which may serve as the point of departure for developing other C−H functionalization reactions using oxime esters and potentially other carbonyl derivatives as the nucleophilic coupling partners.

INTRODUCTION

The development of new synthetic methods to address the need of sustainable growth by modern society is an important goal of organic chemists. Since the early days of organic chemistry, the carbonyl compounds and their derivatives have been among the most frequently used in the development of new reactions.[1] This is not only because these compounds are versatile electrophiles for reaction with nucleophilic reagents in diverse settings but also because these compounds, in the form of enols, enamines, or related tautomeric isomers, are excellent nucleophilic reagents for reaction with electrophilic species, including other carbonyl compounds and derivatives, in a wide range of transformations. Thus, a large body of chemistry has been developed based on the carbonyl derivatives and forms a cornerstone of modern organic chemistry.

During the past two decades, direct C−H functionalization has emerged as a powerful strategy for developing new synthetic methods because of its inherent advantages of bypassing prefunctionalization of the substrates.[2] A commonly used approach to regioselectively functionalize one C−H bond over the others makes use of directing groups to activate neighboring C−H bonds toward transition-metal-mediated functionalization using other reagents.[3] Despite some reports of carbonyl derivatives as electrophilic coupling partners in transition-metal-catalyzed C−H alkylation reactions,[4] nucleophilic carbonyl derivatives (through the forms of enols, enamines, etc.) as the coupling partners in transition-metal-catalyzed C−H alkylation have been rare. Indeed, whereas examples exist for intramolecular C−H alkylation using nucleophilic enamines or related compounds as the coupling partners to synthesize *N*-heterocycles,[5] the intermolecular C−H alkylation using nucleophilic carbonyl derivatives appears to be unknown. Thus, there is a compelling need of developing new approaches for C−H alkylation using carbonyl derivatives. These new approaches would not only significantly increase the scope of C−H functionalization reactions but also provide opportunities to further exploit the rich chemistry of carbonyl derivatives for efficient transformations. Herein, we report that methyl ketone oxime esters are excellent coupling partners for Pd-catalyzed C−H alkylation reactions and we demonstrate the utility of the reaction in the regioselective synthesis of substituted isoquinolines from aryloxime esters (Figure 1, eq 1). Isoquinolines are important heterocycles found in natural products,[6] pharmaceuticals,[7] chiral ligands,[8] and organic materials.[9] Recently, significant progresses have been made in the synthesis of isoquinolines or isoquinolinones using transition-metal catalysis,[10] particularly via transition-metal (Rh, Ru, Ni, Pd, Mn)-catalyzed tandem C−H activation/annulation of aromatic imines, oximes, azides, amides, etc., with internal alkynes or equivalents to give 3,4-disubstituted isoquinolines and isoquinolinones (Figure 1, eq 2).[11−14] In contrast, synthetic methods that allow direct access of 3-substituted isoquinolines have been rare.[15] Our synthesis of

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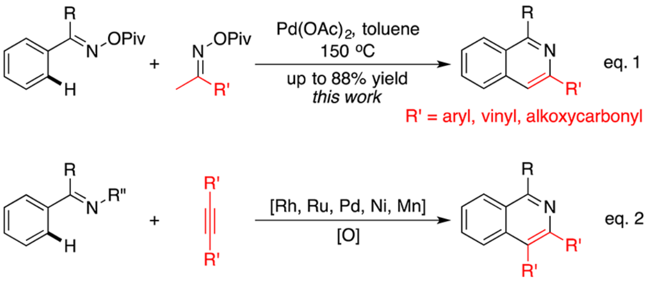


Figure 1. Isoquinolines and isoquinolinones via tandem C−H activation/annulation.

isoquinolines via Pd-catalyzed coupling of oxime esters provides an efficient and operationally simple approach (no external oxidants or any other additives) to this important structural motif using substrates that are readily prepared from commercial ketones.[16,17]

■ RESULTS AND DISCUSSION

We commenced the study using acetophenone oxime acetate (**1a-Ac**, eq 3) as the substrate not only because the oxime is an effective directing group for Pd-catalyzed C−H activation[18] but also because the N−O bond is well-poised for internal oxidation of the transition-metal catalytic center to enable a redox−neutral process without an external oxidant. The initial reaction was carried out using acetophenone as the reaction partner with the anticipation that its enol form may react with the palladacycle C−H activation intermediate and eventually lead to the alkylation product. Indeed, a reaction occurred in the presence of 10 mol % Pd(OAc)$_2$ in toluene at 120 °C to give a product identified as isoquinoline **2a** in 15% yield (eq 3, X = O). Interestingly, a control experiment in the absence of acetophenone showed that **2a** could also be formed by **1a-Ac** itself (eq 3, X = NOAc). Since aryloxime esters could be readily synthesized from commercial aryl ketones, we explored this self-coupling reaction as an entry to Pd-catalyzed C−H alkylation using nucleophilic carbonyl derivatives.In order to improve the efficiency of the reaction, we tested acetophenone oxime benzoate as the substrate, and a slightly improved yield of **2a** was obtained (Table 1, entry 2). The yield was also improved when the reaction was carried out at 150 °C (entry 3). Further improvement of the reaction efficiency was achieved when acetophenone oxime pivalate was used (60% yield, entry 4). The highest yield was obtained when the reaction was carried out using acetophenone oxime pivalate (**1a**) and 10 mol % of Pd(OAc)$_2$ in toluene at 150 °C for 36 h (84% yield, entry 5). Additional experimental parameters, such as common additives and solvents, were also tested (entries 6−13), but none gave better yields.

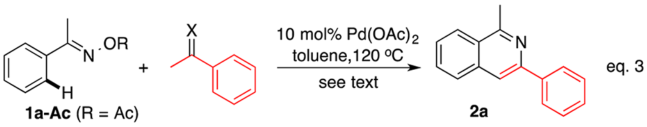
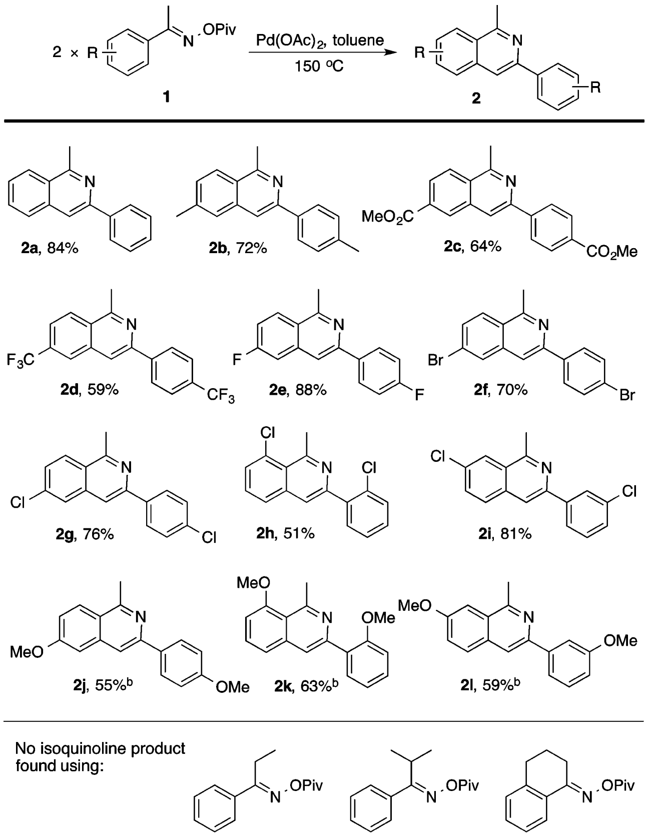


Table 1. Screening of Reaction Conditions for the Pd(II)-Catalyzed Self-Coupling of 1 To Give 2a[a]

entry	R	additive	solvent	T (°C)	conv.[b]/yield[c] (%)
1	Ac		toluene	120	40/15
2	Bz		toluene	120	45/25
3	Bz		toluene	150	60/42
4	Piv		toluene	150	75/60
5[d]	Piv		toluene	150	100/84
6	Piv	AgOAc	toluene	150	30/0
7	Piv	Cu(OAc)$_2$	toluene	150	−/15
8	Piv	NaHCO$_3$	toluene	150	91/29
9	Piv	Cs$_2$CO$_3$	toluene	150	100/41
10	Piv	BzOH	toluene	150	100/42
11	Piv		THF	150	20/<10
12	Piv		1,4-dioxane	150	50/19
13	Piv		DMF	150	30/<10

[a] Unless noted, the reactions were carried out using 0.25 mmol of **1a** and 0.025 mmol of Pd(OAc)$_2$ under the indicated reaction conditions for 24 h. [b] Determined by ^{1}H NMR. [c] Isolated yield. [d] The reaction was carried out for 36 h.

