

RSC Advances

A novel one-pot three-component reaction for the synthesis of 5-arylmino-pyrrolo[2,3-*d*]pyrimidines under microwave irradiation

P. Seetham Naidu and Pulak J. Bhuyan*

*Medicinal Chemistry Division, CSIR-North East Institute of Science & Technology, Jorhat
785006, Assam, India.*

E Mail: Pulak_jyoti@yahoo.com

Electronic Supplementary Information

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General Considerations:

¹H NMR and ¹³C NMR Spectra were recorded on Bruker Avance-DPX 300MHz and 75MHz FT NMR in CDCl₃ using TMS as an internal standard. Chemical shifts were reported in ppm (δ units). [Solvent peak (DMSO-d₆) at around δ 3.36 and δ 2.50 peaks are not considered in all the spectra.]

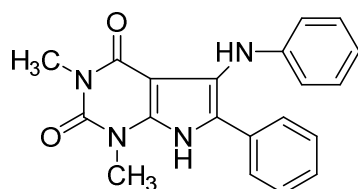
Experimental

General procedure for preparation of 4:

In typical experimental procedure, equimolar amounts of *N,N*-dimethyl-6-amino uracil **1** (1 mmol, 0.155 g), phenyl glyoxal monohydrate **2a** (1 mmol, 0.152 g), and aniline **3a** (1 mmol, 0.093 g) were irradiated in closed vessel in presence of acetic acid (5 mL) in Synthos 3000 microwave reactor at 110 °C for 5 min. The reaction mixture was cooled to room temperature and then added cold water (10 mL) into the mixture. The solid product appeared was filtered and then purified by recrystallization from EtOH to afford the desired product **4a** as a white solid.

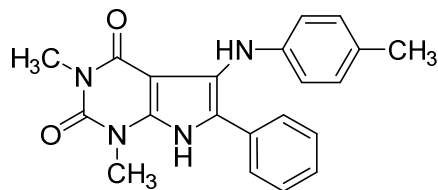
Similarly, compounds **4b-t** were synthesized.

1,3-dimethyl-6-phenyl-5-(phenylamino)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (**4a**):



White solid; yield: 304 mg (88%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.54 (s, 1H), 7.73 (d, 2H), 7.47-7.23 (m, 3H), 7.07 (t, 2H), 6.64 (d, 2H), 6.20 (s, 1H), 3.60 (s, 3H), 3.22 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 159.12, 151.61, 140.01, 136.25, 131.74, 129.98, 128.83, 128.16, 125.59, 117.40, 115.13, 113.57, 107.42, 96.83, 30.82, 27.55; IR (KBr, cm⁻¹): 3454.4, 3352.3, 3189.6, 1698.1, 1635.0, 1592.1, 1561.0, 1509.0, 1437.4, 1330.1, 1035.4, 972.9, 743.9; MS (m/z): 347.3 [M+1]; Anal. Calcd. For C₂₀H₁₈N₄O₂: C, 69.35; H, 5.24; N, 16.17. Found: C, 69.39; H, 5.27; N, 16.14.

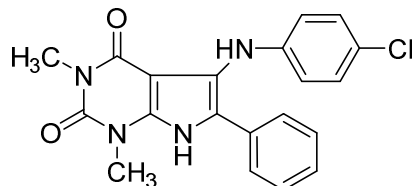
1,3-dimethyl-6-phenyl-5-(*p*-tolylamino)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (**4b**):



White solid; yield: 302 mg (84%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.52 (s, 1H), 7.66 (d, 1H), 7.51 (d, 1H), 7.35 (t, 2H), 7.25-7.07 (m, 3H), 6.84 (d, 1H), 6.49 (d, 1H), 6.15 (s, 1H), 3.54 (s, 3H), 3.17 (s, 3H), 2.12 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 158.08, 151.18, 145.59, 138.81, 131.46, 129.54, 128.74, 127.02, 126.71, 126.29, 125.79, 123.55, 119.89, 113.97, 96.69, 30.82, 27.72, 20.56; IR (KBr, cm⁻¹): 3454.9, 3349.5, 3190.2, 1697.5, 1633.5, 1598.2, 1560.3, 1506.8, 1436.8,

