Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Synthesis of benzofuro[2,3-c]pyridines via a one-pot three-component reaction

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Supporting Information

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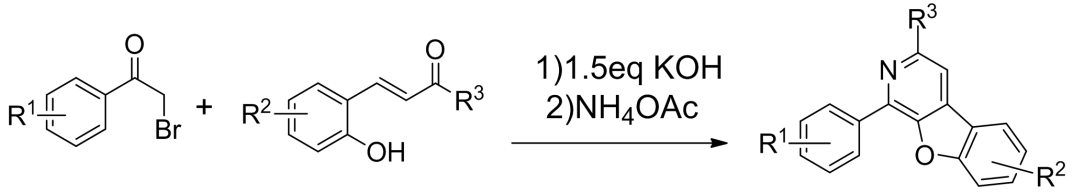
1. General experimental details

All the reactions and manipulations were performed in atmosphere using standard schlenk techniques. All solvents before use did not need any treatment. All reactions were monitored by TLC with silica gel-coated plates.

NMR spectra were recorded on BRUKER DRX 400 spectrometers. Chemical shifts are reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (J) were reported in Hz and refer to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker micrOTOF mass instrument (ESI). IR spectra were recorded on BRUKER TENSOR 27 spectrometers.

2. Synthesis of substituted benzofuro[2,3-c]pyridines

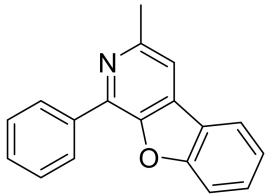


1 **2** **3**

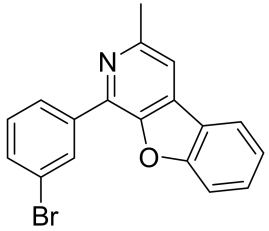
Compound **1** (0.9 mmol) and compound **2** (0.75 mmol) was dissolved in 5 ml dry THF, KOH (1.125 mmol) was slowly

added and the mixture was stirred at room temperature until the reaction was completed (monitored by TLC). Ammonium acetate (4 mmol) and 5 mL C_2H_5OH were added to the reaction mixture and heated to reflux. The reaction mixture was cooled to room temperature, solvent was removed under reduced pressure and the residue was purified by column chromatography.

3. Experimental characterization data for products

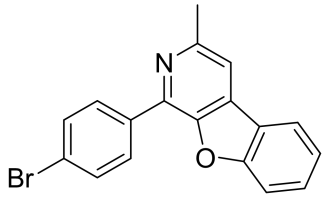


3-methyl-1-phenylbenzofuro[2,3-c]pyridine (3a). The product was obtained as a light yellow solid (140 mg,77%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.1 Hz, 2H, PhH), 8.01 (d, *J* = 7.8 Hz, 1H, PhH), 7.69 (d, *J* = 8.3 Hz, 2H, PhH), 7.63 – 7.57 (m, 3H, PhH, PyH), 7.50 (t, *J* = 7.4 Hz, 1H, PhH), 7.42 (t, *J* = 7.5 Hz, 1H, PhH), 2.81 (s, 3H, CH_3); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 156.9(CH), 151.4(CH), 149.0(CH), 141.3(CH), 136.4(CH), 132.8(CH), 129.6(CH), 129.1(CH), 128.7(CH×2), 128.6(CH×2), 123.2(CH), 122.4(CH), 121.9(CH), 113.2(CH), 112.5(CH), 24.5(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3064, 2956, 2920, 1629, 1577, 1456, 1417, 1193, 1043, 750, 732, 684. UV (CH_2Cl_2): λmax 230, 257, 335 nm. HRMS (ESI) calcd for [$C_{18}H_{13}NO$+H]$^+$: 260.1070, found: 260.1072. MS (EI) m/z: 259, 202, 153, 129, 77.

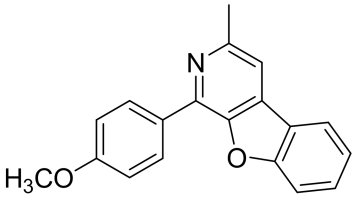


1-(3-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (3b). The product was obtained as a yellow oil (117 mg,46%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H, PhH), 8.44 (d, *J* = 7.7 Hz, 1H, PhH), 8.00 (d, *J* = 7.7 Hz, 1H, PhH), 7.70 (d, *J* = 8.2 Hz, 2H, PhH), 7.62 (t, *J* = 7.9 Hz, 2H, PhH, PyH), 7.48 – 7.40 (m, 2H, PhH), 2.79 (s, 3H, CH_3); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 156.9(CH), 151.5(CH), 148.8(CH), 139.3(CH), 138.2(CH), 133.0(CH), 131.9(CH), 131.4(CH),

130.0(CH), 129.8(CH), 127.1(CH), 123.3(CH), 122.7(CH), 122.2(CH), 121.9(CH), 113.8(CH), 112.4(CH), 24.4(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3053, 1627, 1579, 1461, 1191, 1053, 742, 692, 621. UV (CH_2Cl_2): λmax 245, 289, 325 nm. HRMS (ESI) calcd for $[C_{18}H_{12}NOBr+Na]^+$: 359.9994, found: 359.9996. MS (EI) m/z: 337, 258, 202, 168, 129.

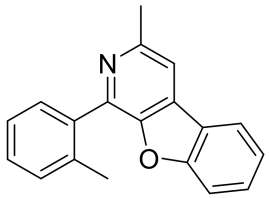


1-(4-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (3c). The product was obtained as a white solid (106 mg,42%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.6 Hz, 2H, PhH), 7.99 (d, *J* = 7.9 Hz, 1H, PhH), 7.68 (d, J = 8.6 Hz, 2H, PhH), 7.62 – 7.54 (m, 3H, PhH, PyH), 7.41 (t, *J* = 7.4 Hz, 1H, PhH), 2.77 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.8(CH), 151.5(CH), 148.8(CH), 139.7(CH), 135.1(CH), 132.7(CH), 131.6(CH×2), 130.2(CH×2), 129.8(CH), 123.5(CH), 123.3(CH), 122.2(CH), 121.9(CH), 113.6(CH), 112.3(CH), 24.1(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3051, 1629, 1583, 1427, 1188, 1045, 736, 626. UV (CH_2Cl_2): λmax 250, 288, 328 nm. HRMS (ESI) calcd for $[C_{18}H_{12}NOBr+Na]^+$: 359.9994, found: 359.9995. MS (EI) m/z: 337, 258, 202, 168, 129.

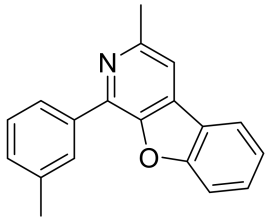


1-(4-methoxyphenyl)-3-methylbenzofuro[2,3-c]pyridine (3d). The product was obtained as a pale yellow solid (119 mg,55%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.50 – 8.43 (m, 2H, PhH), 7.92 (d, *J* = 7.7 Hz, 1H, PhH), 7.63 (d, *J* = 8.3 Hz, 1H, PhH), 7.59 – 7.50 (m, 2H, PhH, PyH), 7.40 – 7.31 (m, 1H, PhH), 7.16 – 7.06 (m, 2H, PhH), 3.92 (s, 3H, OCH_3), 2.77 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 160.4(CH), 156.7(CH), 151.2(CH), 148.7(CH), 141.0(CH), 132.4(CH), 130.1(CH×2), 129.4(CH), 129.1(CH), 123.1(CH), 122.5(CH), 121.8(CH), 114.0(CH×2), 112.4(CH), 112.3(CH), 55.1(OCH_3), 24.4(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3068, 2931, 2866, 1631, 1575, 1460, 1192, 1033, 877, 840, 746, 632. UV (CH_2Cl_2): λmax 252, 293,

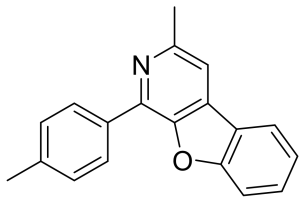
333 nm. HRMS (ESI) calcd for $[C_{19}H_{15}NO_2+Na]^+$: 312.0995, found:312.0994. MS (EI) m/z: 289, 246, 189, 144, 63.



2-methyl-1-(m-tolyl)benzofuro[2,3-c]pyridine (3e). The product was obtained as a yellow solid (152 mg,74%): ^{1}H-NMR (400MHz, $CDCl_3$) δ8.01 (d, *J* = 7.7 Hz, 1H, PhH), 7.72 (s, 1H, PyH), 7.69 – 7.64 (m, 1H, PhH), 7.62 – 7.54 (m, 2H, PhH), 7.46 – 7.38 (m, 4H, PhH), 2.84 (s, 3H, CH_3), 2.42 (s, 3H, CH_3); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.0(CH), 151.4(CH), 149.1(CH), 143.8(CH), 137.0(CH), 136.0(CH), 132.0(CH), 130.7(CH), 130.2(CH), 129.7(CH), 129.0(CH), 125.9(CH), 123.2(CH), 122.6(CH), 122.0(CH), 113.3(CH), 112.5(CH), 24.5(CH_3), 20.1(CH_3). IR ν_{max}(KBr)/cm^{-1}: 3059, 2954, 2920, 1631, 1579, 1460, 1419, 1195, 1043, 879, 740, 622. UV (CH_2Cl_2): λmax 245, 285, 317 nm. HRMS (ESI) calcd for $[C_{19}H_{15}NO+Na]^+$: 296.1046, found: 296.1047. MS (EI) m/z: 273, 244, 218, 120, 63.

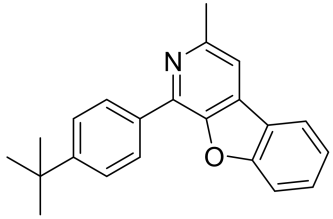


3-methyl-1-(m-tolyl)benzofuro[2,3-c]pyridine (3f). The product was obtained as a light yellow oil (121 mg, 59%): ^{1}H-NMR (400MHz, $CDCl_3$) δ8.29 (d, *J* = 9.8 Hz, 2H, PhH), 7.97 (d, *J* = 7.7 Hz, 1H, PhH), 7.67 (d, *J* = 8.3 Hz, 1H, PhH), 7.60 (m, 2H, PhH, PyH), 7.51 (t, *J* = 7.6 Hz, 1H, PhH), 7.39 (t, J = 7.5 Hz, 1H, PhH), 7.34 (d, J = 7.5 Hz, 1H, PhH), 2.81 (s, 3H, CH_3), 2.56 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.9(CH), 151.3(CH), 149.0(CH), 141.6(CH), 138.2(CH), 136.3(CH), 132.7(CH), 130.0(CH), 129.6(CH), 129.2(CH), 128.4(CH), 126.0(CH), 123.1(CH), 122.4(CH), 121.8(CH), 113.1(CH), 112.4(CH), 24.5(CH_3), 21.7(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3037, 2922, 2856, 1627, 1577, 1458, 1188, 1047, 833, 740, 624. UV (CH_2Cl_2): λmax 248, 290, 327 nm. HRMS (ESI) calcd for $[C_{19}H_{15}NO+Na]^+$: 296.1046, found: 296.1048. MS (EI) m/z: 273, 202, 136, 63.

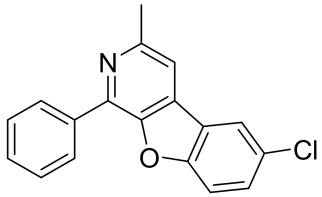


4-methyl-1-(p-tolyl)benzofuro[2,3-c]pyridine (3g). The product was obtained as a light yellow solid (139 mg, 68%):

^{1}H-NMR (400MHz, $CDCl_3$) δ8.41 (d, *J* = 8.2 Hz, 2H, PhH), 7.91 (dd, *J* = 16.5, 6.8 Hz, 1H, PhH), 7.64 (d, *J* = 8.3 Hz, 1H, PhH), 7.60 – 7.54 (m, 2H, PhH, PyH), 7.43 (d, *J* = 8.0 Hz, 2H, PhH), 7.40 – 7.35 (m, 1H, PhH), 2.80 (s, 3H, CH_3), 2.51 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.8(CH), 151.2(CH), 148.8(CH), 141.4(CH), 139.1(CH), 133.6(CH), 132.6(CH), 129.5(CH), 129.3(CH×2), 128.7(CH×2), 123.1(CH), 122.4(CH), 121.8(CH), 112.9(CH), 112.4(CH), 24.5(CH_3), 21.5(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3033, 2925, 2850, 1631, 1581, 1454, 1193, 1047, 875, 827, 742. UV (CH_2Cl_2): λmax 249, 290, 328 nm. HRMS (ESI) calcd for [$C_{19}H_{15}NO$+Na]$^{+}$: 296.1046, found: 296.1047. MS (EI) m/z: 273, 202, 136, 91.

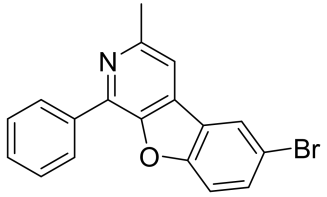


1-(4-(tert-butyl)phenyl)-3-methylbenzofuro[2,3-c]pyridine(3h). The product was obtained as a pale solid (168 mg, 71%): ^{1}H-NMR (400MHz, $CDCl_3$) δ8.43 (d, *J* = 8.4 Hz, 2H, PhH), 7.96 (d, *J* = 7.7 Hz, 1H, PhH), 7.66 (d, *J* = 8.5 Hz, 3H, PhH), 7.59 (m, 2H, PhH, PyH), 7.39 (t, *J* = 7.2 Hz, 1H, PhH), 2.81 (s, 3H, CH_3), 1.47 (s, 9H, $(CH_3)_3$); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.9(CH), 152.2(CH), 151.3(CH), 148.9(CH), 141.5(CH), 133.7(CH), 132.5(CH), 129.5(CH), 128.4(CH×2), 125.6(CH×2), 123.1(CH), 122.5(CH), 121.8(CH), 112.8(CH), 112.4(CH), 34.8(C), 31.4(CH_3×3), 24.6(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3064, 2959, 2864, 1632, 1581, 1460, 1188, 1049, 879, 844, 748, 626. UV (CH_2Cl_2): λmax 247, 290, 327. HRMS (ESI) calcd for [$C_{22}H_{21}NO$+Na]$^{+}$: 338.1515, found: 338.1517. MS (EI) m/z: 315, 300, 202, 136, 77.

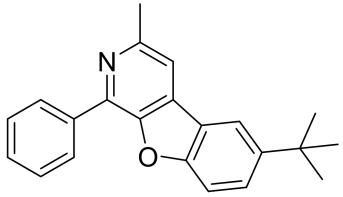


6-chloro-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (**3i).** The product was obtained as a light yellow solid (101 mg, 46%): ^{1}H-NMR (400MHz, $CDCl_3$) δ8.44 – 8.40 (m, 2H, PhH), 7.88 (d, *J* = 1.3 Hz, 1H, PhH), 7.60 (d, *J* = 7.2 Hz, 2H, PhH), 7.53 – 7.50 (m, 4H, PhH, PyH), 2.77 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 155.0(CH), 151.7(CH), 149.4(CH), 141.5(CH), 136.0(CH), 131.7(CH), 129.7(CH), 129.3(CH), 128.7(CH), 128.63(CH×2), 128.57(CH×2),

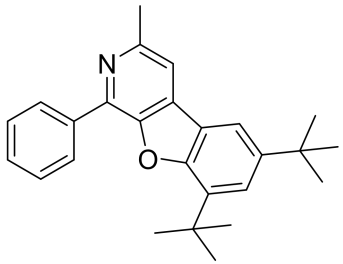
123.8(CH), 121.5(CH), 113.5(CH), 113.1(CH), 24.5(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3043, 1629, 1579, 1452, 1193, 1064, 850, 754, 684, 624. UV (CH_2Cl_2): λmax 245, 299, 329. HRMS (ESI) calcd for $[C_{18}H_{12}NOCl+Na]^+$: 316.0500, found: 316.0501. MS (EI) m/z: 293, 257, 202, 114.



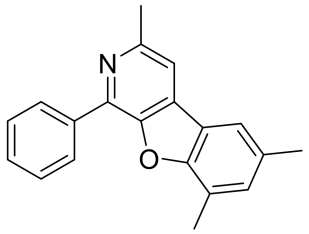
6-bromo-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (**3j**)**.** The product was obtained as a white solid (112 mg, 44%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.3 Hz, 2H, PhH), 8.03 (d, *J* = 1.8 Hz, 1H, PhH), 7.64 (dd, *J* = 8.7, 2.0 Hz, 1H, PhH), 7.61 – 7.55 (m, 2H, PhH), 7.49 (m, 3H, PhH, PyH), 2.76 (s, 3H, CH_3) ; ^{13}C-NMR (100MHz, $CDCl_3$) δ 155.3(CH), 151.7(CH), 149.2(CH), 141.3(CH), 136.0(CH), 132.3(CH), 131.5(CH), 129.3(CH), 128.63(CH×2), 128.58(CH×2), 128.4(CH), 124.6(CH), 116.0(CH), 113.9(CH), 113.1(CH), 24.5(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3057, 1624, 1581, 1450, 1195, 1056, 852, 757, 696, 628. UV (CH_2Cl_2): λmax 247, 298, 332. HRMS (ESI) calcd for $[C_{18}H_{12}NOBr+Na]^+$: 359.9994, found: 359.9993. MS (EI) m/z: 337, 257, 202, 155,129.



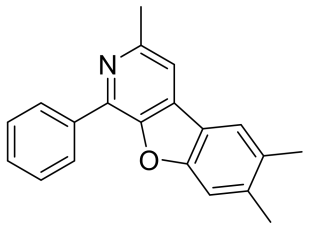
6-(tert-butyl)-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (**3k**)**.** The product was obtained as a white solid (168 mg, 71%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.49 (t, *J* = 7.0 Hz, 2H, PhH), 8.02 (d, *J* = 1.7 Hz, 1H, PhH), 7.71 – 7.65 (m, 2H, PhH), 7.64 – 7.58 (m, 3H, PhH, PyH), 7.55 – 7.47 (t, *J* = 7.4 Hz, 1H, PhH), 2.82 (s, 3H, CH_3), 1.49 (s, 9H, $(CH_3)_3$); ^{13}C-NMR (100MHz, $CDCl_3$) δ 155.1(CH), 151.2(CH), 146.4(CH), 141.1(CH), 136.4(CH), 133.1(CH), 129.1(CH), 128.7(CH×2), 128.6(CH×2), 128.5(CH), 127.6(CH), 122.0(CH), 117.8(CH), 113.2(CH), 111.8(CH), 34.9(C), 31.8(CH_3×3), 24.5(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3060, 2960, 2864, 1633, 1581, 1460, 1195, 1045, 812, 761, 694. UV (CH_2Cl_2): λmax 247, 295, 325. HRMS (ESI) calcd for $[C_{22}H_{21}NO+Na]^+$: 338.1515, found: 338.1515. MS (EI) m/z: 315, 300, 272, 202, 136, 77.



6, 8-di-tert-butyl-3-methyl-1-phenylbenzofuro[2,3-c]-pyridine (3l). The product was obtained as a yellow solid (217 mg, 78%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.55 (d, *J* = 7.4 Hz, 2H, PhH), 7.90 (d, *J* = 1.7 Hz, 1H, PhH), 7.73 (s, 1H, PhH), 7.62 (m, 3H, PhH, PyH), 7.51 (t, *J* = 7.4 Hz, 1H, PhH), 2.83 (s, 3H, CH_3), 1.67 (s, 9H, $(CH_3)_3$), 1.50 (s, 9H, $(CH_3)_3$); ^{13}C-NMR (100MHz, $CDCl_3$) δ 153.3(CH), 150.9(CH), 148.9(CH), 146.2(CH), 140.6(CH), 136.7(CH), 134.9(CH), 133.2(CH), 128.9(CH), 128.6(CH×2), 128.5(CH×2), 124.2(CH), 122.3(CH), 115.6(CH), 113.1(CH), 35.1(C), 34.7(C), 31.9(CH_3×3), 29.9(CH_3×3), 24.6(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3056, 2939, 2868, 1627, 1585, 1453, 1191, 1040, 758, 688. UV (CH_2Cl_2): λmax 249, 297, 329. HRMS (ESI) calcd for $[C_{26}H_{29}NO+Na]^+$: 394.2141, found: 394.2142. MS (EI) m/z: 371, 356, 328, 202, 136, 77.

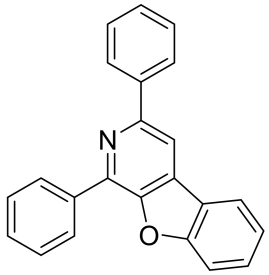


3,6,8-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (3m). The product was obtained as a white solid (123 mg, 57%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.52 ((d, *J* = 7.2 Hz, 2H, PhH), 7.62 (t, *J* = 6.9 Hz, 2H, PhH), 7.53 (d, *J* = 3.9 Hz, 1H, PhH), 7.50 (d, *J* = 7.8 Hz, 2H, PhH, PyH), 7.14 (s, 1H, PhH), 2.79 (s, 3H, CH_3), 2.56 (s, 3H, CH_3), 2.46 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 154.2(CH), 150.9(CH), 149.0(CH), 140.8(CH), 136.6(CH), 133.1(CH), 132.6(CH), 131.7(CH), 129.0(CH), 128.6(CH×2), 128.5(CH×2), 121.9(CH), 121.6(CH), 118.8(CH), 113.2(CH), 24.5(CH_3), 21.3(CH_3), 15.2(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3022, 2922, 2850, 1631, 1577, 1452, 1180, 1093, 846, 757, 692, 634. UV (CH_2Cl_2): λmax 248, 295, 329. HRMS (ESI) calcd for $[C_{20}H_{17}NO+Na]^+$:310.1202, found: 310.1202. MS (EI) m/z: 287, 242, 202, 143, 77.

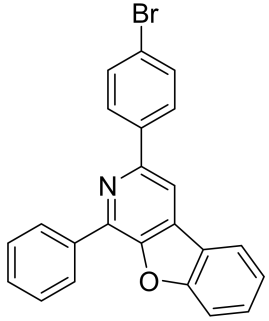


3,6,7-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (3n). The product was obtained as a yellow oil (136 mg, 63%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.3, 2H, PhH), 7.62 (m, 3H, PhH), 7.55 – 7.48 (m, 2H, PhH), 7.37 (s, 1H,

PyH), 2.78 (s, 3H, CH_3), 2.40 (s, 3H, CH_3), 2.38 (s, 3H, CH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 155.8(CH), 151.0(CH), 148.9(CH), 140.8(CH), 139.3(CH), 136.6(CH), 132.9(CH), 131.8(CH), 128.9(CH), 128.7(CH×2), 128.5(CH×2), 121.7(CH), 119.9(CH), 112.9(CH), 112.7(CH), 24.5(CH_3), 20.9(CH_3), 19.9(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3057, 2918, 2852, 1635, 1575, 1454, 1205, 1028, 837, 756, 692. UV (CH_2Cl_2): λmax 249, 300, 327. HRMS (ESI) calcd for $[C_{20}H_{17}NO+Na]^+$:310.1202, found: 310.1201. MS (EI) m/z: 287, 242, 202, 143, 77.

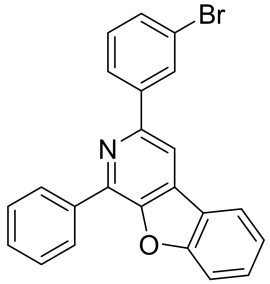


1, 3-diphenylbenzofuro[2,3-c]pyridine (3o). The product was obtained as a white solid (77 mg, 32%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.66 (d, *J* = 7.3 Hz, 2H, PhH), 8.27 (t, *J* = 3.6 Hz, 3H, PhH, PyH), 8.10 (d, *J* = 7.8 Hz, 1H, PhH), 7.73 (d, *J* = 8.4 Hz, 1H, PhH), 7.67 – 7.62 (m, 3H, PhH), 7.59 – 7.53 (m, 3H, PhH), 7.47 (dd, *J* = 7.4, 2.6 Hz, 2H, PhH); ^{13}C-NMR (100MHz, $CDCl_3$) δ 157.0(CH), 150.8(CH), 149.7(CH), 141.3(CH), 139.8(CH), 136.4(CH), 133.2(CH), 129.8(CH), 129.3(CH), 128.8(CH×2), 128.7(CH×2), 128.6(CH×2), 128.4(CH), 127.1(CH×2), 123.3(CH), 122.6(CH), 121.9(CH), 112.6(CH), 110.6(CH); IR ν_{max}(KBr)/cm^{-1}: 3060, 1624, 1570, 1458, 1413, 1191, 1018, 866, 734, 690. UV (CH_2Cl_2): λmax 230, 257, 335. HRMS (ESI) calcd for $[C_{23}H_{15}NO+Na]^+$: 344.1046, found: 344.1047. MS (EI) m/z: 321, 291, 214, 160, 77.

