Supporting Information

Basic Ionic Liquid as Catalysis and Reaction Medium: A Novel and Green Protocol for the Markovnikov Addition of *N*-heterocycles to Vinyl Esters using a Task-Specific Ionic Liquid, [bmIm]OH

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General Procedure for the Markovnikov Addition of 4-nitroimidazole to Vinyl acetate promoted by ionic liquid [bmIm]OH. 4-nitroimidazole (113 mg, 1 mmol) and vinyl acetate (344 mg, 4 mmol) were added to a 10 mL conical flask containing 1 ml [bmim]OH and the mixture was shaken at 200 rpm and 50°C for 2 h. The reaction mixture was extracted from the ionic liquid phase with ethyl ether (10.0 mL×5). The organic layer was dried over anhydrous sodium sulfate and evaporated under reduced pressure. The residue was purified by flash column chromatography (silica gel) to obtain the pure product **3a**, 1-(1-(4-nitroimidazole))-ethyl acetate (186 mg, 93%).

1-(1-(4-Nitro-imidazole))-ethyl acetate (3a**):** white solid, m.p. 82-83°C; IR (KBr): 1748, 1511 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ, ppm): 8.68 (s, 1H), 8.11 (s, 1H), 6.77 (q, 1H, *J*=6.20 Hz), 2.05 (s, 3H), 1.78 (d, 3H, *J*=6.20 Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ, ppm): 169.8, 147.8, 137.2, 120.1, 77.3, 21.1, 20.2. HRMS (ESI) *m/z* calcd. for [M + Na] C₇H₉N₃O₄Na 222.0485, found 222.0476.

1-(1-(4-Nitro-imidazole))-ethyl butyrate (3b**):** yellow oil; IR (neat): 1750, 1514 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ, ppm): 8.66(s, 1H), 8.10 (s, 1H), 6.78 (q, 1H, *J*=6.18Hz), 2.32 (t, 2H), 1.77 (d, 3H, *J*=6.18 Hz), 1.52 (m, 2H), 0.83 (t, 3H). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ,

ppm): 172.1, 147.8, 137.1, 120.0, 77.2, 35.4, 20.2, 18.0, 13.6. HRMS (ESI) m/z calcd. for [M + Na] C₉H₁₃N₃O₄Na 250.0798, found 250.0799.

1-(1-(4-Nitro-imidazole))-ethyl isobutyrate (3c): yellow oil; IR (neat): 1745, 1512 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ , ppm): 8.67(s, 1H), 8.11 (s, 1H), 6.77 (q, 1H, $J=6.12$ Hz), 2.56 (q, 1H), 1.78 (d, 3H, $J=6.12$ Hz), 1.08, 1.04 (d, 6H). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ , ppm): 175.3, 147.8, 137.1, 119.9, 77.4, 33.4, 20.2, 18.8. HRMS (ESI) m/z calcd. for [M + Na] C₉H₁₃N₃O₄Na 250.0798, found 250.0799.

1-(1-(4-Nitro-imidazole))-ethyl valerate (3d): yellow oil; IR (neat): 1749, 1513 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ , ppm): 8.68(s, 1H), 8.11 (s, 1H), 6.79 (q, 1H, $J=6.16$ Hz), 2.34 (t, 2H), 1.78 (d, 3H, $J=6.16$ Hz), 1.48 (m, 2H), 1.26 (m, 2H), 0.85 (t, 3H). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ , ppm): 172.2, 147.8, 137.1, 120.0, 77.3, 33.4, 26.6, 21.9, 20.2, 14.1. HRMS (ESI) m/z calcd. for [M + Na] C₁₀H₁₅N₃O₄Na 264.0955, found 264.0944.

1-(1-(4-Nitro-imidazole))-ethyl caproate (3e): tan oil; IR (neat): 1750, 1513 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ , ppm): 8.66(s, 1H), 8.10 (s, 1H), 6.78 (q, 1H, $J=6.18$ Hz), 2.33 (t, 2H), 1.77 (d, 3H, $J=6.18$ Hz), 1.48 (m, 2H), 1.13-1.24 (m, 4H), 0.80 (t, 3H). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ , ppm): 172.2, 147.8, 137.2, 120.0, 77.2, 33.6, 30.9, 24.2, 22.2, 20.1, 14.2. HRMS (ESI) m/z calcd. for [M + Na] C₁₁H₁₇N₃O₄Na 278.1111, found 278.1103.

