The vinylogous Catellani reaction: A combined computational and experimental study

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Supporting Information

1. General Considerations S2
2. Preparation of Benzylic Alcohol and Sulfonamide S2
3. Preparation of 4-Iodo-2-quinolones S4
4. Vinylogous Catellani Reactions S7
5. Control Experiments S15
6. Single Crystal X-ray Diffraction Study S16
7. DFT Calculations S18
8. NMR Charts S81
1. General considerations

Column chromatography was performed on silica gel (Cica silica gel 60N) with solvents specified below. $^1$H and $^{13}$C NMR spectra were obtained for samples in CDCl$_3$ solutions at 25 °C. $^1$H NMR chemical shifts are reported in terms of chemical shift (δ, ppm) relative to the singlet at 7.26 ppm for chloroform. Splitting patterns are designated as follows: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet. Coupling constants are reported in Hz. $^{13}$C NMR spectra were fully decoupled and are reported in terms of chemical shift (δ, ppm) relative to the triplet at δ 77.0 ppm for CDCl$_3$. Reagents and dry solvents were purchased and used as received. N-protected (o-aminophenyl)propiolates were reported in our previous paper.$^1$ Benzylalcohols 3a,$^2$ 3b,$^3$ 3c,$^4$ 3d,$^5$ 3e,$^4$ 3f,$^6$ 3g,$^2$ 3h,$^2$ 3i,$^2$ 3j,$^5$ 3k,$^6$ 3l,$^6$ 3m,$^7$ 3n,$^8$ 3o,$^9$ and benzylamine 7,$^{10}$ were synthesized according to literature

2. Preparation of benzylalcohols and sulfonamide

**Synthesis of benzyl alcohol 3f:** To a solution of methyl 2-bromo-4-chlorobenzoate (461.9 mg, 1.85 mmol) in Et$_2$O (10.0 mL) was added MeMgl (3.0 M in Et$_2$O, 2.0 mL, 6.0 mmol) at 0 °C. The reaction mixture was stirred for 12 h at room temperature. The reaction was quenched with sat. NH$_4$Cl (10 mL) at 0 °C and the whole mixture was extracted with AcOEt (3 × 20 mL). The combined organic layer was washed with brine (10 mL) and dried over Mg$_2$SO$_4$. After concentration in vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 20:1) to afford 3f (308.3 mg, 86%) as a colorless oil; $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 7.64 (d, J = 8.8 Hz, 1 H), 7.59 (d, J = 1.6 Hz, 1 H), 7.27 (dd, J = 8.8, 1.6 Hz, 1 H), 2.51 (s, 1 H), 1.73 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 144.8, 134.3, 133.1, 128.1, 127.4, 120.5, 73.3, 29.3; IR (neat) 3410 (O–H) cm$^{-1}$; HRMS (DART) m/z calcd for C$_7$H$_9$BrCl 230.9576, found 230.9573 [M–OH]$^+$. 

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Similarly, benzylic alcohol 3d was prepared from the corresponding ester.

**Analytical data for 3d:** 554 mg, 55%; white solid (m.p. 60.1–61.9 °C); ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 7.48 (dd, J = 7.3, 2.3 Hz, 1 H), 7.22–7.13 (m, 2 H), 3.08 (br s, 1 H), 2.45 (s, 3 H), 1.78 (s, 6 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 146.2, 139.8, 129.8, 127.0, 124.9, 123.5, 74.0, 29.7, 24.7; IR (neat) 3423 (O–H) cm⁻¹; HRMS (DART) m/z calced for C₁₀H₁₂Br 211.0122, found 211.0129 [M–OH]⁺.

**Synthesis of benzylic alcohol 3m:** To a suspension of Zn (653.9 mg, 10.0 mmol) in THF (1 mL) was added dibromoethane (32 µL), and this mixture was heated at 65 °C for 1 min. After cooled to room temperature, Me₂SiCl (40 µL) was added. After stirring for 15 min, a solution of o-bromoacetophenone (266.5 µL, 2.0 mmol) and ethyl bromodifluoroacetate (512.9 µL, 4.0 mmol) in THF (3 mL) was added and the resultant mixture was stirred at room temperature for 3 h. The reaction was quenched with sat. NH₄Cl (10 mL) and the whole mixture was extracted with Et₂O (3 × 10 mL). The combined organic layer was washed with brine (10 mL) and dried over MgSO₄. After concentration in vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 8:1) to afford 3m (485.5 mg, 75%) as a colorless oil; ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 7.63 (d, J = 8.0 Hz, 1 H), 7.57 (d, J = 7.6 Hz, 1 H), 7.32 (dt, J = 7.6, 0.8 Hz, 1 H), 7.18 (dt, J = 7.6, 1.2 Hz, 1 H), 4.28 (q, J = 7.2 Hz, 2 H), 4.14 (s, 1 H), 1.93, (s, 3 H), 1.27 (t, J = 7.2 Hz, 3 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 163.2 (t, J = 31.5 Hz), 137.2, 135.7, 130.3, 129.8, 127.2, 120.8, 115.5 (t, J = 261.3 Hz), 77.8 (t, J = 25.3 Hz), 63.1, 23.7, 13.7; ¹⁹F NMR (376 MHz, CDCl₃, 25 °C): δ −112.7 (d, J = 254.2 Hz), −114.1 (d, J = 254.2 Hz); IR (neat) 3521 (O–H), 1761 (C=O) cm⁻¹; HRMS (DART) m/z calced for C₁₂H₁₃BrF₂O₃•NH₄ 340.0356, found 340.0357 [M+NH₄]⁺.

**Synthesis of benzylic alcohol 3n:** The reported procedure for the synthesis of 3j was applied to 6-methyl-5-hepten-2-one (1.2 mL, 10.0 mmol). The crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 100:1–40:1) to afford 3n (200.6 mg, 7%) as a yellow oil; ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 7.72 (dd, J = 8.0, 1.6 Hz, 1 H), 7.58 (dd, J = 8.0, 1.2 Hz, 1 H), 7.30 (dt, J = 7.6, 1.2 Hz, 1 H), 7.09 (dt, J = 7.6, 1.6 Hz, 1 H), 5.10 (t, J = 7.0 Hz, 1 H), 2.54 (s, 1 H), 2.52–2.45 (m, 1 H), 1.97–1.80 (m, 3 H), 1.70 (s, 3 H), 1.65 (s, 3 H), 1.47 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 145.3, 134.9, 132.4, 128.4, 128.3, 127.4, 124.0, 120.1, 76.2, 40.4, 28.0, 25.7, 23.1, 17.6; IR (neat) 3458 (O–H) cm⁻¹; HRMS (DART) m/z calced for C₁₄H₁₉BrO•NH₄ 300.0963, found 300.0943 [M+NH₄]⁺.
Synthesis of benzyl alcohol **3o**: To a solution of 8-bromo-3,4-dihydropyridophen-1(2H)-one\(^{11}\) (596.1 mg, 2.64 mmol) in Et\(_2\)O (5 mL) was added MeMgl (3.0 M in Et\(_2\)O, 1.1 mL, 3.17 mmol) at 0 °C. The reaction mixture was stirred for 1.5 h at room temperature. The reaction was quenched with sat. NH\(_4\)Cl (10 mL) at 0 °C and the whole mixture was extracted with Et\(_2\)O (3 × 10 mL). The combined organic layer was washed with brine (10 mL) and dried over MgSO\(_4\). After concentration in vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 8:1) to afford **3o** (355.5 mg, 56%) as a colorless solid (m.p. 68.0–70.5 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.41 (d, \(J\) = 7.6 Hz, 1 H), 7.06 (d, \(J\) = 7.6 Hz, 1 H), 6.97 (t, \(J\) = 7.6 Hz, 1 H), 3.70 (s, 1 H), 2.89 (ddd, \(J\) = 16.0, 10.8, 5.6 Hz, 1 H), 2.81 (dt, \(J\) = 16.0, 4.4 Hz, 1 H), 2.02–1.97 (m, 2 H), 1.94–1.86 (m, 1 H), 1.82–1.71 (m, 1 H), 1.76 (s, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 140.0, 139.6, 132.7, 128.9, 127.7, 121.7, 72.3, 40.3, 31.4, 28.4, 20.0; IR (neat) 3425 (O–H) cm\(^{-1}\); HRMS (DART) \(m/z\) calcd for C\(_{11}\)H\(_{13}\)BrO•NH\(_4\) 258.0494, found 258.0516 [M+NH\(_4\)]\(^+\).

