Supporting Information

Molecular diversity from the L-proline catalyzed three component reactions of 4-hydroxycoumarin, aldehyde and 3-aminopyrazole or 1, 3-dimethyl-6-aminouracil

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EXPERIMENTAL

All the reagents were commercially available and used without additional purification. Reactions were monitored by TLC. Melting points were determined in a digital melting point apparatus. IR spectra were recorded on a Shimadzu FTIR spectrophotometer in KBr pellet. ^1H NMR and ^{13}C NMR spectra were recorded in $\text{DMSO-}d_6$ and CDCl_3 using Me_4Si as internal standard on Bruker 500 MHz or Bruker Avance II 400 MHz spectrometer and are expressed in parts per million (δ , ppm). Elemental analyses were carried out in a Perkin Elmer 2400 automatic carbon, hydrogen, nitrogen analyzer. All unknown compounds were characterized by usual spectroscopic techniques and known compounds data were compared with the literature data and melting points.

General synthetic procedure of compounds dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridine-6(7*H*)-ones (1a-1j)

A mixture of aromatic aldehyde (1mmol) and 4-hydroxycoumarin (1mmol) in ethanol (3 ml) was stirred at the boiling temperature of ethanol for 30 minutes in presence of L-proline (20 mol%). Then 3-amino-5-methylpyrazole (1mmol) was added to the mixture and stirred under the reflux conditions till the completion of the reaction as per TLC indication. The resulting precipitate was filtered, washed and recrystallized with ethanol and ethylacetate (2:1) mixture to get the pure product.

8-Methyl-7-phenyl-9,11-dihydrochromeno[4,3-b]pyrazolo[4,3-e]pyridine-6(7H)-one **1a**

(Table 2, entry 1): Yield, 79%; White solid; mp = 301-303 °C (Lit.¹ 303-304 °C); IR (KBr): 3171, 3072, 1670, 1612 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆): δ 12.00 (s, 1H), 10.51 (s, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.20-7.26 (m, 3H), 5.12 (s, 1H), 1.93 (s, 3H) ppm; ¹³C NMR (125 MHz, DMSO-*d*₆): δ 161.9, 152.3, 147.8, 146.1, 145.7, 135.3, 132.2, 131.8, 129.5, 128.3, 128.0, 127.7, 126.6, 123.4, 116.3, 114.1, 103.5, 97.5, 37.2, 9.5 ppm; Anal Calcd. for C₂₀H₁₅N₃O₂ (329.35): C, 72.94; H, 4.59; N, 12.76; Found: C, 73.01; H, 4.56; N, 12.68.

8-Methyl-7-p-tolyl-9,11-dihydrochromeno[4,3-b]pyrazolo[4,3-e]pyridine-6(7H)-one **1b**

(Table 2, entry 2): Yield, 67%; White solid; mp = 275-277 °C (Lit.² 276-278 °C); IR (KBr): 3202, 3076, 1680, 1609 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆): δ 11.97 (s, 1H), 10.50 (s, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 8.2 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 1H), 7.01 (d, *J* = 7.9 Hz, 2H), 6.95 (d, *J* = 7.9 Hz, 2H), 5.01 (s, 1H), 2.20 (s, 3H), 1.95 (s, 3H) ppm; ¹³C NMR (125 MHz, DMSO-*d*₆): δ 161.8, 152.9, 146.1, 145.9, 144.3, 135.8, 135.1, 132.7, 129.5, 127.3, 124.8, 123.3, 117.7, 114.2, 103.7, 97.3, 36.4, 21.8, 9.4 ppm; Anal. Calcd. for C₂₁H₁₇N₃O₂ (343.38): C, 73.45; H, 4.99; N, 12.24; Found: C, 73.53; H, 5.02; N, 12.14.