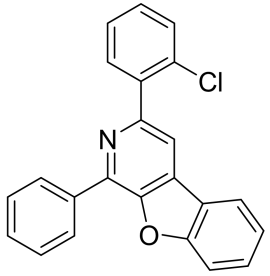


3-(4-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (3p). The product was obtained as a yellow solid (225 mg, 75%): ^{1}H-NMR (400MHz, CDCl3) δ 8.59 (d, *J* = 7.4 Hz, 2H, PhH), 8.10 (s, 1H, PyH), 8.06 (d, *J* = 8.4 Hz, 2H, PhH), 8.00 (d, *J* = 7.6 Hz, 1H, PhH), 7.63 (dd, *J* = 17.1, 8.6 Hz, 7H, PhH), 7.45 – 7.40 (m, 1H, PhH); ^{13}C-NMR (100MHz, $CDCl_3$) δ 157.0(CH), 149.8(CH), 149.2(CH), 141.3(CH), 138.4(CH), 136.1(CH), 133.2(CH), 131.8(CH×2), 129.9(CH), 129.4(CH), 128.7(CH×2), 128.6(CH×2), 128.5(CH×2), 123.5(CH), 122.7(CH), 122.4(CH), 121.8(CH), 112.6(CH), 110.2(CH); IR ν_{max}(KBr)/cm^{-1}: 3053, 1625, 1579, 1452, 1411, 1191, 1006, 877, 748, 688, 624. UV (CH_2Cl_2): λmax 229, 263, 335.

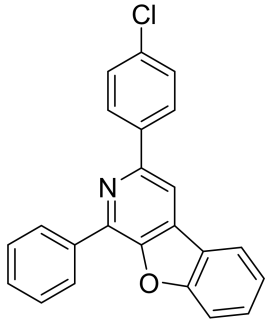
HRMS (ESI) calcd for $[C_{23}H_{14}NOBr+Na]^+$: 422.0151, found: 422.0151. MS (EI) m/z: 399, 320, 290, 263, 214, 187, 160, 77.



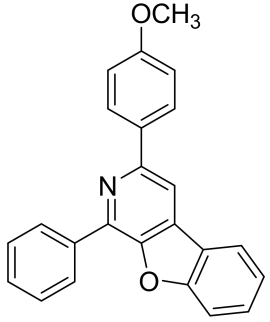
3-(3-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (3q). The product was obtained as a yellow oil (243 mg, 81%): ^{1}H-NMR (400MHz, $CDCl_3$) δ8.57 (d, *J* = 7.7 Hz, 2H, PhH), 8.34 (s, 1H, PyH), 8.08 (d, *J* = 7.8 Hz, 1H, PhH), 8.02 (s, 1H, PhH), 7.95 (d, *J* = 7.7 Hz, 1H, PhH), 7.64 – 7.55 (m, 6H, PhH), 7.42 – 7.35 (m, 2H, PhH); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.9(CH), 149.9(CH), 148.7(CH), 141.6(CH), 141.3(CH), 136.1(CH), 133.1(CH), 131.2(CH), 130.1(CH), 130.0(CH), 129.9(CH), 129.5(CH), 128.7(CH×2), 128.6(CH×2), 125.5(CH), 123.5(CH), 123.0(CH), 122.3(CH), 121.8(CH), 112.5(CH), 110.6(CH); IR ν_{max}(KBr)/cm^{-1}: 3053, 1629, 1554, 1452, 1411, 1191, 1024, 875, 790, 736, 688, 617. UV (CH_2Cl_2): λmax 234, 258, 335. HRMS (ESI) calcd for $[C_{23}H_{14}NOBr+Na]^+$: 422.0151, found: 422.0150. MS (EI) m/z: 399, 320, 290, 214, 187, 160, 87.



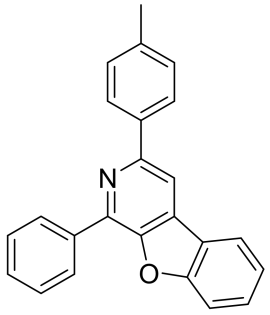
3-(2-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (3r). The product was obtained as a yellow oil (147 mg, 55%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.64 – 8.58 (m, 2H, PhH), 8.19 (s, 1H, PyH), 8.07 (d, *J* = 7.7 Hz, 1H, PhH), 7.85 (dd, *J* = 7.5, 1.8 Hz, 1H, PhH), 7.74 (d, *J* = 8.3 Hz, 1H, PhH), 7.66 – 7.59 (m, 4H, PhH), 7.54 (d, *J* = 7.3 Hz, 1H, PhH), 7.48 – 7.40 (m, 3H, PhH); ^{13}C-NMR (100MHz, $CDCl_3$) δ 157.0(CH), 150.0(CH), 149.7(CH), 141.7(CH), 139.6(CH), 136.2(CH), 132.5(CH), 132.4(CH), 132.2(CH), 130.2(CH), 129.9(CH), 129.4(CH), 129.3(CH), 128.9(CH×2), 128.6(CH×2), 127.1(CH), 123.4(CH), 122.4(CH), 122.0(CH), 115.3(CH), 112.5(CH); IR ν_{max}(KBr)/cm^{-1}: 3063, 3031, 1625, 1579, 1454, 1417, 1191, 1035, 875, 735, 680, 622. UV (CH_2Cl_2): λmax 229, 254, 327. HRMS (ESI) calcd for $[C_{23}H_{14}NOCl+Na]^+$: 378.0656, found: 378.0652. MS (EI) m/z: 355, 320, 263, 189, 160, 77.



3-(4-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (3s). The product was obtained as a yellow solid (168 mg, 63%): ^{1}H-NMR (400MHz, $CDCl_3$) 8.66 – 8.59 (m, 2H, PhH), 8.23 – 8.15 (m, 3H, PhH, PyH), 8.08 (d, *J* = 7.7 Hz, 1H, PhH), 7.73 (d, *J* = 8.3 Hz, 1H, PhH), 7.68 – 7.60 (m, 3H, PhH), 7.55 – 7.44 (m, 4H, PhH); ^{13}C-NMR (100MHz, $CDCl_3$) δ 157.1(CH), 149.9(CH), 149.5(CH), 141.5(CH), 138.2(CH), 136.2(CH), 134.5(CH), 133.3(CH), 129.9(CH), 129.5(CH), 128.84(CH×2), 128.76(CH×2), 128.6(CH×2), 128.3(CH×2), 123.5(CH), 122.5(CH), 121.9(CH), 112.6(CH), 110.4(CH); IR ν_{max}(KBr)/cm^{-1}: 3060, 1629, 1583, 1458, 1421, 1191, 1016, 829, 744, 688, 615. UV (CH_2Cl_2): λmax 230, 261, 337. HRMS (ESI) calcd for $[C_{23}H_{14}NOCl+Na]^+$: 378.0656, found: 378.0655. MS (EI) m/z: 355, 320, 290, 263, 214, 189, 160, 77

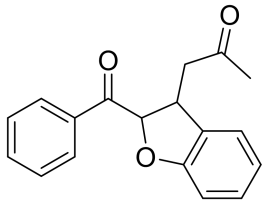


3-(4-methoxyphenyl)-1-phenylbenzofuro[2,3-c]pyridine (3t). The product was obtained as a yellow oil (171 mg, 65%): ^{1}H-NMR (400MHz, $CDCl_3$) δ 8.65 (d, *J* = 7.4 Hz, 2H, PhH), 8.21 (d, *J* = 8.9 Hz, 3H, PhH, PyH), 8.10 (d, *J* = 7.7 Hz, 1H, PhH), 7.73 (d, *J* = 8.3 Hz, 1H, PhH), 7.67 – 7.60 (m, 3H, PhH), 7.54 (d, *J* = 7.2 Hz, 1H, PhH), 7.46 (t, *J* = 7.5 Hz, 1H, PhH), 7.09 (d, *J* = 8.8 Hz, 2H, PhH), 3.93 (s, 3H, OCH_3); ^{13}C-NMR (100MHz, $CDCl_3$) δ 160.0(CH), 156.9(CH), 150.6(CH), 149.5(CH), 141.2(CH), 136.6(CH), 133.1(CH), 132.5(CH), 129.7(CH), 129.3(CH), 128.8(CH×2), 128.5(CH×2), 128.3(CH×2), 123.3(CH), 122.5(CH), 121.7(CH), 114.1(CH×2), 112.6(CH), 109.8(CH), 55.4(OCH_3); IR ν_{max}(KBr)/cm^{-1}: 3062, 2960, 2925, 1610, 1587, 1458, 1415, 1191, 1024, 877, 744, 690, 621. UV (CH_2Cl_2): λmax 231, 265, 341. HRMS (ESI) calcd for $[C_{24}H_{17}NO_2+Na]^+$: 374.1151, found: 374.1152. MS (EI) m/z: 351, 308, 278, 214, 153, 77.



1-phenyl-3-(p-tolyl)benzofuro[2,3-c]pyridine (3u). The product was obtained as a white solid (209 mg, 83%): ^{1}H-NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 7.3 Hz, 2H, PhH), 8.21 (s, 1H, PyH), 8.17 (d, *J* = 8.1 Hz,

2H, PhH), 8.06 (d, *J* = 7.6 Hz, 1H, PhH), 7.71 (d, *J* = 8.3 Hz, 1H, PhH), 7.68 – 7.59 (m, 3H, PhH), 7.55 (t, *J* = 7.3 Hz, 1H, PhH), 7.44 (t, *J* = 7.4 Hz, 1H, PhH), 7.37 (d, *J* = 7.9 Hz, 2H, PhH), 2.49 (s, 3H, $COCH_3$); ^{13}C-NMR (100MHz, $CDCl_3$) δ 156.9(CH), 150.7(CH), 149.7(CH), 141.0(CH), 138.3(CH), 137.0(CH), 136.6(CH), 133.2(CH), 129.7(CH), 129.5(CH×2), 129.3(CH), 128.9(CH×2), 128.6(CH×2), 126.9(CH×2), 123.3(CH), 122.7(CH), 121.8(CH), 112.4(CH), 110.2(CH), 21.4(CH_3); IR ν_{max}(KBr)/cm^{-1}: 3024, 2952, 2916, 1625, 1583, 1452, 1423, 1190, 1020, 875, 738, 690, 619. UV (CH_2Cl_2): λmax 233, 258, 340. HRMS (ESI) calcd for $[C_{24}H_{17}NO+Na]^+$: 358.1202, found: 358.1205. MS (EI) m/z: 335, 290, 189, 167, 77.

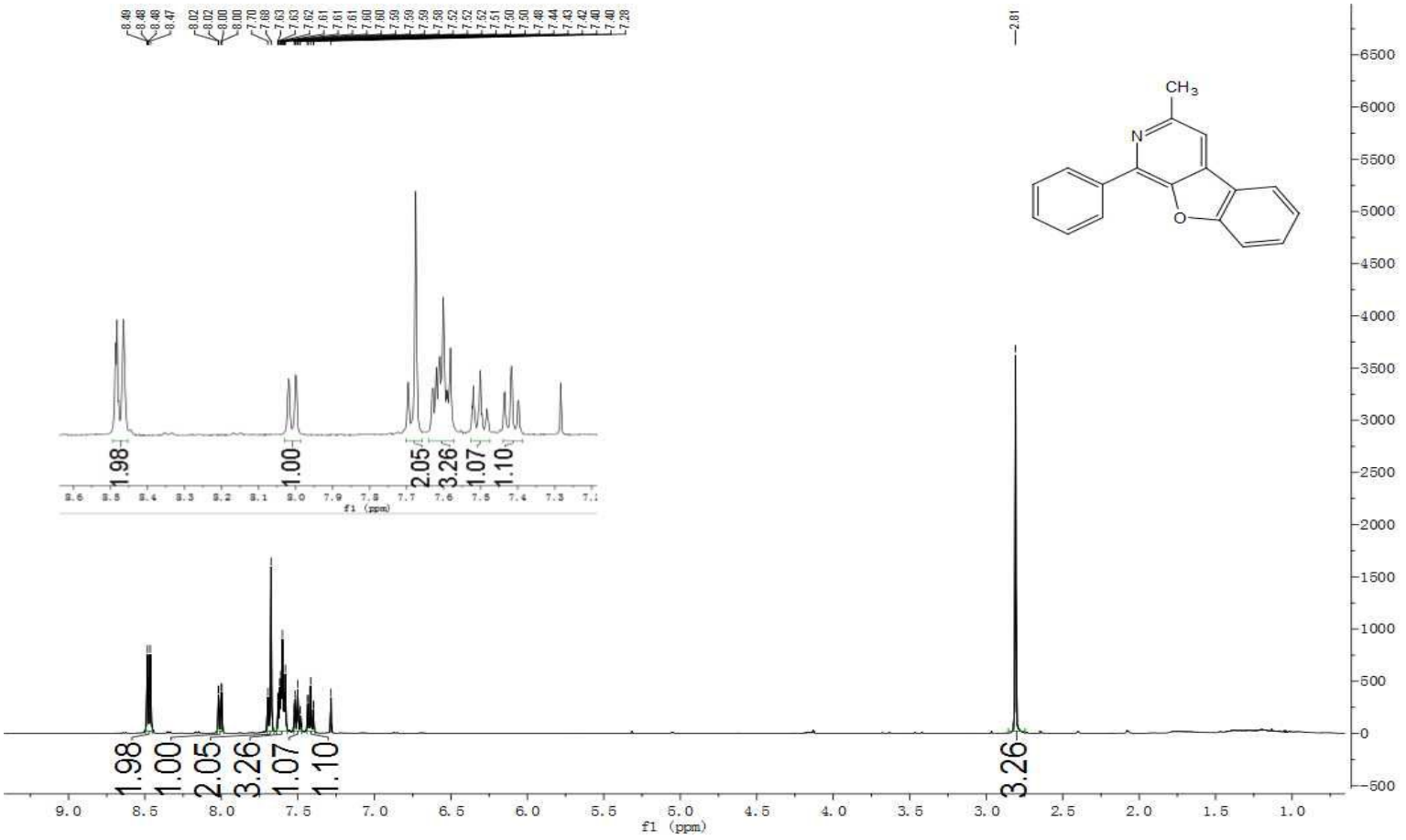


1-(2-benzoyl-2,3-dihydrobenzofuran-3-yl)propan-2-one (4a). The product was obtained as a pale yellow solid (200 mg, 95%): ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.13 – 7.98 (m, 1H, PhH), 7.62 (t, *J* = 7.4 Hz, 1H, PhH), 7.51 (t, *J* = 7.6 Hz, 1H, PhH), 7.18 (t, *J* = 7.2 Hz, 1H, PhH), 6.92 (t, *J* = 7.2 Hz, 1H, PhH), 6.87 (d, *J* = 8.2 Hz, 1H, PhH), 5.56 (d, *J* = 5.8 Hz, 1H, OCHCO), 4.37 (dd, *J* = 13.4, 6.4 Hz, 1H, CH_2CH), 3.09 (dd, *J* = 17.7, 6.3 Hz, 1H, $COCH_2$), 2.91 (dd, *J* = 17.7, 7.8 Hz, 1H, $COCH_2$), 2.19 (s, 3H, $COCH_3$). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 206.6, 194.9, 158.5, 134.9, 133.7, 129.3, 128.8, 128.7, 128.7, 124.7, 121.4, 109.9, 87.4, 48.6, 39.4, 30.2; HRMS (ESI) calcd for $[C_{18}H_{16}O_3+Na]^+$: 303.0992, found: 303.0993.

4 Copies of ^{1}H NMR and ^{13}C NMR of products

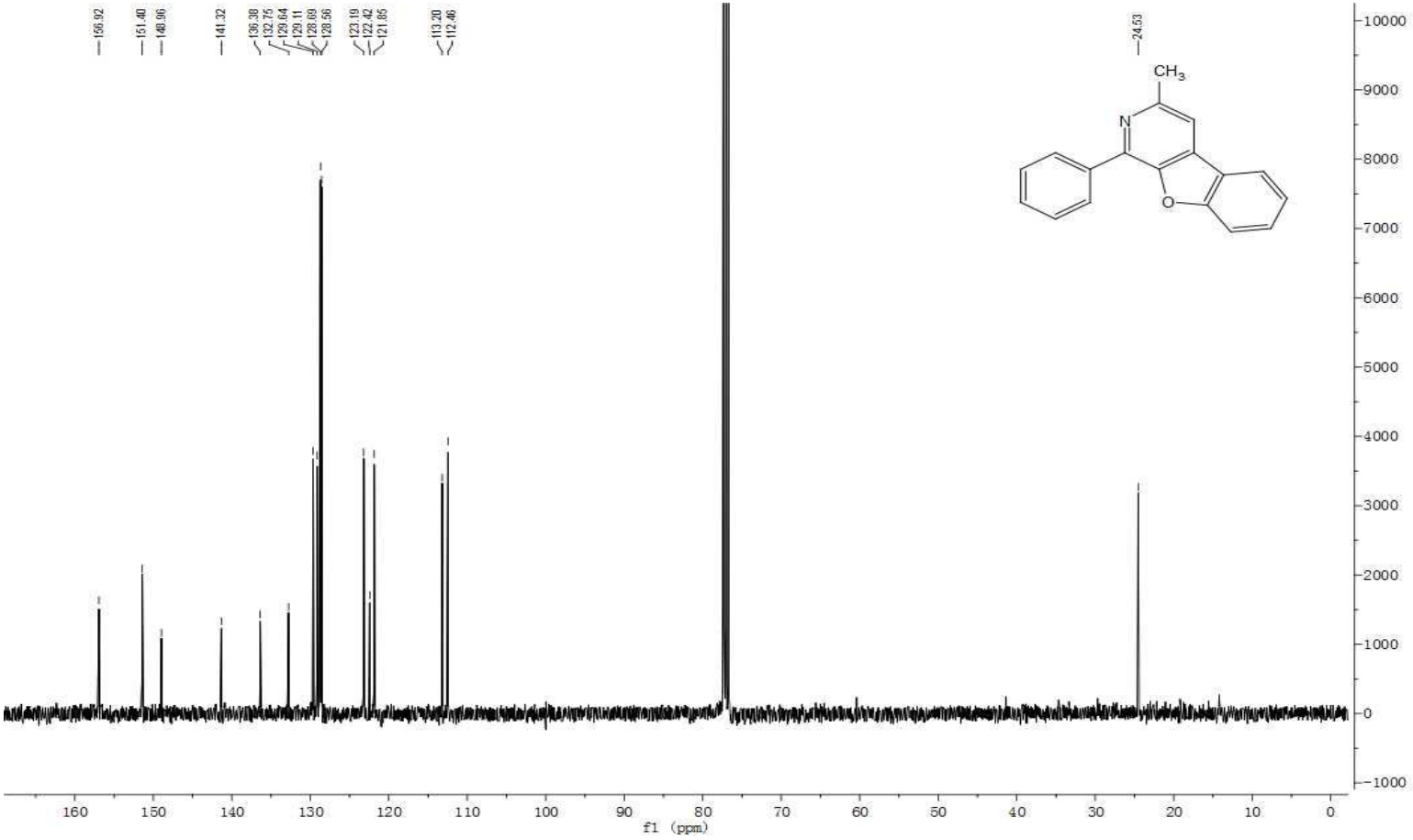
3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 1)

^{1}H NMR



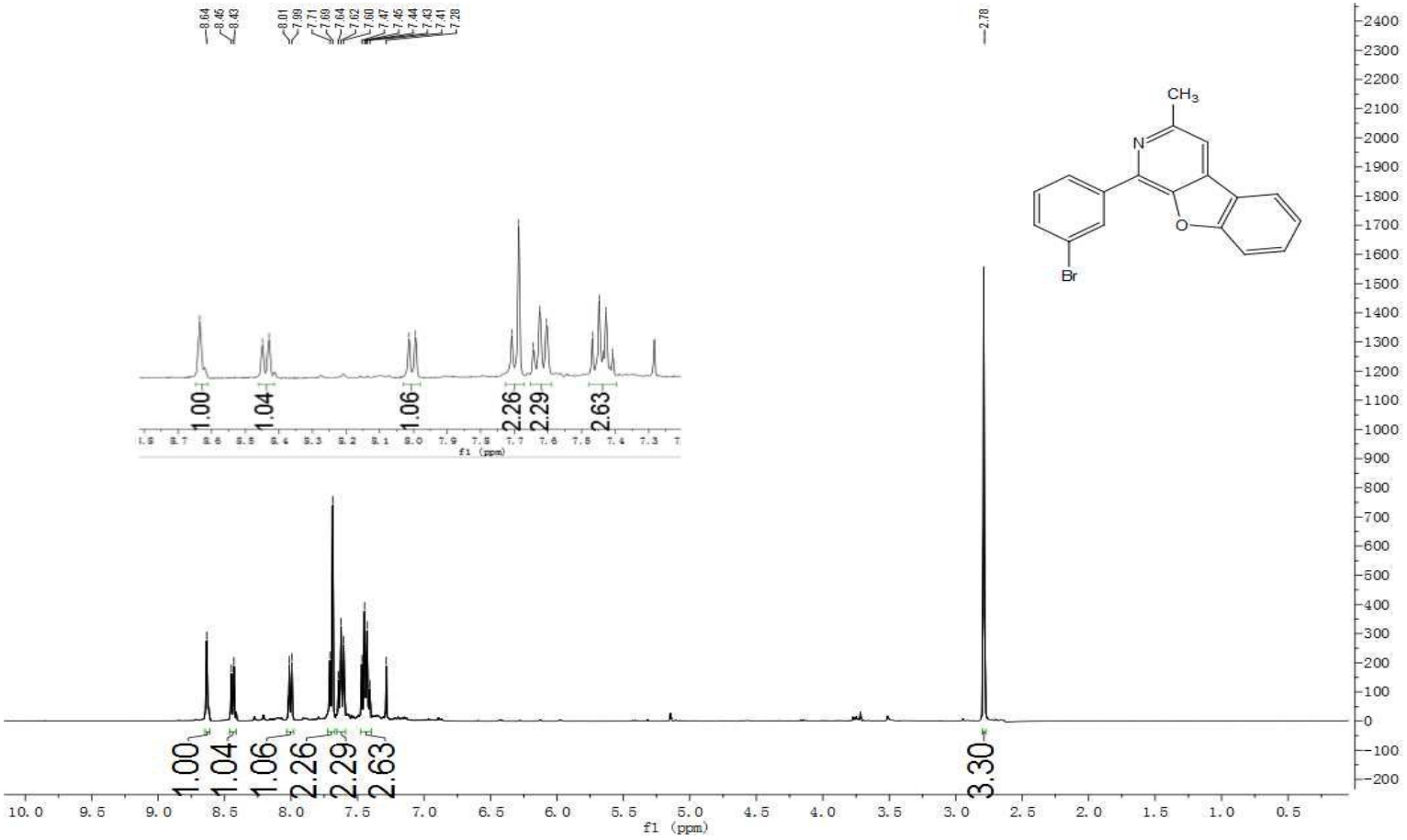
3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 1)

^{13}C NMR



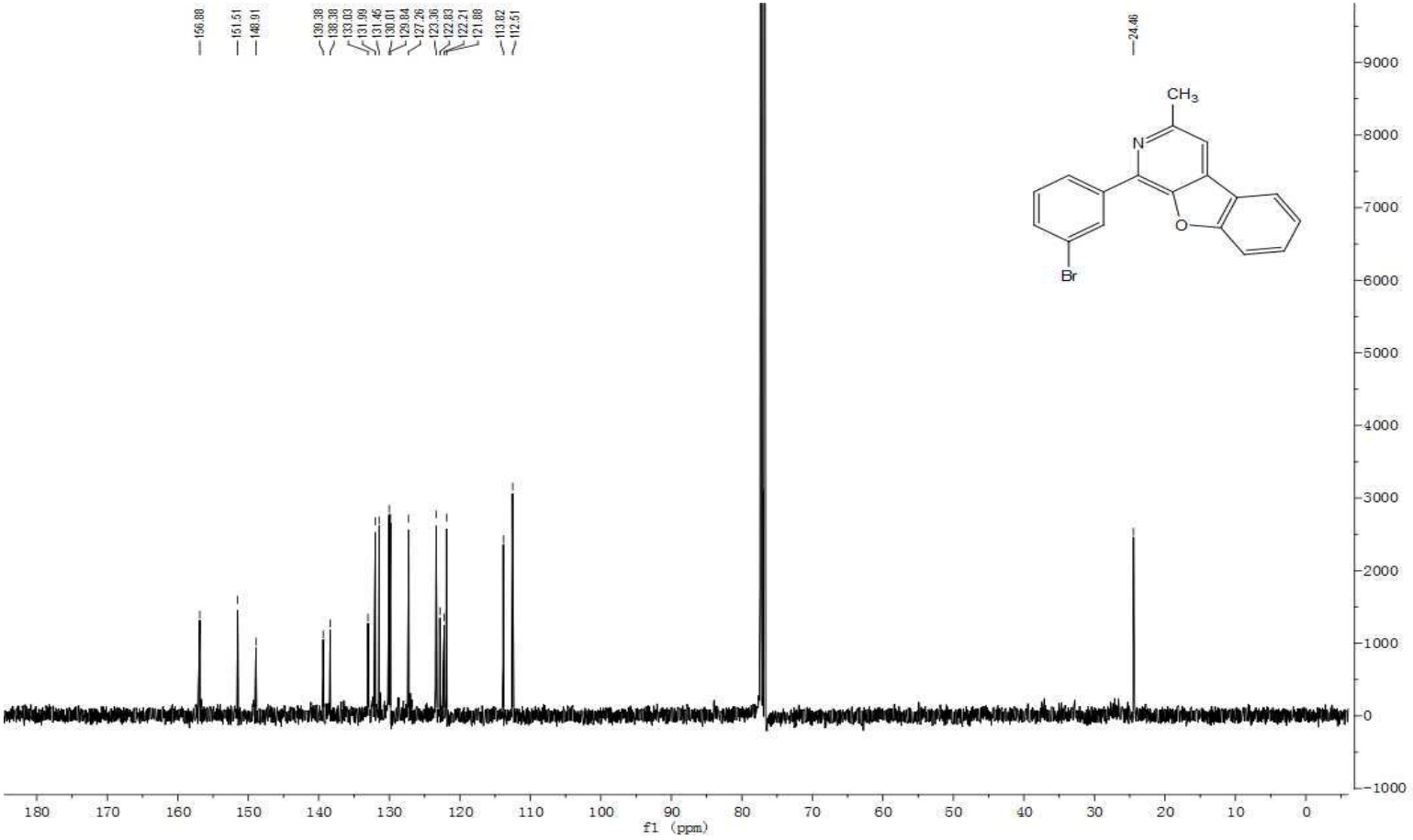
1-(3-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 2)

