Pd(0)-Catalyzed Benzylic Arylation/Oxidation of 4-Methylquinazolines via sp\(^3\) C–H Activation under Air Conditions

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General information
All manipulations were carried out under air atmosphere unless otherwise specified. Pd\((\text{PPh}_3)_4\) and \(\text{Cs}_2\text{CO}_3\) were purchased from Energy Chemical and used without further purification. BINAP was purchased from Adamas-beta and used without further purification. Melting points were measured with an X-4 melting point apparatus (Bei Jing Taike Co., Ltd.). \(^1\)H-NMR and \(^{13}\)C-NMR were determined in CDCl\(_3\) on a Bruker DPX 300 MHz or a Bruker AVANCE III 400 MHz spectrometer at room temperature, respectively, and tetramethylsilane (TMS) served as an internal standard. Spin multiplicities are given as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as brs (broad). Coupling constants \((J)\) are given in hertz (Hz). ESI-MS was carried out on a LCMS-2020 (Shimadzu, Japan). HRMS were recorded on an Agilent 6540Q-TOF LC/MS equipped with electrospray ionization (ESI) probe operating in positive or negative ion mode. All experiments were monitored by thin layer chromatography (TLC). TLC was performed on pre-coated silica gel plates (Qingdao Haiyang Chemical Co., Ltd).

Experimental section
Screening the different palladium catalysts and ligands

\textbf{Table S1} Optimization of the reaction conditions

<table>
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<th>entry</th>
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<th>yield(^b) (%)</th>
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<tr>
<td>1</td>
<td>Pd(OAc)(_2)</td>
<td>P’Bu(_3)-HBF(_4)</td>
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<td>2</td>
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<td>X-Phos</td>
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</tr>
<tr>
<td>6</td>
<td>Pd(\text{PPh}_3)(_2)Cl(_2)</td>
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<td>45</td>
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<tr>
<td>7</td>
<td>Pd(dppf)Cl(_2)</td>
<td></td>
<td>trace</td>
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<tr>
<td>8</td>
<td>Pd(dba)(_2)</td>
<td></td>
<td>trace</td>
</tr>
<tr>
<td>9</td>
<td>Pd(_2)(dba)(_3)</td>
<td></td>
<td>trace</td>
</tr>
<tr>
<td>10</td>
<td>Pd(CH(_3)CN)(_2)Cl(_2)</td>
<td></td>
<td>trace</td>
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</tbody>
</table>

\(^a\)Reaction conditions: 1a (0.3 mmol), 2a (0.6 mmol), catalyst (10 mol%), bidentate ligand (10 mol%) or monodentate ligand (20 mol%), \(\text{Cs}_2\text{CO}_3\) (0.6 mmol) in 3.0 mL of toluene under air atmosphere, 100 °C, 24 h. \(^b\)Isolated yields.

General procedure for the synthesis of products 3a–u:

To a solution of 4-methylquinazoline (0.3 mmol) in toluene (3 mL) was added Pd\((\text{PPh}_3)_4\) (0.1 equiv), BINAP (0.1 equiv), \(\text{Cs}_2\text{CO}_3\) (2.0 equiv) and aryl halide or triflate (2.0 equiv), the
reaction vessel was placed in a preheated oil bath at 100 °C in air. After stirring for 24 h, the reaction mixture was cooled to room temperature, quenched by water (10 mL) and extracted by ethyl acetate (3×10 mL). The organic phase was then washed with brine, dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was then purified by chromatography on silica gel with a eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, ¹H-, ¹³C-NMR and HRMS (ESI).