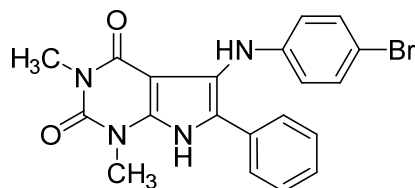
1330.6, 974.0, 742.6; MS (m/z): 361.4 [M+1]; Anal. Calcd. For C₂₁H₂₀N₄O₂: C, 69.98; H, 5.59; N, 15.55. Found: C, 71.05; H, 5.61; N, 15.59.

5-((4-chlorophenyl)amino)-1,3-dimethyl-6-phenyl-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4c):



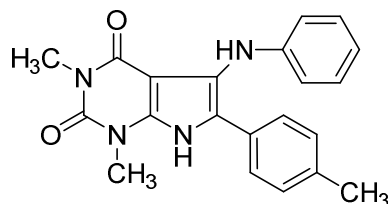
White solid; yield: 323 mg (85%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.53 (s, 1H), 7.65 (d, 1H), 7.52 (t, 1H), 7.39-7.32 (m, 3H), 7.22 (t, 1H), 7.06 (d, 2H), 6.58 (d, 1H), 6.17 (s, 1H), 3.54 (s, 3H), 3.18 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 158.75, 151.06, 149.64, 141.08, 134.17, 130.73, 129.57, 129.16, 128.28, 127.43, 126.51, 116.46, 108.89, 96.49, 30.56, 28.83; IR (KBr, cm⁻¹): 3454.1, 3351.4, 3189.5, 1698.0, 1635.1, 1599.3, 1562.1, 1508.5, 1435.9, 1331.1, 1036.1, 973.6, 742.0; MS (m/z): 381.8 [M+1]; Anal. Calcd. For C₂₀H₁₇N₄O₂Cl: C, 63.08; H, 4.50; N, 14.71. Found: C, 63.04; H, 4.55; N, 14.79.

5-((4-bromophenyl)amino)-1,3-dimethyl-6-phenyl-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4d):



White solid; yield: 357 mg (84%); mp 287-289 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.54 (s, 1H), 7.66 (d, 1H), 7.52 (t, 1H), 7.37 (t, 2H), 7.25-7.15 (m, 3H), 6.54 (d, 2H), 6.16 (s, 1H), 3.54 (s, 3H), 3.16 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 157.84, 151.15, 147.84, 139.01, 131.64, 131.16, 128.86, 127.07, 126.52, 124.45, 118.36, 115.58, 107.83, 96.78, 30.84, 27.77; IR (KBr, cm⁻¹): 3455.0, 3349.2, 3190.1, 1699.5, 1634.3, 1599.6, 1560.9, 1506.5, 1434.8, 1330.9, 1039.6, 974.7, 743.4; MS (m/z): 426.3 [M+1]; Anal. Calcd. For C₂₀H₁₇N₄O₂Br: C, 56.48; H, 4.03; N, 13.17. Found: C, 56.44; H, 4.10; N, 13.24.