1-(1-(4-Nitro-imidazole))-ethyl benzoate (3f): yellow solid, 103-104°C; IR (KBr): 3114, 1724, 1511 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ , ppm): 8.79(s, 1H), 8.22 (s, 1H), 7.98(t, 2H), 7.69(t, 1H), 7.55(t, 2H), 7.03 (q, 1H, $J=6.18$ Hz), 1.92 (d, 3H, $J=6.18$ Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ , ppm): 164.8, 147.7, 138.8, 137.3, 134.6, 129.7, 129.4, 120.1, 78.2, 20.4. HRMS (ESI) m/z calcd. for [M + Na] C₁₂H₁₁N₃O₄Na 284.0642, found 284.0642.

1-(1-imidazole)-ethyl acetate (3g): colorless oil; IR (neat): 1749, 1514 cm⁻¹; ¹H NMR (DMSO-*d*₆, 500 MHz, δ , ppm): 7.86 (s, 1H), 7.39 (s, 1H), 6.93 (s, 1H), 6.72 (q, 1H, $J=6.21$ Hz), 2.01 (s, 3H), 1.71 (d, 3H, $J=6.21$ Hz). ¹³C NMR (DMSO-*d*₆, 125 MHz, δ , ppm): 169.7, 137.3, 129.3, 117.8, 76.2, 21.2, 20.4. HRMS (ESI) m/z calcd. for [M + H] C₇H₁₁N₂O₂ 155.0815, found 155.0813.

1-(1-imidazole)-ethyl butyrate (3h): yellow oil; IR (neat): 1748, 1510 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz, δ , ppm): 7.85 (s, 1H), 7.38 (s, 1H), 6.91 (s, 1H), 6.74 (q, 1H, $J=6.21$ Hz), 2.28 (t, 2H), 1.71 (d, 3H, $J=6.21$ Hz), 1.50 (m, 2H), 0.81 (t, 3H). ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz, δ , ppm): 172.1, 137.3, 129.2, 117.8, 76.0, 35.6, 20.5, 18.2, 13.6. HRMS (ESI) m/z calcd. for $[\text{M} + \text{Na}] \text{C}_9\text{H}_{14}\text{N}_2\text{O}_2\text{Na}$ 205.0947, found 205.0944.

1-(1-imidazole)-ethyl caproate (3i): yellow oil; IR (neat): 1750, 1513 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz, δ , ppm): 7.79 (s, 1H), 7.11 (s, 1H), 7.08 (s, 1H), 6.73 (q, 1H, $J=6.28$), 2.29 (t, 2H), 1.78 (d, 3H, $J=6.28$ Hz), 1.58 (m, 2H), 1.21-1.29 (m, 4H), 0.87 (t, 3H). ^{13}C NMR (CDCl_3 , 125 MHz, δ , ppm): 172.6, 136.6, 139.3, 117.1, 75.3, 34.2, 31.3, 24.5, 22.5, 20.5, 14.1. HRMS (ESI) m/z calcd. for $[\text{M} + \text{Na}] \text{C}_{11}\text{H}_{18}\text{N}_2\text{O}_2\text{Na}$ 233.1260, found 233.1264.

1-(1-imidazole)-ethyl benzoate (3j): yellow solid, 79-80°C; IR (KBr): 3110, 1715, 1513 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz, δ , ppm): 8.00 (dd, 2H), 7.83 (s, 1H), 7.59 (t, 1H), 7.44 (t, 2H), 7.21 (s, 1H), 7.08 (s, 1H), 6.98 (q, 1H, $J=6.29$ Hz), 1.93 (d, 3H, $J=6.29$ Hz). ^{13}C NMR (CDCl_3 , 125 MHz, δ , ppm): 165.3, 136.8, 134.0, 130.0, 129.9, 128.7, 117.1, 76.0, 20.6. HRMS (ESI) m/z calcd. for $[\text{M} + \text{Na}] \text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2\text{Na}$ 239.0791, found 239.0783.

1-(1-(4-methyl-imidazole))-ethyl acetate (3k): yellow oil; IR (neat): 1743, 1509 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz, δ , ppm): 7.71 (s, 1H), 7.07 (s, 1H), 6.64 (q, 1H, $J=6.09$ Hz), 2.07 (s, 3H), 2.01 (s, 3H), 1.68 (d, 3H, $J=6.09$ Hz). ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz, δ , ppm): 170.0, 136.8, 136.0, 114.0, 76.3, 21.4, 20.6, 14.2. HRMS (ESI) m/z calcd. for $[\text{M} + \text{H}] \text{C}_8\text{H}_{13}\text{N}_2\text{O}_2$ 169.0972, found 169.0971.