^{1}H NMR



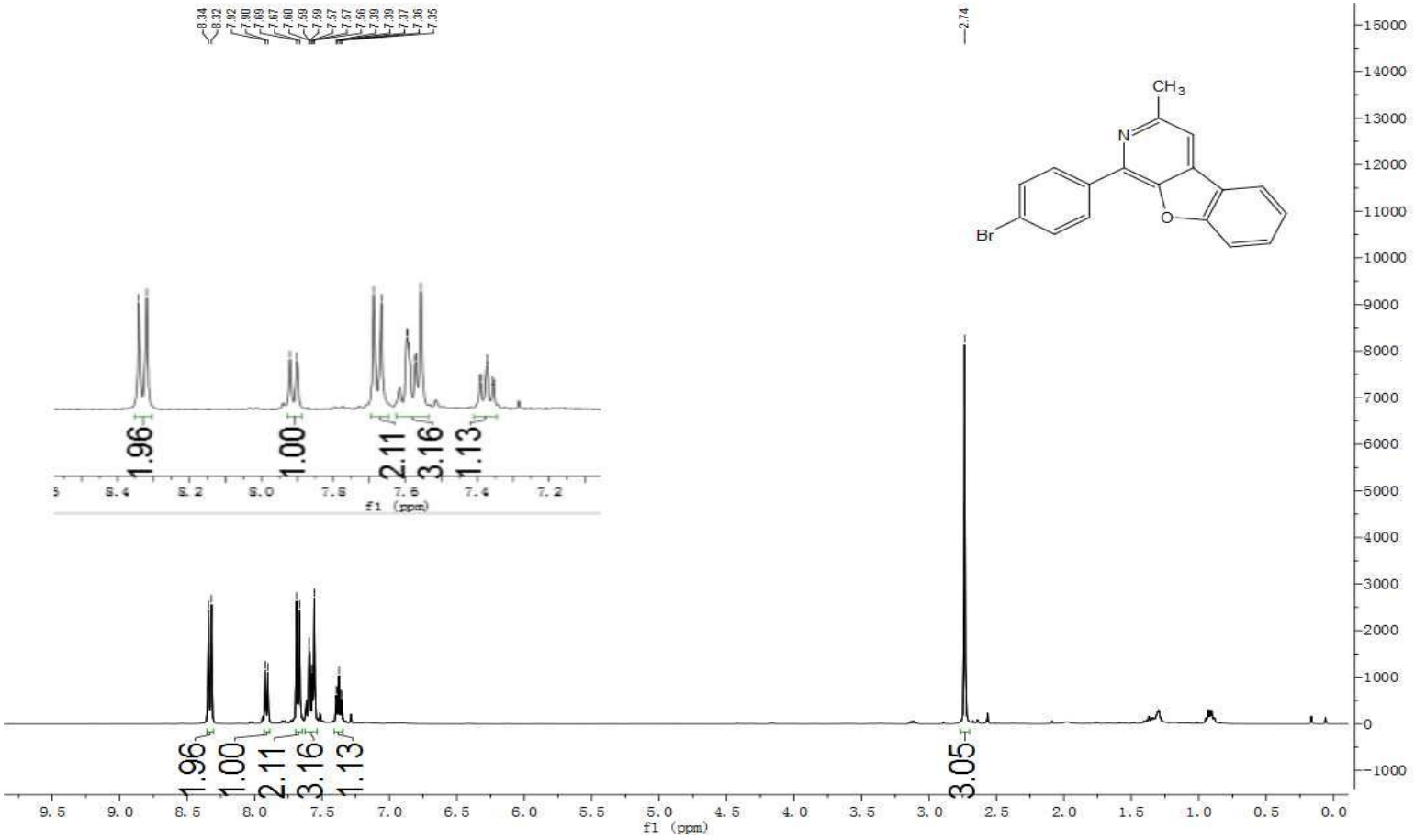
1-(3-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 2)

^{13}C NMR



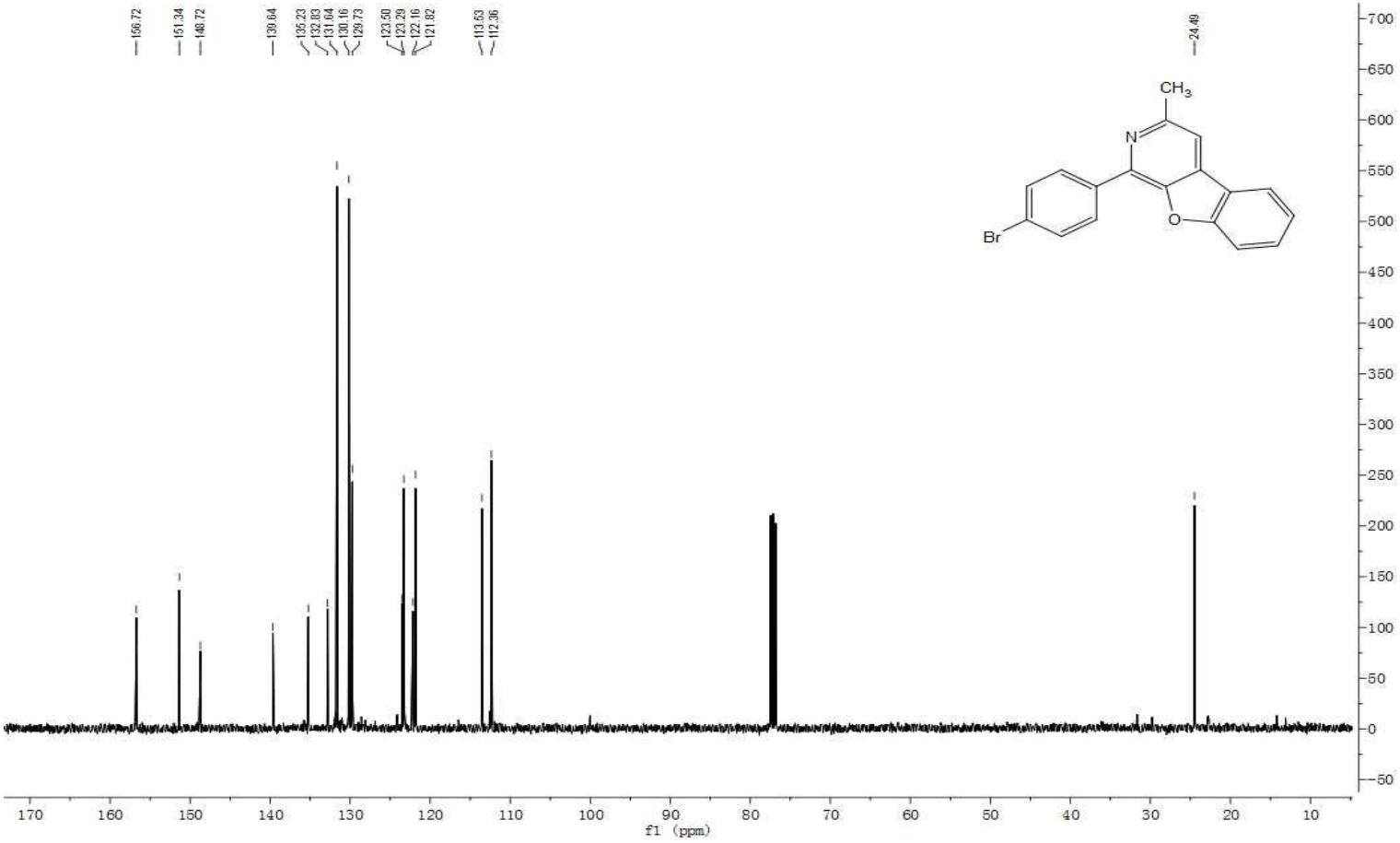
1-(4-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 3)

^{1}H NMR



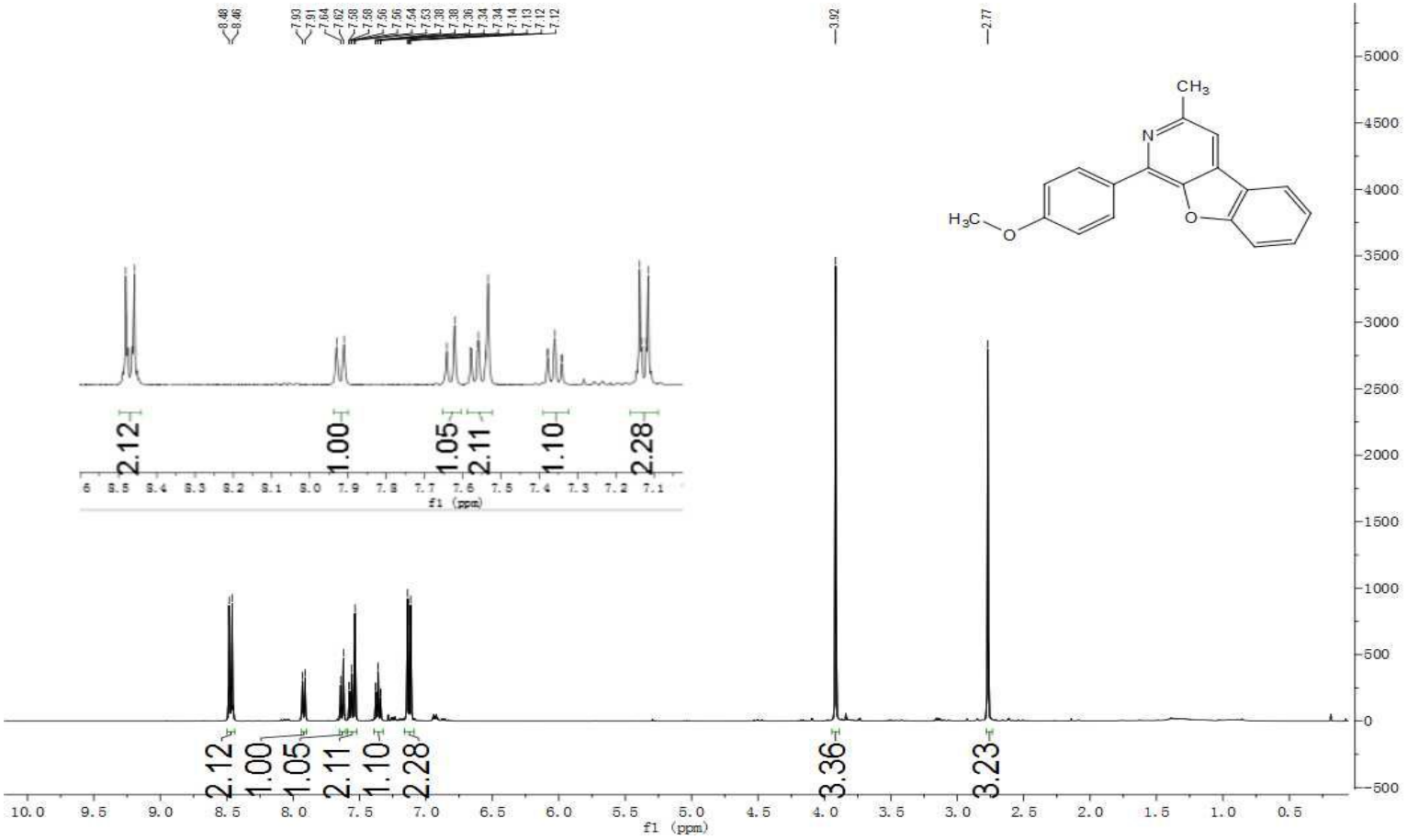
1-(4-bromophenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 3)

^{13}C NMR



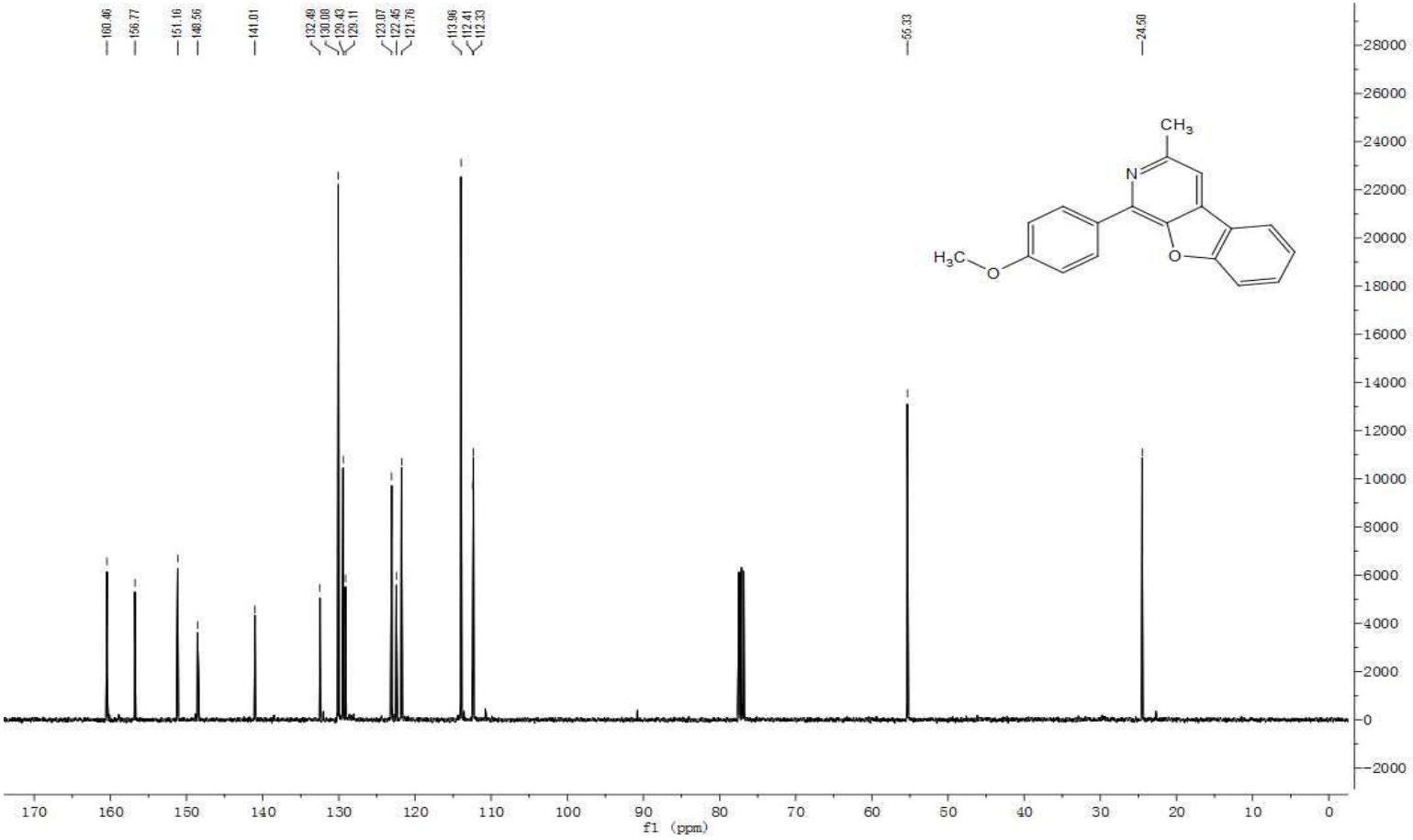
1-(4-methoxyphenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 4)

^{1}H NMR



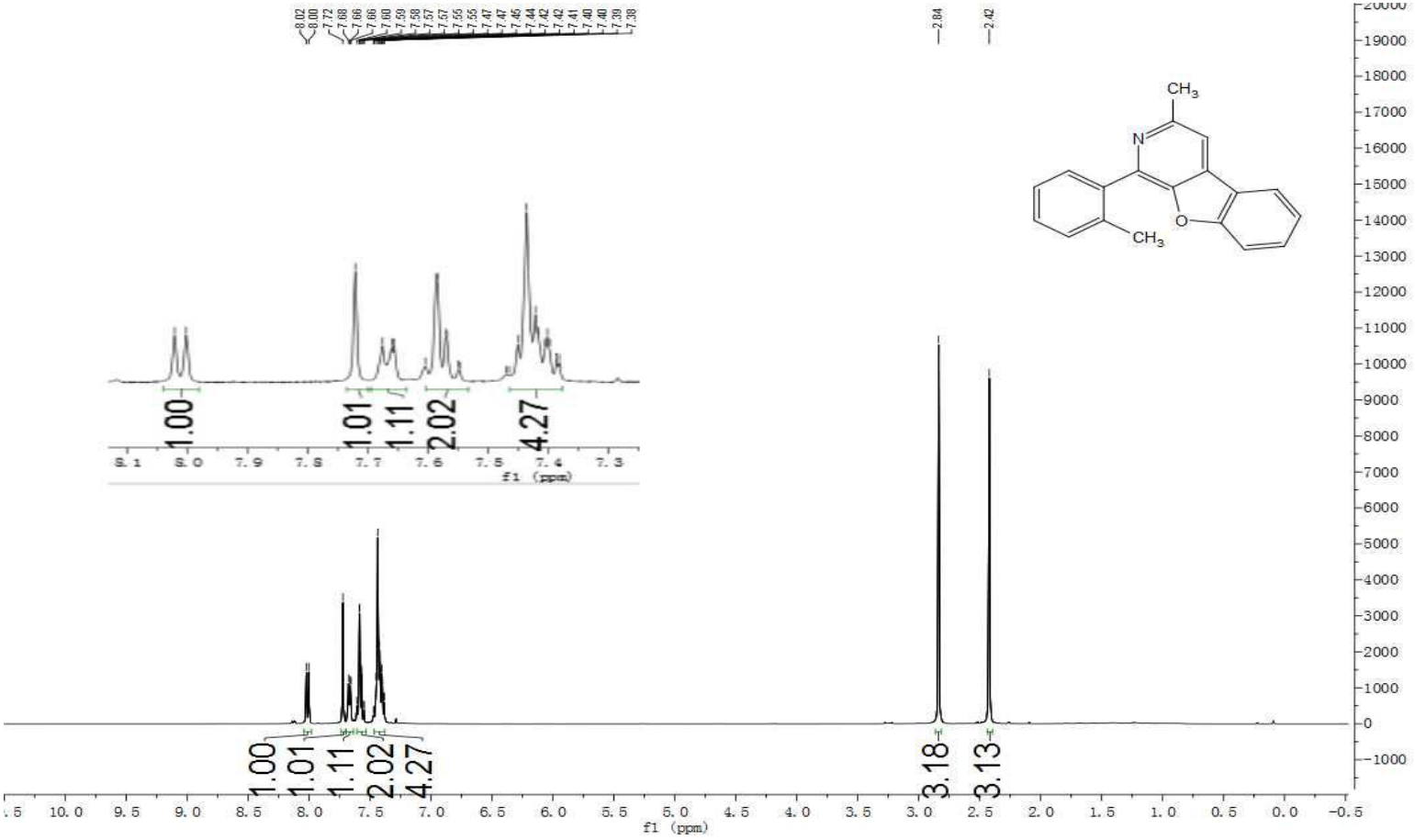
1-(4-methoxyphenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 4)

^{13}C NMR



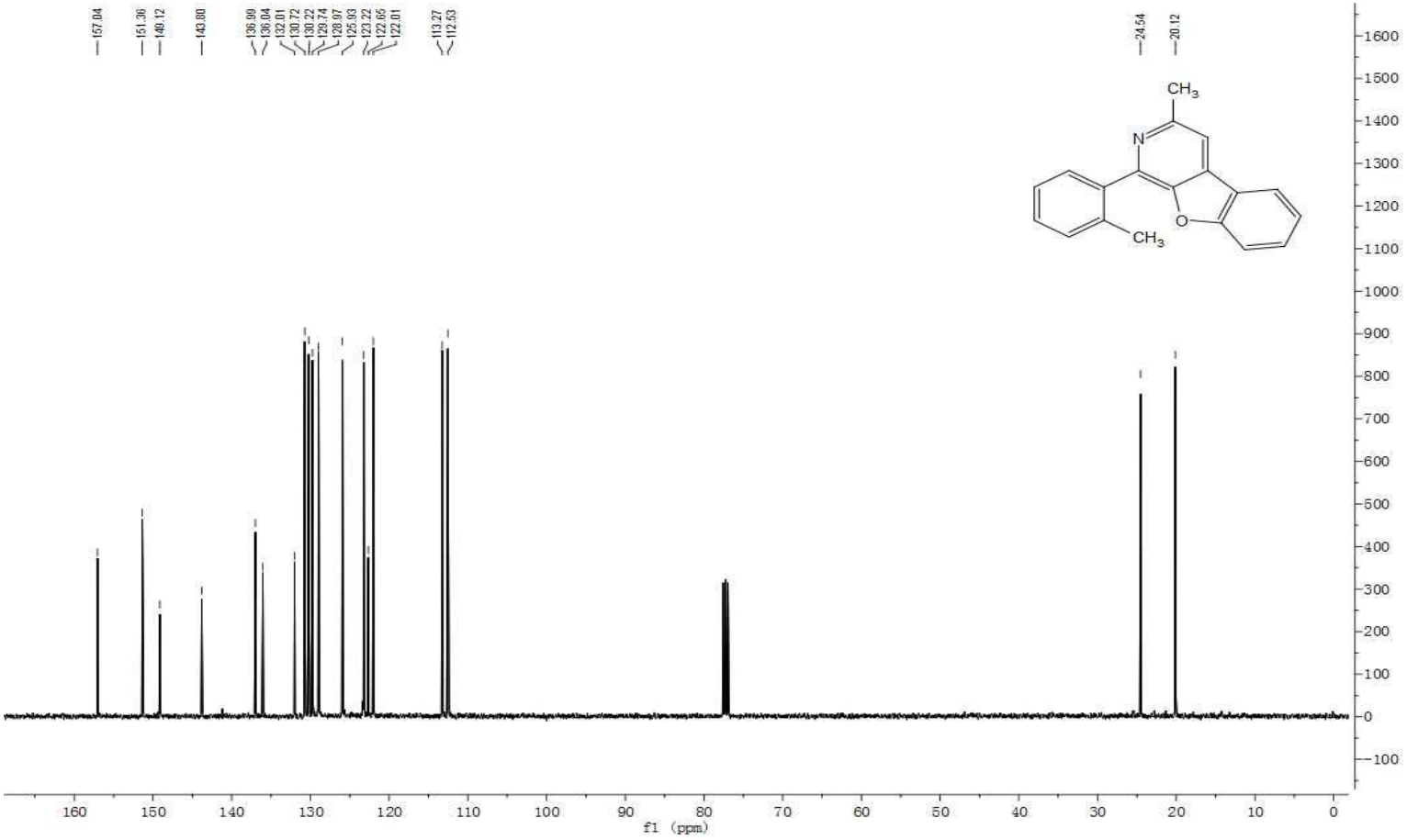
3-methyl-1-(o-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry 5)