General procedure for the synthesis of 4-methylquinazolines 1a–e:

Method A¹:

To a solution of 2-aminoacetophenone (20 mmol) and triethylamine (3.3 mL, 1.2 equiv) in dichloromethane (DCM) (60mL) cooled in an ice-water bath, chloride (1.5 equiv) was added dropwise. The progress of the reaction was monitored by TLC. Upon completion, the solution was washed with diluted hydrochloric acid, saturated NaHCO₃, brine, and dried over anhydrous Na₂SO₄. The organic phase was concentrated in vacuo to give amide as an intermediate without further purification. The amide, 25% ammonia water (20 mL) and isopropanol (20 mL) were added to a 250 mL sealed tube. The tube was located in a preheated 90 °C oil bath and stirred for 10h. The reaction mixture was cooled to room temperature, washed with diluted hydrochloric acid, saturated NaHCO₃, brine, and dried over anhydrous Na₂SO₄, then concentrated in vacuo. The residue was then purified by chromatography on silica gel with a eluent of petroleum ether and ethyl acetate. Products were characterized by Mp, ¹H-, ¹³C-NMR and MS (ESI).

Method B²:

To a mixture of 2-aminoacetophenone (20 mmol) and ZnO (0.8 g, 0.5 equiv) in toluene (50 mL) was added HCO₂H (23 mL, 600 mmol) dropwise. The reaction mixture was heated in an oil bath at 80 °C and stirred for 7h. Upon finished the reaction, the mixture was treated to obtain amide which was further reacted with 25% ammonia water to give a residue as described in Method A. The residue was then purified by chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. Product was characterized by Mp, ¹H-, ¹³C-NMR and MS (ESI).
Procedure for the synthesis of 3uu':

To a Schlenk tube were added 4-methyl-2-phenylquinazoline (1d, 1mmol), 1-fluoro-4-nitrobenzene (2 mmol), t-BuOK (2 mmol) and DMSO (5mL). The reaction mixture was stirred at room temperature for 12h. Upon finished the reaction mixture was quenched by water (20 mL) and extracted by ethyl acetate (3×30 mL). Combined organic phase were dried over anhydrous Na₂SO₄, and concentrated in vacuo. The residue was then purified by chromatography on silica gel with a mixture eluent of petroleum ether, ethyl acetate. Product was characterized by Mp, ¹H-, ¹³C-NMR and HRMS (ESI).

Substrate characterizations

2,4-dimethylquinazoline (1a).³ yellow oil, 45% yield for two steps. ¹H NMR (300 MHz, CDCl₃) δ 8.06 (d, J = 8.3 Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.87–7.80 (m, 1H), 7.57 (t, J = 7.6 Hz, 1H), 2.93 (s, 3H), 2.85 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.0, 163.4, 149.8, 133.5, 128.1, 126.5, 124.8, 122.1, 26.3, 21.6; MS (ESI): 159.00 [M+H]+.

4-methylquinazoline (1b).⁴ yellow oil, 54% yield for two steps. ¹H NMR (400 MHz, CDCl₃) δ 9.18 (s, 1H), 8.15–8.07 (m, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.89 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.65 (sdd, J = 8.2, 6.9, 1.2 Hz, 1H), 2.97 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.1, 154.4, 149.4, 133.5, 128.9, 127.5, 124.9, 124.3, 21.7; MS (ESI): 145.05 [M+H]+.

4-methyl-2-propylquinazoline (1c).⁵ colorless oil, 73% yield for two steps. ¹H NMR (400 MHz, CDCl₃) δ 8.06 (d, J = 8.3 Hz, 1H), 7.96 (d, J = 8.4 Hz, 1H), 7.83 (t, J = 7.7 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 3.08–3.01 (m, 2H), 2.93 (s, 3H), 2.01–1.86 (m, 2H), 1.05 (t, J = 7.4 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.1, 166.8, 149.9, 133.5, 128.5, 126.6, 124.9, 122.5, 42.0, 22.4, 21.7, 14.1; MS (ESI): 187.10 [M+H]+.
4-methyl-2-phenylquinazoline (1d). A white solid, 76% yield for two steps, mp. 84–85 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.63 (dd, $J$ = 7.9, 1.8 Hz, 2H), 8.09 (d, $J$ = 8.3 Hz, 2H), 7.87 (ddd, $J$ = 8.5, 6.9, 1.3 Hz, 1H), 7.46–7.45 (m, 4H), 3.02 (s, 3H); $^{13}$C NMR (75 MHz, CDCl$_3$) 168.1, 160.0, 150.2, 138.2, 133.4, 130.3, 129.1, 128.5, 128.5, 126.7, 124.8, 122.8, 21.9; MS (ESI): 221.00 [M+H]$^+$.

