Supporting Information

Efficient Conversion of Biginelli 3,4-Dihydropyrimidin-2(1*H*)-one to Pyrimidines via PyBroP-mediated Coupling

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I – General Methods

¹H NMR spectra were reported in ppm from tetramethylsilane on the scale. Data are reported as follows: chemical shift, multiplicity, coupling constants (Hz), and relative integration. ¹³C NMR spectra were reported in ppm from the central deuterated solvent peak.

II – Reagents and Starting Materials

PyBOP and PyBroP were purchased from Novabiochem and were recrystallized before use according to the procedure by Alsina¹ et al. Compound **1** was prepared according to the procedure by Hu² et al. Compound **2** was prepared according to the procedure by Kappe³ et al. Interestingly, on its ¹³C NMR spectrum at 25 °C, the four carbon peaks of C₄, C₆ and their directly bonded carbons of the substituents (phenyl and methyl) are missing, due to the tautomerization between pyrimidin-2(1*H*)-one and pyrimidin-2(3*H*)-one. The complete ¹³C NMR data of compound **2** were obtained at 90 °C in DMSO-*d*⁶.

4-Phenyl-6-methyl-3,4-dihydropyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (1). White solid. ¹H NMR (300 MHz, CDCl₃) δ 2.32 (s, 1H), 3.62 (s, 1H), 6.07 (br s, 1H), 7.30 (s, 5H), 8.62 (br s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 18.7, 51.1, 55.5, 101.1, 126.6, 127.4, 128.0, 128.9, 143.6, 146.8, 166.2; LRMS (ES) *m/z* [M+H]⁺ 247.1.

4-Phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (2). White solid. ¹H NMR (300 MHz, CDCl₃) δ 2.61 (s, 3H), 3.59 (s, 3H), 7.45, (m, 3H), 7.58 (m, 2H); ¹³C NMR (100 MHz, CDCl₃, 25 °C) δ 52.7, 111.6, 128.4, 128.8, 131.4, 158.8, 167.1; ¹³C NMR (100 MHz, DMSO-*d*⁶, 90 °C) δ 20.7, 53.5, 111.3, 129.2, 129.9, 131.8, 139.4, 157.5, 164.3, 168.2, 171.2; HRMS (FAB+) *m/z* Calcd for C₁₃H₁₂N₂O₃ [M+H]⁺ 245.0926, Found 245.0918.

III – General Procedures for the PyBroP-mediated Coupling

General Procedure A for the PyBroP-mediated Coupling to Synthesize

Pyrimidines 3a-g: To a stirred solution of compound **2** (48.8 mg, 0.2 mmol) in dioxane (2 mL) at room temperature was added PyBroP (102.5 mg, 0.22 mmol), Et₃N (69.2 μL, 0.5 mmol) and the nucleophile (0.26 mmol). After it was stirred at room temperature for 24-72 h (TLC monitor), it was diluted with EtOAc and washed with saturated NH₄Cl solution, brine and dried with Na₂SO₄. Filtration, evaporation and flash chromatography (5-20% EtOAc in hexane) gave the product **3a-g**.

General Procedure B for the PyBroP-mediated Coupling to Synthesize

Pyrimidines 3h-n: To a stirred solution of compound **2** (48.8 mg, 0.2 mmol) in dioxane (2 mL) at room temperature was added PyBroP (102.5 mg, 0.22 mmol) and Et₃N (69.2 μL, 0.5 mmol); then, the nucleophile (0.26 mmol) and NaOBu^t (23 mg, 0.24 mmol) were

added. After it was stirred at room temperature for 24-72 h (TLC monitor), it was diluted with EtOAc and washed with saturated NH_4Cl solution, brine and dried with Na_2SO_4 . Filtration, evaporation and flash chromatography (5-20% EtOAc in Hexane) gave the product **3h-n**.

