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Supplementary Information

A Convenient and Efficient Protocol for the One Pot Synthesis of 3,4-Dihydropyrimidin-2-(1*H*)-ones Catalyzed by Ionic Liquids under Ultrasound Irradiation

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Spectral data for all synthesized DHPMs

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

IR (KBr) ν_{max}/cm^{-1}: 3224, 2950, 1745, 1670, 1510, 1340, 1125, 780; ^{1}H NMR: δ 9.37 (s,1H), 8.20 (d, 2H), 7.91 (s, 1H), 7.50 (d, 2H), 5.27 (s, 1H), 3.98 (q, *J* 7.1 Hz, 2H), 2.27 (s, 3H), 1.09 (t, *J* 7.1 Hz, 3H); ^{13}C NMR: δ 13.9, 17.8, 53.6, 59.3, 123.7, 127.5, 146.6, 149.3, 151.7, 151.9, 164.9. Calc. for $C_{14}H_{15}N_3O_5$: C, 55.08; H, 4.95; N, 13.76. Found: C, 55.05; H, 4.97; N, 13.74.

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

IR (KBr) ν_{max}/cm^{-1}: 3254, 2966, 1738, 1669, 1170, 1096, 759; ^{1}H NMR: δ 9.24 (s,1H), 7.77 (s, 1H), 7.26 (m, 4H), 5.14 (s, 1H), 3.98 (q, *J* 7.1 Hz, 2H), 2.25 (s, 3H), 1.09 (t, *J* 7.1 Hz, 3H); ^{13}C NMR: δ 14.0, 17.8, 53.6, 59.3, 98.7, 124.9, 126.2, 127.2, 130.4, 132.9, 147.2, 148.9, 151.9, 165.2. Calc. for $C_{14}H_{15}ClN_2O_3$: C, 57.05; H, 5.13; N, 9.50. Found: C, 57.08; H, 5.16; N, 9.48.

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

IR (KBr) ν_{max}/cm^{-1}: 3260, 2980, 1720, 1635, 1248, 1120, 775; ^{1}H NMR: δ 9.15 (s,1H), 7.80 (s, 1H), 7.10 (s, 4H), 5.09 (s, 1H), 3.96 (q, *J* 7.1 Hz, 2H), 2.23 (s, 3H), 1.08 (t, *J* 7.1 Hz, 3H); ^{13}C NMR: δ 14.1, 17.7, 20.6, 53.7, 59.1, 99.4, 126.1, 128.8, 136.3, 141.7, 148.2, 152.2, 165.2. Calc. for $C_{15}H_{18}N_2O_3$: C, 65.68; H, 6.61; N, 10.21. Found: C, 65.64; H, 6.59; N, 10.23.

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*5-Ethoxycarbonyl-6-methyl-4-(2-furyl)-3,4-dihydropyrimidin-2(1H)-one (**2g**)*

IR (KBr) ν_{max}/cm^{-1}: 3234, 2918, 1727, 1648, 1234, 1113; ^{1}H NMR: δ 9.24 (s,1H), 7.75 (s, 1H), 7.54 (s, 1H), 6.34 (s, 1H), 6.08 (s, 1H), 5.19 (s, 1H), 4.01 (q, *J* 6.9 Hz, 2H), 2.22 (s, 3H), 1.12 (t, *J* 6.9 Hz, 3H); ^{13}C NMR: δ 14.1, 17.7, 47.8, 59.1, 96.8, 105.2, 110.3, 142.3, 149.2, 152.2, 155.9, 165.2. Calc. for $C_{12}H_{14}N_2O_4$: C, 57.59; H, 5.64; N, 11.19. Found: C, 57.55; H, 5.62; N, 11.21.

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

IR (KBr) ν_{max}/cm^{-1}: 3109, 2948, 1725, 1698, 1177, 1089, 750; ^{1}H NMR: δ 9.25 (s,1H), 7.70 (s, 1H), 7.33 (m, 4H), 5.61 (s, 1H), 3.87 (q, *J* 6.9 Hz, 2H), 2.28 (s, 3H), 0.98 (t, *J* 6.9 Hz, 3H); ^{13}C NMR: δ 13.9, 17.7, 51.6, 59.1, 98.2, 127.7, 128.8, 129.1, 129.4, 131.8, 141.7, 149.2, 151.4, 165.0. Calc. for $C_{14}H_{15}ClN_2O_3$: C, 57.05; H, 5.13; N, 9.50. Found: C, 57.08; H, 5.15; N, 9.53.