^{1}H NMR



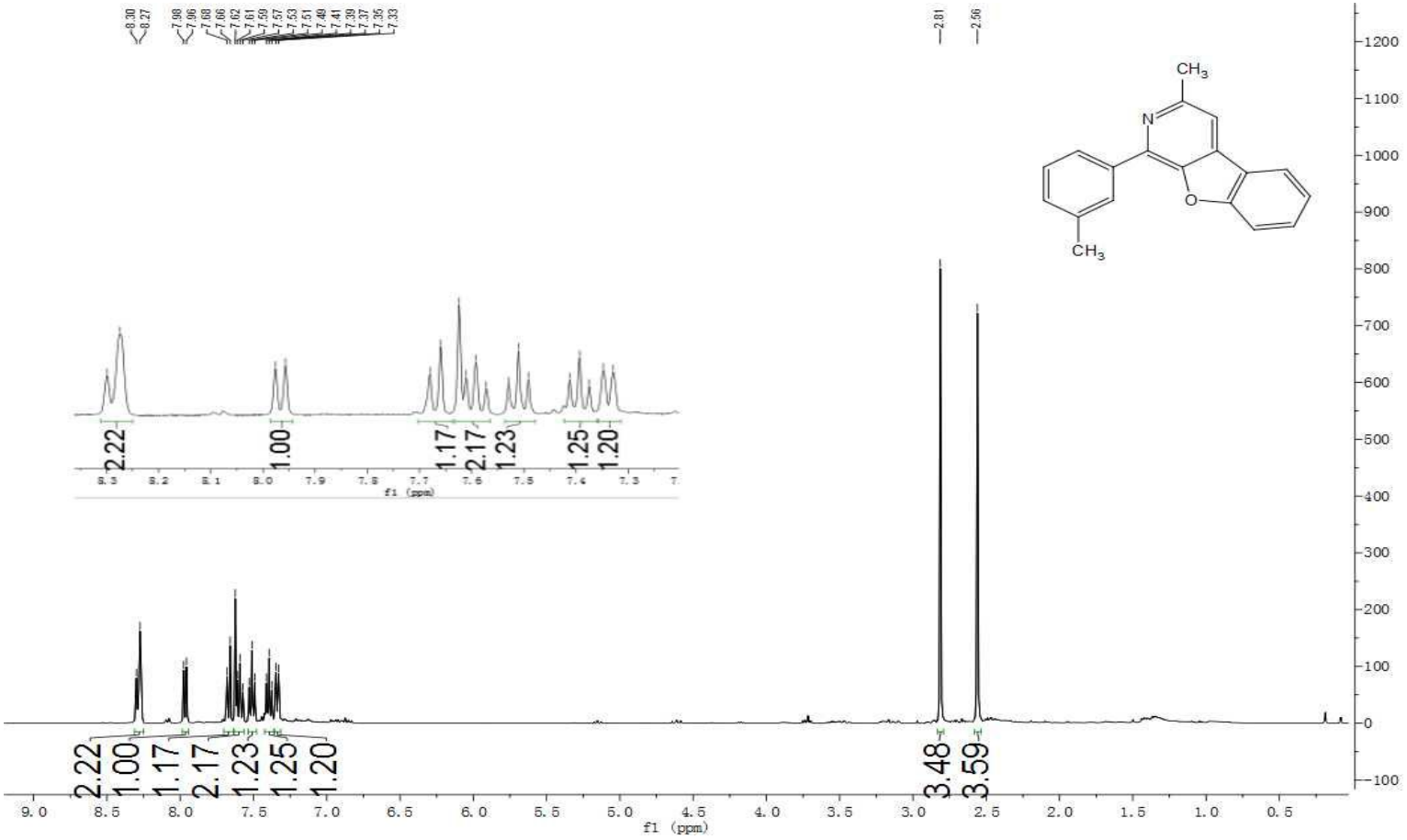
3-methyl-1-(o-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry 5)

^{13}C NMR



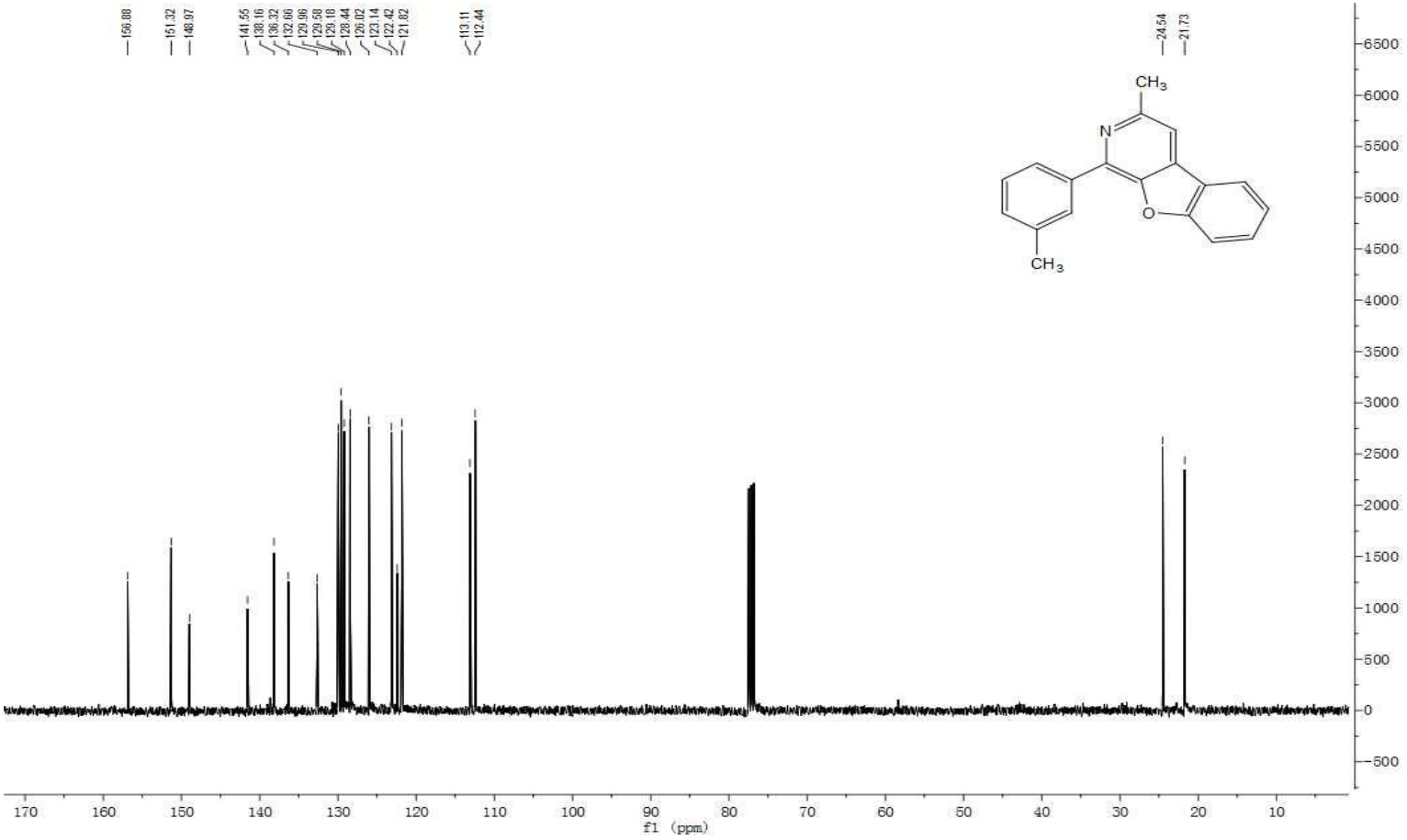
3-methyl-1-(m-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry6)

^{1}H NMR



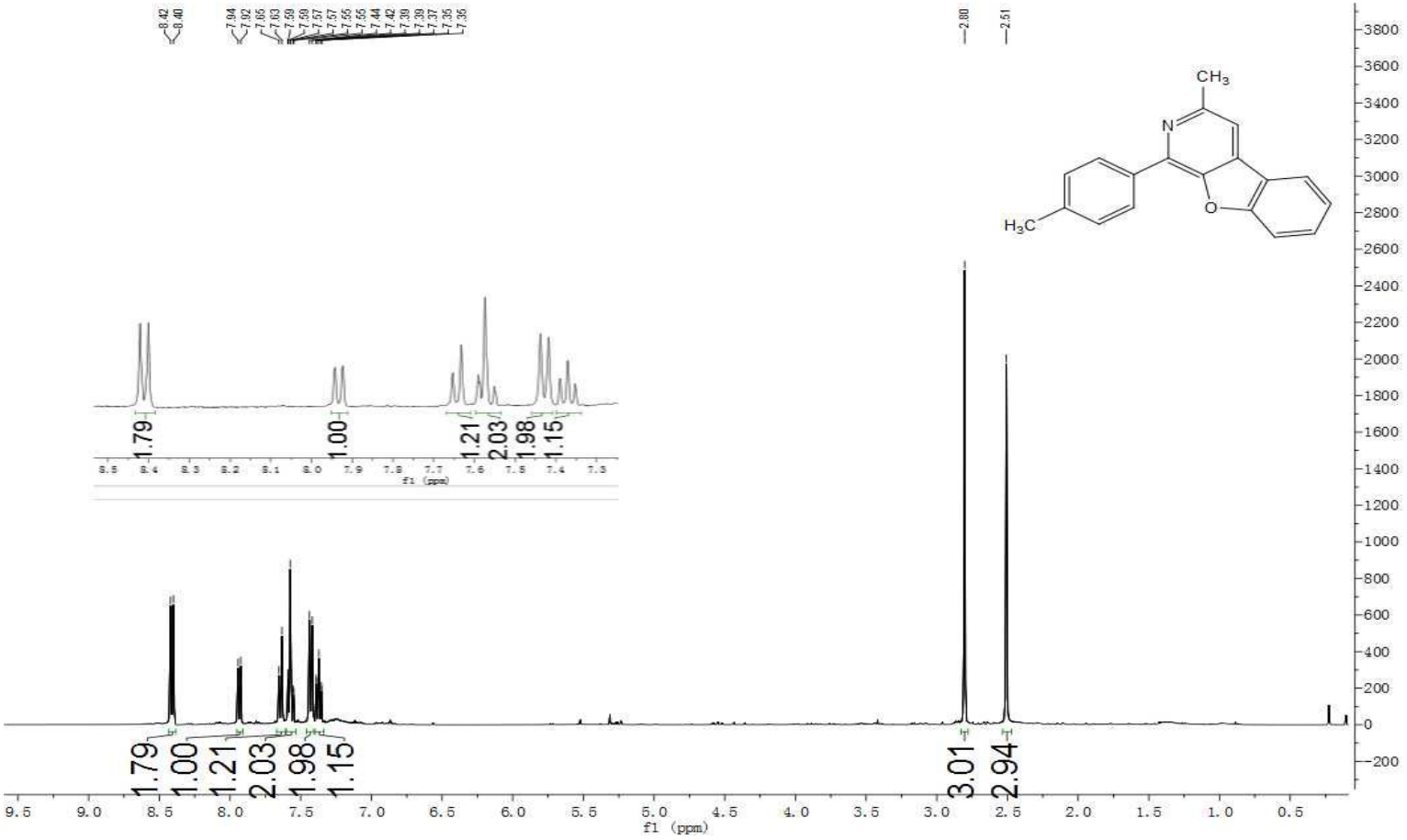
3-methyl-1-(m-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry6)

^{13}C NMR



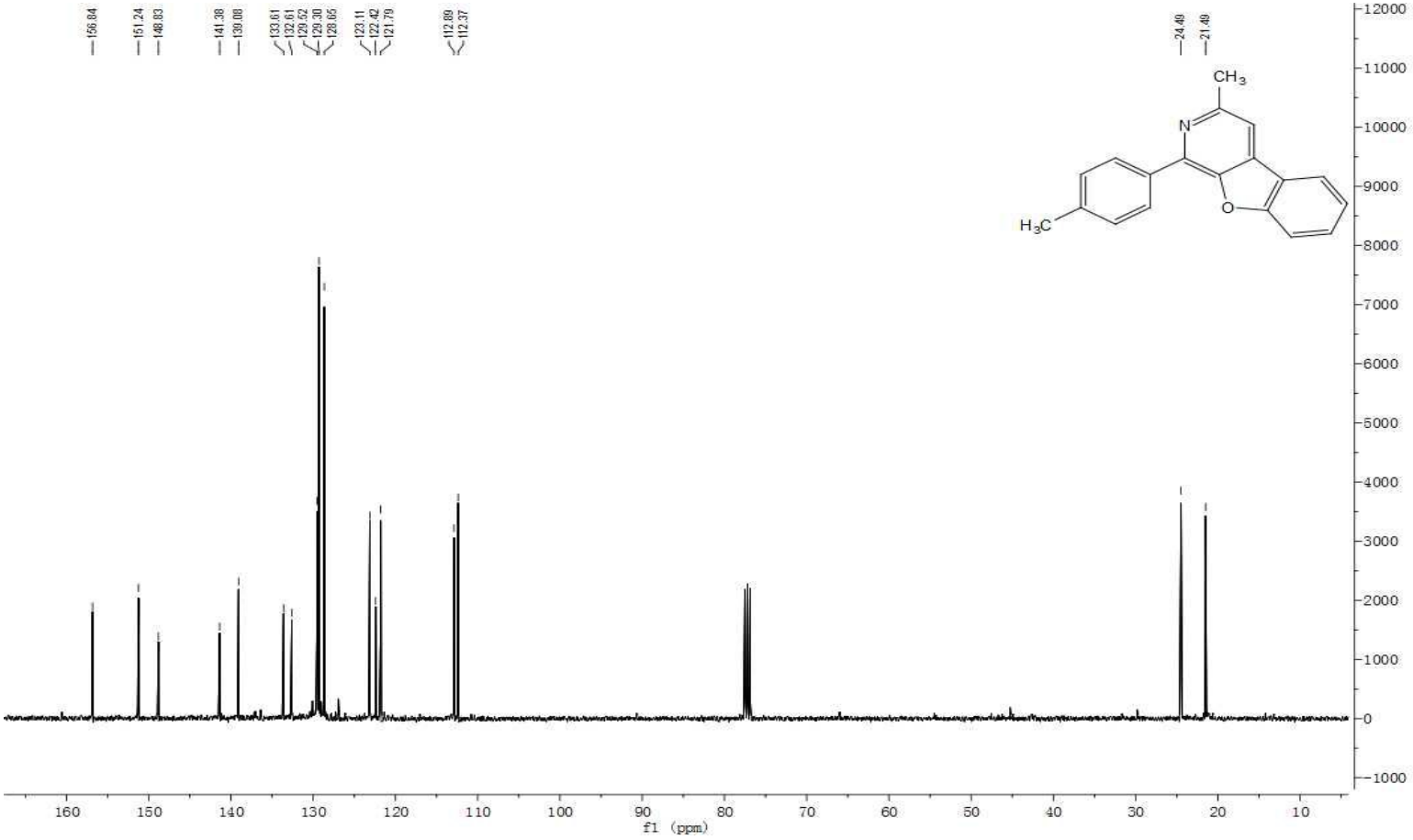
3-methyl-1-(p-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry7)

^{1}H NMR



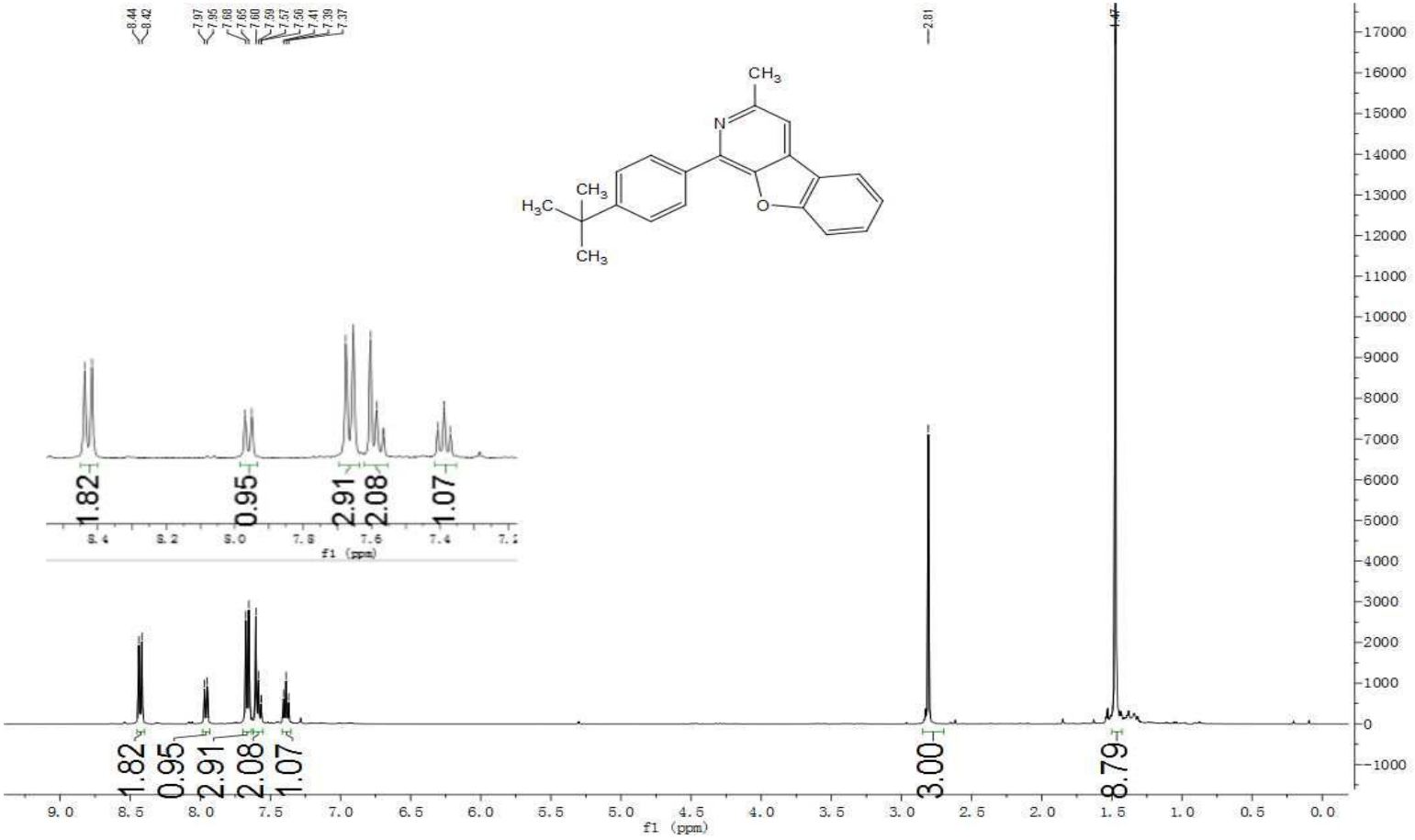
3-methyl-1-(p-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry7)

^{13}C NMR



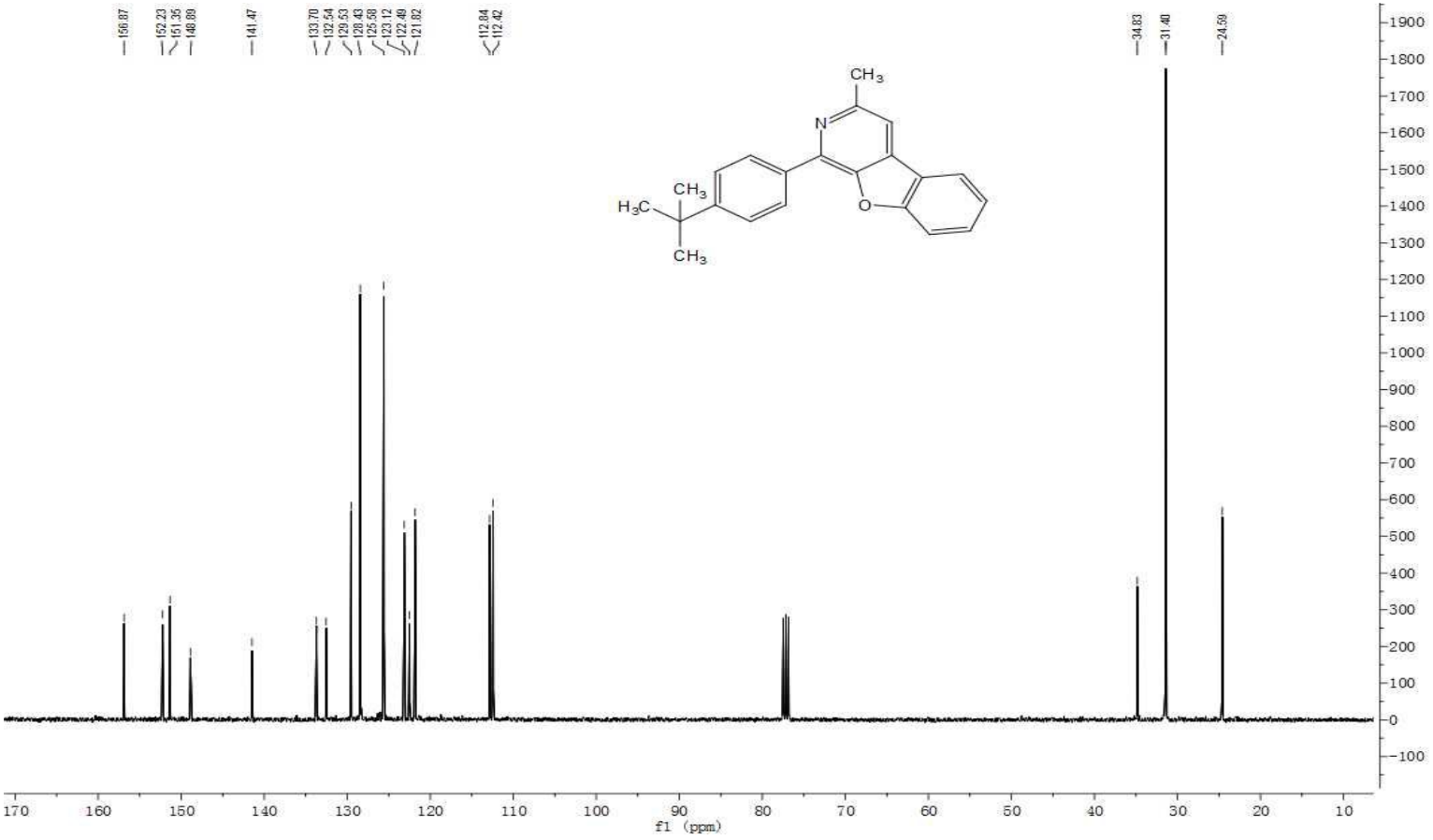
1-(4-(tert-butyl)phenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 8)

^{1}H NMR



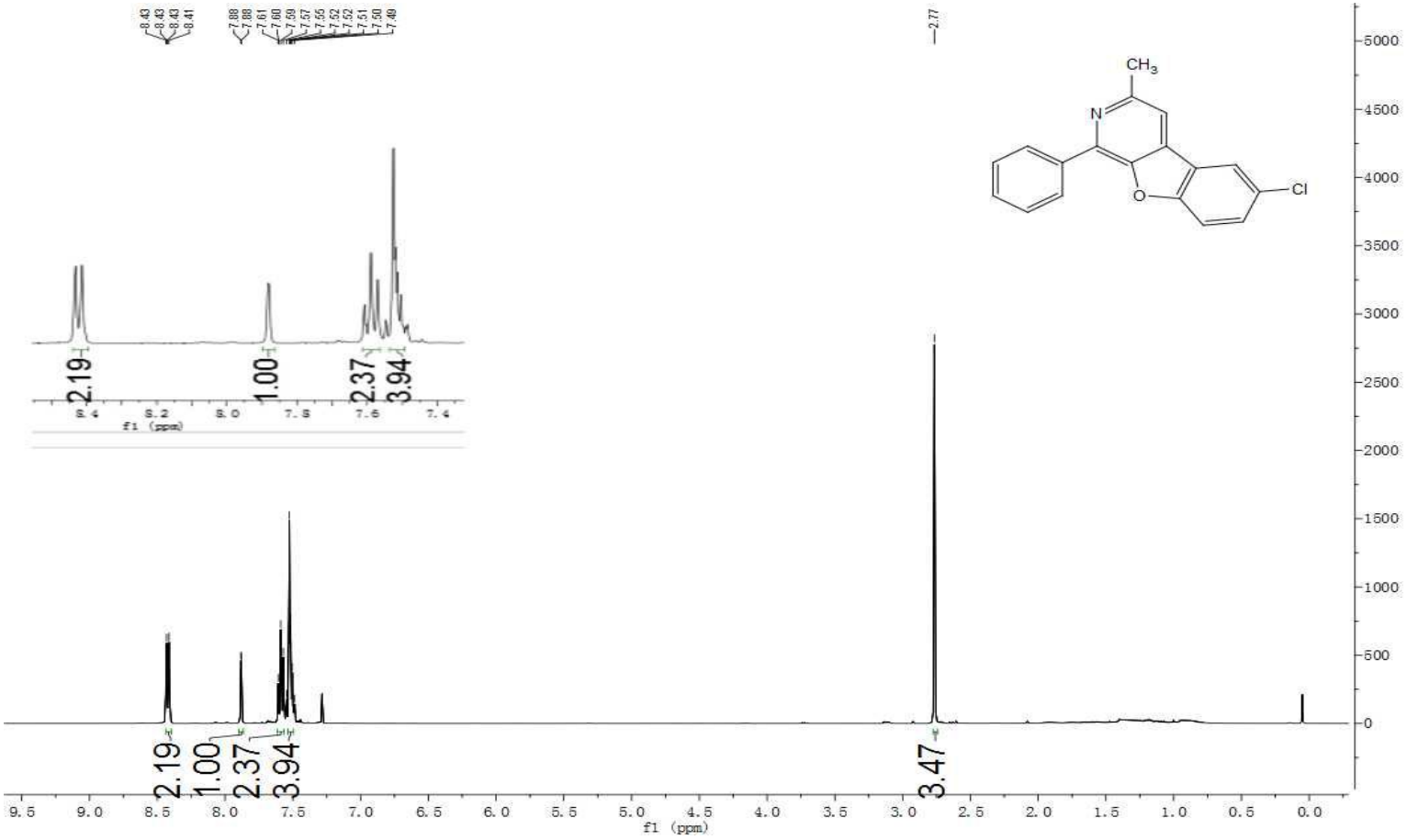
1-(4-(tert-butyl)phenyl)-3-methylbenzofuro[2,3-c]pyridine (Table 3, Entry 8)