Synthesis of sulfonamide **9**: To a solution of o-bromobenzylamine \(^7\) (214.6 mg, 1.0 mmol) in \(\mathrm{CH}_2\mathrm{Cl}_2\) (3.0 mL) was added triethyamine (140 \(\mu\)l, 0.95 mmol) and \(p\)-toluenesulfonyl chloride (180.3 mg, 1.0 mmol) at 0 °C. The reaction mixture was stirred at room temperature for 2 days. The reaction was quenched with 10% HCl (10 mL) and the whole mixture was extracted with \(\mathrm{CH}_2\mathrm{Cl}_2\) (2 × 20 mL). The combined organic layer was washed with brine (10 mL) and dried over Na\(_2\)SO\(_4\). After concentration in vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 4:1) to afford tosylamide **9** (219.6 mg, 60%) as a brown solid (m.p. 96.8–98.9 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.44 (d, \(J\) = 8.4 Hz, 2 H), 7.30 (dd, \(J\) = 8.0, 1.6 Hz, 1 H), 7.25 (dd, \(J\) = 8.4, 1.2 Hz, 1 H), 7.15 (dt, \(J\) = 7.6, 1.6 Hz, 1 H), 6.97 (d, \(J\) = 8.8 Hz, 2 H), 6.96 (dt, \(J\) = 7.6, 1.6 Hz, 1 H), 5.89 (s, 1 H), 2.30 (s, 3 H), 1.81 (s, 6 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 142.5, 141.1, 137.7, 135.4, 128.7, 128.5, 128.2, 127.3, 127.2, 121.7, 58.5, 29.2, 21.3; IR (neat) 3292 (N–H) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{16}\)H\(_{18}\)BrNO\(_2\)S•Na 390.0139, found 390.0141 [M+Na]\(^+\).

3. Synthesis of 4-iodo-2-quinolones

**Synthesis of silylalkyne **S1**: In a sealed tube, a solution of 2-iodo-4-methylaniline (2.33 g, 10.0 mmol) in di-t-butyl dicarbonate (3.68 mL, 16.0 mmol) was heated at 90 °C for 2 days. To a solution of the crude product in DMF (50 mL) was added sodium hydride (60% oil, 0.80 g, 20.0 mmol) at 0 °C. The reaction mixture was stirred at room temperature for 1 h. To the

resultant mixture was added benzyl bromide (1.43 mL, 12.0 mmol). The reaction mixture was stirred at room temperature for 1 h. The reaction was quenched with sat. NH₄Cl (20 mL), and the mixture was extracted with AcOEt (3 × 20 mL). The combined organic layer was washed with water (2 × 20 mL), brine (20 mL), and dried over MgSO₄. After concentration in vacuo, the crude product was purified by flash column chromatography on silica gel (hexane/EtOAc = 50:1~20:1) to afford tert-butyl benzyl(2-iodo-4-methylphenyl)carbamateN-protected o-iodoaniline as a yellow oil.

To a solution of the crude product obtained above (2.01 g, 4.75 mmol) in t-butyl methyl ether (20 mL) and diisopropylamine (4 mL) was added PdCl₂(PPh₃)₃ (33.3 mg, 0.0475 mmol) and Cul (18.1 mg, 0.095 mmol) at room temperature. The reaction mixture was degassed at −78 °C and to this mixture was added trimethylsilylacetylene (0.724 mL, 5.23 mmol). The reaction mixture was stirred at 50 °C for 5 h. Insoluble materials were filtered with a pad of Celite® and the filtrate was concentrated in vacuo. The obtained crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 20:1~15:1) to afford silylalkyne S2 (898 mg, 23% over 3 steps) as a yellow oil; a mixture of two rotamers; ^1^H NMR (CDCl₃, 400 MHz, 25 °C) δ 7.31–7.19 (major+minor) (br m, 6 H), 7.03–6.89 (minor) (br m, 2 H), 6.89 (major) (d, J = 8.0 H, 1 H), 6.70 (major) (d, J = 8.0 H, 1 H), 5.20–4.34 (major+minor) (br m, 2 H), 2.27 (s, 3 H), 1.49 (minor)/1.36 (major) (br s, 9 H), 0.25 (major+minor) (br s, 9 H); ^1^C NMR (CDCl₃, 100 MHz, 25 °C) δ 154.5 (major)/154.2 (minor), 141.8 (minor)/141.4 (major), 138.3 (minor)/137.8 (major), 136.2 (minor)/135.9 (major), 133.5 (minor)/132.9 (major), 129.6 (minor)/129.3 (major), 128.8 (minor)/128.4 (major), 127.8 (major)/127.6 (minor), 126.8 (major/minor), 121.8 (major/minor), 102.0 (major/minor), 97.8 (major+minor), 79.9 (minor)/79.2 (major), 53.7 (minor)/52.6 (major), 28.1 (minor)/27.9 (major), 20.4 (major+minor), −0.4 (major+minor); IR (neat) 2154 (C=O), 1703 (C=O), 1250 (Si–CH₃), 848 (Si–CH₃) cm⁻¹; HRMS (ESI) m/z calcd for C₂₄H₃₁NO₂Si•Na 416.2022, found 416.2012 [M+Na]⁺.

**Synthesis of propiolate S2:** In a flask, CsF (693 g, 4.56 mmol) was heated under vacuum at 120 °C for 1 h. The flask was filled with CO₂ gas (balloon) and then with dry DMF (1 mL). To the resultant suspension was added drop-wise a solution of silylalkyne S1 (898 mg, 2.28 mmol) in dry DMF (6 mL) at room temperature. The reaction mixture was stirred at room temperature for 2 h. After addition of methyl iodide (170 µL, 2.74 mmol), the stirring was continued at room temperature for another 1.5 h. The reaction was quenched with sat. NH₄Cl (10 mL) and the whole mixture was extracted with AcOEt (3 × 10 mL). The combined organic layer was washed with water (2 × 10 mL), brine (10 mL), and dried over MgSO₄. After concentration in vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 30:1~15:1) to afford propiolate S2 (641 mg,
85%) as a yellow oil: a mixture of two rotamers; \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.45–6.81 (major+minor) (br m, 8 H), 5.10–4.30 (major+minor) (br s, 2 H), 3.82 (major+minor) (s, 3 H), 2.29 (major+minor) (s, 3 H), 1.50 (minor)/1.37 (major) (br s, 9 H); \(^1^3\)C NMR (CDCl\(_3\), 100 MHz, 25 °C) \(\delta\) 154.2 (major+minor), 153.9 (major+minor), 143.0 (minor)/142.1 (major), 137.7 (minor)/137.3 (major), 136.4, (major+minor), 134.4 (minor)/134.0 (major), 132.0 (minor)/131.7 (major), 128.4 (major+minor), 128.1 (major+minor), 127.9 (major+minor), 127.7 (minor)/127.0 (major) 118.9 (major or minor), 83.6 (major)/83.2 (minor), 80.7 (minor)/80.1 (major), 54.1 (minor)/53.0 (major), 52.3 (major+minor), 27.8 (major+minor) 20.4 (major+minor); IR (neat) 2218 (C=C), 1712 (C=O) cm\(^{-1}\); HRMS (ESI) m/z calcd for C\(_{23}\)H\(_{25}\)NO\(_2\)•Na 402.1681, found 402.1672 [M+Na]\(^+\).

