Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Palladium-Catalyzed C–S Bond Activation and Functionalization of 3-Sulfenylindoles and Related Electron-Rich Heteroarenes

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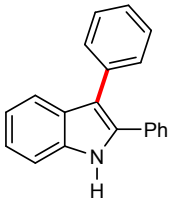
General methods

Melting points were measured using a melting point instrument and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. The chemical shifts are referenced to signals at 7.24 and 77.0 ppm, respectively, and chloroform was used as a solvent with TMS as the internal standard. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC-MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100−400 mesh silica gel plates (GF_{254}). Unless otherwise noted, purchased chemicals were used without further purification.

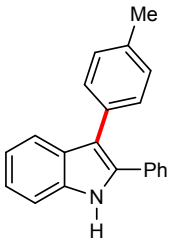
Typical procedure for preparation of 3-arylindoles

A mixture of $Pd(PPh_3)_4$ (5 mol %), CuTC (1.2 equiv), 4Å MS (100 mg), and 1,4-dioxane (2 mL) was added to an Schlenk tube equipped with a stir-bar. A balloon filled with N_2 was connected to the Schlenk tube via the side tube and purged 3 times. Then, 3-sulfenylheteroarenes (0.2 mmol), and arylboronic acids (0.3 mmol) were quickly added to the tube under N_2 atmosphere and stirred at 80 ^{o}C for 12 h. After the reaction was finished, the N_2 gas was released carefully and the reaction was quenched by water and extracted with CH_2Cl_2 three times. The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate) to afford the desired products.

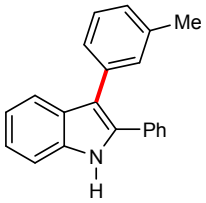
Characterization data for all products



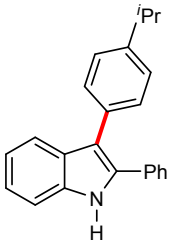
2,3-Diphenyl-1H-indole (**3a**)[1] : Yield: 81% (43.6 mg) as a yellow solid; mp = 120.3 - 121.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 7.2 Hz, 2H), 7.39 - 7.33 (m, 5H), 7.29 -7.25 (m, 5H), 7.13 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 135.2, 134.2, 132.8, 130.3, 128.9, 128.7, 128.6, 128.3, 127.8, 126.3, 122.8, 120.6, 119.8, 115.1, 111.0 ppm; ν_{max}(KBr)/cm^{-1} 3410, 3055, 1602, 1503, 1451, 744; MS (EI) m/z 127, 134, 165, 213, 269; HRMS-ESI (m/z): calcd for $C_{20}H_{16}N$, $[M+H]^+$: 270.1277, found 270.1280.



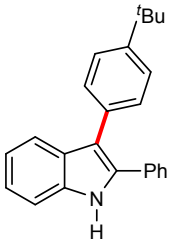
2-Phenyl-3-(*p*-tolyl)-1H-indole (**3b**)[1] : Yield: 83% (46.9 mg) as a white solid; mp = 123.3 - 124.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.40 (d, J = 7.2 Hz, 2H), 7.36 (s, 1H), 7.31 (t, J = 6.5 Hz, 3H), 7.27 (s, 1H), 7.19 (dd, J = 14.4, 7.6 Hz, 3H), 7.12 (d, J = 7.6 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 135.8, 133.9, 132.9, 132.1, 130.1, 129.3, 128.7, 128.2, 127.7, 125.2, 122.7, 120.4, 119.8, 110.9, 100.1, 21.3 ppm; ν_{max}(KBr)/cm^{-1} 3409, 3054, 2922, 1603, 1484, 743; MS (EI) m/z 133, 165, 204, 267, 283; HRMS-ESI (m/z): calcd for $C_{21}H_{18}N$, $[M+H]^+$: 284.1434, found 284.1428.



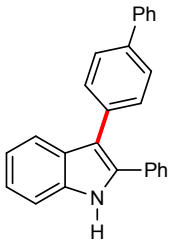
2-Phenyl-3-(*m*-tolyl)-1H-indole (**3c**)[2] : Yield: 80% (45.3 mg) as a white solid; mp = 118.7 - 120.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.36 (dd, J = 13.6, 8.0 Hz, 3H), 7.27 - 7.19 (m, 7H), 7.13 (d, J = 7.6 Hz, 1H), 7.09 (t, J = 7.2 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 136.0, 135.1, 134.1, 132.8, 130.8, 130.3, 128.7, 128.5, 128.2, 127.7, 127.4, 127.1, 122.8, 120.5, 119.9, 115.2, 111.0, 21.6 ppm; ν_{max}(KBr)/cm^{-1} 3409, 3054, 2923, 1604, 1451, 744; MS (EI) m/z 134, 165, 178, 267, 283; HRMS-ESI (m/z): calcd for $C_{21}H_{18}N$, $[M+H]^+$: 284.1434, found 284.1430.



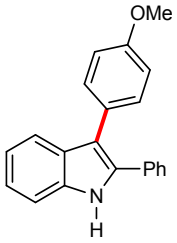
3-(4-Isopropylphenyl)-2-phenyl-1H-indole (**3d**) : Yield: 81% (50.4 mg) as a yellow solid; mp = 74.5 - 76.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.31 (d, J = 7.2 Hz, 2H), 7.26 (d, J = 7.6 Hz, 3H), 7.19 (d, J = 7.6 Hz, 2H), 7.16 - 7.10 (m, 3H), 7.06 - 7.02 (m, 1H), 2.84 (dt, J = 13.6, 6.8 Hz, 1H), 1.20 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 135.9, 133.9, 132.9, 132.4, 130.0, 128.7, 128.2, 127.6, 126.6, 125.2, 122.7, 120.4, 119.9, 115.1, 110.9, 33.9, 24.1 ppm; ν_{max}(KBr)/cm^{-1} 3410, 3055, 2926, 1604, 1484, 1410, 743; MS (EI) m/z 134, 204, 239, 267, 280, 311; HRMS-ESI (m/z): calcd for $C_{23}H_{21}NNa$, $[M+Na]^+$: 334.1566, found 334.1561.



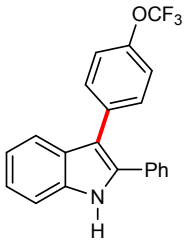
3-(4-(*tert*-Butyl)phenyl)-2-phenyl-1H-indole (**3e**)[3] : Yield: 85% (55.3 mg) as a yellow solid; mp = 62.0 - 63.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.41 (d, J = 7.2 Hz, 2H), 7.38 - 7.35 (m, 5H), 7.28 (q, J = 7.6 Hz, 3H), 7.23 - 7.18 (m, 1H), 7.12 (t, J = 7.2 Hz, 1H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 136.0, 133.9, 132.9, 131.9, 130.2, 129.7, 128.7, 128.3, 127.6, 125.5, 122.7, 120.3, 120.0, 115.0, 110.9, 34.6, 31.5 ppm; ν_{max}(KBr)/cm^{-1} 3409, 3056, 2960, 1603, 1452, 744; MS (EI) m/z 134, 155, 204, 267, 310, 325; HRMS-ESI (m/z): calcd for $C_{24}H_{23}NNa$, $[M+Na]^+$: 348.1723, found 348.1718.



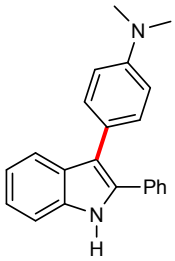
3-([1,1'-Biphenyl]-4-yl)-2-phenyl-1H-indole (**3f**)[3] : Yield: 78% (53.8 mg) as a yellow solid; mp = 103.5 - 104.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.6 Hz, 2H), 7.58 (d, J = 7.2 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.45 - 7.38 (m, 4H), 7.37 - 7.25 (m, 5H), 7.21 (d, J = 7.6 Hz, 1H), 7.15 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 138.9, 136.1, 134.4, 134.3, 132.8, 130.6, 128.9, 128.8, 128.4, 128.2, 127.8, 127.3, 127.2, 127.0, 122.8, 120.6, 119.8, 114.7, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3414, 3055, 2196, 1602, 1488, 1451, 739; MS (EI) m/z 77, 134, 165, 207, 254, 315, 345; HRMS-ESI (m/z): calcd for $C_{26}H_{19}NNa$, $[M+Na]^+$: 368.1410, found 368.1407.



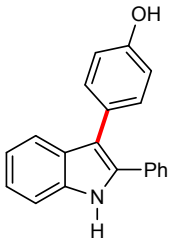
3-(4-Methoxyphenyl)-2-phenyl-1H-indole (**3g**)[4] : Yield: 73% (43.7 mg) as a brown solid; mp = 184.2 - 185.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.4 Hz, 2H), 7.38 - 7.27 (m, 5H), 7.22 (t, J = 7.2 Hz, 2H), 7.13 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 7.2 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 135.9, 133.8, 132.9, 131.2, 129.0, 128.7, 128.1, 127.6, 127.4, 122.7, 120.3, 119.7, 114.7, 114.1, 110.9, 55.3 ppm; ν_{max}(KBr)/cm^{-1} 3409, 3055, 2928, 1606, 1512, 1453, 745; MS (EI) m/z 127, 142, 190, 254, 284, 299; HRMS-ESI (m/z): calcd for $C_{21}H_{17}NNaO$, $[M+Na]^+$: 322.1202, found 322.1201.



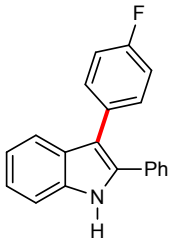
2-Phenyl-3-(4-(trifluoromethoxy)phenyl)-1H-indole (**3h**): Yield: 79% (55.8 mg) as a brown solid; mp = 147.2 - 148.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.36 (dd, J = 12.8, 6.8 Hz, 5H), 7.32 - 7.26 (m, 4H), 7.23 (d, J = 7.6 Hz, 1H), 7.16 (t, J = 7.6 Hz, 1H), 7.11 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 137.3, 135.9, 134.9, 132.2, 129.8, 128.9, 128.5, 128.3, 128.3, 123.0, 122.6, 120.9, 119.3, 118.7, 113.5, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3417, 3062, 1607, 1533, 1451, 747; MS (EI) m/z 134, 165, 190, 267, 353; HRMS-ESI (m/z): calcd for $C_{21}H_{14}F_3NNaO$, $[M+Na]^+$: 376.0920, found 376.0923.



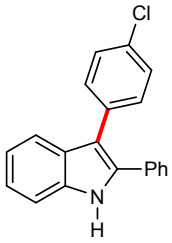
N,*N*-dimethyl-4-(2-phenyl-1H-indol-3-yl)aniline (**3i**): Yield: 66% (41.2 mg) as a yellow solid; mp = 95.6 - 97.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.53 - 7.48 (m, 2H), 7.44 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.6 Hz, 4H), 7.31 (d, J = 7.2 Hz, 1H), 7.25 (d, J = 7.6 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 3.03 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 135.9, 133.4, 133.2, 130.9, 129.2, 128.6, 128.0, 127.4, 122.5, 120.1, 119.9, 115.3, 115.2, 113.0, 110.8, 40.8 ppm; ν_{max}(KBr)/cm^{-1} 3410, 3052, 1606, 1451, 1328, 748; MS (EI) m/z 96, 134, 156, 207, 267, 312; HRMS-ESI (m/z): calcd for $C_{22}H_{21}N_2$, $[M+H]^+$: 313.1699, found 313.1702.



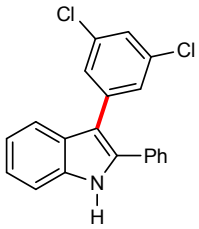
4-(2-Phenyl-1H-indol-3-yl)phenol (**3j**)[6] : Yield: 65% (37.1 mg) as a white solid; mp = 134.6 - 136.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.40 (t, J = 6.8 Hz, 3H), 7.34 - 7.26 (m, 5H), 7.22 (d, J = 8.8 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 8.0 Hz, 2H), 4.92 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 135.9, 133.8, 132.8, 131.4, 129.0, 128.7, 128.1, 127.6, 127.5, 122.7, 120.3, 119.7, 115.6, 114.7, 110.9 ppm; ν_{max}(KBr)/cm^{-1} 3410, 3055, 1608, 1513, 1451, 747; MS (EI) m/z 79, 96, 134, 181, 207, 254, 285; HRMS-ESI (m/z): calcd for $C_{20}H_{15}NNaO$, $[M+Na]^+$: 308.1046, found 308.1038.



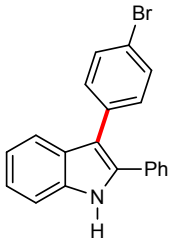
3-(4-Fluorophenyl)-2-phenyl-1H-indole (**3k**)[4] : Yield: 78% (44.8 mg) as a white solid; mp = 163.4 - 164.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.41 - 7.33 (m, 5H), 7.29 (q, J = 7.2 Hz, 3H), 7.24 - 7.19 (m, 1H), 7.18 - 7.10 (m, 1H), 7.05 (t, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.67 (d, J = 245.0 Hz), 135.9, 134.2, 132.6, 131.68 (d, J = 7.8 Hz), 131.04 (d, J = 3.3 Hz), 128.8, 128.2, 127.9, 125.2, 122.8, 120.6, 119.5, 115.55 (d, J = 21.2 Hz), 114.1, 111.0 ppm; ν_{max}(KBr)/cm^{-1} 3413, 3056, 1602, 1452, 746; MS (EI) m/z 132, 165, 183, 257, 272, 287; HRMS-ESI (m/z): calcd for $C_{20}H_{14}FNNa$, $[M+Na]^+$: 310.1002, found 310.1000.



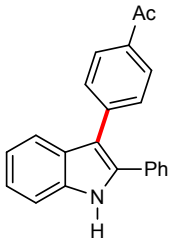
3-(4-Chlorophenyl)-2-phenyl-1H-indole (**3l**)[4] : Yield: 80% (48.5 mg) as a white solid; mp = 145.2 - 146.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.46 (dd, J = 7.6, 1.8 Hz, 3H), 7.44 - 7.37 (m, 7H), 7.33 (t, J = 7.2 Hz, 1H), 7.25 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 134.5, 133.7, 132.4, 132.1, 131.5, 128.8, 128.9, 128.5, 128.3, 128.0, 122.9, 120.7, 119.5, 113.8, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3411, 3048, 1606, 1449, 744; MS (EI) m/z 121, 134, 165, 239, 267, 303; HRMS-ESI (m/z): calcd for $C_{20}H_{14}ClNNa$, $[M+Na]^+$: 326.0707, found 326.0710.



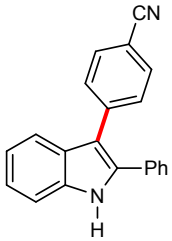
3-(3,5-Dichlorophenyl)-2-phenyl-1H-indole (**3m**): Yield: 72% (48.5 mg) as a yellow solid; mp = 134.5 - 136.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.35 (dd, J = 13.2, 9.6 Hz, 6H), 7.25 (dd, J = 11.4, 9.6 Hz, 4H), 7.17 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 135.8, 135.2, 135.0, 131.8, 129.0, 128.4, 128.3, 128.2, 128.1, 126.3, 123.2, 121.0, 119.2, 112.3, 111.2 ppm; ν_{max}(KBr)/cm^{-1} 3417, 3061, 1587, 1407, 744; MS (EI) m/z 118, 132, 199, 267, 301, 337; HRMS-ESI (m/z): calcd for $C_{20}H_{13}Cl_2NNa$, $[M+Na]^+$: 360.0317, found 360.0315.



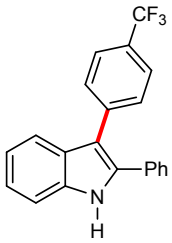
3-(4-Bromophenyl)-2-phenyl-1H-indole (**3n**)[1] : Yield: 76% (52.7 mg) as a yellow solid; mp = 123.8 - 125.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 7.6 Hz, 2H), 7.46 (d, J = 7.6 Hz, 3H), 7.43 - 7.30 (m, 6H), 7.25 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 134.5, 134.2, 132.4, 131.8, 128.9, 128.5, 128.4, 128.3, 128.0, 123.0, 120.7, 120.2, 119.5, 113.8, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3416, 3056, 1601, 1500, 1451, 744; MS (EI) m/z 134, 165, 267, 332, 347; HRMS-ESI (m/z): calcd for $C_{20}H_{14}BrNNa$, $[M+Na]^+$: 370.0202, found 370.0204.



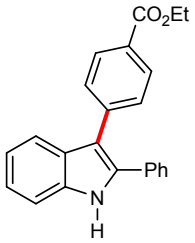
1-(4-(2-Phenyl-1H-indol-3-yl)phenyl)ethanone (**3o**)[2] : Yield: 70% (43.5 mg) as a yellow solid; mp = 203.3 - 204.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.96 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.0 Hz, 1H), 7.53 (d, J = 8.0 Hz, 2H), 7.43 (dd, J = 14.4, 7.6 Hz, 3H), 7.34 (d, J = 6.0 Hz, 3H), 7.28 (d, J = 7.2 Hz, 1H), 7.18 (t, J = 7.6 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 140.7, 136.0, 135.2, 134.8, 132.3, 130.0, 128.9, 128.7, 128.4, 128.2, 128.2, 123.0, 120.9, 119.4, 113.9, 111.1, 26.6 ppm; ν_{max}(KBr)/cm^{-1} 3395, 3057, 1669, 1601, 1552, 1451, 744; MS (EI) m/z 134, 148, 190, 268, 296, 311; HRMS-ESI (m/z): calcd for $C_{22}H_{17}NNaO$, $[M+Na]^+$: 334.1202, found 334.1210.



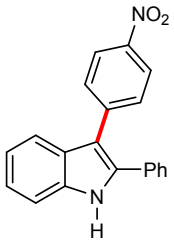
4-(2-Phenyl-1H-indol-3-yl)benzonitrile (**3p**)[2] : Yield: 66% (38.8 mg) as a yellow solid; mp = 211.5 - 213.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.2 Hz, 2H), 7.53 (d, J = 7.6 Hz, 2H), 7.45 (d, J = 8.0 Hz, 1H), 7.43 - 7.32 (m, 5H), 7.28 (t, J = 7.6 Hz, 1H), 7.20 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 136.0, 135.5, 132.3, 132.0, 130.5, 129.0, 128.5, 128.5, 127.9, 123.2, 121.1, 119.3, 119.1, 113.2, 111.3, 109.4 ppm; ν_{max}(KBr)/cm^{-1} 3395, 3057, 2225, 1668, 1552, 1451, 744; MS (EI) m/z 118, 132, 147, 207, 264, 294; HRMS-ESI (m/z): calcd for $C_{21}H_{14}N_2Na$, $[M+Na]^+$: 317.1049, found 317.1049.



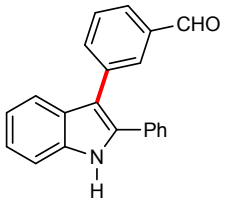
2-Phenyl-3-(4-(trifluoromethyl)phenyl)-1H-indole (**3q**)[4] : Yield: 71% (47.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.41 - 7.28 (m, 6H), 7.24 (t, J = 7.6 Hz, 1H), 7.16 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 136.0, 135.1, 132.3, 130.2, 128.9, 128.4, 128.3 (q, J = 256.8 Hz), 128.2, 128.1, 125.9, 125.50 (q, J = 3.7 Hz), 123.2, 123.1, 120.9, 119.4, 113.6, 111.2 ppm; ν_{max}(KBr)/cm^{-1} 3411, 3058, 1613, 1488, 1406, 744; MS (EI) m/z 77, 134, 165, 239, 267, 322, 337; HRMS-ESI (m/z): calcd for $C_{21}H_{15}F_3N$, $[M+H]^+$: 338.1151, found 338.1150.



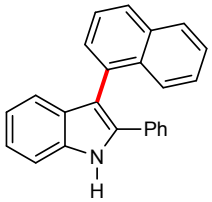
Ethyl 4-(2-phenyl-1H-indol-3-yl)benzoate (**3r**) : Yield: 63% (42.9 mg) as a yellow solid; mp = 134.3 - 135.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.02 (d, J = 8.0 Hz, 2H), 7.68 (d, J = 8.0 Hz, 1H), 7.48 (d, J = 8.0 Hz, 2H), 7.39 (dd, J = 10.4, 6.8 Hz, 3H), 7.28 (d, J = 5.0 Hz, 3H), 7.24 - 7.19 (m, 1H), 7.16 (t, J = 7.6 Hz, 1H), 4.37 (q, J = 7.2 Hz, 2H), 1.38 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 140.4, 136.1, 135.2, 132.4, 129.9, 129.9, 128.8, 128.5, 128.3, 128.1, 127.9, 122.9, 120.8, 119.4, 113.9, 111.2, 61.0, 14.4 ppm; ν_{max}(KBr)/cm^{-1} 3344, 3056, 2982, 1695, 1605, 1452, 1274, 742; MS (EI) m/z 134, 165, 239, 267, 296, 341; HRMS-ESI (m/z): calcd for $C_{23}H_{19}NNaO_2$, $[M+Na]^+$: 364.1308, found 364.1318.



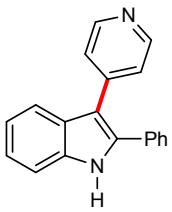
3-(4-Nitrophenyl)-2-phenyl-1H-indole (**3s**) : Yield: 58% (42.9 mg) as a yellow solid; mp = 156.2 - 157.8 °C; ^{1}H NMR (400 MHz, DMSO) δ 11.86 (s, 1H), 8.23 (d, J = 8.0 Hz, 2H), 7.62 (dd, J = 14.4, 8.2 Hz, 3H), 7.45 (ddd, J = 24.8, 14.4, 9.2 Hz, 6H), 7.23 (t, J = 7.6 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ 145.1, 143.0, 136.3, 131.8, 130.2, 130.0, 128.8, 128.7, 128.3, 127.1, 123.9, 122.5, 120.5, 118.3, 111.8, 111.2 ppm; ν_{max}(KBr)/cm^{-1} 3384, 3059, 1668, 1548, 1452, 743; MS (EI) m/z 134, 190, 239, 267, 314; HRMS-ESI (m/z): calcd for $C_{20}H_{14}N_2NaO_2$, $[M+Na]^+$: 337.0947, found 337.0949.



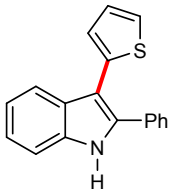
3-(2-Phenyl-1H-indol-3-yl)benzaldehyde (**3t**) : Yield: 54% (32.1 mg) as a yellow solid; mp = 211.3 - 212.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.36 (s, 1H), 7.97 (t, J = 1.6 Hz, 1H), 7.81 (dt, J = 7.6, 1.2 Hz, 1H), 7.67 (ddd, J = 8.0, 3.6, 2.0 Hz, 2H), 7.51 (t, J = 7.6 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.42 - 7.38 (m, 2H), 7.36 - 7.31 (m, 3H), 7.28 (dd, J = 7.2, 1.0 Hz, 1H), 7.20 - 7.16 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 136.9, 136.4, 136.3, 135.9, 134.8, 132.2, 131.8, 129.3, 128.9, 128.4, 128.3, 128.1, 127.1, 123.0, 120.8, 119.2, 113.5, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3390, 3056, 1688, 1494, 1452, 742; MS (EI) m/z 106, 134, 165, 239, 267, 297; HRMS-ESI (m/z): calcd for $C_{21}H_{15}NNaO$, $[M+Na]^+$: 320.1046, found 320.1038



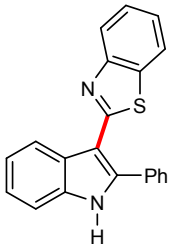
3-(Naphthalen-1-yl)-2-phenyl-1H-indole (**3u**)[4] : Yield: 75% (47.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 7.86 (dd, J = 16.4, 8.0 Hz, 2H), 7.77 (d, J = 8.4 Hz, 1H), 7.48 - 7.37 (m, 4H), 7.28 - 7.17 (m, 5H), 7.13 - 7.07 (m, 3H), 7.03 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 135.1, 134.1, 133.1, 133.1, 132.5, 130.5, 129.2, 128.7, 128.3, 127.6, 127.5, 127.3, 126.8, 125.9, 125.9, 125.8, 122.8, 120.4, 120.4, 113.5, 110.9 ppm; ν_{max}(KBr)/cm^{-1} 3417, 3053, 1597, 1488, 1451, 744; MS (EI) m/z 121, 158, 215, 241, 319; HRMS-ESI (m/z): calcd for $C_{24}H_{18}N$, $[M+H]^+$: 320.1434, found 320.1428.



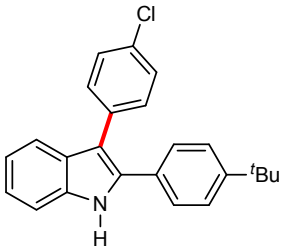
2-Phenyl-3-(pyridin-4-yl)-1H-indole (**3v**) : Yield: 63% (34.0 mg) as a yellow solid; mp = 252.6 - 253.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.56 (s, 2H), 7.74 (d, J = 8.0 Hz, 1H), 7.45 (dd, J = 13.4, 6.4 Hz, 3H), 7.40 - 7.32 (m, 5H), 7.29 (t, J = 7.6 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 143.8, 136.1, 136.0, 131.9, 129.0, 128.6, 128.5, 127.7, 124.7, 123.2, 121.1, 119.2, 112.0, 111.3 ppm; ν_{max}(KBr)/cm^{-1} 3394, 3061, 1661, 1452, 1406, 737; MS (EI) m/z 121, 135, 189, 241, 270; HRMS-ESI (m/z): calcd for $C_{19}H_{15}N_2$, $[M+H]^+$: 271.1230, found 271.1237.



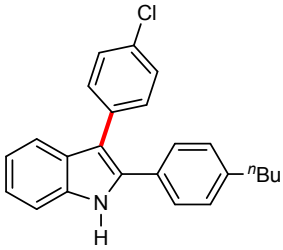
2-Phenyl-3-(thiophen-2-yl)-1H-indole (**3w**)[5] : Yield: 69% (37.9 mg) as a white solid; mp = 126.4 - 127.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.45 (d, J = 7.2 Hz, 2H), 7.31 (dd, J = 6.8, 4.4 Hz, 4H), 7.23 (dd, J = 17.6, 6.4 Hz, 2H), 7.16 (t, J = 7.4 Hz, 1H), 7.03 (d, J = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.5, 135.7, 135.3, 132.4, 128.9, 128.7, 128.5, 128.2, 127.3, 126.3, 124.7, 123.0, 120.8, 120.0, 111.0, 108.0 ppm; ν_{max}(KBr)/cm^{-1} 3406, 3058, 1603, 1485, 1409, 743; MS (EI) m/z 77, 121, 137, 171, 241, 275; HRMS-ESI (m/z): calcd for $C_{18}H_{13}NNaS$, $[M+Na]^+$: 298.0661, found 298.0662.



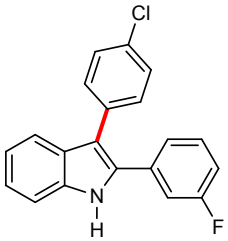
2-(2-Phenyl-1H-indol-3-yl)benzo[d]thiazole (**3x**) : Yield: 57% (37.2 mg) as a brown solid; mp = 215.7 - 217.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.54 (d, J = 7.2 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 7.2 Hz, 2H), 7.42 (m, 5H), 7.34 - 7.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 153.6, 139.7, 135.6, 134.6, 131.5, 129.9, 129.5, 128.9, 127.3, 125.7, 124.3, 123.6, 122.5, 121.9, 121.8, 121.1, 110.9, 109.1 ppm; ν_{max}(KBr)/cm^{-1} 3405, 3058, 1615, 1502, 1446, 749; MS (EI) m/z 146, 163, 207, 292, 326; HRMS-ESI (m/z): calcd for $C_{21}H_{15}N_2S$, $[M+H]^+$: 327.0950, found 327.0953.



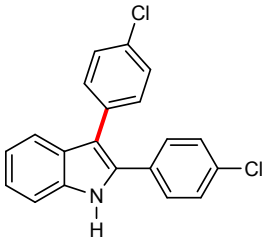
2-(4-(*tert*-Butyl)phenyl)-3-(4-chlorophenyl)-1H-indole (**5a**) : Yield: 83% (59.6 mg) as a yellow solid; mp = 131.2 - 132.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.40 - 7.30 (m, 9H), 7.21 (t, J = 7.6 Hz, 1H), 7.13 (t, J = 7.2 Hz, 1H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 135.9, 134.5, 133.9, 131.9, 131.5, 129.5, 128.8, 128.7, 127.8, 125.8, 122.7, 120.6, 119.3, 113.4, 111.0, 34.7, 31.3 ppm; ν_{max}(KBr)/cm^{-1} 3416, 3055, 2962, 1567, 1485, 1433, 1266, 742; MS (EI) m/z 77, 119, 141, 207, 267, 309, 344, 359; HRMS-ESI (m/z): calcd for $C_{24}H_{22}ClNNa$, $[M+Na]^+$: 382.1333, found 382.1337.



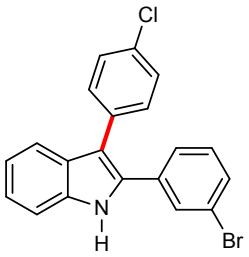
2-(4-Butylphenyl)-3-(4-chlorophenyl)-1H-indole (**5b**): Yield: 80% (57.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.40 - 7.30 (m, 5H), 7.28 (d, J = 7.6 Hz, 2H), 7.21 (d, J = 7.6 Hz, 1H), 7.14 (t, J = 7.2 Hz, 3H), 2.60 (t, J = 7.6 Hz, 2H), 1.66 - 1.55 (m, 2H), 1.42 - 1.31 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 135.8, 134.6, 133.8, 131.9, 131.4, 129.7, 128.9, 128.8, 128.6, 128.1, 122.7, 120.6, 119.3, 113.4, 110.9, 35.4, 33.5, 22.5, 14.0 ppm; ν_{max}(KBr)/cm^{-1} 3410, 3054, 2927, 1644, 1510, 1454, 745; MS (EI) m/z 139, 165, 207, 280, 316, 359; HRMS-ESI (m/z): calcd for $C_{24}H_{22}ClNNa$, $[M+Na]^+$: 382.1333, found 382.1335.



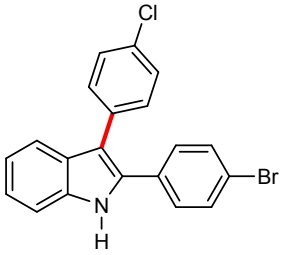
3-(4-Chlorophenyl)-2-(3-fluorophenyl)-1H-indole (**5c**) : Yield: 75% (48.2 mg) as a yellow solid; mp = 121.7 - 123.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.36 - 7.29 (m, 4H), 7.26 (dd, J = 15.6, 8.0 Hz, 2H), 7.18 - 7.11 (m, 2H), 7.07 (d, J = 10.0 Hz, 1H), 6.97 (t, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J = 246.4 Hz), 136.0, 134.5 (d, J = 8.1 Hz), 133.2, 132.9 (d, J = 2.4 Hz), 132.4, 131.4, 130.5 (d, J = 8.5 Hz), 128.9, 128.5, 123.9 (d, J = 3.0 Hz), 123.3, 120.9, 119.6, 115.0 (d, J = 10.9 Hz), 114.8, 114.7 (d, J = 9.3 Hz), 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3416, 3057, 1693, 1612, 1584, 1454, 744; MS (EI) m/z 106, 143, 183, 257, 285, 321; HRMS-ESI (m/z): calcd for $C_{20}H_{13}ClFNNa$, $[M+Na]^+$: 344.0613, found 344.0611.



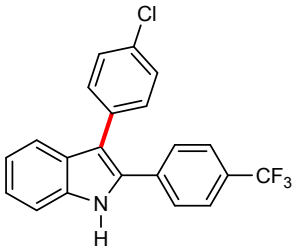
2,3-Bis(4-chlorophenyl)-1H-indole (**5d**)[7] : Yield: 80% (53.9 mg) as a yellow solid; mp = 133.5 - 135.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.32 (dd, J = 13.2, 11.4 Hz, 8H), 7.25 - 7.21 (m, 1H), 7.15 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 133.9, 133.3, 133.1, 132.3, 131.4, 130.9, 129.4, 129.1, 128.9, 128.5, 123.2, 120.8, 119.5, 114.3, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3428, 3054, 1660, 1546, 1453, 743; MS (EI) m/z 134, 165, 239, 267, 301, 337; HRMS-ESI (m/z): calcd for $C_{20}H_{13}Cl_2NNa$, $[M+Na]^+$: 360.0317, found 360.0314.