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

IR (KBr) ν_{max}/cm^{-1}: 3358, 3219, 2930, 1731, 1678, 1171, 819; ^{1}H NMR: δ 9.34 (s,1H), 9.10 (s, 1H), 7.64 (s, 1H), 6.84 (m, 4H), 5.02 (s, 1H), 3.96 (q, *J* 7.0 Hz, 2H), 2.21 (s, 3H), 1.08 (t, *J* 7.0 Hz, 3H); ^{13}C NMR: δ 13.7, 17.45, 54.4, 59.2, 101.1, 115.0, 127.7, 133.8, 146.9, 153.0, 156.8, 165.4. Calc. for $C_{14}H_{16}N_2O_4$: C, 60.86; H, 5.84; N, 10.14. Found: C, 60.84; H, 5.86; N, 10.16.

*5-Ethoxycarbonyl-6-methyl-4-(3,4,5-trimethoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one (**2j**)*

IR (KBr) ν_{max}/cm^{-1}: 3215, 2922, 1732, 1676, 1248, 1126, 821; ^{1}H NMR: δ 9.23 (s,1H), 7.75 (s, 1H), 6.53 (s, 2H),

5.13 (s, 1H), 4.02 (q, *J* 6.6 Hz, 2H), 3.72 (s, 9H), 2.25 (s, 3H), 1.13 (t, *J* 7.0 Hz, 3H); ^{13}C NMR: δ 14.2, 17.8, 54.1, 56.0, 59.4, 60.1, 99.3, 104.3, 140.6, 148.5, 152.5, 152.9, 165.4. Calc. for $C_{17}H_{22}N_2O_6$: C, 58.28; H, 6.33; N, 8.00. Found: C, 58.24; H, 6.30; N, 8.03.

*5-Ethoxycarbonyl-6-methyl-4-(4-hydroxy-3-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one (**2k**)*

IR (KBr) ν_{max}/cm^{-1}: 3384, 3238, 2994, 1726, 1642, 1210, 1140, 756; ^{1}H NMR: δ 9.35 (s,1H), 9.10 (s, 1H), 7.68 (s, 1H), 7.32 (m,3H), 6.10 (s, 1H), 4.12 (q, *J* 7.2 Hz, 2H), 3.45 (s, 3H), 2.32 (s, 3H), 1.10 (t, *J* 7.2 Hz, 3H); ^{13}C NMR: δ 13.6, 18.8, 54.4, 61.7, 101.7, 113.54, 127.8, 128.9, 139.6, 141.8, 146.4, 148.3, 158.8, 165.8. Calc. for $C_{15}H_{18}N_2O_5$: C, 58.82; H, 5.92; N, 9.15. Found: C, 58.79; H, 5.93; N, 9.12.

*5-Ethoxycarbonyl-6-methyl-4-(2-thienyl)-3,4-dihydropyrimidin-2(1H)-one (**2l**)*

IR (KBr) ν_{max}/cm^{-1}: 3228, 2954, 1734, 1664, 1242, 1127, 786; ^{1}H NMR: δ 9.31 (s,1H), 7.88 (s, 1H), 7.35 (d, 1H), 6.90 (m, 2H), 5.39 (s, 1H), 4.05 (q, *J* 7.1 Hz, 2H), 2.20 (s, 3H), 1.15 (t, *J* 7.1 Hz, 3H); ^{13}C NMR: δ 14.2, 17.7, 49.9, 59.3, 99.8, 124.1, 124.9, 126.3, 148.7, 148.9, 152.3, 165.0. Calc. for $C_{12}H_{14}N_2O_3S$: C, 54.12; H, 5.30; N, 10.52. Found: C, 54.15; H, 5.34; N, 10.54.