**Representative procedure for preparation of 4-iodo-2-quinolones 2a –Synthesis of 2a:**

![Methyl 3-(2-(benzyl(tert-butoxycarbonyl)amino)phenyl)propiolate](image)

To a solution of methyl 3-(2-(benzyl(tert-butoxycarbonyl)amino)phenyl)propiolate (365.2 mg, 1.0 mmol) in acetic acid (2 mL) was added sodium iodide (890.0 mg, 6.0 mmol) at room temperature. The reaction mixture was stirred at 110 °C for 1 h. The reaction was quenched with H\(_2\)O (10 mL) and the resultant mixture was extracted with EtOAc (3 × 10 mL). The combined organic layer was washed with sat. Na\(_2\)CO\(_3\) (10 mL), sat. Na\(_2\)S\(_2\)O\(_3\) (10 mL), and brine (10 mL). After dried over MgSO\(_4\), the solvents were removed in vacuo. The obtained crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 7:1) to afford 4-iodo-2-quinoline 2a (340.0 mg, 94%) as a white solid (m.p. 123.6–125.4 °C): \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.85 (dd, \(J = 8.4, 1.6\) Hz, 1 H), 7.61 (s, 1 H), 7.45 (ddd, \(J = 8.4, 7.2, 1.6\) Hz, 1 H) 7.33–7.18 (m, 7 H), 5.54 (s, 2 H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 160.6, 137.8, 135.8, 133.9, 133.1, 131.7, 128.9, 127.4, 126.5, 123.1, 122.2, 115.31, 115.25, 46.3; IR (neat) 1645 (C=O) cm\(^{-1}\); HRMS (ESI) m/z calcd for C\(_{18}\)H\(_{12}\)INO•Na 383.9861, found 383.9851 [M+Na]\(^+\).

**Analytical data for 2b:** 306.7 g, 84%; yellow solid (m.p. 178.7–182.1 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.62 (s, 1 H), 7.58 (s, 1 H), 7.32–7.21 (m, 5 H), 7.19 (d, \(J = 6.8\) Hz, 1 H), 7.10 (d, \(J = 8.8\) Hz, 1 H), 5.52 (s, 2 H), 2.42 (s, 3 H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 160.4, 135.9, 135.7, 133.5, 132.9, 132.8, 132.7, 128.7, 127.3, 126.4, 122.0, 115.14, 115.09, 46.1, 20.6; IR (neat) 1643 (C=O) cm\(^{-1}\); HRMS (ESI) m/z calcd for C\(_{17}\)H\(_{14}\)INO•Na 398.0018, found 398.0013 [M+Na]\(^+\).
Analytical data for 2c: 365.6 mg, 90%; white solid (m.p. 168.3–169.1 °C); 1H NMR (400 MHz, CDCl3, 25 °C) δ 7.85 (d, J = 2.4 Hz, 1 H), 7.62 (s, 1 H), 7.37 (dd, J = 8.8 2.4 Hz, 1 H) 7.34–7.20 (m, 6 H), 5.51 (br s, 2 H); 13C NMR (100 MHz, CDCl3, 25 °C) δ 160.2, 136.4 135.4, 134.3, 133.1, 131.7, 129.0, 128.8, 127.6, 126.4, 123.5, 116.9, 113.3, 46.4; IR (neat) 1647 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C16H11ClINO•Na 417.9472, found 417.9477 [M+Na]⁺.

Analytical data for 2d: 369.7 mg, 95%; white solid (m.p. 151.5–153.2 °C); 1H NMR (400 MHz, CDCl3, 25 °C) δ 7.61 (s, 1 H), 7.35–7.13 (m, 7 H), 7.04 (dd, J = 9.2, 2.8 Hz, 1 H), 5.52 (br s, 2 H), 3.87 (s, 3 H); 13C NMR (100 MHz, CDCl3, 25 °C) δ 160.2, 155.3, 153.9, 135.9, 133.6, 132.2, 128.8, 127.4, 126.4, 123.1, 120.1, 116.8, 116.1, 114.6, 55.7, 46.3; IR (neat) 1639 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C17H14INO•Na 413.9967, found 413.9960 [M+Na]⁺.

Analytical data for 2e: 391.7 mg, 87%; white solid (m.p. 137.6–138.0 °C); 1H NMR (400 MHz, CDCl3, 25 °C) δ 7.59 (s, 1 H) 7.33–7.18 (m, 5 H), 6.47 (s, 1 H), 5.50 (br s, 2 H), 3.95 (s, 3 H), 3.81 (s, 3 H), 3.70 (s, 3 H), 3.60 (s, 3 H); 13C NMR (100 MHz, CDCl3, 25 °C) δ 160.6, 155.8, 150.3, 138.1, 136.1, 136.0, 133.2, 129.0, 127.5, 126.6, 109.2, 101.0, 94.2, 61.5, 60.9, 55.7, 47.0; IR (neat) 1643 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C19H13INO4•Na 474.0178, found 474.0180 [M+Na]⁺.

Analytical data for 2f: 145.2 mg, 89%; pale-yellow solid (m.p. 103.3–104.3 °C); 1H NMR (400 MHz, CDCl3, 25 °C) δ 7.70 (dd, J = 8.4, 1.2 Hz, 1 H) 7.57 (ddd, J = 8.4, 7.2, 1.2 Hz, 1 H), 7.34 (ddd, J = 8.4, 7.2, 1.2 Hz, 1 H), 7.27 (dd, J = 8.4, 1.2 Hz, 1 H), 7.22 (s, 1 H); 13C NMR (100 MHz, CDCl3, 25 °C) δ 158.1, 151.3, 132.9, 132.4, 127.4, 125.1, 120.6, 120.1, 116.9; IR (neat) 1711 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C9H5IO2•Na 294.9232, found 294.9218 [M+Na]⁺.

4. Vinylogous Catellani reactions

Representative procedure (1) – Synthesis of 4aa: A solution of 4-iodo-2-quinoline 2a (72.4 mg, 0.20 mmol), 2-(2-bromophenyl)propan-2-ol 3a (43.2 mg, 0.20 mmol), Pd(OAc)₂ (2.26 mg, 0.01 mmol), norbornene (18.6 mg, 0.20 mmol), and K₂CO₃ (69.3 mg, 0.50 mmol) in dry DMF (4.0 mL) was degassed at –78 °C. The reaction mixture was heated at 105 °C for 2 h. The reaction was quenched with H₂O (10 mL) and the whole mixture was extracted with AcOEt (3 × 20 mL). The combined organic layer was washed with water (2 × 10 mL), brine (10 mL) and dried over MgSO₄. After concentration in
vacuo, the crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 20:1) to afford 4aa (63.7 mg, 87%) as a white solid (m.p. 154.2–157.9 °C):

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$ 9.01 (dd, $J = 8.0$, 1.2 Hz, 1 H), 8.10 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.45 (ddd, $J = 8.8$, 6.8, 1.6 Hz, 1 H), 7.38 (dt, $J = 6.8$, 1.2 Hz, 1 H), 7.35–7.18 (m, 9 H), 5.64 (br s, 2 H), 1.78 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) $\delta$ 161.5, 156.2, 138.8, 137.0, 136.9, 131.2, 128.8, 127.9, 127.8, 127.1, 126.9, 126.6, 125.8, 123.7, 122.1, 121.8, 116.5, 114.7, 106.5, 80.0, 45.9, 27.5; IR (neat) 1634 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{25}$H$_{21}$NO$_2$•Na 390.1470, found 390.1461 [M+Na]$^+$.  