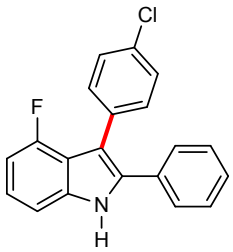
2-(3-Bromophenyl)-3-(4-chlorophenyl)-1H-indole (**5e**): Yield: 76% (57.8 mg) as a yellow solid; mp = 141.5 - 142.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.56 (s, 1H), 7.43 - 7.36 (m, 2H), 7.32 (q, J = 8.6 Hz, 4H), 7.24 (dd, J = 12.4, 7.2 Hz, 2H), 7.14 (dd, J = 17.6, 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 134.5, 133.1, 132.6, 132.4, 131.4, 130.9, 130.7, 130.3, 128.9, 128.4, 127.1, 123.4, 122.9, 120.9, 119.6, 114.7, 111.2 ppm; ν_{max}(KBr)/cm^{-1} 3421, 3056, 1595, 1452, 744; MS (EI) m/z 118, 134, 207, 267, 345, 381; HRMS-ESI (m/z): calcd for $C_{20}H_{13}BrClNNa$, $[M+Na]^+$: 403.9812, found 403.9810.



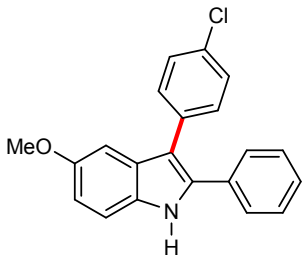
2-(4-Bromophenyl)-3-(4-chlorophenyl)-1H-indole (**5f**): Yield: 73% (55.6 mg) as a yellow solid; mp = 139.3 - 140.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 7.6 Hz, 2H), 7.37 (d, J = 8.0 Hz, 1H), 7.35 - 7.28 (m, 4H), 7.22 (t, J = 7.6 Hz, 3H), 7.14 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.0, 133.3, 133.1, 132.3, 132.1, 131.4, 131.3, 129.7, 128.9, 128.5, 123.3, 122.1, 120.9, 119.5, 114.4, 111.1 ppm; ν_{max}(KBr)/cm^{-1} 3422, 3053, 1544, 1495, 1452, 743; MS (EI) m/z 134, 165, 207, 267, 345, 381; HRMS-ESI (m/z): calcd for $C_{20}H_{13}BrClNNa$, $[M+Na]^+$: 403.9812, found 403.9806.



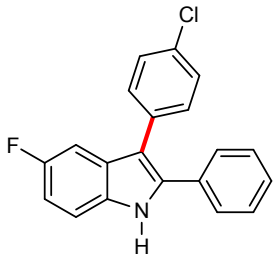
3-(4-Chlorophenyl)-2-(4-(trifluoromethyl)phenyl)-1H-indole (**5g**): Yield: 72% (55.6 mg) as a yellow solid; mp = 115.2 - 116.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.59 (dd, J = 16.8, 8.0 Hz, 3H), 7.48 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.0 Hz, 1H), 7.38 - 7.24 (m, 5H), 7.17 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.2, 135.9, 133.0, 132.6, 132.5, 131.4, 129.7 (q, J = 32.7 Hz), 129.1, 128.5, 128.2, 125.8 (d, J = 3.8 Hz), 123.6, 121.0, 119.7, 115.4, 111.2 ppm; ν_{max}(KBr)/cm^{-1} 3419, 3057, 1616, 1486, 1402, 744; MS (EI) m/z 134, 165, 207, 267, 335, 371; HRMS-ESI (m/z): calcd for $C_{21}H_{13}ClF_3NNa$, $[M+Na]^+$: 394.0581, found 394.0577.



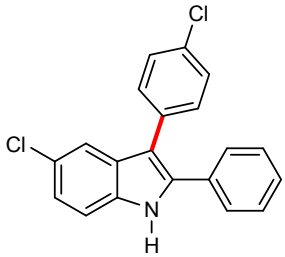
3-(4-Chlorophenyl)-4-fluoro-2-phenyl-1H-indole (**5h**): Yield: 79% (50.7 mg) as a white solid; mp = 107.2 - 108.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.40 - 7.31 (m, 9H), 7.24 (d, J = 8.0 Hz, 1H), 7.17 (td, J = 8.0, 4.8 Hz, 1H), 6.83 (ddd, J = 11.4, 7.6, 0.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0 (d, J = 248.7 Hz), 138.3 (d, J = 10.6 Hz), 134.7 (d, J = 1.2 Hz), 133.4 (d, J = 1.0 Hz), 132.4, 132.2 (d, J = 2.4 Hz), 131.9, 128.8, 128.3, 128.2, 128.1, 123.1 (d, J = 8.1 Hz), 117.1 (d, J = 18.1 Hz), 112.0 (d, J = 2.9 Hz), 107.1 (d, J = 3.7 Hz), 105.9 (d, J = 20.1 Hz) ppm; ν_{max}(KBr)/cm^{-1} 3410, 3052, 1618, 1540, 1438, 746; MS (EI) m/z 96, 134, 143, 207, 285, 321; HRMS-ESI (m/z): calcd for $C_{20}H_{14}ClFN$, $[M+H]^+$: 322.0793, found 322.0796.



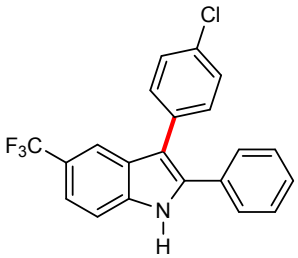
3-(4-Chlorophenyl)-5-methoxy-2-phenyl-1H-indole (**5i**): Yield: 73% (48.6 mg) as a white solid; mp = 218.4 - 219.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.37 - 7.32 (m, 6H), 7.28 (t, J = 8.0 Hz, 4H), 7.05 (s, 1H), 6.89 (d, J = 8.8 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 135.3, 133.8, 132.5, 132.0, 131.4, 131.1, 129.0, 128.9, 128.8, 128.1, 127.9, 113.7, 113.1, 111.9, 101.1, 56.0 ppm; ν_{max}(KBr)/cm^{-1} 3300, 3057, 2924, 1609, 1501, 1471, 1092, 737; MS (EI) m/z 105, 127, 162, 254, 290, 318, 333; HRMS-ESI (m/z): calcd for $C_{21}H_{16}ClNNaO$, $[M+Na]^+$: 356.0813, found 356.0810.



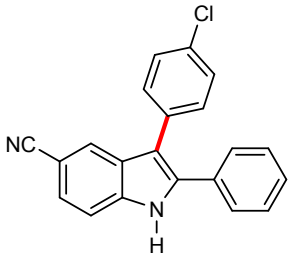
3-(4-Chlorophenyl)-5-fluoro-2-phenyl-1H-indole (**5j**): Yield: 80% (51.4 mg) as a white solid; mp = 105.3 - 106.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.40 - 7.25 (m, 11H), 6.97 (t, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6 (d, J = 235.5 Hz), 136.2, 133.2, 132.4, 132.2, 132.1, 131.2, 129.1 (d, J = 8.4 Hz), 128.9 (d, J = 2.2 Hz), 128.2, 128.0, 125.2, 113.9 (d, J = 4.8 Hz), 111.8 (d, J = 9.6 Hz), 111.2 (d, J = 26.4 Hz), 104.3 (d, J = 24.2 Hz)ppm; ν_{max}(KBr)/cm^{-1} 3440, 3055, 1626, 1480, 1415, 761; MS (EI) m/z 106, 143, 183, 285, 321; HRMS-ESI (m/z): calcd for $C_{20}H_{13}ClFNNa$, $[M+Na]^+$: 344.0613, found 344.0607.



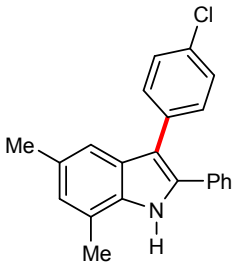
5-Chloro-3-(4-chlorophenyl)-2-phenyl-1H-indole (**5k**): Yield: 83% (55.9 mg) as a yellow solid; mp = 109.8 - 111.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.57 (s, 1H), 7.33 (dt, J = 11.2, 7.0 Hz, 10H), 7.18 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.7, 134.2, 132.9, 132.4, 131.9, 131.3, 129.6, 128.9, 128.9, 128.3, 128.2, 126.4, 123.1, 118.7, 113.5, 112.0 ppm; ν_{max}(KBr)/cm^{-1} 3425, 3060, 1660, 1547, 1501, 1461, 750; MS (EI) m/z 106, 134, 199, 267, 301, 337; HRMS-ESI (m/z): calcd for $C_{20}H_{13}Cl_2NNa$, $[M+Na]^+$: 360.0317, found 360.0318.



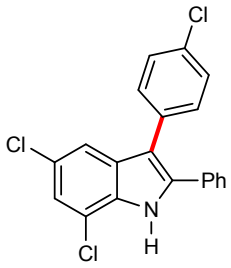
3-(4-Chlorophenyl)-2-phenyl-5-(trifluoromethyl)-1H-indole (**5l**): Yield: 68% (50.5 mg) as a yellow solid; mp = 116.3 - 117.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.88 (s, 1H), 7.50 - 7.44 (m, 2H), 7.41 - 7.30 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 136.1, 132.7, 132.7, 131.7, 131.3, 129.1, 128.9, 128.5, 128.2, 128.0, 123.4 (q, J = 32.9 Hz), 119.5 (q, J = 3.1 Hz), 117.1 (q, J = 4.3 Hz), 114.5, 111.3 ppm; ν_{max}(KBr)/cm^{-1} 3422, 3055, 1594, 1494, 1451, 744; MS (EI) m/z 134, 158, 207, 267, 335, 371; HRMS-ESI (m/z): calcd for $C_{21}H_{14}ClF_3N$, $[M+H]^+$: 372.0761, found 372.0756.



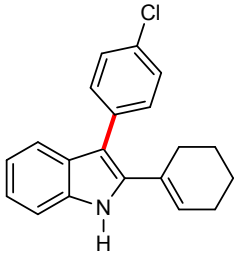
3-(4-Chlorophenyl)-2-phenyl-1H-indole-5-carbonitrile (**5m**): Yield: 60% (39.4 mg) as a yellow solid; mp = 146.8 - 148.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 7.93 (s, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.42 (dd, J = 11.2, 7.6 Hz, 3H), 7.36 (t, J = 7.0 Hz, 5H), 7.30 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 136.6, 132.9, 132.2, 131.2, 129.1, 129.0, 128.7, 128.4, 128.3, 128.0, 125.6, 125.0, 120.7, 114.1, 112.0, 103.5 ppm; ν_{max}(KBr)/cm^{-1} 3416, 3056, 1621, 1588, 1450, 735; MS (EI) m/z 105, 134, 190, 207, 292, 328; HRMS-ESI (m/z): calcd for $C_{21}H_{13}ClN_2Na$, $[M+Na]^+$: 351.0659, found 351.0663.



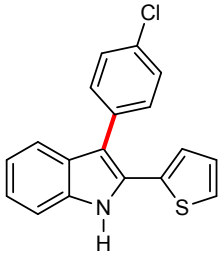
3-(4-Chlorophenyl)-5,7-dimethyl-2-phenyl-1H-indole (**5n**): Yield: 78% (51.6 mg) as a yellow solid; mp = 220.3 - 221.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.41 (d, J = 7.6 Hz, 2H), 7.37 - 7.28 (m, 7H), 7.26 (s, 1H), 6.89 (s, 1H), 2.51 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.3, 134.0, 133.8, 132.7, 131.9, 131.4, 130.3, 128.8, 128.7, 128.4, 128.2, 127.8, 125.2, 119.9, 116.6, 113.9, 21.5, 16.6 ppm; ν_{max}(KBr)/cm^{-1} 3438, 3052, 2920, 1603, 1498, 1447, 741; MS (EI) m/z 140, 178, 207, 281, 295, 331; HRMS-ESI (m/z): calcd for $C_{22}H_{18}ClNNa$, $[M+Na]^+$: 354.1020, found 354.1017.



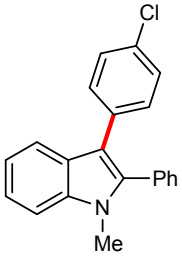
5,7-Dichloro-3-(4-chlorophenyl)-2-phenyl-1H-indole (**5o**): Yield: 66% (48.9 mg) as a yellow solid; mp = 215.5 - 216.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.47 (s, 1H), 7.43 - 7.32 (m, 7H), 7.28 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 132.8, 132.4, 131.7, 131.4, 131.2, 130.3, 129.0, 128.9, 128.7, 128.3, 126.4, 122.2, 117.7, 116.9, 114.4 ppm; ν_{max}(KBr)/cm^{-1} 3432, 3058, 1617, 1501, 1467, 740; MS (EI) m/z 118, 132, 150, 197, 264, 301, 335, 371; HRMS-ESI (m/z): calcd for $C_{20}H_{12}Cl_3NNa$, $[M+Na]^+$: 393.9928, found 393.9924.



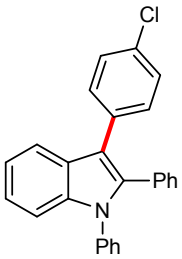
3-(4-Chlorophenyl)-2-(cyclohex-1-en-1-yl)-1H-indole (**5p**): Yield: 65% (36.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.50 - 7.45 (m, 2H), 7.44 - 7.40 (m, 2H), 7.37 (d, J = 8.0 Hz, 1H), 7.25 - 7.20 (m, 1H), 7.17 - 7.11 (m, 1H), 6.12 - 6.06 (m, 1H), 2.24 - 2.14 (m, 4H), 1.71 - 1.66 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 134.8, 134.5, 131.7, 131.0, 130.7, 128.9, 128.5, 122.3, 120.3, 118.9, 112.4, 110.6, 27.8, 25.7, 22.7, 21.9 ppm; ν_{max}(KBr)/cm^{-1} 3408, 3052, 2926, 1602, 1496, 1416, 746; MS (EI) m/z 115, 168, 230, 264, 272, 307; HRMS-ESI (m/z): calcd for $C_{20}H_{19}ClN$, $[M+H]^+$: 308.1201, found 308.1198.



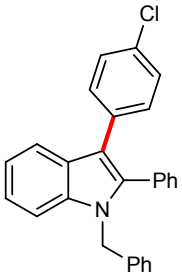
3-(4-Chlorophenyl)-2-(thiophen-2-yl)-1H-indole (**5q**): Yield: 67% (41.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.41 - 7.33 (m, 5H), 7.29 - 7.23 (m, 2H), 7.20 (d, J = 6.0 Hz, 1H), 7.12 (dd, J = 14.8, 7.2 Hz, 1H), 7.01 (t, J = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.7, 133.6, 133.3, 132.3, 131.5, 129.8, 128.8, 128.6, 126.9, 126.3, 122.9, 122.4, 120.7, 119.3, 113.7, 110.9 ppm; ν_{max}(KBr)/cm^{-1} 3419, 3054, 1662, 1511, 1455, 744; MS (EI) m/z 100, 114, 137, 241, 273, 309; HRMS-ESI (m/z): calcd for $C_{18}H_{13}ClNS$, $[M+H]^+$: 310.0452, found 310.0447.



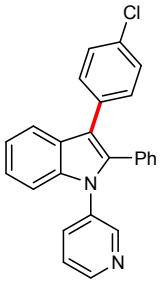
3-(4-Chlorophenyl)-1-methyl-2-phenyl-1H-indole (**5r**): Yield: 86% (54.5 mg) as a yellow solid; mp = 163.5 - 164.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.0 Hz, 1H), 7.41 - 7.34 (m, 4H), 7.32 - 7.26 (m, 3H), 7.22 - 7.16 (m, 5H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 137.4, 133.9, 131.7, 131.3, 131.2, 131.1, 128.6, 128.5, 128.3, 126.8, 122.4, 120.5, 119.4, 113.9, 109.8, 31.0 ppm; ν_{max}(KBr)/cm^{-1} 3048, 2936, 1628, 1486, 1419, 1260, 748; MS (EI) m/z 141, 204, 239, 267, 281, 317; HRMS-ESI (m/z): calcd for $C_{21}H_{17}ClN$, $[M+H]^+$: 318.1044, found 318.1045.



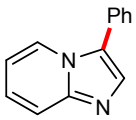
3-(4-Chlorophenyl)-1,2-diphenyl-1H-indole (**5s**): Yield: 82% (62.2 mg) as a white solid; mp = 165.8 - 167.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 - 7.71 (m, 1H), 7.39 - 7.27 (m, 8H), 7.24 - 7.19 (m, 4H), 7.18 - 7.12 (m, 3H), 7.09 - 7.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 137.9, 137.3, 133.5, 131.7, 131.4, 131.3, 131.1, 129.1, 128.8, 128.5, 128.3, 128.0, 127.6, 127.3, 122.9, 121.1, 119.3, 115.5, 110.8 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2922, 1596, 1495, 1453, 743; MS (EI) m/z 77, 113, 164, 239, 267, 343, 379; HRMS-ESI (m/z): calcd for $C_{26}H_{18}ClNNa$, $[M+Na]^+$: 402.1020, found 402.1020.



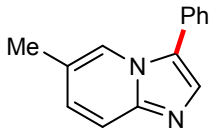
1-Benzyl-3-(4-chlorophenyl)-2-phenyl-1H-indole (**5t**)[8]: Yield: 87% (68.4 mg) as a white solid; mp = 129.0 - 130.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 - 7.74 (m, 1H), 7.31 - 7.21 (m, 10H), 7.19 - 7.14 (m, 5H), 7.01 - 6.94 (m, 2H), 5.26 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 138.0, 137.1, 133.8, 131.6, 131.4, 131.1, 131.1, 128.8, 128.6, 128.5, 128.4, 127.3, 127.2, 126.2, 122.7, 120.7, 119.5, 114.6, 110.7, 47.7 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2922, 1604, 1546, 1445, 740; MS (EI) m/z 91, 163, 239, 267, 302, 393; HRMS-ESI (m/z): calcd for $C_{27}H_{20}ClNNa$, $[M+Na]^+$: 416.1176, found 416.1172.



3-(4-Chlorophenyl)-2-phenyl-1-(pyridin-3-yl)-1H-indole (**5u**): Yield: 56% (68.4 mg) as a yellow solid; mp = 170.4 - 171.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 2H), 7.76 (dd, J = 5.6, 2.8 Hz, 1H), 7.49 (dd, J = 6.6, 4.0 Hz, 1H), 7.36 - 7.26 (m, 8H), 7.23 - 7.15 (m, 3H), 7.06 (dd, J = 8.0, 1.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 148.2, 137.8, 137.1, 135.4, 132.9, 132.1, 131.3, 131.2, 130.6, 128.6, 128.4, 128.0, 127.6, 123.7, 123.4, 121.6, 119.6, 116.5, 110.3 ppm; ν_{max}(KBr)/cm^{-1} 3441, 3053, 1637, 1454, 1426, 740; MS (EI) m/z 105, 171, 241, 267, 344, 380; HRMS-ESI (m/z): calcd for $C_{25}H_{18}ClN_2$, $[M+H]^+$: 381.1153, found 381.1158.



3-Phenylimidazo[1,2-a]pyridine (**12a**)[9] : Yield: 83% (32.2 mg) as a white solid; mp = 135.6 - 136.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 6.8 Hz, 1H), 8.01 - 7.94 (m, 2H), 7.82 (s, 1H), 7.68 - 7.60 (m, 1H), 7.45 (dd, J = 10.4, 4.8 Hz, 2H), 7.34 (ddd, J = 7.6, 4.0, 1.2 Hz, 1H), 7.15 (ddd, J = 9.0, 6.8, 1.2 Hz, 1H), 6.74 (td, J = 6.8, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 145.7, 133.7, 128.7, 127.9, 126.1, 125.6, 124.6, 117.5, 112.4, 108.1 ppm; ν_{max}(KBr)/cm^{-1} 3048, 1636, 1523, 1458, 1407, 746; MS (EI) m/z 78, 96, 139, 167, 194.



6-Methyl-3-phenylimidazo[1,2-a]pyridine (**12b**)[9] : Yield: 80% (33.3 mg) as a white solid; mp = 172.5 - 174.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.96 (d, J = 7.2 Hz, 2H), 7.89 (s, 1H), 7.77 (s, 1H), 7.55 (d, J = 9.2 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.02 (dd, J = 9.2, 1.4 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.8, 133.9, 128.7, 127.8, 127.8, 125.9, 123.3, 122.0, 116.8, 107.8, 18.1 ppm; ν_{max}(KBr)/cm^{-1} 3036, 2928, 1656, 1549, 1473, 1411, 1206, 750; MS (EI) m/z 78, 96, 167, 194, 208.

***References*:**

[1] A. Arcadi, S. Cacchi, G. Fabrizi, A. Goggiamani, A. Iazzetti and F. Marinelli, *Org. Biomol. Chem.*, 2013, **11**, 545.

[2] R. Bernini, S. Cacchi, G. Fabrizi, G. Forte, F. Petrucci, A. Prastaro, S. Niembro, A. Shafir and A. Vallribera, *Green Chem*., 2010, **12**, 150.

[3] K. Sun, S. Liu, P. M. Bec and T. G. Driver, *Angew. Chem. Int. Ed*., 2011, **50**, 1702.

[4] H. Yan, H. Wang, X. Li, X. Xin, C. Wang and B. Wan, *Angew. Chem. Int. Ed*., 2015, **54**, 10613.

[5] T. Tsuchimoto, M. Iwabuchi, Y. Nagase, K. Oki and H. Takahashi, *Angew. Chem. Int. Ed*., 2011, **50**, 1375.

[6] A. Sagadevan, A. Ragupathi and K. C. Hwang, *Angew. Chem. Int. Ed*., 2015, **54**, 13896.

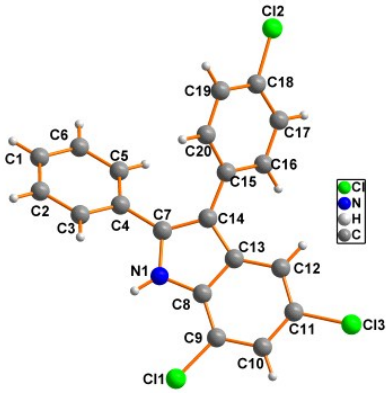
[7] D. Zhao, Z. Shi and F. Glorius, *Angew. Chem. Int. Ed*., 2013, **52**, 12426.

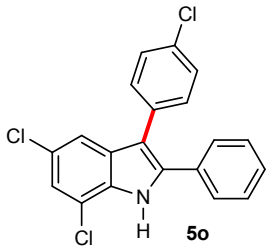
[8] X. Dou, W. Yao, S. Wen and Y. Lu, *Chem. Commun*., 2014, **50**, 9469.

[9] C. He, J. Hao, H. Xu, Y. Mo, H. Liu, J. Han and A. Lei, *Chem. Commun*., 2012, **48**, 11073.

X-ray Crystallographic Analysis for Product 5o

The CCDC number of compound **5o** is 1524656.

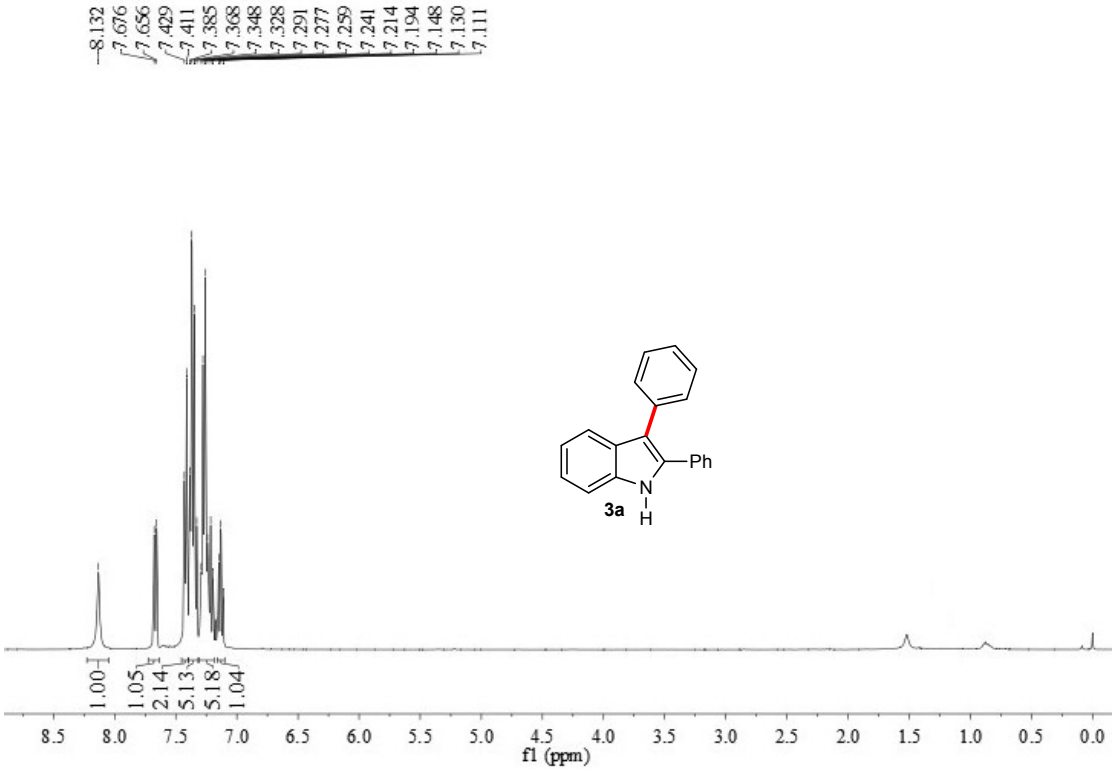


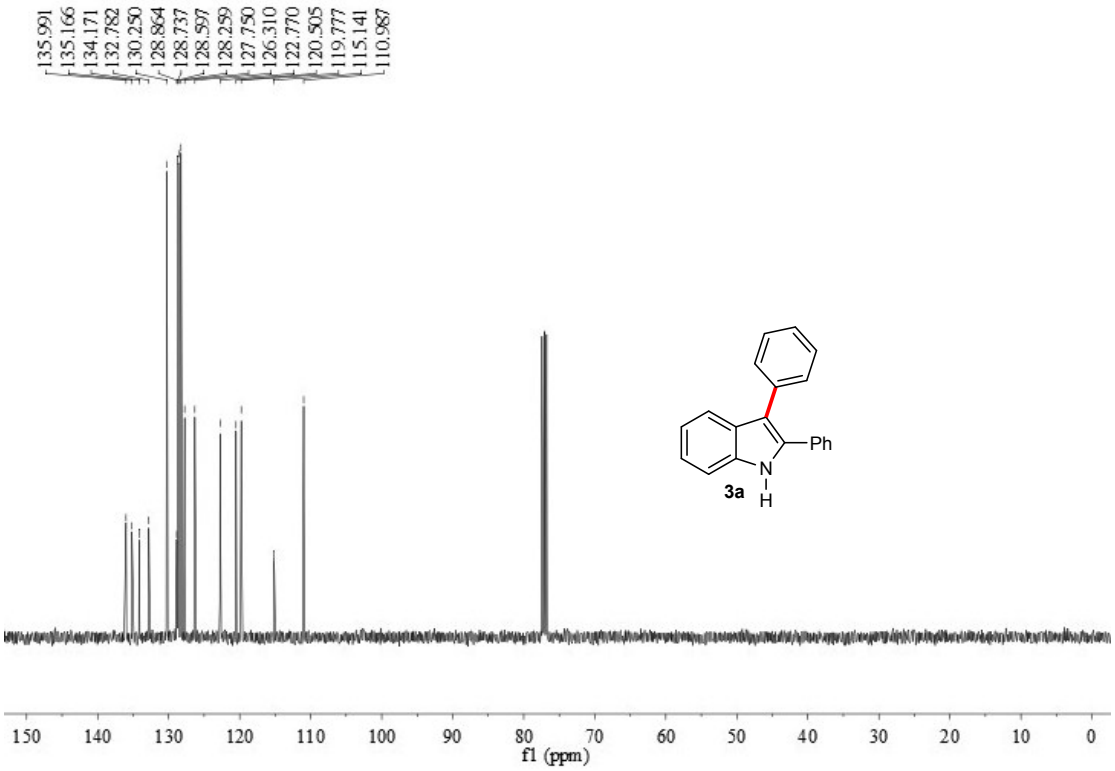


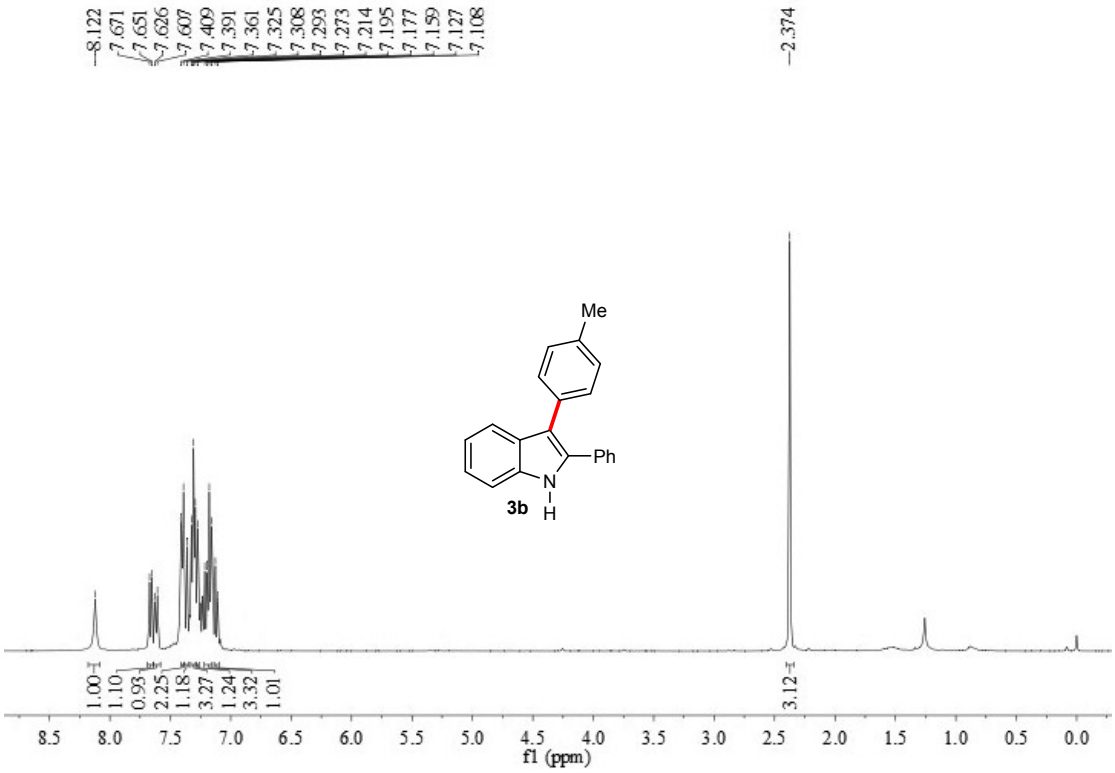
Crystal Data and Structure Refinement for Product **5o**

Empirical formula	$C_{20}H_{12}Cl_3N$
Formula weight	372.66
Temperature	150(10) K
Wavelength	1.54184 Å
Crystal system	monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a= 11.93574(15) Å, α= 90.00°
	b=7.18231(8) Å, β= 94.7142(11)°
	c= 19.3705(2) Å, γ= 90.00°
Density (calculated)	1.496
Absorption coefficient	5.003
F(000)	760.0
Crystal size	0.2×0.1×0.1
Theta range for data collection	4.20 to 74.00
Index ranges	-14<=h<=14, -4<=k<=8, -19<=l<=24
Reflections collected	3260
Independent reflections	3084
Completeness to theta = 25.00°	99.94%
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3260/0/217
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.1081
R indices (all data)	R1 = 0.0414, wR2 = 0.1101