7-(4-methoxyphenyl)-8-methyl-9,11-dihydrochromeno[4,3-b]pyrazolo[4,3-e]pyridine-6(7H)-one **1c**

(Table 2, entry 3): Yield, 72%; White solid; mp = 250-251 °C (Lit.¹ 251-252 °C); IR (KBr): 3250, 3210, 3082, 1672, 1609 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆): δ 11.95 (s, 1H), 10.38 (s, 1H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.59 (t, *J* = 8.2 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 5.01 (s, 1H), 3.61 (s, 3H), 1.95 (s, 3H) ppm; ¹³C NMR (125 MHz, DMSO-*d*₆): δ 161.2, 157.5, 152.3, 146.1, 144.5,

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139.1, 131.0, 128.5, 123.4, 123.1, 116.5, 114.3, 113.2, 103.0, 98.3, 55.6, 36.0, 9.7 ppm; Anal. Calcd for $C_{21}H_{17}N_3O_3$ (359.38): C, 70.18; H, 4.77; N, 11.69; Found: C, 70.10; H, 4.74; N, 11.79.

*7-(4-Chlorophenyl)-8-methyl-9,11-dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridin-6 (7H)-one* **1d** (Table 2, entry 4): Yield, 84%; White solid; mp = 340-342 °C (Lit.¹ 341-342 °C); IR (KBr): 3200, 3076, 1660, 1610 cm^{-1} ; 1H NMR (500 MHz, DMSO- d_6): δ 12.02 (s, 1H), 10.50 (s, 1H), 8.34 (d, J = 7.6 Hz, 1H), 7.52 (t, J = 8.2 Hz, 1H), 7.36 (t, J = 7.9 Hz, 1H), 7.27 (d, J = 8.2 Hz, 1H), 7.20 (d, J = 8.5 Hz, 2H), 7.15 (d, J = 8.5 Hz, 2H), 5.15 (s, 1H), 1.94 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO- d_6): δ 161.5, 152.3, 146.3, 146.0, 145.1, 135.4, 132.1, 129.5, 128.6, 128.1, 125.4, 123.5, 117.6, 114.8, 102.3, 97.5, 36.4, 9.5 ppm; Anal. Calcd for $C_{20}H_{14}ClN_3O_2$ (363.80): C, 66.03; H, 3.88; N, 11.55; Found: C, 65.94; H, 3.85; N, 11.66.

*8-Methyl-7-(3-nitrophenyl)-9,11-dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridin-6(7H)-one* **1e** (Table 2, entry 5): Yield, 60%; White solid; mp = 322-324 °C (Lit.¹ 324-325 °C); IR (KBr): 3302, 3190, 3059, 1662, 1613 cm^{-1} ; 1H NMR (500 MHz, DMSO- d_6): δ 11.82 (s, 1H), 10.32 (s, 1H), 8.22-8.25 (m, 1H), 7.94 (s, 1H), 7.85 (d, J = 7.9 Hz, 1H), 7.58 (d, J = 7.3 Hz, 1H), 7.40 (dd, J_1 = 8.2 Hz, J_2 = 11.6 Hz, 1H), 7.33 (dd, J = 14.9, 7.6 Hz, 1H), 7.20 (t, J = 7.3 Hz, 1H), 7.11 (d, J = 8.2 Hz, 1H), 5.20 (s, 1H), 1.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO- d_6): δ 161.4, 152.5, 149.0, 148.3, 146.7, 145.1, 135.6, 134.4, 131.2, 129.0, 123.6, 123.3, 122.4, 121.0, 116.5, 114.0, 101.6, 96.3, 37.1, 9.5 ppm; Anal. Calcd for $C_{20}H_{14}N_4O_4$ (374.35): C, 64.10; H, 3.77; N, 14.97; Found: C, 64.10; H, 3.74; N, 15.08.

*7-(4-Fluorophenyl)-8-methyl-9,11-dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridin-6 (7H)-one* **1f** (Table 2, entry 6): Yield, 71%; White solid; mp = 351-352 °C (Lit.¹ 353-354 °C); IR

(KBr): 3202, 3071, 1666, 1613 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 12.02 (s, 1H), 10.47 (s, 1H), 8.31 (d, $J = 8.2$ Hz, 1H), 7.55 (t, $J = 7.3$ Hz, 1H), 7.34 (t, $J = 7.3$ Hz, 1H), 7.30 (d, $J = 7.9$ Hz, 1H), 7.20 (dd, $J_1 = 8.5$ Hz, $J_2 = 16.8$ Hz, 2H), 7.00 (t, $J = 8.8$ Hz, 2H), 5.13 (s, 1H), 1.89 (s, 3H) ppm; ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 161.7, 161.5, 160.2, 152.5, 146.3, 145.2, 143.4, 135.5, 131.6, 129.5, 123.8, 123.5, 116.9, 114.8, 114.6, 114.5, 102.6, 97.4, 36.8, 9.9 ppm; Anal. Calcd for $\text{C}_{20}\text{H}_{14}\text{FN}_3\text{O}_2$ (347.34): C, 69.16; H, 4.06; N, 12.10; Found: C, 69.22; H, 4.03; N, 12.19.