Scheme 1. Isoquinolines by Pd(OAc)$_2$-Catalyzed Self-Coupling of 1[a,b]



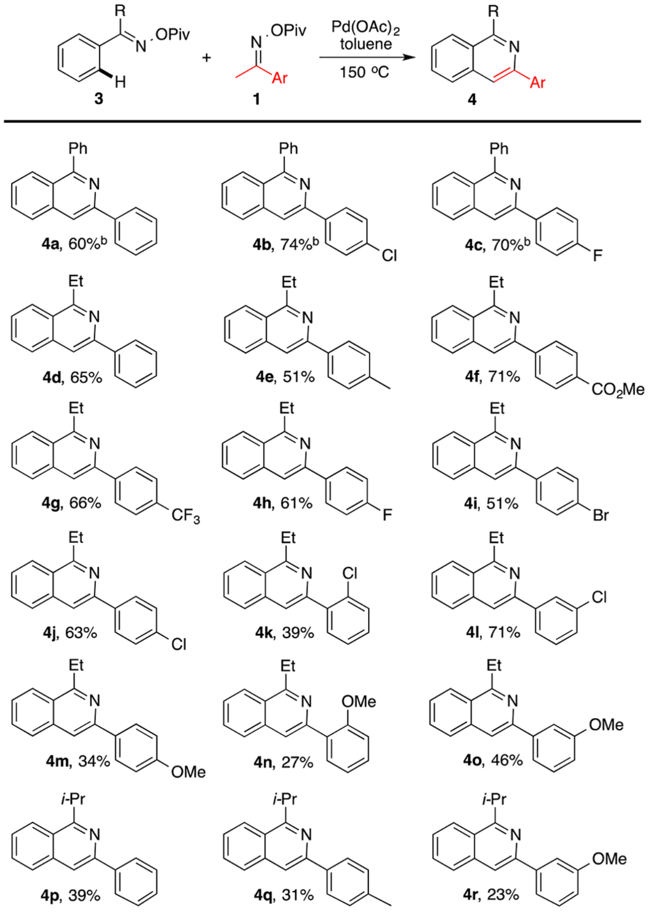
[a] Unless noted, the reaction was carried out using 0.25 mmol of **1**, 0.025 mmol of Pd(OAc)$_2$, and 3 mL of toluene in a sealed tube at 150 °C for 36 h. [b] The reaction was run for 48 h.

We explored the scope of the reaction using various substrates and found the reaction to be general with acetophenone oxime pivalates under the optimized conditions. For example, the reaction of *para*-methyl acetophenone oxime pivalate proceeded smoothly to give isoquinoline **2b** in 72% yield (Scheme 1). *para*-substitution of acetophenone with electron-withdrawing groups, such as ethoxycarbonyl and trifluoromethyl groups, also gave isoquinolines in good yields (**2c** in 64% yield and **2d** in 59% yield) via their oxime pivalates. Substitution of the aryl with halogens, which are valuable handles for further elaboration via conventional Pd(0)-catalyzed reactions, was tolerated in the formation of the fluoro-substituted **2e** (88% yield), bromo-substituted **2f** (70%

yield), and chloro-substituted **2g**−**2i** (76, 51, and 81% yields) from their corresponding substrates. Although regio-isomeric products are possible in the latter two cases, only the sterically more accessible isomer was formed using each of these substrates. The π-donating methoxy group on the aryl was also tolerated and gave the products (i.e., **2j**−**2l**) in good yields with the same regioselectivity as that of their chloro-substituted counterparts. Our attempts of the reaction using the oxime pivalates of other aryl ketones, such as propiophenone, isopropyl phenyl ketone, and tetralone, failed to give the isoquinoline products. These substrates remained intact under the optimized reaction conditions and decomposed at higher reaction temperature.

In order to expand the scope of this process, we explored the reaction using two different aryloxime pivalates. We chose to carry out the reactions using an acetophenone oxime pivalate and another (non-acetophenone, i.e., non-self-coupling) aryloxime pivalate, with the former used in excess because of its competing self-coupling under the reaction conditions. Indeed, when benzophenone oxime pivalate was used as the substrate, isoquinoline **4a** was obtained in 60% yield upon the Pd(II)-catalyzed reaction with acetophenone oxime pivalate (Scheme 2). Similarly, *para*-chloro- and *para*-fluoroacetophenone oxime pivalate underwent the reaction with benzophenone oxime pivalate to give the isoquinolines **4b** (74% yield) and **4c** (70% yield), respectively. Additional aryloxime pivalates were tested, and the reaction was found to be fairly general. For example, the reaction of propiophenone oxime pivalate and acetophenone oxime pivalate or its *para*-methyl analogue gave **4d** and **4e** in 65% and 51% yield, respectively. Substitution of the aryl group of acetophenone with electron-withdrawing groups, such as ethoxylcarbonyl and trifluoromethyl, led to products in somewhat better yields (**4f** for 71% yield, **4g** for 66% yield). The reaction was also found to be compatible with substrates in which the aryl was substituted with halogens, such as with fluoride, chloride, and bromide (**4h**−**4l**). A reduced yield was observed when the chloride substituent was at the *ortho*-position (i.e., **4k**, 39% yield) when compared with the same substituent at the *para*- (i.e., **4j**, 63% yield) or *meta*-position (i.e., **4l**, 71% yield). The isoquinoline products could also be obtained, even though in lower yields, when the π-donating methoxy substituent was present at the aryl, and again, *ortho*-methoxy substitution of the aryl led to reduced yield (i.e., **4n**, 27% yield) compared with those substituted at the *para*- or *meta*-position (i.e., **4m** in 34%, **4o** in 46% yield). The isopropyl phenyl ketone oxime pivalate also participated in the reaction, but affording the isoqunoline products (i.e., **4p**−**4r**) in lower yield, likely due to the increased steric hindrance by the isopropyl group.

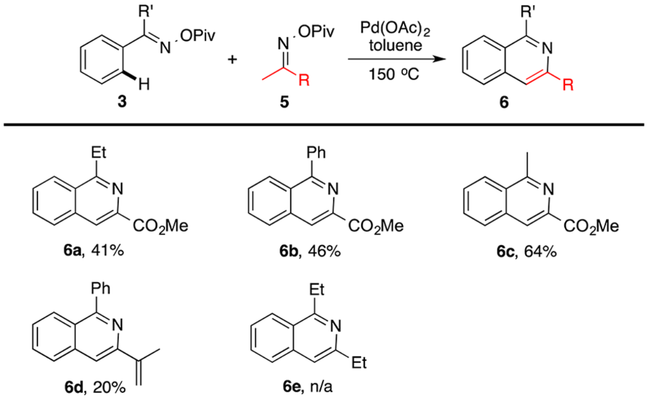
Scheme 2. Isoquinolines by Pd(OAc)$_2$-Catalyzed Coupling of Two Different Aryloxime Pivalates[a,b]



[a]Reaction conditions: 0.375 mmol of **1**, 0.125 mmol of **3**, 0.05 mmol of Pd(OAc)$_2$, and 6 mL of toluene in a sealed tube at 150 °C for 24 h. [b]The reaction was run for 48 h.

The isoquinolines could also be obtained by the reaction of aryloxime pivalates and non-aryl methyl ketone oxime pivalates. For example, methyl pyruvate oxime pivalate reacted with priopiophenone oxime pivalate and benzophenone oxime pivalate to give the isoquinolines **6a** and **6b**, respectively, in useful yields (Scheme 3). When used in excess (3 equiv), acetophenone oxime pivalate also reacted with methyl pyruvate oxime pivalate to give **6c** in 64% yield. The reaction of benzophenone oxime pivalate and **5d** (R = isopropenyl) afforded **6d** in low yield.[19] Instead of affording an isoquinoline product (i.e., **6e**), the reaction of propiophenone oxime pivalate and 2-butanone oxime pivalate led to decomposition of the substrates.

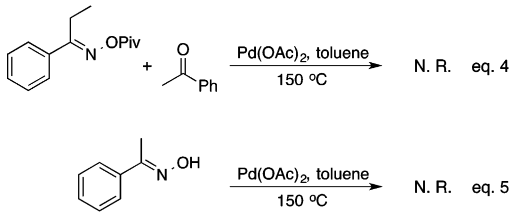
Scheme 3. Isoquinolines by Pd(OAc)$_2$-Catalyzed Coupling of Aryloxime Pivalates and Non-aryl Methyl Ketone Oxime Pivalates[a,b]



[a]Reaction conditions: 0.125 mmol of **3**, 0.125 mmol of **5**, 0.025 mmol of Pd(OAc)$_2$, 3 mL of toluene, 150 °C in a sealed tube for 12 h. [b]0.375 mmol of **3c** was used.