^{1}H and ^{13}C NMR spectra of compounds 3



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7.651
7.626
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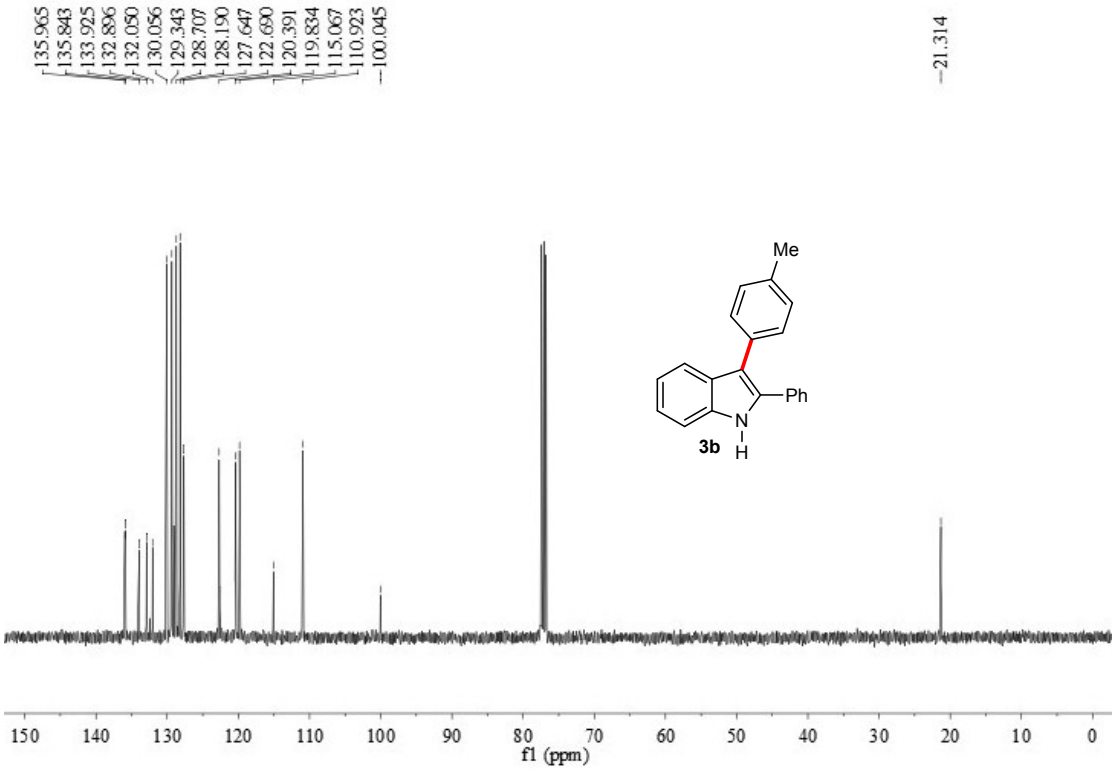
7.409
7.391
7.361
7.325
7.308
7.293
7.273
7.214
7.195
7.177
7.159
7.127
7.108
2.374
Me
Ph
N
H
3b
1.00
1.10
0.93
2.25
1.18
3.27
1.24
3.32
1.01
3.12
f1 (ppm)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132.050
130.056
129.343
128.707
128.190
127.647
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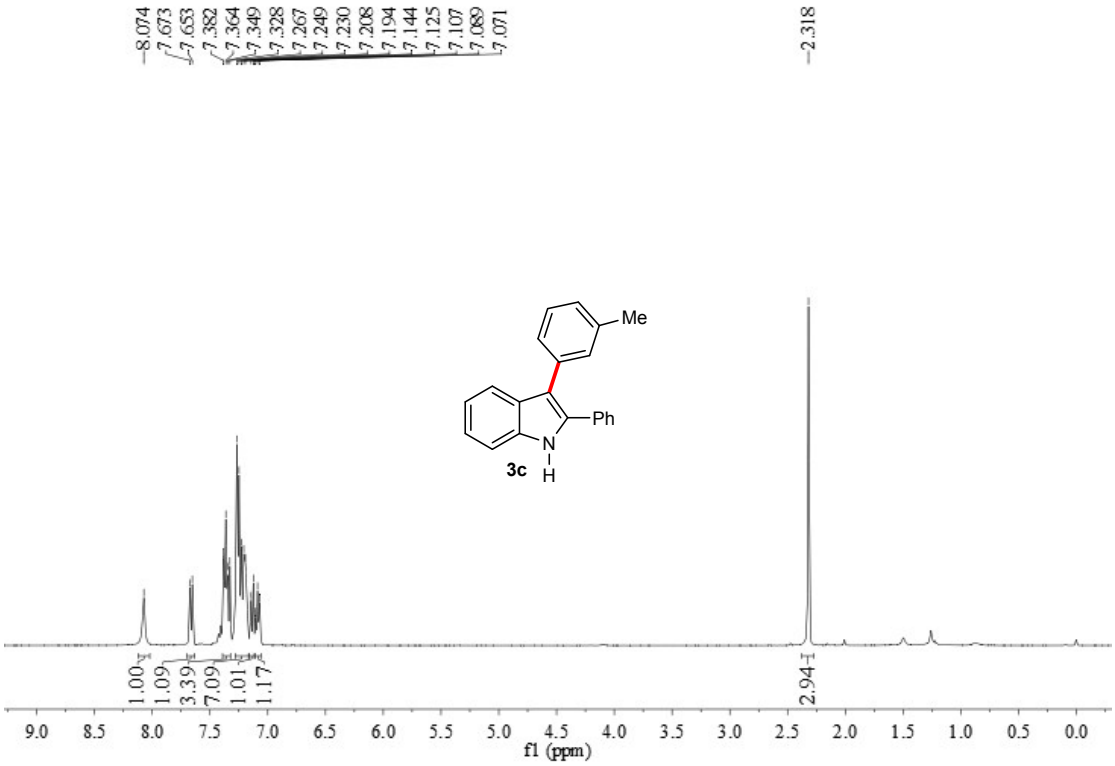
119.834
115.067
110.923
100.045
21.314
Me
Ph
N
H
3b
f1 (ppm)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7.653
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7.267
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7.230
7.208
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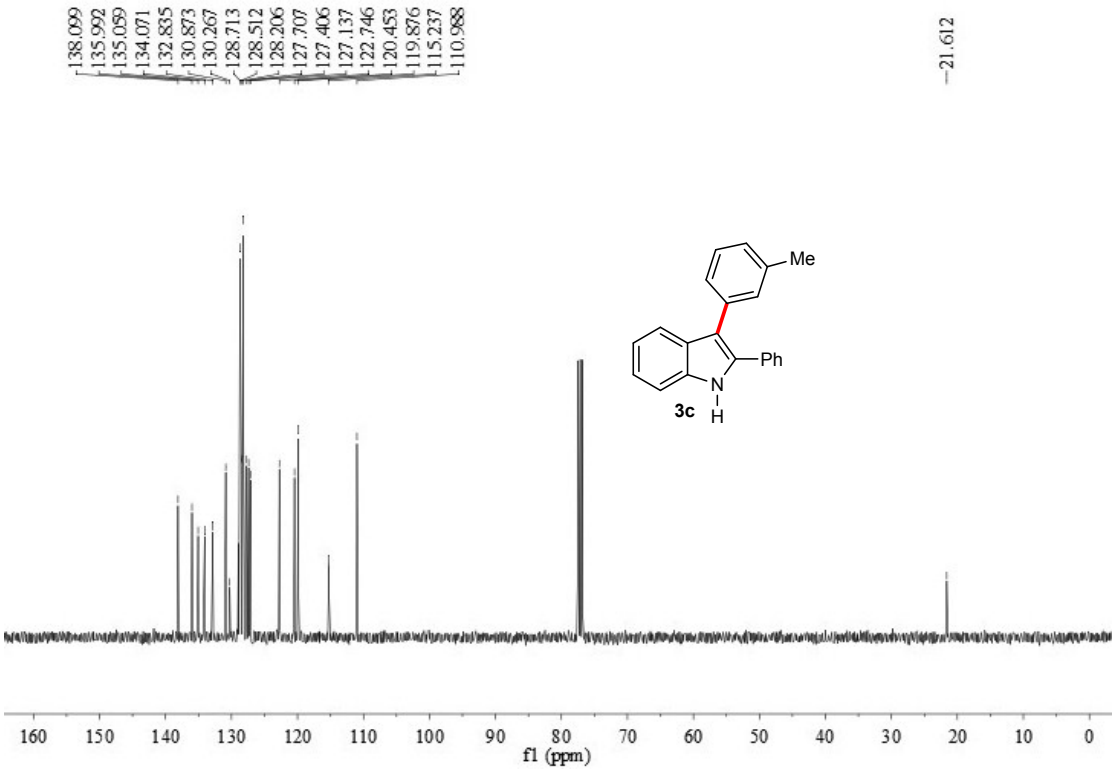
7.144
7.125
7.107
7.089
7.071
2.318
Me
Ph
N
H
3c
1.00
1.09
3.39
7.09
1.01
1.17
2.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.206
127.707
127.406
127.137
122.746
120.453
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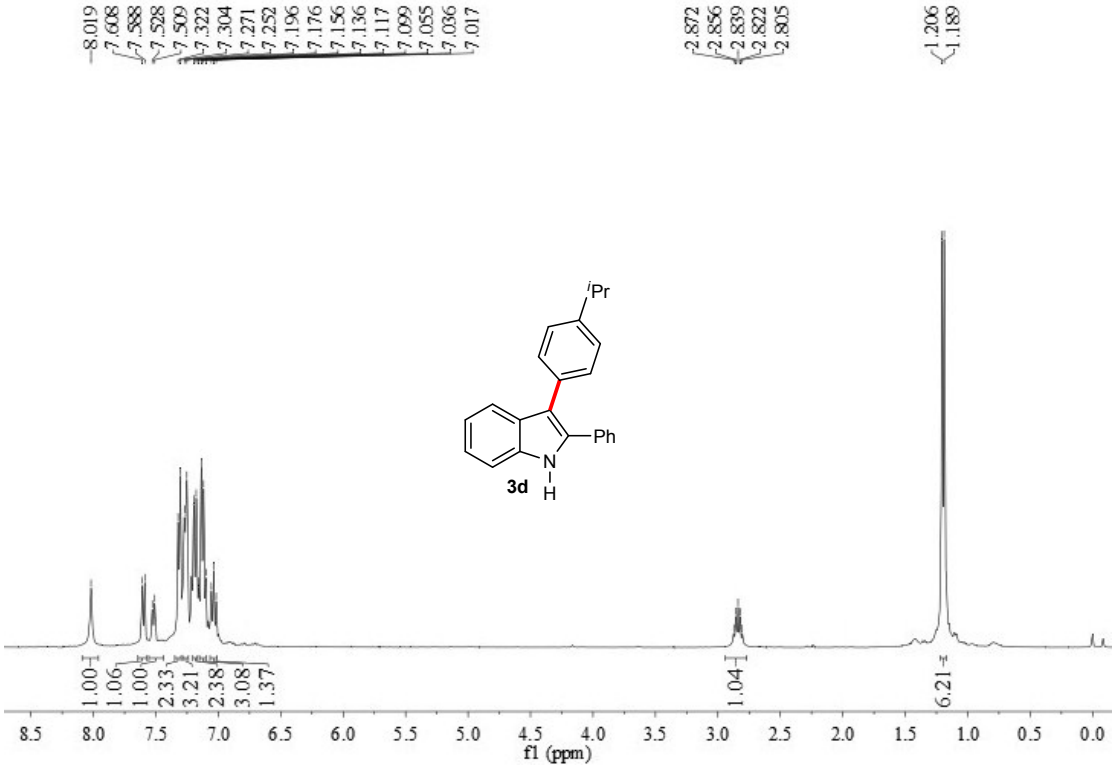
Me
Ph
N
H
3c
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.588
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7.509
7.322
7.304
7.271
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7.196
7.176
7.156
7.136
7.117
7.099
7.055
7.036
7.017
2.872
2.856
2.839
2.822
2.805
1.206
1.189
iPr
Ph
N
H
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2.38
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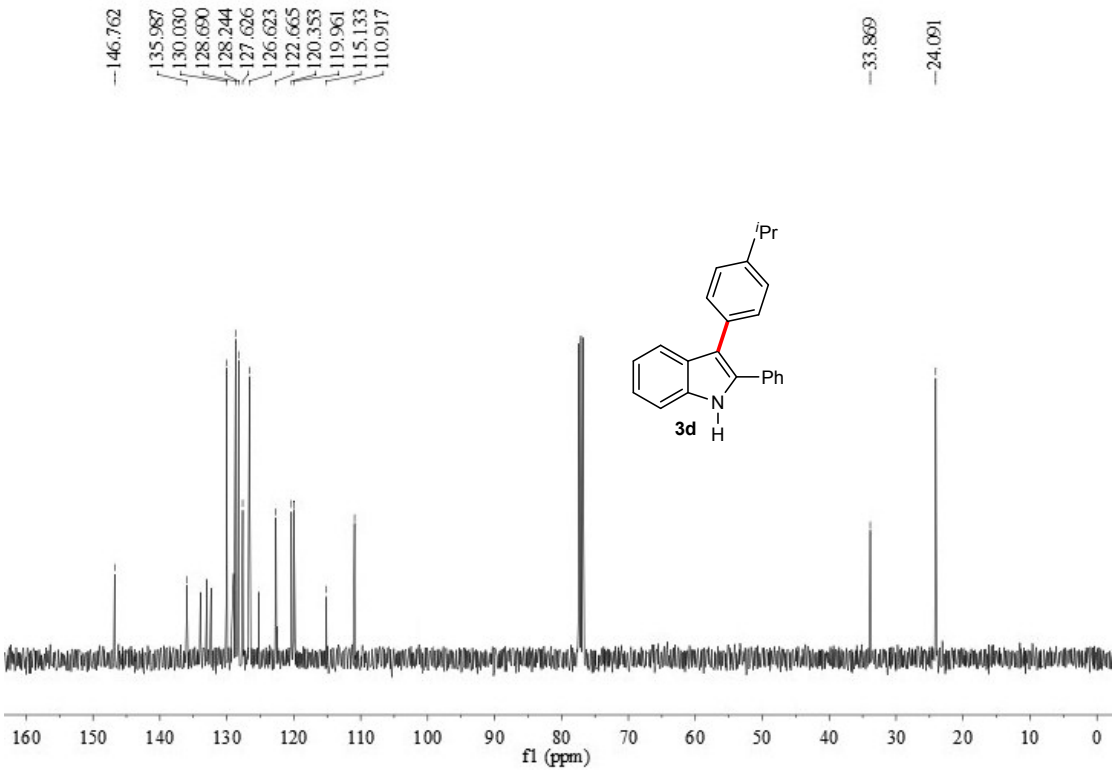
6.21
f1 (ppm)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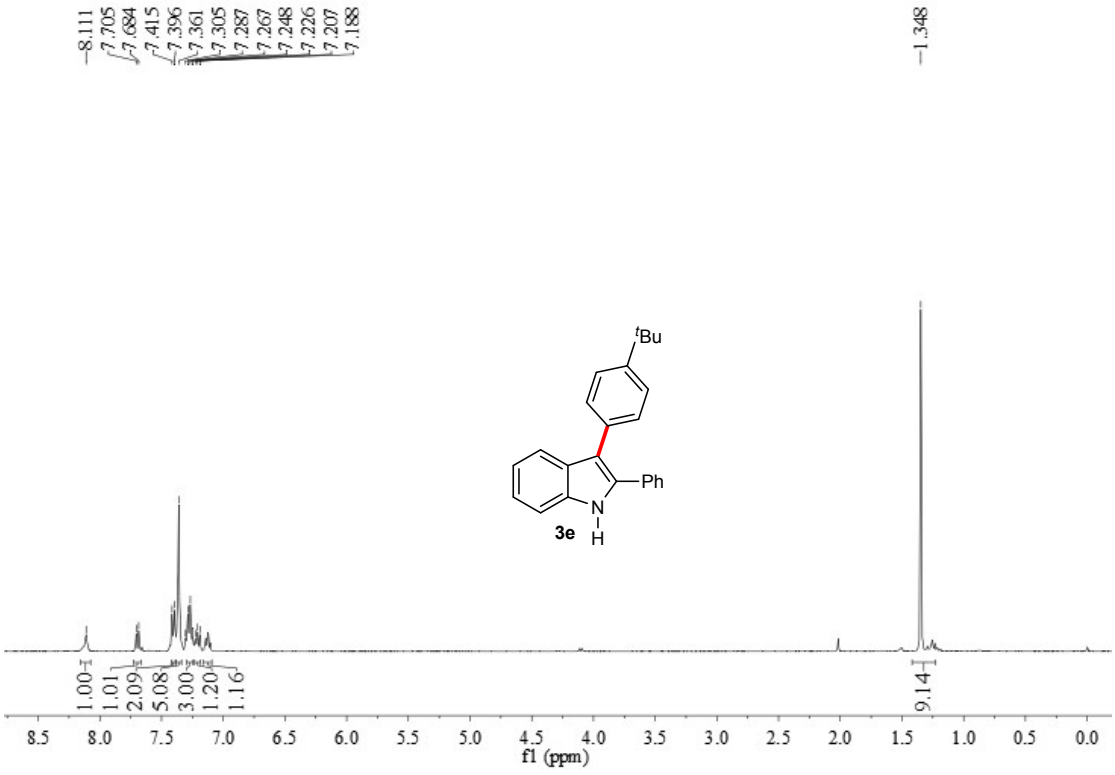
iPr
Ph
N
H
3d
f1 (ppm)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7.287
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7.226
7.207
7.188
1.348
tBu
Ph
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H
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2.09
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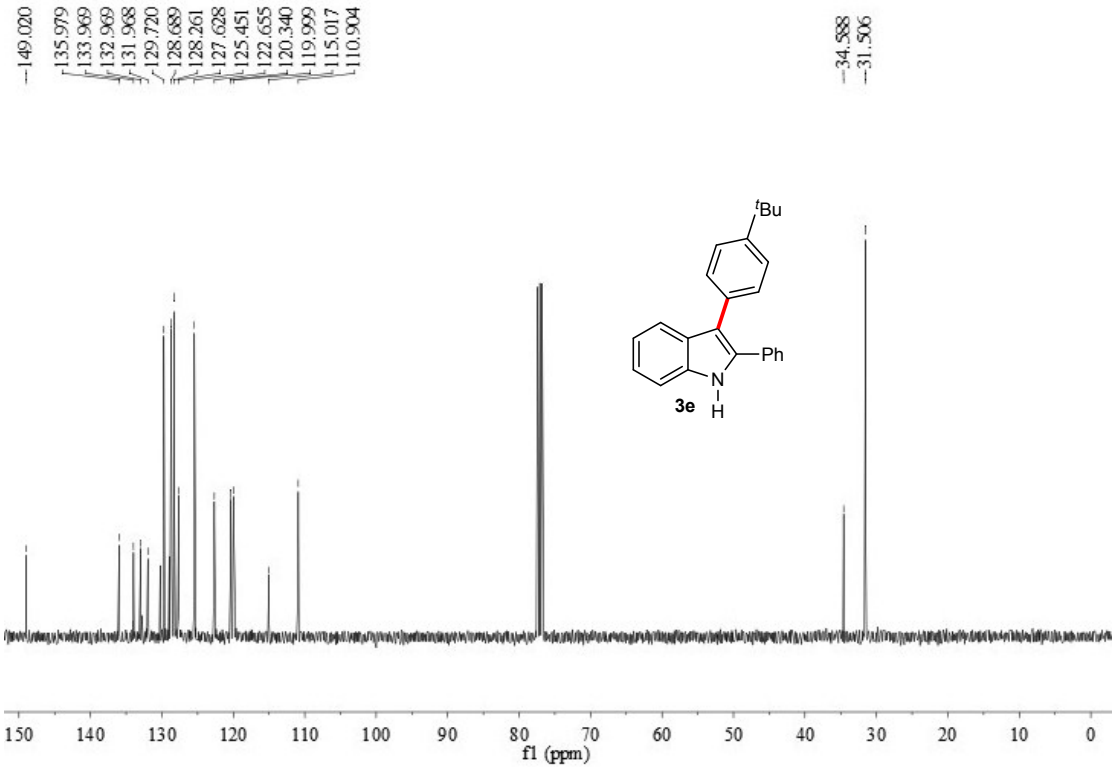
3.00
1.20
1.16
9.14
f1 (ppm)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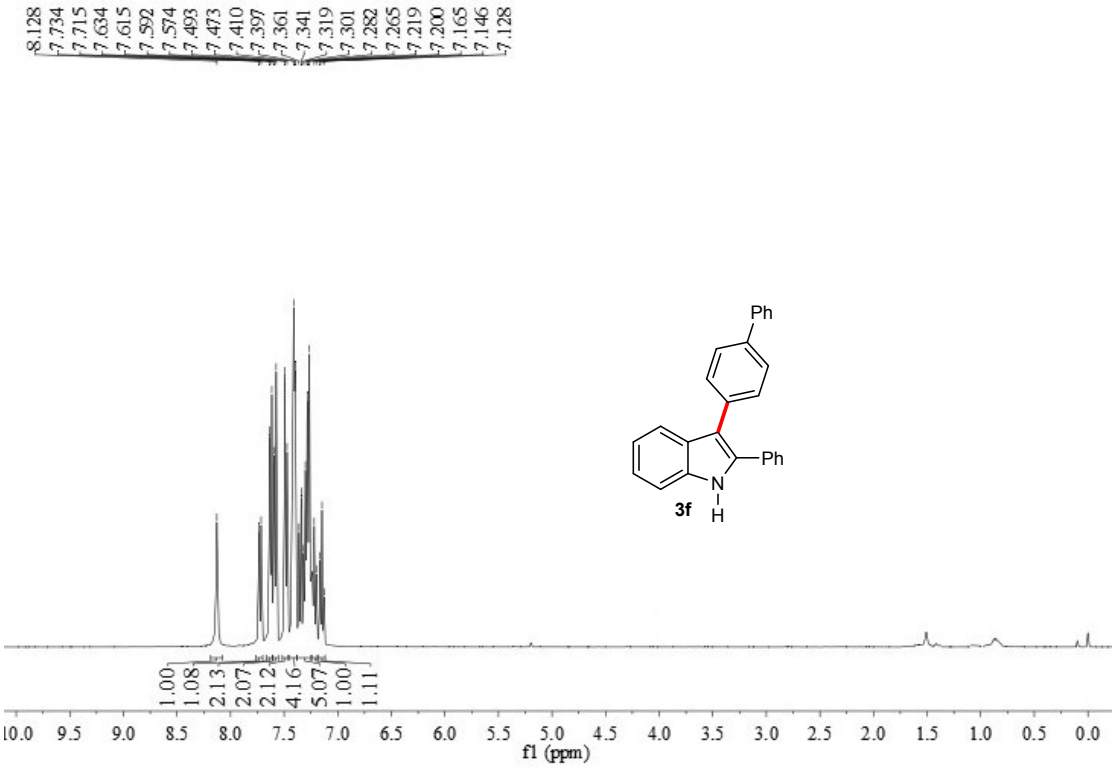
31.506
tBu
Ph
N
H
3e
f1 (ppm)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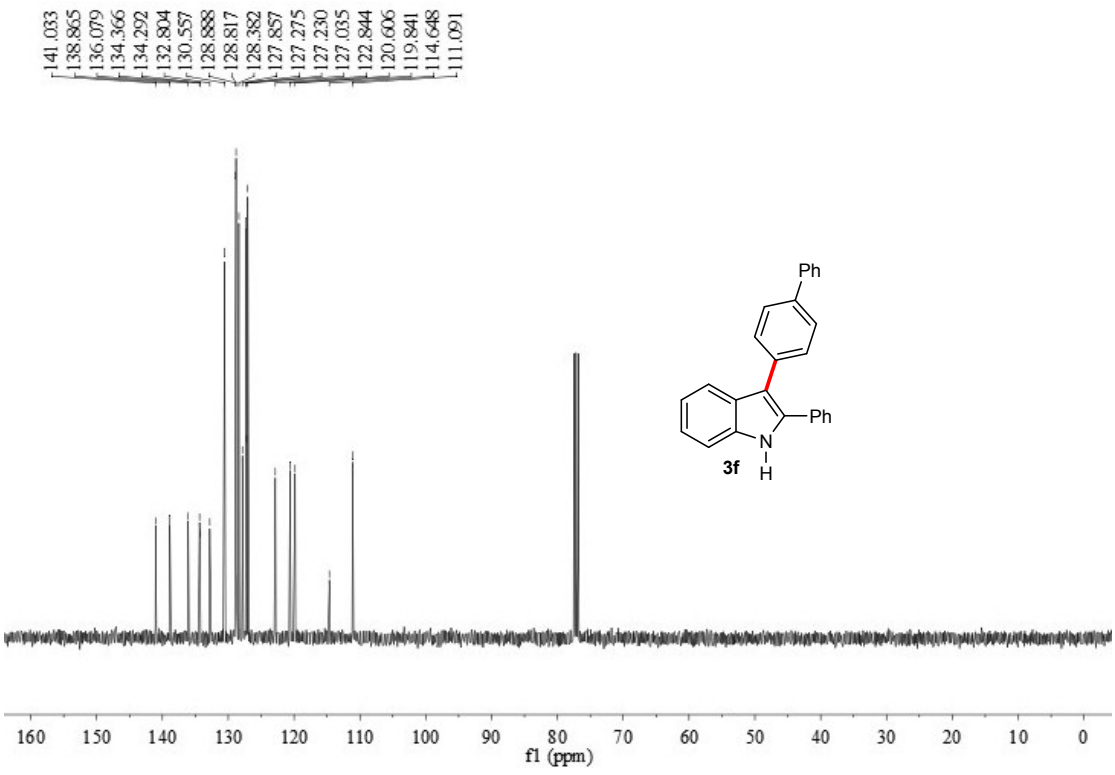
7.341
7.319
7.301
7.282
7.265
7.219
7.200
7.165
7.146
7.128
Ph
Ph
N
H
3f
1.00
1.08
2.13
2.07
2.12
4.16
5.07
1.00
1.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.230
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Ph
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H
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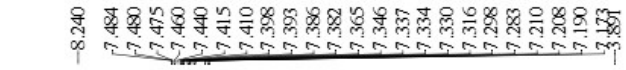
f1 (ppm)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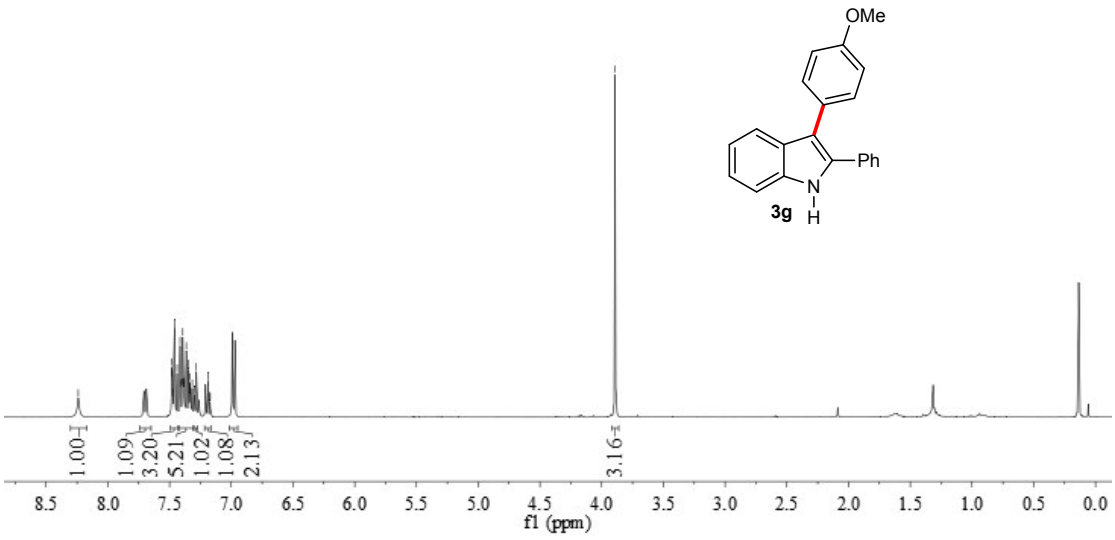