*7-(4-Isopropylphenyl)-8-methyl-9,11-dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridin-6(7H)-one* **1g** (Table 2, entry 7): Yield, 70%; White solid; mp = 323-324 $^\circ\text{C}$ (Lit.¹ 321-322 $^\circ\text{C}$); IR (KBr): 3253, 3208, 3078, 1669, 1613 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 11.98 (s, 1H), 10.45 (s, 1H), 8.34 (d, $J = 8.2$ Hz, 1H), 7.54 (t, $J = 8.2$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.27 (d, $J = 8.2$ Hz, 1H), 7.06 (d, $J = 8.2$ Hz, 2H), 7.04 (d, $J = 8.5$ Hz, 1H), 5.05 (s, 1H), 2.71-2.75 (m, 1H), 1.91 (s, 3H), 1.08 (d, $J = 6.7$ Hz, 6H) ppm; ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 161.4, 152.5, 146.3, 146.1, 145.3, 145.2, 135.6, 132.2, 127.8, 126.4, 124.4, 123.5, 117.2, 114.5, 103.4, 97.8, 36.6, 33.4, 24.3, 9.8 ppm; Anal. Calcd for $\text{C}_{23}\text{H}_{21}\text{N}_3\text{O}_2$ (371.43): C, 74.37; H, 5.70; N, 11.31; Found: C, 74.30; H, 5.64; N, 11.41.

*7-(4-Methoxyphenyl)-9,11-dihydrochromeno[4,3-*b*]pyrazolo[4,3-*e*]pyridin-6(7H)-one* **1h** (Table 2, entry 8): Yield, 74%; White solid; mp = 290-291 $^\circ\text{C}$ (Lit.¹ 292-293 $^\circ\text{C}$); IR (KBr): 3192, 3070, 1670, 1605 cm^{-1} ; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ 12.27 (s, 1H), 10.55 (s, 1H), 8.34 (d, $J = 7.9$ Hz, 1H), 7.56 (t, $J = 7.3$ Hz, 1H), 7.37 (s, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 7.31 (d, $J = 8.2$ Hz, 1H), 7.05 (d, $J = 8.8$ Hz, 2H), 6.72 (d, $J = 8.5$ Hz, 2H), 5.16 (s, 1H), 3.63 (s, 3H) ppm; ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ 161.4, 157.8, 152.5, 146.3, 145.1, 140.8, 132.2,

128.5, 126.5, 124.4, 123.5, 117.1, 114.5, 114.1, 105.8, 97.1, 55.6, 36.5 ppm; Anal. Calcd for $C_{20}H_{15}N_3O_3$ (345.35): C, 69.56; H, 4.38; N, 12.17; Found: C, 69.49; H, 4.35; N, 12.27.

7-(4-Chlorophenyl)-9,11-dihydrochromeno[4,3-b]pyrazolo[4,3-e]pyridin-6(7H)-one **1i**

(Table 2, entry 9): Yield, 77%; White solid; mp = 343-344 °C (Lit.¹ 345-346 °C); IR (KBr): 3192, 3066, 1665, 1605 cm^{-1} ; 1H NMR (500 MHz, DMSO-*d*₆): δ 12.34 (s, 1H), 10.61 (s, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 7.58 (t, *J* = 7.9 Hz, 1H), 7.40 (s, 1H), 7.33 (t, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 5.22 (s, 1H) ppm; ^{13}C NMR (125 MHz, DMSO-*d*₆): δ 161.4, 152.8, 147.4, 145.8, 145.6, 132.4, 131.0, 129.4, 128.7, 126.8, 124.4, 123.8, 117.3, 114.6, 105.4, 96.5, 36.7 ppm; Anal. Calcd for $C_{19}H_{12}ClN_3O_2$ (349.77): C, 65.24; H, 3.46; N, 12.01; Found: C, 65.16; H, 3.49; N, 12.12.

