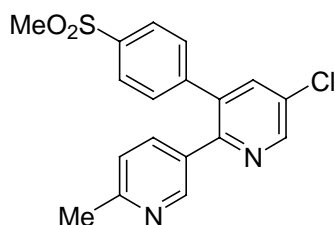


Supporting Information: Annulation of Ketones with Vinamidinium Hexafluorophosphate Salts: An Efficient Preparation of Trisubstituted Pyridines

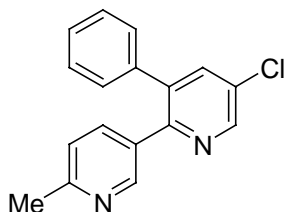
Jean-François Marcoux,* Edward G. Corley,* Kai Rossen, Phil Pye, Jimmy Wu, Michael A. Robbins, Ian W. Davies, Robert D. Larsen, and Paul J. Reider

Department of Process Research, Merck & Co., Inc., P.O. Box 2000, Rahway, NJ 07065

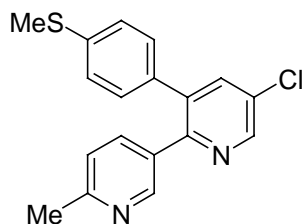
Characterization Data



Data for Table 1, Entry 1. ^1H NMR (400 MHz, CDCl_3) δ 8.71 (d, $J = 2$ Hz, 1H), 8.38 (d, $J = 2$ Hz, 1H), 7.88-7.92 (m, 2H), 7.73 (d, $J = 2$ Hz, 1H), 7.55 (dd, $J = 8, 2$ Hz, 1H), 7.39 (d, $J = 8$ Hz, 2H), 7.08 (d, $J = 8$ Hz, 1H), 3.08 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 158.3, 152.2, 149.7, 148.2, 143.6, 140.0, 137.8, 137.2, 135.2, 131.1, 130.9, 130.2, 127.7, 122.6, 44.3, 24.1. LC-MS ($\text{M}^+ + 1$) 360.0.

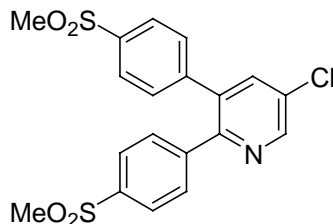


Data for Table 1, Entry 2. ^1H NMR (400 MHz, CDCl_3) δ 8.65 (d, $J = 2$ Hz, 1H), 8.44 (d, $J = 2$ Hz, 1H), 7.73 (d, $J = 2$ Hz, 1H), 7.55 (dd, $J = 8, 2$ Hz, 1H), 7.30-7.34 (m, 3H), 7.14-7.19 (m, 2H), 7.03 (d, $J = 8$ Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 157.8, 152.3, 149.8, 147.3, 138.0, 138.0, 137.4, 137.4, 132.0, 130.8, 129.3, 128.8, 128.1, 122.4, 24.1. LC-MS ($\text{M}^+ + 1$) 282.1.

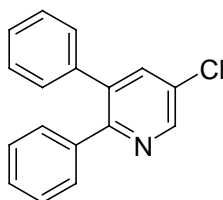


Data for Table 1, Entry 3. ^1H NMR (400 MHz, CDCl_3) δ 8.64 (d, $J = 2$ Hz, 1H), 8.48 (d, $J = 2$ Hz, 1H), 7.72 (d, $J = 2$ Hz, 1H), 7.60 (dd, $J = 8, 2$ Hz, 1H), 7.17-7.20 (m, 2H), 7.05-7.12 (m, 3H), 3.56 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 157.7, 152.0,

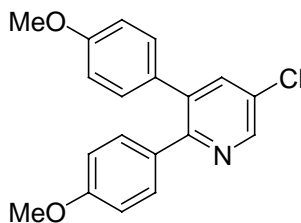
149.5, 147.3, 139.3, 137.9, 137.6, 136.8, 134.3, 132.2, 131.0, 129.6, 126.4, 122.7, 24.0, 15.3. LC-MS ($M^+ + 1$) 328.1.



