
Electronic Supplementary Information (ESI)

**An efficient, Eco-friendly and Sustainable One-Pot Synthesis of
3,4-Dihydropyrimidin-2(1*H*)-ones Directly from Alcohols Catalyzed
by Heteropolyanion-based Ionic Liquids**

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Characterization data of all products

1-(3-Sulfopropyl)pyridine (PyPS)

White solid. Mp: 62.5-64.8 °C; IR (KBr) : 3443, 3159, 3103, 1572, 1459, 1184, 1010, 842, 780, 654, 601, 528 cm⁻¹; ¹H NMR (400 MHz, D₂O) δ 8.86 (d, J = 6.0 Hz, 2H), 8.53 (t, J = 7.8 Hz, 1H), 8.06 (t, J = 7.6 Hz, 2H), 4.75 (t, J = 7.2 Hz, 2H), 2.95 (t, J = 7.2 Hz, 2H), 2.47-2.40 (m, 2H); ¹³C NMR (100 MHz, D₂O) δ 146.0, 144.5, 128.5, 60.0, 47.1, 26.2; HRMS Calcd for C₈H₁₂NO₃S (M + H⁺): 202.0532; Found: 202.0534.

1-Methyl-3-(3-sulfopropyl)imidazole (MIMPS)

White solid. Mp: 55.5-58.8 °C; IR (KBr) : 3433, 3025, 2944, 1631, 1487, 1328, 1197, 1099, 775, 687, 604, 522, 481 cm⁻¹; ¹H NMR (400 MHz, D₂O) δ 8.71 (s, 1H), 7.48 (s, 1H), 7.41 (s, 1H), 4.32 (t, J = 7.2 Hz, 2H), 3.86 (s, 3H), 2.88 (t, J = 7.2 Hz, 2H), 2.31-2.24 (m, 2H); ¹³C NMR (100 MHz, D₂O) δ 136.2, 123.8, 122.2, 47.8, 47.3, 35.8, 25.1; HRMS Calcd for C₇H₁₃N₂O₃S (M + H⁺): 205.0641; Found: 205.0645.

Triethyl-(3-sulfopropyl)amine (TEAPS)

White solid. Mp: 48.5-49.8 °C; ¹H NMR (400 MHz, D₂O) δ 3.27 (q, J = 7.2 Hz, 8H), 2.93 (t, J = 7.2 Hz, 2H), 2.10-2.06 (m, 2H), 1.27-1.20 (m, 9H); ¹³C NMR (100 MHz, D₂O) δ 52.7, 47.3, 46.7, 17.3, 8.3; HRMS Calcd for C₉H₂₂NO₃S (M + H⁺): 224.1315; Found: 224.1318.

1-(3-Sulfopropyl)pyridinium phosphotungstate ([PyPS]₃PW₁₂O₄₀)

White solid. Mp: 142.5-145.8 °C; IR (KBr) : 3409, 3131, 3068, 1633, 1488, 1220, 1182, 1079, 1042, 978, 896, 805, 681, 595, 521 cm⁻¹; ¹H NMR (400 MHz, D₂O) δ 8.87 (brs, 2H), 8.59 (brs, 1H), 8.11 (brs, 2H), 4.78 (brs, 2H), 2.97 (brs, 2H), 2.46 (brs, 2H); ¹³C NMR (100 MHz, D₂O) δ 146.3, 144.4, 128.6, 60.2, 47.2, 26.2; HRMS Calcd for C₈H₁₂NO₃S (M + H⁺): 202.0532; Found: 202.0535.

1-(3-Sulfopropyl)pyridinium hosphomolybdate ([PyPS]₃PMo₁₂O₄₀)

Green solid. Mp: 142.5-145.8 °C; IR (KBr) : 3421, 3066, 1633, 1488, 1181, 1062, 1044, 957, 880, 795, 680, 609, 505 cm⁻¹; ¹H NMR (400 MHz, D₂O) δ 8.87 (brs, 2H), 8.67 (t,

$J = 7.2$ Hz, 1H), 8.20 (t, $J = 7.2$ Hz, 2H), 4.82 (t, $J = 7.2$ Hz, 2H), 2.98 (t, $J = 7.2$ Hz, 2H), 2.51-2.43 (m, 2H); ^{13}C NMR (100 MHz, D_2O) δ 146.4, 144.3, 129.0, 60.3, 47.3, 26.5; HRMS Calcd for $\text{C}_8\text{H}_{12}\text{NO}_3\text{S}$ ($\text{M} + \text{H}^+$): 202.0532; Found: 202.0536.