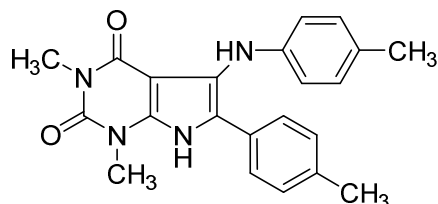
1,3-dimethyl-5-(phenylamino)-6-(p-tolyl)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4e):



White solid; yield: 309 mg (86%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.72 (s, 1H), 8.20 (t, 2H), 7.92 (d, 1H), 7.82 (s, 1H), 7.76 (d, 1H), 7.21 (d, 2H), 6.58 (d, 2H), 6.29 (s, 1H), 3.55 (s, 3H),

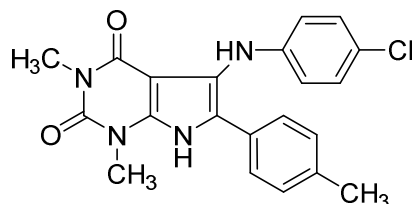
3.24 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 157.58, 151.24, 146.79, 139.98, 131.43, 129.76, 128.78, 127.13, 126.72, 126.25, 123.52, 120.09, 114.06, 96.85, 30.82, 27.69, 20.56; IR (KBr, cm^{-1}): 3454.8, 3352.6, 3189.5, 1698.5, 1635.9, 1592.6, 1561.2, 1509.6, 1340.4, 1331.2, 1038.1, 974.6, 742.5; MS (m/z): 361.4 [M+1]; Anal. Calcd. For $\text{C}_{21}\text{H}_{20}\text{N}_4\text{O}_2$: C, 69.98; H, 5.59; N, 15.55. Found: C, 71.02; H, 5.54; N, 15.50.

1,3-dimethyl-6-(*p*-tolyl)-5-(*p*-tolylamino)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4f):



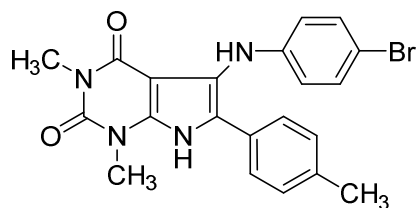
White solid; yield: 314 mg (84%); mp >300 °C; ^1H NMR (300 MHz, DMSO- d_6) δ 11.57 (s, 1H), 7.40 (d, 2H), 7.28 (d, 2H), 7.17 (d, 2H), 7.04 (d, 2H), 6.18 (s, 1H), 3.48 (s, 3H), 3.26 (s, 3H), 2.26 (s, 3H), 2.12 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 161.79, 151.37, 148.00, 139.90, 135.28, 131.31, 129.74, 128.25, 121.63, 121.33, 119.74, 115.68, 97.34, 30.82, 28.08, 21.24, 20.56; IR (KBr, cm^{-1}): 3457.6, 3348.8, 3188.9, 1699.5, 1638.3, 1596.4, 1504.7, 1438.3, 1333.1, 1037.9, 972.9, 744.0; MS (m/z): 375.5 [M+1]; Anal. Calcd. For $\text{C}_{22}\text{H}_{22}\text{N}_4\text{O}_2$: C, 70.57; H, 5.92; N, 14.96. Found: C, 70.69; H, 5.99; N, 14.99.

5-((4-chlorophenyl)amino)-1,3-dimethyl-6-(*p*-tolyl)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4g):



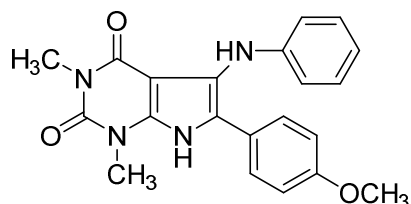
White solid; yield: 334 mg (85%); mp 285-286 °C; ^1H NMR (300 MHz, DMSO- d_6) δ 11.57 (s, 1H), 7.56 (d, 2H), 7.22 (d, 2H), 7.05 (t, 2H), 6.63 (d, 2H), 6.12 (s, 1H), 3.53 (s, 1H), 3.15 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 158.15, 151.80, 148.05, 138.64, 129.45, 128.98, 128.24, 127.54, 126.60, 126.41, 116.50, 115.93, 108.23, 96.21, 30.83, 27.50, 19.01; IR (KBr, cm^{-1}): 3458.1, 3344.6, 3191.5, 1697.8, 1635.2, 1598.6, 1506.0, 1436.1, 1330.6, 1033.4, 973.5, 743.2; MS (m/z): 395.8 [M+1]; Anal. Calcd. For $\text{C}_{21}\text{H}_{19}\text{N}_4\text{O}_2\text{Cl}$: C, 63.88; H, 4.85; N, 14.19. Found: C, 63.85; H, 4.90; N, 14.15.