7-(4-fluorophenyl)-9,11-dihydrochromeno[4,3-b]pyrazolo[4,3-e]pyridin-6(7H)-one **1j**

(Table 2, entry 10): Yield, 75%; White solid; mp = 353-354 °C (Lit.² 355-356 °C); IR (KBr): 3191, 3077, 1662, 1606 cm^{-1} ; 1H NMR (500 MHz, DMSO-*d*₆): δ 12.32 (s, 1H), 10.61 (s, 1H), 8.35 (d, *J* = 8.2 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.40 (s, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.19 (dd, *J* = 8.2, 5.8 Hz, 2H), 6.98 (t, *J* = 8.8 Hz, 2H), 5.24 (s, 1H) ppm; ^{13}C NMR (125 MHz, DMSO-*d*₆): δ 162.2, 161.1, 160.1, 152.7, 146.1, 145.6, 144.5, 132.1, 129.4, 126.7, 124.2, 123.6, 117.1, 115.3, 115.2, 114.4, 105.7, 96.8, 36.7 ppm; Anal. Calcd for $C_{19}H_{12}FN_3O_2$ (333.31): C, 68.46; H, 3.63; N, 12.61; Found: C, 68.54; H, 3.59; N, 12.72.

References

1. L. H. Choudhury et al. *RSC Advances*. **2013**, 3, 15705-15711.
2. A. T. Khan et al. *Tetrahedron Letters*. **2014**, 55, 2006-2009.

General synthetic procedure for the synthesis of 3-benzyl substituted pyrimidino chromen-2-ones (2a-2g)

A mixture of 4- hydroxycoumarin (1 mmol), 4-chloroaldehydes (1 mmol) and L-proline (20 mol%) were dissolved in EtOH (1 ml) and stirred under reflux condition for 15 minutes. Afterwards, 1, 3-dimethyl-6-aminouracils (1 mmol) was added to the solution and stirring was continued till the completion of the reaction as shown by TLC. Then the reaction mixture was allowed to cool at room temperature and the resulting precipitate was filtered, washed and recrystallized with ethanol and ethyl acetate (2:1) mixture to afford the pure product.

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6-amino-5-((4-hydroxy-2-oxo-2H-chromen-3-yl)(p-tolyl)methyl)-1,3-dimethylpyrimidine

-2,4(1H,3H)-dione **2a**: Yield, 80%; White granular solid; mp = 218-220 °C; IR (KBr): 3411, 3361, 3215, 3051, 2951, 1699, 1673, 1659, 1571, 1452, 1066, 1038, 855, 766 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 13.59 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.31-7.25 (m, 2H), 7.11-7.07 (m, 4H), 6.69 (s, 2H), 5.70 (s, 1H), 3.57 (s, 3H), 3.33 (s, 3H), 2.31 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 168.1, 165.4, 164.7, 154.9, 152.3, 150.7, 135.8, 134.4, 132.3, 129.2, 126.2, 124.9, 124.6, 117.4, 116.2, 104.3, 89.3, 36.3, 30.0, 28.7, 21.0 ppm; Anal. Calcd. for C₂₃H₂₁N₃O₅ (419.43): C, 65.86; H, 5.05; N, 10.02; Found C, C, 65.93; H, 5.09; N, 10.14.

Copy of ¹H NMR of Compound 2a

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Copy of ^{13}C NMR of Compound 2a

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6-amino-5-((3-bromophenyl)(4-hydroxy-2-oxo-2H-chromen-3-yl)methyl)-1,3-dimethylpyrimidine-2,4 (1H,3H)-dione **2b**: Yield, 78%; White crystalline solid; mp = 245-247°C; IR (KBr): 3640, 3371, 3225, 3061, 2948, 1699, 1648, 1620, 1567, 1470, 1453, 1065, 853, 761 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ 13.91 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.40-7.32 (m, 4H), 7.31(s, 2H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.16 (s, 1H), 5.65 (s, 1H), 3.40 (s, 3H), 3.18 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 165.6, 164.0, 163.8, 155.2, 151.9, 149.9, 141.5, 132.4, 130.1, 129.1, 128.7, 125.6, 124.2, 123.7, 121.7, 116.9, 116.1, 104.3, 86.4, 35.9, 30.5, 28.2 ppm; Anal. Calcd. for C₂₂H₁₈BrN₃O₅ (484.3): C, 54.56; H, 3.75; N, 8.68; Found C, 54.63; H, 3.79; N, 8.80.