^{13}C NMR



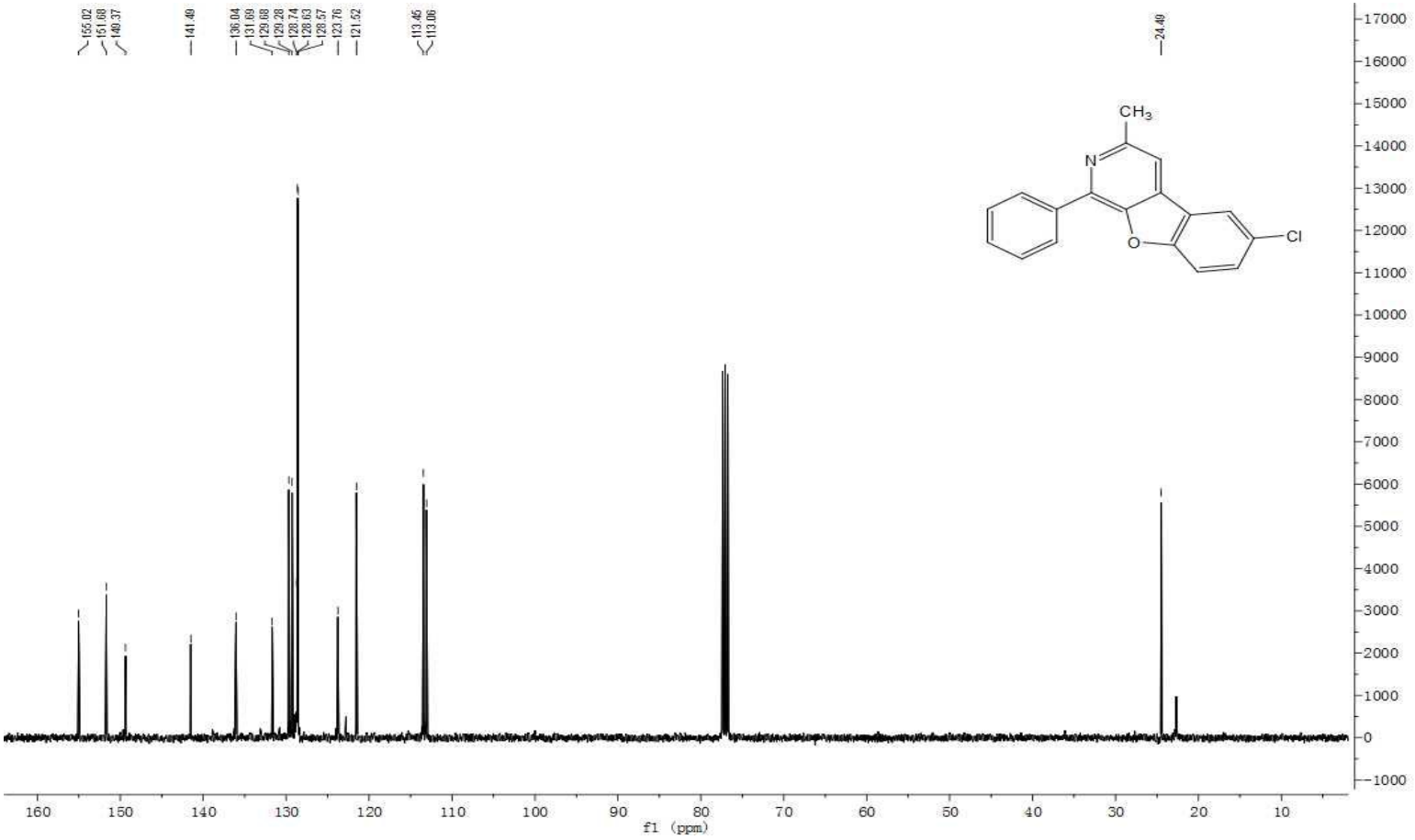
6-chloro-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 9)

^{1}H NMR



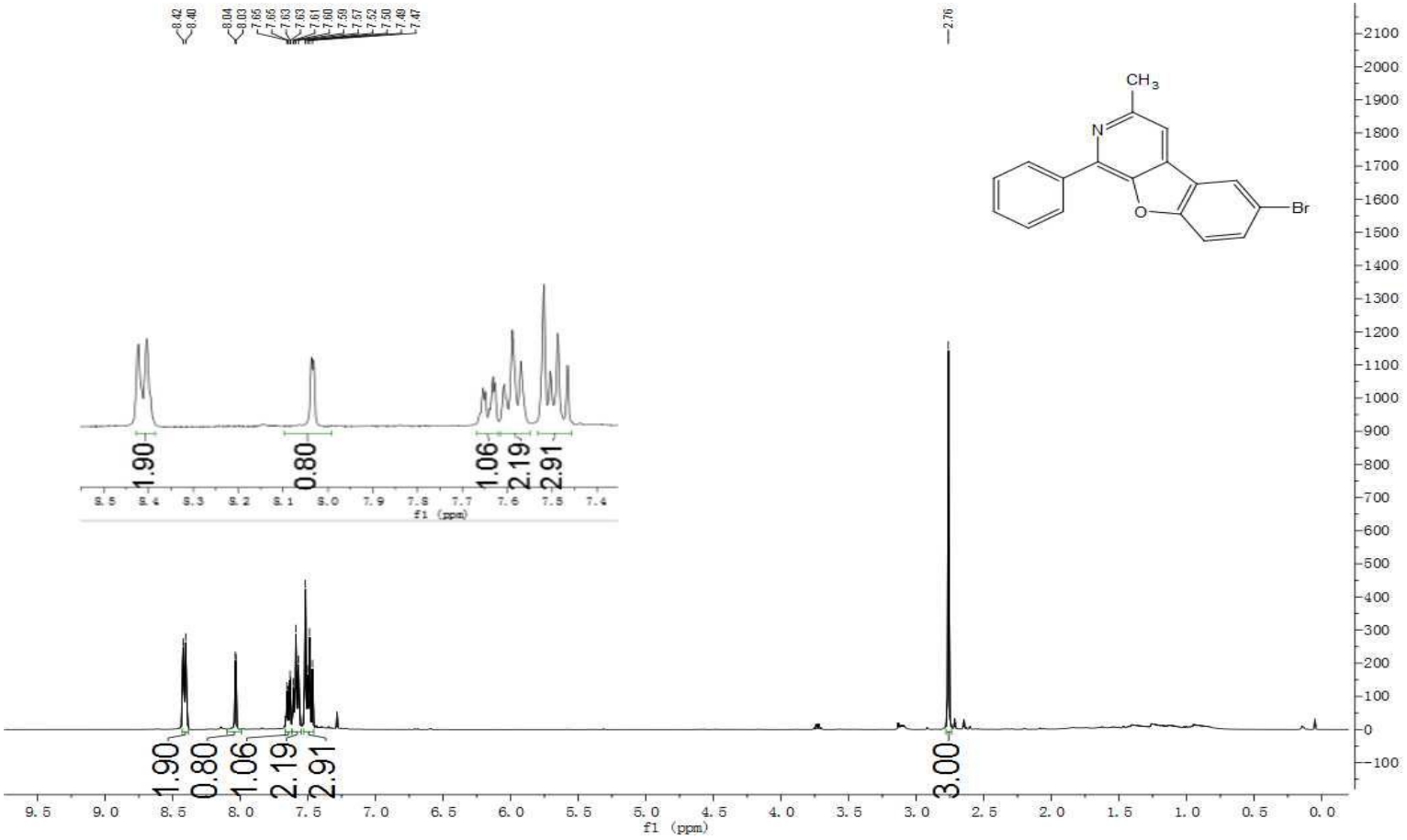
6-chloro-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 9)

^{13}C NMR



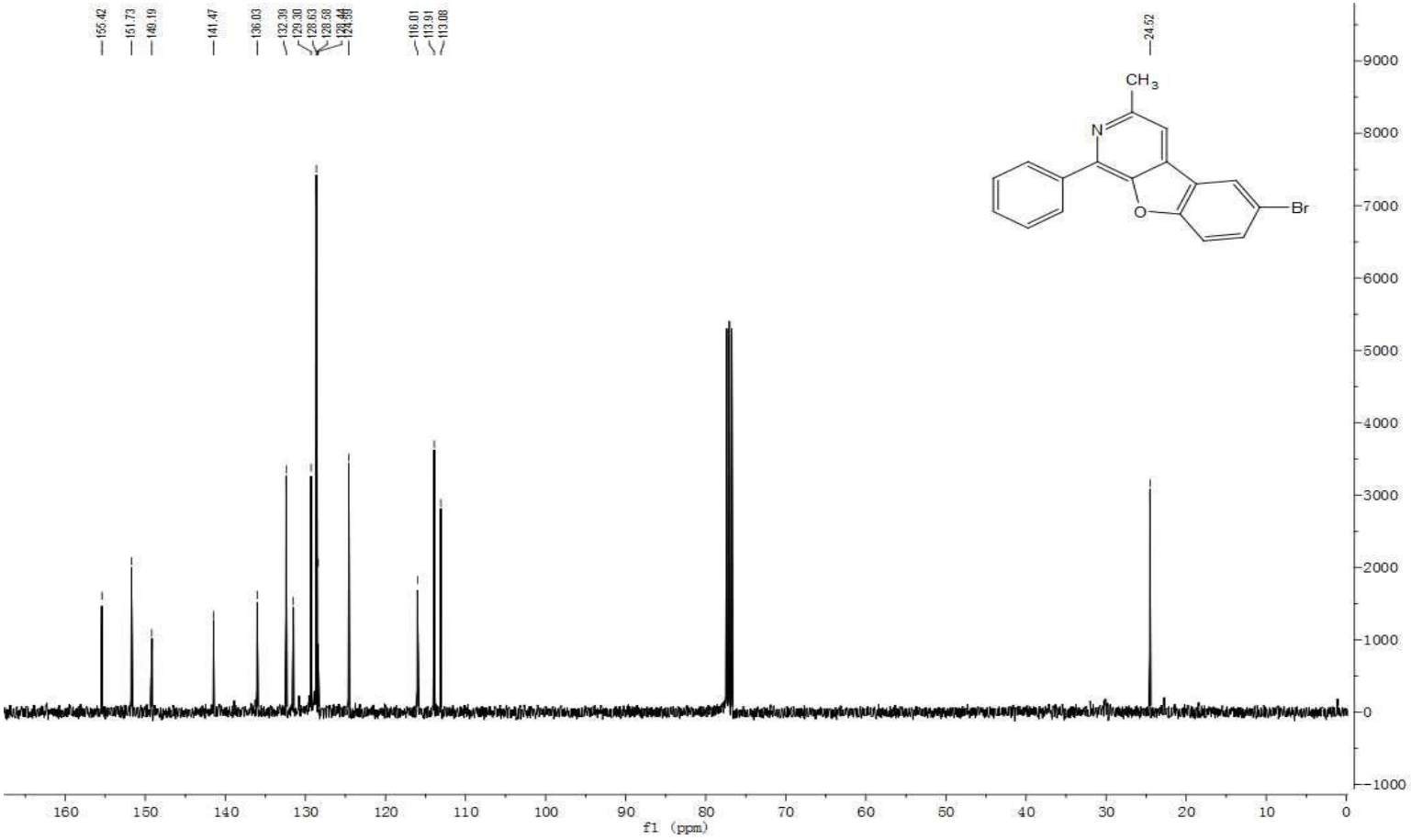
6-bromo-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 10)

^{1}H NMR



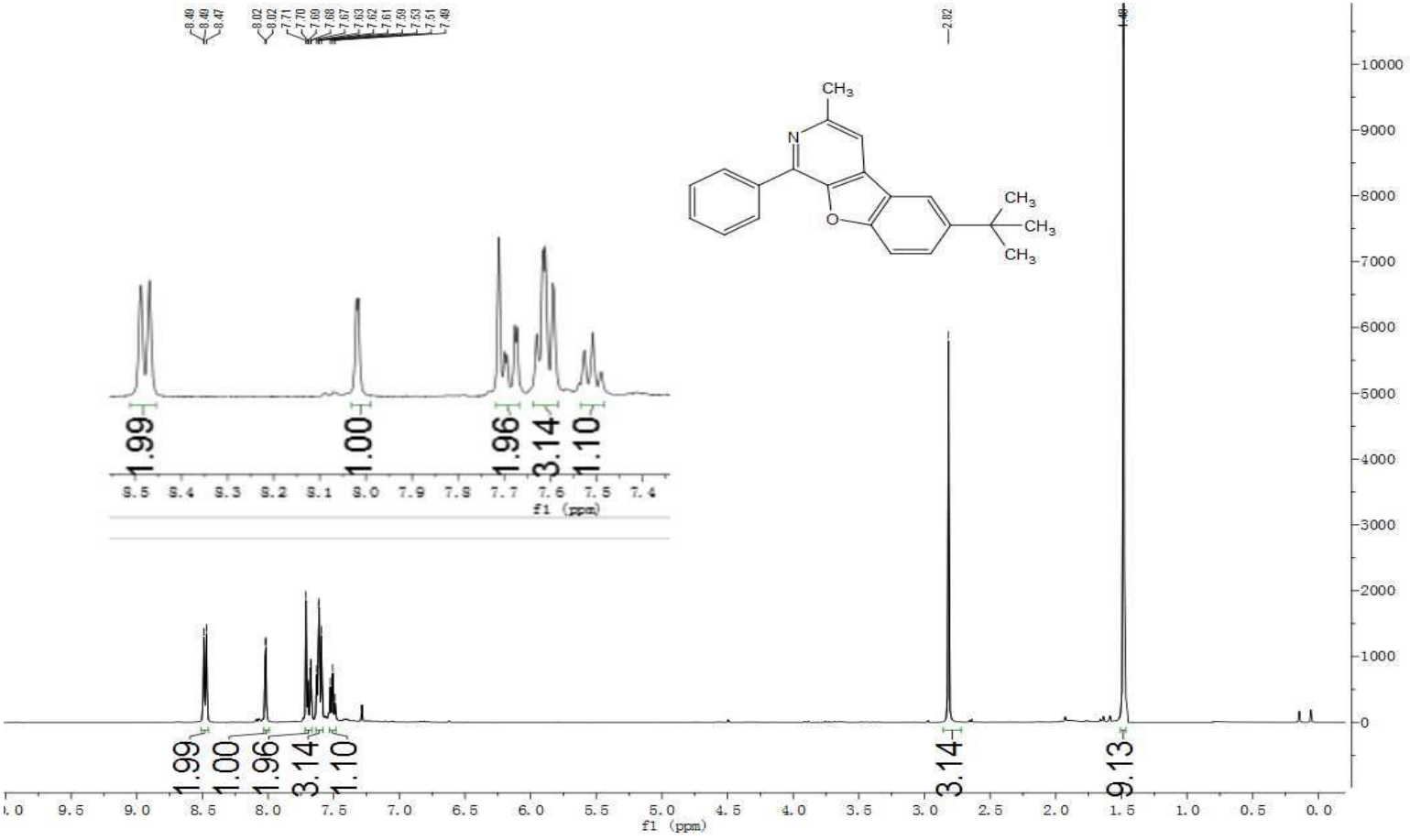
6-bromo-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 10)

^{13}C NMR



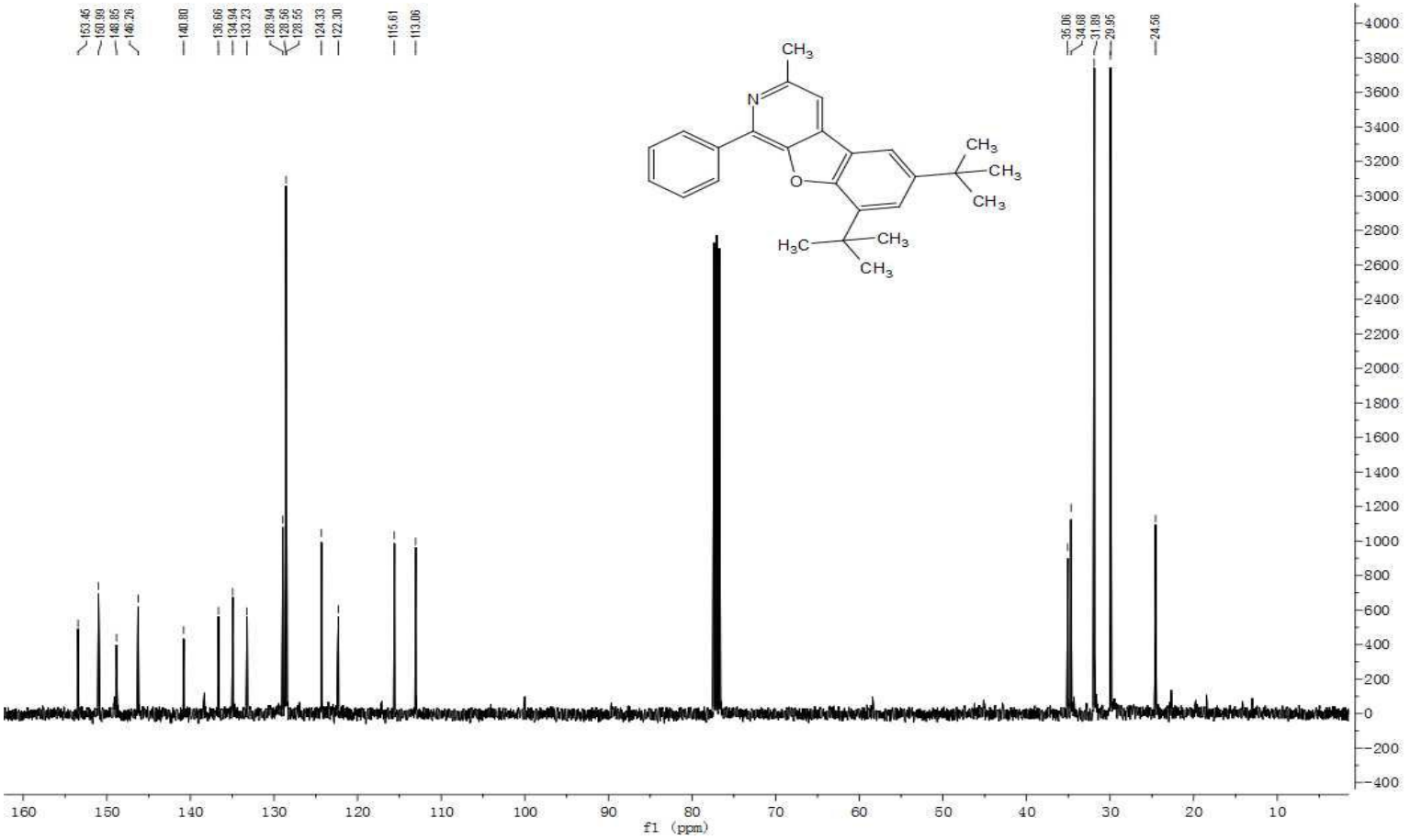
6-(tert-butyl)-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 11)

^{1}H NMR



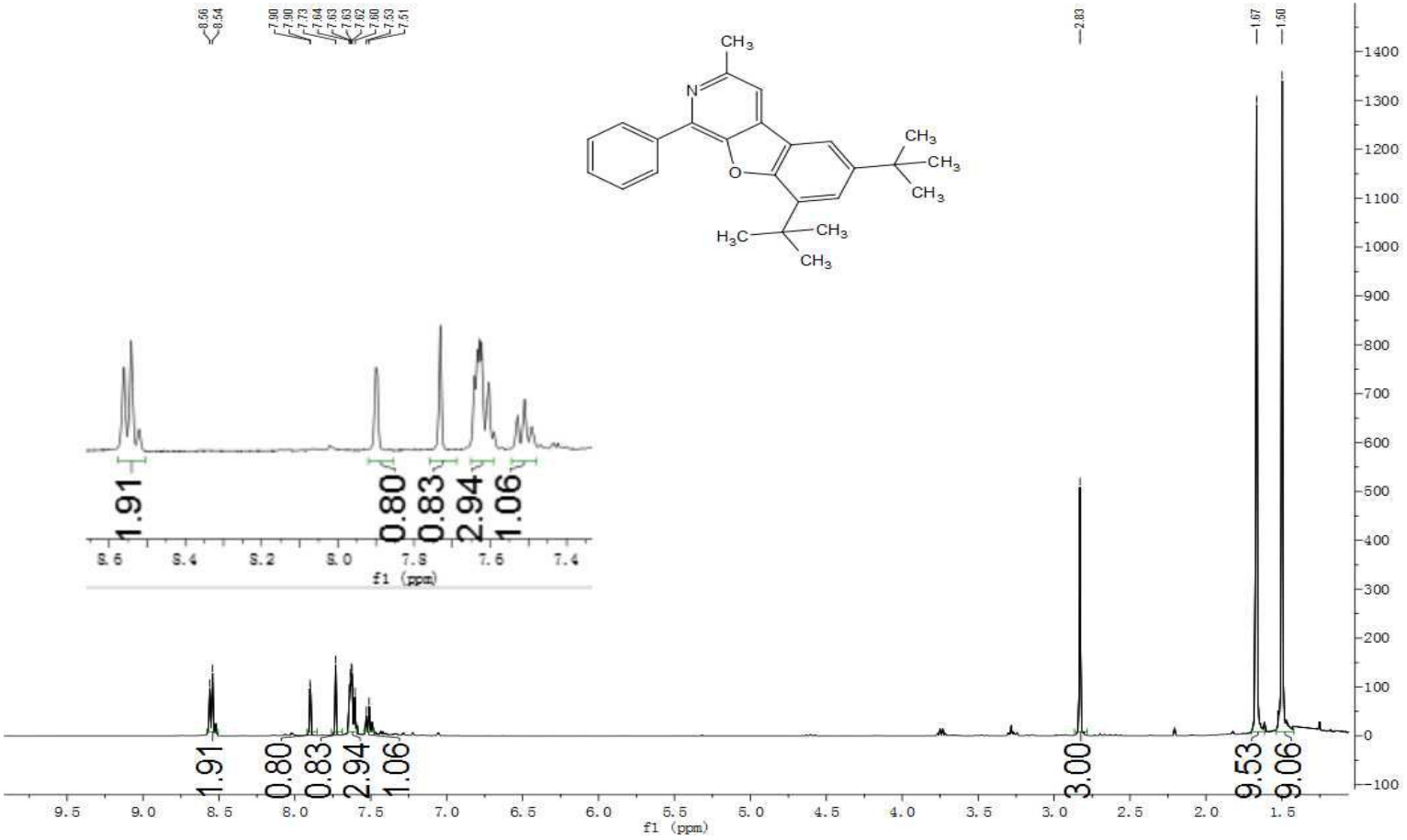
6-(tert-butyl)-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 11)