To better understand this reaction and verify that the oxime esters instead of their potential hydrolysis products, i.e., the ketones and oximes, are the true reaction partners for this C−H alkylation process, a mixture of propiophenone oxime pivalate and acetophenone was subjected to the reaction conditions, but no isoquinoline product was formed (Scheme 4, eq 4). The acetophenone oxime did not undergo the Pd(OAc)$_2$-catalyzed self-coupling either (Scheme 4, eq 5). These results show that the C−H alkylation process indeed occurred with acetophenone oxime pivalates as the substrates.

Scheme 4. Some Control Experiments

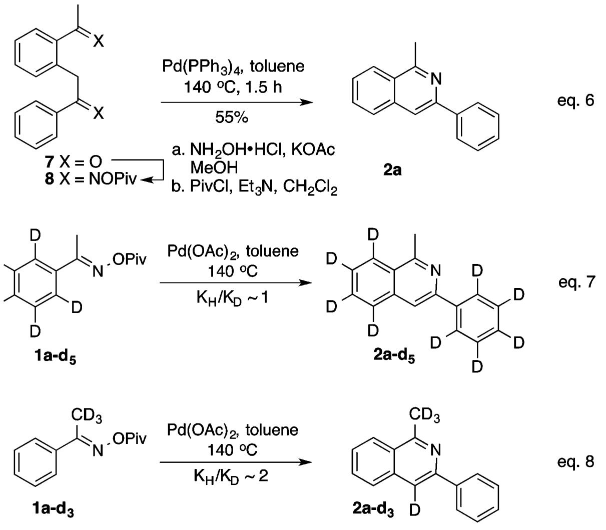


On the basis of these experimental findings, a plausible mechanism for the C−H alkylation of **1a** and formation of isoquinoline **2a** is depicted in Scheme 5. An oxime-directed C−H activation of **1a** with Pd(OAc)$_2$ gives palladacycle **A**.[20] This complex undergoes ligand exchange with another **1a** to form **B** with the oxime ester *N*-bound as an L-type ligand. This is followed by extrusion of the acetate ligand and tautomerization of the Pd-bound oxime ester to its enamine form to give **C**. The *N*-bound Pd(II) complex **C** is expected to be in equilibrium with its *C*-bound form, i.e., **D**, which will undergo reductive elimination to form the C(sp^2)−C(sp^3) bond to give **E**. Oxidative addition of Pd(0) across the N−O bond gives an imido-Pd(II) species **F**, which undergoes intramolecular condensation to give **2a** and concomitantly regenerate the Pd(II) catalyst.

To test this mechanistic hypothesis, the bis-oxime pivalate **8**, prepared from the known bis-ketone **7**,[21] was treated with a stoichiometric amount of Pd(PPh$_3$)$_4$ in toluene at 140 °C (Scheme 6, eq 6). Indeed, isoquinoline **2a** was formed in 55% yield in 1.5 h. In contrast, only a trace amount of **2a** (<5%) was formed under the otherwise identical conditions in the presence of Pd(OAc)$_2$ or in the absence of any catalysts. This result is consistent with the hypothesis of **E** being an intermediate of the reaction.

To gain further insight into the mechanism of the reaction, the deuterated acetophenone oxime pivalates **1a**−**d**$_5$ (with deuterated phenyl) and **1a**−**d**$_3$ (with deuterated methyl) were prepared and their reactions under the optimized conditions were compared with that of **1a**. When the reactions were quenched at 2.5 h (<30% of conversion of **1a** based on TLC), essentially the same conversion and rate of product formation were observed using **1a** and **1a**−**d**$_5$ (**2a**:**2a**−**d**$_5$ = 1:1.03, eq 7). However, approximately 2-fold less of **2a**−**d**$_3$ (**2a**:**2a**−**d**$_3$ = 2.03:1, eq 8) was formed from **1a**−**d**$_3$ during the same interval. Even though the exact kinetics of the reactions using the deuterated and nondeuterated **1a**'s has not been determined, these results do suggest that the tautomerization of **B** but not the Pd(II)-catalyzed C−H activation of **1a** is rate-limiting. This conclusion is also consistent with the experimental observation that only methyl ketone oxime pivalates are competent coupling partners as a more demanding tautomerization step is expected with other oxime esters.

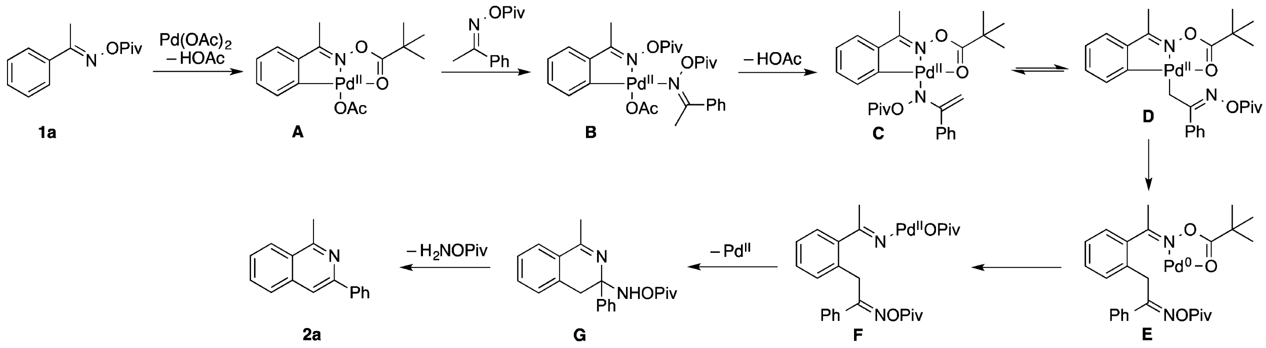
Scheme 6. Some Mechanistic Studies



■ CONCLUSION

In summary, we report methyl ketone oxime esters to be excellent coupling partners in Pd(II)-catalyzed aromatic C−H alkylation reactions. We demonstrate the utility of these C−H alkylation reactions in an efficient and operationally simple procedure for regioselective synthesis of substituted isoquinolines via Pd(II)-catalyzed coupling of readily available aryloxime esters. The oxime group not only served as a directing group for the Pd(II)-catalyzed aromatic C−H activation but also functioned as an internal oxidant to render the reaction redox-neutral without external oxidants. Our study illuminated the scope of this C−H alkylation process which, despite some of its limitations, may serve as the point of departure for developing

Scheme 5. A Proposed Reaction Mechanism



transformations based on transition-metal-catalyzed C−H alkylation using other nucleophilic carbonyl derivatives.

■ EXPERIMENTAL SECTION

General Procedure for Synthesis of the Oxime Esters. All *O*-pivaloyl oxime esters **1**, **3**, and **5** were generated from the corresponding ketones according to the following procedure, adapted from the literature.[22] A suspension of acetophenone (10 mmol), hydroxylamine hydrochloride (1.74 g, 25 mmol), and KOAc (2.45 g, 25 mmol) in 30 mL of methanol was heated gently to reflux for 40 min. Following cooling to rt, the mixture was filtered and the filtrate was evaporated to give a residue, which was dissolved in 40 mL of anhydrous dichloromethane and cooled to 0 °C. After the addition of Et_3N (3.03 g, 30 mmol), a solution of pivaloyl chloride (2.41 g, 20 mmol) in 10 mL of dichloromethane was added dropwise at 0 °C. The mixture was stirred at room temperature for 30 min and quenched with water. The aqueous layer was extracted with dichloromethane three times, and the combined organic layers were washed with saturated $NaHCO_3$ and brine and dried over $NaSO_4$. After evaporation of the solvent, the residue was purified by flash column chromatography to give the oxime ester product.

*1-Phenylethan-1-one O-Pivaloyl Oxime (**1a**).* Isolated as a white amorphous solid (1.86 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.77−7.74 (2H, m), 7.43−7.26 (3H, m), 2.38 (3H, s), 1.34 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.0, 163.1, 134.9, 130.5, 128.5, 127.0, 38.8, 27.3, 14.3 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{18}NO_2$ $[M + H]^+$ 220.1338, found 220.1337.

*1-(p-Tolyl)ethan-1-one O-Pivaloyl Oxime (**1b**).* Isolated as a white amorphous solid (1.98 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.64 (2H, d, J = 8.4 Hz), 7.18 (2H, d, J = 8.4 Hz), 2.35 (3H, s), 2.34 (3H, s), 1.33 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.1, 163.0, 140.7, 132.0, 129.2, 126.9, 38.8, 27.3, 21.8, 14.2 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{20}NO_2$ $[M + H]^+$ 234.1494, found 234.1529.

