**Synthesis of 4,6-diarylpyrimidin-2(1*H*)-one derivatives from benzyl halides and (1-bromoethyl)benzene under solvent free conditions.**

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**SUPPORTING INFORMATION:**

**6-(3,4-Dimethoxyphenyl)-4-phenylpyrimidin-2(1*H*)-one (4b).**

White solid; mp 253-255 oC; IR (ATR, cm-1): 3426 (NH), 1616 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 3.85 (s, 6H, OCH3), 7.18-7.29 (m, 2H, Ar-H), 7.81-7.85 (s, 3H, Ar-H), 8.03-8.11 (m, 4H, Ar-H), 12.17 (s, 1H, NH) ppm; 13C NMR (100 MHz, DMSO-*d6*): *δ* = 56.0, 56.1, 104.4, 113.5, 117.0, 119.7, 122.6, 122.9, 125.0, 126.9, 127.4, 133.5, 139.2, 139.5, 152.5, 153.7, 158.7, 160.0 ppm; Anal. Calcd for C18H16N2O3:C, 70.12; H, 5.23; N, 9.09 found: C, 70.06; H, 5.18; N, 9.01%.

**4,6-Diphenylpyrimidin-2(1*H*)-one (4c).**

White solid; mp 230-232 oC (lit.7 m.p. 231-233 oC); IR (ATR, cm-1): 3418 (NH), 1612 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.30-7.44 (m, 11H, Ar-H ), 12.15 (s, 1H, NH) ppm; Anal. Calcd for C16H12N2O:C, 77.40; H, 4.87; N, 11.28 found: C, 77.33; H, 4.80; N, 11.20%.

**6-(4-Chlorophenyl)-4-phenylpyrimidin-2(1*H*)-one( 4d).**

White solid; mp 260-262 oC (lit.7 m.p. 260–262 oC); IR (ATR, cm-1): 3436 (NH), 1619 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.30-8.27 (m, 10H, Ar-H ), 13.39 (s, 1H, NH) ppm; Anal. Calcd for C16H11ClN2O:C, 67.97; H, 3.92; N, 9.91 found: C, 67.90; H, 3.90; N, 9.89%.

**6-(3-Chlorophenyl)-4-phenylpyrimidin-2(1*H*)-one (4e).**

White solid; mp 208-210 oC (lit.20 m.p. 210–212 oC); IR (ATR, cm-1): 3411 (NH), 1609 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.30-8.21 (m, 10H, Ar-H ), 12.17 (s, 1H, NH) ppm; Anal. Calcd for C16H11ClN2O:C, 67.97; H, 3.92; N, 9.91 found: C, 67.90; H, 3.88; N, 9.88%.

**6-(4-(*Tert*-butyl)phenyl)-4-phenylpyrimidin-2(1*H*)-one (4f).**

White solid; mp 211-213 oC; IR (ATR, cm-1): 3416 (NH), 1621 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 1.33 (s, 9H, *tert*-butyl), 7.37-7.83 (m, 10H, Ar-H), 12.02 (s, 1H, NH) ppm; 13C NMR (100 MHz, DMSO-*d6*): *δ* = 29.9 (3C), 35.3, 105.7, 123.8 (2C), 125.4, 126.6 (2C), 131.4, 132.0, 134.7, 134.9, 139.2, 139.5, 143.7, 152.2, 159.8, 161.9 ppm; LCMS (M+H) = m/z 305.2; Anal. Calcd for C20H20N2O: C, 78.92; H, 6.62; N, 9.20 found: C, 78.89; H, 6.55; N, 9.16%.

**6-(4-Fluorophenyl)-4-phenylpyrimidin-2(1*H*)-one (4g).**

White solid; mp 162-164 oC (lit.20 m.p. 159–161 oC); IR (ATR, cm-1): 3419 (NH), 1621 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.62-8.26 (m, 10H, Ar-H), 12.00 (s, 1H, NH) ppm; Anal. Calcd for C16H11FN2O:C, 72.17; H, 4.16; N, 10.52 found: C, 72.11; H, 4.10; N, 10.48 %.

**6-(4-Nitrophenyl)-4-phenylpyrimidin-2(1*H*)-one (4h).**

White solid; mp >300 oC (lit.47 m.p. >300 oC); IR (ATR, cm-1): 3420 (NH), 1620 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.52-8.58 (m, 10H, Ar-H), 12.07 (s, 1H, NH) ppm; Anal. Calcd for C16H11N3O3:C, 65.53; H, 3.78; N, 14.33 found: C, 65.49; H, 3.70; N, 14.27 %.

**6-(2-Chlorophenyl)-4-phenylpyrimidin-2(1*H*)-one (4i).**

White solid; mp 222-224 oC (lit.20 m.p. 220–223 oC); IR (ATR, cm-1): 3422 (NH), 1611 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.56-8.20 (m, 10H, Ar-H), 12.44 (s, 1H, NH) ppm; Anal. Calcd for C16H11ClN2O:C, 67.97; H, 3.92; N, 9.91 found: C, 67.91; H, 3.87; N, 9.88%.

**6-(4-Bromophenyl)-4-phenylpyrimidin-2(1*H*)-one (4j).**

White solid; mp 255-257 oC (lit.20 m.p. 255–256 oC); IR (ATR, cm-1): 3426 (NH), 1616 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 7.35-8.28 (m, 10H, Ar-H), 12.01 (s, 1H, NH) ppm; Anal. Calcd C16H11BrN2O:C, 58.74; H, 3.39; N, 8.56 found: C, 58.69; H, 3.33; N, 8.51 %.

**6-(4-Methoxyphenyl)-4-phenylpyrimidin-2(1*H*)-one (4k).**

White solid; mp 257-259 oC (lit.26 m.p. 258–260 oC); IR (ATR, cm-1): 3416 (NH), 1619 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 3.74 (s, 3H, OCH3), 6.96-7.71 (m, 10H, Ar-H), 11.43 (s, 1H, NH) ppm; Anal. Calcd for C17H14N2O2:C, 73.37; H, 5.07; N, 10.07 found: C, 73.31; H, 5.00; N, 10.01 %.

**6-(4-Methylphenyl)-4-phenylpyrimidin-2(1*H*)-one (4l).**

White solid; mp 287-289 oC (lit.5 m.p. 288–291 oC); IR (ATR, cm-1): 3426 (NH), 1616 (C=O) cm-1; 1H NMR (400 MHz, DMSO-*d6*): *δ* = 2.55 (s, 3H, CH3), 7.35-8.12 (m, 10H, Ar-H), 12.15 (s, 1H, NH) ppm; Anal. Calcd for C17H14N2O:C, 77.84; H, 5.38; N, 10.68 found: C, 77.77; H, 5.32; N, 10.63 %.

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| Entry | Compounds | Spectra |
| S5 | 4a | 1H |
| S6 | 4a | 13C |
| S7 | 4b | 1H |
| S8 | 4b | 13C |
| S9 | 4c | 1H |
| S10 | 4d | 1H |
| S11 | 4e | 1H |
| S12 | 4f | 1H |
| S13 | 4f | 13C |
| S14 | 4f | mass spectrum |
| S15 | 4g | 1H |
| S16 | 4h | 1H |
| S17 | 4i | 1H |
| S18 | 4j | 1H |
| S19 | 4k | 1H |
| S20 | 4l | 1H |































































