

Supporting Information

Copper-catalyzed cascade reaction: Synthesis of Pyrimido[4,5-*b*]quinolinones from 2-Chloroquinoline-3-carbonitriles with (aryl)methanamines

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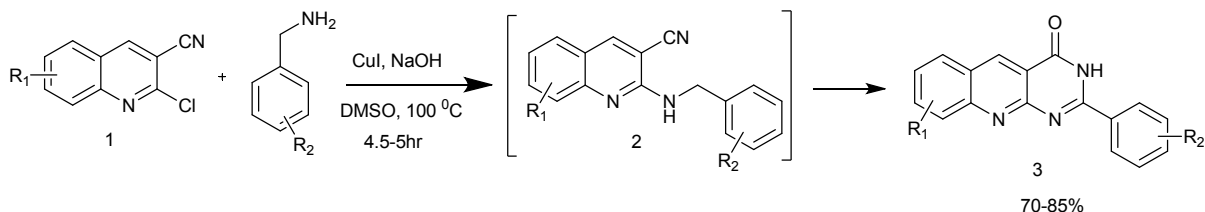
Contents	Page No.
General remarks and representative experimental procedure	2
Characterization Data of final compounds	3-7
¹ H NMR and ¹³ C NMR spectra of final compounds	8-29

General remarks

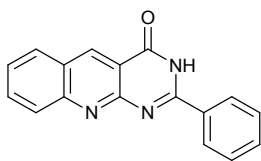
Melting points were measured using Buchi Melting-point apparatus in an open capillary tube and are uncorrected. IR spectra were recorded on VARIAN 3300 FTIR spectrophotometers. ^1H NMR and ^{13}C NMR were recorded on JEOL at 500 and 125 MHz spectrometer respectively. Chemical shifts (δ) are reported relative to TMS (^1H NMR), CDCl_3 (^{13}C NMR) as the internal standards. High resolution mass spectra (HRMS) were obtained on micro TOF QII high-resolution mass spectrometer (ESI) and 6200 series TOF/6500 SRIES QTOF B.05.00 (B5042.0). Thin layer chromatography (TLC) was performed on glass plates (7.5X2.5 and 7.5X5.0 cm) coated with Loba Chemie's silica gel GF254. Visualization of spots was accomplished by exposure to UV light. Commercially available solvents were purified according to literature. Column chromatography was performed using silica gel (100-200).

Representative procedure for the synthesis of 2-phenylpyrimido[4,5-b]quinolin-4(3H)-ones (3):

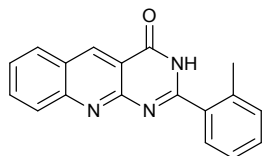
A 25 mL flask equipped with a magnetic stirring bar was charged with substituted 2-chloroquinoline-3-carbonitrile (0.5 mmol), (aryl)methanamine (0.6 mmol), NaOH (1.5 mmol) and CuI (0.005 mmol) in DMSO (2.0 mL). The mixture was allowed to stir under air at 100 °C for 4.5-5 h. After completion of the reaction, the resulting solution was cooled to room temperature, poured into water and extracted with ethyl acetate. The solvent of extract was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using ethyl acetate–hexanes (1:1) as eluent to provide the desired product (3).



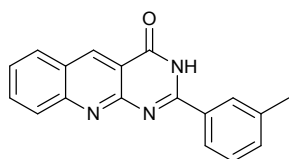
Characterization data of Final compounds:



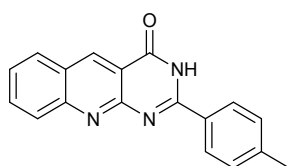
2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3a)^{6b}: Reaction time: 5h; Yield: 78 %; Yellow solid; mp: 354-356 °C; IR (KBr): ν 1294, 1601, 1677 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 7.56 (t, $J=7.0$ Hz, 2H), 7.60-7.64 (m, 2H), 7.90 (t, $J=7.5$ Hz, 1H), 8.05 (d, $J=8.5$ Hz, 1H), 8.23 (t, $J=7.5$ Hz, 3H), 9.25 (s, 1H), 12.62 (s, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 116.65, 127.23, 127.51, 129.17, 129.45, 129.73, 130.53, 133.13, 133.63, 133.89, 139.19, 152.11, 156.84, 157.35, 164.25.