*Methyl 4-(1-((Pivaloyloxy)imino)ethyl)benzoate (**1c**).* Isolated as a white amorphous solid (2.35 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07−8.04 (2H, m), 7.84−7.81 (2H, m), 3.92 (3H, s), 2.39 (3H, s), 1.33 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 166.4, 162.1, 139.1, 131.8, 129.7, 127.0, 52.3, 38.8, 27.3, 14.3 ppm; HRMS (ESI) *m/z* calculated for $C_{15}H_{20}NO_4$ $[M + H]^+$ 278.1392, found 278.1401.

*1-(4-(Trifluoromethyl)phenyl)ethan-1-one O-Pivaloyl Oxime (**1d**).* Isolated as a white amorphous solid (2.44 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83 (2H, d, J = 8.1 Hz), 7.59 (2H, d, J = 8.1 Hz), 2.35 (3H, s), 1.29 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.8, 161.7, 138.4, 132.1 (q, J = 32.6 Hz), 127.4, 125.4 (q, J = 3.8 Hz), 123.8 (q, J = 270.8 Hz), 38.8, 27.1, 14.1 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{17}NO_2F_3$ $[M + H]^+$ 288.1211, found 288.1223.

*1-(4-Fluorophenyl)ethan-1-one O-Pivaloyl Oxime (**1e**).* Isolated as a white amorphous solid (2.01 g, 8.5 mmol, 85% yield); $R_f = 0.2$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.80−7.73 (2H, m), 7.29−7.04 (2H, m), 2.37 (3H, s), 1.34 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.0, 165.9, 162.3 (d, J = 38.7 Hz), 131.0 (d, J = 3.3 Hz), 129.1 (d, J = 8.5 Hz), 115.6 (d, J = 21.7 Hz), 38.8, 27.3, 14.3 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{17}NO_2F$ $[M + H]^+$ 238.1243, found 238.1228.

*1-(4-Bromophenyl)ethan-1-one O-Pivaloyl Oxime (**1f**).* Isolated as a white amorphous solid (2.52 g, 8.5 mmol, 85% yield); $R_f = 0.2$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.61−7.58 (2H, m), 7.49−7.46 (2H, m), 2.31 (3H, s), 1.30 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 162.0, 133.8, 131.7, 128.5, 125.0, 38.8, 27.3, 14.1 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{17}NO_2Br$ $[M + H]^+$ 298.0443, found 298.0430.

*1-(4-Chlorophenyl)ethan-1-one O-Pivaloyl Oxime (**1g**).* Isolated as a white amorphous solid (2.15 g, 8.5 mmol, 85% yield); $R_f = 0.3$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.68 (2H, d, J = 8.7 Hz), 7.34 (2H, d, J = 8.7 Hz), 2.34 (3H, s), 1.32 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 161.9, 136.7, 133.3, 128.8, 128.3, 38.8, 27.3, 14.1 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{17}NO_2Cl$ $[M + H]^+$ 254.0948, found 254.0966.

*1-(2-Chlorophenyl)ethan-1-one O-Pivaloyl Oxime (**1h**).* Isolated as a colorless oil (2.15 g, 8.5 mmol, 85% yield); $R_f = 0.3$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.37−7.19 (4H, m), 2.32 (3H, s), 1.29 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.7, 164.5, 135.2, 132.3, 130.7, 130.4, 129.9, 126.9, 38.8, 27.3, 17.7 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{17}NO_2Cl$ $[M + H]^+$ 254.0948, found 254.0956.

*1-(3-Chlorophenyl)ethan-1-one O-Pivaloyl Oxime (**1i**).* Isolated as a white amorphous solid (2.15 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.73−7.71 (1H, m), 7.60−7.57 (1H, m), 7.37−7.26 (2H, m), 2.32 (3H, s), 1.30 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.8, 161.8, 136.7, 134.6, 130.5, 129.8, 127.0, 125.1, 38.8, 27.2, 14.2 ppm; HRMS (ESI) *m/z* calculated for $C_{13}H_{16}NaNO_2Cl$ $[M + Na]^+$ 276.0767, found 276.0778.

*1-(4-Methoxyphenyl)ethan-1-one O-Pivaloyl Oxime (**1j**).* Isolated as a colorless oil (2.12 g, 8.5 mmol, 85% yield); $R_f = 0.3$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.75−7.71 (2H, m), 6.92−6.88 (2H, m), 3.82 (3H, s), 2.34 (3H, s), 1.33 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.1, 162.5, 161.5, 128.5, 127.2, 113.8, 55.3, 38.8, 27.3, 14.1 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{20}NO_3$ $[M + H]^+$ 250.1443, found 250.1455.

*1-(2-Methoxyphenyl)ethan-1-one O-Pivaloyl Oxime (**1k**).* Isolated as a yellow oil (2.12 g, 8.5 mmol, 85% yield); $R_f = 0.3$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.42−7.34 (2H, m), 6.98−6.89 (2H, m), 3.83 (3H, s), 2.32 (3H, s), 1.33 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.0, 165.4, 157.5, 131.1, 130.0, 125.3, 120.6, 110.9, 55.4, 38.8, 27.3, 17.3 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{20}NO_3$ $[M + H]^+$ 250.1443, found 250.1442.

*1-(3-Methoxyphenyl)ethan-1-one O-Pivaloyl Oxime (**1l**).* Isolated as yellow oil (2.12 g, 8.5 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.25−7.17 (3H, m), 6.90−6.86 (1H, m), 3.72 (3H, s), 2.27 (3H, s), 1.26 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 163.0, 159.6, 136.2, 129.4, 119.5, 116.5, 112.0, 55.2, 38.7, 27.2, 14.3 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{20}NO_3$ $[M + H]^+$ 250.1443, found 250.1455.

*1-(Phenyl-d_5)ethan-1-one O-Pivaloyl Oxime (**1a−d₅**).* Isolated as a white amorphous solid (381 mg, 1.7 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ2.39 (3H, s), 1.34 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.1, 163.1, 38.8, 27.3, 14.4 ppm.

*(Z)-1-Phenylethan-2,2,2-d_3-1-one O-Pivaloyl Oxime (**1a−d_3**).* Isolated as a white amorphous solid (377 mg, 1.7 mmol, 85% yield); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.77−7.74 (2H, m), 7.43−7.26 (3H, m), 1.34 (9H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.1, 134.9, 130.5, 128.5, 127.0, 38.8, 27.3 ppm;

*(Z)-1-Phenylpropan-1-one O-Pivaloyl Oxime (**3a**).* Isolated as a colorless oil (1.98 g, 8.5 mmol, 85% yield); $R_f = 0.5$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.70−7.67 (2H, m), 7.36−7.32 (3H, m), 2.77 (2H, q, J = 7.5 Hz), 1.28 (9H, s), 1.14 (3H, t, J = 7.8 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 167.8, 133.9, 130.4, 128.5, 127.1, 38.7, 27.2, 21.8, 11.2 ppm; HRMS (ESI) *m/z* calculated for $C_{14}H_{20}NO_2$ $[M + H]^+$ 234.1494, found 234.1478.

*(Z)-2-Methyl-1-phenylpropan-1-one O-Pivaloyl Oxime (**3b**).* Isolated as a colorless oil (2.10 g, 8.5 mmol, 85% yield); mixture of two isomers (ratio = 1:1); $R_f = 0.4$ (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40−7.37 (2H, m), 7.33−7.27 (6H, m), 7.08−7.05 (2H, m), 3.48−3.38 (1H, m), 2.98−2.89 (1H, m), 1.27 (9H, s), 1.17 (6H, d, J = 7.5 Hz), 1.12 (6H, d, J = 6.9 Hz), 0.91 (9H, s), ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 175.1, 174.8, 173.8, 173.0, 172.2, 134.1, 133.1, 129.3, 128.6, 128.1, 128.0, 127.9, 126.6, 40.1, 38.6, 38.3, 34.8, 30.0, 27.3, 26.8, 26.4, 19.7, 19.5 ppm; HRMS (ESI) *m/z* calculated for $C_{15}H_{22}NO_2$ $[M + H]^+$ 248.1651, found 248.1681.

*Diphenylmethanone O-Pivaloyl Oxime (**3c**).* Isolated as a white amorphous solid (2.39 g, 8.5 mmol, 85% yield); $R_f = 0.2$ (petroleum ether:EtOAc = 20:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 7.63−7.60 (2H, m), 7.46−7.27 (8H, m), 1.08 (9H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 175.1, 165.6, 134.6, 132.8, 130.9, 129.4, 128.9, 128.5, 128.3, 128.1, 38.5, 26.9 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{20}NO_2$ [M + H]$^+$ 282.1494, found 282.1482.