5-((4-bromophenyl)amino)-1,3-dimethyl-6-(*p*-tolyl)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4h):



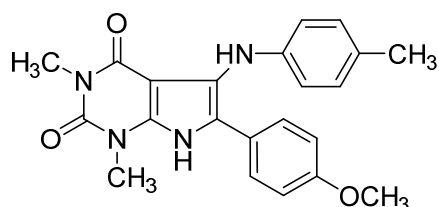
White solid; yield: 368 mg (84%); mp >300 °C; ^1H NMR (300 MHz, DMSO- d_6) δ 11.78 (s, 1H), 8.22 (d, 2H), 7.91 (d, 1H), 7.75 (t, 1H), 7.09 (d, 2H), 6.62 (d, 2H), 6.31 (s, 1H), 3.54 (s, 3H), 3.23 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 158.01, 151.65, 147.85, 139.87, 131.61, 130.36, 128.92, 127.44, 126.53, 123.95, 119.63, 115.54, 107.72, 96.58, 30.79, 27.75, 19.85; IR (KBr, cm^{-1}): 3459.7, 3346.2, 3189.6, 1698.5, 1634.3, 1599.7, 1508.2, 1437.5, 1332.2, 1032.2, 974.0, 744.3; MS (m/z): 440.4 [M+1]; Anal. Calcd. For $\text{C}_{21}\text{H}_{19}\text{N}_4\text{O}_2\text{Br}$: C, 57.41; H, 4.36; N, 12.75. Found: C, 57.49; H, 4.30; N, 12.82.

6-(4-methoxyphenyl)-1,3-dimethyl-5-(phenylamino)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4i):



White solid; yield: 312 mg (83%); mp >300 °C; ^1H NMR (300 MHz, DMSO- d_6) δ 11.54 (s, 1H), 7.99 (d, 2H), 7.61 (d, 1H), 7.18 (s, 1H), 7.01 (t, 1H), 6.94 (d, 2H), 6.55 (t, 2H), 6.11 (s, 1H), 3.73 (s, 3H), 3.53 (s, 3H), 3.15 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 158.39, 150.91, 148.49, 138.44, 131.41, 128.85, 127.45, 123.22, 119.72, 117.01, 114.42, 113.85, 107.28, 96.14, 55.09, 30.31, 27.25; IR (KBr, cm^{-1}): 3419.8, 3342.5, 2814.9, 1689.9, 1632.8, 1595.3, 1519.6, 1384.4, 1351.2, 1246.8, 1182.0, 1025.1, 974.6, 742.4; MS (m/z): 377.5 [M+1]; Anal. Calcd. For $\text{C}_{21}\text{H}_{20}\text{N}_4\text{O}_3$: C, 67.01; H, 5.36; N, 14.88. Found: C, 67.06; H, 5.40; N, 14.83.

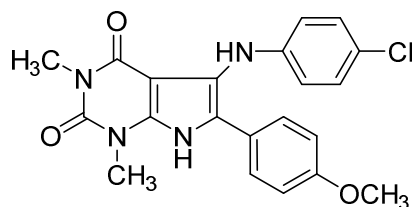
6-(4-methoxyphenyl)-1,3-dimethyl-5-(*p*-tolylamino)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4j):