Copy of ¹H NMR of compound **2b**

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Copy of ^{13}C NMR of Compound 2b

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6-amino-5-((4-chlorophenyl)(4-hydroxy-2-oxo-2H-chromen-3-yl)methyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione **2c**: Yield, 83%; White crystalline solid; mp = 209- 211 °C; IR (KBr): 3445, 3358, 3241, 3063, 2964, 1695, 1660, 1651, 1570, 1509, 1489, 1446, 1095, 1043, 856, 760 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$): δ 13.93 (s, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.61 (t, J = 8.0Hz, 1H), 7.38 – 7.36 (m, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 5.61 (s, 1H), 3.40 (s, 3H), 3.16 (s, 3H) ppm; ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$): δ 165.8, 164.0, 163.9, 155.1, 151.9, 149.9, 137.3, 132.2, 130.4, 128.2, 127.8, 123.7, 116.9, 115.9, 104.2, 86.7, 35.6, 30.4, 28.1 ppm; Anal. Calcd. for $\text{C}_{22}\text{H}_{18}\text{ClN}_3\text{O}_5$ (439.85): C, 60.07; H, 4.12; N, 9.55; Found C, 60.00; H, 4.15; N, 9.66.

Copy of ^1H NMR of Compound **2c**

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Copy of ^{13}C NMR of Compound 2c

Supporting Information

6-amino-5-((4-hydroxy-2-oxo-2H-chromen-3-yl)(phenyl)methyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione **2d**: Yield, 78%; White solid; mp = 188-192 °C; IR (KBr): 3376, 3198, 3049, 2979, 1736, 1707, 1665, 1496, 1445, 1063, 1044, 858, 752 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 13.49 (s, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.18 (m, 3H), 6.52 (s, 2H), 5.75 (s, 1H), 3.57 (s, 3H), 3.33 (s, 3H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 168.1, 165.4, 164.7, 154.9, 152.3, 150.7, 137.5, 132.4, 128.4, 126.3, 124.6, 124.4, 117.4, 116.2, 104.1, 89.3, 36.6, 30.0, 28.7 ppm; Anal. Calcd. for C₂₂H₁₉N₃O₅ (405.4): C, 65.18; H, 4.72; N, 10.37; Found C, 65.25; H, 4.76; N, 10.49.

Copy of ¹H NMR of Compound 2d

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Copy of ^{13}C NMR of Compound 2d

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6-amino-5-(cyclohexyl(4-hydroxy-2-oxo-2H-chromen-3-yl)methyl-1,3-dimethylpyrimidine-2,4 (1H,3H)-dione **2e**: Yield 67%; White solid; mp = 244-245 °C; IR (KBr): 3378, 3220, 2930, 2855, 1707, 1675, 1632, 1598, 1498, 1066, 861, 760 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ 13.98 (s, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 6.62 (s, 2H), 3.81 (d, *J* = 8.0 Hz, 1H), 3.59 (s, 3H), 3.39 (s, 3H), 2.90-2.84 (m, 1H), 1.71-1.63 (m, 5H), 1.32-1.20 (m, 2H), 1.15-1.09 (m, 1H), 0.90-0.80 (m, 2H) ppm; ¹³C NMR (100 MHz, CDCl₃): δ 168.4, 164.9, 164.4, 154.6, 152.1, 150.7, 131.9, 124.3, 124.2, 117.5, 115.9, 105.4, 88.4, 39.9, 34.9, 32.1, 30.1, 28.6, 26.4, 26.0 ppm; Anal. Calcd. for C₂₂H₂₅N₃O₅ (411.45): C, 64.22; H, 6.12; N, 10.21; Found C, 64.28; H, 6.16; N, 10.33.