*Methyl (E)-2-Phenyl-2-((pivaloyloxy)imino)acetate (**5a**).* Isolated as a colorless oil (1.71 g, 8.5 mmol, 85% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 3.86 (3H, s), 2.20 (3H, s), 1.29 (9H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 173.9, 163.6, 156.2, 53.1, 38.8, 27.1, 12.8 ppm; HRMS (ESI) m/z calculated for $C_9H_{15}NaNO_4$ [M + Na]$^+$ 224.0899, found 224.0895.

*(Z)-2-Methyl-1-phenylprop-2-en-1-one O-Pivaloyl Oxime (**5d**).* Compound **5d** was prepared according to Rovis's procedure.[22b] Isolated as a colorless oil (1.56 g, 8.5 mmol, 85% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 5.51 (1H, s), 5.40 (1H, s), 2.09 (3H, s), 2.01 (3H, s), 1.27 (9H, s) ppm.

General Procedure for Self-Coupling of Acetophenone Oxime Pivalates. Oxime ester (0.25 mmol), Pd(OAc)$_2$ (5.7 mg, 0.025 mmol), and 3 mL of anhydrous toluene were added to a sealed tube under N$_2$. The reaction mixture was heated to 150 °C (oil bath) for 36 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford the isoquinoline product.

*1-Methyl-3-phenylisoquinoline (**2a**).* Isolated as a yellow oil (23 mg, 0.11 mmol, 84% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.16−8.11 (3H, m), 7.92 (1H, s), 7.85 (1H, d, J = 8.1 Hz), 7.69−7.64 (1H, m), 7.59−7.37 (4H, m), 3.05 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.5, 150.0, 139.9, 136.8, 130.0, 128.7, 128.3, 127.6, 127.0, 126.7, 126.6, 125.6, 115.2, 22.7 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{14}N$ [M + H]$^+$ 220.1126, found 220.1150.

*1,6-Dimethyl-3-(p-tolyl)isoquinoline (**2b**).* Isolated as a yellow oil (22 mg, 0.09 mmol, 72% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.04−7.80 (3H, m), 7.80 (1H, s), 7.60 (1H, s), 7.39−7.25 (3H, m), 3.00 (3H, s), 2.54 (3H, s), 2.42 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.1, 150.1, 140.1, 138.0, 137.2, 137.1, 129.4, 128.7, 126.8, 126.5, 125.5, 124.9, 114.3, 22.6, 21.8,21.2 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}N$ [M + H]$^+$ 248.1439, found 248.1430.

*Methyl 3-(4-(Methoxycarbonyl)phenyl)-1-methylisoquinoline-6-carboxylate (**2c**).* Isolated as a white amorphous solid (27 mg, 0.08 mmol, 64% yield); R_f = 0.2 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.60 (1H, s), 8.23−8.14 (6H, m), 8.06 (1H, s), 4.01 (3H, s), 3.95 (3H, s), 3.06 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 167.0, 166.4, 159.0, 149.5, 143.5, 136.0, 131.4, 130.5, 130.1, 130.0, 128.4, 126.8, 126.7, 126.0, 116.7, 52.5, 52.1, 22.7 ppm; HRMS (ESI) m/z calculated for $C_{20}H_{18}NO_4$ [M + H]$^+$ 336.1236, found 336.1222.

*1-Methyl-6-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-isoquinoline (**2d**).* Isolated as a yellow oil (26 mg, 0.07 mmol, 59% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.28−8.18 (4H, m), 8.04 (1H, s), 7.79−7.75 (3H, m), 3.08 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 159.2, 149.7, 142.4, 135.8, 132.2, 130.4 (q, J = 198.0 Hz), 129.1 (q, J = 209.8 Hz), 127.2, 126.9, 126.0, 125.7 (q, J = 3.8 Hz), 125.4 (q, J = 4.5 Hz), 123.0 (q, J = 3.0 Hz), 121.9, 116.1, 22.7 ppm; ^{19}F NMR (282 MHz, CDCl$_3$): δ −62.6, −63.1 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{12}NF_6$ [M + H]$^+$ 356.0874, found 356.0881.

*6-Fluoro-3-(4-fluorophenyl)-1-methylisoquinoline (**2e**).* Isolated as a gray amorphous solid (28 mg, 0.11 mmol, 88% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.16−8.08 (3H, m), 7.80 (1H, s), 7.45−7.41 (1H, m), 7.34−7.29 (1H, m), 7.20−7.14 (2H, m), 3.01 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 164.9 (d, J = 9.5 Hz), 161.6 (d, J = 13.3 Hz), 158.5, 150.0, 138.5 (d, J = 10.3 Hz), 135.5, 128.8 (d, J = 8.3 Hz), 128.7 (d, J = 9.6 Hz), 123.7, 117.0 (d, J = 25.0 Hz), 115.6 (d, J = 21.5 Hz), 114.4 (d, J = 5.0 Hz), 110.7 (d, J = 20.5 Hz), 22.7 ppm; ^{19}F NMR (282 MHz, CDCl$_3$): δ −108.5, −113.7 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{12}NF_2$ [M + H]$^+$ 256.0938, found 256.0933.

*6-Bromo-3-(4-bromophenyl)-1-methylisoquinoline (**2f**).* Isolated as a gray amorphous solid (33 mg, 0.09 mmol, 70% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.01−7.95 (4H, m), 7.77 (1H, s), 7.65−7.59 (3H, m), 2.99 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.9, 149.8, 138.2, 137.9, 131.9, 130.4, 129.6, 128.5, 127.4, 125.1, 124.9, 123.1, 113.9, 22.6 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{12}NBr_2$ [M + H]$^+$ 375.9336, found 375.9304.

*6-Chloro-3-(4-chlorophenyl)-1-methylisoquinoline (**2g**).* Isolated as a gray amorphous solid (27 mg, 0.10 mmol, 76% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.09−8.03 (3H, m), 7.82−7.78 (2H, m), 7.52−7.44 (3H, m), 3.00 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.7, 149.9, 137.8, 137.6, 136.3, 134.7, 128.9, 128.2, 127.9, 127.4, 126.3, 124.9, 114.1, 22.6 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{12}NCl_2$ [M + H]$^+$ 288.0347, found 288.0358.

*8-Chloro-3-(2-chlorophenyl)-1-methylisoquinoline (**2h**).* Isolated as a white amorphous solid (18 mg, 0.06 mmol, 51% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 7.86 (1H, s), 7.77−7.65 (3H, m), 7.55−7.48 (2H, m), 7.40−7.30 (2H, m), 3.36 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.1, 148.9, 139.1, 138.6, 132.5, 132.4, 131.9, 130.24, 130.2, 129.6, 129.4, 127.4, 127.0, 124.8, 120.4, 29.4 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{12}NCl_2$ [M + H]$^+$ 288.0347, found 288.0364.

*7-Chloro-3-(3-chlorophenyl)-1-methylisoquinoline (**2i**).* Isolated as a white amorphous solid (29 mg, 0.10 mmol, 81% yield); R_f = 0.7 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.15−8.09 (2H, m), 8.01−7.97 (1H, m), 7.87 (1H, s), 7.80 (1H, d, J = 8.7 Hz), 7.64−7.60 (1H, m), 7.45−7.35 (2H, m), 3.00 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 157.9, 148.8, 141.2, 134.9, 134.8, 132.6, 131.1, 129.9, 129.3, 128.5, 127.3, 127.1, 124.9, 124.8, 115.0, 22.6 ppm; HRMS (ESI) m/z calculated for $C_{16}H_{12}NCl_2$ [M + H]$^+$ 288.0347, found 288.0342.

*6-Methoxy-3-(4-methoxyphenyl)-1-methylisoquinoline (**2j**).* Isolated as a yellow oil (19 mg, 0.07 mmol, 55% yield); R_f = 0.2 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.08−7.98 (3H, m), 7.75 (1H, s), 7.17−7.13 (1H, m), 7.08−7.00 (3H, m), 3.95 (3H, s), 3.87 (3H, s), 2.96 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 160.6, 160.0, 157.7, 150.4, 138.9, 132.7, 128.2, 127.4, 121.9, 119.0, 114.1, 113.7, 105.0, 55.4, 55.3, 22.5 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO_2$ [M + H]$^+$ 280.1338, found 280.1354.