White solid; yield: 319 mg (82%); mp >300 °C; ^1H NMR (300 MHz, DMSO- d_6) δ 11.53 (s, 1H), 7.60 (d, 1H), 7.44 (d, 1H), 6.98-6.91 (m, 3H), 6.83 (d, 1H), 6.47 (d, 2H), 6.11 (s, 1H), 3.74 (s, 3H), 3.53 (s, 3H), 3.16 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 159.39, 149.65, 141.02, 132.89, 129.55, 129.40, 128.26, 127.53, 126.12, 120.24, 116.41, 112.67, 107.99, 96.23, 30.76, 28.18, 20.00; IR (KBr, cm^{-1}): 3445.9, 3349.8, 2810.3, 1689.2, 1632.9, 1594.5, 1554.1, 1519.8, 1383.9, 1349.6,

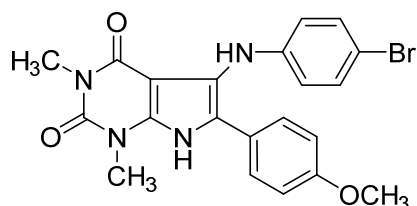
1252.3, 1180.6, 1038.5, 974.0, 744.2; MS (m/z): 391.7 [M+1]; Anal. Calcd. For C₂₂H₂₂N₄O₃: C, 67.68; H, 5.68; N, 14.35. Found: C, 67.65; H, 5.61; N, 14.40.

5-((4-chlorophenyl)amino)-6-(4-methoxyphenyl)-1,3-dimethyl-1,7-dihydro-2H-pyrrolo[2,3-d]-pyrimidine-2,4(3H)-dione (4k):



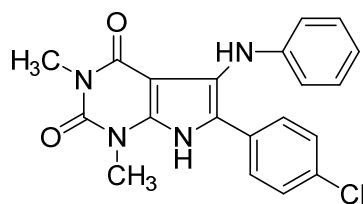
White solid; yield: 348 mg (85%); mp 297-298 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.47 (s, 1H), 7.58 (d, 1H), 7.43 (t, 2H), 7.05 (d, 1H), 6.93 (t, 2H), 6.56 (d, 2H), 3.74 (s, 3H), 3.52 (s, 3H), 3.16 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 158.55, 151.14, 147.64, 138.61, 128.80, 128.38, 127.94, 124.68, 123.72, 120.24, 117.13, 114.94, 114.34, 108.16, 96.64, 55.52, 30.80, 27.75; IR (KBr, cm⁻¹): 3427.6, 3344.6, 2833.3, 1687.0, 1633.5, 1601.7, 1553.0, 1519.1, 1384.2, 1350.9, 1252.1, 1180.9, 1039.3, 973.2, 745.3; MS (m/z): 411.6 [M+1]; Anal. Calcd. For C₂₁H₁₉N₄O₃Cl: C, 61.39; H, 4.66; N, 13.64. Found: C, 61.42; H, 4.70; N, 13.61.

5-((4-bromophenyl)amino)-6-(4-methoxyphenyl)-1,3-dimethyl-1,7-dihydro-2H-pyrrolo[2,3-d]-pyrimidine-2,4(3H)-dione (4l):



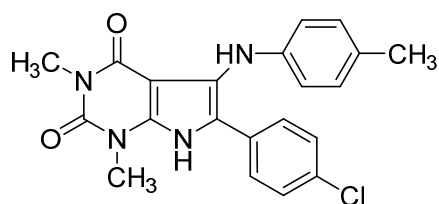
White solid; yield: 377 mg (83%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.48 (s, 1H), 7.58 (d, 1H), 7.48 (t, 2H), 7.16 (d, 2H), 6.93 (t, 2H), 6.51 (d, 1H), 6.12 (s, 1H), 3.74 (s, 3H), 3.53 (s, 3H), 3.16 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 158.57, 151.14, 148.07, 138.62, 131.62, 129.83, 127.96, 124.76, 123.69, 116.97, 115.50, 114.35, 107.68, 96.64, 55.59, 30.81, 27.75; IR (KBr, cm⁻¹): 3427.8, 3344.4, 2835.2, 1686.7, 1633.4, 1599.2, 1519.2, 1384.3, 1351.0, 1251.9, 1181.3, 1039.5, 973.1, 745.2; MS (m/z): 456.2 [M+1]; Anal. Calcd. For C₂₁H₁₉N₄O₃Br: C, 55.40; H, 4.21; N, 12.31. Found: C, 55.46; H, 4.27; N, 12.38.