1-(1-(2-methyl-imidazole))-ethyl acetate (3l): yellow oil; IR (neat): 1746, 1511 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz, δ , ppm): 7.30 (s, 1H), 6.79 (s, 1H), 6.63 (q, 1H, $J=6.14$ Hz), 2.34 (s, 3H), 2.01 (s, 3H), 1.66 (d, 3H, $J=6.14$ Hz). ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz, δ , ppm): 169.7, 144.6, 127.7, 116.6, 75.4, 21.1, 20.8, 13.2. HRMS (ESI) m/z calcd. for $[\text{M} + \text{H}] \text{C}_8\text{H}_{13}\text{N}_2\text{O}_2$ 169.0972, found 169.0967.

1-(1-(2-methyl-4-nitro-imidazole))-ethyl acetate (3m): white solid, m.p. 132-133°C; IR (KBr): 1751, 1514 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz, δ , ppm): 8.64 (s, 1H), 6.78 (q, 1H, $J=5.85$ Hz), 2.46 (s, 3H), 2.07 (s, 3H), 1.75 (d, 3H, $J=5.85$ Hz). ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz, δ ,

ppm): 169.7, 146.8, 148.5, 119.6, 76.3, 21.1, 20.5, 13.5. HRMS (ESI) m/z calcd. for $[M + Na]$ $C_8H_{11}N_3O_4Na$ 236.0642, found 236.0634.

1-(1-pyrrole)-ethyl acetate (5a): colorless oil; IR (neat): 1743, 1676, 1530 cm^{-1} ; 1H NMR (DMSO- d_6 , 500 MHz, δ , ppm): 6.94 (d, 2H), 6.50 (q, 1H, $J=6.02$ Hz), 6.05 (d, 2H), 2.01 (s, 3H), 1.64 (d, 3H, $J=6.02$ Hz). ^{13}C NMR (DMSO- d_6 , 125 MHz, δ , ppm): 169.7, 120.1, 120.0, 109.3, 109.2, 77.9, 21.2, 19.2. HRMS (ESI) m/z calcd. for $[M + Na]$ $C_7H_{10}N_2O_2Na$ 176.0681, found 176.0683.

1-(1-pyrazole)-ethyl acetate (5b): colorless oil; IR (neat): 1744, 1497 cm^{-1} ; 1H NMR (DMSO- d_6 , 500 MHz, δ , ppm): 7.92 (s, 1H), 7.54 (s, 1H), 6.79 (q, 1H, $J=6.20$ Hz), 6.30 (t, 1H), 2.01 (s, 3H), 1.74 (d, 3H, $J=6.20$ Hz). ^{13}C NMR (DMSO- d_6 , 125 MHz, δ , ppm): 169.7, 140.3, 130.6, 106.3, 79.5, 21.2, 19.6). HRMS (ESI) m/z calcd. for $[M + Na]$ $C_7H_{10}N_2O_2Na$ 177.0634, found 177.0634.

1-(1-triazole)-ethyl acetate (5c): light yellow oil; IR (neat): 1748, 1485 cm^{-1} ; 1H NMR (CDCl₃, 500 MHz, δ , ppm): 8.34 (s, 1H), 7.97 (s, 1H), 6.87 (q, 1H, $J=6.24$ Hz), 2.08 (s, 3H), 1.89 (d, 3H, $J=6.24$ Hz). ^{13}C NMR (CDCl₃, 125 MHz, δ , ppm): 169.8, 152.3, 144.2, 76.7, 20.9, 19.2. HRMS (ESI) m/z calcd. for $[M + Na]$ $C_6H_9N_3O_2Na$ 178.0587, found 178.0585.

1-(1-(5-Fluorouracil))-ethyl acetate (5d): white solid, m.p. 171-172°C; IR (KBr): 3434, 1752, 1730, 1663, 1225 cm^{-1} ; 1H NMR (DMSO- d_6 , 500 MHz, δ , ppm): 11.70 (s, 1H), 8.20 (s, 1H), 6.76 (q, 1H, $J=6.20$ Hz), 2.05 (s, 3H), 1.54 (d, 3H, $J=6.20$ Hz). ^{13}C NMR (DMSO- d_6 , 125 MHz, δ , ppm): 169.3, 157.6, 157.7, 148.9, 141.7, 139.8, 125.6, 125.3, 75.6, 21.1, 18.9. HRMS (ESI) m/z calcd. for $[M + Na]$ $C_8H_9N_2O_4FNa$ 239.0439, found 239.0434.

