

Supporting Information

Base-catalyzed cascade synthesis of 2,3-dihydrofuro- [2,3-*b*]pyridines and 2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridines from *N*-propargylic β -enaminones

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General Information

All of the chemicals were obtained from commercially-available sources or prepared according to standard methods. ^1H , ^{19}F and ^{13}C NMR spectra were recorded using a Bruker AV 400 MHz NMR spectrometer. TMS was used as an internal standard. Chemical shifts were reported in ppm downfield from CDCl_3 ($\delta = 7.26$ ppm) or $\text{DMSO-}d_6$ ($\delta = 2.50$ ppm) for ^1H NMR and relative to the central CDCl_3 or $\text{DMSO-}d_6$ resonance ($\delta = 77.0$ ppm or 39.5 ppm) for ^{13}C NMR spectroscopy. Multiplicities were reported as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd) and doublet of triplets (dt). Coupling constants (J) were reported in Hertz (Hz). Melting points were measured on a RY-I apparatus and uncorrected. HRMS were recorded on an IonSpec FT-ICR mass spectrometer with Electron Spray Ionization (ESI) resource.

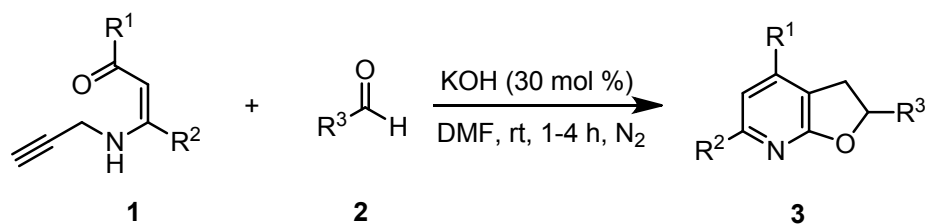
General Procedure for the Preparation *N*-propargyl β -enaminones

All the *N*-propargyl β -enaminones (**1**) were prepared according to the literature procedure¹.

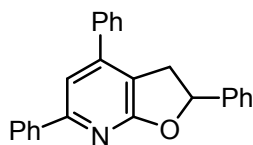
General procedure for the synthesis of *N*-sulfonyl imines

All the *N*-sulfonyl imines (**4**) were prepared according to the literature procedure².

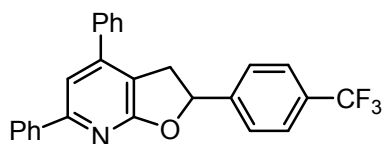
Experimental Procedures and Data for Compounds **3**



A mixture of *N*-propargylic β -enaminones **1** (0.4 mmol), arylaldehydes **2** (0.4 mmol), and KOH (8 mg, 0.12 mmol, 0.3 equiv) in DMF (3 mL) was stirred at room temperature under N_2 for 1-4 h. After **1** was disappeared completely (monitored by TLC), the residue dissolved in H_2O (10 mL) and extracted with EtOAc (3 x 10 mL). The combined EtOAc extracts were dried over Na_2SO_4 and concentrated. Then the solvent was evaporated and the residue was purified by chromatography (silica gel, 1% EtOAc in PE) to give **3**.

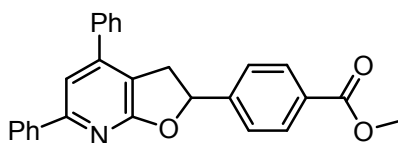


2,4,6-Triphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3a**). Pale yellow solid; 99.2 mg (71% yield); mp 140-141 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.08 (d, $J = 7.2$ Hz, 2H, ArH), 7.56 (d, $J = 7.0$ Hz, 2H, ArH), 7.50-7.37 (m, 11H, ArH), 7.33 (t, $J = 7.2$ Hz, 1H, ArH), 5.90 (t, $J = 8.6$ Hz, 1H, CH), 3.84 (dd, $J = 16.4, 9.4$ Hz, 1H, CH_2), 3.39 (dd, $J = 16.3, 7.8$ Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.7, 155.9, 147.5, 141.3, 138.9, 138.0, 128.8, 128.8, 128.7, 128.7, 128.6, 128.1, 127.7, 126.8, 125.4, 115.2, 113.5, 81.8, 37.1; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{25}H_{20}NO$: 350.1545, found: 350.1543.

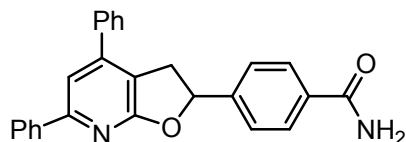


4,6-Diphenyl-2-(4-(trifluoromethyl)phenyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3b**).

Yellow solid; 130.2 mg (78% yield); mp 113-114 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (dd, *J* = 8.5, 1.5 Hz, 2H, ArH), 7.65 (d, *J* = 8.3 Hz, 2H, ArH), 7.59 (d, *J* = 8.4 Hz, 2H, ArH), 7.54 (dd, *J* = 8.2, 1.5 Hz, 2H, ArH), 7.51-7.39 (m, 7H, ArH), 5.96 (t, *J* = 8.5 Hz, 1H, CH), 3.90 (dd, *J* = 16.3, 9.5 Hz, 1H, CH₂), 3.35 (dd, *J* = 16.3, 7.7 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.5, 156.1, 147.8, 145.4, 138.7, 137.8, 130.2 (q, *J*_{C-F} = 32.8 Hz), 129.0, 128.9, 128.8, 128.6, 127.7, 126.8, 125.7 (q, *J*_{C-F} = 3.8 Hz), 125.7, 124.0 (q, *J*_{C-F} = 270.6 Hz), 114.6, 113.8, 80.8, 37.1; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₁₉F₃NO: 418.1419, found: 418.1421.

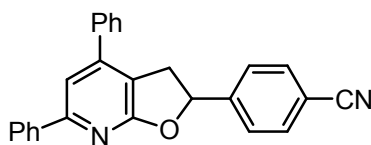


Methyl 4-(4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridin-2-yl)benzoate (**3c**). Pale yellow solid; 123.8 mg (76% yield); mp 157-158 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08-8.04 (m, 4H, ArH), 7.54 (d, *J* = 7.9 Hz, 4H, ArH), 7.49-7.38 (m, 7H, ArH), 5.93 (t, *J* = 8.6 Hz, 1H, CH), 3.91 (s, 3H, OCH₃), 3.86 (dd, *J* = 16.4, 9.6 Hz, 1H, CH₂), 3.33 (dd, *J* = 16.3, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): 168.5, 166.6, 156.0, 147.6, 146.3, 138.7, 137.8, 130.0, 129.8, 128.9, 128.8, 128.8, 128.6, 127.6, 126.8, 125.3, 114.7, 113.7, 81.1, 52.1, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₇H₂₂NO₃: 408.1600, found: 408.1593.

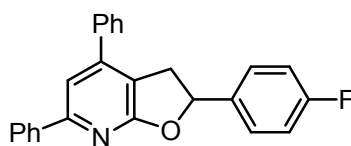


4-(4,6-Diphenyl-2,3-dihydrofuro[2,3-*b*]pyridin-2-yl)benzamide (**3d**). Pale yellow solid; 116.1 mg (74% yield); mp 164-165 °C; ¹H NMR (DMSO-*d*₆, 400 MHz) δ 8.12 (d, *J* = 7.6 Hz, 2H, ArH), 8.01 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 2H, ArH), 7.76 (d, *J* = 7.4 Hz, 1H, ArH), 7.65 (s, 1H, ArH), 7.55 (d, *J* = 7.8 Hz, 2H, ArH), 7.52 (d, *J* = 7.8 Hz, 2H, ArH), 7.48 (d, *J* = 7.5 Hz, 2H, ArH), 7.44-7.39 (m, 2H, ArH), 5.99 (t, *J* = 8.5 Hz,

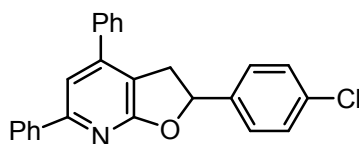
1H, CH), 3.94 (dd, $J = 16.4, 9.4$ Hz, 1H, CH₂), 3.38 (dd, $J = 16.3, 8.0$ Hz, 1H, CH₂); ¹³C NMR (DMSO-*d*₆, 100 MHz): δ 168.3, 167.5, 154.5, 146.9, 144.2, 138.3, 137.2, 134.0, 128.9, 128.9, 128.9, 128.7, 128.0, 127.9, 126.5, 125.5, 115.8, 113.0, 80.9, 36.2; HRMS (ESI) m/z [M + H]⁺ calculated for C₂₆H₂₁N₂O₂: 393.1603, found: 393.1596.



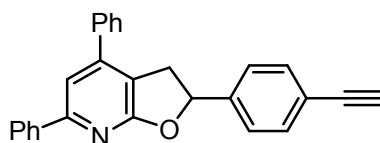
4-(4,6-Diphenyl-2,3-dihydrofuro[2,3-*b*]pyridin-2-yl)benzonitrile (**3e**). Yellow solid; 107.8 mg (72% yield); mp 138-139 °C; ¹H NMR (DMSO, 400 MHz) δ 8.06 (d, $J = 7.2$ Hz, 2H, ArH), 7.67 (d, $J = 8.1$ Hz, 2H, ArH), 7.57 (d, $J = 8.1$ Hz, 2H, ArH), 7.54-7.39 (m, 9H, ArH), 5.92 (t, $J = 8.5$ Hz, 1H, CH), 3.89 (dd, $J = 16.2, 9.6$ Hz, 1H, CH₂), 3.31 (dd, $J = 16.2, 7.6$ Hz, 1H, CH₂); ¹³C NMR (DMSO, 100 MHz): δ 168.3, 156.2, 147.8, 146.6, 138.6, 137.7, 132.5, 129.0, 128.9, 128.9, 128.6, 127.6, 126.8, 126.0, 118.5, 114.3, 113.9, 111.9, 80.5, 36.9; HRMS (ESI) m/z [M + H]⁺ calculated for C₂₆H₁₉N₂O: 375.1497, found: 375.1492.