2-(N-Benzylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3a). White solid. ^1H NMR (400 MHz, CDCl_3) δ 2.47 (s, 3H), 3.58 (s, 3H), 4.69 (d, $J = 6.0$, 2H), 5.99 (br s, 1H), 7.2-7.6 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.0, 45.4, 52.0, 115.3, 127.3, 127.6, 127.9, 128.3, 128.6, 129.6, 138.9, 139.0, 161.2, 165.9, 167.4, 169.5; HRMS (FAB+) m/z Calcd for $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 334.1556, Found 334.1546.

2-(N-Benzyl-N-methylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3b). Colorless oil. ^1H NMR (300 MHz, CDCl_3) δ 2.50 (s, 3H), 3.20 (s, 3H), 3.59 (s, 3H), 4.99 (s, 2H), 7.3-7.7 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.7, 35.1, 52.3, 52.7, 114.0, 127.5, 128.0, 128.5, 128.6, 128.9, 129.9, 138.7, 139.8, 161.4, 165.8, 167.5, 170.3; HRMS (FAB+) m/z Calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 348.1712, Found 348.1715.

2-(Pyrrolidin-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3c). White solid. ^1H NMR (300 MHz, CDCl_3) δ 1.98 (m, 4H), 2.49 (s, 3H), 3.58 (s, 3H), 3.62 (m, 4H), 7.37 (m, 3H), 7.57 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.7, 25.8, 47.1, 52.2, 113.5, 128.5, 128.6, 129.8, 140.0, 159.6, 165.9, 167.3, 170.4; HRMS (FAB+) m/z Calcd for $\text{C}_{17}\text{H}_{19}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 298.1556, Found 298.1553.

2-(Morpholin-4-yl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3d). White solid. ^1H NMR (300 MHz, CDCl_3) δ 2.49 (s, 3H), 3.58 (s, 3H), 3.75 (m, 4H), 3.90 (m, 4H), 7.40 (m, 3H), 7.55 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.6, 44.5, 52.3, 67.3, 114.6, 128.4, 128.6, 130.0, 139.6, 160.7, 165.9, 167.5, 170.0; **HRMS** (FAB+) m/z Calcd for $\text{C}_{17}\text{H}_{19}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$ 314.1504, Found 314.1496.

2-((S)-1-Ethoxycarbonyl-2-phenyl-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3e). Colorless oil. ^1H NMR (300 MHz, CDCl_3) δ 1.20 (t, 3H), 2.46 (s, 1H), 3.18 (m, 2H), 3.59 (s, 3H), 4.15 (m, 2H), 5.04 (m, 1H), 5.72 (br d, $J = 7.6$, 1H), 7.1-7.6 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ 14.6, 23.3, 38.6, 52.4, 55.8, 61.6, 116.3, 127.4, 128.4, 128.7, 128.9, 129.8, 130.1, 136.7, 139.1, 160.6, 167.7, 169.8, 172.6; **HRMS** (FAB+) m/z Calcd for $\text{C}_{24}\text{H}_{25}\text{N}_3\text{O}_4$ $[\text{M}+\text{H}]^+$ 420.1923, Found 420.1927.

2-((RS)-1-Benzyl-2-hydroxy-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3f). Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 2.46 (s, 3H), 2.95 (m, 2H), 3.58 (s, 3H), 3.66 (dd, $J = 11.0$, 5.5, 1H), 3.79 (dd, $J = 11.0$, 3.2, 1H), 4.34 (m, 1H), 5.69 (br d, $J = 6.7$, 1H), 7.1-7.6 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.4, 37.9, 52.4, 55.1, 60.8, 64.9, 115.7, 127.0, 128.3, 128.8, 129.0, 129.7, 130.2, 138.4, 139.1, 161.4, 166.3, 167.8, 169.5; **HRMS** (FAB+) m/z Calcd for $\text{C}_{22}\text{H}_{23}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$ 378.1818, Found 378.1824.