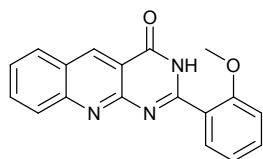
2-(o-tolyl)pyrimido[4,5-b]quinolin-4(3H)-one (3b)^{6b}: Reaction time: 4.5 h; Yield: 84 %; yellow solid; mp: 258-260 °C; IR (KBr): ν 754, 1597, 1675 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 2.43 (s, 3H), 7.31-7.35 (m, 2H), 7.43 (t, $J=7.0$ Hz, 1H), 7.56 (d, $J=7.5$ Hz, 1H), 7.63 (t, $J=7.5$ Hz, 1H), 7.90 (t, $J=8.0$ Hz, 1H), 8.05 (d, $J=8.5$ Hz, 1H), 8.24 (d, $J=8.5$ Hz, 1H), 9.28 (s, 1H), 12.53 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 20.20, 116.15, 126.26, 126.82, 127.01, 128.99, 129.65, 130.03, 130.75, 131.21, 133.34, 134.68, 136.80, 138.69, 151.44, 156.84, 158.63, 163.31.



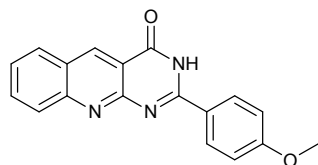
2-(m-tolyl)pyrimido[4,5-b]quinolin-4(3H)-one (3c): Reaction time: 4.5 h; Yield: 82 %; White solid; mp: 306-308 °C; IR (KBr): ν 807, 1294, 1600, 1678 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 2.38 (s, 3H), 7.39-7.43 (m, 2H), 7.59-7.63 (m, 1H), 7.87-7.91 (m, 1H), 8.02 (d, $J=4.5$ Hz, 2H), 8.08 (s, 1H), 8.21 (t, $J=7.0$ Hz, 1H), 9.24 (d, $J=7.0$ Hz, 1H), 12.54 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 21.49, 116.13, 125.76, 126.70, 126.95, 128.94, 129.10, 129.24, 130.02, 133.03, 133.22, 133.34, 138.54, 138.64, 151.61, 156.33, 156.87, 163.70; HRMS (ESI) exact mass calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{OH}$: 288.1137 ($\text{M}+\text{H}$)⁺, found: 288.1131 ($\text{M}+\text{H}$)⁺.



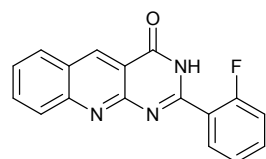
2-(p-tolyl)pyrimido[4,5-b]quinolin-4(3H)-one (3d)^{6b}: Reaction time: 4.5 h; Yield: 80 %; Yellow solid; mp: 302-304 °C; IR (KBr): ν 1249, 1599, 1670 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 2.36 (s, 3H), 7.35 (d, $J=7.0$ Hz, 2H), 7.59 (t, $J=7.0$ Hz, 1H), 7.88 (t, $J=7.0$ Hz, 1H), 8.02 (d, $J=8.0$ Hz, 1H), 8.14 (d, $J=8.0$ Hz, 2H), 8.20 (d, $J=8.0$ Hz, 1H), 9.21 (s, 1H), 12.55 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 21.58, 116.01, 126.66, 126.85, 128.63, 128.86, 129.81, 130.01, 130.27, 133.32, 138.63, 142.88, 151.54, 156.34, 159.16, 163.88.



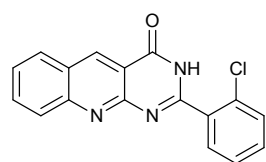
2-(2-methoxyphenyl)pyrimido[4,5-b]quinolin-4(3H)-one (3e): Reaction time: 4.5h; Yield: 83 %; Orange solid; mp: 216-218 °C; IR (KBr): ν 744, 1234, 1588, 1692 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 3.86 (s, 3H), 7.10 (t, $J=7.0$ Hz, 1H), 7.19 (d, $J=8.5$ Hz, 1H), 7.53-7.56 (m, 1H), 7.62 (t, $J=7.5$ Hz, 1H), 7.81 (d, $J=7.5$ Hz, 1H), 7.90 (t, $J=8.0$ Hz, 1H), 8.03 (d, $J=8.5$ Hz, 1H), 8.23 (d, $J=8.0$ Hz, 1H), 9.26 (s, 1H), 12.16 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 56.36, 112.52, 116.07, 121.06, 122.86, 126.70, 126.94, 128.93, 129.99, 131.19, 133.31, 138.67, 151.44, 156.47, 156.98, 157.82, 162.70; HRMS (ESI) exact mass calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{OH}$: 304.1086 ($\text{M}+\text{H}$)⁺, found: 304.1081 ($\text{M}+\text{H}$)⁺.