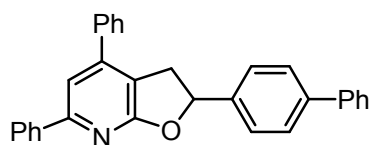
2-(4-Fluorophenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3f**). Yellow solid; 107.2 mg (73% yield); mp 129-130 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (d, $J = 7.4$ Hz, 2H, ArH), 7.55 (d, $J = 7.3$ Hz, 2H, ArH), 7.51-7.40 (m, 9H, ArH), 7.07 (td, $J = 8.4, 1.4$ Hz, 2H, ArH), 5.86 (t, $J = 8.3$ Hz, 1H, CH), 3.81 (dd, $J = 16.3, 9.4$ Hz, 1H, CH₂), 3.35 (dd, $J = 16.3, 7.8$ Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.5, 162.5 (d, $J_{C-F} = 247.3$ Hz), 155.9, 147.5, 138.7, 137.9, 137.0 (d, $J_{C-F} = 3.2$ Hz), 128.9, 128.8, 128.8, 128.6, 127.7, 127.3 (d, $J_{C-F} = 8.0$ Hz), 126.8, 115.5 (d, $J_{C-F} = 21.7$ Hz), 115.0, 113.6, 81.2, 37.1; HRMS (ESI) m/z [M + H]⁺ calculated for C₂₅H₁₉FNO: 368.1451, found: 368.1450.



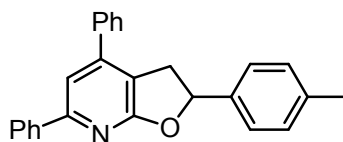
2-(4-Chlorophenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3g**). Yellow solid; 107.4 mg (70% yield); mp 105-106 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (d, *J* = 7.5 Hz, 2H, ArH), 7.55 (d, *J* = 7.3 Hz, 2H, ArH), 7.50-7.39 (m, 9H, ArH), 7.35 (d, *J* = 8.4 Hz, 2H, ArH), 5.86 (t, *J* = 8.5 Hz, 1H, CH), 3.82 (dd, *J* = 16.3, 9.4 Hz, 1H, CH₂), 3.32 (dd, *J* = 16.3, 7.7 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): 168.5, 156.0, 147.6, 139.8, 138.7, 137.8, 133.8, 128.9, 128.8, 128.8, 128.8, 128.6, 127.7, 126.9, 126.8, 114.9, 113.6, 81.0, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₅H₁₉ClNO: 384.1155, found: 384.1162.



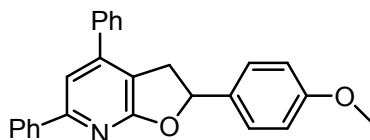
2-(4-Ethynylphenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3h**). Pale yellow solid; 97.1 mg (65% yield); mp 134-135 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (dd, *J* = 7.1, 1.5 Hz, 2H, ArH), 7.55 (dd, *J* = 8.2, 1.3 Hz, 2H, ArH), 7.52-7.49 (m, 4H, ArH), 7.47-7.38 (m, 7H, ArH), 5.90 (t, *J* = 8.5 Hz, 1H, CH), 3.85 (dd, *J* = 16.3, 9.5 Hz, 1H, CH₂), 3.35 (dd, *J* = 16.3, 7.7 Hz, 1H, CH₂), 3.08 (s, 1H, CH); ¹³C NMR (CDCl₃, 100 MHz): δ 168.6, 156.0, 147.6, 142.0, 138.8, 137.9, 132.5, 128.9, 128.9, 128.8, 128.6, 127.7, 126.9, 125.4, 121.9, 114.9, 113.7, 83.2, 81.3, 77.5, 37.1; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₇H₂₀NO: 374.1545, found: 374.1536.



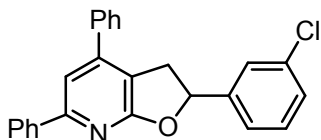
2-([1,1'-Biphenyl]-4-yl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3i**). Yellow solid; 110.6 mg (65% yield); mp 154-155 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.09 (dd, *J* = 7.2, 1.4 Hz, 2H, ArH), 7.62-7.53 (m, 8H, ArH), 7.51-7.38 (m, 9H, ArH), 7.35 (tt, *J* = 7.3, 1.9 Hz, 1H, ArH), 5.95 (t, *J* = 8.5 Hz, 1H, CH), 3.87 (dd, *J* = 16.4, 9.4 Hz, 1H, CH₂), 3.43 (dd, *J* = 16.4, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.7, 155.9, 147.5, 141.0, 140.6, 140.3, 138.8, 138.0, 128.8, 128.8, 128.8, 128.7, 128.6, 127.7, 127.4, 127.4, 127.1, 126.8, 125.9, 115.2, 113.5, 81.6, 37.1; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₁H₂₄NO: 426.1858, found: 426.1851.



4,6-Diphenyl-2-(p-tolyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3j**). Pale yellow solid; 72.7 mg (50% yield); mp 66-67 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (d, *J* = 7.3 Hz, 2H, ArH), 7.56 (d, *J* = 7.0 Hz, 2H, ArH), 7.50-7.40 (m, 7H, ArH), 7.36 (d, *J* = 7.9 Hz, 2H, ArH), 7.19 (d, *J* = 7.8 Hz, 2H, ArH), 5.87 (t, *J* = 8.5 Hz, 1H, CH), 3.80 (dd, *J* = 16.3, 9.3 Hz, 1H, CH₂), 3.38 (dd, *J* = 16.3, 7.8 Hz, 1H, CH₂), 2.36 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 168.8, 155.9, 147.4, 138.9, 138.3, 138.1, 137.9, 129.3, 128.8, 128.8, 128.7, 128.6, 127.7, 126.8, 125.5, 115.4, 113.4, 81.8, 37.1, 21.1; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO: 364.1701, found: 364.1695.

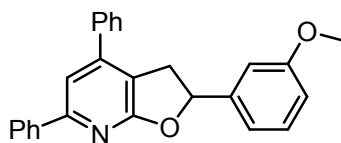


2-(4-Methoxyphenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3k**). Yellow solid; 60.7 mg (40% yield); mp 122-123 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.06 (dd, *J* = 7.2, 1.3 Hz, 2H, ArH), 7.57 (dd, *J* = 6.9, 1.5 Hz, 2H, ArH), 7.50-7.42 (m, 6H, ArH), 7.41-7.38 (m, 3H, ArH), 6.91 (d, *J* = 8.7 Hz, 2H, ArH), 5.84 (t, *J* = 8.6 Hz, 1H, CH), 3.81 (s, 3H, OCH₃), 3.78 (dd, *J* = 16.4, 9.3 Hz, 1H, CH₂), 3.38 (dd, *J* = 16.4, 7.9 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.7, 159.5, 155.8, 147.4, 138.9, 138.1, 133.2, 128.8, 128.8, 128.7, 128.6, 127.7, 127.0, 126.8, 115.4, 114.0, 113.4, 81.8, 55.3, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO₂: 380.1651, found: 380.1650.

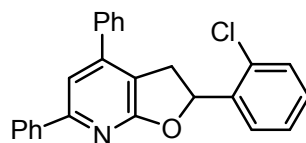


2-(3-Chlorophenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3l**). Pale yellow solid; 104.5 mg (68% yield); mp 87-88 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.06 (d, *J* = 7.4 Hz, 2H, ArH), 7.55 (d, *J* = 7.4 Hz, 2H, ArH), 7.51-7.39 (m, 8H, ArH), 7.35-7.30 (m, 3H, ArH), 5.87 (t, *J* = 8.6 Hz, 1H, CH), 3.85 (dd, *J* = 16.3, 9.5 Hz, 1H, CH₂), 3.35 (dd, *J* = 16.3, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.5, 156.0, 147.6, 143.4, 138.7, 137.8, 134.6, 130.0, 128.9, 128.9, 128.8, 128.6, 128.2, 127.7, 126.8,

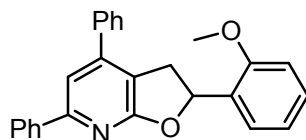
125.6, 123.5, 114.7, 113.7, 80.8, 37.0; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{25}H_{19}ClNO$: 384.1155, found: 384.1160.



2-(3-Methoxyphenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3m**). White solid; 91.0 mg (60% yield); mp 115-116 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.07 (dd, $J = 7.2$, 1.4 Hz, 2H, ArH), 7.56 (dd, $J = 8.4$, 1.6 Hz, 2H, ArH), 7.51-7.39 (m, 7H, ArH), 7.30 (t, $J = 7.9$ Hz, 1H, ArH), 7.05-7.02 (m, 2H, ArH), 6.86 (dd, $J = 8.1$, 2.0 Hz, 1H, ArH), 5.88 (t, $J = 8.6$ Hz, 1H, CH), 3.82 (dd, $J = 16.3$, 9.4 Hz, 1H, CH_2), 3.81 (s, 3H, OCH_3), 3.38 (dd, $J = 16.3$, 8.0 Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.7, 159.8, 155.9, 147.4, 143.0, 138.8, 138.0, 129.7, 128.8, 128.8, 128.7, 128.6, 127.7, 126.8, 117.6, 115.2, 113.6, 113.5, 110.8, 81.6, 55.3, 37.1; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{26}H_{22}NO_2$: 380.1651, found: 380.1648.