2-Phenylsulfanyl-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3g). Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 2.50 (s, 3H), 3.69 (s, 3H), 7.3-7.7 (m, 10H); ^{13}C NMR (100 MHz, CDCl_3) δ 22.8, 52.7, 121.2, 128.4, 128.6, 129.1, 129.3, 129.4, 130.5, 135.4, 137.3, 163.5, 166.2, 168.8, 172.4; HRMS (FAB+) m/z Calcd for $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 337.1011, Found 337.1024.

2-(*N*-Methyl-methanesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3h). White solid. ^1H NMR (300 MHz, CDCl_3) δ 2.59 (s, 3H), 3.52 (s, 3H), 3.59 (s, 3H), 3.69 (s, 3H), 7.47 (m, 3H), 7.67 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.3, 33.5, 42.9, 53.0, 120.0, 128.7, 129.0, 130.8, 137.9, 158.7, 164.8, 167.4, 169.0; HRMS (FAB+) m/z Calcd for $\text{C}_{15}\text{H}_{17}\text{N}_3\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$ 336.1018, Found 336.1004.

2-(*N*-Methyl-benzenesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3i). White solid. ^1H NMR (300 MHz, CDCl_3) δ 2.47 (s, 3H), 3.63 (s, 3H), 3.77 (s, 3H), 7.3-7.6 (m, 8H), 8.02 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 22.9, 34.0, 52.9, 120.0, 128.7, 129.9, 130.6, 133.2, 133.3, 137.8, 140.9, 157.8, 164.8, 167.0, 169.0; HRMS (FAB+) m/z Calcd for $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$ 398.1175, Found 398.1167.

2-(Imidazol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3j). White solid. ^1H NMR (300 MHz, CDCl_3) δ 2.65 (s, 3H), 3.73 (s, 3H), 7.17 (s, 1H), 7.50 (m, 3H), 7.78 (m, 2H), 7.95 (s, 1H), 8.68 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.2, 53.2, 117.1, 123.4, 128.7, 129.1, 131.1, 131.2, 136.9, 137.3, 154.0, 165.9, 168.5, 168.6; HRMS (FAB+) m/z Calcd for $\text{C}_{16}\text{H}_{14}\text{N}_4\text{O}_2$ $[\text{M}+\text{H}]^+$ 295.1195, Found 295.1193.

2-(Indol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3k). White solid. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 2.96 (s, 3H), 3.71 (s, 3H), 6.70 (d, $J = 3.7$, 1H), 7.24 (m, 1H), 7.34 (m, 1H), 7.52 (m, 3H), 7.61 (d, $J = 7.7$, 1H), 7.74 (m, 2H), 8.36 (d, $J = 3.7$, 1H), 8.86 (d, $J = 8.3$, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 23.4, 52.9, 107.7, 117.0, 120.6, 121.3, 122.8, 124.2, 126.5, 128.7, 129.0, 130.7, 131.9, 135.9, 138.4, 157.0, 165.7, 167.8, 169.2; **HRMS** (FAB+) m/z Calcd for $\text{C}_{21}\text{H}_{17}\text{N}_3\text{O}_2$ $[\text{M}+\text{H}]^+$ 343.1321, Found 343.1327.

2-Bis(Ethoxycarbonylmethyl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3l). Colorless oil. $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 1.29 (t, $J = 7.1$, 6H), 2.59 (s, 3H), 3.73 (s, 3H), 4.28 (q, $J = 7.1$, 4H), 5.11 (s, 1H), 7.43 (m, 3H), 7.62 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 14.4, 23.0, 53.2, 62.2, 62.4, 124.4, 128.8, 129.0, 130.7, 137.6, 163.2, 163.9, 166.3, 166.9, 168.9; **HRMS** (FAB+) m/z Calcd for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_6$ $[\text{M}+\text{H}]^+$ 387.1556, Found 387.1564.