^{13}C NMR



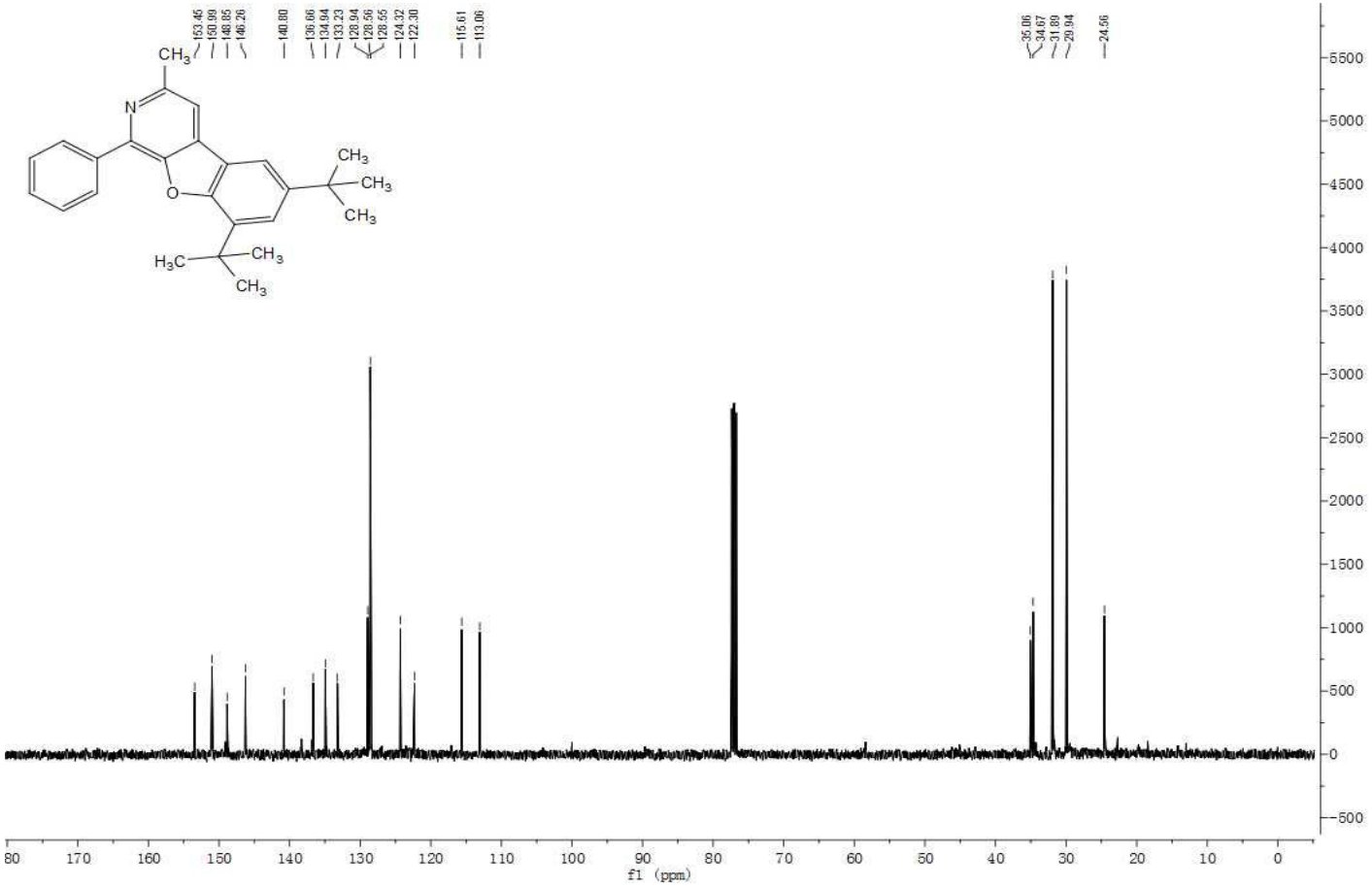
6,8-di-tert-butyl-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry12)

^{1}H NMR



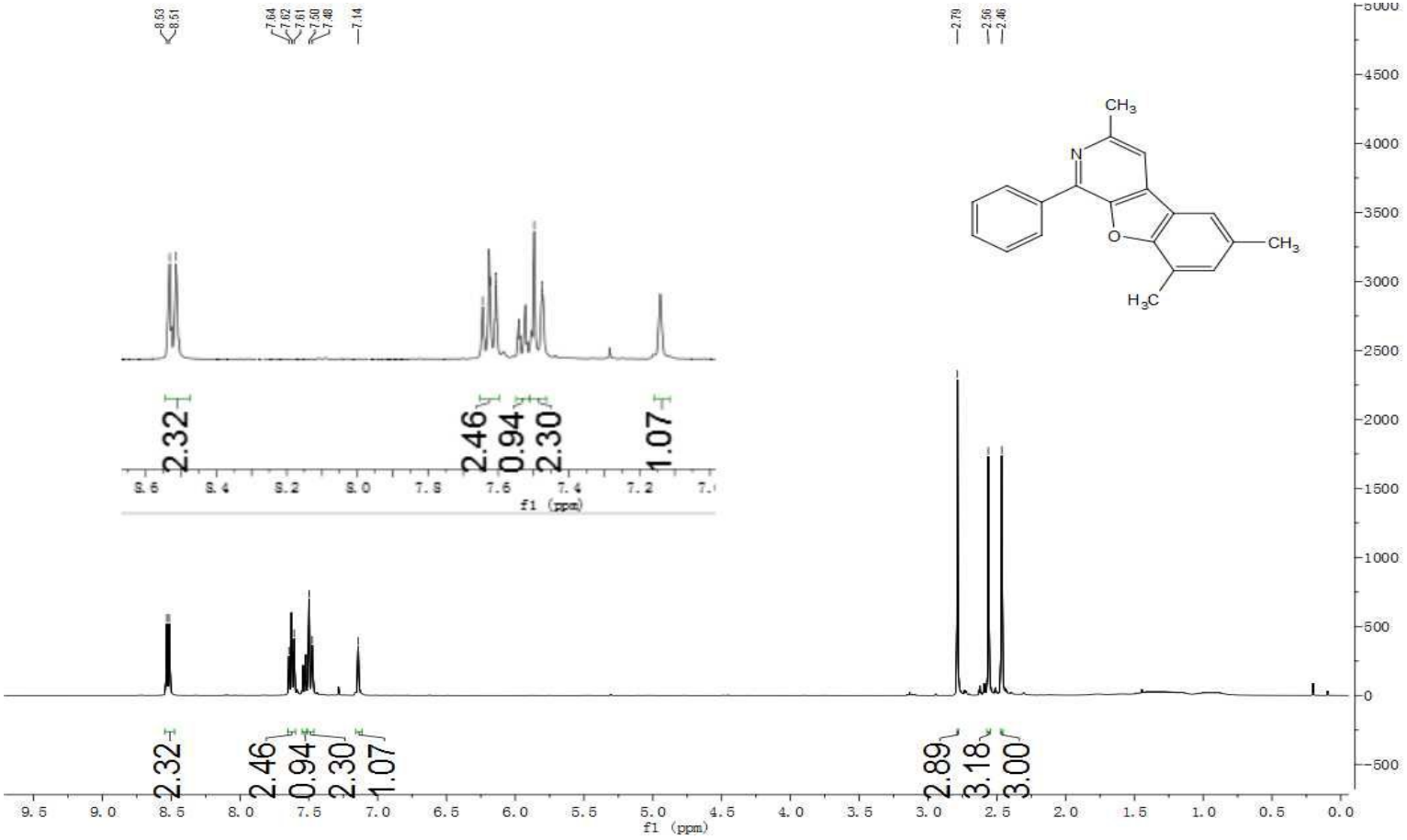
6,8-di-tert-butyl-3-methyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 12)

^{13}C NMR



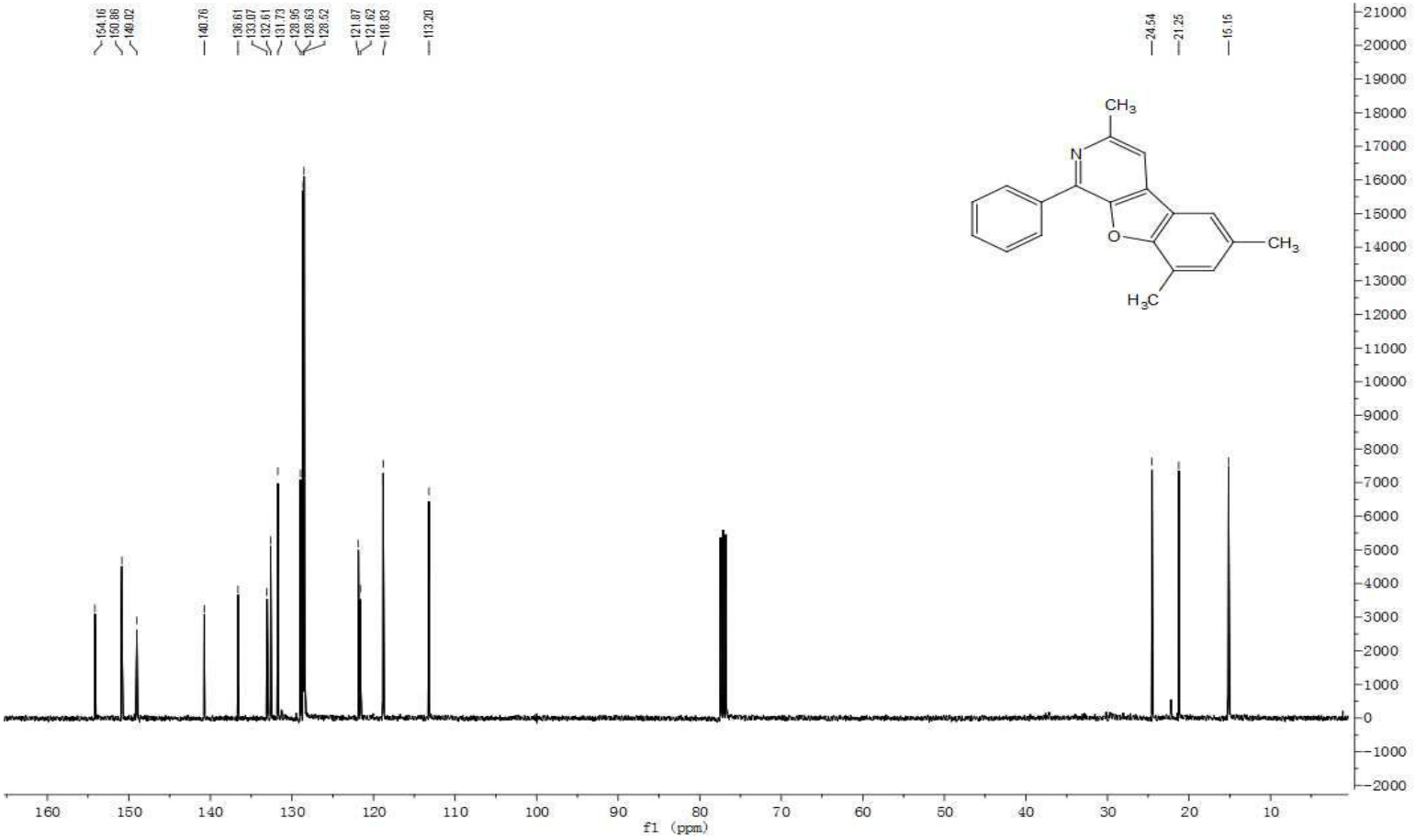
3,6,8-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 13)

^{1}H NMR



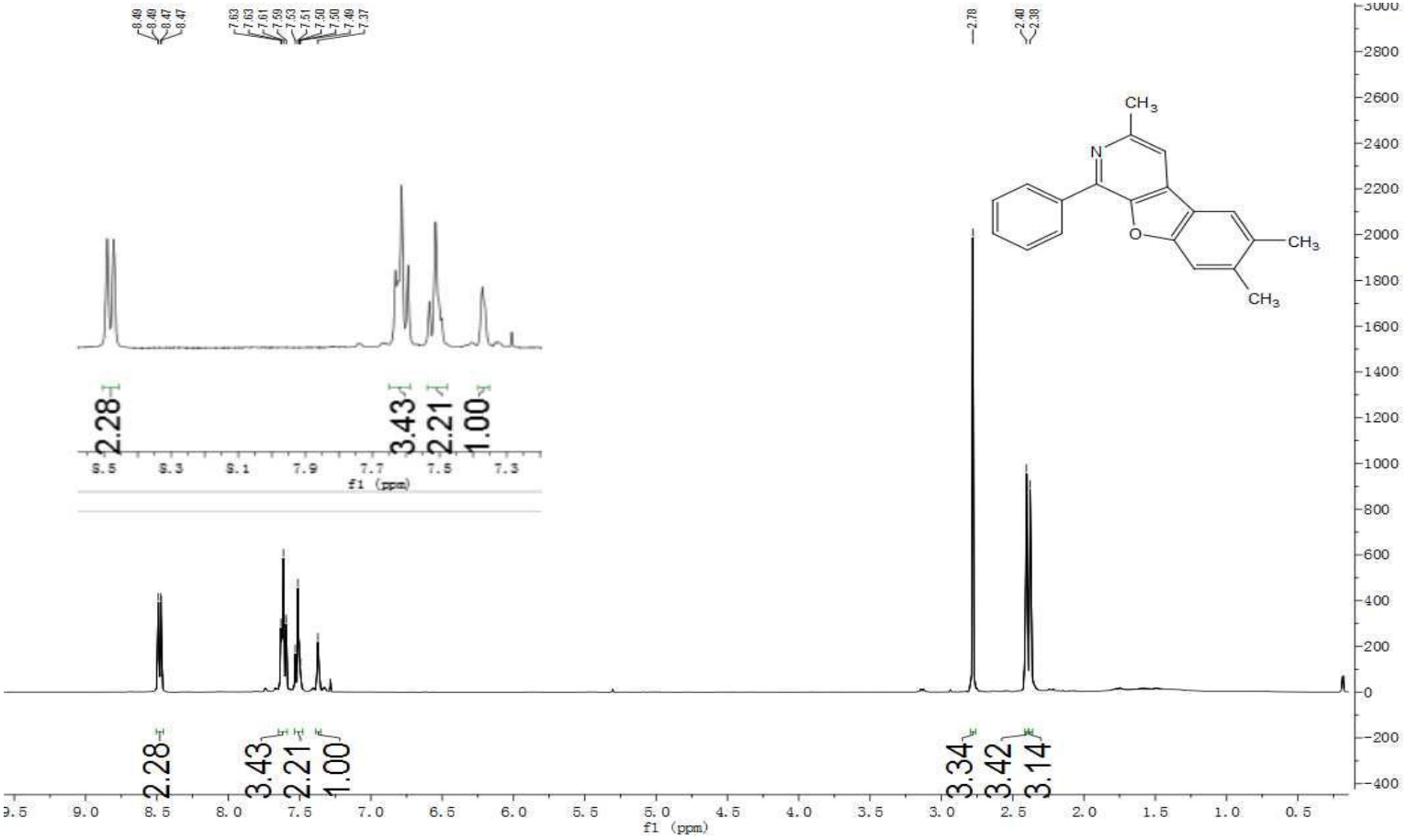
3,6,8-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 13)

^{13}C NMR



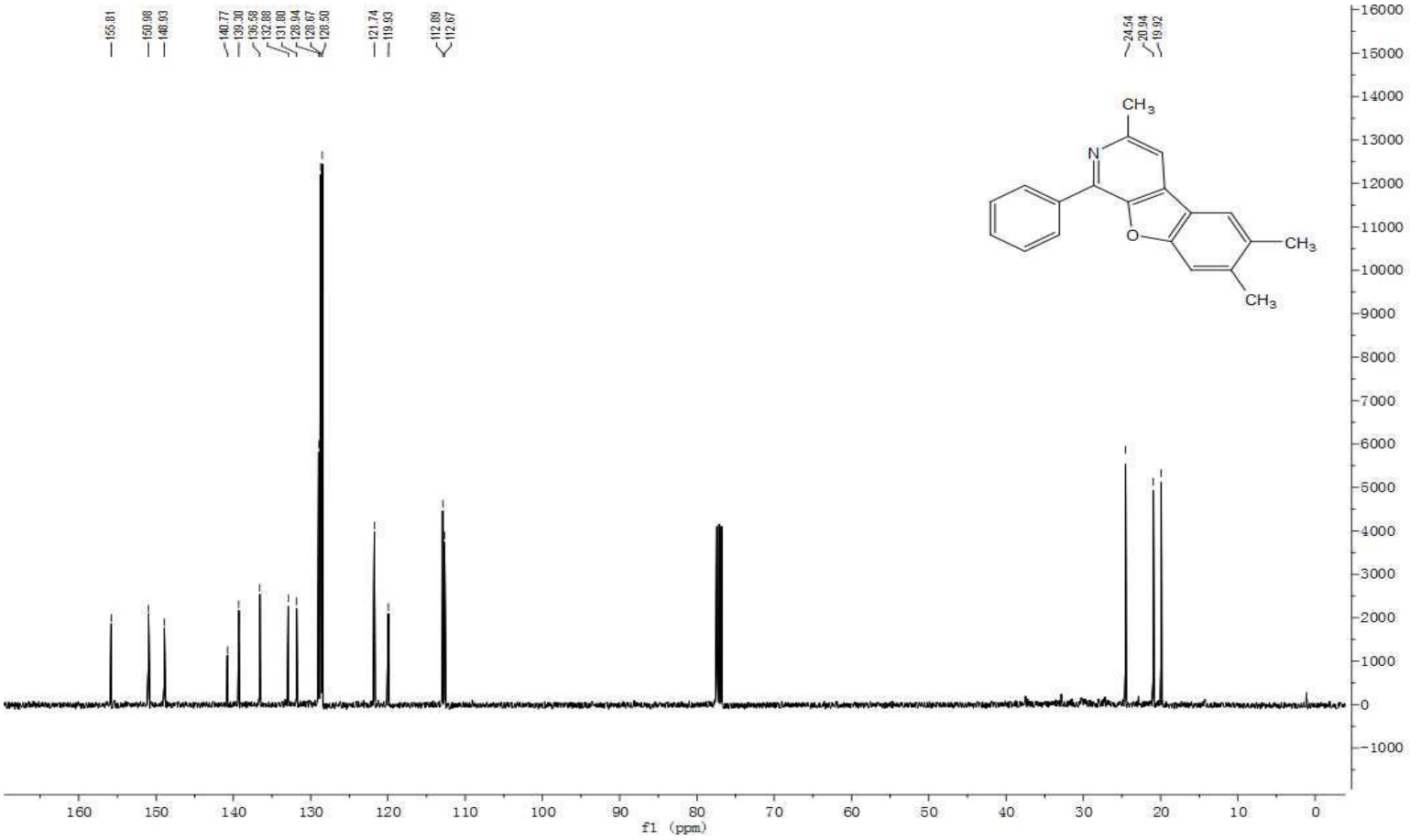
3,6,7-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 14)

^{1}H NMR



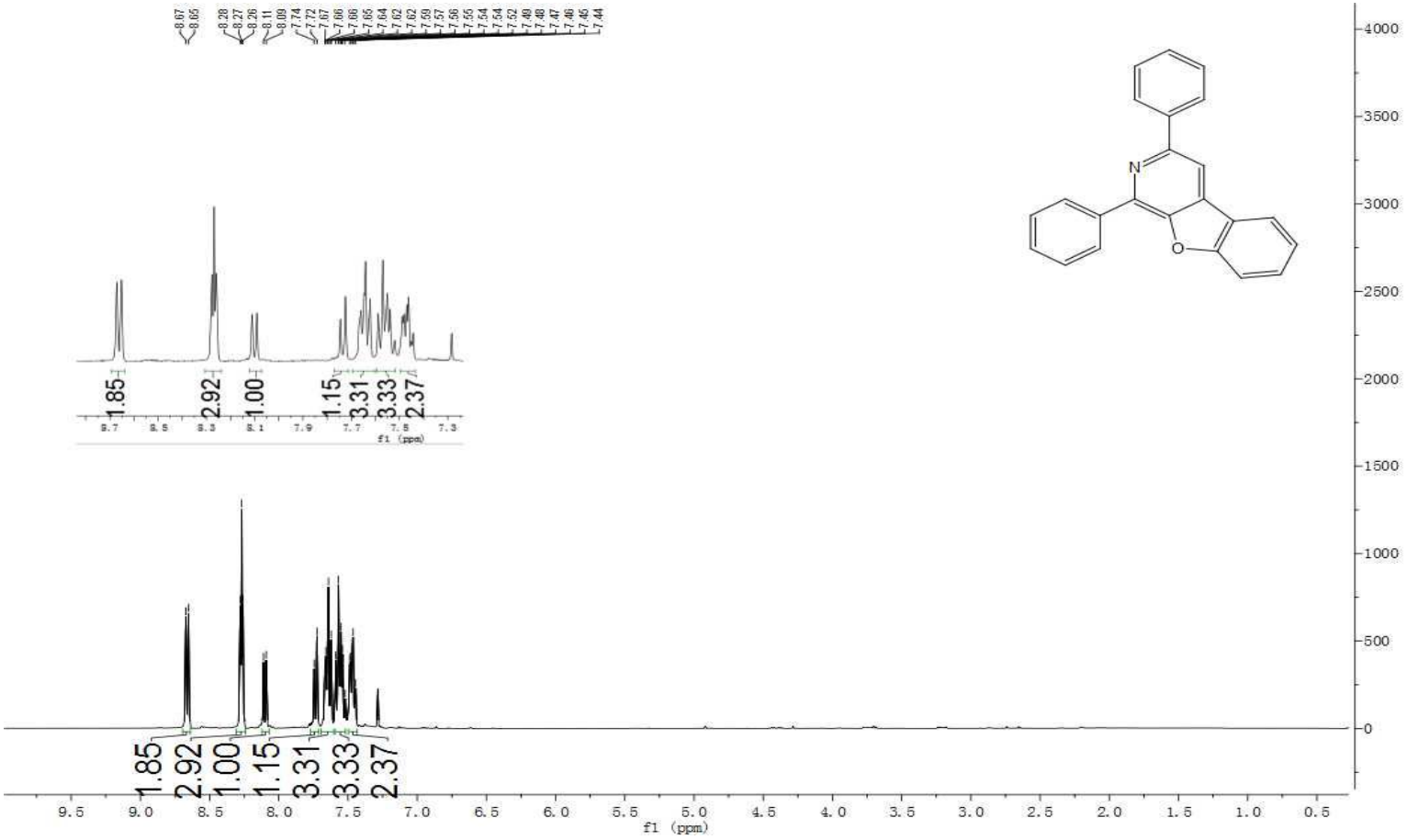
3,6,7-trimethyl-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 14)

^{13}C NMR



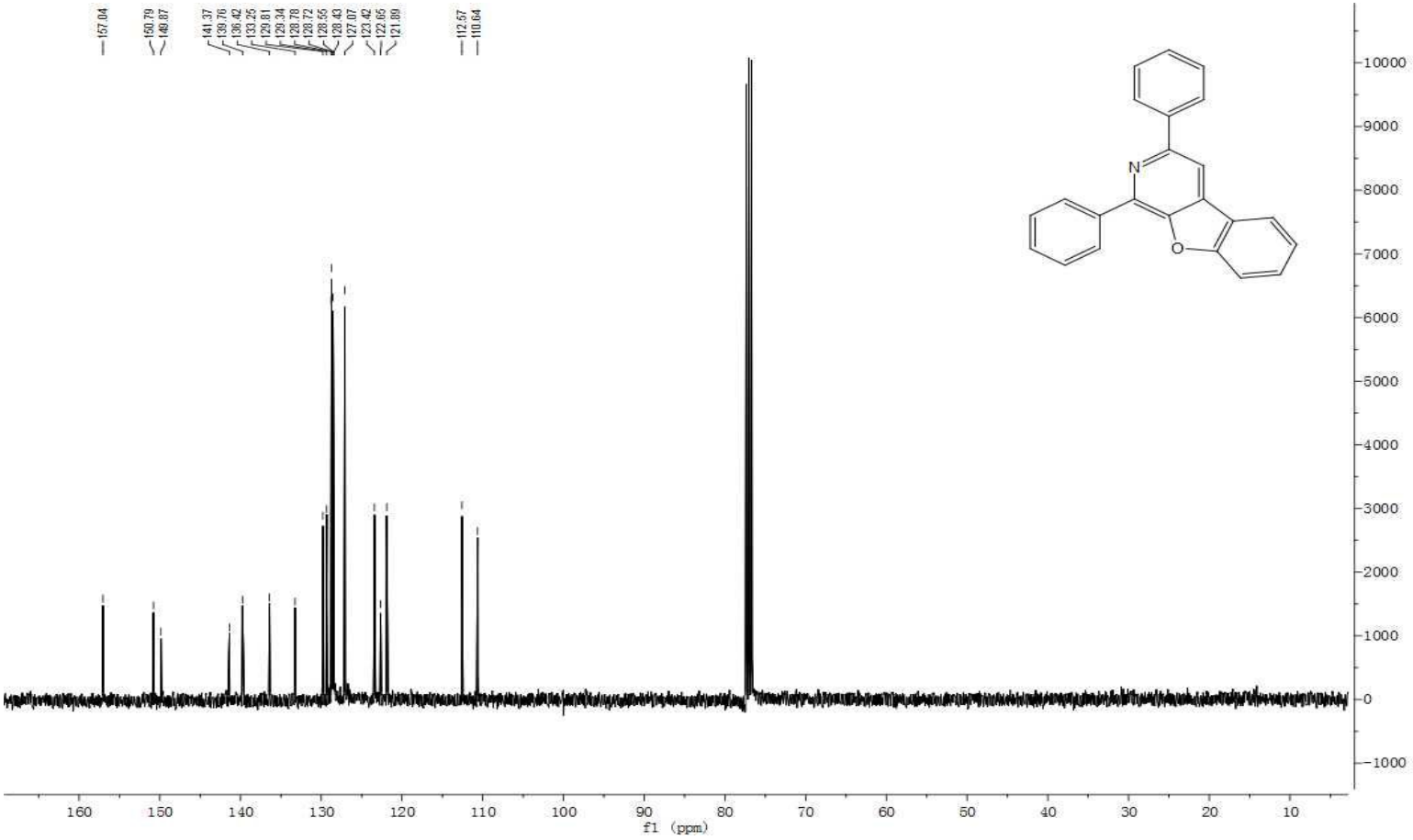
1,3-diphenylbenzofuro[2,3-c]pyridine (Table 3, Entry 15)