3.891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7.0
6.5
6.0
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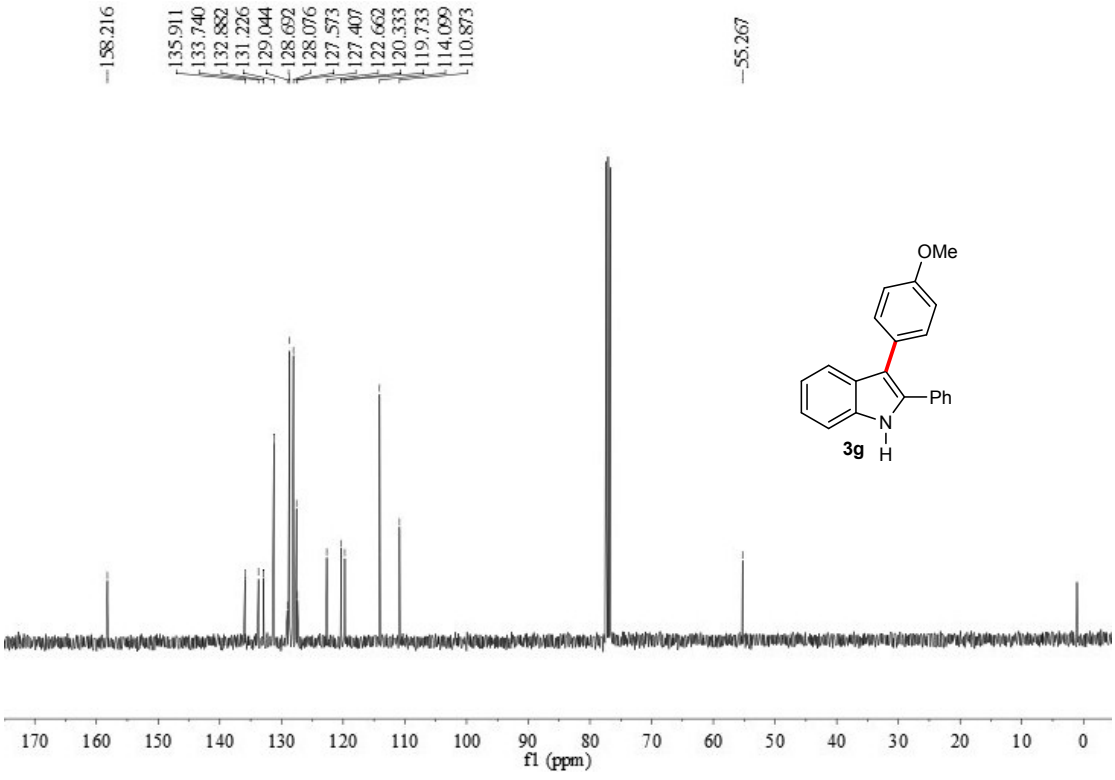
f1 (ppm)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OMe
Ph
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H
3g
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10
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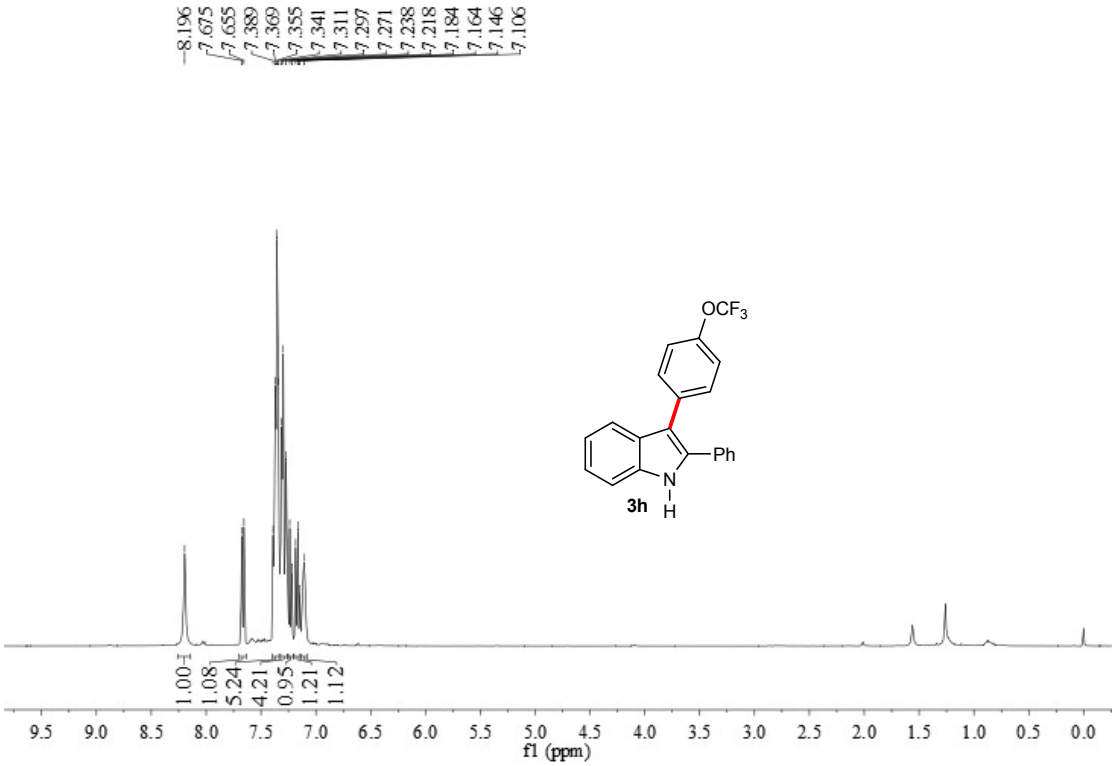
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7.164
7.146
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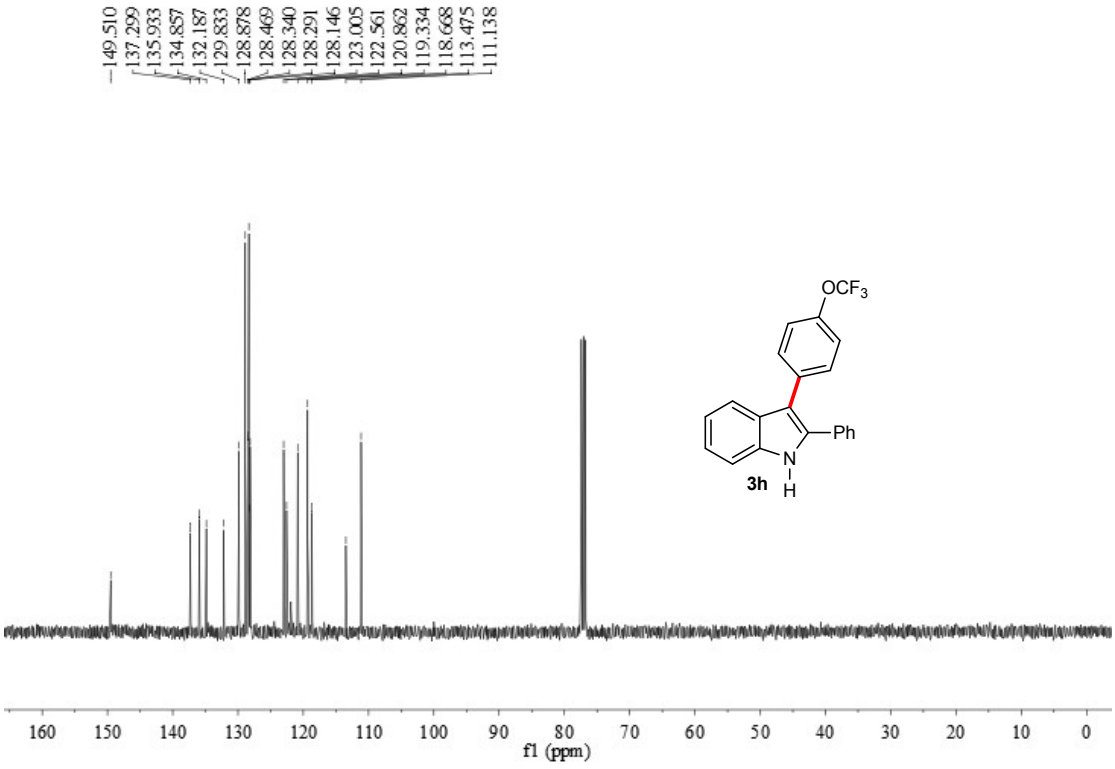
1.12
f1 (ppm)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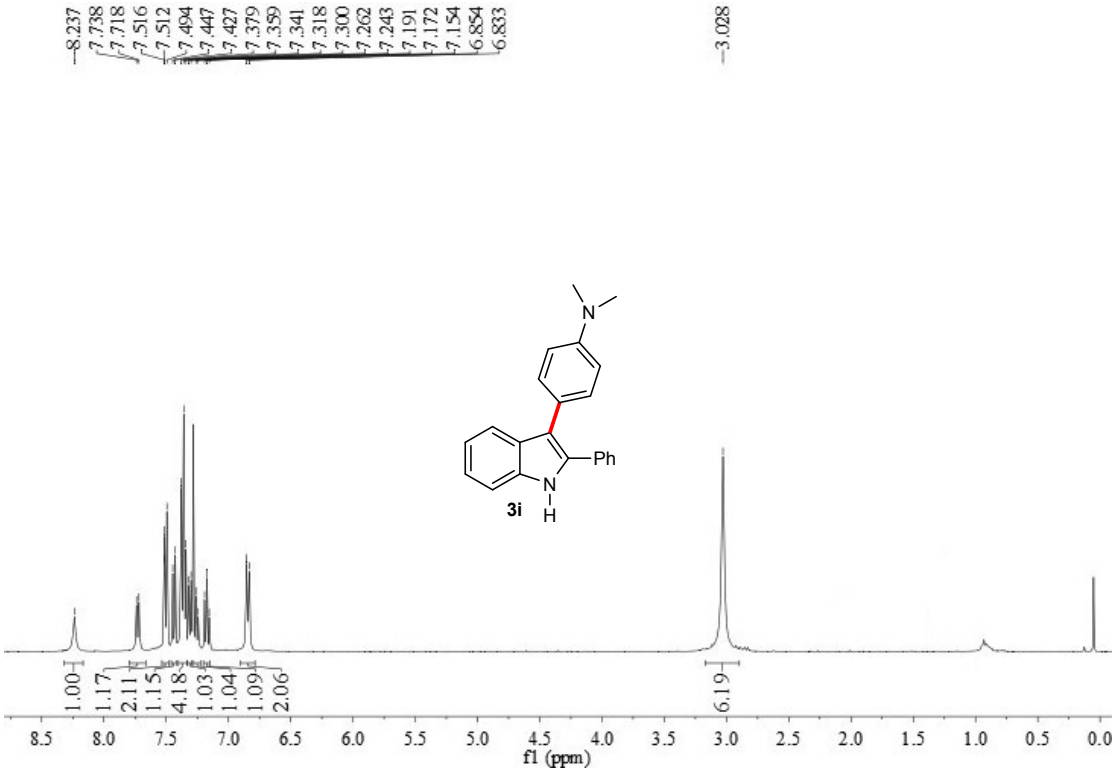
H
3h
f1 (ppm)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7.243
7.191
7.172
7.154
6.854
6.833
3.028
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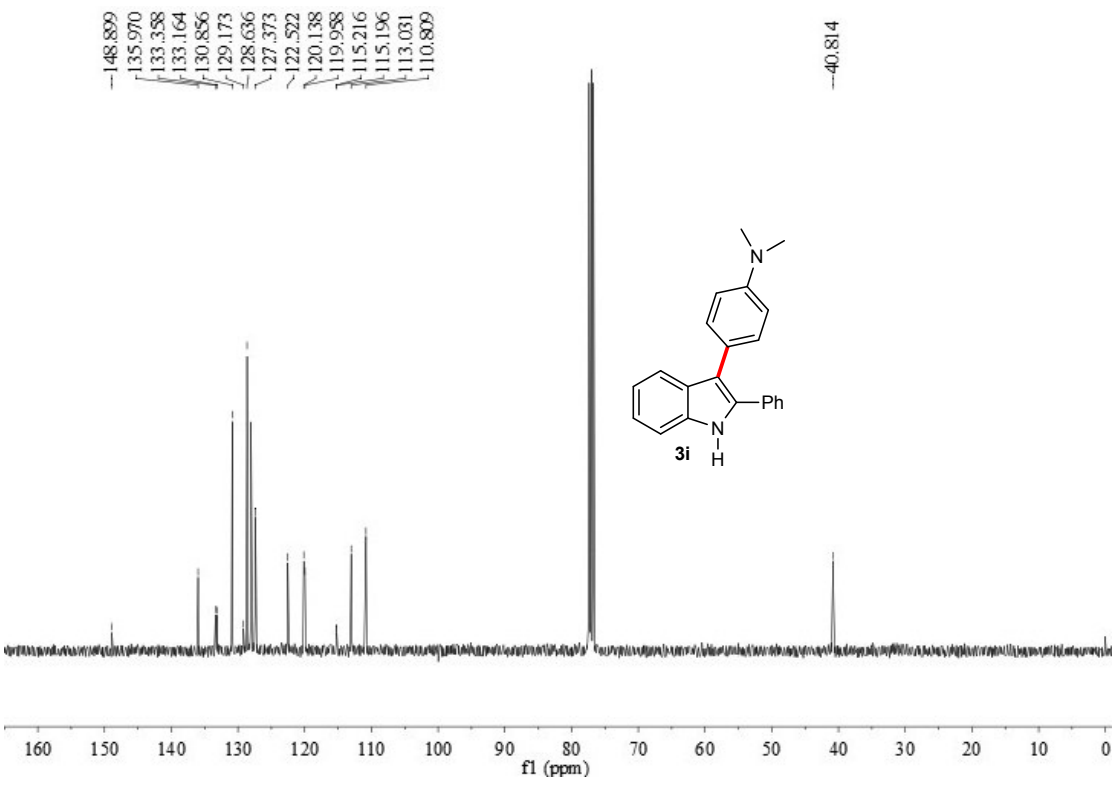
N
H
3i
1.00
1.17
2.11
1.15
4.18
1.03
1.04
1.09
2.06
6.19
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.373
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120.138
119.958
115.216
115.196
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40.814
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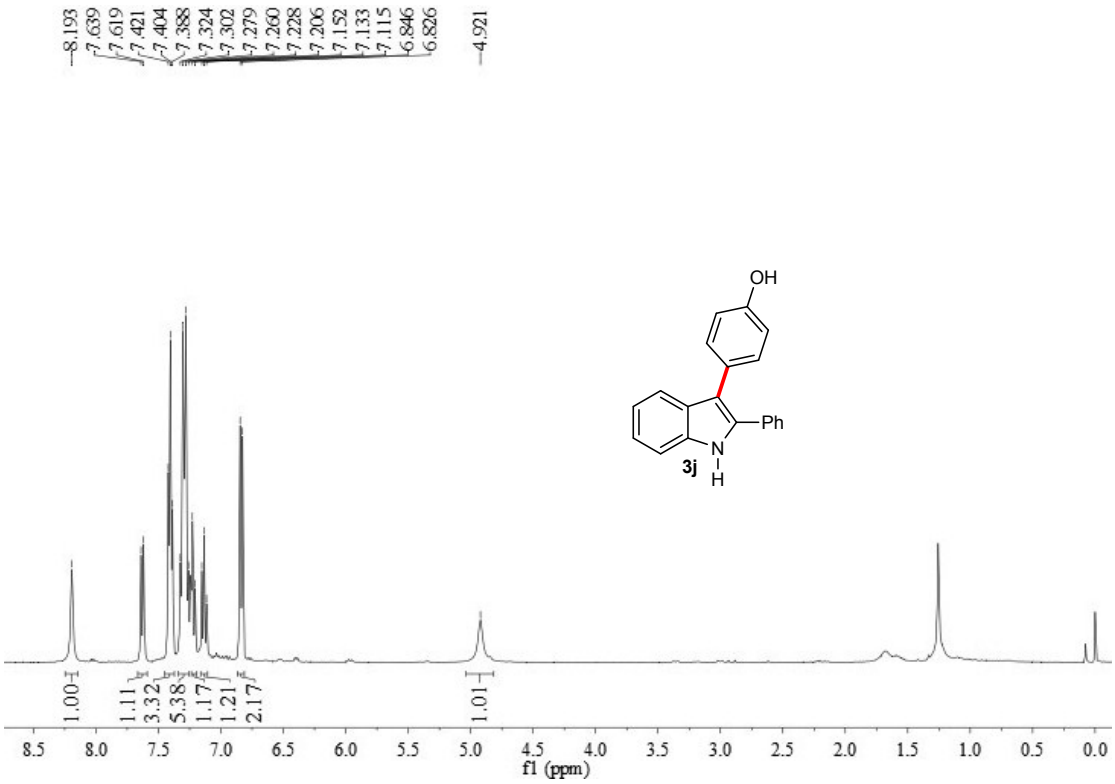
Ph
N
H
3i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.133
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6.826
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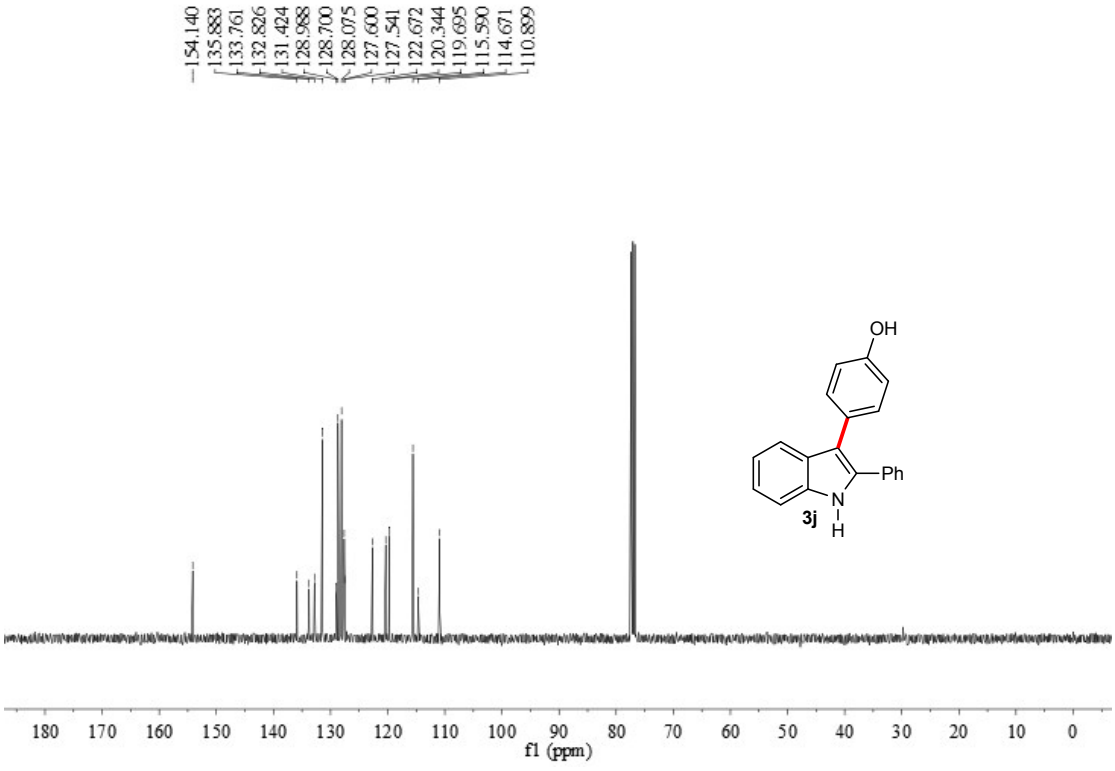
1.01
f1 (ppm)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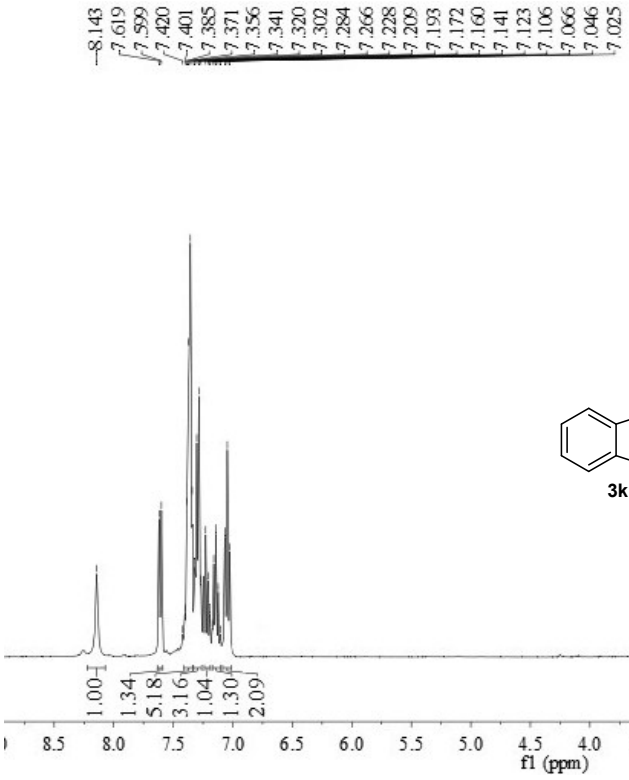
OH
Ph
N
H
3j
f1 (ppm)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7.228
7.209
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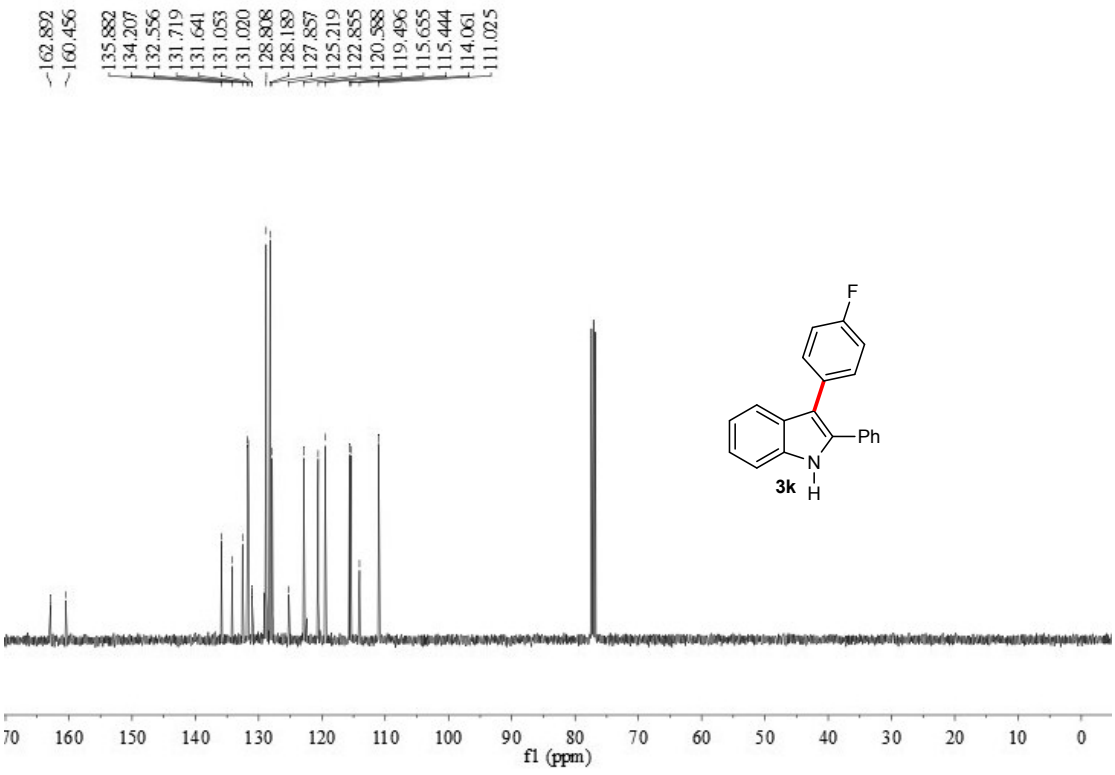
f1 (ppm)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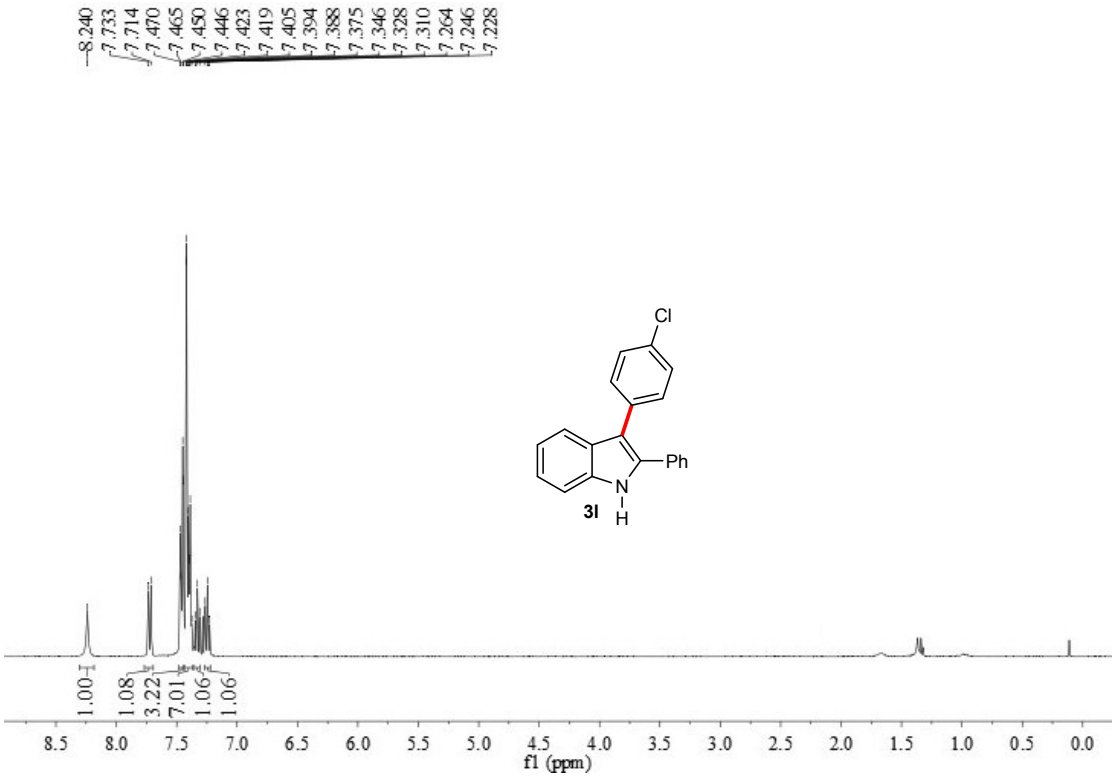
3k
f1 (ppm)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7.733
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7.465
7.450
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7.423
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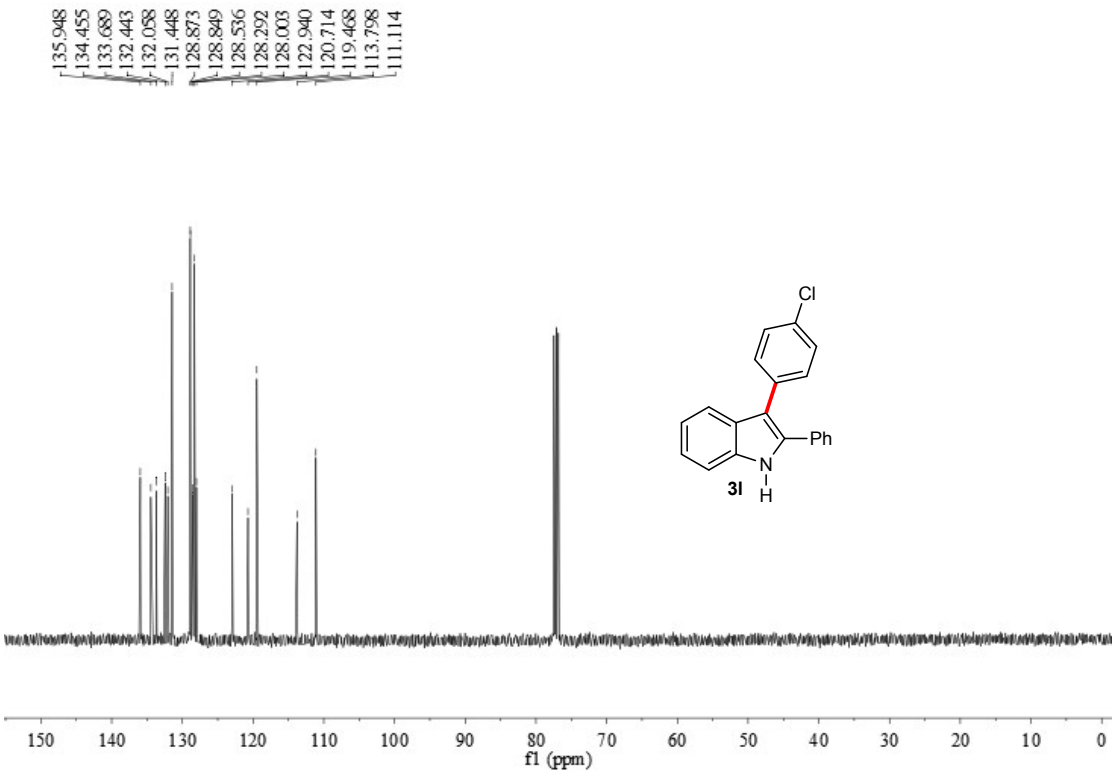
7.388
7.375
7.346
7.328
7.310
7.264
7.246
7.228
Cl
Ph
N
H
3l
1.00
1.08
3.22
7.01
1.06
1.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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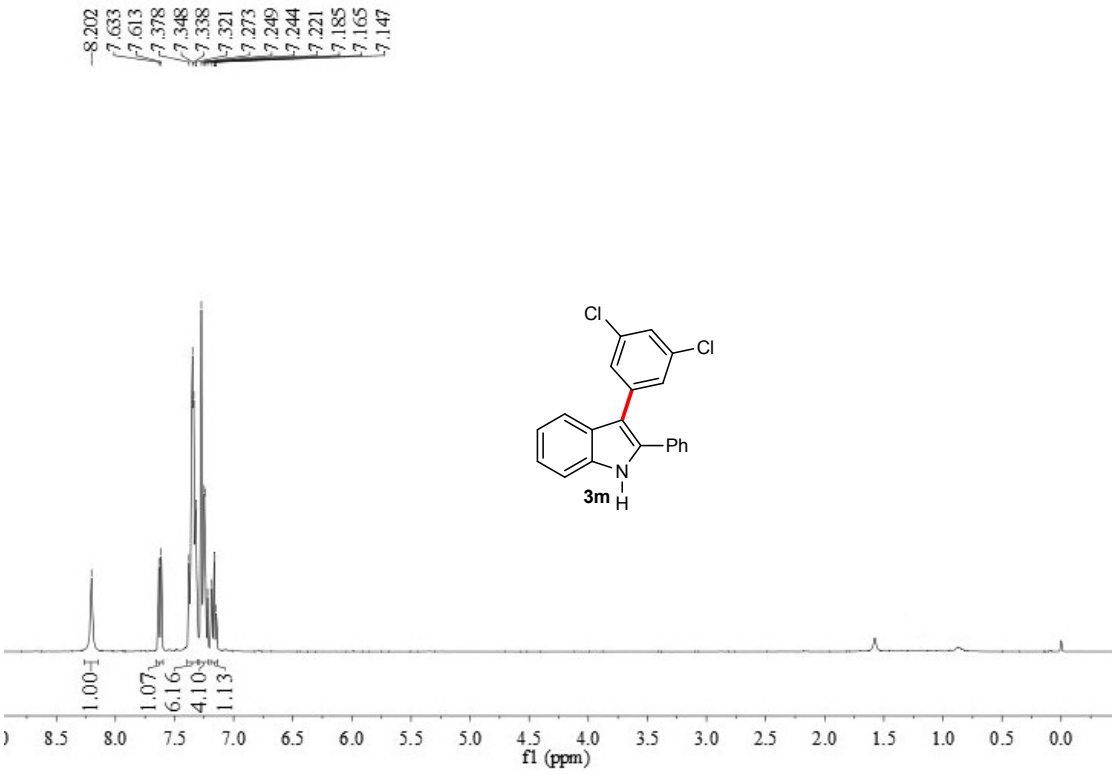
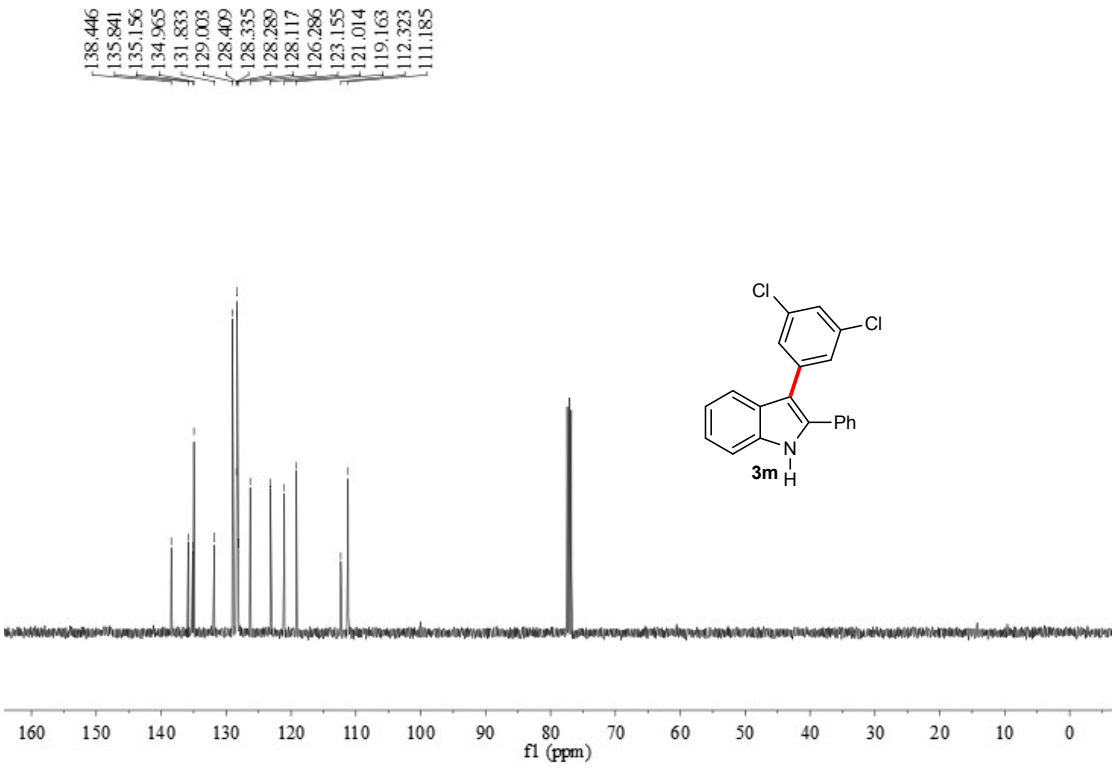
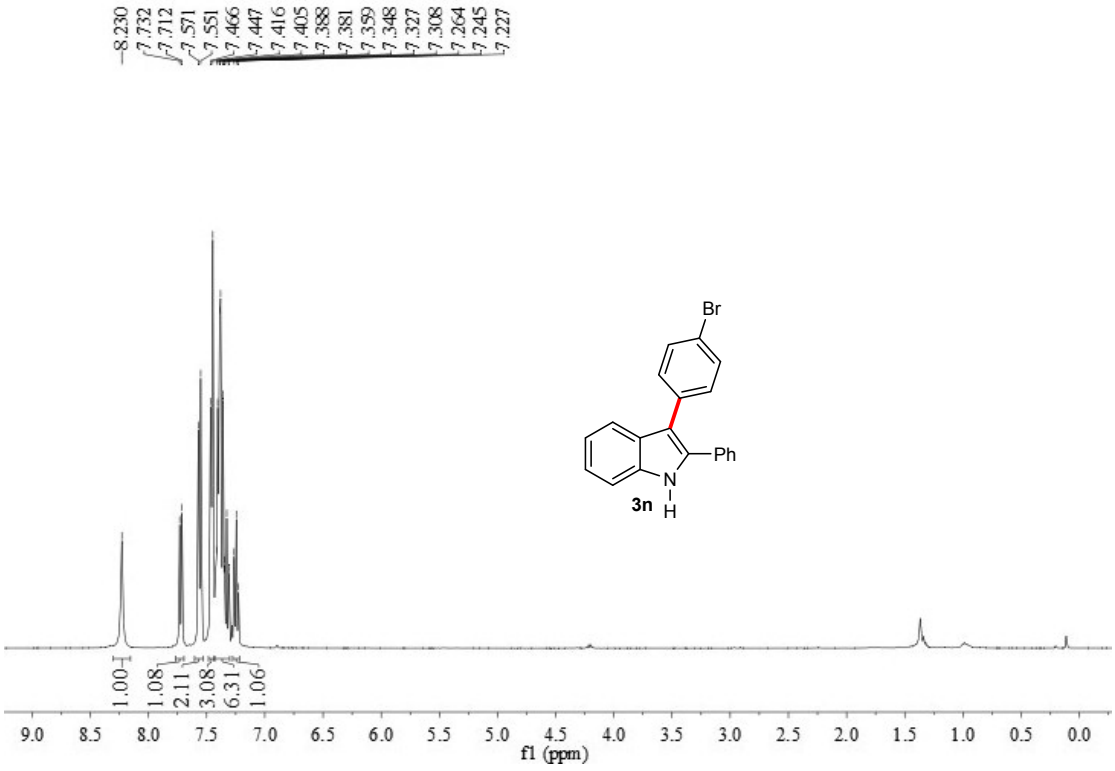
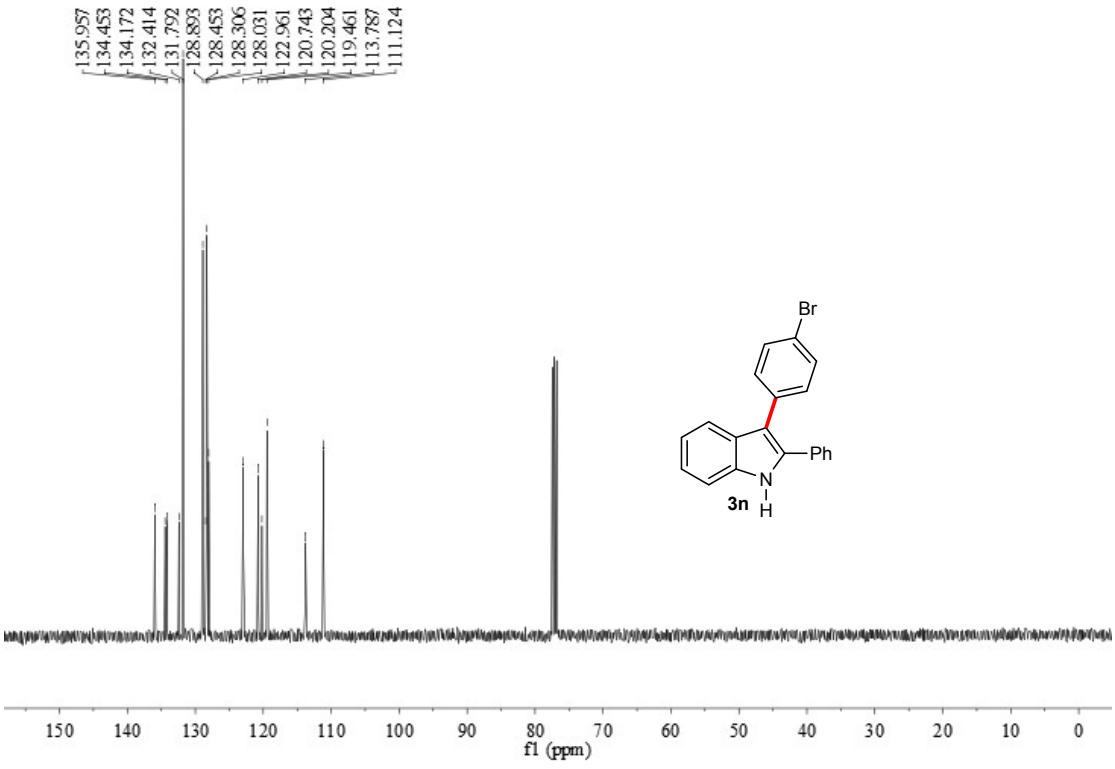
134.455
133.689
132.443
132.058
131.448
128.873
128.849
128.536
128.292
128.003
122.940
120.714
119.468
113.798
111.114
Cl
Ph
N
H
3l
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.202
7.633
7.613
7.378
7.348
7.338
7.321
7.273
7.249
7.244
7.221
7.185
7.165
7.147
Cl
Cl
Ph
N
H
3m
1.00
1.07
6.16
4.10
1.13
f1 (ppm)