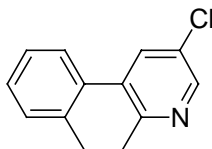
Data for Table 1, Entry 4. ^1H NMR (400 MHz, CDCl_3) δ 8.75 (d, $J = 2$ Hz, 1H), 7.93 (d, $J = 8$ Hz, 2H), 7.87 (d, $J = 8$ Hz, 2H), 7.78 (d, $J = 2$ Hz, 1H), 7.53 (d, $J = 8$ Hz, 2H), 7.41 (d, $J = 8$ Hz, 2H), 3.11 (s, 3H), 3.06 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 153.1, 148.4, 143.8, 143.3, 140.6, 140.5, 138.2, 135.5, 131.8, 130.7, 130.3, 128.0, 127.4, 44.4, 44.4. LC-MS ($M^+ + 1$) 422.0.



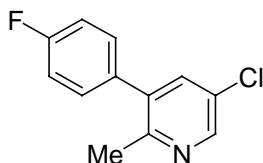
Data for Table 1, Entry 5. ^1H NMR (300 MHz, CDCl_3) δ 8.64 (s, 1H), 7.72 (d, $J = 2$ Hz, 1H), 7.14-7.32 (m, 10H); ^{13}C NMR (75 MHz CDCl_3) δ 155.3, 146.9, 139.0, 138.6, 137.9, 137.1, 130.3, 129.8, 129.4, 128.5, 128.1, 127.9, 127.7. LC-MS ($M^+ + 1$) 266.9.



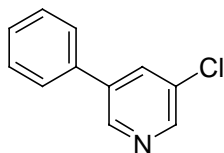
Data for Table 1, Entry 6. ^1H NMR (300 MHz, CDCl_3) δ 8.50 (d, $J = 2$ Hz, 1H), 7.77 (d, $J = 2$ Hz, 1H), 7.41-7.49 (m, 3H), 7.27 (d, $J = 8$ Hz, 1H), 7.08 (d, $J = 8$ Hz, 2H), 7.02 (d, $J = 2$ Hz, 2H), 4.73 (s, 3H), 4.68 (s, 3H); ^{13}C NMR (75 MHz CDCl_3) δ 159.5, 159.2, 154.9, 146.5, 137.9, 136.4, 131.7, 131.1, 131.1, 130.5, 129.8, 114.0, 113.5, 55.3, 55.2. LC-MS ($M^+ + 1$) 326.1.



Data for Table 1, Entry 7. ^1H NMR (300 MHz, CDCl_3) δ 8.37 (bs, 1H), 7.96 (d, $J = 2$ Hz, 1H), 7.61-7.68 (m, 1H), 7.24-7.36 (m, 3H), 2.89-3.13 (m, 4H); ^{13}C NMR (75 MHz CDCl_3) δ 155.6, 146.1, 136.8, 131.6, 130.8, 130.3, 130.1, 128.9, 128.3, 127.2, 123.8, 30.9, 28.3. LC-MS ($M^+ + 1$) 217.1.

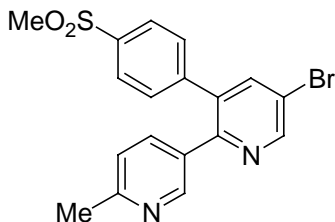


Data for Table 1, Entry 8. ^1H NMR (300 MHz, CDCl_3) δ 8.45 (s, 1H), 7.49 (s, 1H), 7.21-7.28 (m, 2H), 7.10-7.16 (m, 2H), 2.45 (s, 3H); ^{13}C NMR (75 MHz CDCl_3) δ 147.1, 145.9, 137.7, 136.2, 133.9, 132.0, 129.1, 128.6, 127.0. LC-MS (M^+ +1) 223.1.

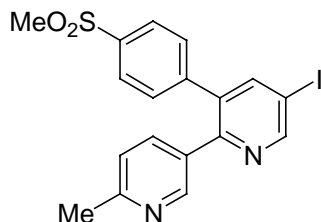


Data for Table 1, Entry 9. ^1H NMR (300 MHz, CDCl_3) δ 8.69 (d, $J=2$ Hz, 1H), 8.52 (d, $J=2$ Hz, 1H), 7.82 (t, $J=2$ Hz, 1H), 7.36-7.55 (m, 5H); ^{13}C NMR (75 MHz CDCl_3) δ 147.1, 145.9, 137.7, 136.2, 133.9, 132.0, 129.1, 128.6, 127.0. LC-MS (M^+ +1) 191.1.