*8-Methoxy-3-(2-methoxyphenyl)-1-methylisoquinoline (**2k**).* Isolated as a yellow oil (22 mg, 0.08 mmol, 63% yield); R_f = 0.2 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 7.98−7.95 (2H, m), 7.54−7.49 (1H, m), 7.38−7.32 (2H, m), 7.13−7.08 (1H, m), 7.01 (1H, d, J = 8.4 Hz), 6.86 (1H, d, J = 7.8 Hz), 3.99 (3H, s), 3.88 (3H, s), 3.16 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 158.1, 157.8, 157.3, 147.8, 139.2, 131.4, 129.9, 129.2, 121.1, 120.1, 119.5, 119.1, 111.6, 106.0, 55.7, 55.4, 28.9 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO_2$ [M + H]$^+$ 280.1338, found 280.1322.

*7-Methoxy-3-(3-methoxyphenyl)-1-methylisoquinoline (**2i**).* Isolated as a yellow oil (21 mg, 0.07 mmol, 59% yield); R_f = 0.2 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 7.89 (1H, s), 7.82−7.69 (3H, m), 7.45−7.30 (3H, m), 6.98−6.95 (1H, m), 4.01 (3H, s), 3.95 (3H, s), 3.03 (3H, s) ppm; ^{13}C NMR (75 MHz, CDCl$_3$): δ 160.1, 158.2, 156.8, 148.1, 141.5, 132.2, 129.7, 129.2, 127.7, 122.7, 119.2, 115.2, 113.9, 112.1, 103.6, 55.5, 55.4, 22.8 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO_2$ [M + H]$^+$ 280.1338, found 280.1328.

General Procedure for Cross-Coupling of the Oxime Esters. Ethyl or phenyl aryl oxime ester (0.125 mmol), acetophenone oxime ester (0.375 mmol), Pd(OAc)$_2$ (11.4 mg, 0.05 mmol), and 6 mL of anhydrous toluene were added to a sealed tube under N$_2$. The reaction mixture was heated to 150 °C (oil bath) for 24 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford the isoquinoline product.

*1,3-Diphenylisoquinoline (**4a**).* Isolated as a yellow oil (21 mg, 0.08 mmol, 60% yield); R_f = 0.6 (petroleum ether:EtOAc = 20:1); ^{1}H NMR (300 MHz, CDCl$_3$): δ 8.24−8.20 (2H, m), 8.15−8.12 (1H, m), 8.08 (1H, s), 7.95−7.92 (1H, m), 7.84−7.80 (2H, m), 7.71−7.66 (1H, m), 7.57−7.45 (6H, m), 7.44−7.38 (1H, m) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 160.4, 150.2, 139.9, 139.6, 137.8, 130.2, 130.0, 128.7, 128.6, 128.4, 128.3, 127.5, 127.4, 127.1, 126.9, 125.8, 115.7 ppm; HRMS (ESI) m/z calculated for $C_{21}H_{16}N$ $[M + H]^+$ 282.1283, found 282.1282.

3-(4-Chlorophenyl)-1-phenylisoquinoline (***4b***). Isolated as a yellow oil (29 mg, 0.09 mmol, 74% yield); R_f = 0.5 (petroleum ether:EtOAc = 20:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.19−8.11 (3H, m), 8.04 (1H, s), 7.92 (1H, d, J = 6 Hz), 7.81−7.78 (2H, m), 7.71−7.66 (1H, m), 7.59−7.44 (6H, m), ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 160.5, 148.9, 139.7, 138.0, 137.7, 134.5, 130.2, 130.1, 128.8, 128.7, 128.29, 128.28, 127.6, 127.4, 127.1, 125.9, 115.6 ppm; HRMS (ESI) m/z calculated for $C_{21}H_{15}NCl$ $[M + H]^+$ 316.0893, found 316.0908.

3-(4-Fluorophenyl)-1-phenylisoquinoline (***4c***). Isolated as a yellow oil (26 mg, 0.09 mmol, 70% yield); R_f = 0.3 (petroleum ether:EtOAc = 20:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22−8.11 (3H, m), 8.02 (1H, s), 7.92 (1H, d, J = 8.4 Hz), 7.82−7.78 (2H, m), 7.71−7.66 (1H, m), 7.59−7.48 (4H, m), 7.20−7.15 (2H, m) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 164.9, 161.6, 160.4, 149.2, 139.7, 137.8, 135.7 (d, J = 3.2 Hz), 130.14, 130.13, 128.8, 128.7 (d, J = 6.8 Hz), 128.3, 127.5 (d, J = 15.4 Hz), 126.9, 125.7, 115.5 (d, J = 21.5 Hz) 115.3 (d, J = 0.8 Hz) ppm; ^{19}F NMR (282 MHz, $CDCl_3$): δ −114.0 ppm; HRMS (ESI) m/z calculated for $C_{21}H_{15}NF$ $[M + H]^+$ 300.1189, found 300.1179.

1-Ethyl-3-phenylisoquinoline (***4d***). Isolated as a yellow oil (19 mg, 0.08 mmol, 65% yield); R_f = 0.7 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.20−8.16 (3H, m), 7.92 (1H, s), 7.86 (1H, d, J = 8.1 Hz), 7.68−7.63 (1H, m), 7.59−7.47 (3H, m), 7.42−7.37 (1H, m), 3.41 (2H, q, J = 7.5 Hz), 1.53 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.7, 149.8, 140.0, 137.1, 129.7, 128.7, 128.2, 127.8, 126.9, 126.6, 125.9, 125.2, 114.9, 28.5, 13.3 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{16}N$ $[M + H]^+$ 234.1283, found 234.1282.

1-Ethyl-3-(p-tolyl)isoquinoline (***4e***). Isolated as a white amorphous solid (16 mg, 0.06 mmol, 51% yield); R_f = 0.8 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.19 (1H, d, J = 8.4 Hz), 8.11 (2H, d, J = 8.1 Hz), 7.92 (1H, s), 7.88 (1H, d, J = 8.1 Hz), 7.70−7.55 (2H, m), 7.33 (2H, d, J = 8.4 Hz), 3.43 (2H, q, J = 7.5 Hz), 2.46 (3H, s), 1.55 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.0, 162.7, 149.9, 138.2, 137.1, 129.7, 129.4, 127.8, 126.8, 126.5, 125.7, 125.2, 114.5, 28.5, 21.3, 13.4 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}N$ $[M + H]^+$ 248.1439, found 248.1423.

Methyl 4-(1-Ethylisoquinolin-3-yl)benzoate (***4f***). Isolated as a colorless oil (26 mg, 0.09 mmol, 71% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.29−8.14 (5H, m), 7.99 (1H, s), 7.88 (1H, d, J = 7.8 Hz), 7.70−7.56 (2H, m), 3.95 (3H, s), 3.41 (2H, q, J = 7.5 Hz), 1.53 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.1, 163.0, 148.4, 144.2, 136.8, 130.0, 129.6, 128.0, 127.2, 126.7, 126.2, 125.2, 115.8, 52.1, 28.4, 13.2 ppm; HRMS (ESI) m/z calculated for $C_{19}H_{18}NO_2$ $[M + H]^+$ 292.1338, found 292.1331.

1-Ethyl-3-(4-(trifluoromethyl)phenyl)isoquinoline (***4g***). Isolated as a yellow oil (25 mg, 0.08 mmol, 66% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.35−8.26 (2H, m), 8.25−8.15 (1H, m), 7.97−7.85 (2H, m), 7.76−7.55 4H, m), 3.41 (2H, q, J = 7.5 Hz), 1.53 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.1, 148.1, 143.3, 136.8, 130.0, 128.0 (q, J = 275.7 Hz), 127.9, 127.3, 127.1 (2C), 126.3, 125.6 (q, J = 3.8 Hz), 125.2, 115.7, 28.4, 13.2 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): δ −62.5 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{15}NF_3$ $[M + H]^+$ 302.1157, found 302.1148.

1-Ethyl-3-(4-fluorophenyl)isoquinoline (***4h***). Isolated as a yellow oil (19 mg, 0.08 mmol, 61% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.25−8.10 (3H, m), 7.95−7.80 (2H, m), 7.74−7.58 (2H, m), 7.25−7.15 (2H, m), 3.51 (2H, q, J = 7.2 Hz, 6.9 Hz), 1.54 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.0, 163.2, 161.7, 148.0, 137.3, 130.8, 129.1 (d, J = 8.4 Hz), 128.5 (d, J = 9.1 Hz), 127.9, 127.3, 126.7, 125.7, 125.5, 115.7 (d, J = 21.5 Hz) 27.8, 13.7 ppm; ^{19}F NMR (282 MHz, $CDCl_3$): δ −113.6 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{15}NF$ $[M + H]^+$ 252.1189, found 252.1186.