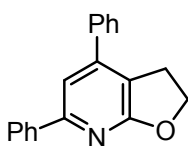


2-(2-Chlorophenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3n**). Yellow solid; 112.1 mg (73% yield); mp 163-164 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.07 (d, $J = 7.2$ Hz, 2H, ArH), 7.69 (dd, $J = 7.4$, 1.7 Hz, 1H, ArH), 7.54 (dd, $J = 7.0$, 1.5 Hz, 2H, ArH), 7.49-7.37 (m, 8H, ArH), 7.31-7.22 (m, 2H, ArH), 6.17 (dd, $J = 9.5$, 7.1 Hz, 1H, CH), 4.04 (dd, $J = 16.6$, 9.6 Hz, 1H, CH_2), 3.23 (dd, $J = 16.6$, 7.0 Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.6, 156.0, 147.8, 139.5, 138.8, 137.9, 130.9, 129.5, 129.0, 128.9, 128.9, 128.8, 128.6, 127.7, 127.1, 126.9, 126.3, 114.8, 113.8, 78.9, 36.2; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{25}H_{19}ClNO$: 384.1155, found: 384.1163.

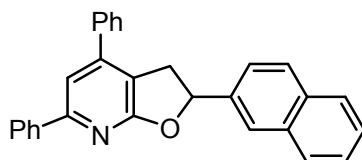


2-(2-Methoxyphenyl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3o**). Pale yellow solid; 75.9 mg (50% yield); mp 152-153 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.08 (dd, $J = 7.2$, 1.4 Hz, 2H, ArH), 7.59 (dd, $J = 7.6$, 0.9 Hz, 1H, ArH), 7.55 (dd, $J = 7.0$, 1.5

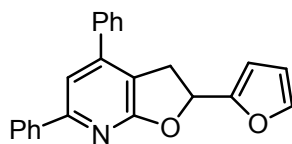
Hz, 2H, ArH), 7.49-7.38 (m, 7H, ArH), 7.28 (td, $J = 7.8, 1.3$ Hz, 1H, ArH), 6.97 (t, $J = 7.3$ Hz, 1H, ArH), 6.90 (d, $J = 8.2$ Hz, 1H, ArH), 6.13 (dd, $J = 9.3, 7.4$ Hz, 1H, CH), 3.90 (dd, $J = 16.6, 9.5$ Hz, 1H, CH₂), 3.84 (s, 3H, OCH₃), 3.22 (dd, $J = 16.6, 7.2$ Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.8, 155.6, 155.5, 147.4, 138.9, 138.1, 130.0, 128.7, 128.7, 128.5, 128.5, 128.5, 127.7, 126.8, 125.5, 120.5, 115.7, 113.3, 110.1, 77.9, 55.2, 36.2; HRMS (ESI) m/z [M + H]⁺ calculated for C₂₆H₂₂NO₂: 380.1651, found: 380.1644.



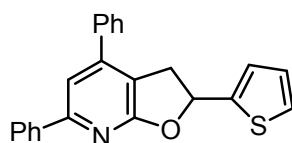
4,6-Diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3p**). Yellow viscous liquid; 28.4 mg (26% yield); ¹H NMR (CDCl₃, 400 MHz): δ 8.03 (dd, $J = 7.9, 1.4$ Hz, 2H, ArH), 7.57 (dd, $J = 7.8, 1.5$ Hz, 1H, ArH), 7.50 (t, $J = 7.3$ Hz, 2H, ArH), 7.46-7.37 (m, 5H, ArH), 4.69 (t, $J = 8.5$ Hz, 2H, CH₂), 3.41 (t, $J = 8.5$ Hz, 2H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): 169.3, 155.6, 147.5, 138.9, 138.2, 128.8, 128.8, 128.7, 128.6, 127.7, 126.8, 115.4, 113.2, 69.1, 28.2; HRMS (ESI) m/z [M + H]⁺ calculated for C₁₉H₁₆NO: 274.1232, found: 274.1231.



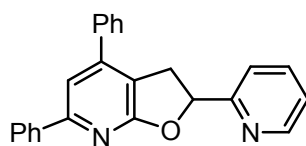
2-(Naphthalen-2-yl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3s**). Yellow solid; 123.0 mg (77% yield); mp 76-77 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.09 (dd, $J = 7.1, 1.4$ Hz, 2H, ArH), 7.97 (s, 1H, ArH), 7.88 (d, $J = 8.6$ Hz, 1H, ArH), 7.86-7.83 (m, 2H, ArH), 7.58-7.39 (m, 12H, ArH), 6.07 (t, $J = 8.5$ Hz, 1H, CH), 3.92 (dd, $J = 16.4, 9.5$ Hz, 1H, CH₂), 3.47 (dd, $J = 16.4, 7.8$ Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.8, 155.9, 147.5, 138.8, 138.6, 138.0, 133.1, 133.0, 128.8, 128.8, 128.7, 128.7, 128.6, 128.0, 127.7, 127.7, 126.8, 126.4, 126.1, 124.3, 123.2, 115.2, 113.5, 81.8, 37.1; HRMS (ESI) m/z [M + H]⁺ calculated for C₂₉H₂₂NO: 400.1701, found: 400.1696.



2-(Furan-2-yl)-4,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3t**). Yellow viscous liquid; 76.1 mg (56% yield); ¹H NMR (CDCl₃, 400 MHz): δ 8.05 (d, *J* = 7.3 Hz, 2H, ArH), 7.59 (d, *J* = 7.1 Hz, 2H, ArH), 7.51 (t, *J* = 7.2 Hz, 2H, ArH), 7.47-7.31 (m, 6H, ArH), 6.48 (d, *J* = 2.8 Hz, 1H, ArH), 6.37 (s, 1H, ArH), 5.85 (t, *J* = 8.4 Hz, 1H, CH), 3.68 (d, *J* = 8.4 Hz, 2H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.1, 155.8, 152.2, 147.4, 143.2, 138.8, 138.0, 128.9, 128.8, 128.7, 128.5, 127.7, 126.8, 115.0, 113.5, 110.4, 108.7, 75.0, 32.9; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₃H₁₈NO₂: 340.1338, found: 340.1332.

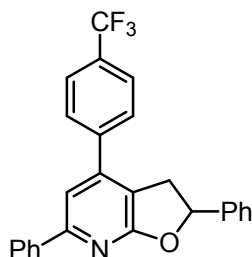


4,6-Diphenyl-2-(thiophen-2-yl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3u**). Pale yellow solid; 82.5 mg (58% yield); mp 122-123 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.06 (td, *J* = 7.0, 1.5 Hz, 2H, ArH), 7.58 (td, *J* = 8.2, 1.5 Hz, 2H, ArH), 7.51 (tt, *J* = 7.3, 1.5 Hz, 2H, ArH), 7.48-7.43 (m, 4H, ArH), 7.40 (tt, *J* = 7.2, 1.4 Hz, 1H, ArH), 7.31 (dd, *J* = 5.0, 1.2 Hz, 1H, ArH), 7.16 (dt, *J* = 3.4, 0.9 Hz, 1H, ArH), 7.00 (dd, *J* = 5.0, 3.6 Hz, 2H, ArH), 6.09 (dd, *J* = 8.5, 7.8 Hz, 1H, CH), 3.82 (dd, *J* = 16.4, 9.1 Hz, 1H, CH₂), 3.55 (dd, *J* = 16.3, 7.5 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.0, 156.0, 147.5, 143.7, 138.7, 137.9, 128.9, 128.8, 128.7, 128.5, 127.7, 126.8, 126.8, 125.7, 125.3, 114.9, 113.6, 78.0, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₃H₁₈NOS: 356.1109, found: 356.1102.

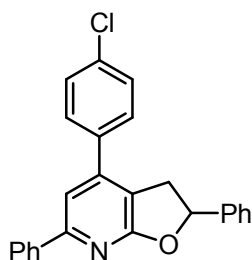


4,6-Diphenyl-2-(pyridin-2-yl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3v**). Yellow solid; 112.1 mg (80% yield); mp 127-128 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.60 (d, *J* = 4.7 Hz, 1H, ArH), 8.06 (dd, *J* = 7.1, 1.4 Hz, 2H, ArH), 7.75-7.69 (m, 2H, ArH), 7.58 (dd, *J* = 6.9, 1.5 Hz, 2H, ArH), 7.50-7.38 (m, 7H, ArH), 7.23 (tt, *J* = 6.7, 1.6 Hz, 1H, ArH), 5.99 (dd, *J* = 9.8, 6.8 Hz, 1H, CH), 3.95 (dd, *J* = 16.6, 9.9 Hz, 1H, CH₂), 3.66 (dd, *J* = 16.6, 6.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.6, 160.3, 155.8, 149.3,

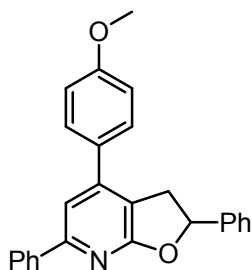
147.6, 138.8, 137.8, 136.9, 128.8, 128.8, 128.7, 128.6, 127.7, 126.8, 122.8, 120.3, 115.0, 113.7, 81.5, 35.1; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{24}H_{19}N_2O$: 351.1497, found: 351.1497.