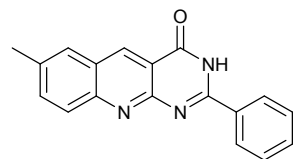
2-(4-methoxyphenyl)pyrimido[4,5-b]quinolin-4(3H)-one (3f)^{6b}: Reaction time: 4.5h; Yield: 80 %; Yellow solid; mp: 302-304 °C; IR (KBr): ν 1264, 1599 1667 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 3.83 (s, 3H), 7.10 (d, J = 8.0 Hz, 2H), 7.60 (t, J = 7.0 Hz, 1H), 7.89 (t, J = 7.5 Hz, 1H), 8.02 (d, J = 8.5 Hz, 1H), 8.21 (d, J =8.0 Hz, 1H), 8.26 (d, J = 8.0 Hz, 2H), 9.22 (s, 1H), 12.50 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 56.06, 106.51, 114.64, 116.26, 116.41, 118.19, 123.45, 125.07, 126.74, 129.89, 130.54, 133.29, 134.49, 138.58, 140.59, 150.22, 159.16, 163.02.



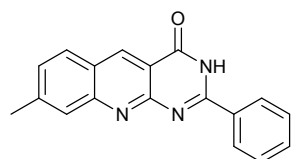
2-(2-fluorophenyl)pyrimido[4,5-b]quinolin-4(3H)-one (3g)^{6b}: Reaction time: 5h; Yield: 75 %; Yellow solid; mp: 234-236 °C; IR (KBr): ν 1600, 1687 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 7.37-7.42 (m, 2H), 7.62-7.66 (m, 2H), 7.85 (t, J = 7.5 Hz, 1H), 7.72 (t, J =7.0 Hz, 1H), 8.05 (d, J =8.5 Hz, 1H), 8.26 (d, J =8.0 Hz, 1H), 9.29 (s, 1H), 12.65 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 116.22, 116.86 (J = 21.12 Hz), 122.75 (J = 12.5 Hz), 125.25, 126.91, 127.22, 129.040, 130.07, 131.67, 133.48, 133.90 (J = 8.25 Hz), 138.85, 151.43, 154.22, 156.71, 160.15 (J = 249.75 Hz), 163.06; ^{19}F NMR (500 MHz, CDCl_3): δ -113.66.



2-(2-chlorophenyl)pyrimido[4,5-b]quinolin-4(3H)-one (3h): Reaction time: 5h; Yield: 77 %; Yellow solid; mp: 292-296°C; IR (KBr): ν 1492, 1599, 1682 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 7.51 (t, J = 7.5 Hz, 1H), 7.55-7.58(m, 1H), 7.61-7.67 (m, 2H), 7.71 (d, J =7.5 Hz, 1H), 7.92 (t, J =7.0 Hz, 1H), 8.05 (d, J =8.5 Hz, 1H), 8.27 (d, J =8.0 Hz, 1H), 9.31 (s, 1H), 12.75 (s, 1H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ 106.53, 116.27, 123.45, 127.27, 127.84, 130.27, 131.33, 131.81, 132.41, 133.55, 134.32, 138.97, 150.24, 151.34, 156.57, 159.16, 162.97; HRMS (ESI) exact mass calcd. for $\text{C}_{17}\text{H}_{10}\text{ClN}_3\text{O}$: 308.0591 ($\text{M}+\text{H}$)⁺, found: 308.0585 ($\text{M}+\text{H}$)⁺. Crystal Data: Bond precision: C-C = 0.0039 Å; Wavelength= 0.71073; Cell: a = 19.7298(7) b = 19.7298(7) c = 19.0360(7); α =90 β =90 γ =120; Temperature: 293 K; Volume: 6417.3(6); Space group: R 3 c; Hall group: R 3 -2¹c; Moiety formula: $\text{C}_{17}\text{H}_{10}\text{ClN}_3\text{O}$; Sum formula: $\text{C}_{17}\text{H}_{10}\text{ClN}_3\text{O}$; Mr: 307.73; D (g/cm^3): 1.433; Z: 14; μ (mm^{-1}): 0.272; F000: 2844.0, F000': 2847.66; h,k,l max: 26,26,25; Nref: 3417[1715]; Correction method= Not given; Data completeness= 1.98/0.99; Theta(max)= 27.930; R(reflections)= 0.0458(2805); wR_2 (reflections)= 0.1033(3388); S= 1.022; Npar= 199.