1-Methyl-3-(3-sulfopropyl)imidazolium phosphotungstate ([MIMPS] $_3$ PW $_{12}$ O $_{40}$)

White solid. Mp: 119.5-120.8 °C; IR (KBr) : 3417, 3147, 1636, 1571, 1459, 1418, 1173, 1080, 980, 897, 800, 516 cm^{-1} ; ^1H NMR (400 MHz, D_2O) δ 8.68 (s, 1H), 7.55 (s, 1H), 7.51 (s, 1H), 4.42 (t, $J = 7.2$ Hz, 2H), 4.02 (s, 3H), 2.91 (t, $J = 7.2$ Hz, 2H), 2.36-2.28 (m, 2H); ^{13}C NMR (100 MHz, D_2O) δ 135.9, 124.2, 122.6, 48.1, 47.4, 36.1, 25.3; HRMS Calcd for $\text{C}_7\text{H}_{13}\text{N}_2\text{O}_3\text{S}$ ($\text{M} + \text{H}^+$): 205.0641; Found: 205.0645.

1-Methyl-3-(3-sulfopropyl)imidazolium hosphomolybdate ([MIMPS] $_3$ PMo $_{12}$ O $_{40}$)

Green solid. Mp: 105.5-108.8 °C; IR (KBr) : 3422, 3149, 3100, 1630, 1569, 1454, 1405, 1217, 1171, 1059, 963, 882, 796, 610, 504 cm^{-1} ; ^1H NMR (400 MHz, D_2O) δ 8.63 (s, 1H), 7.48 (s, 1H), 7.42 (s, 1H), 4.35 (brs, 2H), 3.92 (s, 3H), 2.86 (brs, 2H), 2.26 (brs, 2H); ^{13}C NMR (100 MHz, D_2O) δ 136.3, 124.3, 122.6, 48.2, 47.4, 36.1, 25.3; HRMS Calcd for $\text{C}_7\text{H}_{13}\text{N}_2\text{O}_3\text{S}$ ($\text{M} + \text{H}^+$): 205.0641; Found: 205.0643.

Triethyl-(3-sulfopropyl)aminium phosphotungstate ([TEAPS] $_3$ PW $_{12}$ O $_{40}$)

White solid. Mp: 185.5-187.8 °C; IR (KBr) : 3440, 1485, 1460, 1400, 1230, 1170, 1080, 978, 893, 810 cm^{-1} ; ^1H NMR (400 MHz, D_2O) δ 3.29-3.28 (m, 8H), 2.98-2.93 (m, 2H), 2.17-2.01 (m, 2H), 1.28-1.25 (m, 9H); ^{13}C NMR (100 MHz, D_2O) δ 60.2, 52.9, 48.0, 24.3, 6.7; HRMS Calcd for $\text{C}_9\text{H}_{22}\text{NO}_3\text{S}$ ($\text{M} + \text{H}^+$): 224.1315; Found: 224.1318.

Triethyl-(3-sulfopropyl)aminium hosphomolybdate ([TEAPS] $_3$ PMo $_{12}$ O $_{40}$)

Green solid. Mp: 165.5-167.8 °C; ^1H NMR (400 MHz, D_2O) δ 3.37-3.21 (m, 8H), 2.97-2.87 (m, 2H), 2.16-2.06 (m, 2H), 1.28-1.25 (m, 9H); ^{13}C NMR (100 MHz, D_2O) δ 60.2, 52.9, 48.0, 24.3, 6.7; HRMS Calcd for $\text{C}_9\text{H}_{22}\text{NO}_3\text{S}$ ($\text{M} + \text{H}^+$): 224.1315; Found: 224.1318.