![Image of 4aa](image_url)

**Analytical data for 4aa:** 61.7 mg, 81%; yellow solid (m.p. 177.1–179.5 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$ 9.00 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.86 (s, 1 H), 7.37 (dt, $J = 7.6$, 1.2 Hz, 1 H), 7.33–7.19 (m, 8 H), 7.14 (d, $J = 8.4$ Hz, 1 H), 5.61 (br s, 2 H), 2.40 (s, 3 H), 1.77 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) $\delta$ 161.3, 156.0, 137.0, 136.9, 132.5, 131.4, 128.7, 127.80, 127.78, 127.0, 126.5, 125.8, 123.2, 122.1, 116.4, 114.6, 106.5, 79.9, 45.8, 27.4, 20.7; IR (neat) 1631 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{26}$H$_{23}$NO$_2$•Na 404.1627, found 404.1620 [M+Na]$^+$.  

![Image of 4ca](image_url)

**Analytical data for 4ca:** 64.9 mg, 81%; white solid (m.p. 175.8–179.4 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$ 8.99 (d, $J = 7.6$ Hz, 1 H), 8.04 (d, $J = 2.4$ Hz, 1 H), 7.42–7.22 (m, 9 H), 7.18 (d, $J = 8.8$ Hz, 1 H), 5.60 (br s, 2 H), 1.78 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) $\delta$ 161.1, 155.0, 137.2, 137.1, 136.5, 131.1, 128.8, 128.3, 127.9, 127.6, 127.3, 126.5, 125.9, 123.0, 122.2, 117.6, 116.2, 107.3, 80.4, 46.0, 27.5; IR (neat) 1637 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{25}$H$_{20}$ClNO$_2$•Na 424.1080, found 424.1085 [M+Na]$^+$.  

![Image of 4da](image_url)

**Analytical data for 4da:** 72.6 mg, 90%; white solid (m.p. 199.2–201.2 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$ 9.02 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.50 (d, $J = 2.4$ Hz, 1 H), 7.37 (dt, $J = 7.6$, 1.6 Hz, 1 H), 7.34–7.20 (m, 7 H), 7.18 (d, $J = 9.6$ Hz, 1 H), 7.06 (dd, $J = 9.2$, 2.8 Hz, 1 H), 5.61 (br s, 2 H), 3.87 (s, 3 H), 1.77 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) $\delta$ 161.0, 155.6, 154.6, 137.04, 136.98, 133.5, 128.7, 127.9, 127.8, 127.09, 126.97, 126.5, 125.9, 122.1, 119.9, 117.2, 116.1, 106.9, 105.4, 80.0, 55.7, 45.9, 27.5; IR (neat) 1631 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{26}$H$_{23}$NO$_2$•Na 420.1576, found 420.1576 [M+Na]$^+$.  

S8
**Analytical data for 4ea:** 39.3 mg, 44%; white solid (m.p. 158.0–158.5 °C); ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 8.92 (dd, J = 8.0, 1.2 Hz, 1 H), 7.36 (dt, J = 7.6, 1.2 Hz, 1 H), 7.33–7.19 (m, 7 H), 6.53 (s, 1 H), 5.60 (br s, 2 H), 3.93 (s, 3 H); 13C NMR (100 MHz, CDCl₃, 25 °C) δ 163.1, 157.6, 155.8, 151.8, 138.9, 137.1, 137.0, 136.7, 128.9, 127.7, 127.4, 127.3, 127.2, 126.7, 125.6, 121.7, 105.5, 105.4, 94.6, 79.5, 62.1, 61.2, 55.8, 46.8, 27.0; IR (neat) 1631 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₂₅H₂₇NO₃•Na 480.1787, found 480.1789 [M+Na]⁺.

**Analytical data for 4ab:** 66.5 mg, 87%; white solid (m.p. 172.0–172.7 °C); ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 8.86 (s, 1 H), 8.10 (dd, J = 8.0, 1.2 Hz, 1 H), 7.44 (ddd, J = 8.8, 7.2, 1.6 Hz, 1 H), 7.34–7.18 (m, 7 H), 7.14 (d, J = 1.2 Hz, 2 H), 5.64 (br s, 2 H), 2.41 (s, 3 H); 13C NMR (100 MHz, CDCl₃, 25 °C) δ 161.5, 156.3, 138.7, 137.4, 136.8, 134.3, 131.1, 128.7, 128.6, 127.1, 126.7, 126.5, 126.2, 123.7, 122.1, 121.8, 116.6, 114.6, 106.5, 80.0, 45.8, 27.6, 21.5; IR (neat) 1633 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₂₆H₂₃NO₂•Na 404.1627, found 404.1619 [M+Na]⁺.

**Analytical data for 4ac:** 63.6 mg, 83%; white solid (m.p. 128.2–129.1 °C); ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 8.90 (d, J = 8.4 Hz, 1 H), 8.09 (dd, J = 7.6, 1.2 Hz, 1 H), 7.43 (ddd, J = 8.8, 6.8, 1.6 Hz, 1 H), 7.34–7.17 (m, 8 H), 7.04 (d, J = 1.2 Hz, 1 H), 5.63 (br s, 2 H), 2.40 (s, 3 H), 1.76 (s, 6 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 161.5, 155.6, 138.6, 137.7, 137.1, 136.9, 130.9, 128.7, 128.4, 127.1, 126.5, 125.8, 124.1, 123.6, 122.8, 121.7, 116.6, 114.6, 106.6, 79.9, 45.8, 27.6, 21.5; IR (neat) 1633 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₂₆H₂₃NO₂•Na 404.1627, found 404.1615 [M+Na]⁺.

**Analytical data for 4ad:** This compound was obtained as an inseparable mixture with remained 3d as a yellow foam. Thus, the yield was estimated as 74% by internal standard. Analytical sample was obtained by purification with HPLC; ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 8.06 (dd, J = 8.0, 1.2 Hz, 1 H), 7.44 (ddd, J = 8.8, 6.8, 1.6 Hz, 1 H), 7.35–7.17 (m, 9 H), 7.14–7.08 (m, 1 H), 5.65 (br s, 2 H), 2.42 (s, 3 H), 1.74 (s, 6 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 160.3, 158.0, 140.7, 139.0, 137.1, 135.6, 131.2, 131.0, 128.8, 127.4, 127.1, 126.5, 126.0, 123.2, 121.6, 119.5, 117.0, 114.6, 109.9, 81.6, 46.0, 26.5, 22.9; IR (neat) 1641 (C=O) cm⁻¹; HRMS (DART) m/z calcd for C₂₆H₂₃NO₂•H 382.1807, found 382.1821 [M+H]⁺.
Analytical data for 4ae: 69.2 mg, 90%; white solid (m.p. 159.9–160.2 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 8.82 (dd, $J = 7.6$, 2.8 Hz, 1 H), 8.10 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.47 (dd, $J = 8.8$, 7.2, 2.0 Hz, 1 H), 7.34–7.16 (m, 8 H), 7.00 (dt, $J = 8.0$, 2.8 Hz, 1 H), 5.63 (br s, 2 H), 1.77 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 162.4 (d, $J = 242.2$ Hz), 161.3, 156.8, 139.0, 136.7, 132.6 (d, $J = 2.8$ Hz), 131.6, 129.1 (d, $J = 10.5$ Hz), 128.8, 127.2, 126.5, 123.9, 123.6 (d, $J = 8.6$ Hz), 121.9, 116.2, 114.7, 114.3 (d, $J = 22.9$ Hz), 112.8 (d, $J = 25.8$ Hz), 105.7 (d, $J = 1.9$ Hz), 80.1, 46.0, 27.7; $^{19}$F NMR (376 MHz, CDCl$_3$, 25 °C): δ –113.7; IR (neat) 1763 (C=O), 1637 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{25}$H$_{20}$FNO$_2$•Na 408.1376, found 408.1369 [M+Na]$^+$.