Copy of ¹H NMR of Compound **2e**

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Copy of ^{13}C NMR of Compound 2e

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6-amino-5-((4-hydroxy-2-oxo-2H-chromen-3-yl)(4-nitrophenyl)methyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione **2f**: Yield, 76%; Light yellow solid; mp = 240-242 °C; IR (KBr): 3539, 3387, 3211, 3077, 2886, 1709, 1698, 1621, 1573, 1446, 1067, 854, 762 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ 13.94 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.41 (s, 2H), 7.37 (t, *J* = 8.0 Hz, 1H), 5.76 (s, 1H), 3.43 (s, 3H), 3.19 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 168.1, 165.7, 164.1, 155.2, 151.9, 149.9, 147.0, 145.7, 132.4, 127.7, 124.1, 123.8, 123.0, 116.9, 115.9, 103.9, 86.5, 36.5, 30.5, 28.2 ppm; Anal. Calcd. for C₂₂H₁₈N₄O₇ (450.4): C, 58.67; H, 4.03; N, 12.44; Found C, 58.75; H, 4.06; N, 12.55.

Copy of ¹H and ¹³C NMR of Compound **2f**

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Copy of ^{13}C NMR of Compound 2f

Supporting Information

6-amino-5-((4-hydroxy-2-oxo-2H-chromen-3-yl)(4-isopropylphenyl)methyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione **2g**: Yield 81%; White solid; m.p. 257-259 °C; IR (KBr): 3464, 3322, 3232, 3047, 2957, 1672, 1650, 1619, 1573, 1461, 1067, 1017, 857, 761 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): δ 13.88 (s, 1H), 7.87 (s, 1H), 7.61 (s, 1H), 7.35 (s, 4H), 7.09 (s, 4H), 5.63 (s, 1H), 3.45 (s, 3H), 3.22 (s, 3H), 2.85 (s, 1H), 1.20 (s, 6H) ppm; ¹³C NMR (100 MHz, DMSO-*d*₆): δ 168.3, 164.1, 163.8, 155.0, 151.9, 149.9, 145.5, 135.2, 131.9, 126.1, 125.8, 123.9, 123.7, 116.9, 115.8, 104.4, 87.1, 35.6, 32.9, 30.3, 28.1, 23.8 ppm; Anal. Calcd. for C₂₅H₂₅N₃O₅ (447.48): C, 67.10; H, 5.63; N, 9.39; Found C, 67.17; H, 5.67; N, 9.51.

Copy of ¹H NMR of Compound **2g**

Supporting Information

Copy of ^{13}C NMR of Compound 2g

Single X-ray Crystallographic structure of 6-amino-5-((4-hydroxy-2-oxo-2*H*-chromen-3-yl)(4-isopropylphenyl)methyl)-1,3-dimethyl pyrimidine-2,4(1*H*,3*H*)-dione 2g (CCDC 1024914) which showing free –OH, -NH₂ and CO groups.

Supporting Information

Table 1. Crystal data and structure refinement for 2g

Identification code	shelxl
Empirical formula	C ₂₅ H ₂₅ N ₃ O ₅
Formula weight	447.48
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 16.2625(9) Å alpha = 90 deg. b = 14.4341(8) Å beta = 129.177(4) deg. c = 12.3554(7) Å gamma = 90 deg.
Volume	2248.3(2) Å ³
Z, Calculated density	4, 1.322 Mg/m ³
Absorption coefficient	0.093 mm ⁻¹
F(000)	944
Crystal size	0.30 x 0.30 x 0.25 mm
Theta range for data collection	2.19 to 26.00 deg.
Limiting indices	-20 ≤ h ≤ 20, -17 ≤ k ≤ 17, -15 ≤ l ≤ 15
Reflections collected / unique	11898 / 4109 [R(int) = 0.0509]
Completeness to theta = 26.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9794 and 0.9701
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4109 / 47 / 326
Goodness-of-fit on F ²	1.041
Final R indices [I > 2sigma(I)]	R1 = 0.0441, wR2 = 0.1111
R indices (all data)	R1 = 0.0578, wR2 = 0.1255
Absolute structure parameter	0.1(11)
Largest diff. peak and hole	0.186 and -0.243 e.Å ⁻³