3-(4-Bromophenyl)-1-ethylisoquinoline (***4i***). Isolated as a yellow oil (20 mg, 0.06 mmol, 51% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18−8.15 (1H, m), 8.09−8.04 (2H, m), 7.89 (1H, s), 7.84 (1H, d, J = 8.1 Hz), 7.68−7.54 (4H, m), 3.39 (2H, q, J = 7.5 Hz), 1.52 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.9, 148.5, 138.8, 136.9, 131.7, 129.9, 128.5, 127.8, 126.9, 126.0, 125.2, 122.6, 114.8, 28.4, 13.2 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{15}NBr$ $[M + H]^+$ 312.0386, found 312.0388.

3-(4-Chlorophenyl)-1-ethylisoquinoline (***4j***). Isolated as a slightly yellow oil (21 mg, 0.08 mmol, 63% yield); R_f = 0.7 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18−8.11 (3H, m), 7.89 (1H, s), 7.87−7.84 (1H, m), 7.69−7.55 (2H, m), 7.48−7.44 (2H, m), 3.39 (2H, q, J = 7.5 Hz), 1.52 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.9, 148.5, 138.4, 136.9, 134.3, 129.9, 128.8, 128.1, 127.8, 126.9, 126.0, 126.2, 114.8, 28.4, 13.2 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{15}NCl$ $[M + H]^+$ 268.0893, found 268.0884.

3-(2-Chlorophenyl)-1-ethylisoquinoline (***4k***). Isolated as a yellow oil (13 mg, 0.05 mmol, 39% yield); R_f = 0.3 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.20 (1H, d, J = 8.4 Hz), 7.88 (1H, s), 7.85 (1H, s), 7.74−7.59 (3H, m), 7.52−7.49 (1H, m), 7.41−7.29 (2H, m), 3.40 (2H, q, J = 7.5 Hz, 7.8 Hz), 1.49 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.0, 149.1, 139.6, 136.3, 132.6, 132.0, 130.2, 129.9, 129.0, 127.8, 127.2, 126.9, 125.6, 125.2, 119.8, 28.6, 14.0 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{15}NCl$ $[M + H]^+$ 268.0893, found 268.0866.

3-(3-Chlorophenyl)-1-ethylisoquinoline (***4l***). Isolated as a slightly yellow oil (24 mg, 0.09 mmol, 71% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.21−8.19 (1H, m), 8.16 (1H, s), 8.07−8.03 (1H, m), 7.91 (1H, s), 7.86 (1H, d, J = 7.8 Hz), 7.69−7.55 (2H, m), 7.44−7.35 (2H, m), 3.39 (2H, q, J = 7.5 Hz), 1.52 (3H, t, J = 7.8 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.0, 148.2, 141.8, 136.9, 134.7, 129.94, 129.85, 128.2, 127.9, 127.1, 127.0, 126.1, 125.2, 124.9, 115.2, 28.4, 13.3 ppm; HRMS (ESI) m/z calculated for $C_{17}H_{15}NCl$ $[M + H]^+$ 268.0893, found 268.0888.

1-Ethyl-3-(4-methoxyphenyl)isoquinoline (***4m***). Isolated as a slightly yellow oil (11 mg, 0.04 mmol, 34% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15−8.11 (3H, m), 7.83 (1H, s), 7.81 (1H, s), 7.65−7.49 (2H, m), 7.04−7.01 (2H, m), 3.87 (3H, s), 3.38 (2H, q, J = 7.5 Hz), 1.51 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.2, 160.0, 149.5, 137.2, 132.0, 129.7, 128.1, 127.6, 126.3, 125.5, 125.1, 114.1, 113.8, 55.4, 28.4, 13.3 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO$ $[M + H]^+$ 264.1383, found 264.1398.

1-Ethyl-3-(2-methoxyphenyl)isoquinoline (***4n***). Isolated as a yellow oil (9 mg, 0.03 mmol, 27% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (1H, d, J = 8.4 Hz), 8.09 (1H, s), 8.02−7.99 (1H, m), 7.84 (1H, d, J = 8.1 Hz), 7.67−7.53 (2H, m), 7.39−7.33 (1H, m), 7.14−7.02 (2H, m), 3.90 (3H, s), 3.39 (2H, q, J = 7.5 Hz), 1.49 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.4, 157.2, 136.7, 131.5, 129.51, 129.49, 129.47, 129.2, 128.0, 126.6, 125.4, 125.1, 121.1, 119.8, 111.6, 55.7, 28.5, 13.8 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO$ $[M + H]^+$ 264.1383, found 264.1379.

1-Ethyl-3-(3-methoxyphenyl)isoquinoline (***4o***). Isolated as a slightly yellow oil (15 mg, 0.06 mmol, 46% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (1H, d, J = 8.4 Hz), 7.91 (1H, s), 7.86 (1H, d, J = 8.1 Hz), 7.80−7.72 (2H, m), 7.68−7.53 (2H, m), 7.43−7.38 (1H, m), 6.97−6.93 (1H, m), 3.92 (3H, s), 3.40 (2H, q, J = 7.5 Hz), 1.52 (3H, t, J = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.7, 160.1, 149.5, 137.0, 129.82, 129.78, 129.6, 127.8, 126.7, 126.0, 125.2, 119.3, 115.1, 114.0, 112.5, 55.3, 28.4, 13.3 ppm; HRMS (ESI) m/z calculated for $C_{18}H_{18}NO$ $[M + H]^+$ 264.1383, found 264.1408.

1-Isopropyl-3-phenylisoquinoline (***4p***). Isolated as a yellow oil (12 mg, 0.05 mmol, 39% yield); R_f = 0.5 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.32−8.22 (3H, m), 7.97 (1H, s), 7.90 (1H, d, J = 8.1 Hz), 7.70−7.65 (1H, m), 7.61−7.50 (3H, m), 7.48−7.38 (1H, m), 4.06−3.97 (1H, m), 1.55 (6H, d, J = 6.9 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.8, 165.0, 149.3, 137.3, 129.5, 128.7, 128.3, 128.0, 126.8, 126.6, 125.4, 124.8, 114.4, 31.4, 22.3 ppm; HRMS (ESI) *m*/*z* calculated for $C_{18}H_{18}N$ $[M + H]^+$ 248.1439, found 248.1449.

1-Isopropyl-3-(p-tolyl)isoquinoline (**4q**). Isolated as a yellow oil (10 mg, 0.04 mmol, 31% yield); R_f = 0.8 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22–8.12 (3H, m), 7.89 (1H, s), 7.84 (1H, d, *J* = 8.1 Hz), 7.65–7.50 (2H, m), 7.32–7.29 (2H, m), 4.01–3.92 (1H, m), 2.42 (3H, s), 1.50 (6H, d, *J* = 6.6 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.6, 149.3, 138.1, 137.3, 129.4, 129.3, 127.9, 126.7, 126.3, 125.2, 124.7, 113.9, 105.0, 31.4, 22.3, 21.3 ppm; HRMS (ESI) *m*/*z* calculated for $C_{19}H_{20}N$ $[M + H]^+$ 262.1596, found 262.1585.

1-Isopropyl-3-(3-methoxyphenyl)isoquinoline (**4r**). Isolated as a yellow oil (8 mg, 0.03 mmol, 23% yield); R_f = 0.4 (petroleum ether:EtOAc = 20:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.21 (1H, d, *J* = 8.4 Hz), 7.92 (1H, s), 7.89–7.78 (3H, m), 7.66–7.53 (2H, s), 7.43–7.38 (1H, m), 6.97–6.93 (1H, m), 4.02–3.93 (1H, m), 3.93 (3H, s), 1.51 (6H, d, *J* = 6.9 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.7, 160.0, 148.9, 141.5, 137.2, 129.6, 129.5, 128.0, 126.6, 125.4, 124.7, 119.2, 114.5, 113.9, 112.5, 55.3, 31.4, 22.3 ppm; HRMS (ESI) *m*/*z* calculated for $C_{19}H_{20}NO$ $[M + H]^+$ 278.1545, found 278.1536.

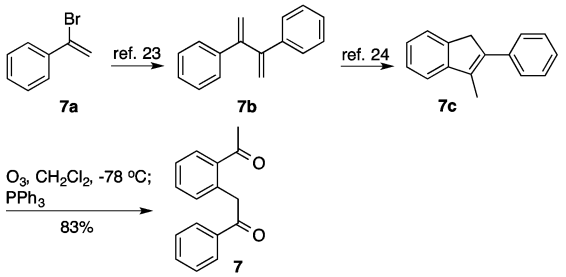
General Procedure for Synthesis of 6a and 6b. Ethyl or phenyl aryl oxime ester (0.125 mmol), methyl pyruvate oxime ester (25 mg, 0.125 mmol), $Pd(OAc)_2$ (5.7 mg, 0.025 mmol), and 3 mL of anhydrous toluene were added to a sealed tube under N_2. The reaction mixture was heated to 150 °C (oil bath) for 12 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford the isoquinoline product.