1-(9-(allopurinol))-ethyl acetate (5e): white solid, m.p. 170-171°C; IR (KBr): 3435, 1746, 1677 cm^{-1} ; 1H NMR (DMSO- d_6 , 500 MHz, δ , ppm): 11.76(s, 1H), 8.70 (s, 1H), 7.97 (s, 1H), 6.91 (q, 1H, $J=6.00$ Hz), 2.05 (s, 3H), 1.79 (d, 3H, $J=6.00$ Hz). ^{13}C NMR (DMSO- d_6 , 125 MHz, δ , ppm): 169.7, 159.3, 159.1, 148.1, 129.9, 107.6, 80.8, 21.1, 19.8. HRMS (ESI) m/z calcd. for $[M + Na]$ $C_9H_{10}N_4O_3Na$ 245.0645, found 245.0639

1-(9-(6-benzylamino-purine))-ethyl acetate (5f): yellow oil; IR (neat): 3031, 1750, 16

20, 1580 cm^{-1} ; ^1H NMR ($\text{DMSO-}d_6$, 500 MHz, δ , ppm): 8.40 (s, 1H), 8.38 (s, 1H), 8.22 (s, 1H), 7.34-7.19 (m, 5H), 6.96 (q, 1H, $J=6.23$), 2.01 (s, 3H), 1.90 (d, 3H, $J=6.23$ Hz). ^{13}C NMR ($\text{DMSO-}d_6$, 125 MHz, δ , ppm): 169.6, 155.5, 153.2, 152.3, 145.0, 138.3, 128.7, 128.4, 127.6, 127.3, 127.1, 99.0, 75.2, 49.8, 21.1, 19.6. HRMS (ESI) m/z calcd. for $[\text{M} + \text{Na}]$ $\text{C}_{16}\text{H}_{17}\text{N}_5\text{O}_2\text{Na}$ 334.1274, found 334.1280.

1-(1-(4-Nitro-imidazole))-ethyl acetate (3a).

^1H NMR (500 MHz, $\text{DMSO-}d_6$)

^{13}C NMR (125 MHz, $\text{DMSO-}d_6$)

1-(1-(4-Nitro-imidazole))-ethyl butyrate (3b).

¹H NMR (500 MHz, DMSO-*d*₆)

¹³C NMR (125 MHz, DMSO-*d*₆)

1-(1-(4-Nitro-imidazole))-ethyl isobutyrate (3c).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-(4-Nitro-imidazole))-ethyl valerate (3d).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-(4-Nitro-imidazole))-ethyl caproate (3e).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-(4-Nitro-imidazole))-ethyl benzoate (3f).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-imidazole)-ethyl acetate (3g).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-imidazole)-ethyl butyrate (3h).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-imidazole)-ethyl caproate (3i).

¹H NMR (500 MHz, CDCl₃)

¹³C NMR (125 MHz, CDCl₃)

1-(1-(4-methyl-imidazole))-ethyl acetate (3k).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-(2-methyl-imidazole))-ethyl acetate (3I).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-(2-methyl-4-nitro-imidazole))-ethyl acetate (3m).

^1H NMR (500 MHz, $\text{DMSO-}d_6$)

^{13}C NMR (125 MHz, $\text{DMSO-}d_6$)

1-(1-pyrrole)-ethyl acetate (5a).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-pyrazole)-ethyl acetate (5b).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(1-triazole)-ethyl acetate (5c).

^1H NMR (500 MHz, CDCl_3)

^{13}C NMR (125 MHz, CDCl_3)

1-(1-(5-Fluorouracil))-ethyl acetate (5d).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(9-allylpurinol)-ethyl acetate (5e).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

1-(9-(6-benzylamino-purine))-ethyl acetate (5f).

^1H NMR (500 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (125 MHz, $\text{DMSO}-d_6$)

Imidazole ^{13}C -NMR.

Imidazole + [bmIm]OH (1:1, molar ratio) ^{13}C -NMR.

Imidazole + [bmIm]OH (1:1, molar ratio) ^{13}C -NMR (amplified figure).

Vinyl butyrate ^{13}C -NMR

Vinyl butyrate + [bmIm]OH (1:1, molar ratio) ^{13}C -NMR.

Vinyl butyrate + [bmIm]BF₄ (1:1, molar ratio) ^{13}C -NMR.

The ^1H -NMR figure of partially deuterated compound **3a**.

The ESI-MS figure of partially deuterated compound **3a**.