

Supporting Information

An efficient one pot three-component synthesis of 2,4,6-triarylpyridines using triflimide as a metal-free catalyst under solvent-free conditions

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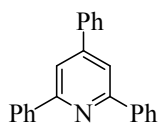
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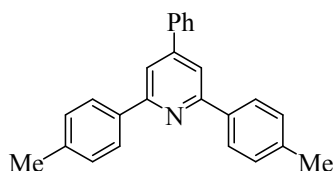
Characterization data of compounds 3a-u

¹H and ¹³C NMR Spectra of all compounds 3a-u

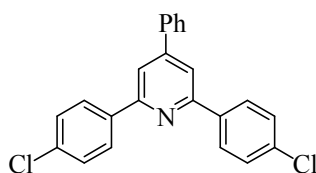
Characterization data of compounds 3a-u



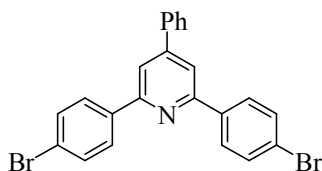
2,4,6-triphenylpyridine (**3a**): white solid; MP: 133-134 °C (lit.^[22] 134-135 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.25 (4H, d, *J* = 7.8 Hz), 7.95 (2H, s), 7.81 (2H, d, *J* = 7.2 Hz), 7.55-7.60 (6H, m), 7.53 (1H, d, *J* = 7.2 Hz), 7.48 (2H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 150.4, 139.5, 139.0, 129.18, 129.16, 129.1, 128.8, 127.2, 117.3. Anal. Calcd for C₂₃H₁₇N: C, 89.90; H, 5.54; N, 4.56. Found: C, 89.65; H, 5.33; N, 4.75.



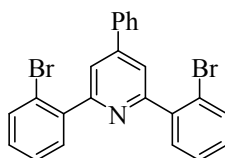
2,6-bis(4-methylphenyl)-4-phenylpyridine (**3b**): white solid; MP: 159-160 °C (lit.^[7] 158-159 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.16 (4H, s), 7.88-7.89 (2H, m), 7.79 (2H, d, *J* = 4.8 Hz), 7.57 (2H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz), 7.51 (1H, dd, *J* = 6.6 Hz, *J* = 7.8 Hz), 7.37 (4H, m), 2.48 (6H, s); ¹³C NMR (100 MHz, CDCl₃) δ 157.4, 150.1, 139.3, 139.0, 136.9, 129.5, 129.1, 128.9, 127.2, 127.1, 116.6, 21.4. Anal. Calcd for C₂₅H₂₁N: C, 89.55; H, 6.27; N, 4.18. Found: C, 89.31; H, 6.03; N, 4.40.



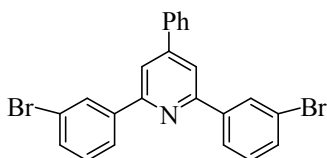
2,6-bis(4-chlorophenyl)-4-phenylpyridine (**3c**): white solid; MP: 184-185 °C (lit.^[22] 186-187 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.16 (4H, d, *J* = 8.4 Hz), 7.87 (2H, s), 7.76 (2H, d, *J* = 7.2 Hz), 7.57 (2H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.50-7.53 (5H, m); ¹³C NMR (100 MHz, CDCl₃) δ 156.3, 150.7, 138.6, 137.6, 135.4, 129.3, 129.2, 128.9, 128.4, 127.2, 117.2. Anal. Calcd for C₂₃H₁₅NCl₂: C, 73.40; H, 3.99; N, 3.72. Found: C, 73.59; H, 3.75; N, 3.94.



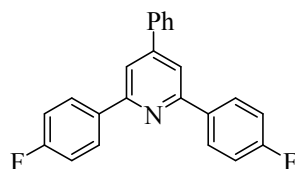
2,6-bis(4-bromophenyl)-4-phenylpyridine (**3d**): white solid; MP: 106-108 °C (lit.^[19] 104-106 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.09 (4H, d, *J* = 6.6 Hz), 7.90 (2H, s), 7.77 (2H, d, *J* = 6.0 Hz), 7.68 (4H, d, *J* = 6.6 Hz), 7.57 (2H, dd, *J* = 6.6 Hz, *J* = 7.2 Hz), 7.53 (1H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 156.4, 150.7, 138.6, 138.1(2C), 131.9, 129.3, 129.2, 128.7, 127.3, 123.7, 117.3. Anal. Calcd for C₂₃H₁₅NBr₂: C, 59.38; H, 3.23; N, 3.01. Found: C, 59.61; H, 3.44; N, 2.75.