5-Ethoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one

White solid. Mp: 201.1-203.6 °C; IR (KBr): 3244, 3109, 2933, 1710, 1650, 1222, 1089 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO}-d_6$) δ 9.20 (s, 1H), 7.74 (s, 1H), 7.35-7.30 (m, 2H),

7.25-7.21 (m, 3H), 5.15 (d, $J = 3.0$ Hz, 1H), 3.98 (q, $J = 7.0$ Hz, 2H), 2.25 (s, 3H), 1.09 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.4, 152.2, 148.4, 144.9, 128.4, 127.3, 126.3, 99.3, 59.2, 54.0, 17.8, 14.1; HRMS Calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}^+$): 261.1234; Found: 261.1238.

5-Ethoxycarbonyl-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one
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White solid. Mp: 203.1-205.7 °C; IR (KBr): 3243, 3111, 2930, 1709, 1649, 1223, 1089 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 9.16 (s, 1H), 7.67 (s, 1H), 7.15 (d, $J = 8.7$ Hz, 2H), 6.87 (d, $J = 8.7$ Hz, 2H), 5.10 (d, $J = 3.0$ Hz, 1H), 3.97 (q, $J = 7.0$ Hz, 2H), 3.71 (s, 3H), 2.24 (s, 3H), 1.10 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.4, 158.5, 152.2, 148.1, 137.1, 127.5, 113.7, 99.6, 59.2, 55.1, 53.4, 17.8, 14.2; HRMS Calcd for $\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}_4$ ($\text{M} + \text{H}^+$): 291.1339; Found: 291.1337.

5-Ethoxycarbonyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 216.1-217.1 °C; IR (KBr): 3231, 3094, 2916, 1701, 1649, 1456, 1285, 1219, 1082, 777 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 9.16 (s, 1H), 7.69 (s, 1H), 7.12 (s, 4H), 5.10 (d, $J = 2.1$ Hz, 1H), 3.98 (q, $J = 7.2$ Hz, 2H), 2.26 (s, 3H), 2.24 (s, 3H), 1.10 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.4, 152.2, 148.2, 142.0, 136.4, 128.9, 126.2, 99.4, 59.2, 53.6, 20.7, 17.8, 14.1; HRMS Calcd for $\text{C}_{15}\text{H}_{19}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}^+$): 275.1390; Found: 275.1394.

5-Ethoxycarbonyl-6-methyl-4-(4-chlorophenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 214.8-216.6 °C; IR (KBr): 3245, 3119, 2972, 1650, 1487, 1471, 1287, 1220, 1084, 778, 484 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 9.32 (s, 1H), 9.11 (s, 1H), 7.39 (d, $J = 8.4$ Hz, 2H), 7.25 (d, $J = 8.4$ Hz, 2H), 5.14 (d, $J = 3.3$ Hz, 1H), 3.98 (q, $J = 7.2$ Hz, 2H), 2.25 (s, 3H), 1.09 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.2, 152.0, 148.7, 143.8, 131.8, 128.4, 128.2, 98.8, 59.3, 53.4, 17.8, 14.1; HRMS Calcd for $\text{C}_{14}\text{H}_{16}\text{ClN}_2\text{O}_3$ ($\text{M} + \text{H}^+$): 295.0844; Found: 295.0841.

5-Ethoxycarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 201.1-202.7 °C; IR (KBr): 3230, 3109, 2977, 1701, 1641, 1591, 1520 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.37 (s, 1H), 8.22 (d, *J* = 8.7 Hz, 2H), 7.90 (s, 1H), 7.50 (d, *J* = 8.7 Hz, 2H), 5.27 (d, *J* = 3.0 Hz, 1H), 3.98 (q, *J* = 6.9 Hz, 2H), 2.26 (s, 3H), 1.09 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.1, 152.0, 151.8, 149.4, 146.7, 127.7, 123.9, 98.2, 59.4, 53.7, 17.9, 17.8, 14.1; HRMS Calcd for C₁₄H₁₆N₃O₅ (M + H⁺): 306.1084; Found: 306.1086.

5-Ethoxycarbonyl-6-methyl-4-(4-hydroxyphenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 198.4-200.1 °C; IR (KBr): 3520, 3230, 3150, 1705, 1690 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.25 (s, 1H), 7.78 (s, 1H), 7.62 (s, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 8.4 Hz, 2H), 5.04 (d, *J* = 2.7 Hz, 1H), 3.97 (q, *J* = 7.2 Hz, 2H), 2.23 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.4, 156.5, 152.2, 147.8, 135.5, 127.4, 115.0, 99.7, 59.1, 53.4, 17.8, 14.1; HRMS Calcd for C₁₄H₁₇N₂O₄ (M + H⁺): 277.1183; Found: 277.1186.