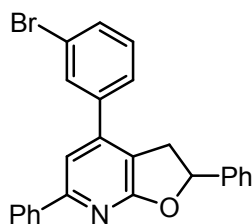
2,6-Diphenyl-4-(4-(trifluoromethyl)phenyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3w**). Yellow solid; 83.4 mg (50% yield); mp 173-174 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, $J = 7.2$ Hz, 2H, ArH), 7.74 (d, $J = 8.2$ Hz, 2H, ArH), 7.66 (d, $J = 8.1$ Hz, 2H, ArH), 7.49-7.37 (m, 8H, ArH), 7.33 (t, $J = 7.2$ Hz, 1H, ArH), 5.92 (t, $J = 8.5$ Hz, 1H, CH), 3.82 (dd, $J = 16.4, 9.4$ Hz, 1H, CH_2), 3.37 (dd, $J = 16.4, 7.8$ Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.8, 156.3, 146.0, 141.6, 141.1, 138.5, 130.7 (q, $J_{C-F} = 32.5$ Hz), 129.1, 128.7, 128.6, 128.2, 128.1, 126.8, 125.8 (q, $J_{C-F} = 3.5$ Hz), 125.4, 123.9 (q, $J_{C-F} = 271.1$ Hz), 115.5, 113.2, 81.8, 36.9; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{26}H_{19}F_3NO$: 418.1419, found: 418.1425



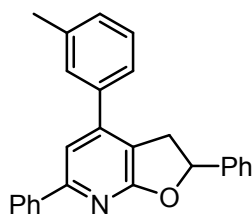
4-(4-Chlorophenyl)-2,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3x**). Pale yellow solid; 95.0 mg (62% yield); mp 111-112 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, $J = 7.2$ Hz, 2H, ArH), 7.49-7.38 (m, 12H, ArH), 7.33 (t, $J = 7.2$ Hz, 1H, ArH), 5.90 (t, $J = 8.5$ Hz, 1H, CH), 3.79 (dd, $J = 16.3, 9.4$ Hz, 1H, CH_2), 3.35 (dd, $J = 16.3, 7.8$ Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.8, 156.0, 146.2, 141.1, 138.6, 136.4, 134.8, 129.0, 129.0, 128.9, 128.7, 128.6, 128.1, 126.8, 125.4, 115.1, 113.1, 81.7, 37.0; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{25}H_{19}ClNO$: 384.1155, found: 384.1160.



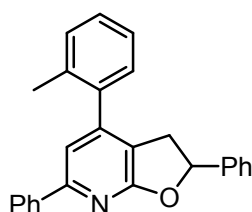
4-(4-Methoxyphenyl)-2,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3y**). Yellow solid; 83.4 mg (55% yield); mp 75-76 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (dd, *J* = 7.2, 1.4 Hz, 2H, ArH), 7.51 (d, *J* = 8.8 Hz, 2H, ArH), 7.49-7.44 (m, 4H, ArH), 7.41-7.37 (m, 11H, ArH), 7.32 (tt, *J* = 7.2, 2.4 Hz, 1H, ArH), 7.00 (dd, *J* = 8.8 Hz, 2H, ArH), 5.89 (t, *J* = 8.5 Hz, 1H, CH), 3.86 (s, 3H, OCH₃), 3.83 (dd, *J* = 16.2, 9.4 Hz, 1H, CH₂), 3.38 (dd, *J* = 16.2, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.8, 160.0, 155.8, 147.0, 141.4, 139.0, 130.3, 129.0, 128.7, 128.6, 128.6, 128.0, 126.8, 125.4, 114.7, 114.2, 113.2, 81.7, 55.4, 37.3; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO₂: 380.1651, found: 380.1648.



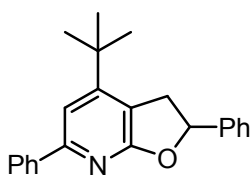
4-(3-Bromophenyl)-2,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3z**). White solid; 114.7mg (66% yield); mp 125-126 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.13 (d, *J* = 7.2 Hz, 2H, ArH), 7.69 (s, 1H, ArH), 7.56 (d, *J* = 7.7 Hz, 1H, ArH), 7.47-7.33 (m, 4H, ArH), 5.91 (t, *J* = 8.5 Hz, 1H, CH), 3.82 (dd, *J* = 16.4, 9.4 Hz, 1H, CH₂), 3.36 (dd, *J* = 16.4, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.8, 156.2, 146.0, 141.1, 140.1, 138.6, 131.7, 130.7, 130.4, 129.0, 128.7, 128.6, 128.2, 126.9, 126.3, 125.5, 123.0, 115.3, 113.2, 81.9, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₅H₁₉BrNO: 428.0650, found: 428.0652.



2,6-Diphenyl-4-(*m*-tolyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3aa**). Pale yellow viscous liquid; 95.9mg (67% yield); ¹H NMR (CDCl₃, 400 MHz): δ 8.02 (d, *J* = 7.5 Hz, 2H, ArH), 7.40 (t, *J* = 7.3 Hz, 4H, ArH), 7.37-7.24 (m, 8H, ArH), 7.19-7.17 (m, 1H, ArH), 5.82 (t, *J* = 8.6 Hz, 1H, CH), 3.76 (dd, *J* = 16.3, 9.4 Hz, 1H, CH₂), 3.31 (dd, *J* = 16.3, 7.8 Hz, 1H, CH₂), 2.37 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 168.7, 155.8, 147.6, 141.3, 138.9, 138.5, 137.9, 129.4, 128.8, 128.7, 128.6, 128.5, 128.3, 128.0, 126.8, 125.4, 124.8, 115.2, 113.5, 81.8, 37.1, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO: 364.1701, found: 364.1699.

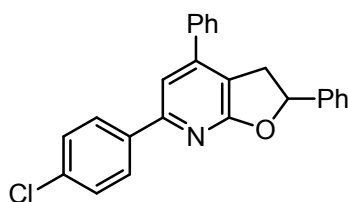


2,6-Diphenyl-4-(*o*-tolyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3ab**). Pale yellow solid; 88.7 mg (61% yield); mp 44-45 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.04 (d, *J* = 7.4 Hz, 2H, ArH), 7.46-7.30 (m, 10H, ArH), 7.24 (d, *J* = 8.1 Hz, 2H, ArH), 7.19 (d, *J* = 7.3 Hz, 1H, ArH), 5.89 (t, *J* = 8.6 Hz, 1H, CH), 3.52 (dd, *J* = 16.4, 9.5 Hz, 1H, CH₂), 3.07 (dd, *J* = 16.4, 7.8 Hz, 1H, CH₂), 2.23 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 168.3, 155.3, 148.5, 141.4, 138.8, 137.9, 134.9, 130.5, 128.8, 128.7, 128.6, 128.4, 128.3, 128.0, 126.8, 125.9, 125.4, 116.7, 114.8, 81.8, 36.4, 19.8; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO: 364.1701, found: 364.1696.

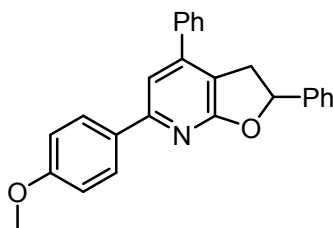


4-(Tert-butyl)-2,6-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ac**). Yellow viscous liquid; 54.0mg (41% yield); ¹H NMR (CDCl₃, 400 MHz): δ 8.02 (d, *J* = 7.2 Hz, 2H, ArH), 7.48-7.33 (m, 9H, ArH), 5.81 (t, *J* = 8.7 Hz, 1H, CH), 3.88 (dd, *J* = 16.0, 9.4 Hz, 1H, CH₂), 3.38 (dd, *J* = 16.0, 8.2 Hz, 1H, CH₂), 1.39 (s, 9H, 3×CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 168.9, 157.9, 155.4, 141.5, 139.3, 128.6, 128.6, 128.5, 128.0, 126.8, 125.5, 114.5, 111.4, 81.1, 38.8, 35.7, 29.7; HRMS (ESI) *m/z* [M + H]⁺

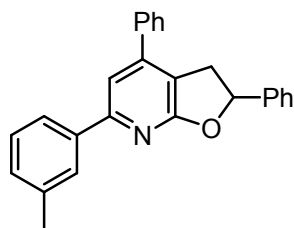
calculated for C₂₃H₂₄NO: 330.4428, found: 330.4421.



6-(4-Chlorophenyl)-2,4-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ad**). Yellow solid; 99.8 mg (65% yield); mp 118-119 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.02 (d, *J* = 8.6 Hz, 2H, ArH), 7.55 (dd, *J* = 8.4, 1.5 Hz, 2H, ArH), 7.51-7.37 (m, 10H, ArH), 7.32 (tt, *J* = 7.2, 2.4 Hz, 1H, ArH), 5.91 (t, *J* = 8.65 Hz, 1H, CH), 3.84 (dd, *J* = 16.4, 9.4 Hz, 1H, CH₂), 3.39 (dd, *J* = 16.4, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.7, 154.5, 147.5, 141.1, 137.7, 137.2, 134.8, 128.8, 128.8, 128.7, 128.6, 128.1, 128.0, 127.6, 125.4, 115.6, 113.2, 81.8, 37.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₅H₁₉ClNO: 384.1155, found: 384.1159.