2-cyclohexyl-4-methylquinazoline (1e). A yellow solid, 66% yield for two steps, mp. 46–48 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.08–8.00 (m, 1H), 7.96 (d, $J$ = 8.4 Hz, 1H), 7.54 (ddd, $J$ = 8.2, 6.9, 1.1 Hz, 1H), 3.04–2.95 (m, 1H), 2.92 (s, 3H), 2.08–2.04 (m, 2H), 1.95–1.67 (m, 5H), 1.57–1.31 (m, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 170.0, 167.8, 150.0, 133.1, 128.6, 126.3, 124.8, 122.6, 47.9, 31.9, 26.4, 26.0, 21.7; MS (ESI): 227.15 [M+H]$^+$.

Product characterizations

(2-methylquinazolin-4-yl)(4-nitrophenyl)methanone (3a). A yellow solid, 73% yield, mp. 158–161 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.33 (d, $J$ = 8.7 Hz, 2H), 8.16 (d, $J$ = 8.6 Hz, 2H), 8.08 (dd, $J$ = 8.6, 3.9 Hz, 2H), 8.00–7.92 (m, 1H), 7.63 (t, $J$ = 7.6 Hz, 1H), 2.94 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.4, 163.2, 162.0, 152.0, 150.8, 139.9, 134.9, 131.8, 128.6, 128.3, 125.4, 123.7, 119.8, 26.3; HRMS (ESI) m/z calcd for C$_{16}$H$_{12}$N$_3$O$_3$ [M+H]$^+$ 294.0879, found 294.0873.

(2-methylquinazolin-4-yl)(phenyl)methanone (3b). A yellow solid, 76% yield, mp. 143–145 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.05 (d, $J$ = 8.5 Hz, 1H), 7.96–7.89 (m, 4H), 7.68–7.62 (m, 1H),...
7.59–7.53 (m, 1H), 7.49 (t, J = 7.9 Hz, 2H), 2.95 (s, 3H); ^13^C NMR (100 MHz, CDCl$_3$) δ 193.2, 164.6, 163.4, 151.4, 135.2, 134.6, 134.5, 130.6, 128.8, 128.3, 127.7, 125.6, 119.8, 26.4; HRMS (ESI) m/z calcd for C$_{16}$H$_{13}$N$_2$O [M+H]$^+$ 249.1028, found 249.1021.

(2-methylquinazolin-4-yl)(o-tolyl)methanone (3c). yellow solid, 57% yield, mp. 120–123 °C. ^1^H NMR (400 MHz, CDCl$_3$) δ 8.04 (d, J = 8.5 Hz, 1H), 7.99 (dd, J = 8.4, 0.6 Hz, 1H), 7.91 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.57 (ddd, J = 8.2, 6.9, 1.1 Hz, 1H), 7.48 (td, J = 7.5, 1.3 Hz, 1H), 7.37 (dd, J = 7.8, 1.2 Hz, 2H), 7.19 (t, J = 7.5 Hz, 1H), 2.91 (s, 3H), 2.70 (s, 3H); ^13^C NMR (100 MHz, CDCl$_3$) δ 195.6, 165.7, 163.6, 151.5, 141.3, 134.53, 134.45, 133.3, 133.2, 132.4, 128.3, 127.7, 125.693, 125.686, 119.8, 26.4, 22.0; HRMS (ESI) m/z calcd for C$_{17}$H$_{15}$N$_2$O [M+H]$^+$ 263.1184, found 263.1179.