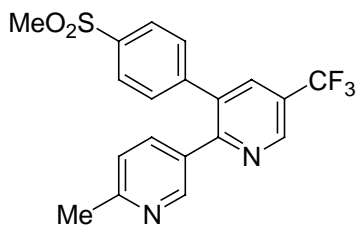
Data for Table 2, Entry 1, see Data for Table 1, Entry 1.



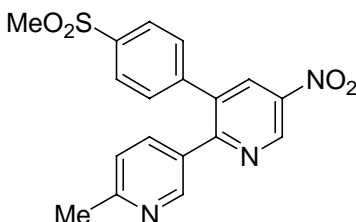
Data for Table 2, Entry 2. ^1H NMR (400 MHz, CDCl_3) δ 8.82 (s, 1H), 8.40 (s, 1H), 7.88-7.94 (m, 3H), 7.59 (d, $J=8$ Hz, 1H), 7.41 (d, $J=7$ Hz, 2H), 7.11 (d, $J=8$ Hz, 1H), 3.10 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 158.5, 152.6, 150.6, 149.6, 143.7, 140.7, 140.3, 137.4, 135.7, 131.3, 130.4, 128.0, 122.9, 119.7, 44.5, 24.2. LC-MS (M^+ +1) 404.0.



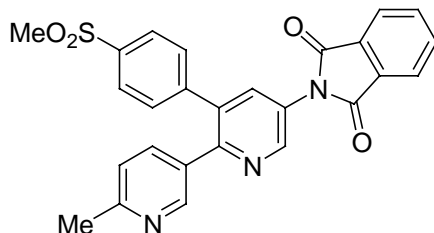
Data for Table 2, Entry 3. ^1H NMR (400 MHz, CDCl_3) δ 9.06 (s, 1H), 8.41 (s, 1H), 7.87-7.93 (m, 3H), 7.58 (d, $J=8$ Hz, 1H), 7.41 (d, $J=7$ Hz, 2H), 7.13 (d, $J=8$ Hz, 1H), 3.10 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 158.6, 152.3, 150.1, 148.7, 143.6, 140.3, 139.1, 137.1, 135.5, 131.1, 130.6, 128.1, 122.8, 121.4, 44.4, 24.1. LC-MS (M^+ +1) 451.1.



Data for Table 2, Entry 4. ^1H NMR (400 MHz, CDCl_3) δ 9.03 (s, 1H), 8.46 (s, 1H), 7.92-7.98 (m, 3H), 7.63 (d, J = 8 Hz, 1H), 7.43-7.49 (m, 2H), 7.13 (d, J = 8 Hz, 1H), 3.10 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 158.9, 157.3, 149.5, 146.2, 146.2, 143.5, 140.5, 137.7, 135.6, 134.3, 131.2, 130.0, 128.0, 123.0, 44.4, 24.0, -0.1. LC-MS (M^+ +1) 393.1.



Data for Table 2, Entry 5. ^1H NMR (400 MHz, CDCl_3) δ 9.52 (d, J = 2 Hz, 1H), 8.51 (d, J = 2 Hz, 1H), 7.95 (d, J = 8 Hz, 2H), 7.62 (dd, J = 8, 2 Hz, 1H), 7.43-7.49 (m, 3H), 7.12 (d, J = 8 Hz, 1H), 3.09 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 159.8, 159.5, 149.9, 144.3, 142.8, 142.8, 140.7, 137.5, 134.7, 133.4, 130.5, 130.4, 128.1, 122.8, 44.4, 24.3. LC-MS (M^+ +1) 370.1.



Data for Table 2, Entry 6. ^1H NMR (400 MHz, CDCl_3) δ 8.98 (d, J = 2 Hz, 1H), 8.48 (d, J = 2 Hz, 1H), 8.02 (dd, J = 5, 3 Hz, 2H), 7.90-7.94 (m, 3H), 7.87 (dd, J = 5, 3 Hz, 2H), 7.67 (dd, J = 8, 2 Hz, 1H), 7.48 (dd, J = 7, 2 Hz, 2H), 7.67 (d, J = 8 Hz, 1H), 3.10 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz CDCl_3) δ 173.7, 166.6, 158.3, 152.9, 149.7, 146.5, 144.1, 140.0, 137.6, 135.5, 134.9, 134.5, 131.6, 130.5, 127.9, 127.8, 124.1, 122.9, 44.4, 24.0. LC-MS (M^+ +1) 470.0.