5-Ethoxycarbonyl-6-methyl-4-(2-hydroxyphenyl)-3,4-dihydropyrimidin-2(1H)-one

White solid. Mp: 223.1-224.5 °C; IR (KBr): 3354, 3268, 1683, 1597 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.57 (brs, 1H), 9.09 (s, 1H), 7.10 (s, 1H), 7.05 (td, *J* = 7.5, 1.5 Hz, 1H), 6.97 (dd, *J* = 7.5, 1.5 Hz, 1H), 6.79 (dd, *J* = 7.5, 0.6 Hz, 1H), 6.71 (td, *J* = 7.5, 0.6 Hz, 1H), 5.46 (d, *J* = 3.0 Hz, 1H), 3.92 (q, *J* = 7.2 Hz, 2H), 2.27 (s, 3H), 1.04 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.5, 154.7, 152.4, 148.6, 129.9, 128.3, 127.3, 118.8, 115.4, 97.8, 59.1, 49.2, 17.8, 14.1; HRMS Calcd for C₁₄H₁₇N₂O₄ (M + H⁺): 277.1183; Found: 277.1186.

5-Ethoxycarbonyl-6-methyl-4-(furan-2-yl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 207.2-208.9 °C; IR (KBr): 3364, 3221, 3120, 2970, 1699, 1638, 1457, 1372, 1299, 1229, 1092, 1014, 793, 742, 449 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.24 (s, 1H), 7.76 (s, 1H), 7.55 (dd, *J* = 1.8, 0.9 Hz, 1H), 6.35 (dd, *J* = 3.0, 1.8 Hz, 1H), 6.09

(d, $J = 3.3$ Hz, 1H), 5.21 (d, $J = 3.6$ Hz, 1H), 4.02 (qd, $J = 7.2, 0.9$ Hz, 2H), 2.23 (s, 3H), 1.13 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.1, 156.0, 152.5, 149.4, 142.2, 110.4, 105.3, 96.8, 59.3, 47.8, 17.8, 14.2; HRMS Calcd for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{O}_4$ ($\text{M} + \text{H}^+$): 251.1026; Found: 251.1024.

5-Ethoxycarbonyl-6-methyl-4-(n-hexyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 229.8-231.2 °C; IR (KBr): 3248, 3121, 2957, 2936, 2855, 1724, 1703, 1647, 1383, 1288, 1223, 1086, 779 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 8.92 (s, 1H), 7.32 (s, 1H), 4.11-3.99 (m, 3H), 2.15 (m, 3H), 1.38 (m, 10H), 1.18 (t, $J = 6.9$ Hz, 3H), 0.84 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.5, 152.8, 148.3, 99.5, 59.1, 50.1, 36.7, 31.3, 28.5, 23.7, 22.1, 17.7, 14.2, 14.0; HRMS Calcd for $\text{C}_{14}\text{H}_{25}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}^+$): 269.1860; Found: 269.1863.

5-Ethoxycarbonyl-6-methyl-4-isopropyl-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 193.4-194.8 °C; IR (KBr): 3234, 2985, 1710, 1642 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 8.90 (s, 1H), 7.30 (s, 1H), 4.11-4.00 (m, 2H), 3.94 (t, $J = 3.6$ Hz, 1H), 2.17 (s, 3H), 1.70-1.62 (m, 1H), 1.18 (t, $J = 7.1$ Hz, 1H), 0.81 (d, $J = 6.9$ Hz, 3H), 0.74 (d, $J = 6.9$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 165.8, 153.2, 148.5, 98.1, 59.0, 55.5, 34.6, 18.5, 17.7, 16.0, 14.2; HRMS Calcd for $\text{C}_{11}\text{H}_{19}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}^+$): 227.1390; Found: 227.1387.