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

IR (KBr) ν_{max}/cm^{-1}: 3200, 2956, 1720, 1678, 1180, 1097, 694; ^{1}H NMR: δ 10.32 (s,1H), 9.64 (s, 1H), 7.27 (m, 5H), 5.15 (d, 1H), 4.01 (q, *J* 7.0 Hz, 2H), 2.27 (s, 3H), 1.09 (t, *J* 7.0 Hz, 3H); ^{13}C NMR: δ 14.4, 17.6, 54.4, 60.0, 101.1, 126.8, 128.1, 129.2, 140.4, 143.9, 153.7, 165.5. Calc. for $C_{14}H_{16}N_2O_2S$: C, 60.85; H, 5.84; N, 10.14. Found: C, 60.84; H, 5.80; N, 10.16.

*5-Ethoxycarbonyl-6-methyl-4-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-thione (**2n**)*

IR (KBr) ν_{max}/cm^{-1}: 3088, 2933, 1730, 1687, 1247, 1175, 944; ^{1}H NMR: δ 10.28 (s,1H), 9.59 (s, 1H), 7.01 (m, 4H), 5.10 (s, 1H), 3.98 (q, *J* 7.0 Hz, 2H), 3.70 (s, 3H), 2.27 (s, 3H), 1.09 (t, *J* 7.0 Hz, 3H); ^{13}C NMR: δ 14.1, 17.6, 53.9, 55.2, 59.6, 101.2, 113.7, 127.5, 135.3, 144.7, 158.2, 165.2, 174.2. Calc. for $C_{15}H_{18}N_2O_3S$: C, 58.80; H, 5.92; N, 9.14. Found: C, 58.78; H, 5.95; N, 9.11.

Copies of ^{13}C NMR spectra in evidence for bonding of IL with p-tolualdehyde

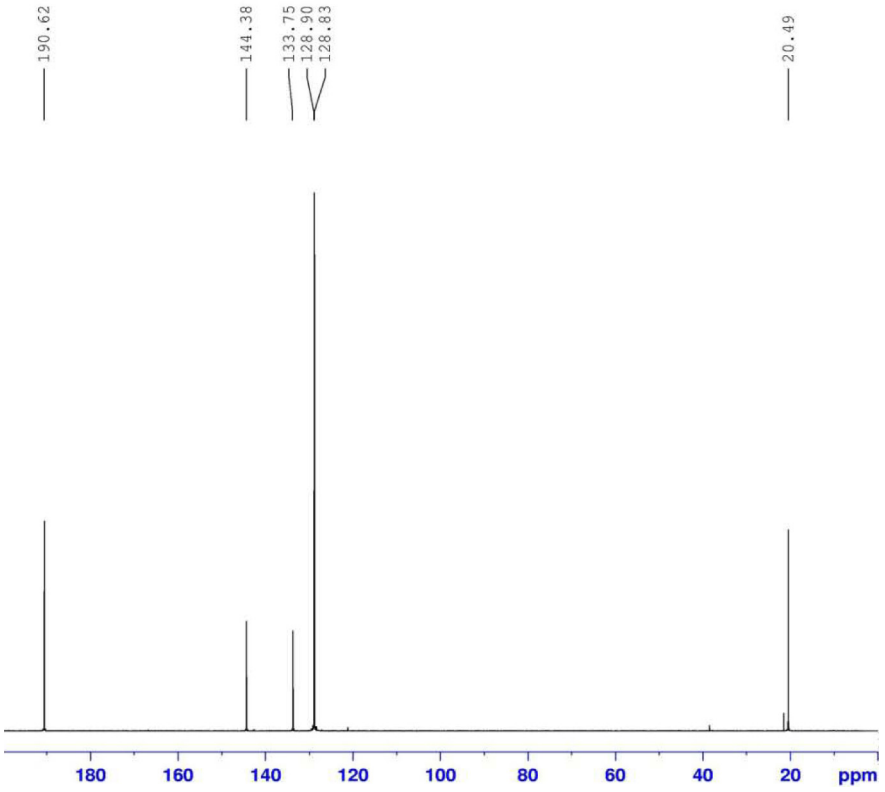

Figure S1. ^{13}C NMR spectrum of neat *p*-tolualdehyde.