6-(4-chlorophenyl)-1,3-dimethyl-5-(phenylamino)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4m):



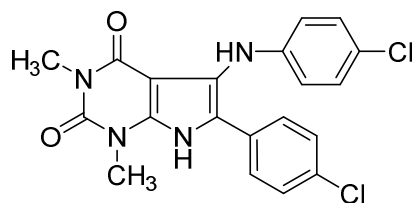
Yellow solid; yield: 345 mg (91%); mp 297–298 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.50 (s, 1H), 7.70 (d, 2H), 7.42 (d, 2H), 7.31 (s, 1H), 7.02 (t, 2H), 6.60 (d, 2H), 6.19 (s, 1H), 3.53 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 158.69, 151.40, 147.70, 139.09, 130.26, 129.13, 128.79, 127.76, 122.61, 120.06, 113.88, 96.80, 30.87, 27.74; IR (KBr, cm^{-1}): 3475.5, 3343.5, 3195.9, 1693.8, 1633.1, 1599.6, 1560.9, 1507.3, 1436.1, 1317.2, 1266.9, 1033.3, 974.4, 742.7; MS (m/z): 381.6 [M+1]; Anal. Calcd. For $\text{C}_{20}\text{H}_{17}\text{N}_4\text{O}_2\text{Cl}$: C, 63.08; H, 4.50; N, 14.71. Found: C, 63.15; H, 4.56; N, 14.67.

6-(4-chlorophenyl)-1,3-dimethyl-5-(*p*-tolylamino)-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4n):



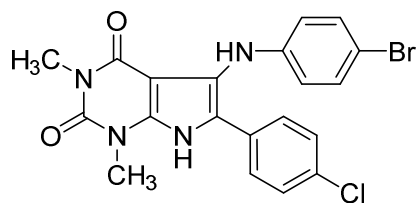
Light yellow solid; yield: 342 mg (87%); mp >300 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.64 (s, 1H), 7.69 (d, 2H), 7.42 (d, 2H), 6.85 (d, 2H), 6.49 (d, 2H), 6.19 (s, 1H), 3.53 (s, 3H), 3.15 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 157.23, 153.14, 145.14, 139.02, 130.33, 129.59, 128.76, 128.52, 127.65, 122.16, 120.67, 114.05, 96.65, 30.87, 27.72, 20.56; IR (KBr, cm^{-1}): 3463.0, 3344.6, 3193.2, 1695.2, 1632.2, 1595.0, 1560.4, 1509.3, 1437.8, 1317.4, 1268.1, 1034.6, 973.8, 743.1; MS (m/z): 395.4 [M+1]; Anal. Calcd. For $\text{C}_{21}\text{H}_{19}\text{N}_4\text{O}_2\text{Cl}$: C, 63.88; H, 4.85; N, 14.19. Found: C, 63.80; H, 4.81; N, 14.15.

6-(4-chlorophenyl)-5-((4-chlorophenyl)amino)-1,3-dimethyl-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4o):