Methyl 1-Ethylisoquinoline-3-carboxylate (**6a**). Isolated as a yellow oil (11 mg, 0.05 mmol, 41% yield); R_f = 0.4 (petroleum ether:EtOAc = 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.44 (1H, s), 8.24–8.21 (1H, m), 7.97–7.94 (1H, m), 7.77–7.69 (2H, m), 4.04 (3H, s), 3.41 (2H, q, *J* = 7.5 Hz), 1.45 (3H, t, *J* = 7.5 Hz) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.6, 164.1, 140.6, 135.9, 130.4, 129.3, 128.9, 128.1, 125.5, 122.9, 52.8, 29.0, 14.1 ppm; HRMS (ESI) *m*/*z* calculated for $C_{13}H_{14}NO_2$ $[M + H]^+$ 216.1025, found 216.1020.

Methyl 1-Phenylisoquinoline-3-carboxylate (**6b**). Isolated as a gray amorphous solid (15 mg, 0.06 mmol, 59% yield); R_f = 0.4 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.59 (1H, s), 8.13 (1H, d, *J* = 8.4 Hz), 8.02 (1H, d, *J* = 8.1 Hz), 7.80–7.63 (4H, m), 7.56–7.49 (3H, m), 4.04 (3H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.6, 161.2, 140.9, 138.9, 136.6, 130.7, 130.1, 129.4, 128.9, 128.43, 128.38, 128.2, 127.8, 123.3, 52.8 ppm; HRMS (ESI) *m*/*z* calculated for $C_{17}H_{14}NO_2$ $[M + H]^+$ 264.1025, found 264.1024.

Methyl 1-Methylisoquinoline-3-carboxylate (6c). Acetophenone oxime ester (82 mg, 0.375 mmol), methyl pyruvate oxime ester (25 mg, 0.125 mmol), $Pd(OAc)_2$ (11.4 mg, 0.05 mmol), and 6 mL of anhydrous toluene were added to a sealed tube under N_2. The reaction mixture was heated to 150 °C (oil bath) for 12 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford **6c** as a gray amorphous solid (16 mg, 0.08 mmol, 64% yield); R_f = 0.2 (petroleum ether:EtOAc = 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.46 (1H, s), 8.20–8.16 (1H, m), 7.96–7.93 (1H, m), 7.79–7.70 (2H, m), 4.04 (3H, s), 3.04 (3H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.5, 159.4, 140.4, 135.5, 130.7, 129.4, 129.0, 128.7, 125.8, 123.0, 52.8, 22.7 ppm; HRMS (ESI) *m*/*z* calculated for $C_{12}H_{12}NO_2$ $[M + H]^+$ 202.1079, found 202.1074.

1-Phenyl-3-(prop-1-en-2-yl)isoquinoline (6d). Benzophenone oxime ester (35 mg, 0.125 mmol), compound **5d** (25 mg, 0.125 mmol), $Pd(OAc)_2$ (5.7 mg, 0.025 mmol), and 3 mL of anhydrous toluene were added to a sealed tube under N_2. The reaction mixture was heated to 150 °C (oil bath) for 12 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford **6d** as a yellow oil (6 mg, 0.03 mmol, 20% yield); R_f = 0.6 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15–8.07 (1H, m), 7.95–7.82 (1H, m), 7.80–7.60 (4H, m), 7.56–7.45 (4H, m), 6.27 (1H, s), 5.34 (1H, s), 2.33 (3H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.5, 150.7, 142.3, 139.9, 137.6, 130.2, 129.8, 128.5, 128.2, 127.5, 127.4, 126.7, 125.8, 115.8, 114.9, 20.5 ppm; HRMS (ESI) *m*/*z* calculated for $C_{18}H_{16}N$ $[M + H]^+$ 246.1283, found 246.1280.



2-(2-Acetylphenyl)-1-phenylethan-1-one (7). Compound **7b** was prepared according to Ogoshi's procedure.[23] Compound **7c** was prepared according to Lee's procedure.[24] A solution of **7c** (206 mg, 1 mmol) in 5 mL of dichloromethane was bubbled with O_3 at −78 °C. After the color of the solution turned to blue (about 5 min), the O_3 was turned off. To the solution was added a solution of PPh_3 (786 mg, 3 mmol) in 10 mL of dichloromethane at −78 °C under a N_2 atmosphere. After 30 min at that temperature, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford **7** (198 mg, 0.83 mmol, 83% yield) as a white amorphous solid; R_f = 0.2 (petroleum ether:EtOAc = 8:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07–8.03 (2H, m), 7.88–7.85 (1H, m), 7.60–7.39 (5H, m), 7.27–7.24 (1H, m), 4.66 (2H, s), 2.58 (3H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 201.2, 197.3, 137.3, 137.1, 135.2, 133.0, 132.9, 132.0, 130.1, 128.6, 128.1, 127.2, 44.6, 28.7 ppm.

2,2-Dimethyl-1-(((1-(2-(2-oxo-2-phenylethyl)phenyl)-ethylidene)amino)oxy)propan-1-one *O*-Pivaloyl Oxime (8). Prepared using the general procedures as described above. Isolated as a colorless gum; mixture of (*E*,*Z*)-isomers (66 mg, 0.15 mmol, 75% yield); R_f = 0.4 (petroleum ether:EtOAc = 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.70–7.58 (3.1H, m), 7.37–7.15 (12.5H, m), 7.05–7.02 (0.6H, m), 4.47 (1.9H, s), 4.41 (0.6H, s), 2.30 (1.4H, s), 2.28 (0.9H, s), 2.23 (2.8H, s), 2.21 (1H, s), 2.16 (2.8H, s), 1.33 (9H, s), 1.22 (4.3H, s), 1.16 (2.6H, s), 0.98 (4.1H, s) ppm; ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.9, 174.7, 168.6, 166.5, 164.7, 164.3, 164.0, 163.6, 135.3, 135.1, 134.9, 134.1, 133.9, 133.7, 133.5, 130.7, 130.6, 130.5, 129.9, 129.8, 129.4, 129.2, 128.8, 128.61, 128.58, 128.53, 127.9, 127.7, 127.6, 127.4, 127.04, 126.95, 126.89, 125.6, 38.8, 38.6, 38.3, 32.6, 32.3, 32.2, 27.3, 27.13, 27.06, 26.9, 22.1, 19.7, 17.6 ppm; HRMS (ESI) *m*/*z* calculated for $C_{26}H_{32}KN_2O_4$ $[M + K]^+$ 475.1999, found 475.1967.

Synthesis of 2a from 8. Bis-oxime ester **8** (66 mg, 0.15 mmol), $Pd(PPh_3)_4$ (175 mg, 0.15 mmol), and 3 mL of anhydrous toluene were added to a sealed tube under N_2. The reaction mixture was heated to 140 °C (oil bath) for 1.5 h. Following cooling to rt, the solvent was evaporated to give a residue, which was purified by flash column chromatography to afford **2a** (18 mg, 0.08 mmol, 55% yield).

Single Time Point Kinetic Experiments Using 1a, 1a–d$_3$, and 1a–d$_5$. The $Pd(OAc)_2$-catalyzed self-coupling of **1a**, **1a–d$_3$**, and **1a–d$_5$** in toluene was carried out under the optimized reaction conditions except for that the reaction was cooled to rt after 2.5 h. The reaction mixture was spotted on a TLC plate and developed using a solvent of hexanes:ethyl acetate (4:1). The TLC plate was air-dried and imaged using the ChemiDoc XRS+ system (Bio-Rad, Hercules, CA, USA) equipped with a trans-UV light source (302 nm) and a supercooled high-resolution CCD camera with 1.44 megapixel resolution. Both **1a**'s and **2a**'s are UV-active. Their UV images were acquired and analyzed by Image Lab software version 3.0 (Bio-Rad, Hercules, CA, USA) using the manufacturer-programed imaging quantification function. The UV adsorption of **2a**'s was quantified and normalized against that of **1a**'s before the relative quantities of **2a**'s were compared. The following ratios were observed: **2a**:**2a–d$_5$** = 1:1.03, **2a**:**2a–d$_3$** = 2.03:1.

■ ASSOCIATED CONTENT

Supporting Information

Experimental procedures and spectra data for all new compounds. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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