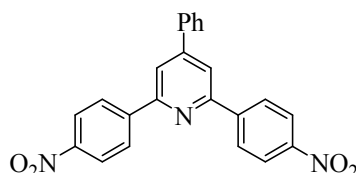
2,6-bis(2-bromophenyl)-4-phenylpyridine (**3e**): white solid; MP: 162-164 °C (lit.^[13] 161-164 °C); ¹H NMR (400 MHz, CDCl₃) δ 7.88 (2H, s), 7.79-7.80 (2H, m), 7.73-7.75 (4H, m), 7.55 (2H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.50 (1H, d, *J* = 7.2 Hz), 7.46 (2H, ddd, *J* = 7.2 Hz, *J* = 0.6 Hz), 7.30 (2H, ddd, *J* = 7.8 Hz, *J* = 1.8 Hz); ¹³C NMR(10 MHz, CDCl₃) δ 158.4, 148.3, 141.2, 138.2, 133.4, 131.8, 129.8, 129.22, 129.20, 127.7, 127.3, 122.0, 121.5. Anal. Calcd for C₂₃H₁₅NBr₂: C, 59.38; H, 3.23; N, 3.01. Found: C, 59.11; H, 3.01; N, 3.25.



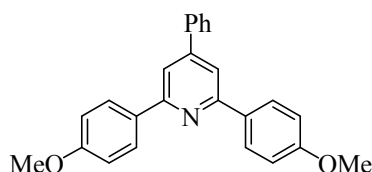
2,6-bis(3-bromophenyl)-4-phenylpyridine (**3f**): white solid; MP: 174-176 °C (lit.^[13] 175-177 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.34 (2H, s), 8.14 (2H, d, *J* = 7.8 Hz), 7.88 (2H, s), 7.76 (2H, d, *J* = 7.2 Hz), 7.61 (2H, dd, *J* = 7.8 Hz, *J* = 1.2 Hz), 7.57 (2H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.53 (1H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.42 (2H, dd, *J* = 7.8 Hz, *J* = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 156.1, 150.7, 141.3, 138.5, 132.1, 130.3, 130.2, 129.32, 129.25, 127.2, 125.8, 123.1, 117.7. Anal. Calcd for C₂₃H₁₅NBr₂: C, 59.38; H, 3.23; N, 3.01. Found: C, 59.69; H, 3.42; N, 3.28.



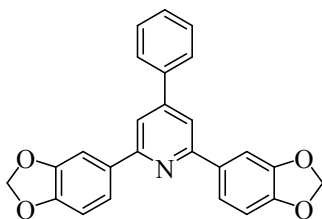
2,6-bis(4-fluorophenyl)-4-phenylpyridine (**3g**): white solid; MP: 102-104 °C (lit.^[7] 100-102 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.19–8.22 (4H, m), 7.85 (2H, d, *J* = 6.0 Hz), 7.76 (2H, d, *J* = 7.2 Hz), 7.57 (2H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz), 7.52 (1H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz), 7.23 (4H, dd, *J* = 8.6 Hz, *J* = 8.4 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 163.7, 156.5, 150.5, 138.8, 135.6, 129.2, 129.1, 128.94, 128.89, 127.2, 116.7, 115.7. Anal. Calcd for C₂₃H₁₅NF₂: C, 80.47; H, 4.37; N, 4.08. Found: C, 80.66; H, 4.59; N, 3.84.



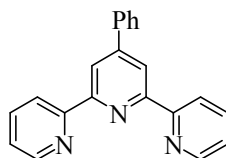
2,6-bis(4-nitrophenyl)-4-phenylpyridine (**3h**): white solid; MP: 315-316 °C (lit.^[19] 316-318 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.39-8.43 (8H, m), 8.08 (2H, s), 7.80 (2H, d, *J* = 8.4 Hz), 7.61(2H, dd, *J* = 7.2 Hz, *J* = 7.2 Hz), 7.56-7.58 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 155.5, 151.4, 148.5, 144.8, 137.9, 129.7, 129.4, 128.0, 127.2, 124.1, 119.1. Anal. Calcd for C₂₃H₁₅N₃O₄: C, 69.52; H, 3.78; N, 10.58. Found: C, 69.76; H, 3.53; N, 10.77.