^{1}H NMR



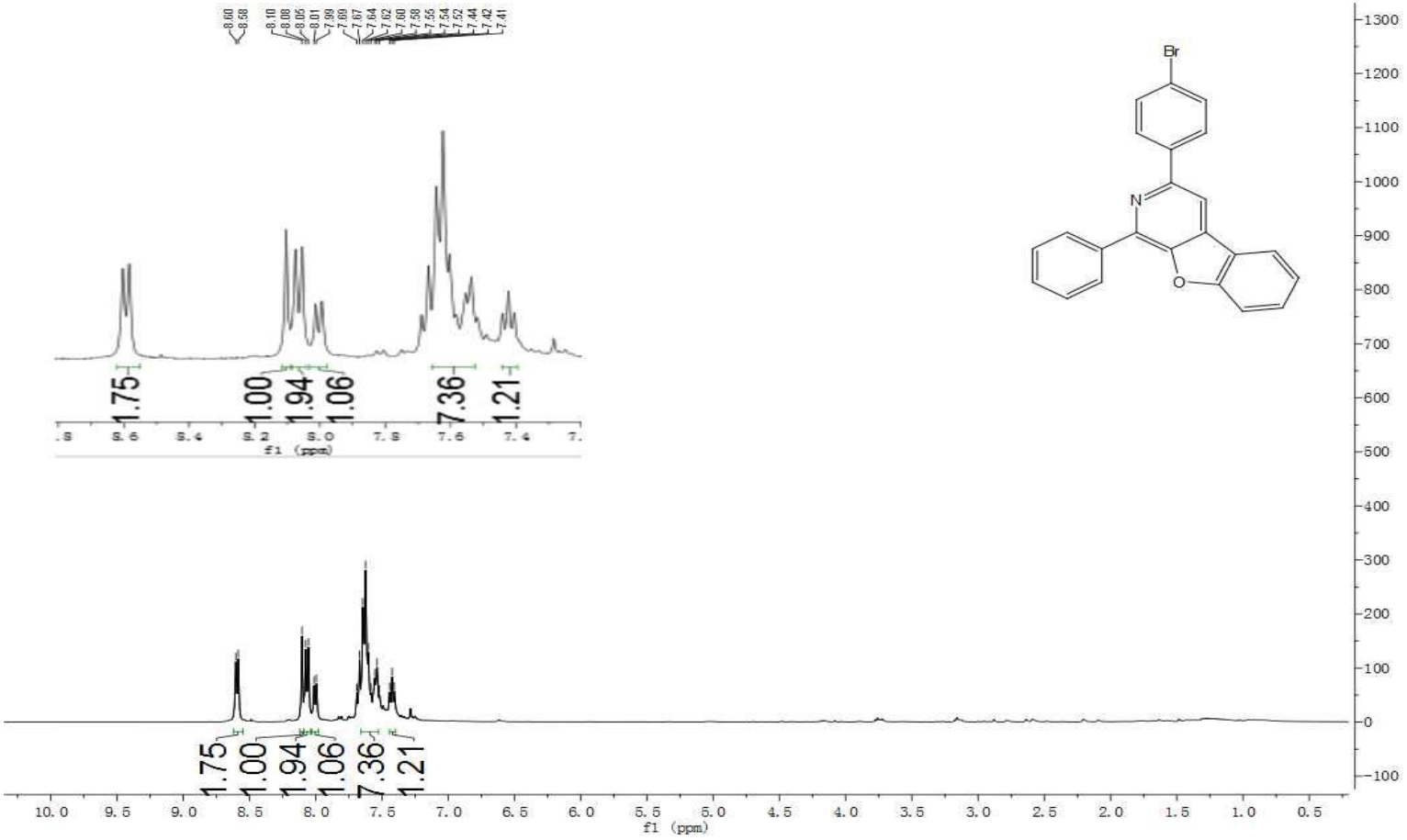
1,3-diphenylbenzofuro[2,3-c]pyridine (Table 3, Entry 15)

^{13}C NMR



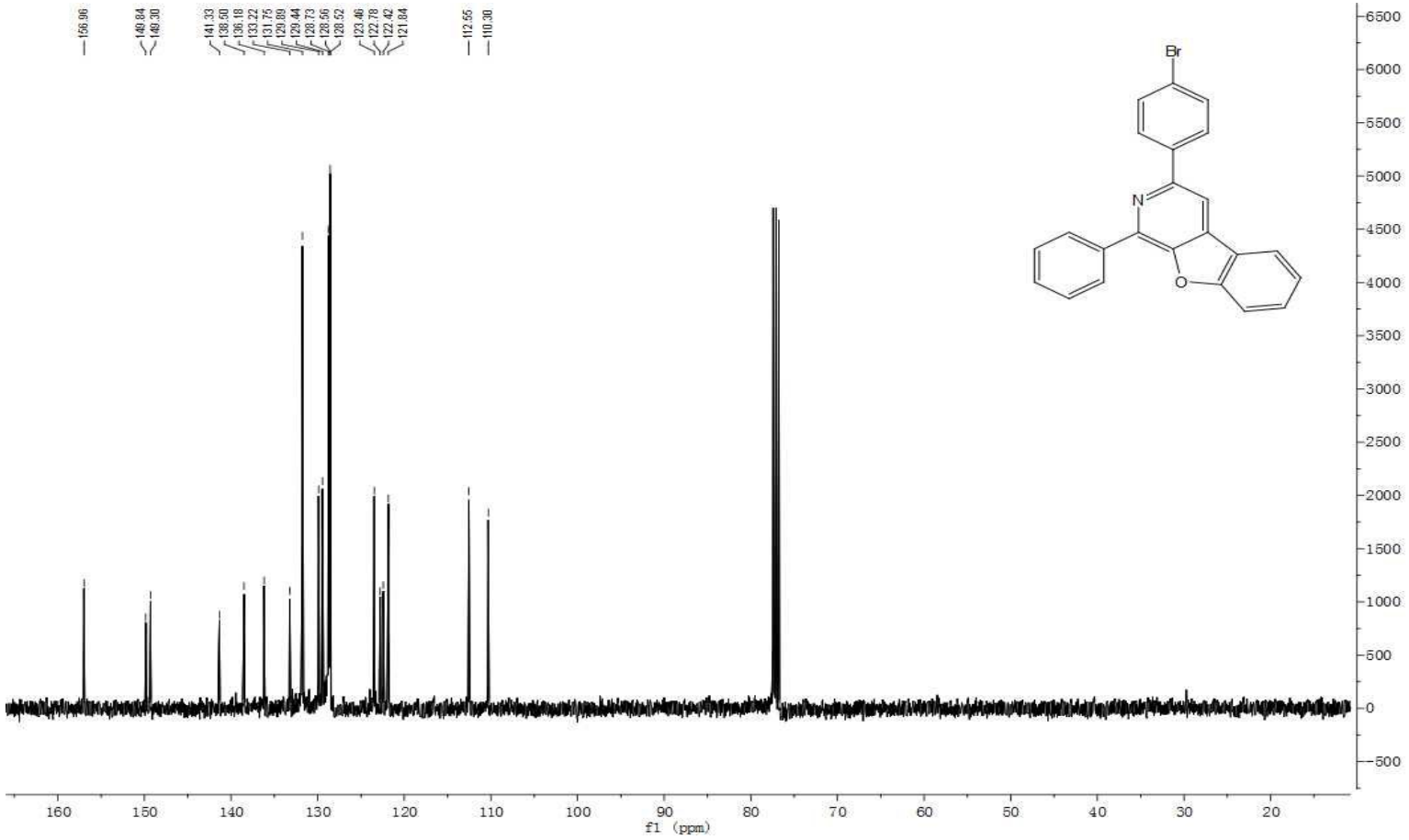
3-(4-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 16)

^{1}H NMR



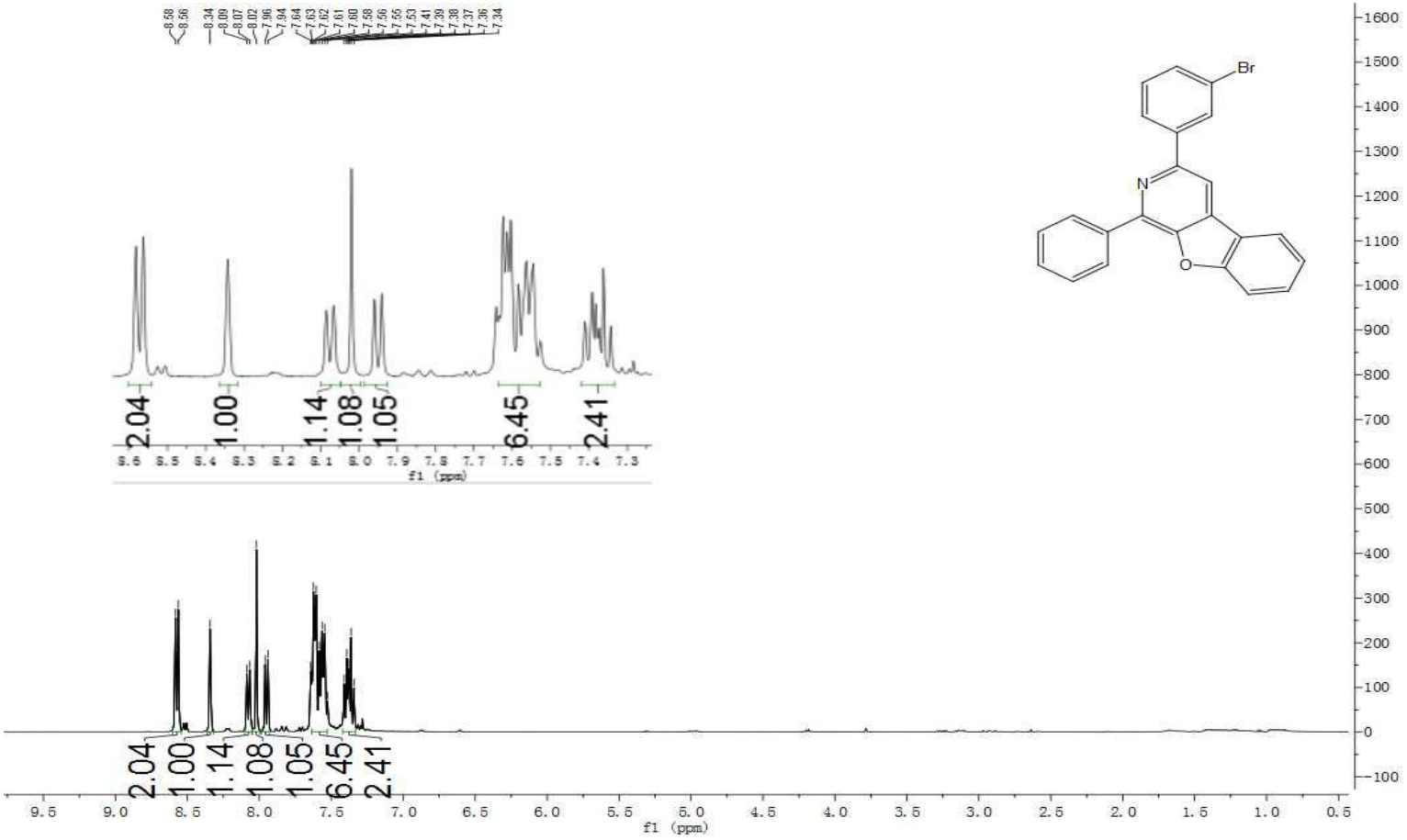
3-(4-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 16)

^{13}C NMR



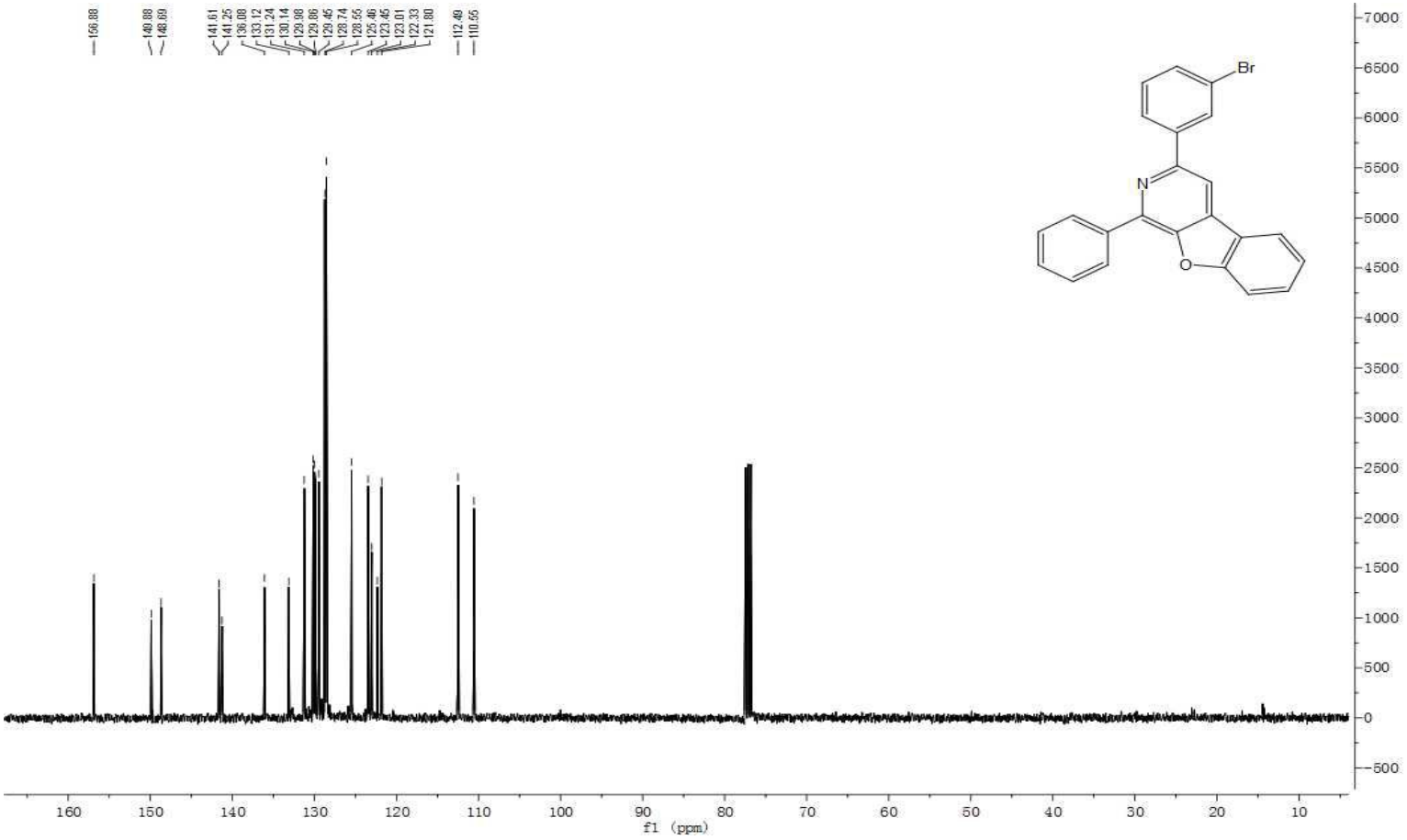
3-(3-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 17)

^{1}H NMR



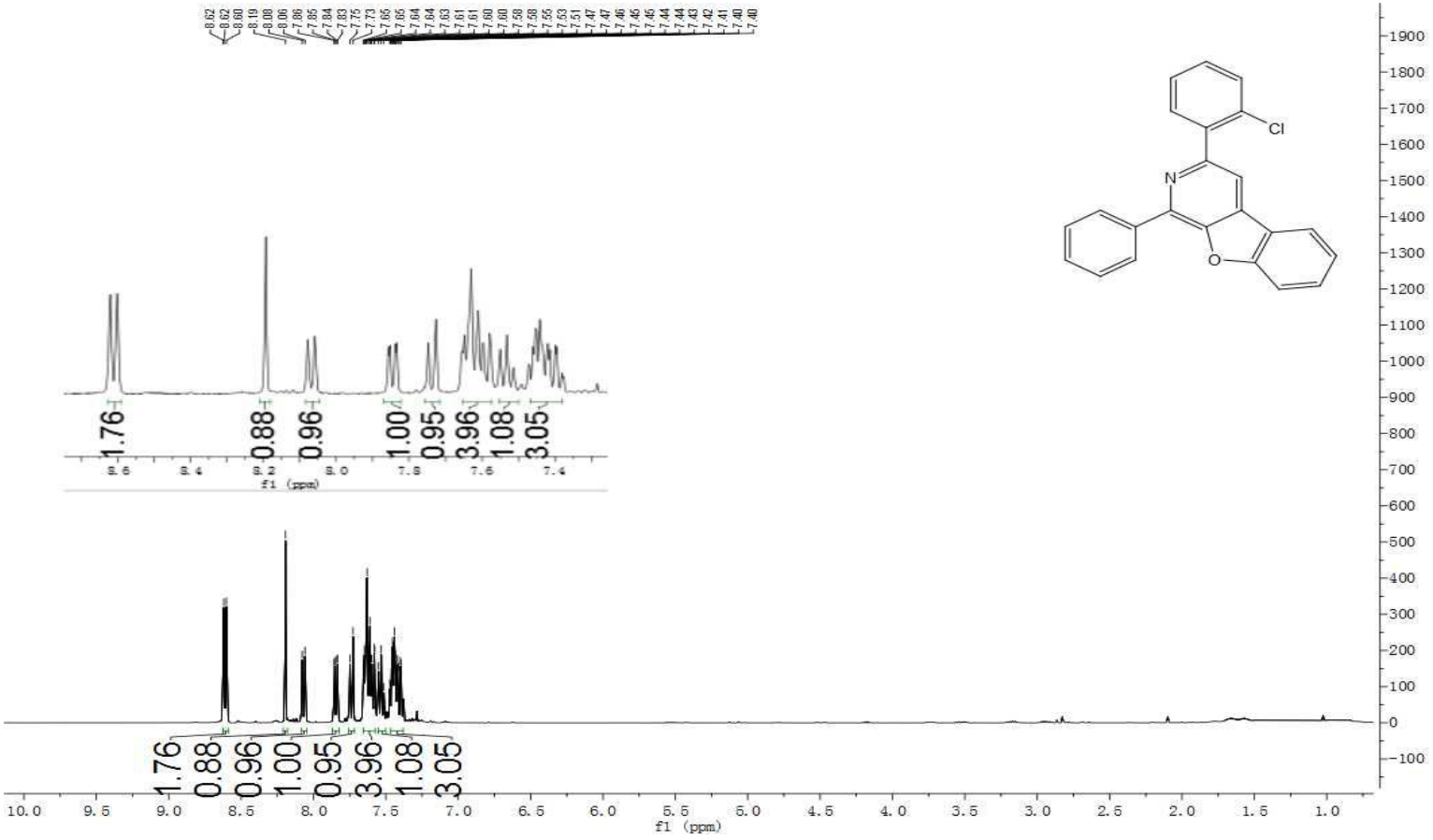
3-(3-bromophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 17)

^{13}C NMR



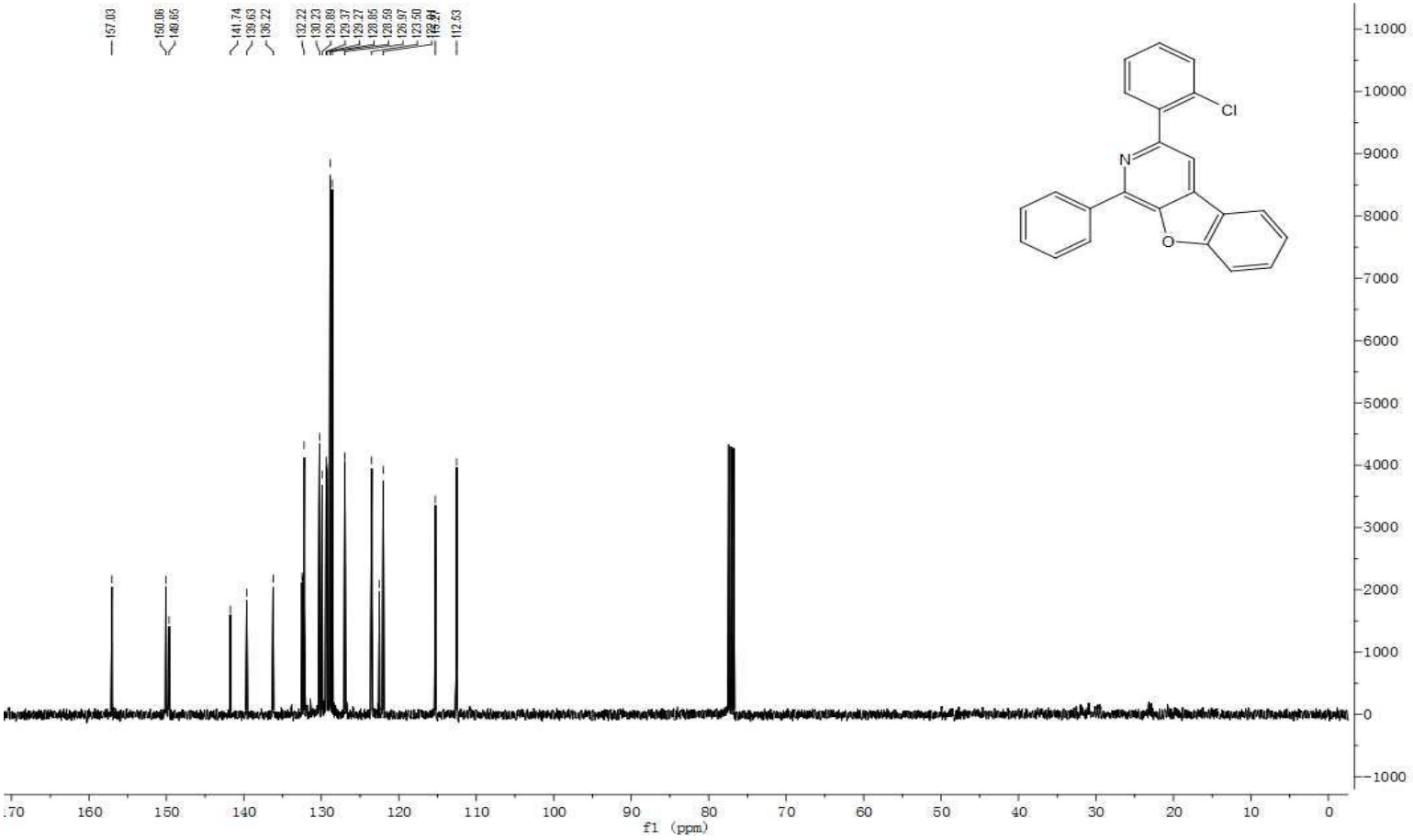
3-(2-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 18)

^{1}H NMR



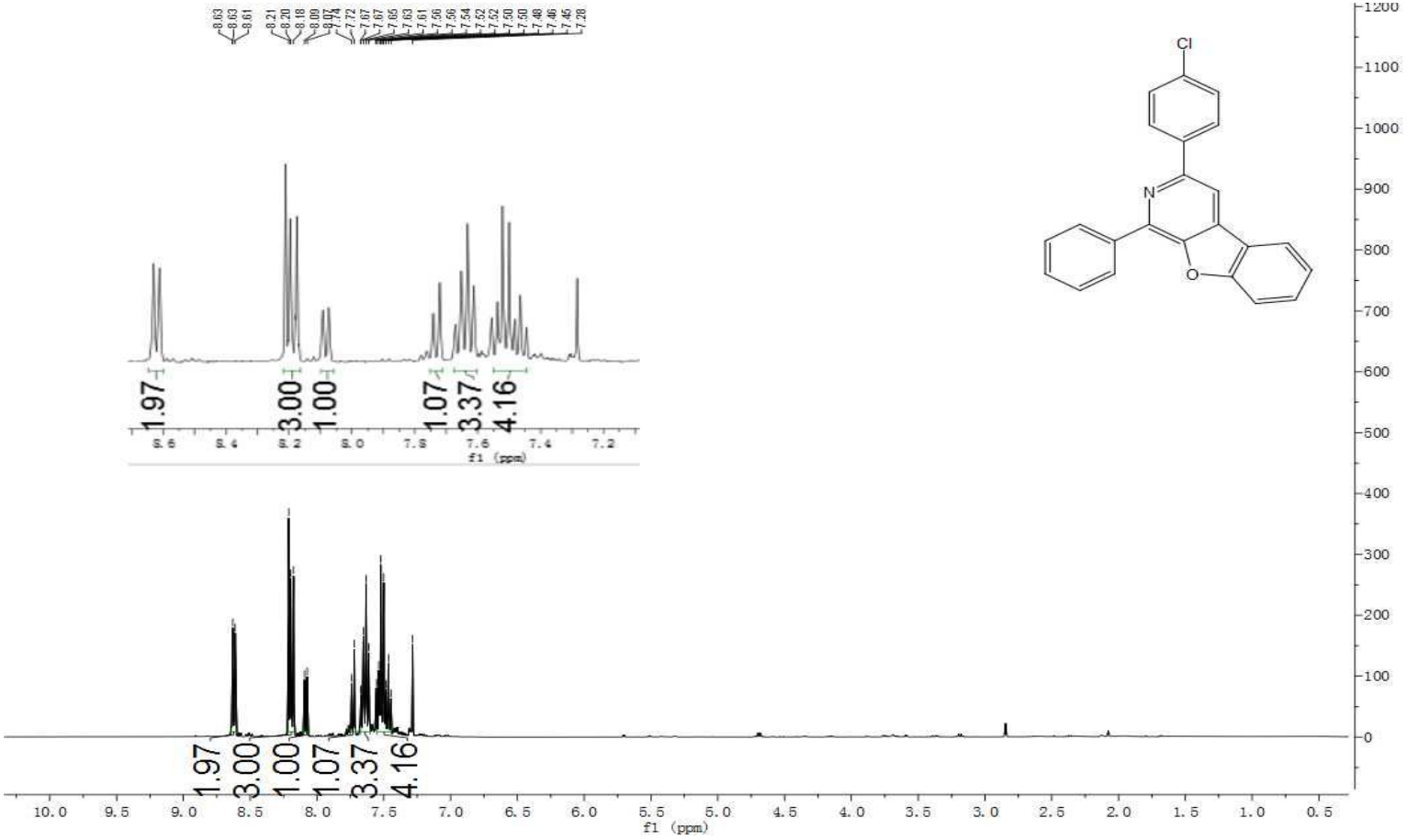
3-(2-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 18)