5-Ethoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 200.4-202.5 °C; IR (KBr): 3322, 3466, 3176, 3111, 1670, 1575, 1470, 1277, 1197, 1105, 696 cm^{-1} ; ^1H NMR (300 MHz, DMSO- d_6) δ 10.34 (s, 1H), 9.65 (s, 1H), 7.37-7.21 (m, 5H), 5.18 (d, $J = 3.6$ Hz, 1H), 4.01 (q, $J = 6.9$ Hz, 2H), 2.29 (s, 3H), 1.10 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 174.2, 165.1, 145.0, 143.5, 128.6, 127.7, 126.4, 100.7, 59.6, 54.1, 17.2, 14.0; HRMS Calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_2\text{S}$ ($\text{M} + \text{H}^+$): 277.1005; Found: 277.1006.

5-Ethoxycarbonyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 192.3-194.1 °C; IR (KBr): 3255, 1659, 1562 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.30 (s, 1H), 9.61 (d, *J* = 1.8 Hz, 1H), 7.16 (m, 4H), 5.13 (d, *J* = 3.6 Hz, 1H), 4.00 (q, *J* = 7.2 Hz, 2H), 2.28 (s, 3H), 2.26 (s, 3H), 1.10 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.2, 165.2, 144.9, 140.6, 136.9, 129.1, 126.3, 100.8, 59.6, 53.8, 20.7, 17.2, 14.1; HRMS Calcd for C₁₅H₁₉N₂O₂S (M + H⁺): 291.1162; Found: 291.1160.

5-Ethoxycarbonyl-6-methyl-4-(4-chlorophenyl)-3,4-dihydropyrimidin-2(1H)-thione

Colorless solid. Mp: 168.1-169.6 °C; IR (KBr): 3331, 3167, 3105, 2978, 1668, 1570, 1197, 747 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.39 (s, 1H), 9.67 (s, 1H), 7.44-7.40 (m, 2H), 7.25-7.20 (m, 2H), 5.17 (d, *J* = 3.6 Hz, 1H), 4.00 (q, *J* = 7.0 Hz, 2H), 2.29 (s, 3H), 1.09 (t, *J* = 7.0 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.3, 165.0, 145.4, 142.4, 132.3, 128.6, 128.3, 100.3, 59.7, 53.5, 17.2, 14.0; HRMS Calcd for C₁₄H₁₆ClN₂O₂S (M + H⁺): 311.0616; Found: 311.0619.

5-Ethoxycarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydro-pyrimidin-2-thione

Yellow solid. Mp: 200.0-202.1 °C; IR (KBr): 3324, 3173, 2918, 1679, 1655, 1576, 1522, 1466, 1350, 1201, 1176, 1123 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.50 (s, 1H), 9.77 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 8.7 Hz, 2H), 5.30 (d, *J* = 3.6 Hz, 1H), 4.01 (q, *J* = 6.9 Hz, 2H), 2.31 (s, 3H), 1.10 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.4, 164.8, 150.4, 147.0, 146.0, 127.8, 124.0, 99.7, 59.8, 53.7, 17.3, 14.0; HRMS Calcd for C₁₄H₁₆N₃O₄S (M + H⁺): 322.0856; Found: 322.0854.

5-Methoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 211.3-213.7 °C; IR (KBr): 3238, 3117, 2933, 1719, 1645, 1222, 1092 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.23 (s, 1H), 7.77 (s, 1H), 7.35-7.30 (m, 2H), 7.26-7.21 (m, 3H), 5.15 (d, *J* = 3.3 Hz, 1H), 3.53 (s, 3H), 2.26 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.9, 152.2, 148.7, 144.7, 128.5, 127.4, 126.2, 99.1, 53.9, 50.9, 17.9; HRMS Calcd for C₁₃H₁₅N₂O₃ (M + H⁺): 247.1077; Found: 247.1079.

5-Methoxycarbonyl-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-o

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Yellow solid. Mp: 192.1-194.2 °C; IR (KBr): 3232, 3104, 3003, 2950, 2837, 1698, 1645, 1609, 1512 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.19 (s, 1H), 7.69 (s, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 5.09 (d, *J* = 3.0 Hz, 1H), 3.72 (s, 3H), 3.52 (s, 3H), 2.25 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.9, 158.5, 152.2, 148.4, 136.9, 127.3, 113.8, 99.3, 55.1, 53.2, 50.8, 17.8; HRMS Calcd for C₁₄H₁₇N₂O₄ (M + H⁺): 277.1183; Found: 277.1186.