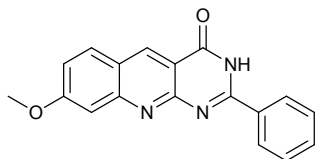


7-methyl-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3i): Reaction time: 5h; Yield: 85 %; Brown solid; mp: 234-236°C; IR (KBr): ν 1291, 1596, 1667 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 2.48 (s, 3H), 7.54-7.57 (m, 3H), 7.73 (d, J =8.5 Hz, 1H), 7.94 (d, J =8.0 Hz, 2H), 8.24 (d, J =7.0 Hz, 2H), 9.09 (s, 1H), 12.58 (s, 1H); ^{13}C NMR (125MHz, $\text{DMSO}-d_6$): δ 21.67, 106.39, 116.09, 126.76, 128.25, 128.65, 129.20, 132.48, 133.39, 135.75, 136.58, 137.54, 150.26, 156.25, 169.09, 164.21; HRMS (ESI) exact mass calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}$: 288.1137 ($\text{M}+\text{H}$)⁺, found: 288.1131 ($\text{M}+\text{H}$)⁺.

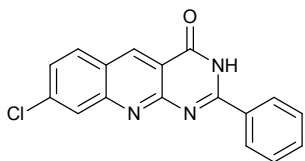


8-methyl-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3j)^{6b}: Reaction time: 5h; Yield: 82 %; Yellow solid; mp: 310-312°C; IR (KBr): ν 1293, 1594, 1664 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ 2.53 (s, 3H), 7.46 (d, J =8.0 Hz, 1H), 7.55 (t, J = 8.0 Hz, 2H), 7.59-7.62 (m, 1H), 7.82 (s, 1H), 8.11 (d, J =8.5Hz, 1H), 8.24 (d,

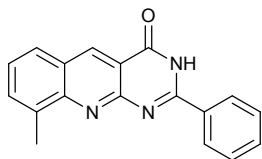
$J=7.5$ Hz, 2H), 9.17(s, 1H), 12.60 (s, 1H) ; ^{13}C NMR (125MHz, DMSO- D_6): δ 22.37, 115.37, 124.98, 127.56, 128.67, 129.21, 129.40, 129.66, 132.56, 133.22, 138.18, 143.94, 151.88, 156.31, 156.92, 163.96.



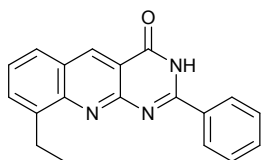
8-methoxy-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3k): Reaction time: 4.5h; Yield: 83 %; Yellow solid; mp: 296-298°C; IR (KBr): ν 1223, 1382, 1573, 1595, 1677 cm^{-1} ; ^1H NMR (500 MHz, DMSO- D_6): δ 3.92 (s, 3H), 7.23 (d, $J=9.0$ Hz, 1H), 7.36 (s, 1H), 7.53-7.59 (m, 3H), 8.08 (d, $J=9.0$ Hz, 1H), 8.22 (d, $J=7.0$ Hz, 2H), 9.09 (s, 1H), 12.53 (s, 1H) ; ^{13}C NMR (125 MHz, DMSO- D_6): δ 56.27, 106.53, 113.88, 120.66, 122.37, 128.62, 129.19, 131.27, 132.51, 133.20, 137.83, 153.93, 156.12, 157.35, 163.42, 163.72; HRMS (ESI) exact mass calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}_2\text{H}$: 304.1086 (M+H) $^+$, found: 304.1081 (M+H) $^+$.