138.446
135.841
135.156
134.965
131.833
129.003
128.409
128.335
128.289
128.117
126.286
123.155
121.014
119.163
112.323
111.185
Cl
Cl
Ph
N
H
3m
f1 (ppm)


8.230
7.732
7.712
7.571
7.551
7.466
7.447
7.416
7.405
7.388
7.381
7.359
7.348
7.327
7.308
7.264
7.245
7.227
Br
Ph
N
H
3n
1.00
1.08
2.11
3.08
6.31
1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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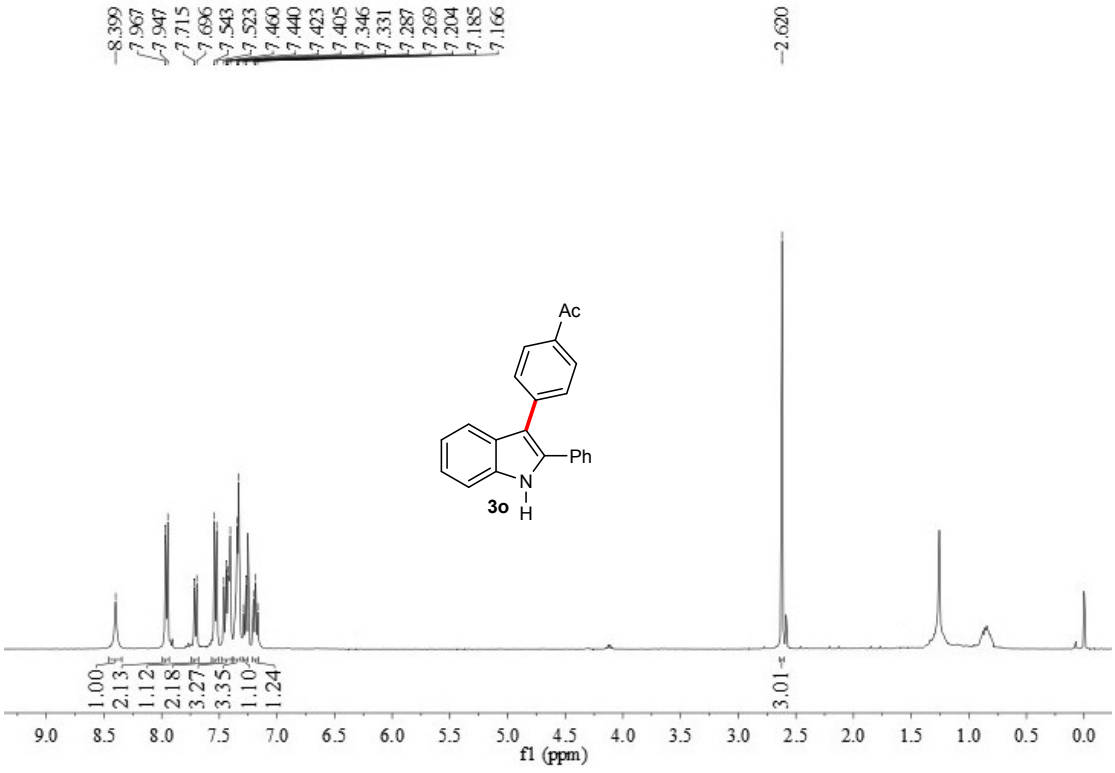
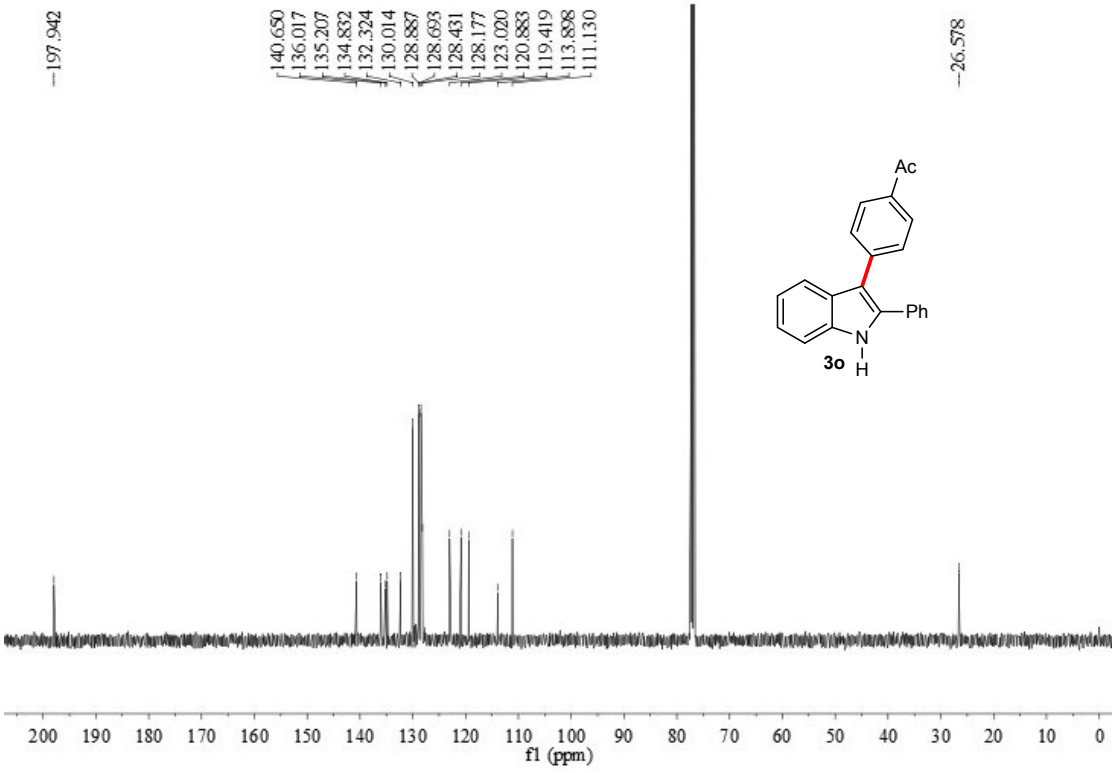
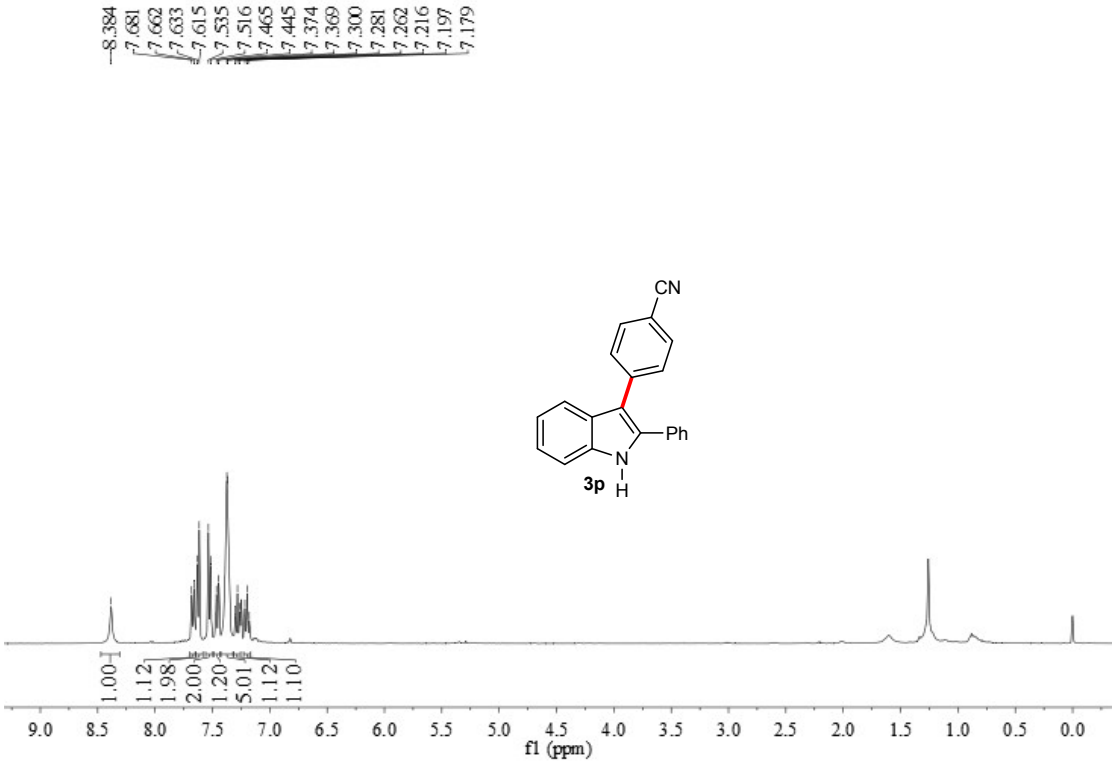
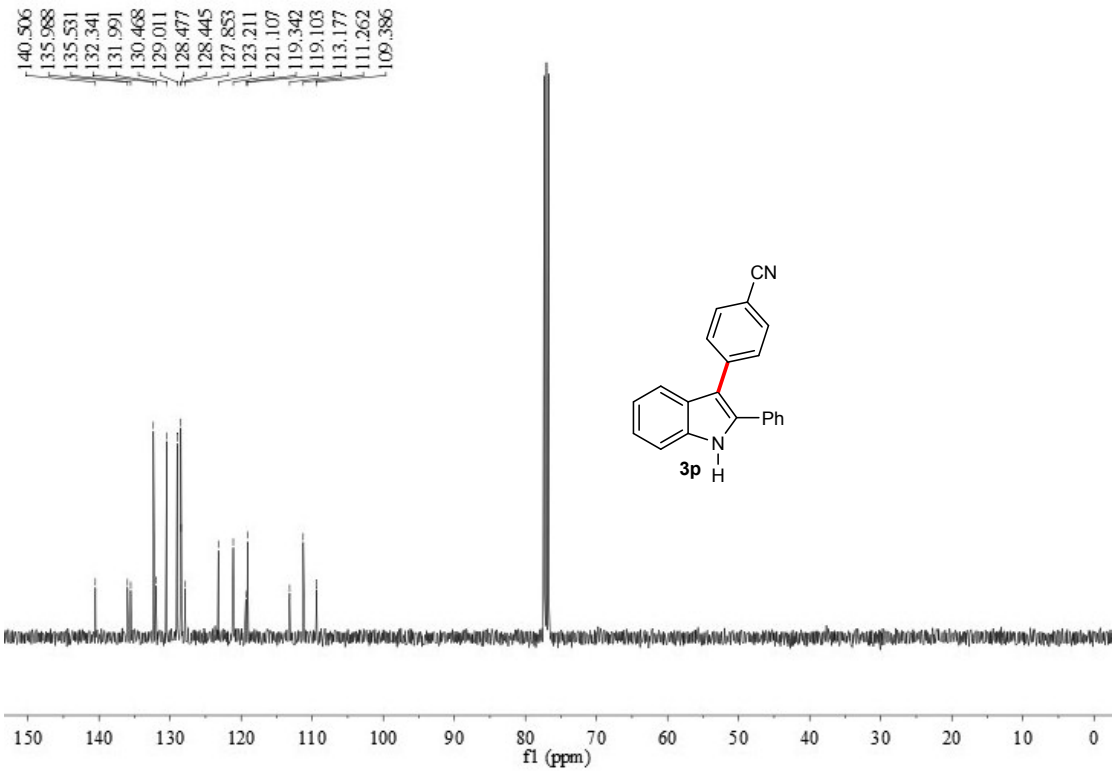
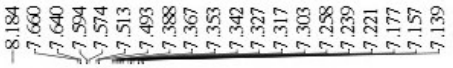
134.453
134.172
132.414
131.792
128.893
128.453
128.306
128.031
122.961
120.743
120.204
119.461
113.787
111.124
Br
Ph
N
H
3n
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

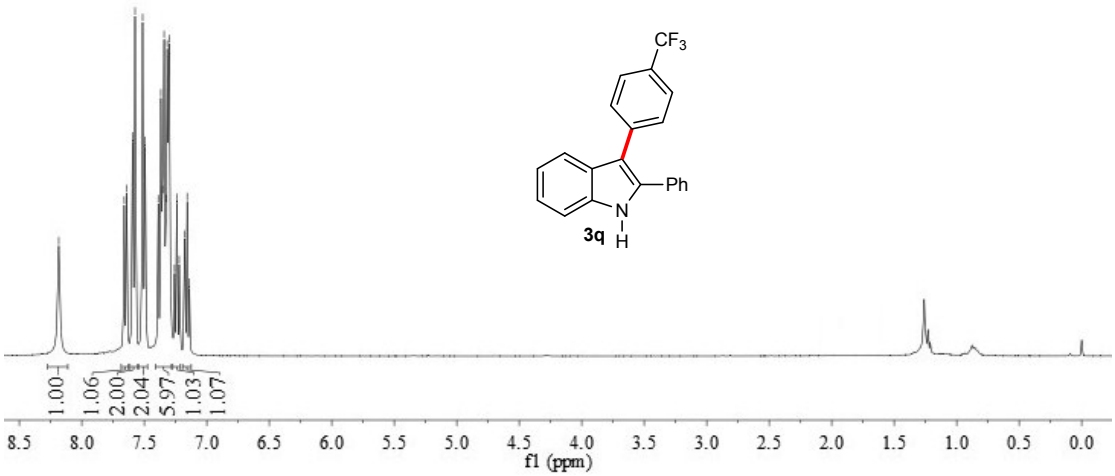

8.399
7.967
7.947
7.715
7.696
7.543
7.523
7.460
7.440
7.423
7.405
7.346
7.331
7.287
7.269
7.204
7.185
7.166
2.620
Ac
Ph
N
H
3o
1.00
2.13
1.12
2.18
3.27
3.35
1.10
1.24
3.01
f1 (ppm)

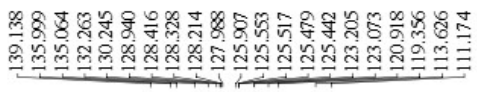

197.942
140.650
136.017
135.207
134.832
132.324
130.014
128.887
128.693
128.431
128.177
123.020
120.883
119.419
113.898
111.130
26.578
Ac
Ph
N
H
3o
f1 (ppm)

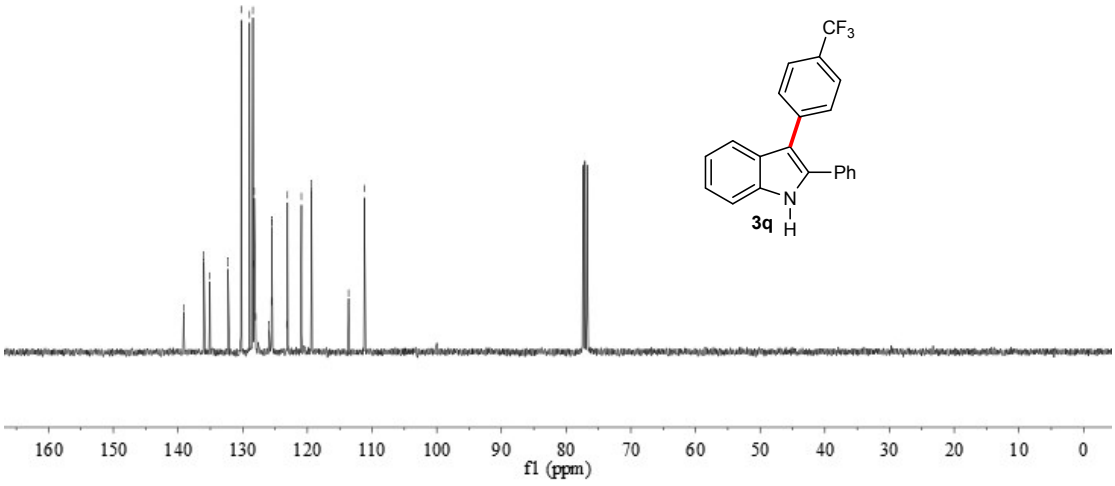

8.384
7.681
7.662
7.633
7.615
7.535
7.516
7.465
7.445
7.374
7.369
7.300
7.281
7.262
7.216
7.197
7.179
CN
Ph
N
H
3p
1.00
1.12
1.98
2.00
1.20
5.01
1.12
1.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

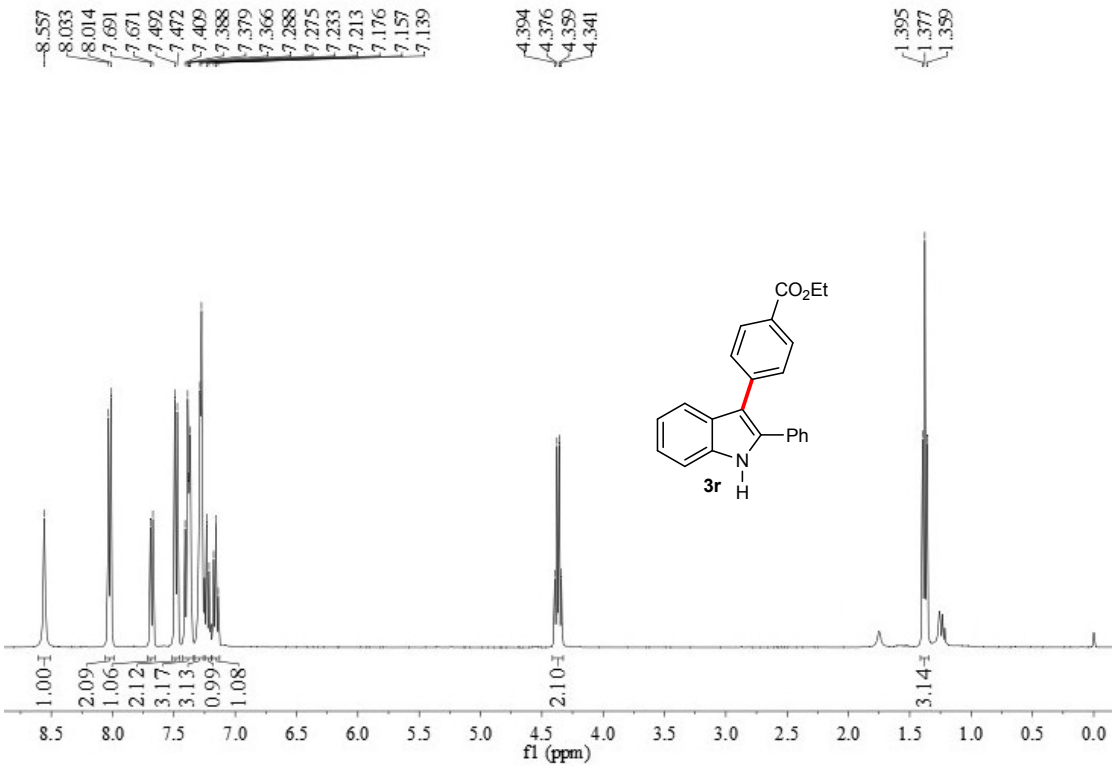

140.506
135.988
135.531
132.341
131.991
130.468
129.011
128.477
128.445
127.853
123.211
121.107
119.342
119.103
113.177
111.262
109.386
CN
Ph
N
H
3p
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

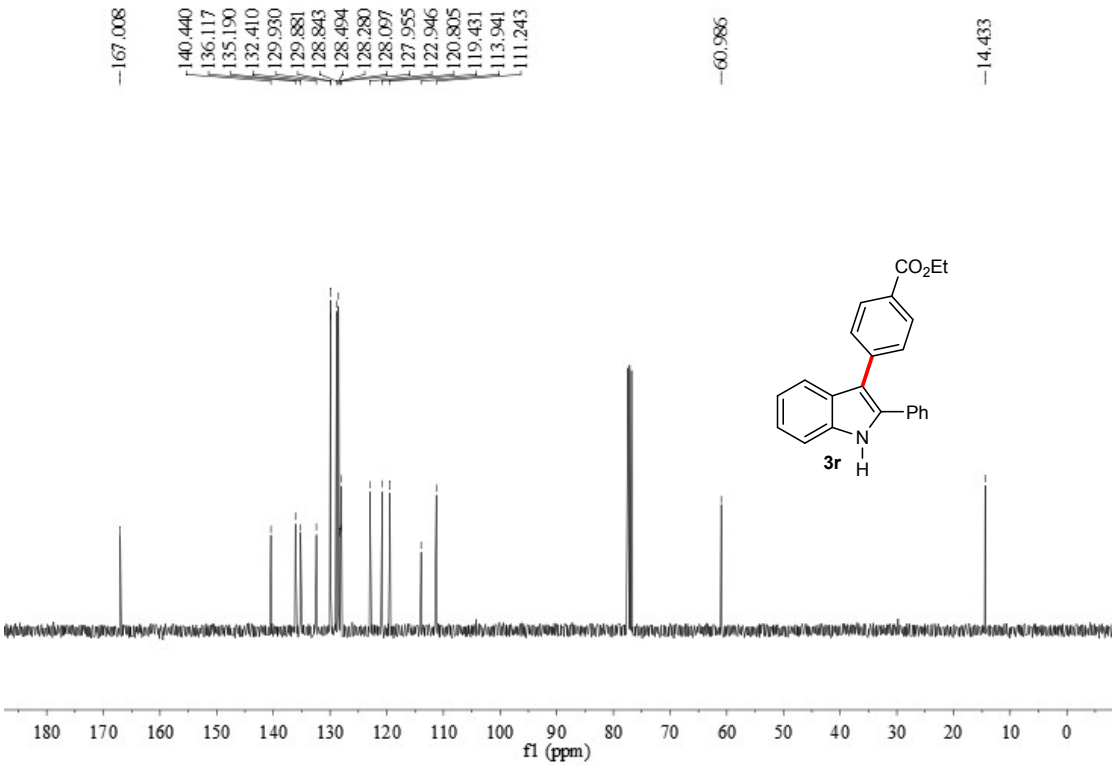

8.184
7.660
7.640
7.594
7.574
7.513
7.493
7.388
7.367
7.353
7.342
7.327
7.317
7.303
7.258
7.239
7.221
7.177
7.157
7.139

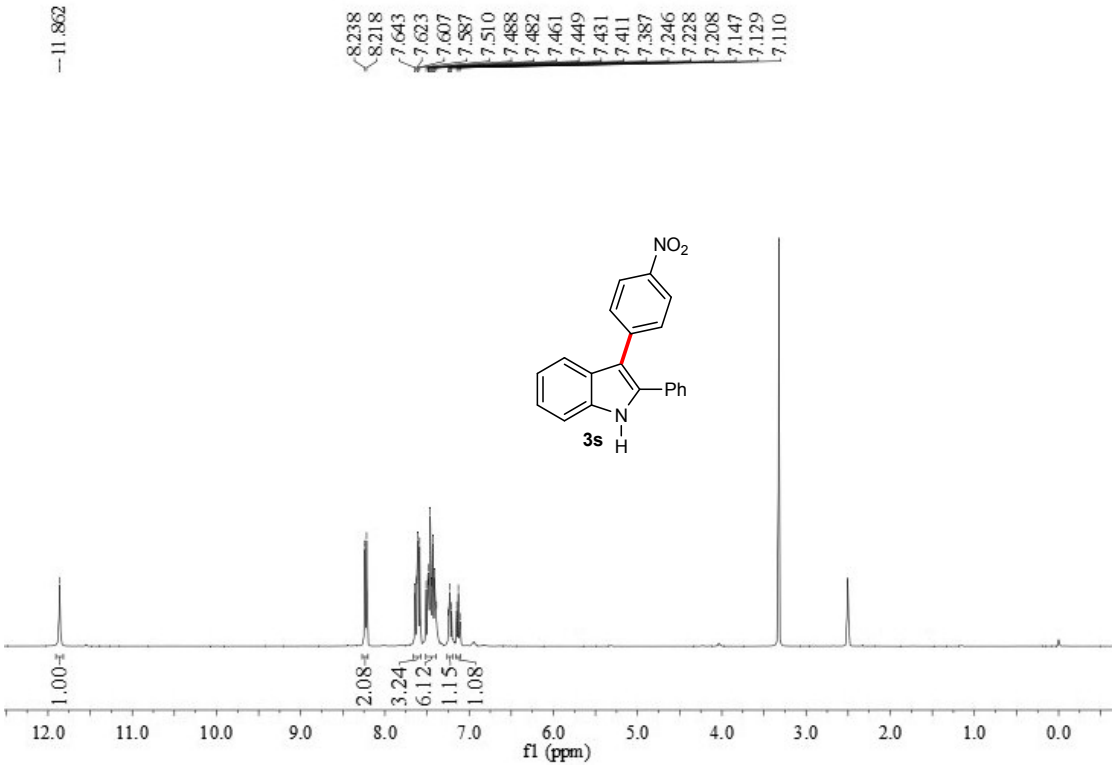

CF3
Ph
N
H
3q
1.00
1.06
2.00
2.04
5.97
1.03
1.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

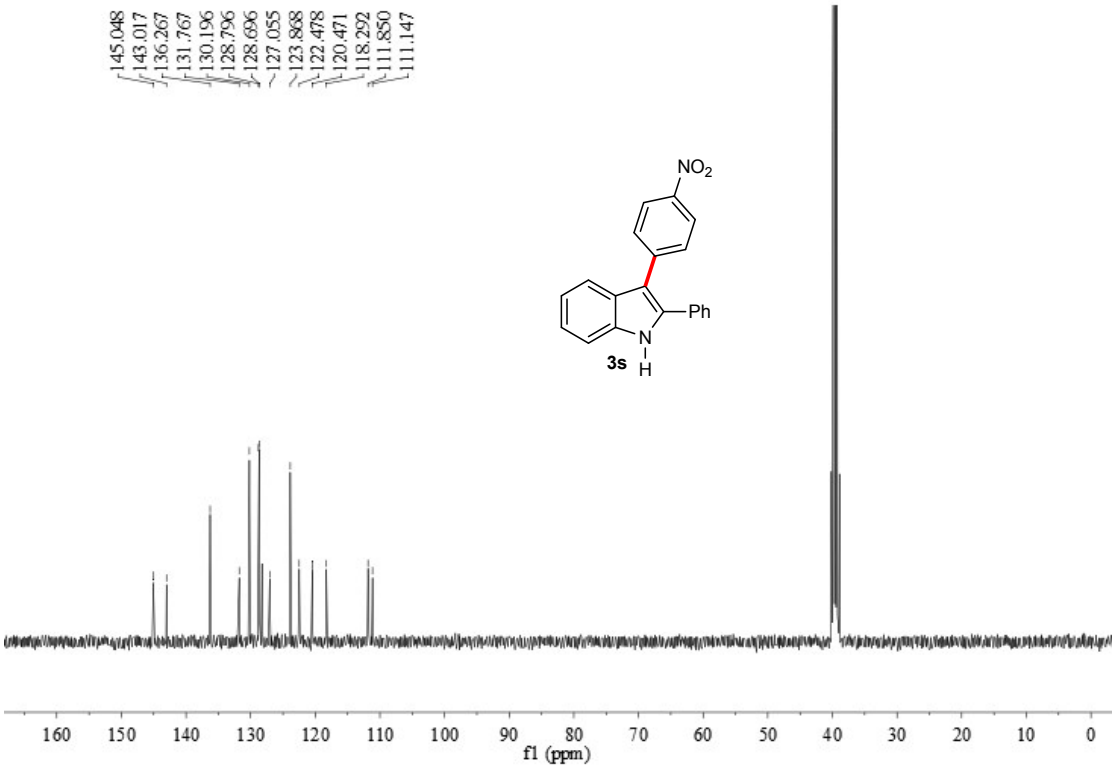

139.138
135.999
135.064
132.263
130.245
128.940
128.416
128.328
128.214
127.988
125.907
125.553
125.517
125.479
125.442
123.205
123.073
120.918
119.356
113.626
111.174

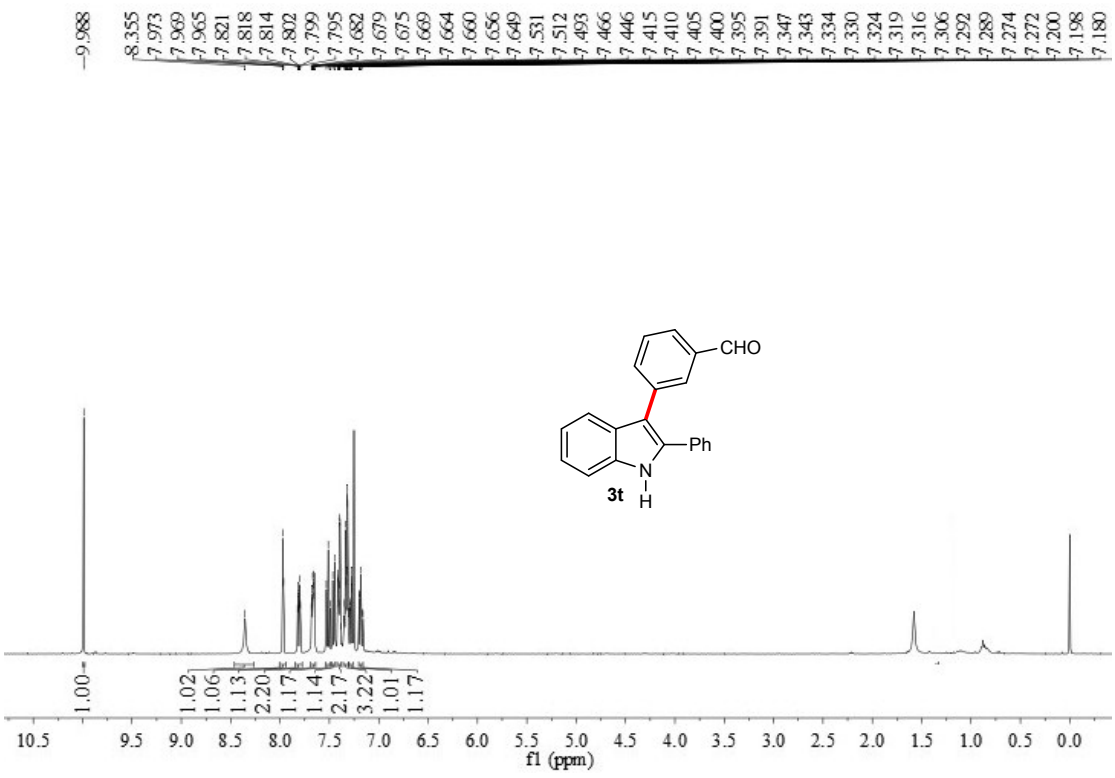

CF3
Ph
N
H
3q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.557
8.033
8.014
7.691
7.671
7.492
7.472
7.409
7.388
7.379
7.366
7.288
7.275
7.233
7.213
7.176
7.157
7.139
4.394
4.376
4.359
4.341
1.395
1.377
1.359
CO2Et
Ph
N
H
3r
1.00
2.09
1.06
2.12
3.17
3.13
0.99
1.08
2.10
3.14
f1 (ppm)