Analytical data for 4af: 67.7 mg, 84%; white solid (m.p. 157.5–158.7 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 9.10 (d, $J = 2.0$ Hz, 1 H), 8.10 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.47 (dd, $J = 8.4$, 5.6, 1.2 Hz, 1 H), 7.35–7.20 (m, 8 H), 7.16 (d, $J = 8.8$ Hz, 1 H), 5.63 (br s, 2 H), 1.76 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.2, 156.8, 139.0, 136.6, 135.1, 134.0, 131.7, 128.8, 128.6, 127.7, 127.2, 126.5, 125.7, 123.8, 123.5, 122.0, 116.2, 114.7, 105.5, 79.9, 45.9, 27.5; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{25}$H$_{20}$ClNO$_2$•Na 424.1073, found 424.1080 [M+Na]$^+$.

Analytical data for 4ag: 65.1 mg, 82%; white solid (m.p. 172.8–173.9 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 8.97 (d, $J = 7.2$ Hz, 1 H), 8.07 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.42 (dd, $J = 8.4$, 6.8, 1.6 Hz, 1 H), 7.34–7.18 (m, 7 H), 6.90 (dd, $J = 7.2$, 2.8 Hz, 1 H), 6.79 (d, $J = 2.8$ Hz, 1 H), 5.62 (br s, 2 H), 3.86 (s, 3 H), 1.74 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.5, 159.4, 154.7, 139.1, 138.4, 136.9, 130.7, 128.7, 127.5, 127.1, 126.5, 123.4, 121.8, 119.8, 116.6, 114.6, 111.6, 109.2, 106.5, 79.7, 55.3, 45.9, 27.4; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{25}$H$_{23}$NO$_3$•Na 420.1576, found 420.1563 [M+Na]$^+$.

Analytical data for 4ah: 65.5 mg, 81%; pale-brown solid (m.p. 216.3–221.4 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 8.62 (s, 1 H), 8.07 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.43 (ddd, $J = 8.6$, 7.0, 1.6 Hz, 1 H), 7.32–7.19 (m, 7 H), 6.75 (s, 1 H), 5.98 (s, 2 H), 5.63 (br s, 2 H), 1.73 (s, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.4, 155.0, 147.2, 146.9, 138.4, 136.8, 131.4, 130.9, 128.7, 127.1, 126.5, 123.4, 121.8, 121.2, 116.4, 114.6, 106.7, 106.6, 103.1, 101.1, 79.8, 45.9, 27.5; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{26}$H$_{21}$NO$_4$•Na 434.1368, found 434.1367 [M+Na]$^+$.
**Analytical data for 4ai:** 62.7 mg, 79%; white solid (m.p. 158.9–159.2 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 9.10 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 8.06 (dd, $J$ = 8.0, 1.6 Hz, 1 H), 7.44 (dd, $J$ = 8.8, 7.2, 1.6 Hz, 1 H), 7.36 (dt, $J$ = 8.0, 1.6 Hz, 1 H), 7.33–7.18 (m, 8 H), 7.11 (dd, $J$ = 7.2, 1.6 Hz, 1 H), 5.62 (br s, 2 H), 2.10 (q, $J$ = 7.6 Hz, 4 H), 0.95 (t, $J$ = 7.6 Hz, 6 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.6, 156.5, 138.9, 136.9, 133.7, 131.1, 128.7, 128.0, 127.6, 127.3, 127.1, 126.6, 126.0, 123.8, 123.6, 121.8, 116.3, 114.7, 105.5, 85.7, 45.9, 31.1, 8.1; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) $m/z$ calcld for C$_{27}$H$_{25}$NO$_2$•Na 418.1783, found 418.1778 [M+Na]$^+$. 

**Analytical data for 4aj:** 59.5 mg, 74%; pale-brown solid (m.p. 219.6–221.5 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 9.00 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 8.17 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 7.46 (dd, $J$ = 8.0, 7.6, 1.2 Hz, 1 H), 7.40–7.21 (m, 10 H), 5.63 (br s, 2 H), 2.37 (br d, $J$ = 13.6 Hz, 2 H), 2.00–1.76 (m, 5 H), 1.71 (br d, $J$ = 13.6 Hz, 2 H), 1.43–1.32 (m, 1 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.4, 155.6, 138.9, 137.2, 136.9, 131.1, 128.7, 127.9, 127.7, 127.14, 127.09, 126.6, 125.8, 123.5, 121.92, 121.88, 116.6, 114.7, 107.0, 80.4, 45.9, 34.8, 25.3, 21.7; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) $m/z$ calcld for C$_{28}$H$_{25}$NO$_2$•Na 430.1783, found 430.1775 [M+Na]$^+$. 

**Analytical data for 4ak:** 60.0 mg, 72%; yellow solid (m.p. 171.5–177.4 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 9.01 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 8.24 (dd, $J$ = 8.0, 1.6 Hz, 1 H), 7.48–7.42 (m, 2 H), 7.39 (dt, $J$ = 7.2, 1.6 Hz, 1 H), 7.33–7.19 (m, 13 H), 5.72 (br d, $J$ = 16.8 Hz, 1 H), 5.39 (br d, $J$ = 16.8 Hz, 1 H), 2.18 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.2, 156.3, 144.1, 138.8, 136.7, 135.0, 131.2, 128.7, 128.3, 128.0, 127.9, 127.7, 127.6, 127.1, 126.4, 125.9, 125.8, 124.5, 123.5, 122.0, 116.3, 114.7, 107.6, 83.2, 45.9, 28.3; IR (neat) 1633 (C=O) cm$^{-1}$; HRMS (ESI) $m/z$ calcld for C$_{30}$H$_{23}$NO$_2$•Na 452.1627, found 452.1619 [M+Na]$^+$. 

**Analytical data for 4al:** 51.8 mg, 60%; pale-yellow solid (m.p. 192.5–195.3 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 9.06 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 8.18 (dd, $J$ = 8.0, 1.2 Hz, 1 H), 7.52–7.40 (m, 2 H), 7.37 (dt, $J$ = 7.6, 1.2 Hz, 1 H), 7.32–7.18 (m, 9 H), 6.80 (dd, $J$ = 5.2, 3.6 Hz, 1 H), 6.70 (dd, $J$ = 3.6, 1.2 Hz, 1 H), 5.73 (br d, $J$ = 16.8 Hz, 1 H), 5.43 (br d, $J$ = 16.8 Hz, 1 H), 2.29 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 161.2, 155.8, 148.6, 138.7, 136.7, 134.8, 131.2, 128.7, 128.6, 127.8, 127.6, 127.0, 126.4, 126.2, 126.0,
125.9, 125.7, 123.8, 123.7, 121.9, 116.2, 114.6, 107.3, 80.8, 45.8, 29.0; IR (neat) 1633 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{28}H\(_{21}\)NO\(_2\)S•Na 458.1191, found 458.1172 [M+Na]\(^+\).