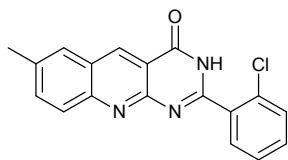
8-chloro-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3l): Reaction time: 5h; Yield: 80 %; Orange solid; mp: 370-372°C; IR (KBr): ν 1291, 1597, 1676 cm^{-1} ; ^1H NMR (500 MHz, DMSO- D_6): δ 7.52-7.58 (m, 4H), 8.02 (s, 1H), 8.21 (d, $J=6.0$ Hz, 3H), 9.21 (s, 1H), 12.64 (s, 1H) ; ^{13}C NMR (125 MHz, DMSO- D_6): δ 116.34, 125.22, 127.39, 127.55, 128.74, 129.19, 131.94, 132.73, 132.95, 138.07, 138.89, 151.76, 156.90, 157.62, 163.48; HRMS (ESI) exact mass calcd. for $\text{C}_{17}\text{H}_{10}\text{ClN}_3\text{OH}$: 308.0591 (M+H) $^+$, found: 308.0585 (M+H) $^+$.



9-methyl-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3m): Reaction time: 5h; Yield: 82 %; yellow solid; mp: 376-378°C; IR (KBr): ν 1291, 1599, 1682 cm^{-1} ; ^1H NMR (500 MHz, DMSO- D_6): δ 2.74(s, 3H), 7.48-7.52 (m, 1H), 7.56 (t, $J=7.5$ Hz, 2H), 7.61 (t, $J=7.5$ Hz, 1H), 7.76 (d, $J=6.5$ Hz, 1H), 8.05 (d, $J=8.5$ Hz, 1H), 8.25 (d, $J=8.0$ Hz, 2H), 9.21 (s, 1H), 12.63 (s, 1H); ^{13}C NMR (125 MHz, DMSO- D_6): δ 18.58, 115.83, 123.24, 126.71, 127.93, 128.73, 129.19, 132.54, 132.92, 133.21, 136.67, 138.79, 150.68, 156.19, 159.71, 163.79; HRMS (ESI) exact mass calcd. for $\text{C}_{18}\text{H}_{13}\text{N}_3\text{OH}$: 288.1137 (M+H) $^+$, found: 288.1131 (M+H) $^+$.

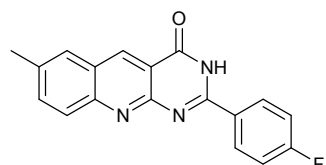


9-ethyl-2-phenylpyrimido[4,5-b]quinolin-4(3H)-one (3n): Reaction time: 5h; Yield: 80 %; White solid; mp: 234-236°C; IR (KBr): ν 1224, 1601, 1664 cm^{-1} ; ^1H NMR (500 MHz, DMSO- D_6): δ 1.30(t, $J=6.0$ Hz, 3H), 3.22-3.24 (m, 2H), 7.54-7.61 (m, 4H), 7.73 (d, $J=5.0$ Hz, 1H), 8.05 (d, $J=7.0$ Hz, 1H), 8.24 (d, $J=6.0$ Hz, 1H), 9.20 (s, 1H), 12.62 (s, 1H); ^{13}C NMR (125 MHz, DMSO- D_6): δ 15.57, 24.55, 115.83, 126.85, 127.92, 128.74, 128.94, 129.19, 131.41, 132.52, 133.24, 138.90, 142.35, 150.01, 156.06, 156.32, 163.86; HRMS (ESI) exact mass calcd. for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{OH}$: 302.1293 (M+H) $^+$, found: 302.1288 (M+H) $^+$.



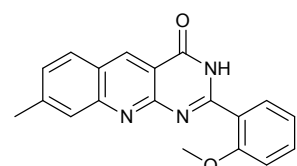
2-(2-chlorophenyl)-7-methylpyrimido[4,5-b]quinolin-4(3H)-one (3o): Reaction time: 5h; Yield: 78 %; Yellow solid; mp: 240-240°C; IR (KBr): ν 1327, 1593, 1680 cm^{-1} ; ^1H NMR (500 MHz, DMSO- D_6): δ 2.50 (s, 3H), 7.50(t, $J=7.0$ Hz, 1H), 7.56 (t, $J=7.0$ Hz, 1H), 7.61 (d, $J=8.0$ Hz, 1H), 7.70 (d, $J=7.0$ Hz, 1H), 7.76 (d, $J=8.5$ Hz, 1H), 7.95 (d, $J=8.8$ Hz, 1H), 8.00 (s, 1H), 9.16 (s, 1H), 12.70 (s, 1H); ^{13}C NMR (125MHz, DMSO- D_6): δ 21.68, 116.20, 126.97, 127.82, 128.28, 128.83, 130.25, 131.33,