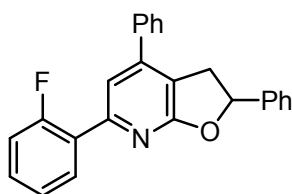


6-(4-Methoxyphenyl)-2,4-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ae**). Yellow solid; 78.9 mg (52% yield); mp 132-133 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.04 (d, *J* = 8.7 Hz, 2H, ArH), 7.55 (d, *J* = 7.2 Hz, 2H, ArH), 7.50-7.35 (m, 8H, ArH), 7.32 (t, *J* = 7.1 Hz, 1H, ArH), 6.99 (d, *J* = 8.7 Hz, 2H, ArH), 5.88 (t, *J* = 8.6 Hz, 1H, CH), 3.86 (s, 3H, OCH₃), 3.81 (dd, *J* = 16.2, 9.5 Hz, 1H, CH₂), 3.37 (dd, *J* = 16.2, 7.8 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 168.6, 160.3, 155.6, 147.4, 141.4, 138.1, 131.5, 128.8, 128.6, 128.6, 128.1, 128.0, 127.7, 125.4, 114.3, 113.9, 112.6, 81.7, 55.3, 37.1; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₂NO₂: 380.1651, found: 380.1646.

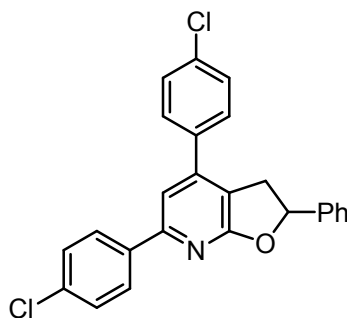


2,4-Diphenyl-6-(*m*-tolyl)-2,3-dihydrofuro[2,3-*b*]pyridine (**3af**). Pale yellow viscous

liquid; 88.7 mg (61% yield); ^1H NMR (CDCl_3 , 400 MHz): δ 8.04 (d, $J = 7.4$ Hz, 2H, ArH), 7.44-7.23 (m, 12H, ArH), 7.19 (d, $J = 7.3$ Hz, 1H, ArH), 5.89 (t, $J = 8.6$ Hz, 1H, CH), 3.52 (dd, $J = 16.4, 9.5$ Hz, 1H, CH_2), 3.07 (dd, $J = 16.4, 7.8$ Hz, 1H, CH_2), 2.23 (s, 3H, CH_3); ^{13}C NMR (CDCl_3 , 100 MHz): δ 168.3, 155.3, 148.5, 141.4, 138.8, 137.9, 134.9, 130.5, 128.8, 128.7, 128.6, 128.4, 128.3, 128.0, 126.8, 125.9, 125.4, 116.7, 114.8, 81.8, 36.4, 19.8; HRMS (ESI) m/z $[\text{M} + \text{H}]^+$ calculated for $\text{C}_{26}\text{H}_{22}\text{NO}$: 364.1701, found: 364.1697.

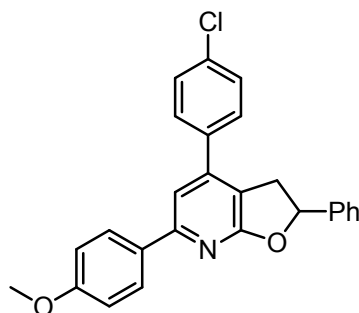


6-(2-Fluorophenyl)-2,4-diphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ag**). Pale yellow solid; 79.5 mg (54% yield); mp 92-93 °C; ^1H NMR (CDCl_3 , 400 MHz): δ 8.14 (td, $J = 7.9, 1.8$ Hz, 1H, ArH), 7.57-7.55 (m, 3H, ArH), 7.50-7.31 (m, 9H, ArH), 7.27 (td, $J = 7.6, 1.0$ Hz, 1H, ArH), 7.16 (ddd, $J = 11.6, 8.2, 0.9$ Hz, 1H, ArH), 5.91 (t, $J = 8.6$ Hz, 1H, CH), 3.86 (dd, $J = 16.4, 9.4$ Hz, 1H, CH_2), 3.41 (dd, $J = 16.4, 7.8$ Hz, 1H, CH_2); ^{13}C NMR (CDCl_3 , 100 MHz): δ 168.6, 160.4 (d, $J_{\text{C-F}} = 248.4$ Hz), 151.1, 151.1 (d, $J_{\text{C-F}} = 2.7$ Hz), 147.2, 141.2, 137.8, 131.0 (d, $J_{\text{C-F}} = 2.7$ Hz), 130.1 (d, $J_{\text{C-F}} = 8.7$ Hz), 128.8, 128.7, 128.7, 128.1, 127.8, 126.9 (d, $J_{\text{C-F}} = 10.9$ Hz), 125.4, 124.3 (d, $J_{\text{C-F}} = 3.4$ Hz), 117.6 (d, $J_{\text{C-F}} = 10.7$ Hz), 116.1 (d, $J_{\text{C-F}} = 23.3$ Hz), 115.6, 81.7, 37.2; HRMS (ESI) m/z $[\text{M} + \text{H}]^+$ calculated for $\text{C}_{25}\text{H}_{19}\text{FNO}$: 368.1451, found: 368.1448.



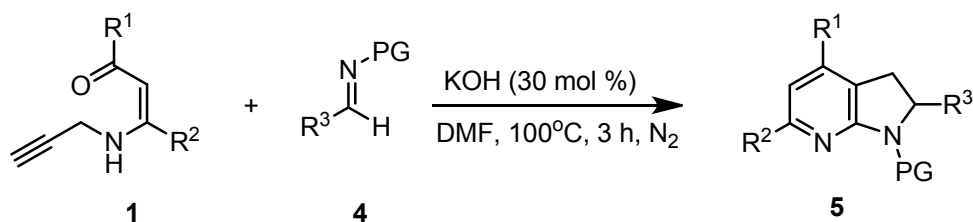
4,6-Bis(4-chlorophenyl)-2-phenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ah**). Yellow solid; 110.3 mg (66% yield); mp 157-158 °C; ^1H NMR (CDCl_3 , 400 MHz): δ 8.00 (d, $J = 7.6$ Hz, 2H, ArH), 7.49-7.33 (m, 12H, ArH), 5.90 (t, $J = 8.5$ Hz, 1H, CH), 3.80 (dd, $J = 16.3, 9.4$ Hz, 1H, CH_2), 3.35 (dd, $J = 16.3, 7.7$ Hz, 1H, CH_2); ^{13}C NMR (CDCl_3 , 100

MHz): δ 168.8, 154.8, 146.4, 141.0, 137.1, 136.2, 135.0, 135.0, 129.1, 129.0, 128.8, 128.7, 128.2, 128.1, 125.4, 115.5, 113.0, 81.9, 37.0; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{25}H_{18}Cl_2NO$: 418.0765, found: 418.0770.



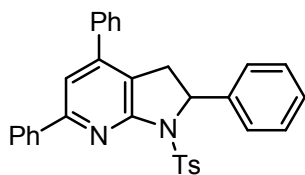
4-(4-Chlorophenyl)-6-(4-methoxyphenyl)-2-phenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3ai**). Brick red solid; 99.3 mg (60% yield); mp 126-127 °C; 1H NMR ($CDCl_3$, 400 MHz): δ 8.01 (d, $J = 8.7$ Hz, 1H, ArH), 7.49-7.43 (m, 6H, ArH), 7.39 (t, $J = 7.4$ Hz, 1H, ArH), 7.33 (d, $J = 7.2$ Hz, 1H, ArH), 7.31 (s, 1H, ArH), 6.98 (d, $J = 8.7$ Hz, 1H, ArH), 5.89 (t, $J = 8.5$ Hz, 1H, CH), 3.86 (s, 3H, OCH_3), 3.78 (dd, $J = 16.3, 9.4$ Hz, 1H, CH_2), 3.34 (dd, $J = 16.2, 7.8$ Hz, 1H, CH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.7, 160.4, 155.8, 146.2, 141.2, 136.6, 134.8, 131.3, 129.0, 129.0, 128.7, 128.1, 128.1, 125.4, 114.2, 114.0, 112.3, 81.8, 55.3, 37.1; HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{26}H_{21}ClNO_2$: 414.1261, found: 414.1260.

Experimental Procedures and Data for Compounds 5

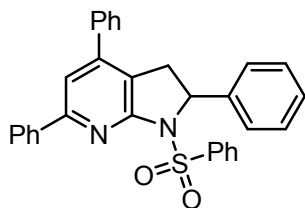


A mixture of *N*-propargylic β -enaminones **1** (0.4 mmol), *N*-sulfonyl imines **4** (0.8 mmol), and KOH (8 mg, 0.12 mmol, 0.3 equiv) in DMF (3 mL) was stirred at 100 °C under N_2 for 3 h. After **1** was disappeared completely (monitored by TLC), the residue dissolved in H_2O (10 mL) and extracted with EtOAc (3 x 10 mL). The combined EtOAc extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 2%

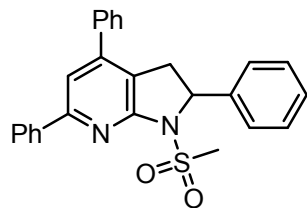
EtOAc in PE) to give **5**.



2,4,6-Triphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5a**). Yellow solid; 130.7 mg (65% yield); mp 209-210 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08 (d, *J* = 7.3 Hz, 2H, ArH), 7.70 (d, *J* = 8.2 Hz, 2H, ArH), 7.49 (t, *J* = 7.4 Hz, 2H, ArH), 7.44-7.36 (m, 7H, ArH), 7.26-7.23 (m, 5H, ArH), 7.09 (d, *J* = 8.2 Hz, 2H, ArH), 5.74 (dd, *J* = 10.3, 3.1 Hz, 1H, CH), 3.85 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.10 (dd, *J* = 16.8, 3.1 Hz, 1H, CH₂), 2.33 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.7, 155.7, 146.9, 143.6, 142.3, 138.9, 137.8, 136.9, 128.9, 128.8, 128.8, 128.7, 128.7, 128.6, 128.4, 128.0, 127.8, 126.9, 126.2, 118.6, 114.6, 63.3, 36.0, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₇N₂O₂S: 503.1793, found: 503.1789.