5-Methoxycarbonyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-one

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Yellow solid. Mp: 204.0-206.4 °C; IR (KBr): 3175, 1691, 1634 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.19 (s, 1H), 7.71 (s, 1H), 7.11 (s, 4H), 5.11 (d, *J* = 3.3 Hz, 1H), 3.52 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.9, 152.2, 148.5, 141.8, 136.4, 129.0, 126.1, 99.2, 53.5, 50.8, 20.7, 17.8; HRMS Calcd for C₁₄H₁₇N₂O₃ (M + H⁺): 261.1234; Found: 261.1236.

5-Methoxycarbonyl-6-methyl-4-(4-chlorophenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 204.3-207.1 °C; IR (KBr): 3238, 3114, 2950, 2875, 1702, 1645 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.28 (s, 1H), 7.80 (s, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.7 Hz, 2H), 5.14 (d, *J* = 3.3 Hz, 1H), 3.53 (s, 3H), 2.25 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.7, 152.0, 149.0, 143.6, 131.9, 128.5, 128.1, 98.6, 53.3, 50.9, 17.9; HRMS Calcd for C₁₃H₁₄ClN₂O₃ (M + H⁺): 281.0687; Found: 281.0689.

5-Methoxycarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 235.5-237.3 °C; IR (KBr): 3366, 3233, 3113, 2951, 1703, 1643, 1598, 1520 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.38 (s, 1H), 8.21 (d, *J* = 8.9 Hz, 2H), 7.91 (s, 1H), 7.50 (d, *J* = 8.9 Hz, 2H), 5.27 (d, *J* = 3.3 Hz, 1H), 3.53 (s, 3H), 2.27 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 165.6, 151.8, 151.7, 149.6, 146.7, 127.6, 123.9, 98.0, 53.5, 50.9, 17.9; HRMS Calcd for C₁₃H₁₄N₃O₅ (M + H⁺): 292.0928; Found: 292.0925.

5-Methoxycarbonyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 202.1-204.5 °C; IR (KBr): 3340, 1662, 1600, 1566 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.37 (s, 1H), 9.68 (d, *J* = 1.8 Hz, 1H), 7.38-7.32 (m, 2H), 7.30-7.26 (m, 1H), 7.25-7.21 (m, 2H), 5.18 (d, *J* = 3.6 Hz, 1H), 3.56 (s, 3H), 2.30 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.3, 165.7, 145.3, 143.3, 128.7, 127.7, 128.3, 100.5, 53.9, 51.1, 17.3; HRMS Calcd for C₁₃H₁₅N₂O₂S (M + H⁺): 263.0849; Found: 263.0846.

5-Methoxycarbonyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 155.3-156.9 °C; IR (KBr): 3334, 3200, 2970, 1669, 1570, 1470, 1183 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.34 (s, 1H), 9.65 (d, *J* = 1.8 Hz, 1H), 7.16-7.08 (m, 4H), 5.13 (d, *J* = 3.6 Hz, 1H), 3.54 (s, 3H), 2.29 (s, 3H), 2.26 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.2, 165.7, 145.2, 140.4, 136.9, 129.1, 126.2, 100.5, 53.6, 51.1, 20.7, 17.2; HRMS Calcd for C₁₄H₁₇N₂O₂S (M + H⁺): 277.1005; Found: 277.1001.

5-Methoxycarbonyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 122.2-124.7 °C; IR (KBr): 3178, 3105, 2997, 2952, 1693, 1567, 1516 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.52 (s, 1H), 9.78 (s, 1H), 8.23 (d, *J* = 8.7 Hz, 2H), 7.49 (d, *J* = 8.7 Hz, 2H), 5.31 (d, *J* = 3.6 Hz, 1H), 3.56 (s, 3H), 2.31 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 174.5, 165.4, 150.2, 147.0, 146.2, 127.8, 124.1, 99.5, 53.6, 51.3, 17.4; HRMS Calcd for C₁₃H₁₄N₃O₄S (M + H⁺): 308.0700; Found: 308.0702.