2-Phenoxy-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3m). Colorless oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 2.56 (s, 3H), 3.70 (s, 3H), 7.40-7.65 (m, 10H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 22.8, 52.6, 120.7, 121.6, 128.3, 128.4, 128.5, 128.6, 129.5, 137.2, 152.8, 164.1, 166.5, 168.7, 169.3; **HRMS** (FAB+) m/z Calcd for $\text{C}_{19}\text{H}_{16}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$ 321.1239, Found 321.1241.

2-(3,4-Dimethoxy-phenylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3n). Light yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 2.54 (s, 3H), 3.63 (s, 3H), 3.87 (s, 3H), 3.89 (s, 3H), 6.84 (d, $J = 8.0$, 1H), 6.97 (dd, $J = 8.0$, 3.0, 1H), 7.21 (br s, 1H), 7.45 (m, 3H), 7.63 (m, 2H), 7.68 (d, $J = 3.0$, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 23.3, 52.4, 55.9, 56.3, 104.7, 111.3, 111.9, 116.5, 128.1, 128.6, 130.1, 132.9, 138.8, 145.0, 149.0, 159.0, 165.8, 167.5, 169.3; **HRMS** (FAB+) m/z Calcd for $\text{C}_{21}\text{H}_{21}\text{N}_3\text{O}_4$ $[\text{M}+\text{H}]^+$ 380.1610, Found 380.1616.

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**4-Phenyl-6-methyl-3,4-dihydropyrimidin-2(1H)-one-5-carboxylic acid methyl ester
(1) (¹H NMR)**

**4-Phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (2)
(¹H NMR)**

4-Phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (2)
 (^{13}C NMR, CDCl_3 , 25°C)

4-Phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (2)
 (^{13}C NMR, $\text{DMSO}-d_6$, 90°C)

**2-(*N*-Benzylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3a) (¹H NMR)**

**2-(*N*-Benzylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3a) (¹³C NMR)**

2-(*N*-Benzyl-*N*-methylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3b) (¹H NMR)

2-(*N*-Benzyl-*N*-methylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3b) (¹³C NMR)

**2-(Pyrrolidin-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3c) (¹H NMR)**

**2-(Pyrrolidin-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3c) (¹³C NMR)**

**2-(Morpholin-4-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3d) (¹H NMR)**

**2-(Morpholin-4-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid
methyl ester (3d) (¹³C NMR)**

2-((S)-1-Ethoxycarbonyl-2-phenyl-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3e) (¹H NMR)

2-((S)-1-Ethoxycarbonyl-2-phenyl-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3e) (¹³C NMR)

2-((*RS*)-1-Benzyl-2-hydroxy-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3f) (¹H NMR)

2-((*RS*)-1-Benzyl-2-hydroxy-ethylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3f) (¹³C NMR)

2-Phenylsulfanyl-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3g) (¹H NMR)

2-Phenylsulfanyl-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3g) (¹³C NMR)

2-(*N*-Methyl-methanesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3h) (¹H NMR)

2-(*N*-Methyl-methanesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3h) (¹³C NMR)

2-(*N*-Methyl-benzenesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3i) (¹H NMR)

2-(*N*-Methyl-benzenesulfonyl-amino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3i) (¹³C NMR)

2-(Imidazol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3j) (¹H NMR)

2-(Imidazol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3j) (¹³C NMR)

2-(Indol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3k) (¹H NMR)

2-(Indol-1-yl)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3k) (¹³C NMR)

2-Bis(Ethoxycarbonylmethyl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3l) (¹H NMR)

2-Bis(Ethoxycarbonylmethyl)-4-phenyl-6-methyl-pyrimidin-2(1H)-one-5-carboxylic acid methyl ester (3l) (¹³C NMR)

**2-Phenoxy-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester
(3m) (¹H NMR)**

**2-Phenoxy-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester
(3m) (¹³C NMR)**

2-(3,4-Dimethoxy-phenylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3n) (¹H NMR)

2-(3,4-Dimethoxy-phenylamino)-4-phenyl-6-methyl-pyrimidin-2(1*H*)-one-5-carboxylic acid methyl ester (3n) (¹³C NMR)