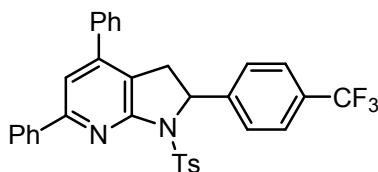


2,4,6-Triphenyl-1-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5b**). Yellow solid; 97.7 mg (50% yield); mp 248-249 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.07 (d, *J* = 7.6 Hz, 2H, ArH), 7.83 (d, *J* = 7.6 Hz, 2H, ArH), 7.50-7.37 (m, 10H, ArH), 7.29 (t, *J* = 7.8 Hz, 2H, ArH), 7.25-7.19 (m, 5H, ArH), 5.75 (dd, *J* = 10.3, 3.0 Hz, 1H, CH), 3.86 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.11 (dd, *J* = 16.8, 3.0 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 156.7, 155.8, 147.0, 142.1, 139.8, 138.9, 137.8, 132.7, 128.9, 128.8, 128.7, 128.7, 128.6, 128.3, 128.1, 128.1, 127.8, 126.9, 126.2, 118.6, 114.7, 63.33, 36.00; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₁H₂₅N₂O₂S: 489.1637, found: 489.1623.

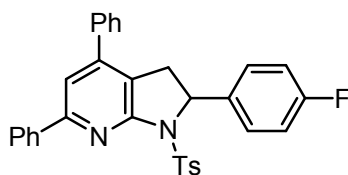


1-(Methylsulfonyl)-2,4,6-triphenyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5c**).

White solid; 90.4 mg (53% yield); mp 228-229 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.10 (d, *J* = 7.2 Hz, 2H, ArH), 7.51-7.41 (m, 9H, ArH), 7.35-7.29 (m, 5H, ArH), 5.69 (dd, *J* = 10.2, 3.1 Hz, 1H, CH), 3.90 (dd, *J* = 16.8, 10.2 Hz, 1H, CH₂), 3.31 (s, 3H, CH₃), 3.15 (dd, *J* = 16.8, 3.1 Hz, 1H, CH₂); ¹³C NMR (CDCl₃, 100 MHz): δ 157.0, 155.8, 147.4, 142.3, 138.6, 137.7, 129.1, 129.0, 128.9, 128.8, 128.7, 128.2, 127.8, 126.8, 125.7, 118.9, 114.7, 62.5, 41.9, 36.0; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₆H₂₃N₂O₂S: 427.1480, found: 427.1468.

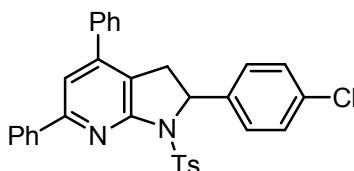


4,6-Diphenyl-1-tosyl-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5d**). Yellow solid; 102.7 mg (45% yield); mp 198-199 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.10 (d, *J* = 7.2 Hz, 2H, ArH), 7.76 (d, *J* = 8.3 Hz, 2H, ArH), 7.52-7.39 (m, 11H, ArH), 7.35 (d, *J* = 8.0 Hz, 2H, ArH), 7.12 (d, *J* = 8.1 Hz, 2H, ArH), 5.76 (dd, *J* = 10.4, 3.4 Hz, 1H, CH), 3.86 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.06 (dd, *J* = 16.8, 3.5 Hz, 1H, CH₂), 2.34 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.6, 156.0, 147.3, 146.2, 144.0, 138.7, 137.6, 136.6, 130.2 (q, *J*_{C-F} = 32.3 Hz), 129.1, 128.9, 129.0, 128.8, 128.7, 128.3, 127.7, 126.9, 126.5, 125.7 (q, *J*_{C-F} = 3.6 Hz), 123.9 (q, *J*_{C-F} = 270.4 Hz), 118.0, 114.8, 62.7, 35.9, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₃H₂₆F₃N₂O₂S: 571.1667, found: 571.1661.



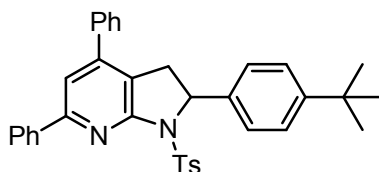
2-(4-Fluorophenyl)-4,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5e**).

Pale yellow solid; 102.0 mg (49% yield); mp 211-212 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.09 (d, *J* = 8.0 Hz, 2H, ArH), 7.74 (d, *J* = 8.1 Hz, 2H, ArH), 7.50 (t, *J* = 7.3 Hz, 2H, ArH), 7.44-7.39 (m, 7H, ArH), 7.21 (dd, *J* = 7.9, 5.5 Hz, 2H, ArH), 7.13 (d, *J* = 8.0 Hz, 2H, ArH), 6.93 (t, *J* = 8.5 Hz, 2H, ArH), 5.73 (dd, *J* = 10.2, 2.7 Hz, 1H, CH), 3.85 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.06 (dd, *J* = 16.8, 2.9 Hz, 1H, CH₂), 2.34 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 162.4 (d, *J*_{C-F} = 245.2 Hz), 156.5, 155.8, 147.0, 143.7, 138.8, 138.2 (d, *J*_{C-F} = 3.1 Hz), 137.7, 136.8, 128.9, 128.8, 128.8, 128.2, 128.6, 128.3, 128.0 (d, *J*_{C-F} = 8.2 Hz), 127.7, 126.9, 118.3, 115.5 (d, *J*_{C-F} = 21.5 Hz), 114.7, 62.6, 36.0, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₆FN₂O₂S: 521.1699, found: 521.1692.



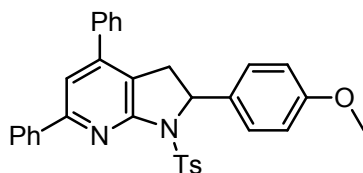
2-(4-Chlorophenyl)-4,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5f**).

Pale yellow solid; 122.4 mg (57% yield); mp 120-121 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08 (d, *J* = 7.4 Hz, 2H, ArH), 7.76 (d, *J* = 8.2 Hz, 2H, ArH), 7.49 (t, *J* = 7.4 Hz, 2H, ArH), 7.45-7.39 (m, 7H, ArH), 7.22-7.13 (m, 6H, ArH), 5.70 (dd, *J* = 10.3, 3.2 Hz, 1H, CH), 3.83 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.03 (dd, *J* = 16.8, 3.3 Hz, 1H, CH₂), 2.35 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.5, 155.8, 147.1, 143.8, 140.9, 138.7, 137.6, 136.7, 133.7, 128.9, 128.9, 128.8, 128.8, 128.7, 128.6, 128.3, 127.7, 127.6, 126.9, 118.2, 114.7, 62.6, 36.0, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₆ClN₂O₂S: 537.1404, found: 537.1403.



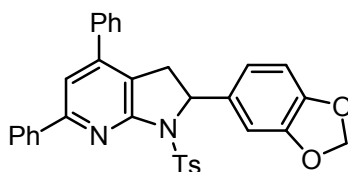
2-(4-(*tert*-Butyl)phenyl)-4,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5g**). Yellow solid; 120.7 mg (54% yield); mp 224-225 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.11 (dd, *J* = 7.2, 1.3 Hz, 2H, ArH), 7.64 (d, *J* = 8.3 Hz, 2H, ArH), 7.50 (t, *J* = 7.4 Hz, 2H, ArH), 7.45-7.36 (m, 7H, ArH), 7.23 (d, *J* = 8.4 Hz, 2H, ArH), 7.12 (d, *J*

= 8.4 Hz, 2H, ArH), 7.04 (d, $J = 8.2$ Hz, 2H, ArH), 5.71 (dd, $J = 10.2, 2.7$ Hz, 1H, CH), 3.84 (dd, $J = 16.7, 10.3$ Hz, 1H, CH₂), 3.13 (dd, $J = 16.8, 2.8$ Hz, 1H, CH₂), 2.31 (s, 3H, CH₃), 1.29 (s, 9H, 3×CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.7, 155.6, 151.0, 146.8, 143.3, 139.0, 138.9, 137.8, 136.9, 128.8, 128.8, 128.6, 128.6, 128.6, 128.4, 127.8, 126.9, 126.0, 125.5, 118.9, 114.4, 63.2, 35.8, 34.5, 31.3, 21.5; HRMS (ESI) m/z [M + H]⁺ calculated for C₃₆H₃₅N₂O₂S: 559.2419, found: 559.2406.



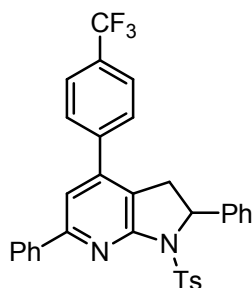
2-(4-Methoxyphenyl)-4,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine

(**5h**). Pale yellow solid; 134.2 mg (63% yield); mp 216-217 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08 (d, $J = 7.4$ Hz, 2H, ArH), 7.70 (d, $J = 8.2$ Hz, 2H, ArH), 7.49 (t, $J = 7.4$ Hz, 2H, ArH), 7.44-7.39 (m, 7H, ArH), 7.15 (d, $J = 8.6$ Hz, 2H, ArH), 7.10 (d, $J = 8.1$ Hz, 2H, ArH), 6.76 (d, $J = 8.6$ Hz, 2H, ArH), 5.71 (dd, $J = 10.3, 2.8$ Hz, 1H, CH), 3.83 (dd, $J = 16.8, 10.3$ Hz, 1H, CH₂), 3.79 (s, 3H, OCH₃), 3.09 (dd, $J = 16.8, 2.8$ Hz, 1H, CH₂), 2.33 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 159.3, 156.6, 155.7, 146.9, 143.5, 138.9, 137.8, 137.0, 134.5, 128.8, 128.8, 128.7, 128.6, 128.6, 128.4, 127.8, 127.6, 126.9, 118.7, 114.5, 113.9, 62.9, 55.3, 36.1, 21.5; HRMS (ESI) m/z [M + H]⁺ calculated for C₃₃H₂₉N₂O₂S: 533.1899, found: 533.1890.