5-Acetyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 238.5-240.9 °C; IR (KBr): 3287, 3241, 2914, 1706, 603, 1466, 1248, 764 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 9.21 (s, 1H), 7.86 (s, 1H), 7.35-7.30 (m, 2H), 7.26-7.22 (m, 3H), 5.26 (d, *J* = 3.3 Hz, 1H), 3.54 (s, 3H), 2.29 (s, 3H), 2.10 (s, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 194.3, 152.2, 148.2, 144.3, 128.6, 127.4, 126.5, 109.6, 53.9, 30.4, 19.0; HRMS Calcd for C₁₃H₁₅N₂O₂ (M + H⁺): 231.1128; Found: 231.1124.

5-Acetyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 204.2-206.5 °C; IR (KBr): 3288, 3120, 2920, 1699, 1616, 1236,

1139, 765, 561 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 9.16 (s, 1H), 7.78 (s, 1H), 7.13 (s, 4H), 5.22 (d, $J = 3.0$ Hz, 1H), 2.28 (s, 3H), 2.26 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 194.4, 152.2, 148.0, 141.3, 136.5, 129.1, 126.4, 109.6, 53.6, 30.3, 20.7, 18.9; HRMS Calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}^+$): 245.1285; Found: 245.1288.

5-Acetyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-one

Yellow solid. Mp: 263.3-264.8 $^{\circ}\text{C}$; IR (KBr): 3339, 3254, 3138, 1709, 1672, 1607, 1514, 1445, 1348, 1236, 1103, 762 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 9.34 (s, 1H), 9.20 (d, $J = 8.7$ Hz, 2H), 7.99 (s, 1H), 7.50 (d, $J = 8.7$ Hz, 2H), 5.38 (d, $J = 3.6$ Hz, 1H), 2.31 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 193.9, 152.0, 151.6, 149.1, 146.7, 127.7, 123.8, 109.5, 53.2, 30.7, 19.1; HRMS Calcd for $\text{C}_{13}\text{H}_{14}\text{N}_3\text{O}_3$ ($\text{M} + \text{H}^+$): 276.0979; Found: 276.0981.

5-Acetyl-6-methyl-4-phenyl-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 228.1-230.3 $^{\circ}\text{C}$; IR (KBr): 3323, 3180, 2984, 1669, 1578, 1463, 1272, 1201, 758 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 10.28 (s, 1H), 9.76 (s, 1H), 7.38-7.22 (m, 5H), 5.29 (d, $J = 3.9$ Hz, 1H), 2.33 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 194.8, 174.1, 144.6, 142.9, 128.6, 127.7, 126.6, 110.5, 53.8, 30.4, 18.3; HRMS Calcd for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{OS}$ ($\text{M} + \text{H}^+$): 247.0900; Found: 247.0901.

5-Acetyl-6-methyl-4-(4-methylphenyl)-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 215.7-217.3 $^{\circ}\text{C}$; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 10.25 (s, 1H), 9.72 (s, 1H), 7.16-7.09 (m, 4H), 5.25 (d, $J = 3.9$ Hz, 1H), 2.32 (s, 3H), 2.26 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 194.8, 174.0, 144.4, 140.0, 137.0, 129.2, 126.5, 110.4, 53.6, 30.3, 20.7, 18.2; HRMS Calcd for $\text{C}_{14}\text{H}_{17}\text{N}_2\text{OS}$ ($\text{M} + \text{H}^+$): 261.1056; Found: 261.1059.

5-Acetyl-6-methyl-4-(4-nitrophenyl)-3,4-dihydropyrimidin-2(1H)-thione

Yellow solid. Mp: 207.3-209.5 $^{\circ}\text{C}$; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ 10.46 (s, 1H), 9.89 (d, $J = 2.4$ Hz, 1H), 8.22 (d, $J = 8.7$ Hz, 2H), 7.48 (d, $J = 8.7$ Hz, 2H), 5.41 (d, $J = 3.9$ Hz, 1H), 2.36 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (75 MHz, $\text{DMSO-}d_6$) δ 194.6, 174.6, 150.0,

146.9, 145.6, 127.8, 124.0, 110.3, 53.1, 30.8, 18.5; HRMS Calcd for C₁₃H₁₄N₃O₃S (M + H⁺):
292.0750; Found: 292.0753.







































