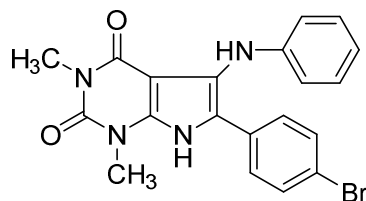
Light yellow solid; yield: 369 mg (89%); mp >300 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.79 (s, 1H), 8.17 (q, 2H), 7.91 (d, 1H), 7.75 (d, 1H), 7.05 (t, 2H), 6.63 (d, 2H), 6.29 (s, 1H), 3.54 (s, 3H), 3.23 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 157.87, 151.16, 147.39, 139.00, 131.18, 128.84, 127.03, 126.50, 124.36, 120.39, 118.53, 115.03, 108.13, 96.78, 30.84, 27.77; IR (KBr, cm^{-1}): 3468.4, 3345.1, 3192.9, 1696.7, 1633.5, 1597.6, 1561.3, 1508.5, 1436.4, 1316.7, 1268.5, 1033.9, 974.4, 742.8; MS (m/z): 416.3 [M+1]; Anal. Calcd. For $\text{C}_{20}\text{H}_{16}\text{N}_4\text{O}_2\text{Cl}_2$: C, 57.85; H, 3.88; N, 13.49. Found: C, 57.90; H, 3.93; N, 13.55.

5-((4-bromophenyl)amino)-6-(4-chlorophenyl)-1,3-dimethyl-1,7-dihydro-2*H*-pyrrolo[2,3-*d*]pyrimidine-2,4(3*H*)-dione (4p):



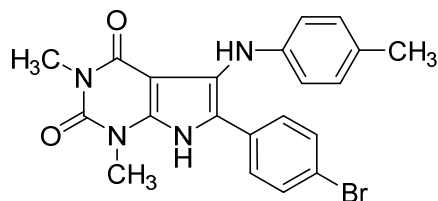
Light yellow solid; yield: 403 mg (88%); mp >300 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.57 (s, 1H), 7.68 (q, 2H), 7.51-7.39 (m, 4H), 7.18 (d, 1H), 6.53 (d, 1H), 6.20 (s, 1H), 3.52 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 157.82, 151.48, 147.30, 139.27, 131.70, 131.38, 128.90, 128.53, 127.92, 118.40, 115.68, 107.57, 96.62, 30.87, 27.62; IR (KBr, cm^{-1}): 3460.4, 3349.2, 3190.1, 1690.0, 1633.5, 1602.2, 1552.5, 1510.9, 1438.2, 1318.5, 1269.4, 1033.1, 974.6, 743.1; MS (m/z): 459.7 [M+1]; Anal. Calcd. For $\text{C}_{20}\text{H}_{16}\text{N}_4\text{O}_2\text{BrCl}$: C, 52.25; H, 3.51; N, 12.19. Found: C, 52.29; H, 3.47; N, 12.12.

6-(4-bromophenyl)-1,3-dimethyl-5-(phenylamino)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4q):



Light yellow solid; yield: 382 mg (90%); mp >300 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.53 (s, 1H), 7.61 (d, 1H), 7.44 (d, 2H), 7.01 (t, 2H), 6.94 (d, 2H), 6.56 (d, 2H), 6.11 (s, 1H), 3.53 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 158.67, 151.16, 148.99, 139.11, 131.10, 128.74, 127.28, 126.50, 124.33, 120.19, 118.99, 115.25, 107.43, 96.68, 30.80, 27.75; IR (KBr, cm^{-1}): 3463.0, 3341.4, 3172.4, 1694.8, 1664.8, 1633.1, 1596.2, 1561.0, 1436.6, 1317.1, 1033.6, 973.0, 743.4; MS (m/z): 426.3 [M+1]; Anal. Calcd. For $\text{C}_{20}\text{H}_{17}\text{N}_4\text{O}_2\text{Br}$: C, 56.48; H, 4.03; N, 13.17. Found: C, 56.54; H, 4.08; N, 13.21.