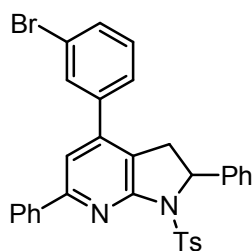


2-(Benzo[*d*][1,3]dioxol-5-yl)-4,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5i**). Pale yellow solid; 146.5 mg (67% yield); mp 203-204 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.09 (dd, $J = 7.2, 1.4$ Hz, 2H, ArH), 7.78 (d, $J = 8.3$ Hz, 2H, ArH), 7.49 (t, $J = 7.4$ Hz, 2H, ArH), 7.44-7.37 (m, 7H, ArH), 7.13 (d, $J = 8.1$ Hz, 2H, ArH), 6.76 (dd, $J = 8.0, 1.5$ Hz, 1H, ArH), 6.69 (d, $J = 8.0$ Hz, 1H, ArH), 6.59 (d, $J = 1.5$ Hz, 1H, ArH), 5.89 (d, $J = 5.2$ Hz, 2H, ArH), 5.65 (dd, $J = 10.2, 3.0$ Hz, 1H, CH), 3.81 (dd, $J = 16.8, 10.3$ Hz, 1H, CH₂), 3.06 (dd, $J = 16.8, 3.1$ Hz, 1H, CH₂), 2.34 (s,

3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.6, 155.8, 147.9, 147.3, 147.0, 143.7, 138.9, 137.8, 137.0, 136.3, 128.9, 128.8, 128.8, 128.7, 128.6, 128.4, 127.8, 126.9, 120.0, 118.5, 114.6, 108.2, 106.4, 101.0, 63.3, 36.1, 21.6; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₃H₂₇N₂O₄S: 547.1692, found: 547.1683.

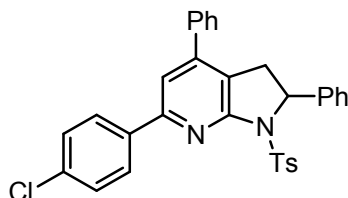


2,6-Diphenyl-1-tosyl-4-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5j**). Pale yellow solid; 152.9 mg (67% yield); mp 103-104 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08 (dd, *J* = 8.5, 1.4 Hz, 2H, ArH), 7.70 (dd, *J* = 8.4, 1.9 Hz, 4H, ArH), 7.54 (d, *J* = 8.1 Hz, 2H, ArH), 7.50 (t, *J* = 7.3 Hz, 2H, ArH), 7.44 (t, *J* = 7.2 Hz, 1H, ArH), 7.39 (s, 1H, ArH), 7.28-7.19 (m, 5H, ArH), 7.10 (d, *J* = 8.2 Hz, 2H, ArH), 5.76 (dd, *J* = 10.4, 3.2 Hz, 1H, CH), 3.83 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.07 (dd, *J* = 16.8, 3.2 Hz, 1H, CH₂), 2.33 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.8, 156.0, 145.4, 143.7, 142.0, 141.3, 138.5, 136.7, 130.6 (q, *J*_{C-F} = 32.5 Hz), 129.0, 128.8, 128.7, 128.6, 128.4, 128.2, 128.0, 126.8, 126.1, 125.7 (q, *J*_{C-F} = 3.7 Hz), 123.8 (q, *J*_{C-F} = 270.7 Hz), 118.7, 114.2, 63.3, 35.8, 21.4; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₃H₂₆F₃N₂O₂S: 571.1667, found: 571.1660.

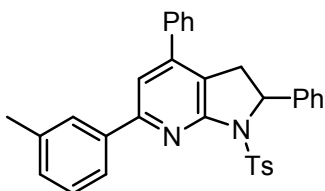


4-(3-Bromophenyl)-2,6-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5k**). Pale yellow solid; 141.9 mg (61% yield); mp 205-206 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.08 (d, *J* = 7.3 Hz, 2H, ArH), 7.70 (d, *J* = 8.2 Hz, 2H, ArH), 7.56 (s, 1H, ArH), 7.52-7.47 (m, 3H, ArH), 7.43 (t, *J* = 7.2 Hz, 1H, ArH), 7.36 (s, 1H, ArH), 7.34 (d, *J* = 7.9 Hz, 1H, ArH), 7.29 (t, *J* = 7.7 Hz, 1H, ArH), 7.27-7.20 (m, 5H, ArH), 7.09 (d, *J* = 8.1 Hz, 2H, ArH), 5.74 (dd, *J* = 10.3, 3.1 Hz, 1H, CH), 3.83 (dd, *J* = 16.8, 10.4

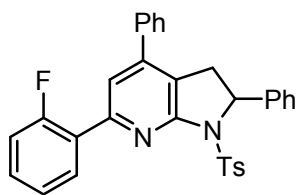
Hz, 1H, CH₂), 3.06 (dd, *J* = 16.8, 3.2 Hz, 1H, CH₂), 2.32 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.8, 156.0, 145.4, 143.6, 142.1, 139.8, 138.6, 136.7, 131.7, 130.7, 130.3, 129.0, 128.8, 128.7, 128.6, 128.4, 128.1, 126.9, 126.4, 126.2, 122.9, 118.6, 114.2, 63.3, 35.9, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₆BrN₂O₂S: 581.0898, found: 581.0898.



6-(4-Chlorophenyl)-2,4-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5l**). Yellow solid; 118.1 mg (55% yield); mp 241-242 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.01 (d, *J* = 8.4 Hz, 2H, ArH), 7.66 (d, *J* = 8.1 Hz, 2H, ArH), 7.45-7.37 (m, 8H, ArH), 7.25-7.22 (m, 5H, ArH), 7.09 (d, *J* = 8.1 Hz, 2H, ArH), 5.74 (dd, *J* = 10.3, 2.9 Hz, 1H, CH), 3.84 (dd, *J* = 16.9, 10.4 Hz, 1H, CH₂), 3.09 (dd, *J* = 16.9, 2.9 Hz, 1H, CH₂), 2.32 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.7, 154.4, 147.0, 143.7, 142.1, 137.6, 137.3, 136.8, 134.8, 128.8, 128.8, 128.7, 128.7, 128.7, 128.3, 128.1, 128.0, 127.7, 126.2, 119.0, 114.4, 63.3, 36.0, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₆ClN₂O₂S: 537.1404, found: 537.1397.

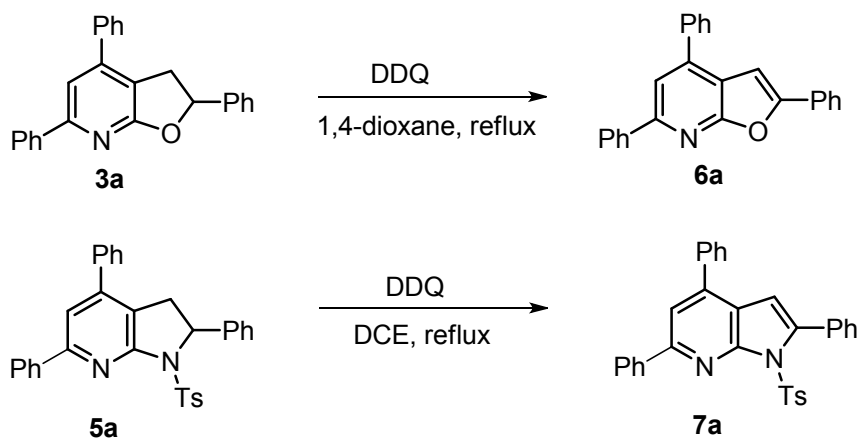


2,4-Diphenyl-6-(*m*-tolyl)-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5m**). Yellow solid; 121.9 mg (59% yield); mp 197-198°C; ¹H NMR (CDCl₃, 400 MHz): δ 7.87-7.85 (m, 2H, ArH), 7.71 (d, *J* = 8.1 Hz, 2H, ArH), 7.43-7.35 (m, 7H, ArH), 7.26-7.23 (m, 6H, ArH), 7.11 (d, *J* = 8.0 Hz, 2H, ArH), 5.75 (dd, *J* = 10.3, 2.9 Hz, 1H, CH), 3.85 (dd, *J* = 16.8, 10.4 Hz, 1H, CH₂), 3.10 (dd, *J* = 16.8, 3.0 Hz, 1H, CH₂), 2.47 (s, 3H, CH₃), 2.33 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 156.7, 155.9, 146.9, 143.5, 142.3, 138.9, 138.0, 137.8, 136.9, 129.6, 128.8, 128.8, 128.7, 128.6, 128.5, 128.5, 128.0, 127.8, 127.6, 126.2, 124.1, 118.5, 114.6, 63.2, 36.0, 21.6, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₃H₂₉N₂O₂S: 517.1950, found: 517.1945.