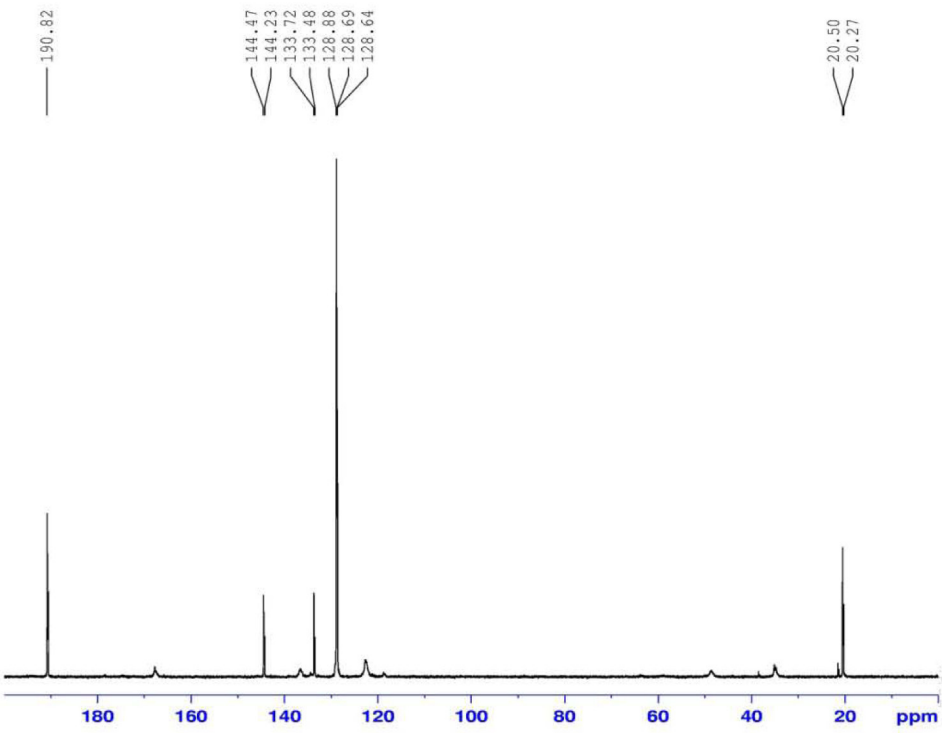

Figure S2. ^{13}C NMR spectrum of *p*-tolualdehyde + [cmmim][BF_4].

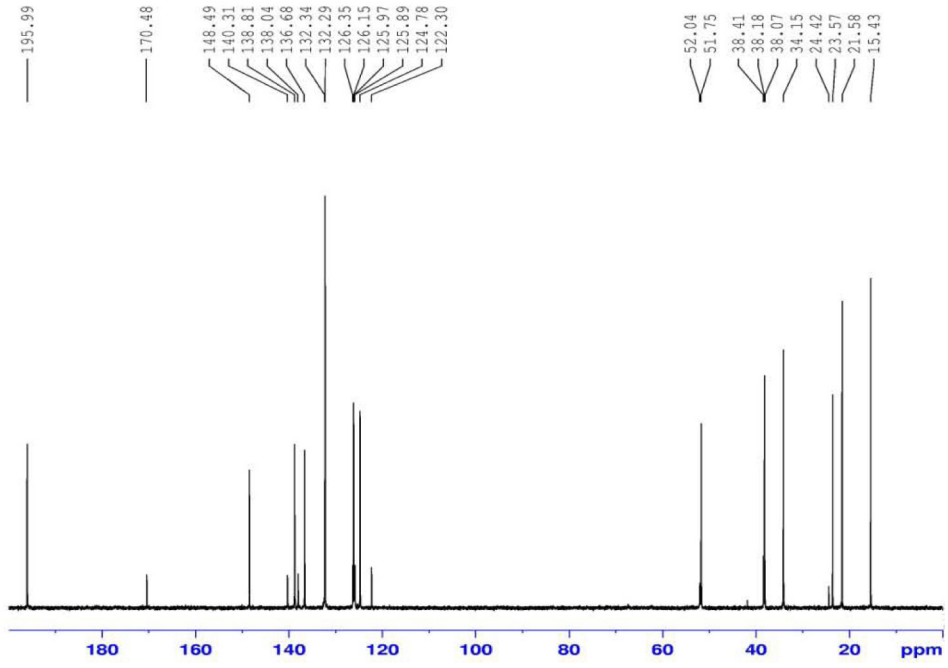

Figure S3. ^{13}C NMR spectrum of *p*-tolualdehyde + [cmmim][BF_4] + [bmim][BF_4].