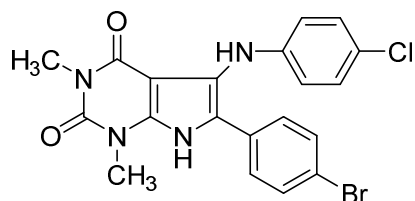
6-(4-bromophenyl)-1,3-dimethyl-5-(*p*-tolylamino)-1,7-dihydro-2H-pyrrolo[2,3-d]pyrimidine-2,4(3H)-dione (4r):



Light yellow solid; yield: 390 mg (89%); mp >300 °C; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 11.34 (s, 1H), 7.31-7.16 (m, 5H), 6.93 (d, 2H), 6.84 (d, 1H), 6.20 (s, 1H), 3.53 (s, 3H), 3.18 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 158.37, 151.19, 140.36, 135.82, 134.11, 128.94, 128.55, 127.60, 127.07, 126.70, 120.16, 118.63, 113.81, 107.09, 96.91, 31.04, 27.93, 19.94; IR (KBr, cm^{-1}): 3463.4, 3331.2, 3171.0, 1694.6, 1667.1, 1629.0, 1597.2, 1548.8, 1440.2, 1317.4, 1060.6, 973.8,

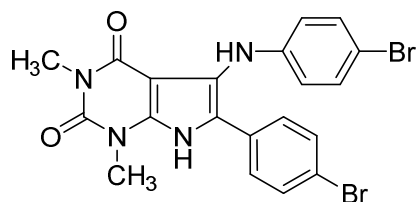
743.1; MS (m/z): 440.4 [M+1]; Anal. Calcd. For C₂₁H₁₉N₄O₂Br: C, 57.41; H, 4.36; N, 12.75. Found: C, 57.48; H, 4.30; N, 12.81.

6-(4-bromophenyl)-5-((4-chlorophenyl)amino)-1,3-dimethyl-1,7-dihydro-2H-pyrrolo[2,3-d]-pyrimidine-2,4(3H)-dione (4s):



Light yellow solid; yield: 403 mg (88%); mp 299-300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.56 (s, 1H), 7.59 (d, 3H), 7.45 (d, 1H), 7.06 (d, 2H), 6.57 (d, 2H), 6.20 (s, 1H), 3.53 (s, 3H), 3.15 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 159.12, 151.61, 147.81, 138.66, 131.74, 130.13, 128.83, 128.16, 117.40, 115.13, 113.57, 109.81, 97.04, 30.80, 27.75; IR (KBr, cm⁻¹): 3463.6, 3338.5, 3176.9, 1694.6, 1667.6, 1633.0, 1597.2, 1561.0, 1437.2, 1316.9, 1032.1, 973.1, 744.0; MS (m/z): 459.5 [M+1]; Anal. Calcd. For C₂₀H₁₆N₄O₂BrCl: C, 52.25; H, 3.51; N, 12.19. Found: C, 52.21; H, 3.54; N, 12.22.

6-(4-bromophenyl)-5-((4-bromophenyl)amino)-1,3-dimethyl-1,7-dihydro-2H-pyrrolo[2,3-d]-pyrimidine-2,4(3H)-dione (4t):



Light yellow solid; yield: 437 mg (87%); mp >300 °C; ¹H NMR (300 MHz, DMSO-*d*₆) δ 11.46 (s, 1H), 7.58 (d, 2H), 7.43 (t, 1H), 7.16 (d, 1H), 6.96 (d, 2H), 6.52 (d, 2H), 6.11 (s, 1H), 3.52 (s, 3H), 3.16 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 158.75, 151.20, 140.68, 136.83, 132.81, 128.63, 127.61, 127.12, 126.70, 120.20, 119.15, 115.63, 105.39, 96.22, 31.10, 27.91; IR (KBr, cm⁻¹): 3463.3, 3334.5, 3176.3, 1694.8, 1666.7, 1631.2, 1595.1, 1549.0, 1438.0, 1317.4, 1032.2, 973.1, 743.5; MS (m/z): 505.4 [M+1]; Anal. Calcd. For C₂₀H₁₆N₄O₂Br₂: C, 47.65; H, 3.20; N, 11.12. Found: C, 47.68; H, 3.25; N, 11.18.