**Analytical data for 4am:** Because of instability under the reaction conditions, 2.5 equivs of 3m was used. The title compound was purified by short column chromatography and recrystallization; 54.6 mg, 61%; white solid (m.p. 126.8–128.5 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 9.21 (d, \(J = 7.6\) Hz, 1 H), 8.01 (dd, \(J = 8.0, 1.6\) Hz, 1 H), 7.52–7.44 (m, 2 H), 7.39–7.34 (m, 2 H), 7.32–7.20 (m, 7 H), 5.69 (br d, \(J = 16.8\) Hz, 1 H), 5.54 (br d, \(J = 16.8\) Hz, 1 H), 4.13 (dq, \(J = 10.8, 7.2\) Hz, 1 H), 4.08 (dq, \(J = 10.8, 7.2\) Hz, 1 H), 2.11 (s, 3 H), 1.02 (t, \(J = 7.2\) Hz, 3 H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 162.7 (t, \(J = 31.5\) Hz), 161.0, 155.3, 138.7, 136.6, 131.6, 129.5, 128.7, 128.0, 127.8, 127.7, 127.1, 126.5, 126.0, 125.3, 123.6, 121.9, 115.1, 114.7, 114.2 (t, \(J = 262.2\) Hz), 105.2, 81.5 (t, \(J = 26.2\) Hz), 63.2, 45.9, 22.7, 13.4; \(^19\)F NMR (376 MHz, CDCl\(_3\), 25 °C): \(\delta\) –115.3; IR (neat) 1763 (C=O), 1637 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{28}H\(_{23}\)F\(_2\)NO\(_4\)•Na 498.1493, found 498.1495 [M+Na]\(^+\).

**Analytical data for 4an:** 82.4 mg, 94%; yellow oil; \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 9.04 (d, \(J = 8.0\) Hz, 1 H), 8.10 (d, \(J = 8.0\) Hz, 1 H), 7.44 (ddd, \(J = 8.0, 7.2, 1.2\) Hz, 1 H), 7.37 (dt, \(J = 7.2, 1.6\) Hz, 1 H), 7.34–7.18 (m, 9 H), 5.63 (br s, 2 H), 5.06 (br s, 1 H), 2.16–2.08 (m, 3 H), 2.01–1.96 (m, 1 H), 1.78 (s, 3 H), 1.62 (s, 3 H), 1.48 (s, 3 H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 161.4, 156.0, 138.7, 136.8, 135.9, 132.0, 131.1, 128.7, 127.7, 127.6, 127.1, 127.0, 126.5, 125.8, 123.53, 123.49, 122.8, 121.8, 116.3, 114.6, 106.1, 82.2, 45.8, 39.7, 25.8, 25.5, 22.6, 17.4; IR (neat) 1636 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{30}H\(_{29}\)NO\(_2\)•Na 458.2096, found 458.2091 [M+Na]\(^+\).

**Analytical data for 4ao:** 25.0 mg, 34%; white solid (m.p. 188.2–191.9 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 8.77 (d, \(J = 8.0\) Hz, 1 H), 8.11 (dd, \(J = 8.0, 1.6\) Hz, 1 H), 7.44 (ddd, \(J = 8.8, 7.2, 1.6\) Hz, 1 H), 7.45–7.18 (m, 8 H), 7.10 (d, \(J = 7.2\) Hz, 1 H), 5.75 (br d, \(J = 16.8\) Hz, 1 H), 5.54 (br d, \(J = 16.8\) Hz, 1 H), 2.92–2.88 (m, 2 H), 2.40–2.28 (m, 2 H), 2.18–1.96 (m, 2 H), 1.51 (s, 3 H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 161.5, 156.0, 138.7, 136.9, 133.3, 131.3, 131.1, 128.7, 128.4, 127.7, 127.1, 127.0, 126.6, 123.7, 123.2, 121.8, 116.6, 114.6, 107.6, 78.4, 45.9, 35.9, 28.1, 24.5, 20.1; IR (neat) 1633 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{27}H\(_{23}\)NO\(_2\)•Na 416.1627, found 416.1628 [M+Na]\(^+\).
Analytical data for 4ap: 27.9 mg, 39%; orange solid (m.p. 157.6–159.1 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 8.92 (dd, \(J = 8.0, 1.2\) Hz, 1 H), 8.09 (dd, \(J = 8.0, 1.6\) Hz, 1 H), 7.45 (ddd, \(J = 8.4, 7.2, 1.6\) Hz, 1 H), 7.40 (dt, \(J = 8.0, 1.2\) Hz, 1 H), 7.35–7.14 (m, 9 H), 5.80–5.43 (br m, 2 H), 5.53 (q, \(J = 6.4\) Hz, 1 H), 1.73 (d, \(J = 6.4\) Hz, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 161.5, 156.9, 138.8, 136.8, 133.1, 131.3, 128.8, 128.3, 127.8, 127.6, 127.1, 126.6, 125.6, 123.6, 123.1, 121.9, 116.3, 114.7, 107.0, 75.3, 45.9, 20.1; IR (neat) 1633 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{24}\)H\(_{19}\)NO\(_2\)\(\cdot\)Na 376.1314, found 376.1303 [M+Na]\(^+\).

Analytical data for 4aq: 11.9 mg, 17%; orange solid (m.p. 130.4–132.3 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 8.86 (d, \(J = 8.0\) Hz, 1 H), 8.06 (dd, \(J = 7.6, 1.6\) Hz, 1 H), 7.45 (ddd, \(J = 8.4, 7.2, 1.6\) Hz, 1 H), 7.42 (t, \(J = 6.8\), 1 H), 7.35–7.14 (m, 9 H), 5.64 (br s, 2 H), 5.34 (s, 2 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 161.4, 158.3, 138.7, 136.8, 131.4, 128.8, 128.7, 128.6, 128.5, 127.7, 127.2, 126.6, 125.4, 123.8, 123.6, 121.9, 115.8, 114.8, 107.7, 69.5, 45.8; IR (neat) 1633 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{23}\)H\(_{17}\)NO\(_2\)\(\cdot\)Na 362.1157, found 362.1149 [M+Na]\(^+\).

Analytical data for 8: 64.6 mg, 88%; white solid (m.p. 150.2–153.8 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 9.05 (d, \(J = 8.4\) Hz, 1 H), 7.60 (dd, \(J = 7.2, 1.2\) Hz, 1 H), 7.42 (ddd, \(J = 8.8, 7.2, 1.6\) Hz, 1 H), 7.37–7.15 (m, 10 H), 5.61 (br s, 2 H), 4.91 (br s, 1 H), 1.63 (s, 6 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) (one overlapping Csp\(^2\) signal) \(\delta\) 160.9, 145.2, 138.9, 137.6, 137.3, 130.6, 129.6, 128.7, 127.0, 126.9, 126.5, 126.0, 122.0, 121.3, 120.3, 115.7, 114.3, 102.3, 53.7, 45.7, 29.6; IR (neat) 3338 (N=H), 1606 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{25}\)H\(_{22}\)NO\(_3\)\(\cdot\)Na 389.1630, found 389.1622 [M+Na]\(^+\).

Three-component coupling products 10a,b and 11 were also obtained under the Catellani reaction condition.