(2-methylquinazolin-4-yl)(m-tolyl)methanone (3d). brown solid, 55% yield, mp. 113–114 °C. ^1^H NMR (400 MHz, CDCl$_3$) δ 8.07–8.03 (m, 1H), 7.93–7.88 (m, 2H), 7.76 (s, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.58–7.52 (m, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 2.95 (s, 3H), 2.39 (s, 3H); ^13^C NMR (100 MHz, CDCl$_3$) δ 193.4, 165.0, 163.4, 151.5, 141.3, 134.53, 134.45, 133.3, 133.2, 132.4, 128.3, 127.7, 130.8, 128.7, 128.3, 128.1, 127.6, 125.7, 119.8, 26.4, 21.3; HRMS (ESI) m/z calcd for C$_{17}$H$_{15}$N$_2$O [M+H]$^+$ 263.1184, found 263.1181.

(2-methylquinazolin-4-yl)(p-tolyl)methanone (3e). yellow solid, 62% yield, mp. 147–150 °C. ^1^H NMR (400 MHz, CDCl$_3$) δ 8.04 (d, J = 8.5 Hz, 1H), 7.95–7.87 (m, 2H), 7.83 (d, J = 8.3 Hz, 2H), 7.58–7.52 (m, 1H), 7.29 (d, J = 8.1 Hz, 2H), 2.95 (s, 3H), 2.43 (s, 3H); ^13^C NMR (100 MHz, CDCl$_3$) δ 192.8, 165.0, 163.4, 151.4, 145.8, 134.5, 132.8, 130.8, 129.5, 128.3, 127.6, 125.7, 119.8, 26.4, 21.9; HRMS (ESI) m/z calcd for C$_{17}$H$_{15}$N$_2$O [M+H]$^+$ 263.1184, found 263.1181.
(4-methoxyphenyl)(2-methylquinazolin-4-yl)methanone (3f). White solid, 63% yield, mp. 135–137 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.03 (d, $J$ = 8.4 Hz, 1H), 7.95–7.84 (m, 4H), 7.54 (t, $J$ = 7.6 Hz, 1H), 6.95 (d, $J$ = 8.9 Hz, 2H), 3.87 (s, 3H), 2.94 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.7, 165.2, 164.8, 163.4, 151.4, 134.5, 133.1, 128.3, 128.2, 127.5, 125.8, 119.9, 114.1, 55.6, 26.4; HRMS (ESI) m/z calcd for C$_{17}$H$_{15}$N$_2$O$_2$ [M+H]+ 279.1134, found 279.1129.

(4-chlorophenyl)(2-methylquinazolin-4-yl)methanone (3g). White solid, 79% yield, mp. 133–135 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.04 (d, $J$ = 8.5 Hz, 1H), 7.98–7.86 (m, 4H), 7.57 (t, $J$ = 7.6 Hz, 1H), 7.49–7.44 (m, 2H), 2.93 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.8, 163.7, 163.3, 151.6, 141.1, 134.6, 133.6, 132.0, 129.1, 128.4, 127.8, 125.5, 119.8, 26.4; HRMS (ESI) m/z calcd for C$_{16}$H$_{12}$ClN$_2$O [M+H]+ 283.0638, found 283.0632.

(4-fluorophenyl)(2-methylquinazolin-4-yl)methanone (3h). White solid, 61% yield, mp. 156–158 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.09–7.87 (m, 5H), 7.61–7.53 (m, 1H), 7.17 (t, $J$ = 8.6 Hz, 2H), 2.94 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.5, 167.9, 165.3, 164.1, 163.3, 151.6, 134.7, 133.5, 133.4, 131.68, 131.65, 128.4, 127.8, 125.6, 119.8, 116.2, 116.0, 26.4; HRMS (ESI) m/z calcd for C$_{16}$H$_{12}$FN$_2$O [M+H]+ 267.0934, found 267.0927.