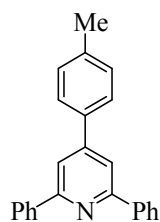
2,6-bis(4-methoxyphenyl)-4-phenylpyridine (**3i**): white solid; MP: 125-126 °C (lit.^[22] 124-125 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.20 (4H, d, *J* = 8.4 Hz), 7.81 (2H, s), 7.77 (2H, d, *J* = 7.2 Hz), 7.54-7.57 (2H, m), 7.49-7.51 (1H, m), 7.08 (4H, d, *J* = 8.4 Hz), 3.92 (6H, s); ¹³C NMR (100 MHz, CDCl₃) δ 160.5, 157.0, 150.1, 139.4, 132.3, 129.1, 128.9, 128.4, 127.2, 115.7, 114.1, 55.4. Anal. Calcd for C₂₅H₂₁NO₂: C, 81.74; H, 5.72; N, 3.81. Found: C, 81.53; H, 5.49; N, 4.07.



2,6-bis(benzo[d][1,3]dioxol-5-yl)-4-phenylpyridine (**3j**): white solid; MP: 140-142 °C (lit.^[6] 141-143 °C); ¹H NMR (400 MHz, CDCl₃) δ 7.77 (2H, d, *J* = 1.8 Hz), 7.76 (2H, s), 7.75 (2H, d, *J* = 9.6 Hz), 7.71 (2H, dd, *J* = 8.4 Hz, *J* = 1.8 Hz), 7.55 (2H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.50 (1H, dd, *J* = 7.8 Hz, *J* = 7.2 Hz), 6.97 (1H, s), 6.95 (1H, s), 6.06 (4H, s); ¹³C NMR (100 MHz, CDCl₃) δ 156.7, 150.2, 148.5, 148.3, 139.1, 134.0, 129.1, 129.0, 127.2, 121.1, 116.1, 108.4, 107.6, 101.3. Anal. Calcd for C₂₅H₁₇NO₄: C, 75.95; H, 4.30; N, 3.54. Found: C, 75.71; H, 4.59; N, 3.24.

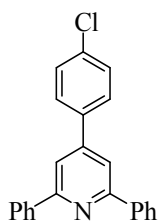


2,6-bis(2-pyridyl)-4-phenylpyridine (**3k**): yellow solid; MP: 207-209 °C (lit.^[6] 208-210 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.77 (2H, s), 8.76 (2H, d, *J* = 4.2 Hz), 8.70 (2H, d, *J* = 7.8 Hz), 7.93-7.94 (2H, m), 7.87-7.90 (2H, m), 7.53 (2H, dd, *J* = 7.2 Hz, *J* = 7.8 Hz), 7.47 (1H, dd, *J* = 7.8 Hz, *J* = 7.2 Hz), 7.36 (2H, dd, *J* = 7.2 Hz, *J* = 4.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 156.3, 155.9, 150.3, 149.1, 138.5, 136.9, 129.0, 128.9, 127.4, 123.8, 121.4, 119.0. Anal. Calcd for C₂₁H₁₅N₃: C, 81.55; H, 4.85; N, 13.59. Found: C, 81.79; H, 4.68; N, 13.75.

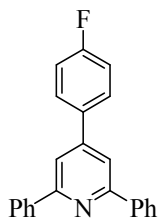


2,6-diphenyl-4-(4-methylphenyl)pyridine (**3l**): yellow solid; MP: 116-117 °C (lit.^[22] 117-118 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.20 (4H, d, *J* = 7.6 Hz), 7.88 (2H, s), 7.65 (2H, d, *J* = 8.0 Hz), 7.51 (4H, t, *J* = 7.6 Hz), 7.44 (2H, t, *J* = 7.0 Hz), 7.33 (2H, d, *J* = 8.2 Hz), 2.44 (1H, s); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 150.1, 139.7, 139.1, 136.1, 129.8, 129.0, 128.7, 127.2, 127.0, 116.9,

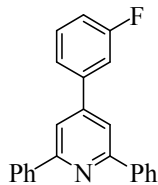
21.3. Anal. Calcd for C₂₄H₁₉N: C, 89.72; H, 5.92; N, 4.36. Found: C, 89.41; H, 5.70; N, 4.57.