167.008
140.440
136.117
135.190
132.410
129.930
129.881
128.843
128.494
128.280
128.097
127.955
122.946
120.805
119.431
113.941
111.243
60.986
14.433
CO2Et
Ph
N
H
3r
f1 (ppm)


11.862
8.238
8.218
7.643
7.623
7.607
7.587
7.510
7.488
7.482
7.461
7.449
7.431
7.411
7.387
7.246
7.228
7.208
7.147
7.129
7.110
NO2
Ph
N
H
3s
1.00
2.08
3.24
6.12
1.15
1.08
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


145.048
143.017
136.267
131.767
130.196
128.796
128.696
127.055
123.868
122.478
120.471
118.292
111.850
111.147
NO2
Ph
N
H
3s
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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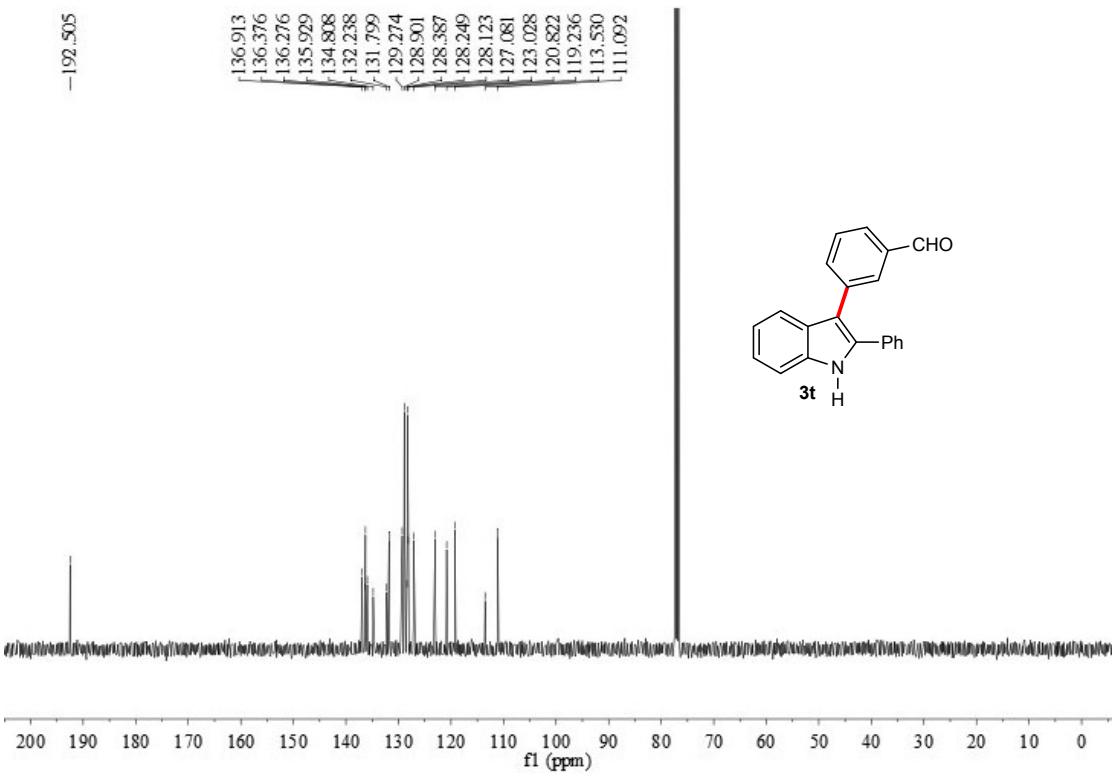
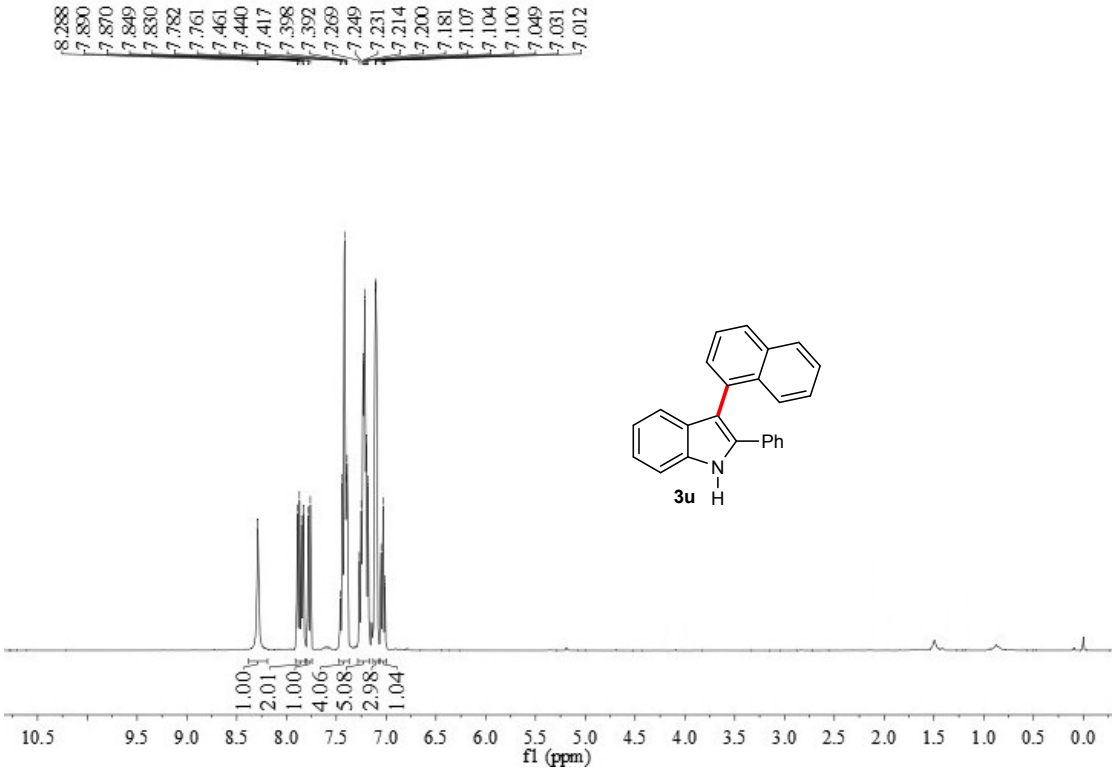
8.355
7.973
7.969
7.965
7.821
7.818
7.814
7.802
7.799
7.795
7.682
7.679
7.675
7.669
7.664
7.660
7.656
7.649
7.531
7.512
7.493
7.466
7.446
7.415
7.410
7.405
7.400
7.395
7.391
7.347
7.343
7.334
7.330
7.324
7.319
7.316
7.306
7.292
7.289
7.274
7.272
7.200
7.198
7.180
CHO
Ph
N
H
3t
1.00
1.02
1.06
1.13
2.20
1.17
1.14
2.17
3.22
1.01
1.17
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


192.505
136.913
136.376
136.276
135.929
134.808
132.238
131.799
129.274
128.901
128.387
128.249
128.123
127.081
123.028
120.822
119.236
113.530
111.092
CHO
Ph
N
H
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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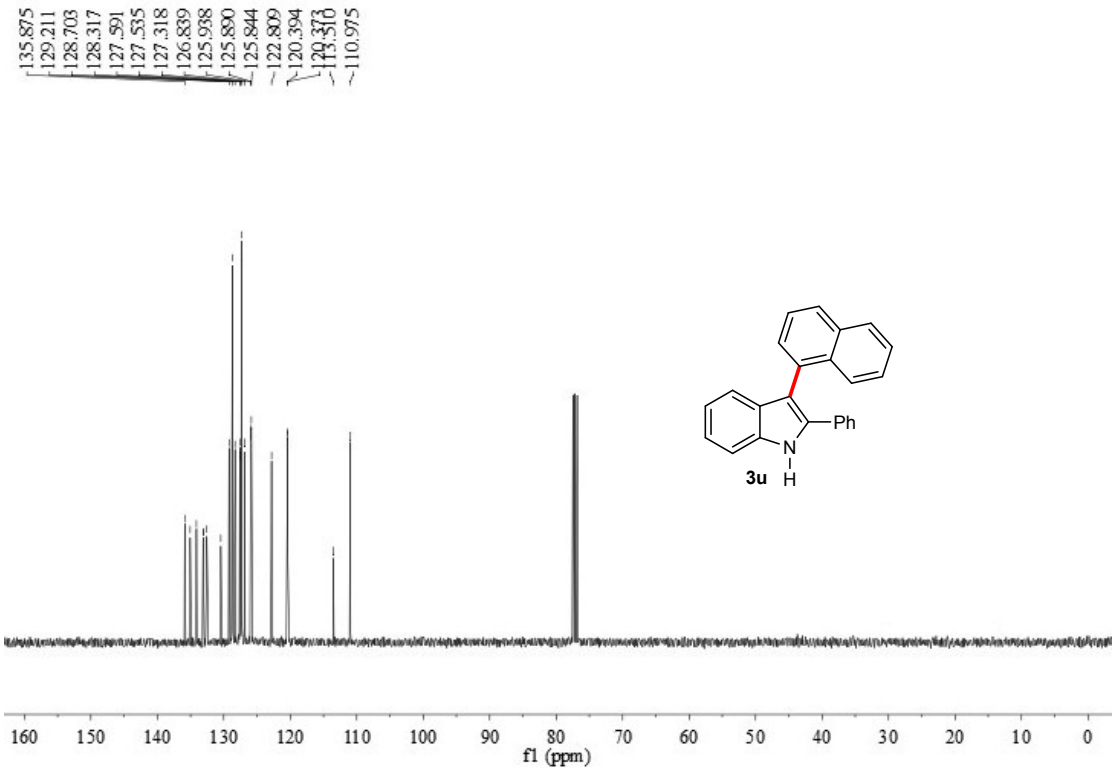
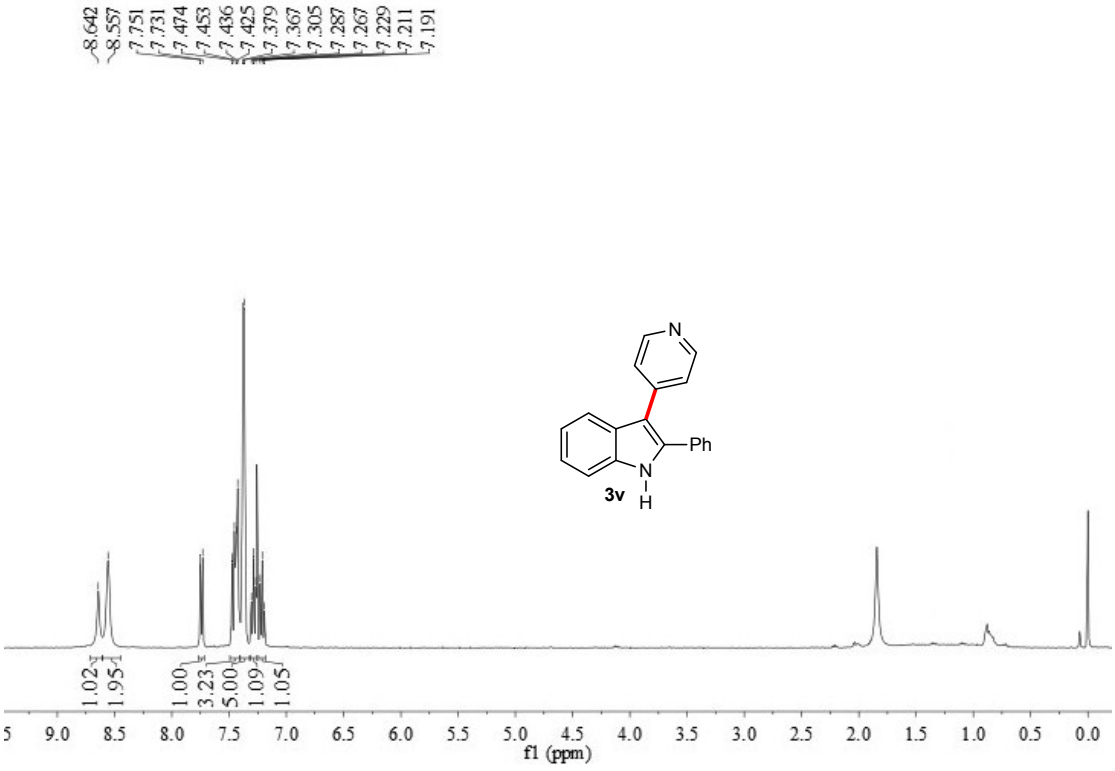
7.890
7.870
7.849
7.830
7.782
7.761
7.461
7.440
7.417
7.398
7.392
7.269
7.249
7.231
7.214
7.200
7.181
7.107
7.104
7.100
7.049
7.031
7.012
Ph
N
H
3u
1.00
2.01
1.00
4.06
5.08
2.98
1.04
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


135.875
129.211
128.703
128.317
127.991
127.535
127.318
126.839
125.938
125.890
125.844
122.809
120.394
120.373
113.310
110.975
Ph
N
H
3u
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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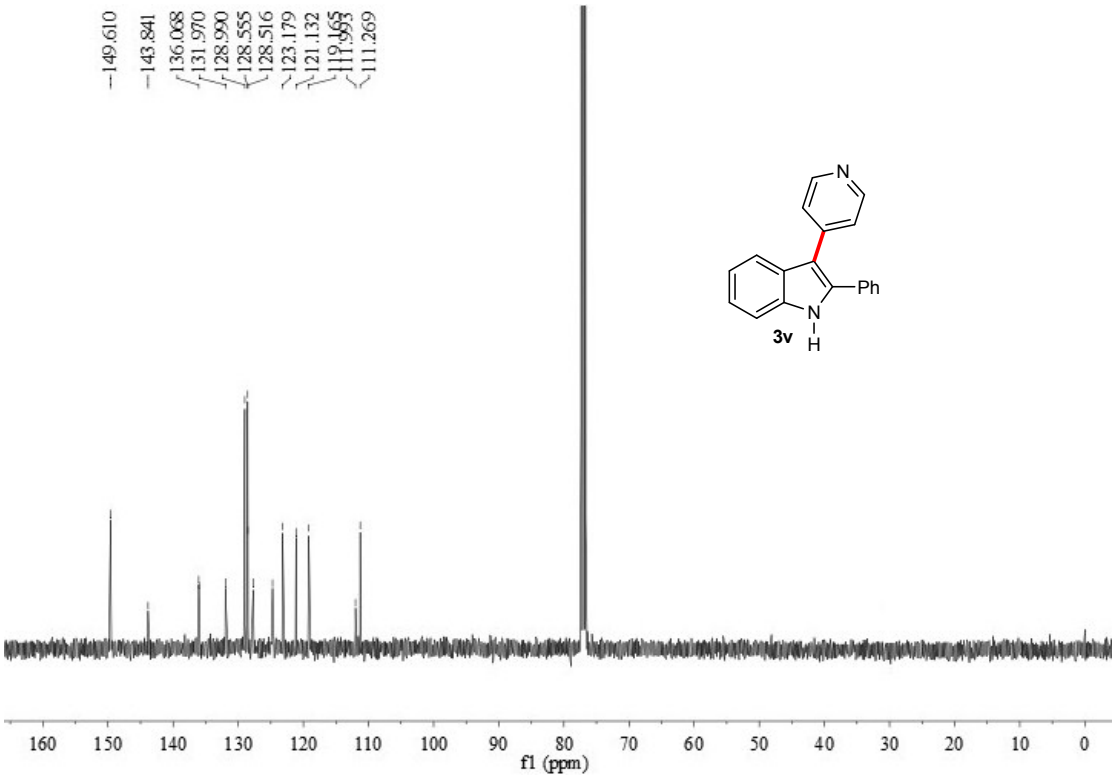
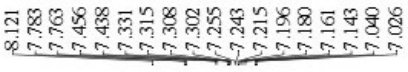
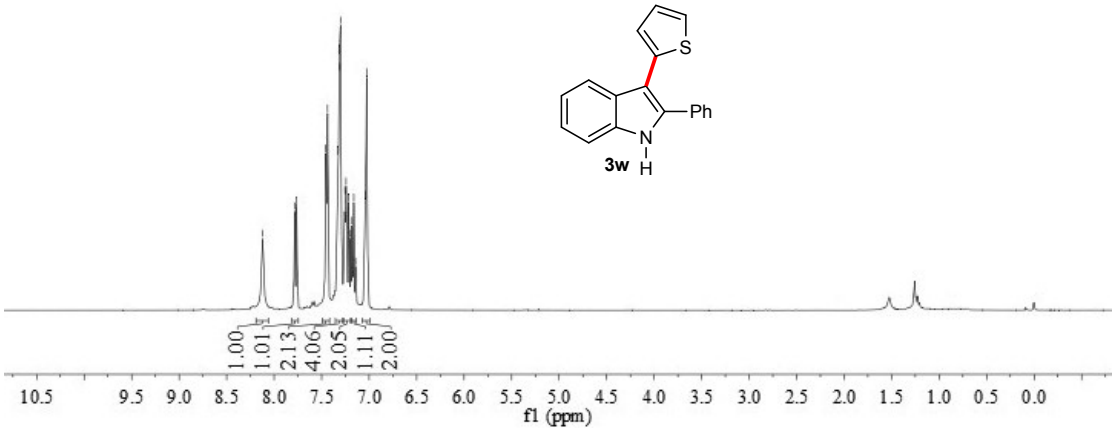
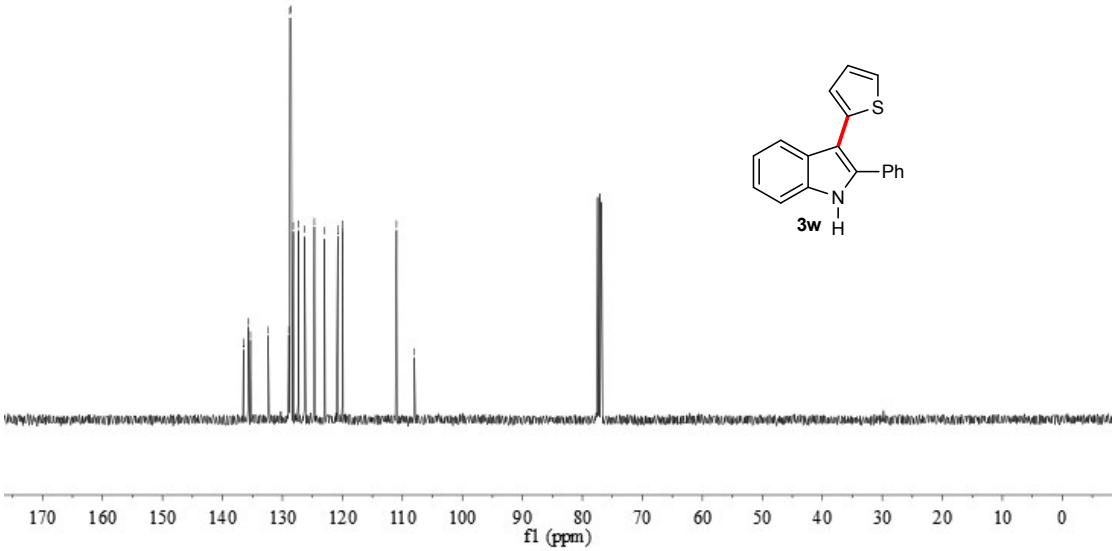
7.731
7.474
7.453
7.436
7.425
7.379
7.367
7.305
7.287
7.267
7.229
7.211
7.191
N
Ph
N
H
3v
1.02
1.95
1.00
3.23
5.00
1.09
1.05
f1 (ppm)

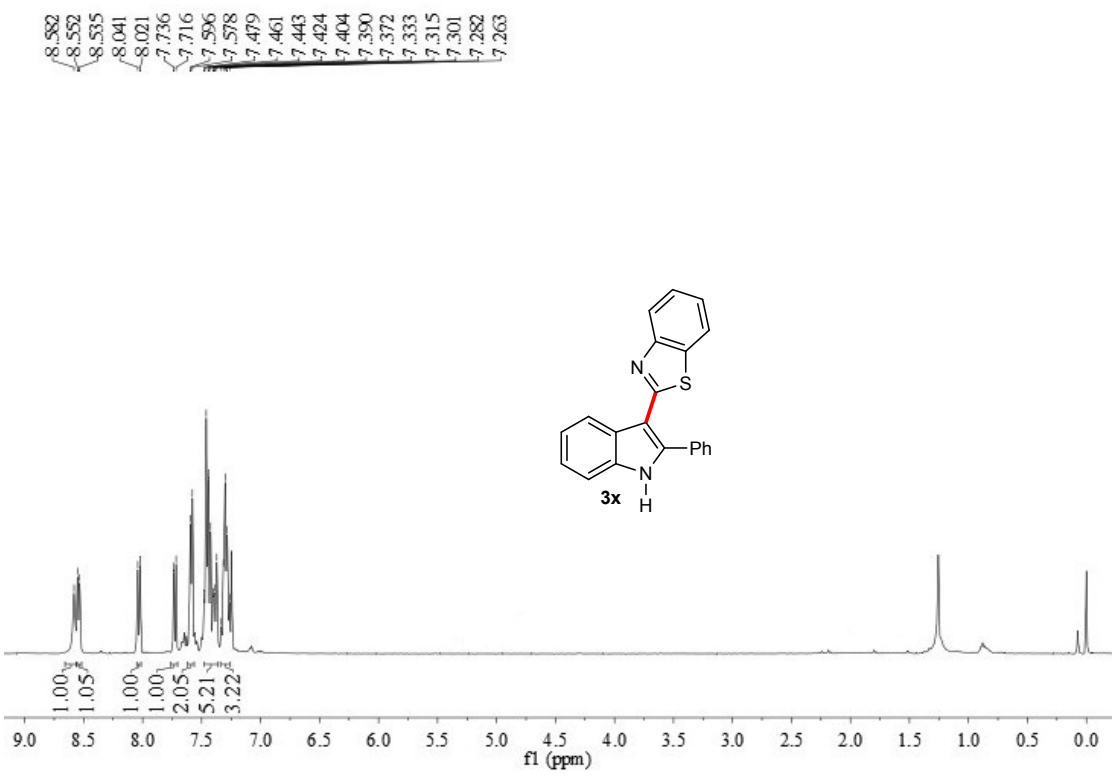

149.610
143.841
136.068
131.970
128.900
128.555
128.516
123.179
121.132
119.165
111.993
111.269
N
Ph
N
H
3v
f1 (ppm)

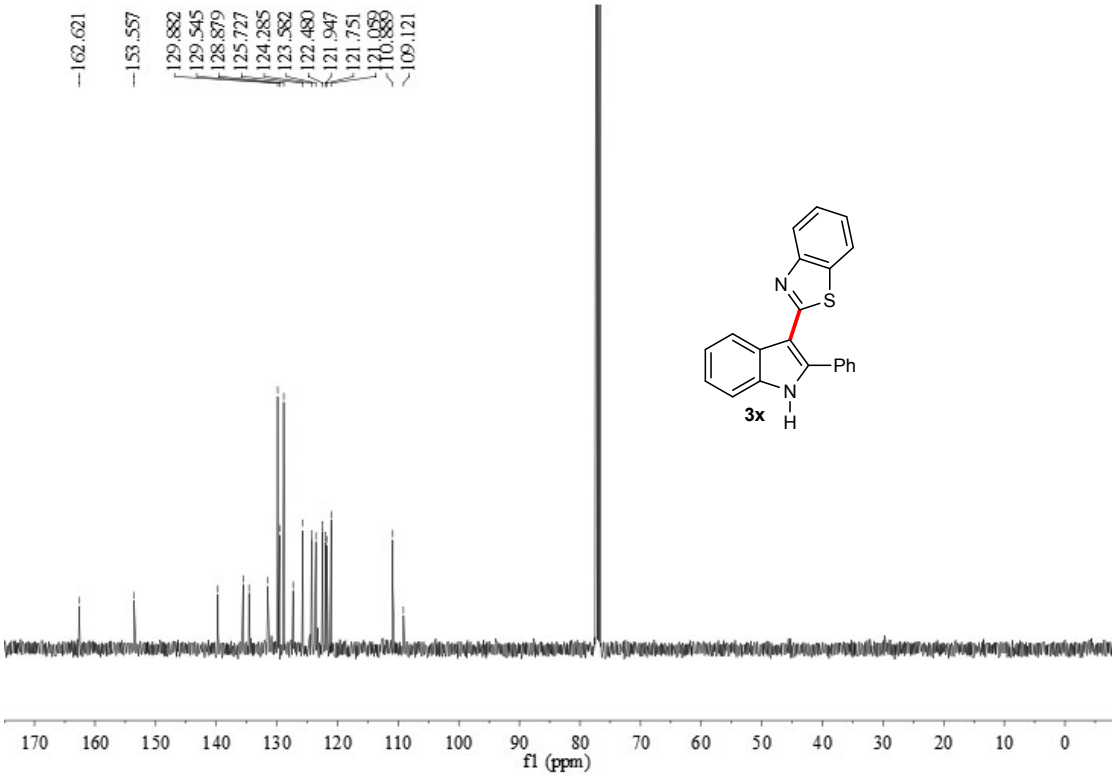

8.121
7.783
7.763
7.456
7.438
7.331
7.315
7.308
7.302
7.255
7.243
7.215
7.196
7.180
7.161
7.143
7.040
7.026


S
Ph
N
H
3w
1.00
1.01
2.13
4.06
2.05
1.11
2.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

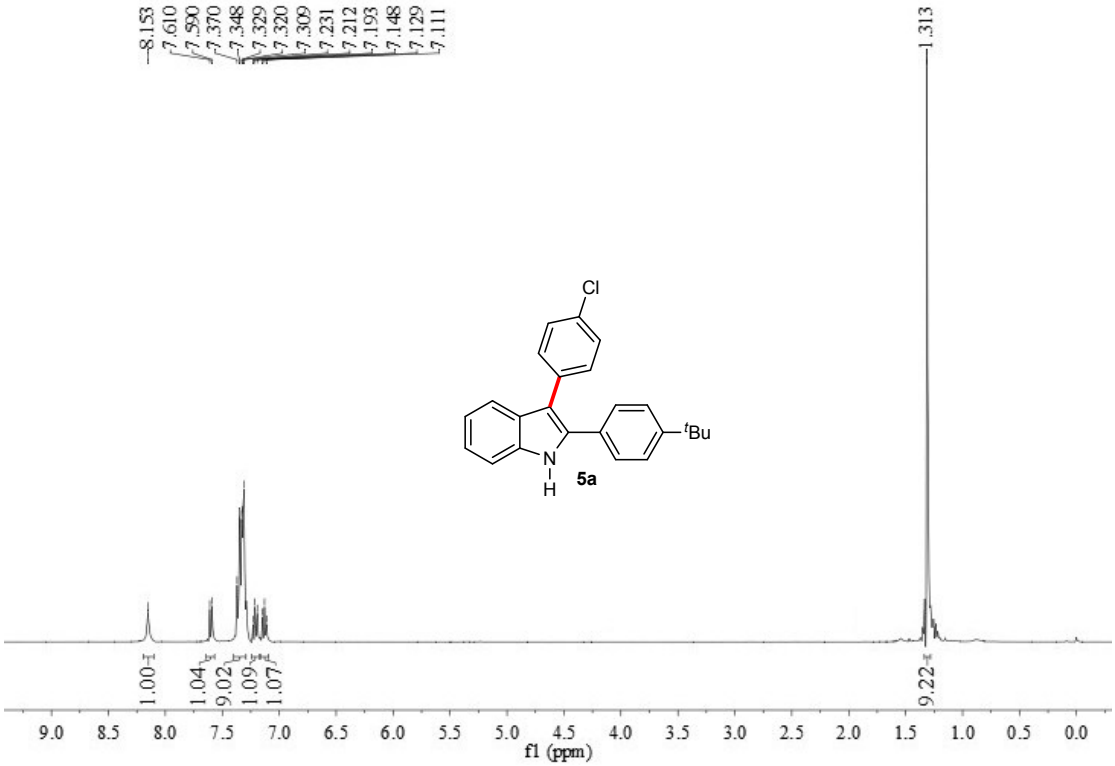

136.510
135.702
135.331
132.376
128.941
128.744
128.535
128.205
127.325
126.295
124.679
122.996
120.784
119.961
110.990
108.003

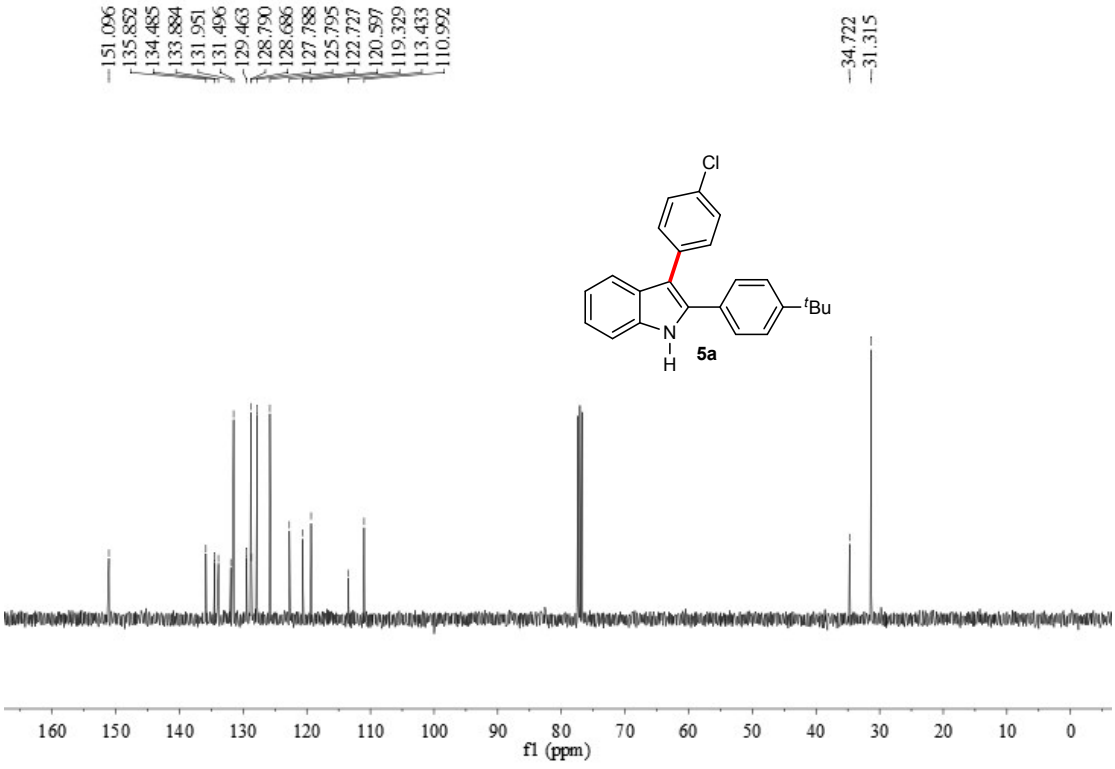

S
Ph
N
H
3w
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

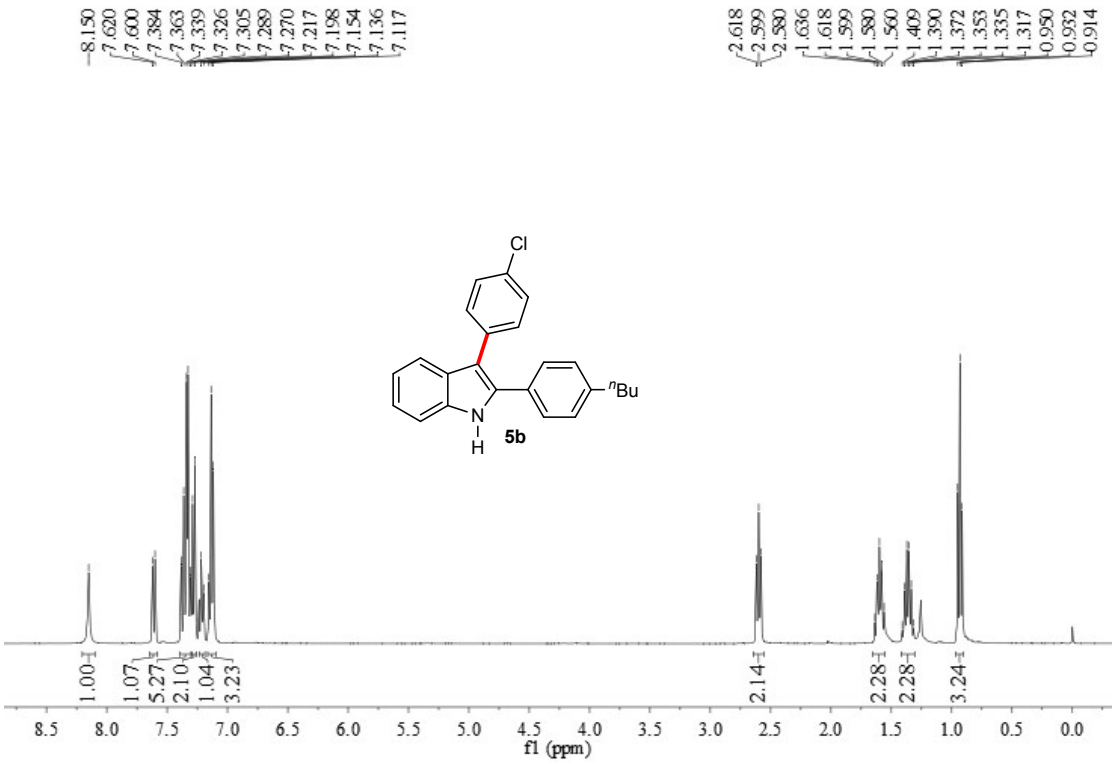

8.582
8.552
8.535
8.041
8.021
7.736
7.716
7.596
7.578
7.479
7.461
7.443
7.424
7.404
7.390
7.372
7.333
7.315
7.301
7.282
7.263
N
S
Ph
N
H
3x
1.00
1.05
1.00
1.00
2.05
5.21
3.22
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.621
153.557
129.882
129.545
128.879
125.727
124.285
123.382
122.480
121.947
121.751
109.121
N
S
Ph
N
H
3x
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{1}H and ^{13}C NMR spectra of compounds 5