(2-methylquinazolin-4-yl)(4-(trifluoromethyl)phenyl)methanone (3i). White solid, 66% yield, mp. 143–145 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.14–8.05 (m, 3H), 8.04–8.00 (m, 1H), 7.94 (ddd, $J$
= 8.5, 6.9, 1.4 Hz, 1H), 7.76 (d, J = 8.2 Hz, 2H), 7.60 (ddd, J = 8.2, 7.0, 1.1 Hz, 1H), 2.94 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 192.0, 163.3, 163.0, 151.8, 137.99, 137.98, 135.8, 135.5, 135.2, 134.9, 134.7, 131.0, 128.5, 128.0, 127.5, 125.74, 125.71, 125.67, 125.63, 125.4, 124.8, 122.1, 119.8, 119.4, 26.3; HRMS (ESI) m/z calcd for C\(_{17}\)H\(_{12}\)F\(_3\)N\(_2\)O \([M+H]^+\) 317.0902, found 317.0897.

![Image](image-url)

4-(2-methylquinazoline-4-carbonyl)benzonitrile (3j). yellow solid, 37% yield, mp. 191–193 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 8.14–8.02 (m, 4H), 8.01–7.91 (m, 1H), 7.80 (d, \(J = 8.6\) Hz, 2H), 7.62 (t, \(J = 7.6\) Hz, 1H), 2.94 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 191.6, 163.2, 162.3, 151.9, 138.4, 134.8, 132.4, 131.0, 128.5, 128.2, 125.3, 119.8, 117.8, 117.3, 26.3; HRMS (ESI) m/z calcd for C\(_{17}\)H\(_{12}\)N\(_3\)O \([M+H]^+\) 274.0980, found 274.0977.

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4-(2-methylquinazoline-4-carbonyl)benzaldehyde (3k). yellow solid, 32% yield, mp. 153–155 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 10.14 (s, 1H), 8.18–7.90 (m, 7H), 7.61 (ddd, \(J = 8.2, 6.9, 1.1\) Hz, 1H), 2.95 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 192.4, 191.5, 163.3, 163.1, 151.8, 139.7, 139.6, 134.8, 131.2, 129.7, 128.5, 128.0, 125.4, 119.8, 26.4; HRMS (ESI) m/z calcd for C\(_{17}\)H\(_{13}\)N\(_2\)O\(_2\) \([M+H]^+\) 277.0977, found 277.0967.

![Image](image-url)

methyl 4-(2-methylquinazoline-4-carbonyl)benzoate (3l). white solid, 38% yield, mp. 142–143 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 8.15 (d, \(J = 8.5\) Hz, 2H), 8.09–7.97 (m, 4H), 7.94 (ddd, \(J = 8.4, 6.9, 1.4\) Hz, 1H), 7.63–7.55 (m, 1H), 3.96 (s, 3H), 2.94 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 192.6, 166.0, 163.5, 163.3, 151.7, 138.5, 134.9, 134.7, 130.6, 129.8, 128.4, 127.9, 125.5, 119.8, 52.6, 26.4; HRMS (ESI) m/z calcd for C\(_{18}\)H\(_{15}\)N\(_2\)O\(_3\) \([M+H]^+\) 307.1083, found 307.1086.
benzo[d][1,3]dioxol-5-yl(2-methylquinazolin-4-yl)methanone (3m). yellow solid, 50% yield, mp. 178–180 °C. 1H NMR (400 MHz, CDCl3) δ 8.04 (dd, J = 8.8, 0.8 Hz, 1H), 7.94–7.87 (m, 2H), 7.59–7.53 (m, 1H), 7.52 (d, J = 1.7 Hz, 1H), 7.41 (dd, J = 8.2, 1.7 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 6.08 (s, 2H), 2.95 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 191.3, 165.0, 163.4, 153.2, 151.4, 148.5, 134.5, 130.0, 128.6, 128.3, 127.6, 125.7, 119.8, 109.3, 108.2, 102.2, 26.4; HRMS (ESI) m/z calcd for C17H13N2O3 [M+H]+ 293.0926, found 293.0922.