4-(4-chlorophenyl)-2,6-diphenylpyridine (**3m**): white solid; MP: 126-127 °C (lit.^[22] 124-126 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.16-8.26 (4H, m), 7.83-7.89 (m, 2H), 7.67-7.75 (m, 2H), 7.43-7.60 (m, 8H); ¹³C NMR (100 MHz, CDCl₃) δ 157.7, 149.0, 139.4, 137.5, 135.2, 129.3, 129.2, 128.7, 128.5, 127.1, 116.8. Anal. Calcd for C₂₃H₁₆NCl: C, 80.82; H, 4.69; N, 4.10. Found: C, 80.58; H, 4.51; N, 4.33.

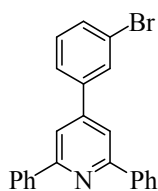


2,6-diphenyl-4-(4-fluorophenyl)pyridine (**3n**): white solid; MP: 128-129 °C (lit.^[17] 127-128 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.23 (4H, d, *J* = 7.8 Hz), 7.87 (2H, s), 7.75 (2H, dd, *J* = 7.9 Hz, *J* = 5.5 Hz), 7.55 (4H, t, *J* = 7.6 Hz), 7.48 (2H, t, *J* = 6.8 Hz), 7.26 (2H, dd, *J* = 15.0 Hz, *J* = 6.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 163.4, 157.6, 149.2, 139.5, 135.2, 129.1, 128.9, 128.7, 127.1, 116.9, 116.1. Anal. Calcd for C₂₃H₁₆NF: C, 84.92; H, 4.92; N, 4.31. Found: C, 84.61; H, 4.67; N, 4.59.

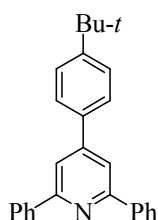


2,6-diphenyl-4-(3-fluorophenyl)pyridine (**3o**): white solid; MP: 137-138 °C (lit.^[4] 136-137 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.25 (4H, d, *J* = 7.3 Hz), 7.89 (2H, s), 7.45-7.60 (9H, m), 7.21 (1H, t, *J* = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 163.3, 157.7, 157.7, 148.9, 141.3, 139.4, 139.4, 130.72, 129.2, 129.2, 128.8, 128.8, 127.2, 127.2, 122.9, 116.9, 116.9, 115.8, 114.2. Anal. Calcd

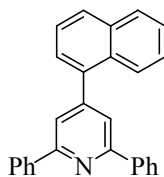
for C₂₃H₁₆NF: C, 84.92; H, 4.92; N, 4.31. Found: C, 84.73; H, 4.71; N, 4.59.



4-(3-bromophenyl)-2,6-diphenylpyridine (**3p**): white solid; MP: 135-136 °C (lit.^[13] 135-136 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.24 (4H, d, *J* = 7.6 Hz), 7.91 (1H, s), 7.86 (2H, s), 7.69 (1H, d, *J* = 7.5 Hz), 7.64 (1H, d, *J* = 7.89 Hz), 7.56 (4H, t, *J* = 7.4 Hz), 7.46-7.51 (2H, m), 7.42 (1H, t, *J* = 7.8 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 157.7, 157.7, 148.7, 141.2, 139.3, 139.3, 131.9, 130.6, 130.2, 129.2, 129.2, 128.8, 128.8, 127.2, 127.2, 125.8, 123.3, 116.9, 116.9. Anal. Calcd for C₂₃H₁₆NBr: C, 71.52; H, 4.15; N, 3.63. Found: C, 71.29; H, 4.41; N, 6.78.

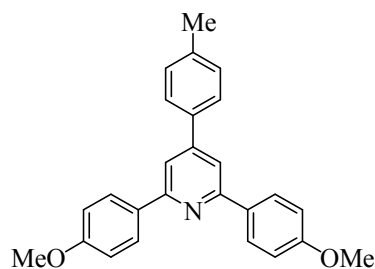


2,6-diphenyl-4-[4-(*tert*-butyl)phenyl]pyridine (**3q**): yellow oil (lit.^[4]); ¹H NMR (400 MHz, CDCl₃) δ 8.23 (4H, d, *J* = 8.0 Hz), 7.92 (2H, s), 7.73 (2H, d, *J* = 8.0 Hz), 7.52-7.62 (6H, m), 7.43-7.50 (2H, m), 1.43 (9H, s); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 152.3, 150.0, 139.7, 136.1, 129.0, 128.7, 127.1, 126.9, 126.1, 117.0, 34.8, 31.3, 31.3, 31.3. Anal. Calcd for C₂₇H₂₅N: C, 89.26; H, 6.89; N, 3.86. Found: C, 89.01; H, 6.62; N, 4.09.