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7.305
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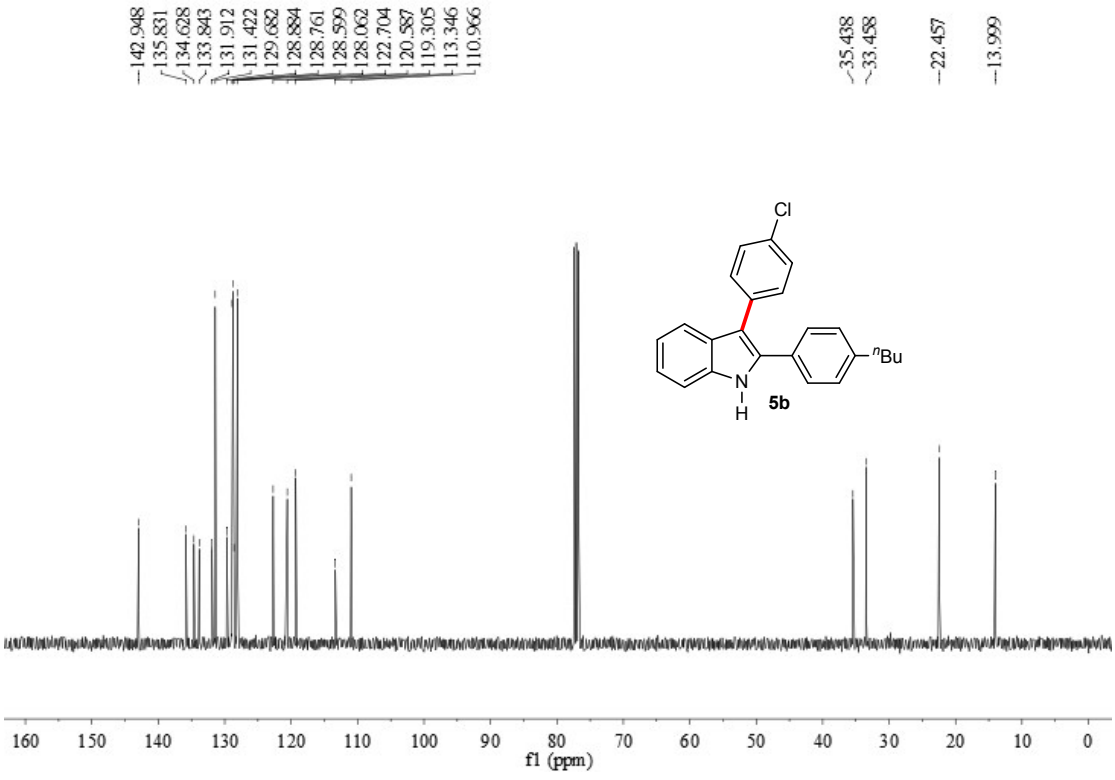
7.198
7.154
7.136
7.117
2.618
2.599
2.580
1.636
1.618
1.599
1.580
1.560
1.409
1.390
1.372
1.353
1.335
1.317
0.950
0.932
0.914
Cl
nBu
N
H
5b
1.00
1.07
5.27
2.10
1.04
3.23
2.14
2.28
2.28
3.24
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.062
122.704
120.587
119.305
113.346
110.966
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13.999
Cl
nBu
N
H
5b
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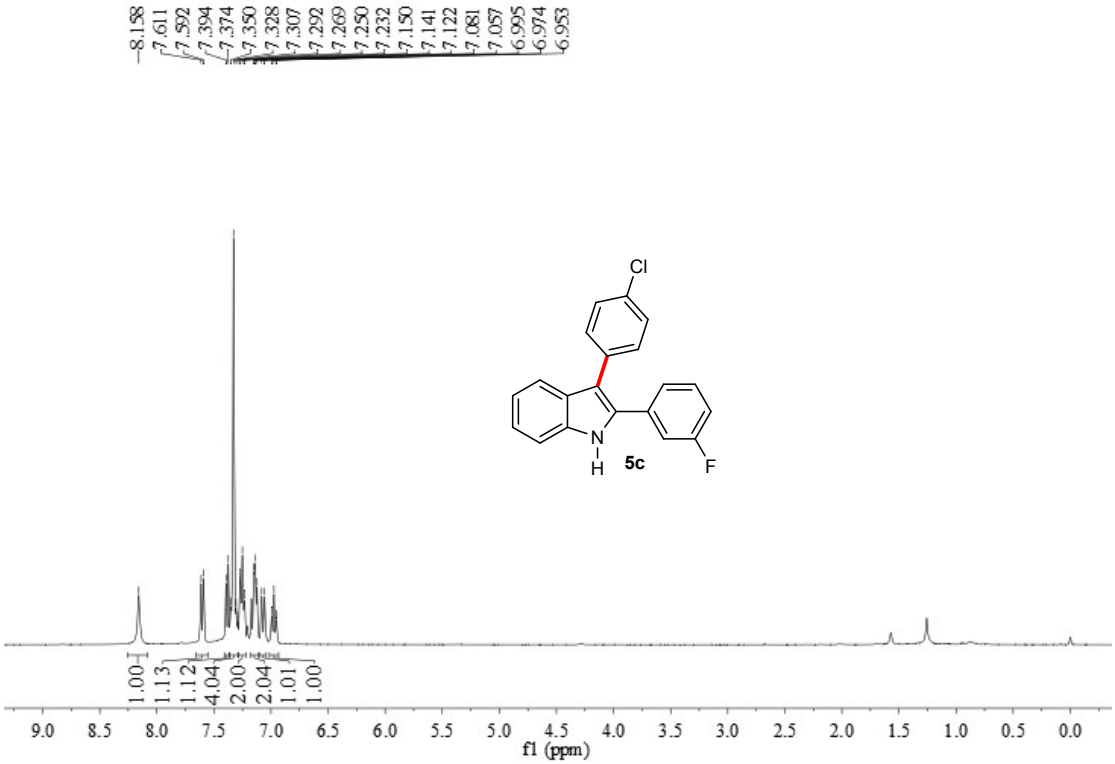
f1 (ppm)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7.394
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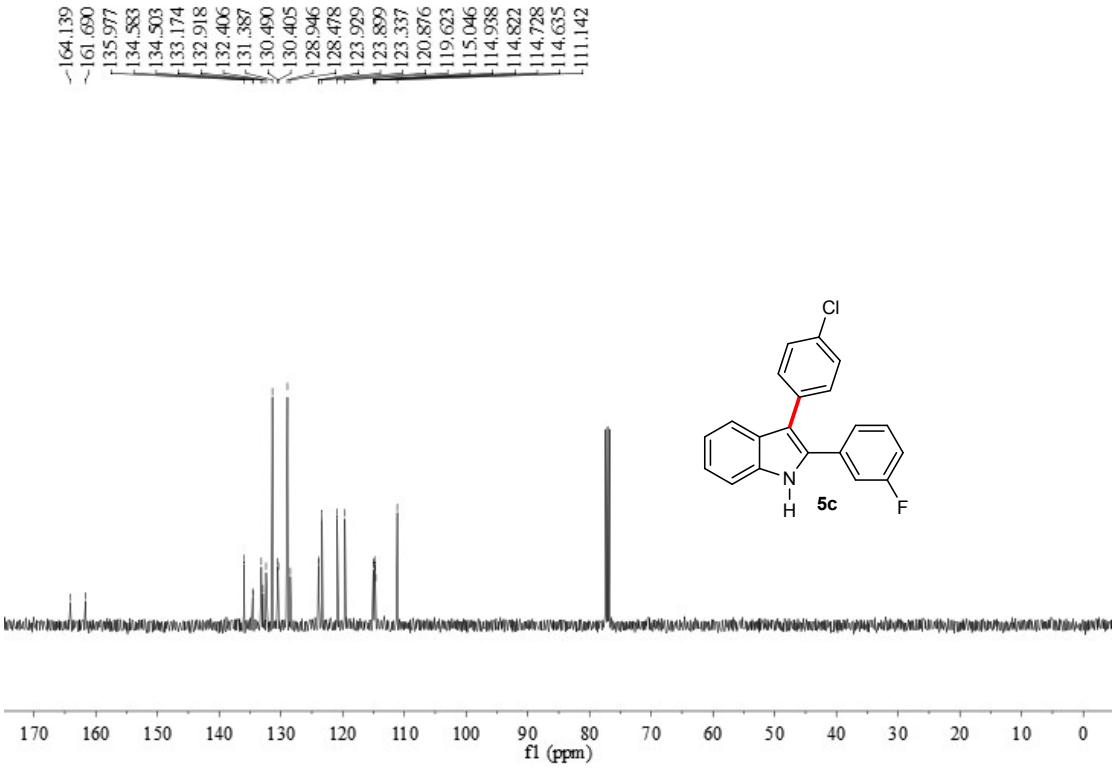
7.350
7.328
7.307
7.292
7.269
7.250
7.232
7.150
7.141
7.122
7.081
7.057
6.995
6.974
6.953
Cl
N
H
5c
F
1.00
1.13
1.12
4.04
2.00
2.04
1.01
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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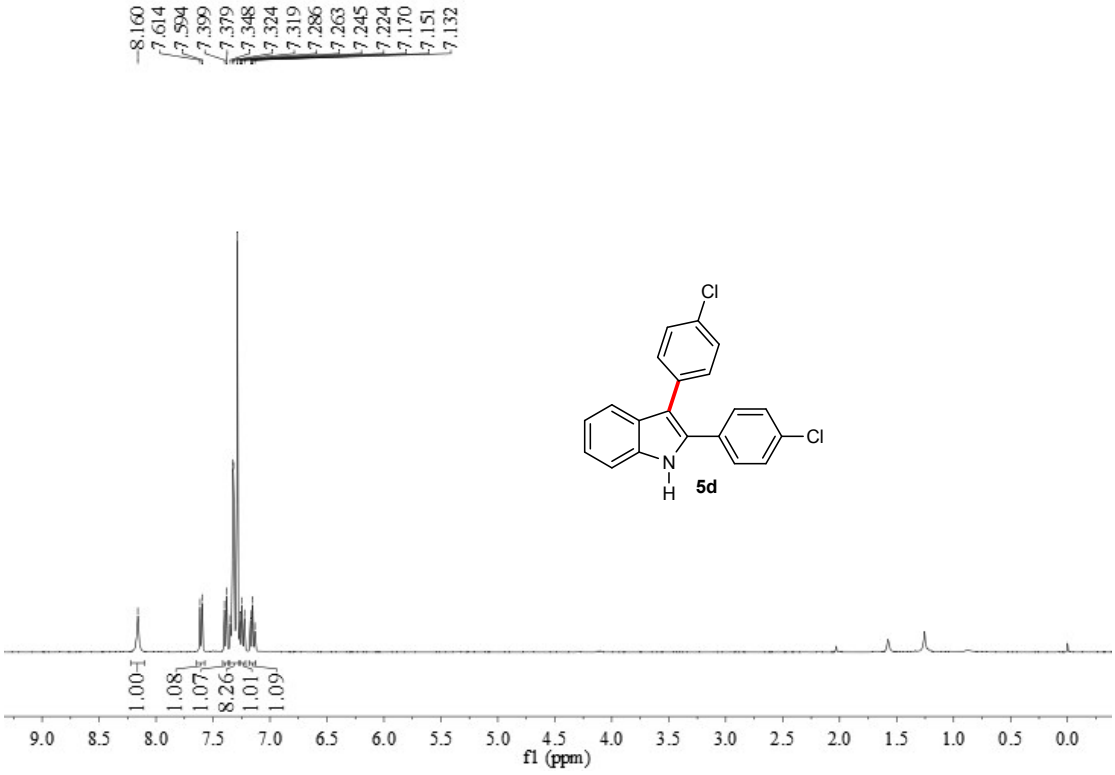
133.174
132.918
132.406
131.387
130.490
130.405
128.946
128.478
123.929
123.899
123.337
120.876
119.623
115.046
114.938
114.822
114.728
114.635
111.142
Cl
N
H
5c
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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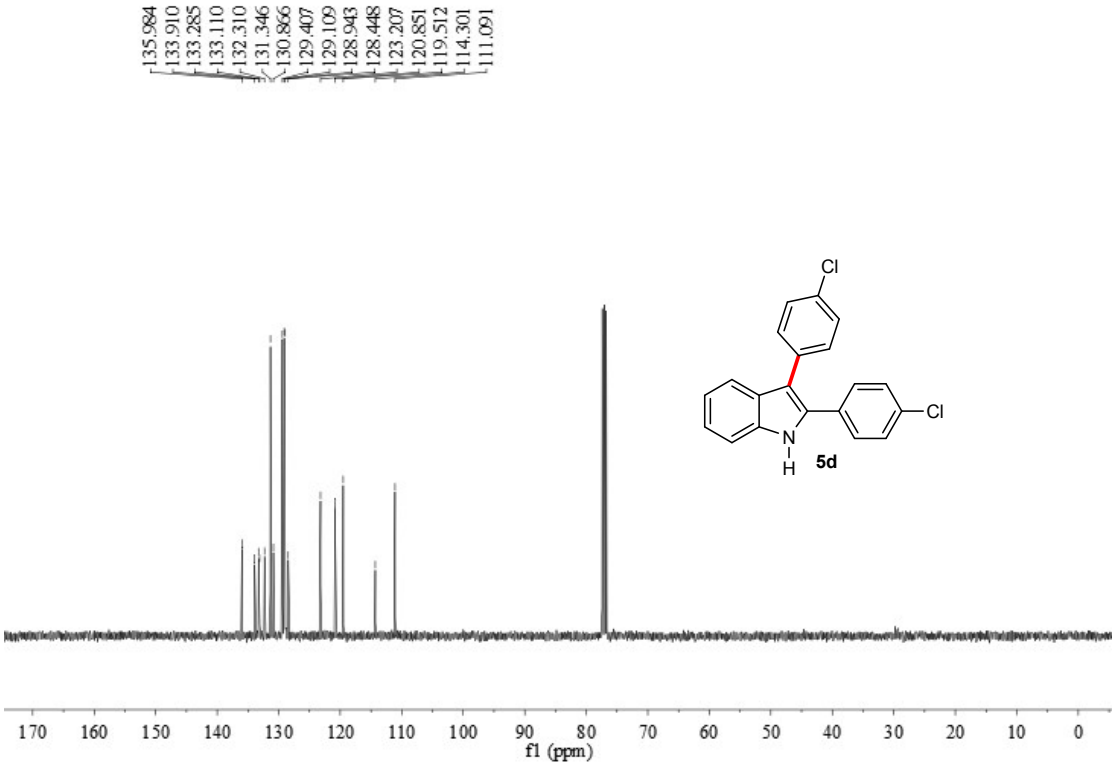
7.614
7.594
7.399
7.379
7.348
7.324
7.319
7.286
7.263
7.245
7.224
7.170
7.151
7.132
Cl
Cl
N
H
5d
1.00
1.08
1.07
8.26
1.01
1.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.285
133.110
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129.407
129.109
128.943
128.448
123.207
120.851
119.512
114.301
111.091
Cl
Cl
N
H
5d
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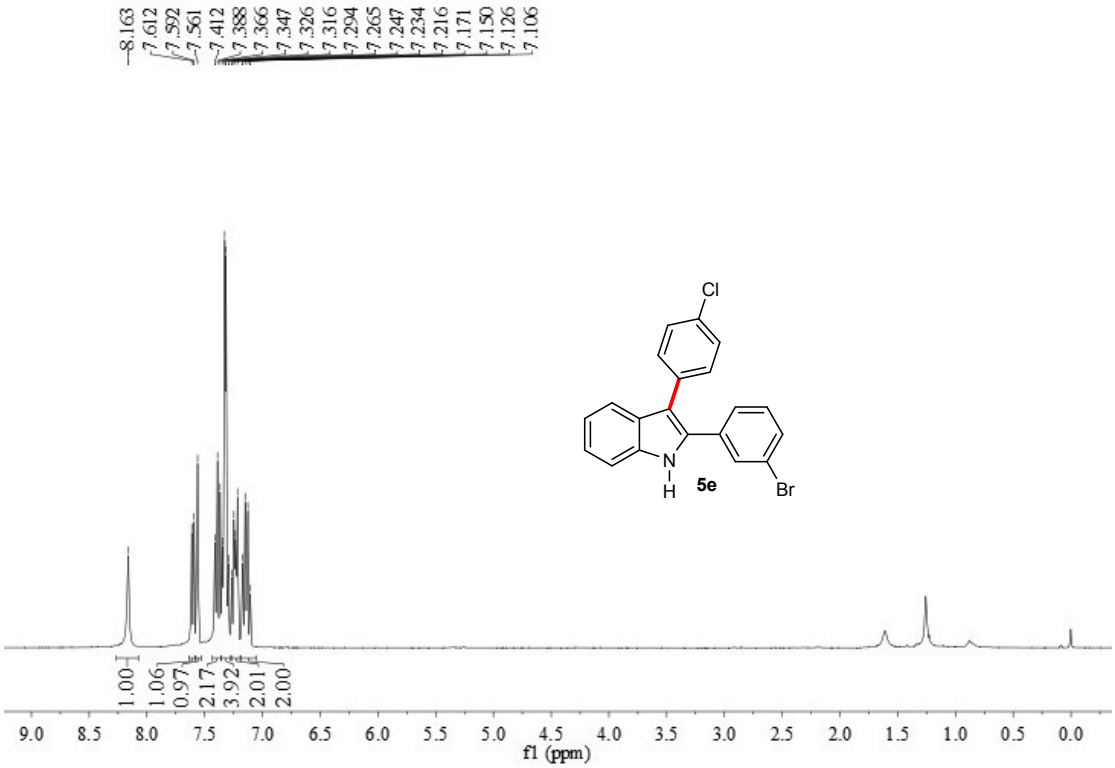
f1 (ppm)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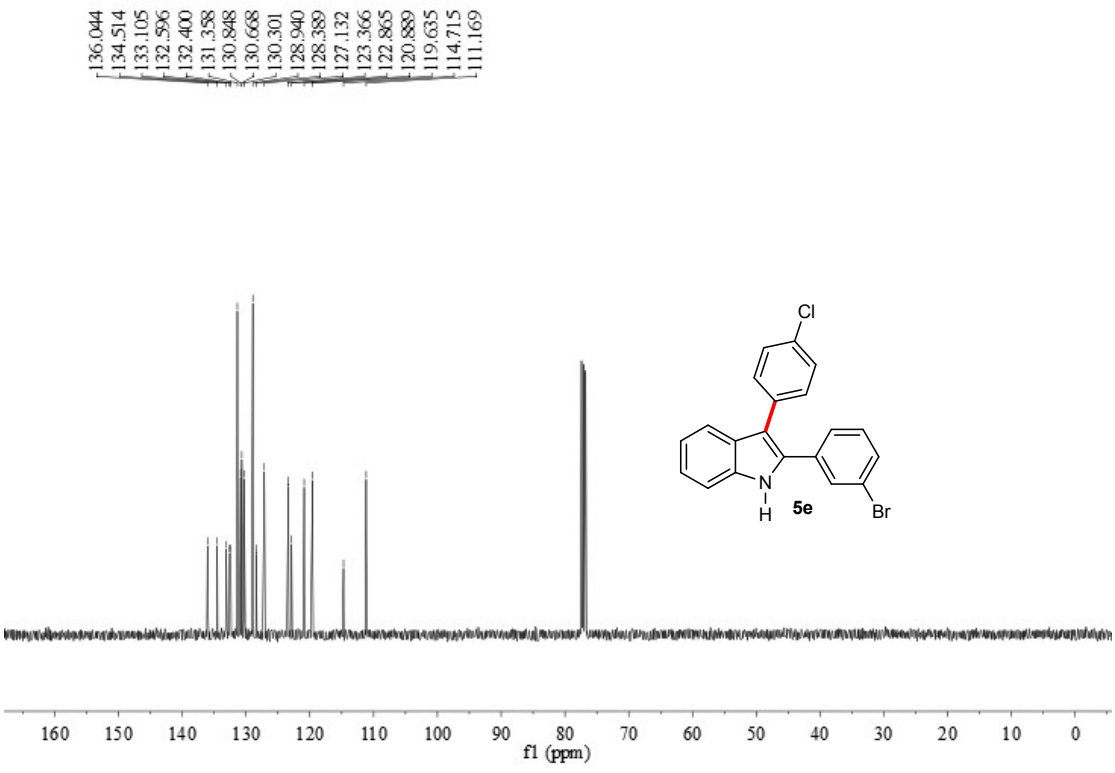
7.592
7.561
7.412
7.388
7.366
7.347
7.326
7.316
7.294
7.265
7.247
7.234
7.216
7.171
7.150
7.126
7.106
Cl
N
H
5e
Br
1.00
1.06
0.97
2.17
3.92
2.01
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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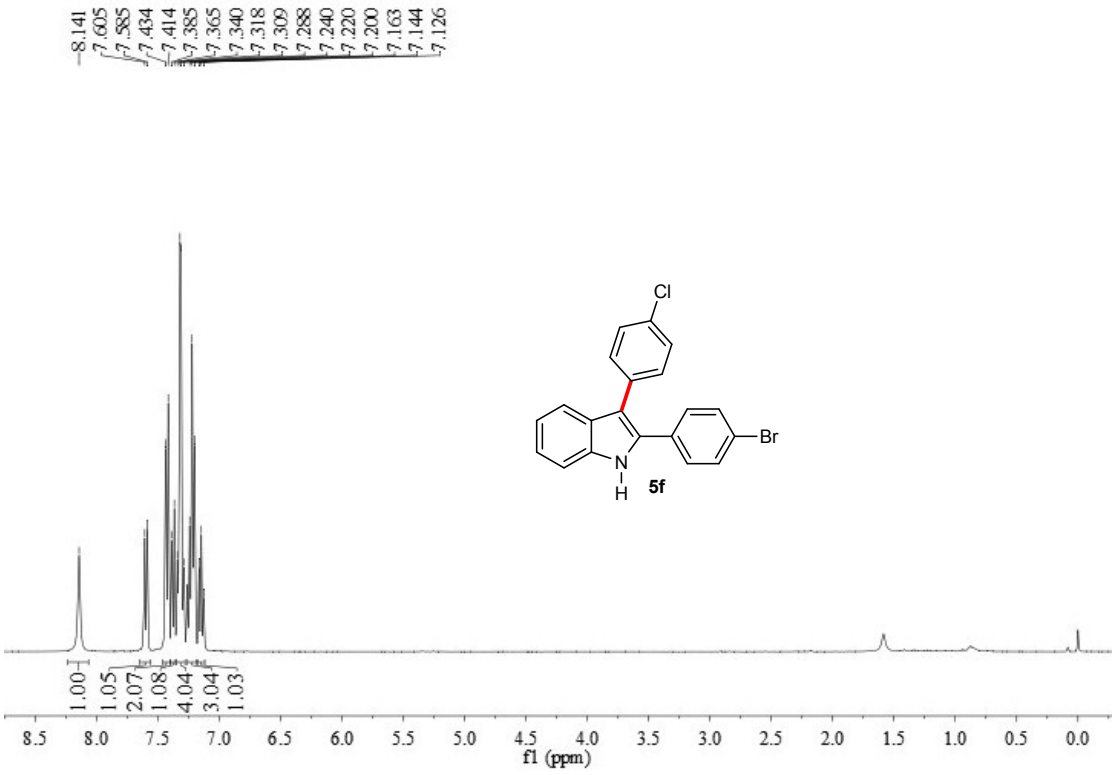
131.358
130.848
130.668
130.301
128.940
128.389
127.132
123.366
122.865
120.889
119.635
114.715
111.169
Cl
N
H
5e
Br
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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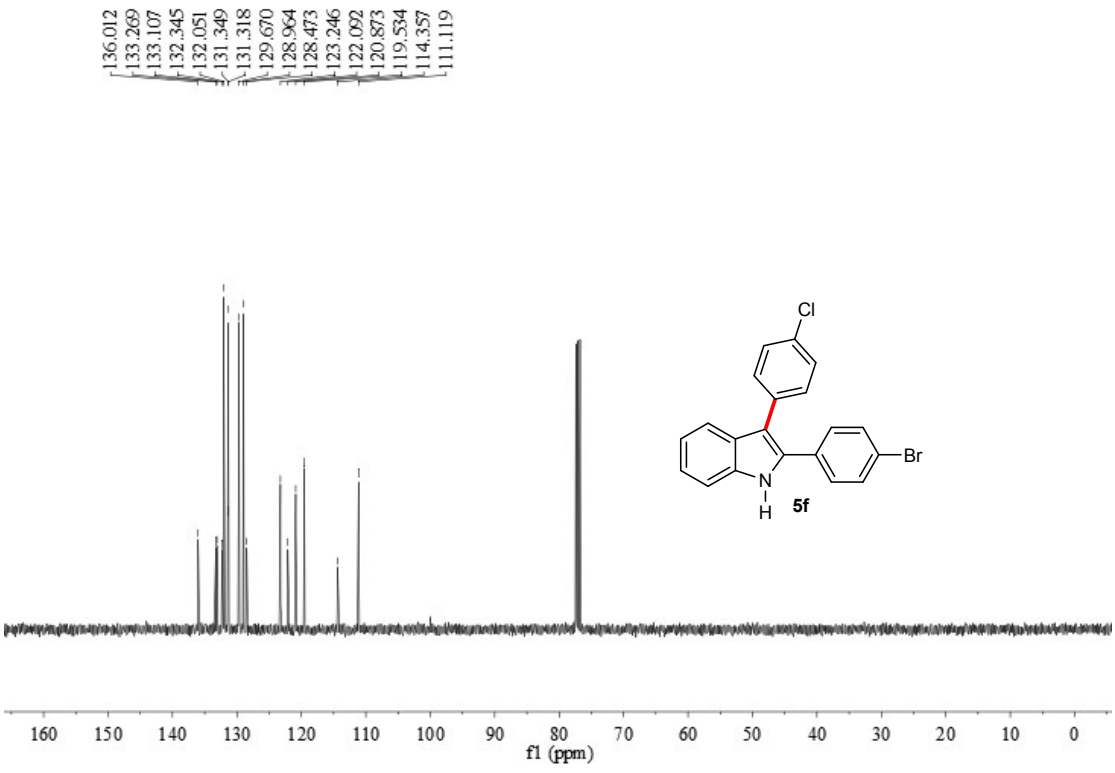
7.414
7.385
7.365
7.340
7.318
7.309
7.288
7.240
7.220
7.200
7.163
7.144
7.126
Cl
Br
N
H
5f
1.00
1.05
2.07
1.08
4.04
3.04
1.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.107
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131.318
129.670
128.964
128.473
123.246
122.092
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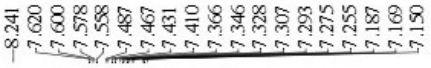
111.119
Cl
Br
N
H
5f
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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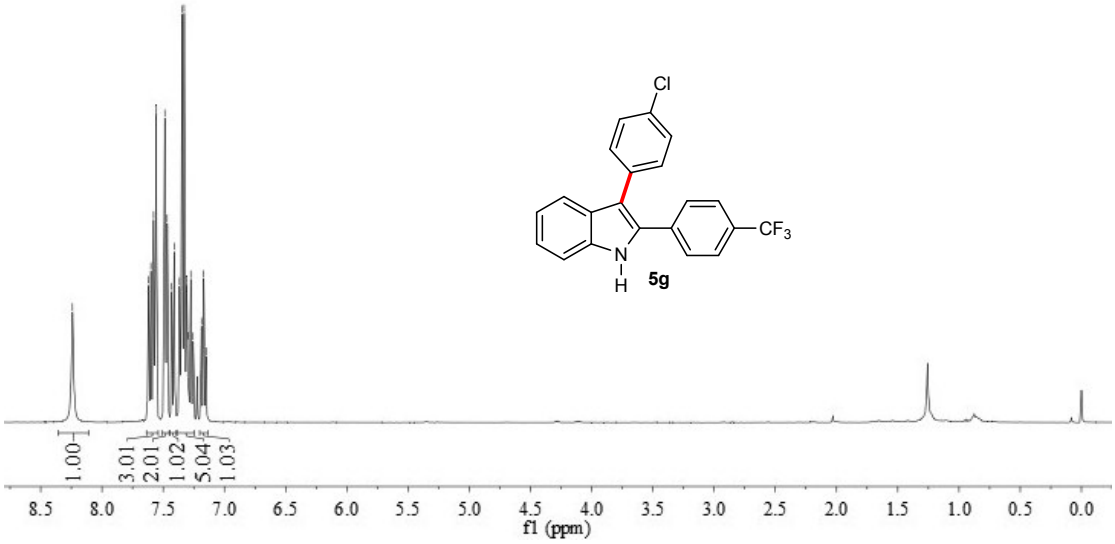
7.346
7.328
7.307
7.293
7.275
7.255
7.187
7.169
7.150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CF3
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H
5g
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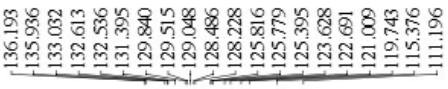
3.01
2.01
1.02
5.04
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.515
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121.009
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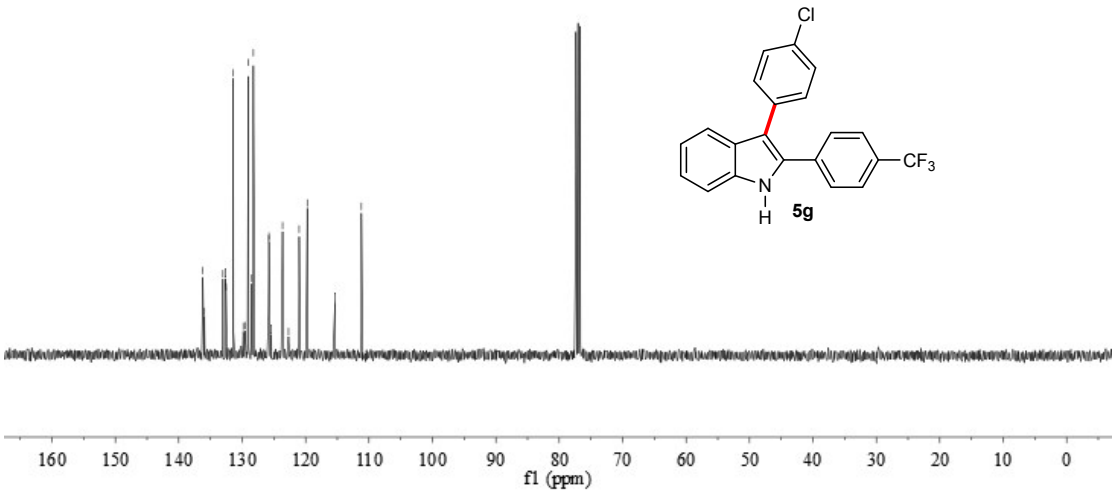
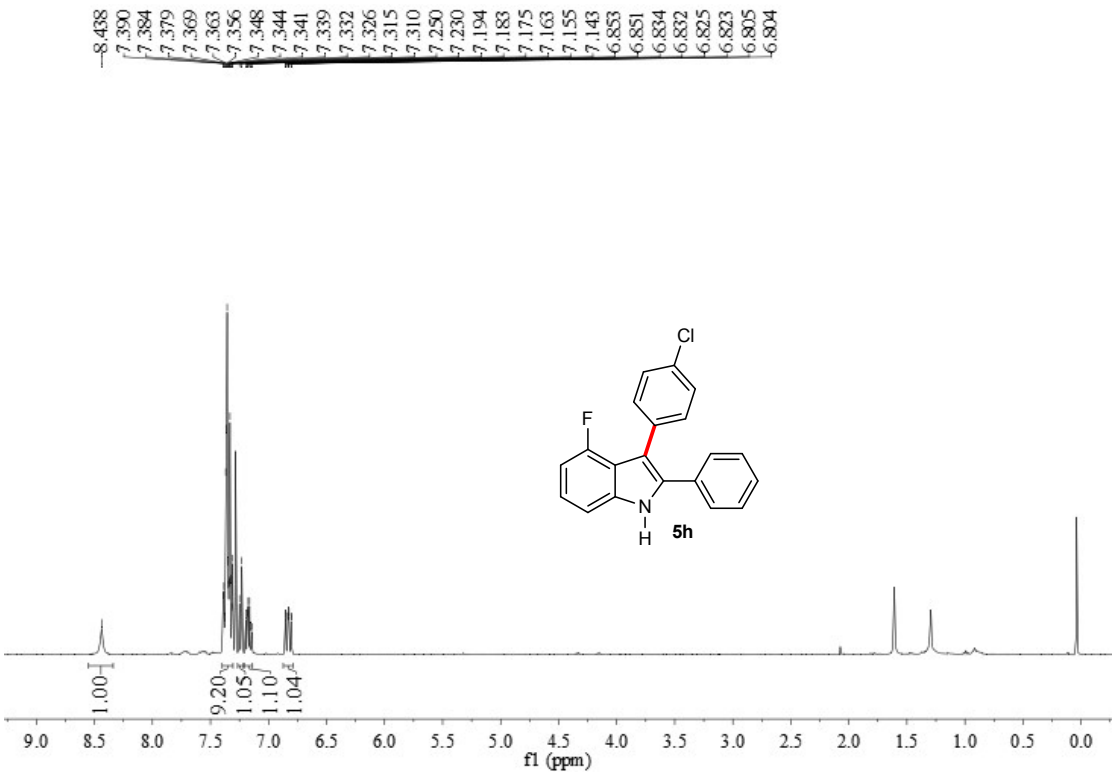
115.376
111.196