(2-methylquinazolin-4-yl)(naphthalen-2-yl)methanone (3n). yellow solid, 52% yield, mp. 133–135 °C. 1H NMR (300 MHz, CDCl3) δ 8.29 (s, 1H), 8.14 (dd, J = 8.6, 1.7 Hz, 1H), 8.08 (d, J = 8.5 Hz, 1H), 8.00–7.82 (m, 5H), 7.68–7.47 (m, 3H), 2.98 (s, 3H); 13C NMR (100 MHz, CDCl3) δ 193.2, 164.9, 163.5, 151.5, 136.2, 134.6, 134.1, 132.6, 132.3, 129.9, 129.4, 128.8, 128.3, 127.9, 127.7, 127.0, 125.7, 124.6, 120.0, 26.5; HRMS (ESI) m/z calcd for C20H15N2O [M+H]+ 299.1184, found 299.1182.

(1-ethyl-1H-indol-5-yl)(2-methylquinazolin-4-yl)methanone (3o). yellow solid, 43% yield, mp. 112–114 °C. 1H NMR (300 MHz, CDCl3) δ 8.12–8.00 (m, 2H), 7.98–7.80 (m, 3H), 7.51 (t, J = 7.3 Hz, 1H), 7.41 (d, J = 8.8 Hz, 1H), 7.18 (d, J = 3.2 Hz, 1H), 6.55 (d, J = 3.2 Hz, 1H), 4.20 (q, J = 7.3 Hz, 2H), 2.97 (s, 3H), 1.47 (t, J = 7.3 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 193.3, 166.5, 163.6, 151.2, 139.0, 134.4, 129.1, 128.2, 128.1, 127.4, 127.3, 126.8, 126.0, 123.2, 120.0, 109.7, 103.8, 41.3, 26.5, 15.4; HRMS (ESI) m/z calcd for C20H18N3O [M+H]+ 316.1450, found 316.1450.
(1-ethyl-1H-pyrrolo[2,3-b]pyridin-5-yl)(2-methylquinazolin-4-yl)methanone (3p). Yellow solid, 48% yield, mp. 124–125 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.90 (d, $J$ = 2.0 Hz, 1H), 8.49 (d, $J$ = 2.0 Hz, 1H), 8.05 (d, $J$ = 8.5 Hz, 1H), 8.01 (d, $J$ = 8.4 Hz, 1H), 7.91 (ddd, $J$ = 8.4, 7.0, 1.2 Hz, 1H), 7.56 (t, $J$ = 7.6 Hz, 1H), 7.32 (d, $J$ = 3.6 Hz, 1H), 6.57 (d, $J$ = 3.6 Hz, 1H), 4.37 (q, $J$ = 7.3 Hz, 2H), 2.95 (s, 3H), 1.48 (t, $J$ = 7.3 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 192.4, 164.7, 163.4, 151.6, 149.3, 146.5, 134.6, 132.0, 129.6, 128.3, 127.7, 125.8, 124.0, 120.2, 119.9, 102.0, 39.8, 26.4, 15.6; HRMS (ESI) m/z calcd for C$_{19}$H$_{17}$N$_4$O$_3$ [M+H]$^+$ 317.1402, found 317.1402.

Phenyl(quinazolin-4-yl)methanone (3q). White solid, 35% yield, mp. 91–93 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 9.44 (s, 1H), 8.18 (d, $J$ = 8.5 Hz, 1H), 8.08 (d, $J$ = 8.4 Hz, 1H), 8.04–7.92 (m, 3H), 7.67 (td, $J$ = 7.5, 2.5 Hz, 2H), 7.51 (t, $J$ = 7.8 Hz, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 193.0, 164.1, 153.8, 151.3, 135.2, 134.7, 134.5, 130.7, 129.1, 128.81, 128.78, 125.9, 122.1; HRMS (ESI) m/z calcd for C$_{15}$H$_{11}$N$_2$O [M+H]$^+$ 235.0871, found 235.0863.