131.83, 132.36, 134.35, 135.96, 136.99, 137.76, 150.09, 156.05, 156.09, 163.00; HRMS (ESI) exact mass calcd. for $C_{18}H_{12}ClN_3OH$: 322.0747 ($M+H$)⁺, found: 322.0742 ($M+H$)⁺.



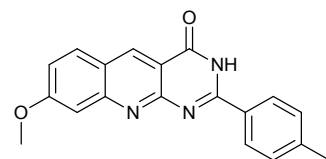
2-(4-fluorophenyl)-7-methylpyrimido[4,5-b]quinolin-4(3H)-one (3p):

Reaction time: 5h; Yield: 77 %; Yellow solid; mp: 344-346°C; IR (KBr): ν 1294, 1598, 1675 cm^{-1} ; 1H NMR (500 MHz, DMSO- D_6): δ 2.52 (s, 3H), 7.39 (t, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz, 1H), 7.79 (s, 1H), 8.08 (d, J =8.0 Hz, 1H) 8.28-8.31 (m, 2H), 9.14 (s, 1H), 12.60 (s, 1H); ^{13}C NMR (125MHz, DMSO- D_6): δ 22.36, 105.15, 115.83, 116.25 (J = 22.00 Hz), 125.00 (J = 11.5 Hz), 127.55, 129.40, 129.64, 129.68, 131.34 (J = 8.87 Hz), 138.14, 143.95, 145.47, 149.87, 159.38, 164.96 (J = 248.87 Hz); HRMS (ESI) exact mass calcd. for $C_{18}H_{12}FN_3OH$: 306.1043 ($M+H$)⁺, found: 306.1037 ($M+H$)⁺.



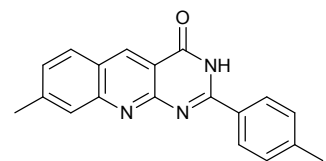
2-(2-methoxyphenyl)-8-methylpyrimido[4,5-b]quinolin-4(3H)-one (3q):

Reaction time: 4.5h; Yield: 80 %; Yellow solid; mp: 240-242°C; IR (KBr): ν 1475, 1567, 1589, 1698 cm^{-1} ; 1H NMR (500 MHz, DMSO- D_6): δ 2.57 (s, 3H), 3.90 (s, 3H), 7.14 (t, J =7.5 Hz, 1H), 7.23 (d, J = 8.5 Hz, 1H), 7.50 (d, J = 8.0 Hz, 1H), 7.56-7.59 (m, 1H), 7.83-7.85 (m, 2H), 8.15 (d, J =8.0 Hz, 1H), 9.21 (s, 1H), 12.14 (s, 1H); ^{13}C NMR (125 MHz, DMSO- D_6): δ 22.35, 56.41, 112.56, 115.38, 121.08, 122.95, 124.97, 127.62, 129.41, 129.63, 131.21, 133.28, 138.15, 143.92, 151.81, 156.30, 157.14, 157.85, 162.75; HRMS (ESI) exact mass calcd. for $C_{19}H_{15}N_3O_2H$: 318.1243 ($M+H$)⁺, found: 318.1237 ($M+H$)⁺.



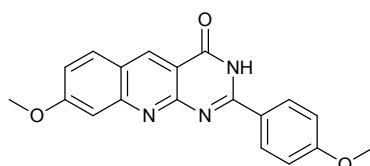
8-methoxy-2-(p-tolyl)pyrimido[4,5-b]quinolin-4(3H)-one (3r):