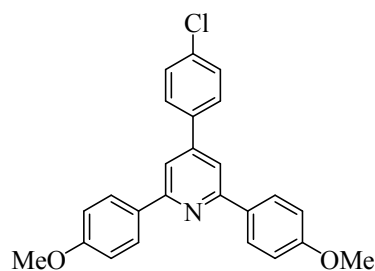


2,6-diphenyl-4-(naphthalen-1-yl)pyridine (**3r**): white solid; MP: 132-133 °C (lit.^[4] 133-134 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.28(5H, d, *J* = 7.3 Hz), 7.96-8.08 (4H, m), 7.93-7.96 (1H, m), 7.90 (1H, dd, *J* = 8.5, 1.5 Hz), 7.53-7.62 (6H, m), 7.49 (2H, t, *J* = 7.3 Hz); ¹³C NMR (100 MHz, CDCl₃) δ 157.6, 150.1, 139.6, 136.4, 133.6, 133.5, 129.1, 129.0, 128.7, 128.5, 127.8, 127.2, 126.8, 126.7, 126.5, 124.9, 117.3. Anal. Calcd for C₂₇H₁₉N: C, 90.76; H, 5.32; N, 3.92. Found: C, 90.48;

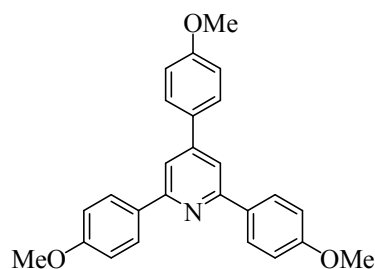
H, 5.04; N, 4.15.



2,6-bis(4-methoxyphenyl)-4-(4-methylphenyl)pyridine (**3s**): white solid; MP: 129-130 °C (lit.^[22] 128-129 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.20 (4H, d, *J* = 8.4 Hz), 7.79 (2H, s), 7.68 (2H, d, *J* = 7.8 Hz), 7.37 (2H, d, *J* = 7.8 Hz), 7.08 (4H, d, *J* = 9.0 Hz), 3.92 (6H, s), 2.47 (3H, s); ¹³C NMR (100 MHz, CDCl₃) δ 160.5, 156.9, 149.9, 138.9, 136.4, 132.4, 129.8, 128.4, 127.0, 115.5, 114.0, 55.4, 21.3. Anal. Calcd for C₂₆H₂₃NO₂: C, 81.89; H, 6.04; N, 3.67. Found: C, 81.62; H, 6.32; N, 3.43.



2,6-bis(4-methoxyphenyl)-4-(4-chlorophenyl)pyridine (**3t**): white solid; MP: 115-117 °C (lit.^[13] 113-115 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.18 (4H, d, *J* = 8.6 Hz), 7.73 (2H, s), 7.68 (2H, d, *J* = 7.9 Hz), 7.52 (2H, d, *J* = 8.2 Hz), 7.05-7.07 (4H, m), 3.91 (6H, s); ¹³C NMR (100 MHz, CDCl₃) δ 160.6, 157.0, 148.8, 137.7, 135.1, 132.0, 129.3, 128.45, 128.44, 115.4, 114.1, 55.4. Anal. Calcd for C₂₅H₂₀NO₂Cl: C, 74.72; H, 4.98; N, 3.49. Found: C, 74.51; H, 4.72; N, 3.68.



2,4,6-tris(4-methoxyphenyl)pyridine (**3u**): white solid; white solid; MP: 133-134 °C (lit.^[22] 134-135 °C); ¹H NMR (400 MHz, CDCl₃) δ 8.19 (4H, d, *J* = 8.6 Hz), 7.77 (2H, s), 7.73 (2H, d, *J*

= 8.6 Hz), 7.05-7.08 (6H, m), 3.91 (9H, s); ^{13}C NMR (100 MHz, CDCl_3) δ 160.5 160.4, 156.9, 149.5, 132.4, 131.6, 128.4, 128.3, 115.3, 114.5, 114.0, 55.44, 55.39. Anal. Calcd for $\text{C}_{26}\text{H}_{23}\text{NO}_3$: C, 78.59; H, 5.79; N, 3.53. Found: C, 78.31; H, 5.55; N, 3.75.

^1H and ^{13}C NMR Spectra of all compounds 3a-u