(4-methoxyphenyl)(quinazolin-4-yl)methanone (3r). Yellow solid, 34% yield, mp. 115–117 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 9.42 (s, 1H), 8.15 (d, $J$ = 8.5 Hz, 1H), 8.05 (d, $J$ = 8.4 Hz, 1H), 8.01–7.91 (m, 3H), 7.65 (t, $J$ = 7.7 Hz, 1H), 6.97 (d, $J$ = 9.0 Hz, 2H), 3.89 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.4, 164.8, 164.7, 153.9, 151.2, 134.6, 133.1, 129.0, 128.6, 128.3, 126.0, 122.1, 114.1, 55.7. MS (ESI): 265.05 [M+H]$^+$.
phenyl(2-propylquinazolin-4-yl)methanone (3s). yellow solid, 21% yield, mp. 74–77 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.08 (d, J = 8.5 Hz, 1H), 8.02–7.87 (m, 4H), 7.66 (t, J = 7.4 Hz, 1H), 7.60–7.53 (m, 1H), 7.50 (t, J = 7.7 Hz, 2H), 3.22–3.04 (m, 2H), 2.06–1.85 (m, 2H), 1.05 (t, J = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 193.3, 166.6, 164.5, 151.5, 135.3, 134.42, 134.41, 130.7, 128.7, 128.5, 127.6, 125.6, 120.0, 41.8, 22.3, 14.0; HRMS (ESI) m/z calcd for C$_{18}$H$_{17}$N$_2$O $\text{[M+H]}^+$ 277.1341, found 277.1345.

(4-nitrophenyl)(2-propylquinazolin-4-yl)methanone (3t). yellow solid, 41% yield, mp. 121–123 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.38–8.31 (m, 2H), 8.23–8.05 (m, 4H), 7.96 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.64 (ddd, J = 8.2, 7.0, 0.9 Hz, 1H), 3.40–2.93 (m, 2H), 2.19–1.80 (m, 2H), 1.04 (t, J = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.5, 166.4, 161.8, 152.0, 150.8, 140.1, 134.7, 131.8, 128.8, 128.2, 125.3, 123.7, 112.0, 41.6, 22.2, 14.0; HRMS (ESI) m/z calcd for C$_{18}$H$_{16}$N$_3$O$_3$ $\text{[M+H]}^+$ 322.1192, found 322.1188.

(4-nitrophenyl)(2-phenylquinazolin-4-yl)methanone (3u). yellow solid, 35% yield, mp. 197–199 °C. $^1$H NMR (400 MHz, CDCl$_3$) δ 8.59–8.53 (m, 2H), 8.37 (d, J = 8.9 Hz, 2H), 8.27 (d, J = 8.9 Hz, 2H), 8.23 (ddd, J = 8.8, 4.1 Hz, 2H), 7.99 (ddd, J = 8.5, 6.9, 1.3 Hz, 1H), 7.67 (ddd, J = 8.1, 7.0, 1.0 Hz, 1H), 7.54–7.47 (m, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.4, 161.4, 159.5, 152.6, 150.8, 140.3, 137.1, 134.8, 131.9, 131.2, 129.5, 128.8, 128.61, 128.59, 125.5, 123.7, 120.5; HRMS (ESI) m/z calcd for C$_{21}$H$_{14}$N$_3$O$_3$ $\text{[M+H]}^+$ 356.1035, found 356.0996.

4-(4-nitrobenzyl)-2-phenylquinazoline (3uu'). yellow solid, 49% yield, mp. 148–150 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.66–8.60 (m, 2H), 8.28 (d, J = 8.7 Hz, 1H), 8.19 (d, J = 8.8 Hz, 2H), 8.10 (d, J = 8.5 Hz, 1H), 7.91 (ddd, J = 8.4, 7.0, 1.3 Hz, 1H), 7.66 – 7.49 (m, 6H), 4.81 (s, 2H); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 167.5, 160.1, 151.2, 146.8, 145.2, 137.8, 133.7, 130.6, 129.9, 129.6, 128.5, 127.3, 124.3, 123.7, 122.2, 40.7; HRMS (ESI) m/z calcd for C$_{21}$H$_{16}$N$_3$O$_2$
[M+H]$^+$ 342.1243, found 342.1239.

References:
Spectral copies of $^1$H- and $^{13}$C-NMR of products
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