^{13}C NMR



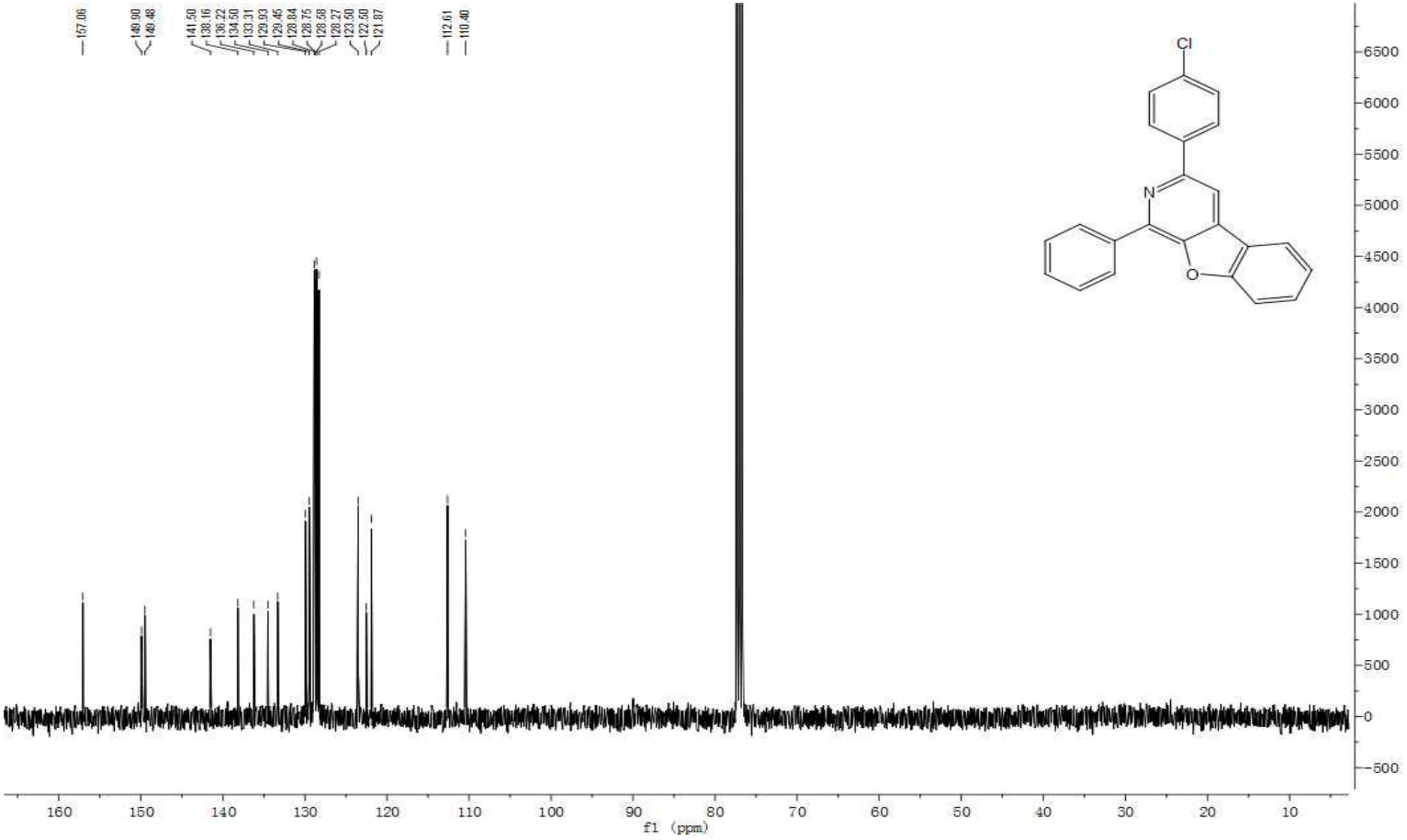
3-(4-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 19)

^{1}H NMR



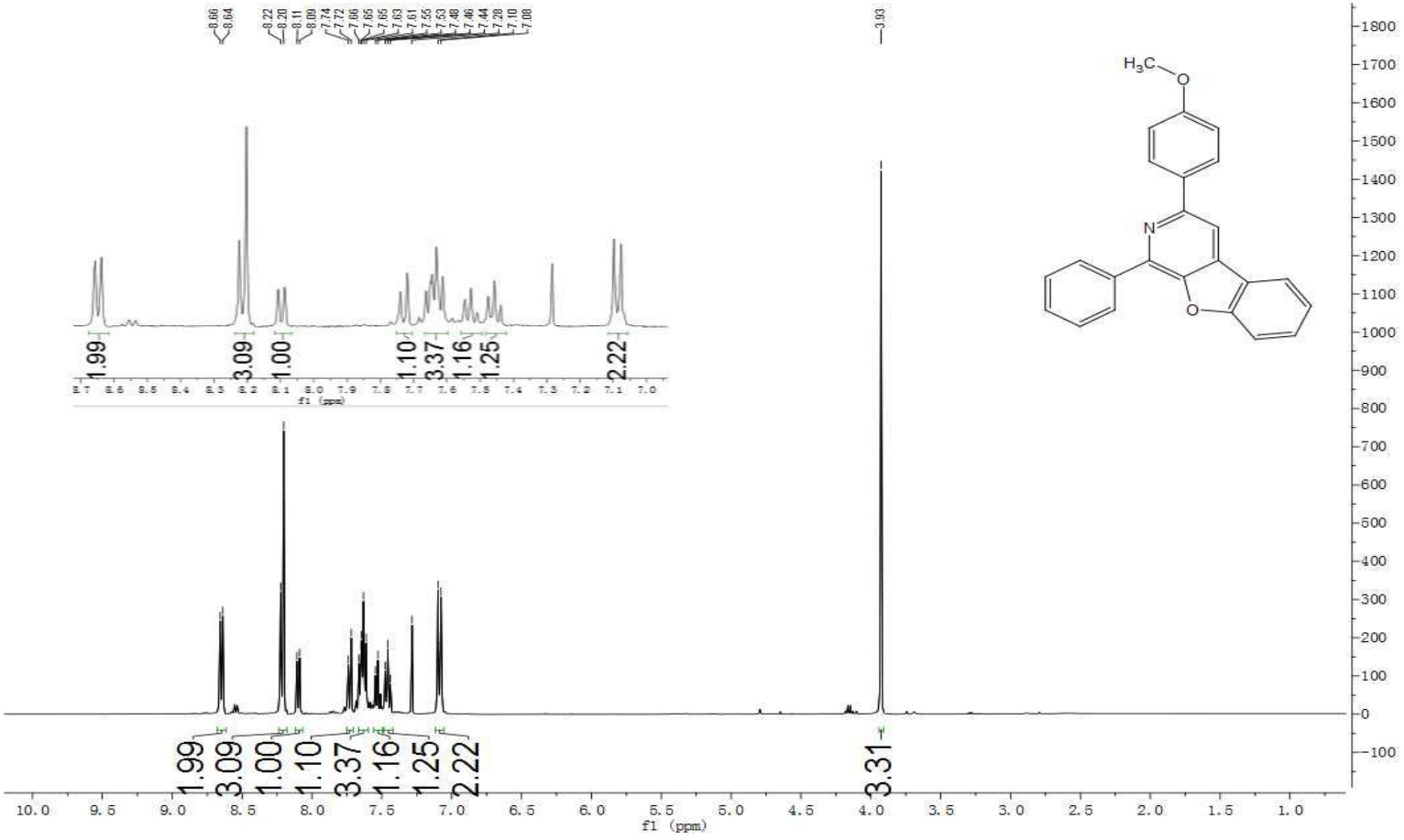
3-(4-chlorophenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 19)

^{13}C NMR



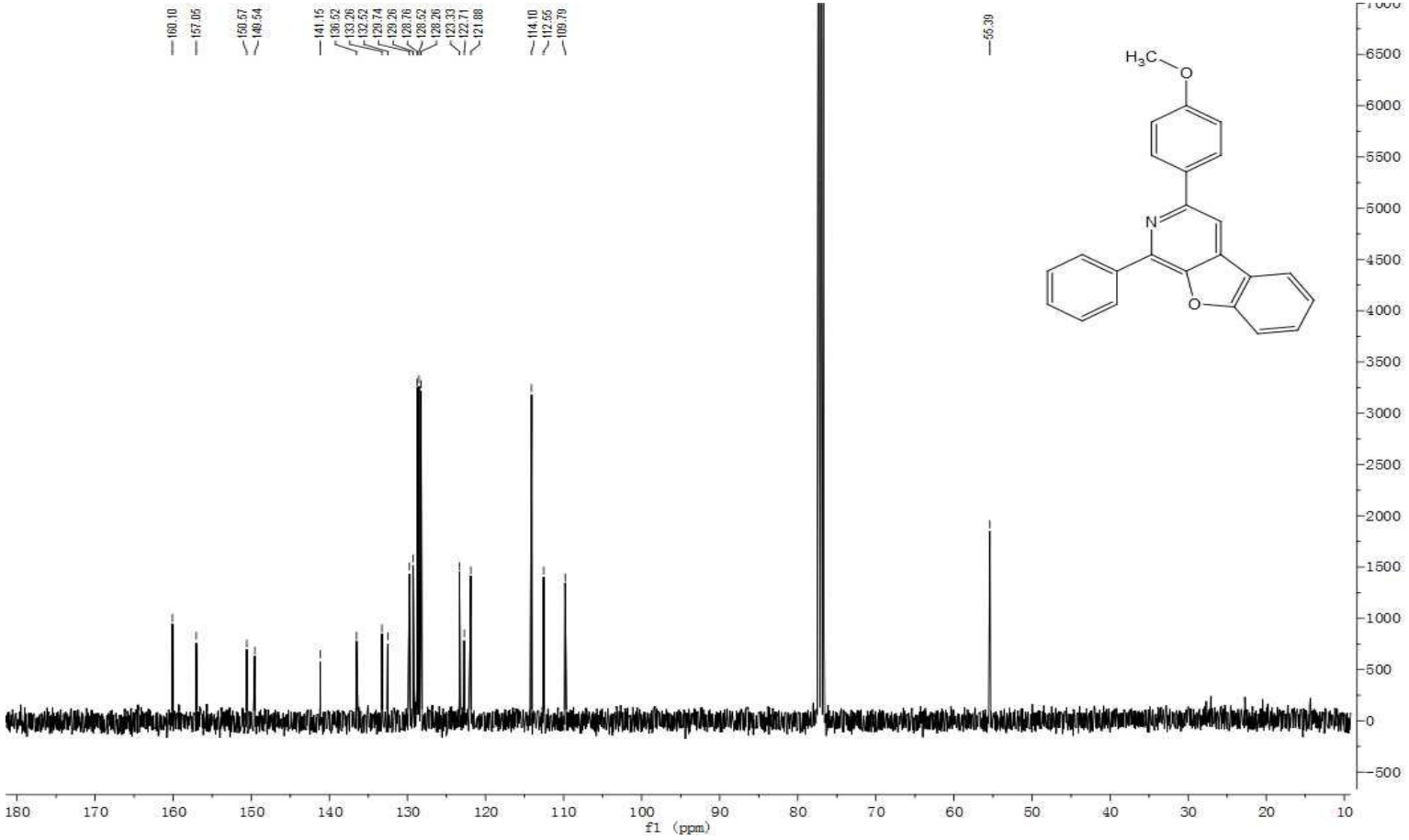
3-(4-methoxyphenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 20)

^{1}H NMR



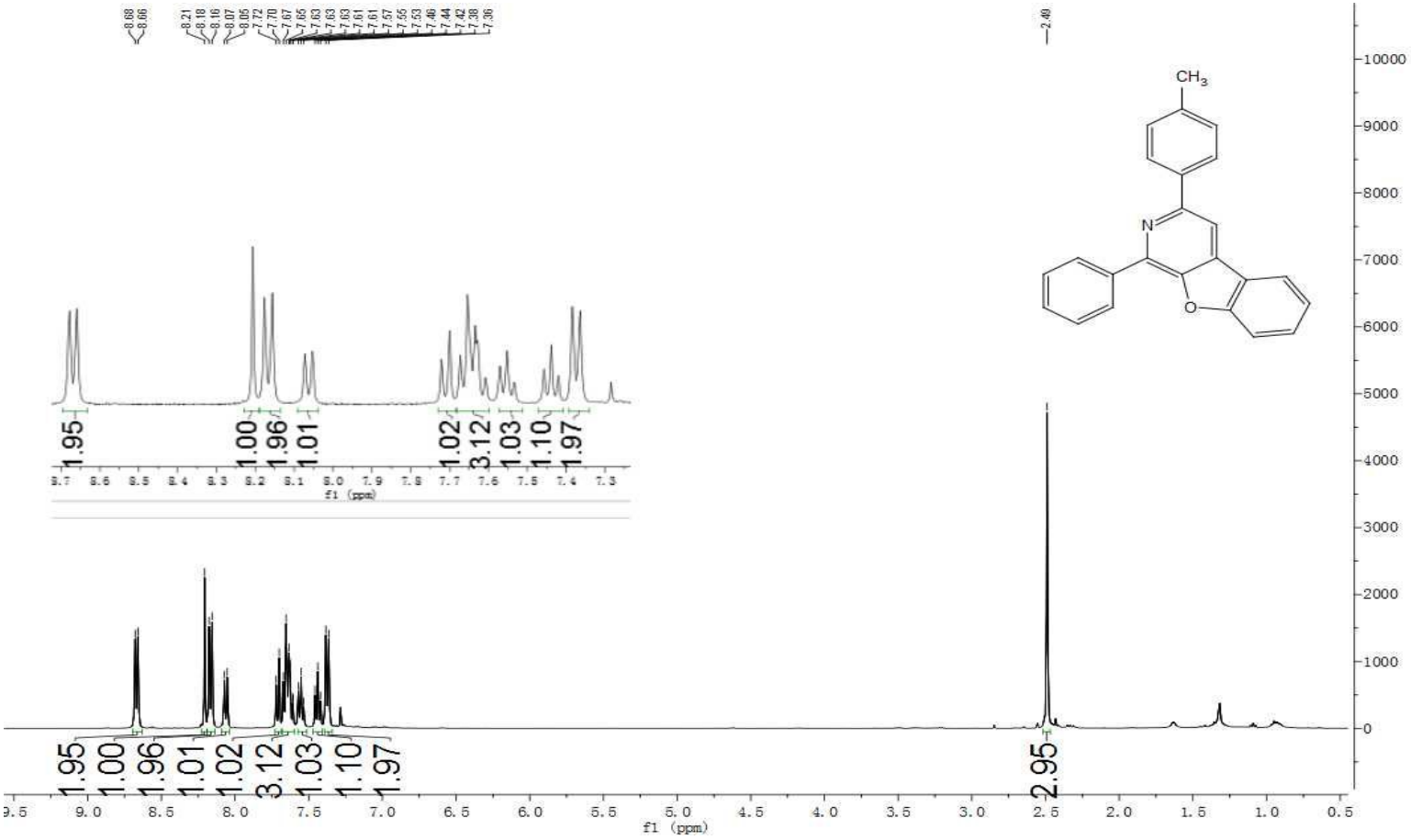
3-(4-methoxyphenyl)-1-phenylbenzofuro[2,3-c]pyridine (Table 3, Entry 20)

^{13}C NMR



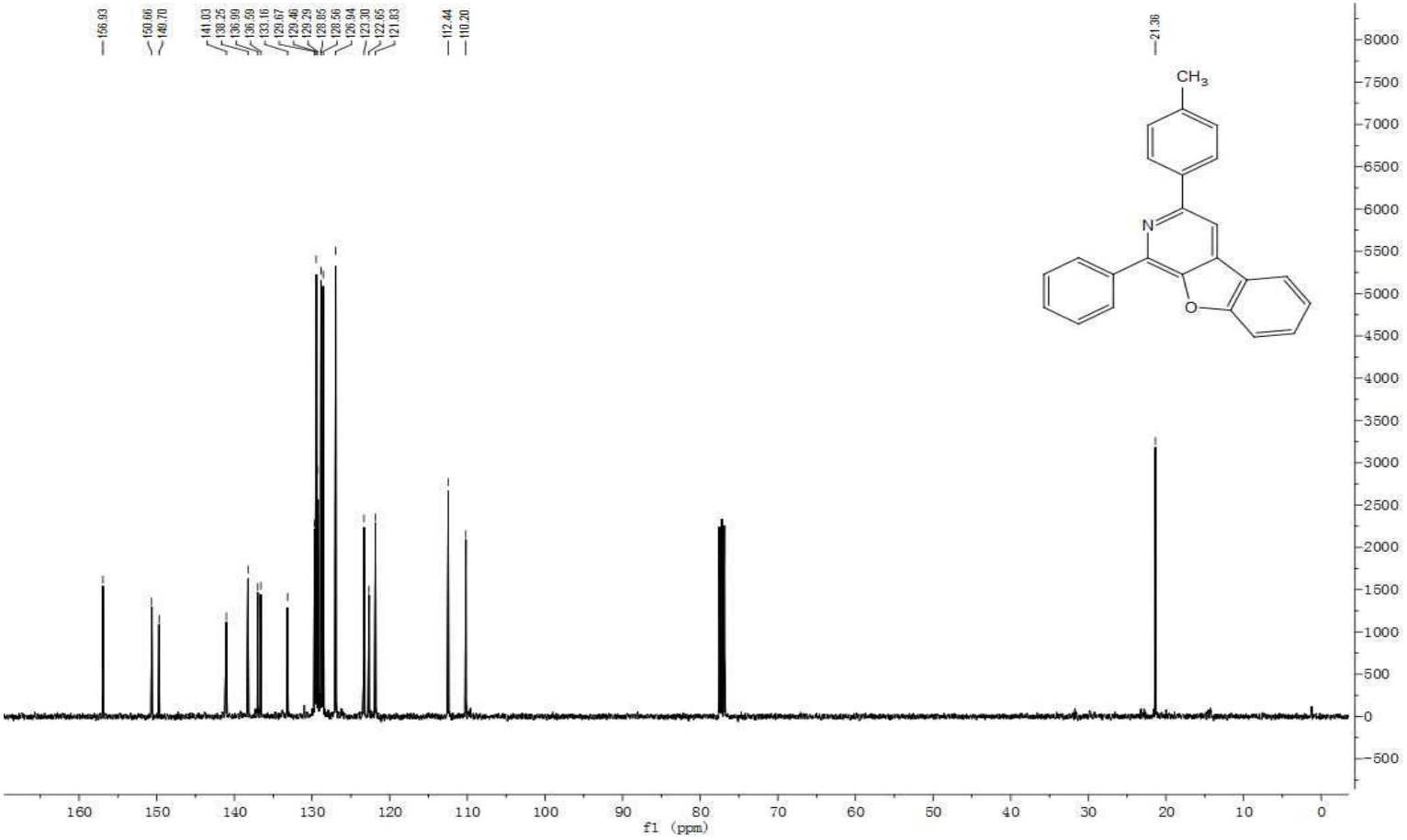
1-phenyl-3-(p-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry 21)

^{1}H NMR



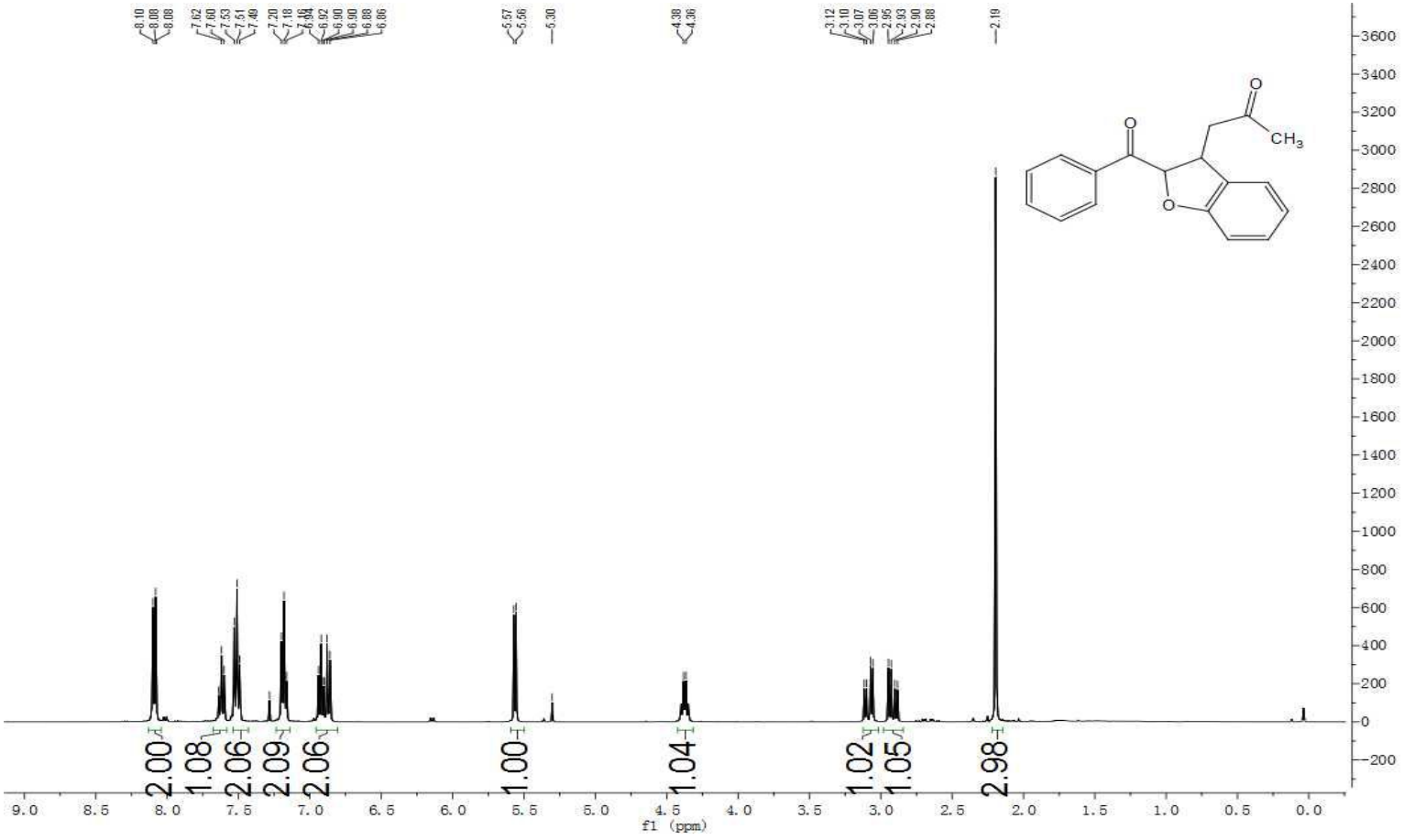
1-phenyl-3-(p-tolyl)benzofuro[2,3-c]pyridine (Table 3, Entry21)

^{13}C NMR



1-(2-benzoyl-2, 3-dihydrobenzofuran-3-yl)propan-2-one (compound 4a)

^{1}H NMR



1-(2-benzoyl-2, 3-dihydrobenzofuran-3-yl)propan-2-one (compound 4a)

^{13}C NMR