Analytical data for 10a: 103.3 mg, 85%; white solid (m.p. 203.4–205.3 °C); \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 9.27 (dd, \(J = 8.4, 1.2\) Hz, 1 H), 7.69 (dd, \(J = 7.2, 1.2\) Hz, 1 H), 7.48–7.21 (m, 11 H), 7.20 (t, \(J = 8.0\) Hz, 1 H), 6.92 (d, \(J = 8.0\) Hz, 2 H), 5.86 (br d, \(J = 13.6\) Hz, 1 H), 5.42 (br d, \(J = 13.6\) Hz, 1 H), 4.72 (s, 1 H), 3.80 (d, \(J = 9.2\) Hz, 1 H), 3.29 (d, \(J = 9.6\) Hz, 1 H), 2.19 (d, \(J = 3.2\) Hz, 1 H), 2.00 (s, 1 H), 1.98 (s, 3 H), 1.80 (s, 6 H), 1.79–1.51 (m, 4 H), 1.65 (d, \(J = 11.0\) Hz, 1 H), 1.00 (d, \(J = 11.0\) Hz, 1 H); \(^{13}\)C NMR (100 MHz,
CDCl₃, 25 °C) δ 160.3, 143.2, 142.7, 139.4, 139.1, 138.8, 136.8, 136.6, 132.3, 129.8, 129.0, 128.8, 128.1, 127.5, 127.2, 127.0, 126.6, 125.7, 124.9, 123.8, 122.0, 120.0, 115.0, 60.3, 51.5, 46.8, 46.5, 44.9, 42.6, 33.6, 33.4, 31.2, 30.6, 29.2, 20.8; IR (neat) 3271 (N–H), 1630 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₃₉H₃₈N₂O₃S•Na 637.2501, found 637.2494 [M+Na]⁺.

Analytical data for 10b: 76.5 mg, 51%; brown solid (m.p. 114.2–115.4 °C); ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 9.20 (d, J = 8.0 Hz, 1 H), 7.85 (d, J = 8.0 Hz, 1 H), 7.47 (d, J = 8.0 Hz, 2 H), 7.41–7.14 (m, 10 H), 7.03 (d, J = 8.0 Hz, 2 H), 5.84 (br s, 1 H), 5.44 (br s, 1 H), 5.15 (s, 1 H), 4.73 (dd, J = 10.4, 6.0 Hz, 1 H), 4.68 (d, J = 9.2 Hz, 1 H), 4.61–4.55 (m, 1 H), 4.41 (dd, J = 12.0, 6.4 Hz, 1 H), 4.19 (t, J = 11.4 Hz, 1 H), 3.60 (d, J = 9.6 Hz, 1 H), 2.57 (br s, 1 H), 2.45 (br s, 1 H), 2.31 (s, 2 H), 2.21 (s, 3 H), 2.14 (s, 3 H), 2.07 (s, 3 H), 1.98 (d, J = 11.2 Hz, 1 H), 1.85 (s, 3 H), 1.70 (s, 3 H), 1.22 (d, J = 12.0 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 171.0, 170.5, 160.1, 142.8, 140.7, 139.8, 138.7, 136.6, 135.0, 133.2, 129.7, 129.4, 128.7, 128.2, 127.1 (2C), 126.7, 126.5, 125.9, 125.2, 124.7, 121.7, 119.8, 114.9, 62.5, 62.3, 60.7, 52.8, 49.2, 46.5, 42.2, 39.7, 38.2, 36.5, 35.7, 33.4, 32.1, 21.18, 21.11; IR (neat) 3253 (N–H), 1739 (C=O), 1633 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₄₃H₄₆N₂O₇S•Na 781.2923, found 781.2904 [M+Na]⁺.

The reaction of 2a with 3o afforded an inseparable mixture of S₃ and S₄ (35.5 mg) in a ratio of S₃/S₄ = 2:1. Analytically pure sample of S₄ was obtained by partial separation using preparative HPLC. In comparison with the spectral data of 10, S₄ was tentatively assigned as the three-component annulation product. Although S₄ was obtained as a single diastereomer, its stereochemistry could not be elucidated. The structure of S₃ was tentatively assigned as a singlet of the C4 proton of the quinolone ring was observed at δ 7.69 ppm.

Analytical data for S₃: 21.9 mg, 28% based on ¹H NMR analysis; colorless oil; ¹H NMR (400 MHz, CDCl₃, 25 °C) δ 7.69 (s, 1 H), 7.59 (dd, J = 8.0, 1.2 Hz, 1 H), 7.44 (ddd, J = 8.8, 7.2, 1.6 Hz, 1 H), 7.34 (d, J = 8.8 Hz, 1 H), 7.33–7.22 (m, 5 H), 7.22 (d, J = 6.8 Hz, 1 H), 7.21 (d, J = 6.8 Hz, 1 H), 7.17 (d, J = 7.2 Hz, 1 H), 6.97 (dd, J = 7.2, 1.2 Hz, 1 H), 5.72 (br d, J = 15.8 Hz, 1 H), 5.52 (br d, J = 15.8 Hz, 1 H), 3.01–2.84 (m, 2 H), 2.09–1.76 (m, 4 H), 1.75 (br s, 1 H), 1.40 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 164.1, 141.8, 138.8, 137.9, 137.5, 137.3, 136.4, 136.2, 130.2, 130.1, 128.8, 128.7, 127.3, 126.9, 126.8, 122.5, 121.1, 115.1, 71.1, 46.8, 41.8, 31.1, 30.2, 20.0; IR (neat) 3365 (O–H), 1631 (C=O) cm⁻¹; HRMS (ESI) m/z calcd for C₂₇H₂₅NO₂•Na 418.1783, found 418.1792 [M+Na]⁺.
5. Control Experiments

Reaction of 2a with 3a in the absence of norbornene. Homo coupling product 5 was obtained under the Catellani reaction conditions, except for using 10 mol % of Pd(OAc)\(_2\) in the absence of norbornene.

**Analytical data for 5:**

- **S15**: 64.6 mg, 88%; white solid (m.p. 246.8–249.7 °C);
- \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 7.47 (ddd, \(J = 8.4, 7.2, 1.2\) Hz, 2 H), 7.42–7.27 (m, 14 H), 7.08 (ddd, \(J = 8.0, 7.2, 0.8\) Hz, 2 H), 6.87 (s, 2 H), 5.70 (br d, \(J = 15.6\) Hz, 2 H), 5.62 (br d, \(J = 15.6\) Hz, 2 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 161.6, 146.6, 139.6, 136.1, 131.3, 128.9, 127.5, 126.7, 122.5, 121.8, 119.9, 115.5, 46.3; IR (neat) 1652 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{32}\)H\(_{24}\)N\(_2\)O\(_2\)•Na 491.1736, found 491.1747 [M+Na]^+.