6-(2-Fluorophenyl)-2,4-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5n**). Yellow solid; 104.1 mg (50% yield); mp 143-144 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.19 (t, *J* = 7.4 Hz, 1H, ArH), 7.66 (d, *J* = 7.8 Hz, 2H, ArH), 7.56 (s, 1H, ArH), 7.43-7.13 (m, 13H, ArH), 7.07 (d, *J* = 7.8 Hz, 2H, ArH), 5.74 (d, *J* = 8.5 Hz, 1H, CH), 3.87 (dd, *J* = 16.7, 10.4 Hz, 1H, CH₂), 3.12 (d, *J* = 16.9 Hz, 1H, CH₂), 2.32 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 167.7, 160.6 (d, *J*_{C-F} = 248.6 Hz), 156.5, 151.1 (d, *J*_{C-F} = 3.0 Hz), 146.6, 143.6, 142.1, 137.6, 136.7, 131.3 (d, *J*_{C-F} = 2.6 Hz), 130.2 (d, *J*_{C-F} = 8.5 Hz), 128.8, 128.7, 128.7, 128.6, 128.4, 128.0, 127.8, 126.9 (d, *J*_{C-F} = 10.6 Hz), 126.2, 124.3 (d, *J*_{C-F} = 3.4 Hz), 118.9, 118.7 (d, *J*_{C-F} = 11.3 Hz), 116.1 (d, *J*_{C-F} = 23.3 Hz), 63.2, 36.1, 21.5; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₆FN₂O₂S: 521.1699, found: 521.1696.

Synthetic Transformations



To a solution of 2,4,6-triphenyl-2,3-dihydrofuro[2,3-*b*]pyridine (**3a**; 104.8 mg, 0.3 mmol, 1.0 equiv) in anhydrous 1,4-dioxane (3 mL) was added 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (204.3 mg, 0.9 mmol, 3.0 equiv) and the reaction mixture was stirred under reflux for 20 h. Then it was quenched with a sat. aq. NaHCO₃ solution and

extracted with EtOAc (3 × 15 mL). The combined organic layers were washed with a sat. aq. NaCl solution, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude product by flash chromatography (SiO₂, 1% EtOAc in PE) afforded **6a**.

2,4,6-Triphenylfuro[2,3-*b*]pyridine (**6a**). White solid; 90.7 mg (87% yield); mp 176-177 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.16 (d, *J* = 7.5 Hz, 2H, ArH), 7.94 (d, *J* = 7.5 Hz, 2H, ArH), 7.79 (s, 1H, ArH), 7.76 (d, *J* = 7.4 Hz, 2H, ArH), 7.58 (t, *J* = 7.2 Hz, 2H, ArH), 7.53-7.44 (m, 6H, ArH), 7.38 (t, *J* = 7.0 Hz, 1H, ArH), 7.20 (s, 1H, ArH); ¹³C NMR (CDCl₃, 100 MHz): δ 162.7, 155.9, 152.5, 143.6, 139.0, 137.9, 129.6, 129.1, 129.0, 128.9, 128.8, 128.8, 128.7, 128.2, 127.0, 125.0, 118.2, 115.6, 99.7; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₂₅H₁₈NO: 348.1388, found: 348.1383.

To a solution of 2,4,6-triphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrolo[2,3-*b*]pyridine (**5a**; 150.8 mg, 0.3 mmol, 1.0 equiv) in anhydrous DCE (4 mL) was added DDQ (204.3 mg, 0.9 mmol, 3.0 equiv) and the reaction mixture was stirred under reflux for 24 h. Then it was quenched with a sat. aq. NaHCO₃ solution and extracted with CH₂Cl₂ (3 × 15 mL). The combined organic layers were washed with a sat. aq. NaCl solution, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude product by flash chromatography (SiO₂, 2% EtOAc in PE) afforded **7a**.

2,4,6-Triphenyl-1-tosyl-1*H*-pyrrolo[2,3-*b*]pyridine (**7a**). White solid; 129.2 mg (86% yield); mp 194-195 °C; ¹H NMR (CDCl₃, 400 MHz): δ 8.25 (dd, *J* = 7.3, 1.2 Hz, 2H, ArH), 7.94 (d, *J* = 8.3 Hz, 2H, ArH), 7.77 (s, 1H, ArH), 7.67-7.60 (m, 4H, ArH), 7.55 (t, *J* = 7.6 Hz, 2H, ArH), 7.52-7.43 (m, 7H, ArH), 7.18 (d, *J* = 8.2 Hz, 2H, ArH), 6.72 (s, 1H, ArH), 2.32 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 100 MHz): δ 152.5, 150.6, 144.7, 142.7, 142.4, 139.2, 137.9, 135.9, 133.0, 129.7, 129.2, 129.0, 128.8, 128.7, 128.7, 128.7, 128.4, 128.2, 127.7, 127.0, 119.0, 115.4, 108.3, 21.57; HRMS (ESI) *m/z* [M + H]⁺ calculated for C₃₂H₂₅N₂O₂S: 501.1637, found: 501.1633.

References

- 1 (a) R. J. Cox, D. J. Ritson, T. A. Dane, J. Berge, J. P. H. Charmant and A. Kantacha, *Chem. Commun.*, 2005, 1037; (b) S. Cacchi, G. Fabrizi and E. Filisti, *Org. Lett.*, 2008, **10**, 2629.
- 2 S. Morales, F. G. Guijarro, J. L. G. Ruano and M. B. Cid, *J. Am. Chem. Soc.*, 2014, **136**, 1082.

X-Ray Structure of **3a**

Crystal data

Crystallographic data for compound **3a** (CCDC-1544842) has been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of charge, on application to CCDC (Email:deposit@ccdc.cam.ac.uk).

Datablock: **3a**

Bond precision: C-C = 0.0015 Å Wavelength=0.71073
Cell: a=9.3863(16) b=17.598(3) c=11.455(2)
alpha=90 beta=106.320(4) gamma=90
Temperature: 113 K

	Calculated	Reported
Volume	1815.9(5)	1815.9(5)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	-P 2ybc

Moiety formula	C ₂₅ H ₁₉ N O	C ₂₅ H ₁₉ N O
Sum formula	C ₂₅ H ₁₉ N O	C ₂₅ H ₁₉ N O
Mr	349.41	349.41
Dx,g cm ⁻³	1.278	1.278
Z	4	4
Mu (mm ⁻¹)	0.077	0.077
F000	736.0	736.0
F000'	736.29	
h,k,lmax	12,22,14	12,22,14
Nref	4183	4121
Tmin,Tmax	0.985,0.991	0.985,0.991
Tmin'	0.985	

Correction method= # Reported T Limits: Tmin=0.985 Tmax=0.991

AbsCorr = MULTI-SCAN

Data completeness= 0.985

Theta(max)= 27.540

R(reflections)= 0.0367(3514)

wR2(reflections)= 0.1049(4121)

S = 1.039

Npar= 244

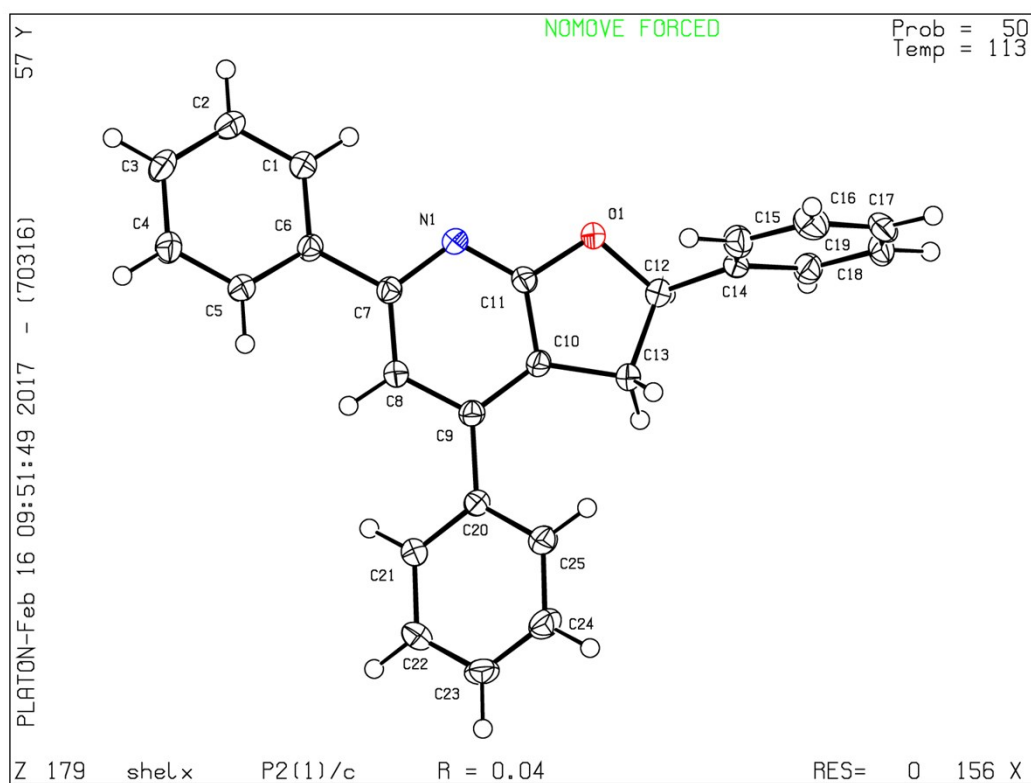


Figure 1. Ortep view of the complex **3a** (Color scheme: C, gray; N, blue; O, red)

¹H and ¹³C NMR spectra