Reaction time: 4.5h; Yield: 81 %; White solid; mp: 342-344°C; IR (KBr): ν 1219, 1593, 1685 cm^{-1} ; 1H NMR (500 MHz, DMSO- D_6): δ 2.39 (s, 3H), 3.95 (s, 3H), 7.24 (dd, J =2.00, 9.00 Hz, 1H), 7.35 (t, J =8.0 Hz, 3H), 8.06 (d, J = 9.0 Hz, 1H), 8.16 (d, J =8.0 Hz, 2H), 9.06 (s, 1H), 12.20 (s, 1H); ^{13}C NMR (125 MHz, DMSO- D_6): δ 21.47, 56.29, 106.96, 113.92, 120.34, 122.41, 128.59, 129.69, 130.61, 131.19, 137.68, 142.66, 153.98, 156.36, 157.22, 163.54, 163.92; HRMS (ESI) exact mass calcd. For $C_{19}H_{15}N_3O_2H$: 318.1243 ($M+H$)⁺, found: 318.1237 ($M+H$)⁺.



8-methyl-2-(p-tolyl)pyrimido[4,5-b]quinolin-4(3H)-one (3s):

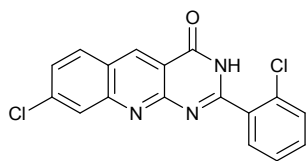
Reaction time: 5h; Yield: 85 %; Yellow solid; mp: 322-324°C; IR (KBr): ν 1294, 1595, 1677 cm^{-1} ; 1H NMR (500 MHz, DMSO- D_6): δ 2.40 (s, 3H), 2.55 (s, 3H), 7.38 (d, J = 8.0 Hz, 2H), 7.46 (d, J =9.0 Hz, 1H), 7.82 (s, 1H), 8.11 (d, J =8.5 Hz, 1H), 8.18 (d, J =8.0 Hz, 2H), 9.16 (s, 1H), 12.53 (s, 1H); ^{13}C NMR (125 MHz, DMSO- D_6): δ 21.58, 22.36, 115.30, 124.88, 127.54, 128.60, 129.27, 129.62, 129.78, 130.33, 138.08, 142.77, 143.84, 151.91, 155.97, 157.02, 163.77; HRMS (ESI) exact mass calcd. for $C_{19}H_{15}N_3OH$: 302.1293 ($M+H$)⁺, found: 302.1288 ($M+H$)⁺.



8-methoxy-2-(4-methoxyphenyl)pyrimido[4,5-b]quinolin-4(3H)-one (3t):

Reaction time: 4.5h; Yield: 85 %; White solid; mp: 274-276°C; IR (KBr): ν 1500, 1593, 1685 cm^{-1} ; 1H NMR (500 MHz, DMSO- D_6): δ 3.85 (s, 3H), 3.95 (s, 3H), 7.08 (d, J = 9.0 Hz, 2H), 7.23 (dd, J = 2.5, 9.5 Hz, 1H), 7.36 (s, 1H),

8.05 (d, $J=9.0$ Hz, 1H), 8.25 (d, $J=8.5$ Hz, 2H), 9.04 (s, 1H), 12.14 (s, 1H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 56.11, 56.27, 106.91, 113.77, 114.01, 114.70, 120.19, 122.31, 125.50, 130.49, 131.18, 137.65, 153.98, 155.98, 163.13, 163.52, 163.99; HRMS (ESI) exact mass calcd. for $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_3\text{H}$: 334.1192 ($\text{M}+\text{H}$) $^+$, found: 334.1186 ($\text{M}+\text{H}$) $^+$.



8-chloro-2-(2-chlorophenyl)pyrimido[4,5-b]quinolin-4(3H)-one(3u):

Reaction time: 5h; Yield: 70 %; Yellow solid; mp: 304-306°C; IR (KBr): ν 1484, 1598, 1683 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 6.93-7.02 (m, 1H), 7.56 (t, $J=7.0$ Hz, 1H), 7.60-7.65 (m, 2H), 8.23-8.28 (m, 3H), 9.29 (s, 1H), 12.67 (s, 1H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 116.49, 123.81, 125.32, 127.48, 127.69, 128.78, 129.27, 132.04, 132.81, 133.02, 138.17, 139.01, 149.68, 151.88, 157.02, 157.75, 163.58; HRMS (ESI) exact mass for $\text{C}_{17}\text{H}_9\text{Cl}_2\text{N}_3\text{OH}$: 342.0201 ($\text{M}+\text{H}$) $^+$, found: 342.0202 ($\text{M}+\text{H}$) $^+$.