**Synthesis of 4fa:** A solution of 4-iodocoumarin 2f (30.0 mg, 0.11 mmol), 2-(2-bromophenyl)propan-2-ol 3a (23.7 mg, 0.11 mmol), Pd(OAc)\(_2\) (1.2 mg, 0.006 mmol), P(2-furyl)\(_3\) (2.6 mg, 0.011 mmol), norbornene (10.4 mg, 0.11 mmol), and K\(_2\)CO\(_3\) (38.1 mg, 0.28 mmol) in dry m-xylene (2.2 mL) was degassed at −78 °C. The reaction mixture was heated at 140 °C for 18 h. After cooling to room temperature, the crude mixture was purified by flash column chromatography on silica gel (hexane/EtOAc = 20:1~8:1) to afford 4fa (25.0 mg, 82%) as a yellow foam:

- \(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \(\delta\) 8.68 (d, \(J = 8.0\) Hz, 1 H), 7.91 (dd, \(J = 8.0, 1.2\) Hz, 1 H), 7.57 (ddd, \(J = 8.0, 7.2, 1.2\) Hz, 1 H), 7.40 (dt, \(J = 8.0, 1.2\) Hz, 1 H), 7.36–7.29 (m, 3 H), 7.22 (d, \(J = 8.0\) Hz, 1 H), 1.78 (s, 6 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \(\delta\) 160.2, 159.2, 152.9, 136.0, 132.3, 128.3, 128.1, 125.1, 125.0, 123.9, 123.1, 122.3, 116.3, 115.8, 101.4, 81.5, 27.8; IR (neat) 1714 (C=O) cm\(^{-1}\); HRMS (ESI) \(m/z\) calcd for C\(_{18}\)H\(_{14}\)O\(_3\)•Na 301.0841, found 301.0864 [M+Na]^+.
Reaction of 2a with o-bromophenol. 4-aryloxy-2-quinolone 6b was obtained under the Catellani reaction conditions, except for using 10 mol % of Pd(OAc)$_2$ and 1 equiv of norbornene.

Analytical data for 6b: 21.7 mg, 27%; white solid (m.p. 246.8–249.7 °C); $^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ 8.23 (dd, $J = 7.6$, 1.2 Hz, 1 H), 7.71 (dd, $J = 8.0$, 1.2 Hz, 1 H), 7.51 (dt, $J = 7.6$, 1.6 Hz, 1 H), 7.43 (dt, $J = 7.6$, 1.6 Hz, 1 H), 7.34–7.18 (m, 9 H), 5.76 (s, 1 H), 5.53 (br s, 2 H); $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ 163.5, 161.7, 150.3, 139.6, 136.5, 134.3, 131.7, 129.2, 128.8, 127.7, 127.2, 126.5, 123.6, 116.4, 116.0, 115.1, 100.0, 45.7; IR (neat) 1647 (C=O) cm$^{-1}$; HRMS (ESI) m/z calcd for C$_{22}$H$_{16}$BrNO$_2$•Na 428.0262 found 428.0268 [M+Na]$^+$. 

Preparation of 2a-d$_1$: To a solution of methyl 3-(2-(benzyl(tert-butoxycarbonyl)amino)phenyl)propiolate (182.9 mg, 0.5 mmol) in acetic acid-d$_4$ (1 mL) was added sodium iodide (448.7 mg, 3.0 mmol) at room temperature. The reaction mixture was stirred at 110 °C for 1 h. The reaction was quenched with H$_2$O (10 mL) and the resultant mixture was extracted with EtOAc (3 × 10 mL). The combined organic layer was washed with sat. Na$_2$CO$_3$ (10 mL), sat. Na$_2$S$_2$O$_3$ (10 mL), and brine (10 mL). After dried over MgSO$_4$, the solvents were removed in vacuo. The obtained crude material was purified by flash column chromatography on silica gel (hexane/EtOAc = 8:1) to afford 4-iodo-2-quinolone 2a-d$_1$ (85%D, 169.2 mg, 94%) as a white solid (m.p. 125.1–127.1 °C).

Competition experiment using 2a-d$_1$: In a similar manner with the reaction of 2a with 3a, the reaction of 4-iodo-2-quinolone 2a (51.1 mg, 0.14 mmol) and 2a-d$_1$ (85%D, 72.4 mg, 0.20 mmol) with 2-(2-bromophenyl)propan-2-ol 3a (37.0 mg, 0.17 mmol) was performed in the presence of Pd(OAc)$_2$ (1.97 mg, 0.009 mmol), norbornene (37.0 mg, 0.17 mmol), and K$_2$CO$_3$ (58.8 mg, 0.42 mmol) in dry DMF (3.4 mL) at 105 °C for 1 h. After an usual purification, 2a-d$_1$ (51%D, 60.0 mg, 49%) was recovered along with 4aa (52.9 mg, 42%).

6. Single Crystal X-ray Diffraction Study
A single crystal of 10a was mounted on a glass fiber, and diffraction data were collected in $\theta$ ranges specified in Table S1 at 123 K on a Bruker D8 QUEST diffractometer with graphite monochromatized Mo Kα radiation ($\lambda = 0.71073$ Å). The absorption correction was made using SADABS. The structure was solved by direct methods and refined by the full-matrix least-squares on $F^2$ by using SHELXL-2013.$^{12}$ All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions. Final refinement details are compiled in Table S1. The supplementary crystallographic data

for this paper (CCDC 1557549) can also be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; or deposit@ccdc.cam.ac.uk).

Table S1. Selected crystallographic data and collection parameters for 10a.

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<th>Value</th>
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<td>R₁, wR₂ (all data)</td>
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<td>Weighting scheme</td>
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<td>Where P = (Fo² + 2Fc²)/3</td>
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<tr>
<td>extinction coefficient</td>
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<td>largest diff. peak and hole, e Å⁻³</td>
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<td>R.M.S. deviation from mean, e Å⁻³</td>
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7. DFT Calculations

The Gaussian 09 program package was used for all geometry optimizations.\(^{13}\) The geometries of the stationary points and transition states were fully optimized using the Becke’s three-parameter hybrid density functional method (B3LYP)\(^{14}\) with a double-$\zeta$ basis set with the relativistic effective core potential of Hay and Wadt (LanL2DZ)\(^{15}\) for PD, K, Br, and I and the 6-31G(d)\(^{16}\) basis sets for other elements. The vibrational frequencies and thermal correction to Gibbs free energy (TCGFE) including zero-point energy were calculated at the same level of theory. The obtained structures were characterized by the number of imaginary frequencies (IF, one or zero for transition or ground states, respectively). The connectivity of each step was also confirmed by intrinsic reaction coordinate (IRC) calculation\(^{17}\) from the transition states followed by optimization of the resultant geometries. Single-point energies for geometries obtained by the above method were calculated using the Truhlar’s M06L functional\(^{18}\) with the basis sets including the Stuttgart-Dresden-Bonn energy-consistent pseudopotential (SDD)\(^{19}\) for Pd, K, Br, and I, and the 6-311++G(d,p) basis sets\(^{20}\) for other elements. To examine the solvent effect, the above single-point energy calculations were performed using the polarizable continuum model (PCM)\(^{21}\) method with


dielectric constants (e) of 37.219 for DMF. The obtained energies, ZPEs, TCGFEs, and IF are summarized in Tables S1 and S2.

Table S1. Summary of theoretical calculations.

<table>
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<tr>
<th>Model</th>
<th>Energy/au</th>
<th>TCGFE/au</th>
<th>IF/cm⁻¹</th>
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**Table S2.** Summary of theoretical calculations.

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*Residual imaginary frequency due to the twist motion of one of two methyl groups at the benzylic position.

**Scheme S1**  CMD step of model complex a leading to palladacycle complex b. Relative Gibbs free energies in DMF at 298 K, 1 atm are indicated in parentheses.
Scheme S2  Oxidative addition/reductive elimination steps of model complex $sG$ and subsequent deinsertion of NBE from intermediate complex $sI$. Relative Gibbs free energies in DMF at 298 K, 1 atm are indicated in parentheses.
Scheme S3  Deprotonation of benzylic alcohol of model complex sK and subsequent bromide dissociation from intermediate complex sL. Relative Gibbs free energies in DMF at 298 K, 1 atm are indicated in parentheses.

Scheme S4  Reductive elimination from model complex sO affording the final product complex sP. Relative Gibbs free energies in DMF at 298 K, 1 atm are indicated in parentheses.
Standard orientations

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