Cl
CF3
N
H
5g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.348
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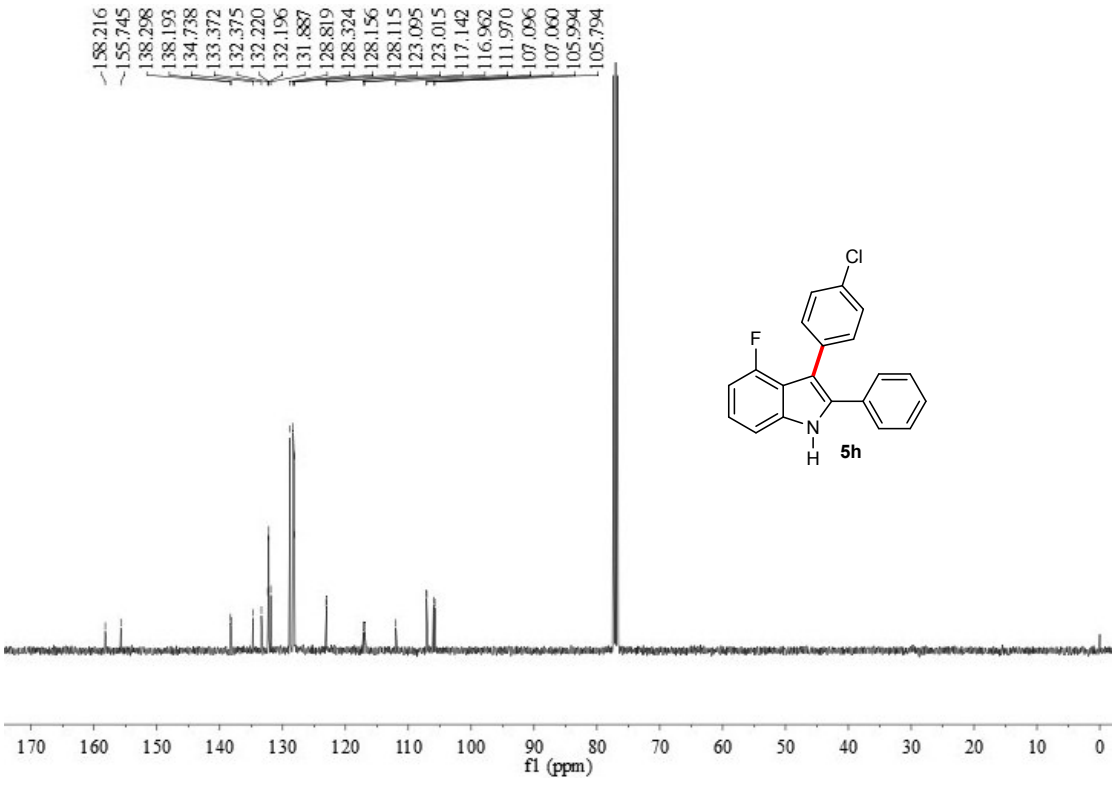
7.332
7.326
7.315
7.310
7.250
7.230
7.194
7.183
7.175
7.163
7.155
7.143
6.853
6.851
6.834
6.832
6.825
6.823
6.805
6.804
Cl
F
N
H
5h
1.00
9.20
1.05
1.10
1.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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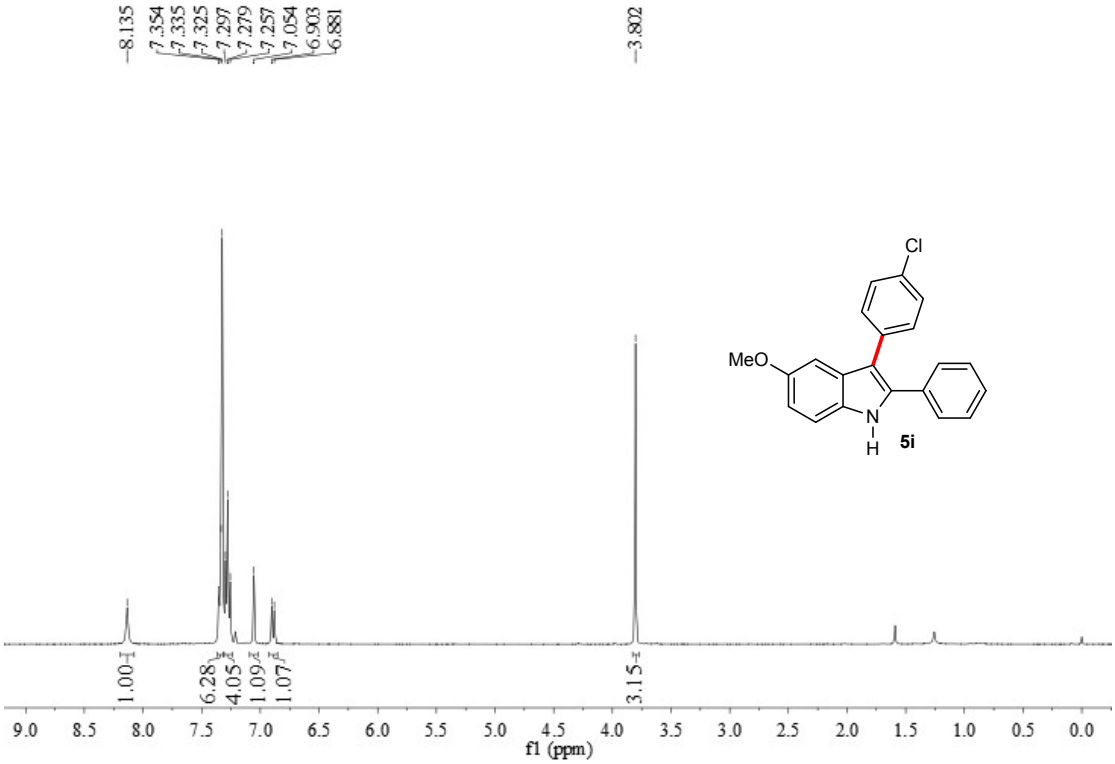
133.372
132.375
132.220
132.196
131.887
128.819
128.324
128.156
128.115
123.095
123.015
117.142
116.962
111.970
107.096
107.060
105.994
105.794
Cl
F
N
H
5h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.325
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7.257
7.054
6.903
6.881
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MeO
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H
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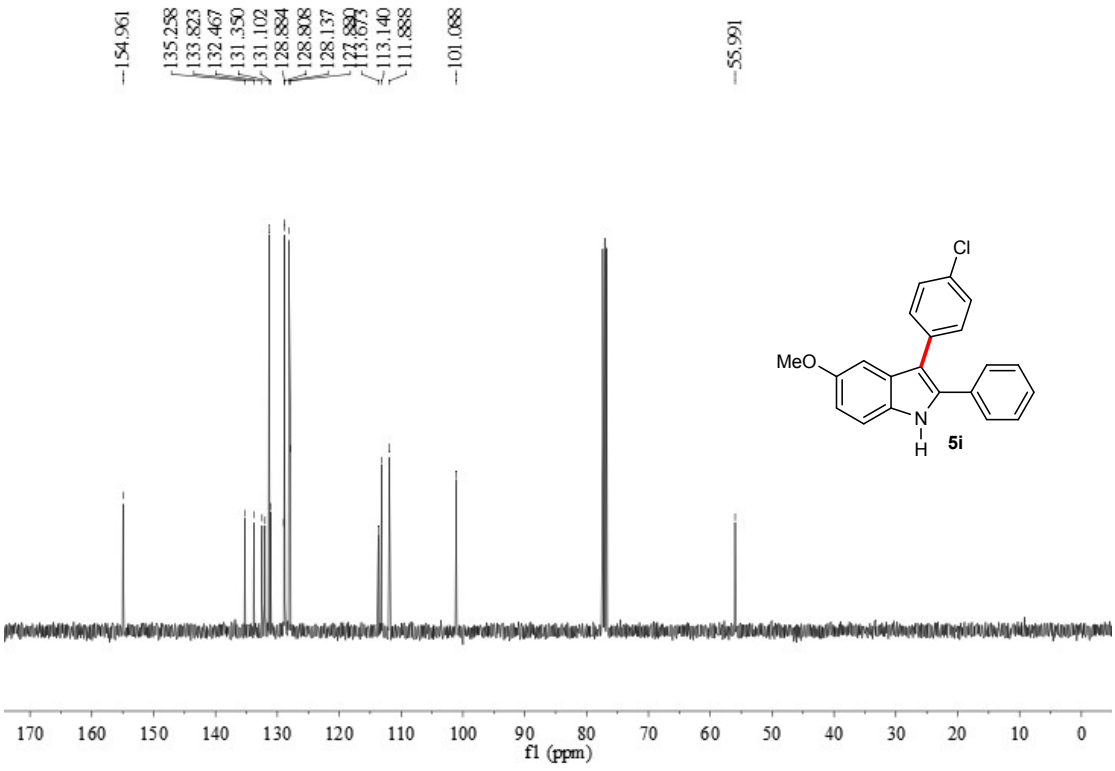
1.00
6.28
4.05
1.09
1.07
3.15
f1 (ppm)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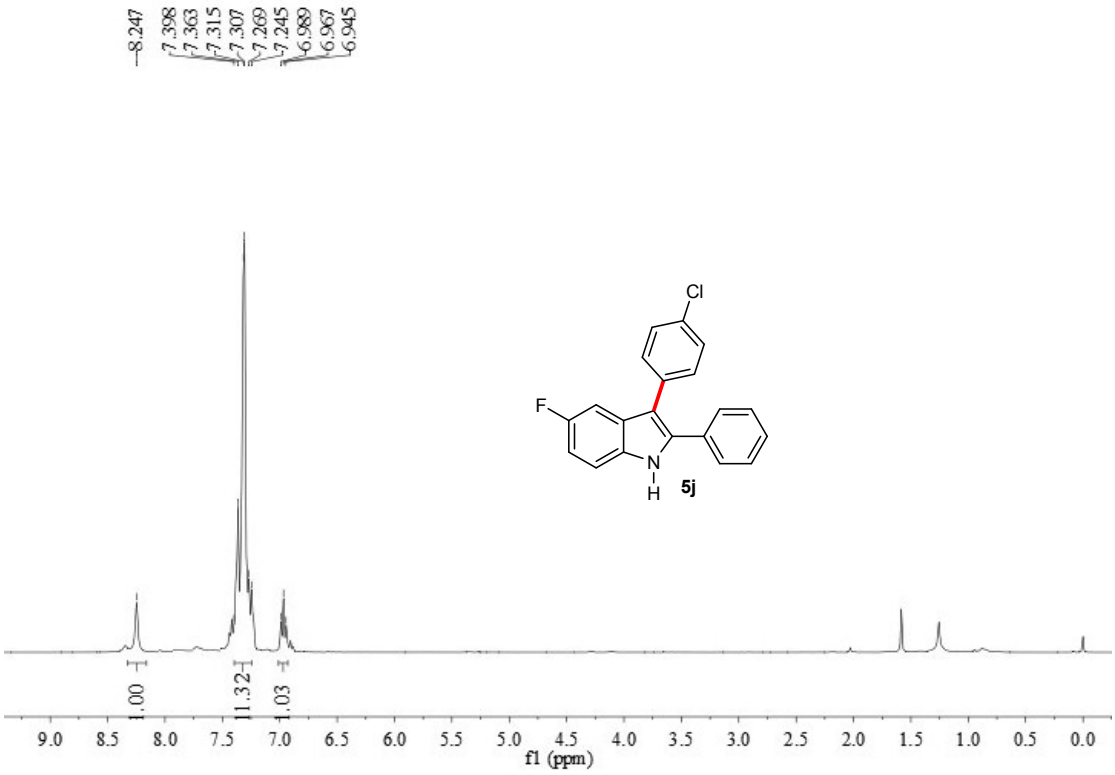
Cl
MeO
N
H
5i
f1 (ppm)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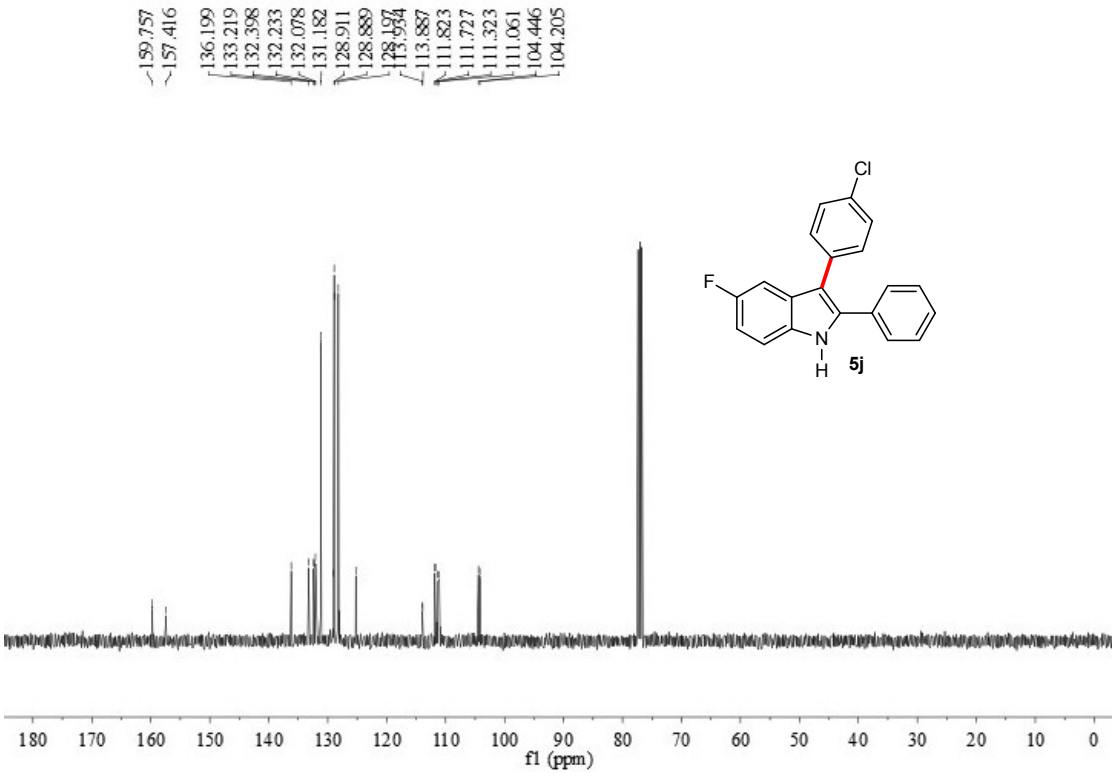
7.269
7.245
6.989
6.967
6.945
Cl
F
N
H
5j
1.00
11.32
1.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.182
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128.889
128.187
123.934
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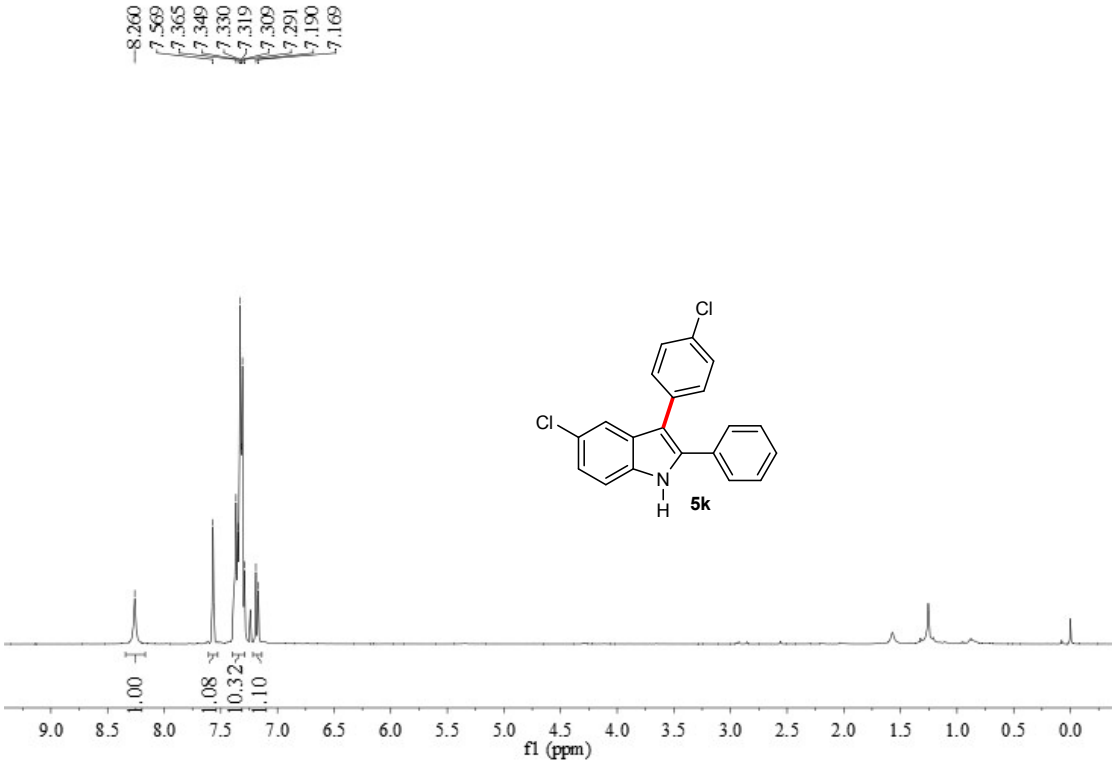
111.823
111.727
111.323
111.061
104.446
104.205
Cl
F
N
H
5j
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.260
7.569
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7.319
7.309
7.291
7.190
7.169
Cl
Cl
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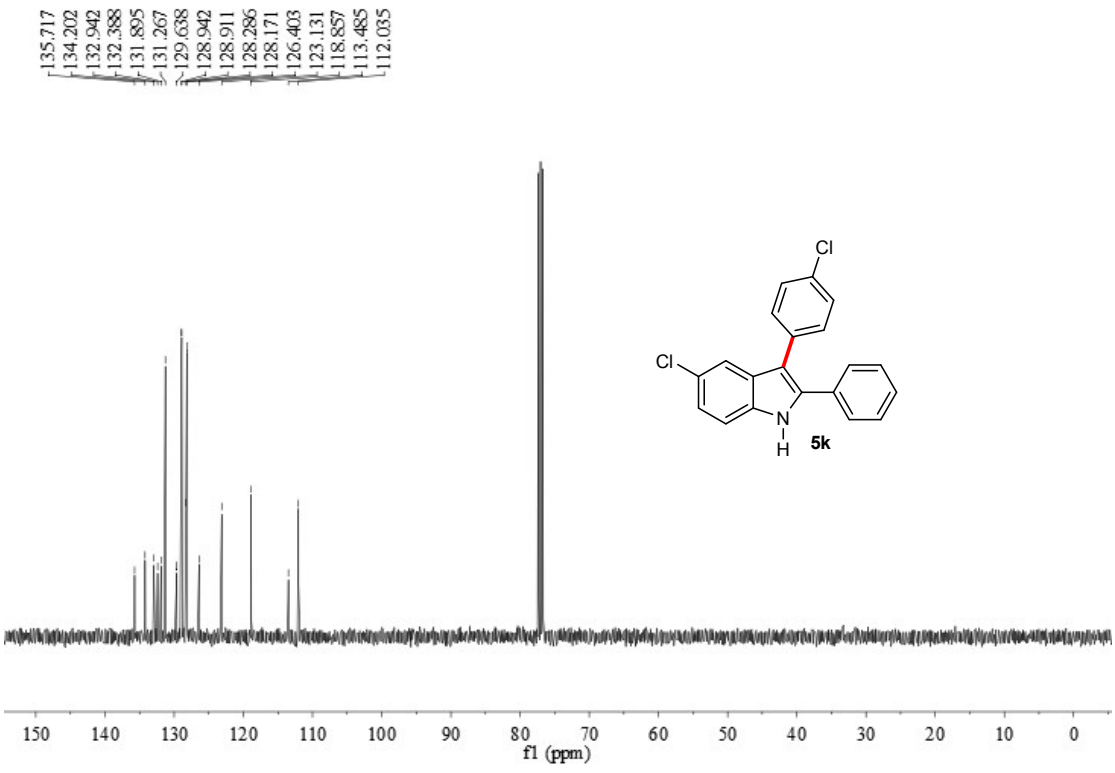
H
5k
1.00
1.08
10.32
1.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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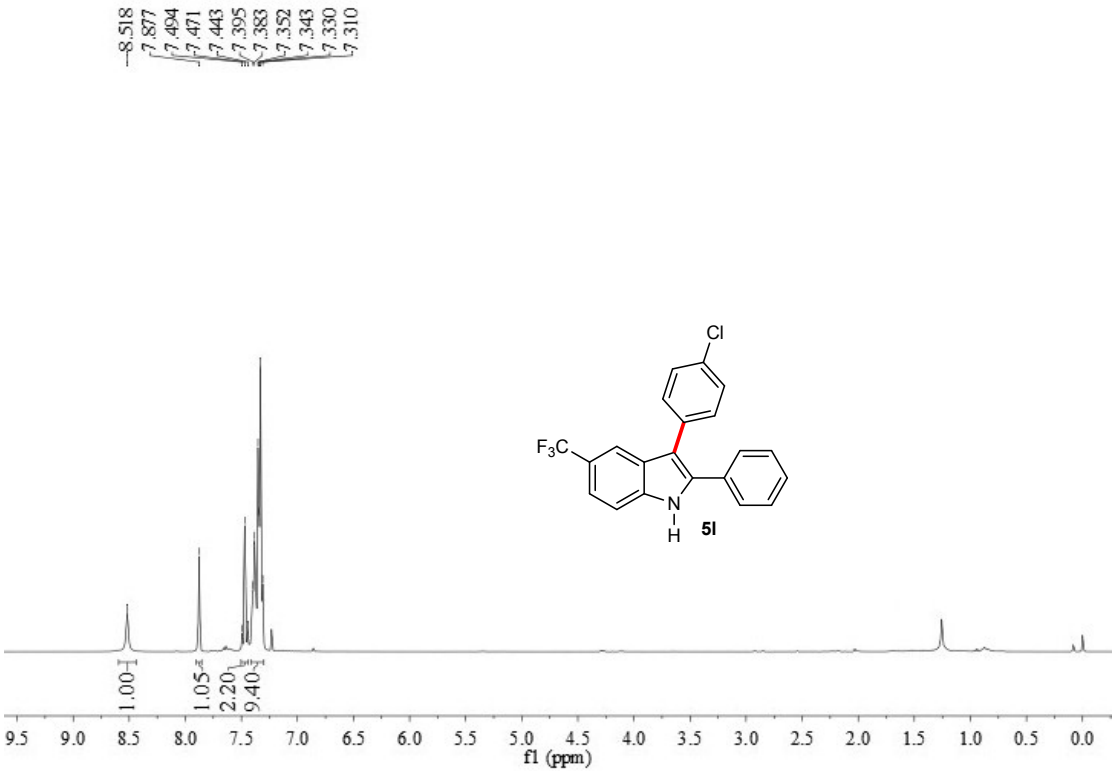
128.942
128.911
128.286
128.171
126.403
123.131
118.857
113.485
112.035
Cl
Cl
N
H
5k
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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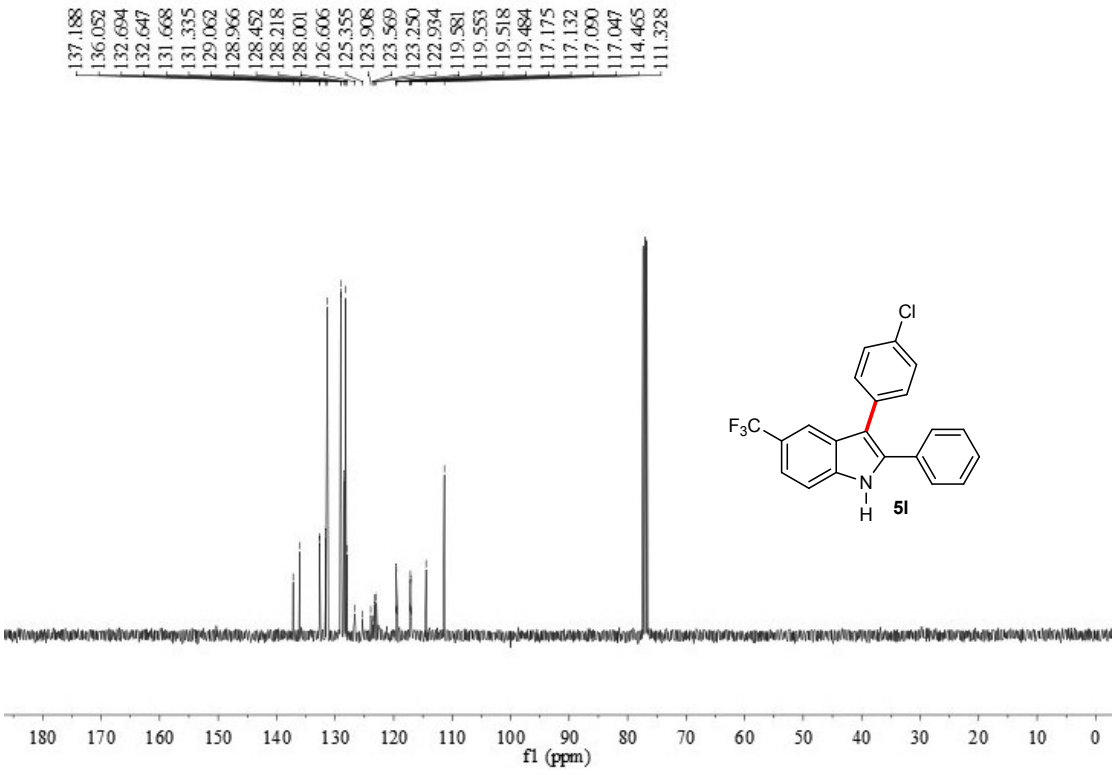
7.494
7.471
7.443
7.395
7.383
7.352
7.343
7.330
7.310
Cl
F3C
N
H
5l
1.00
1.05
2.20
9.40
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.218
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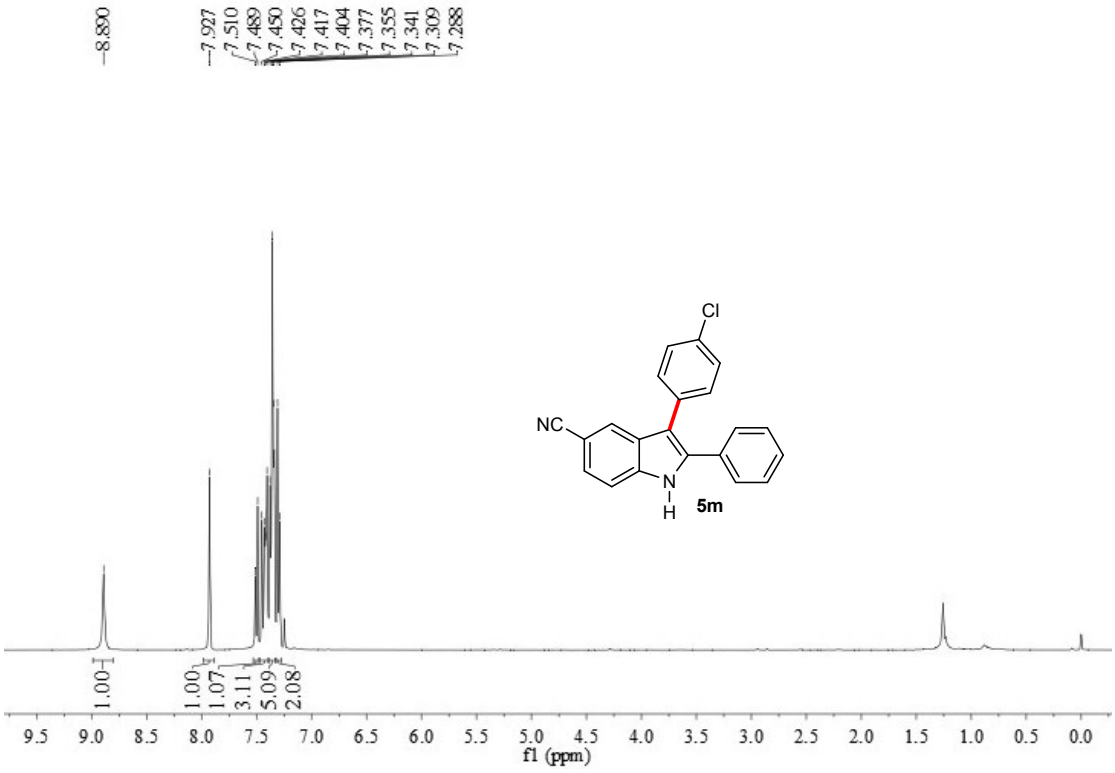
125.355
123.908
123.569
123.250
122.934
119.581
119.553
119.518
119.484
117.175
117.132
117.090
117.047
114.465
111.328
Cl
F3C
N
H
5l
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.404
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7.355
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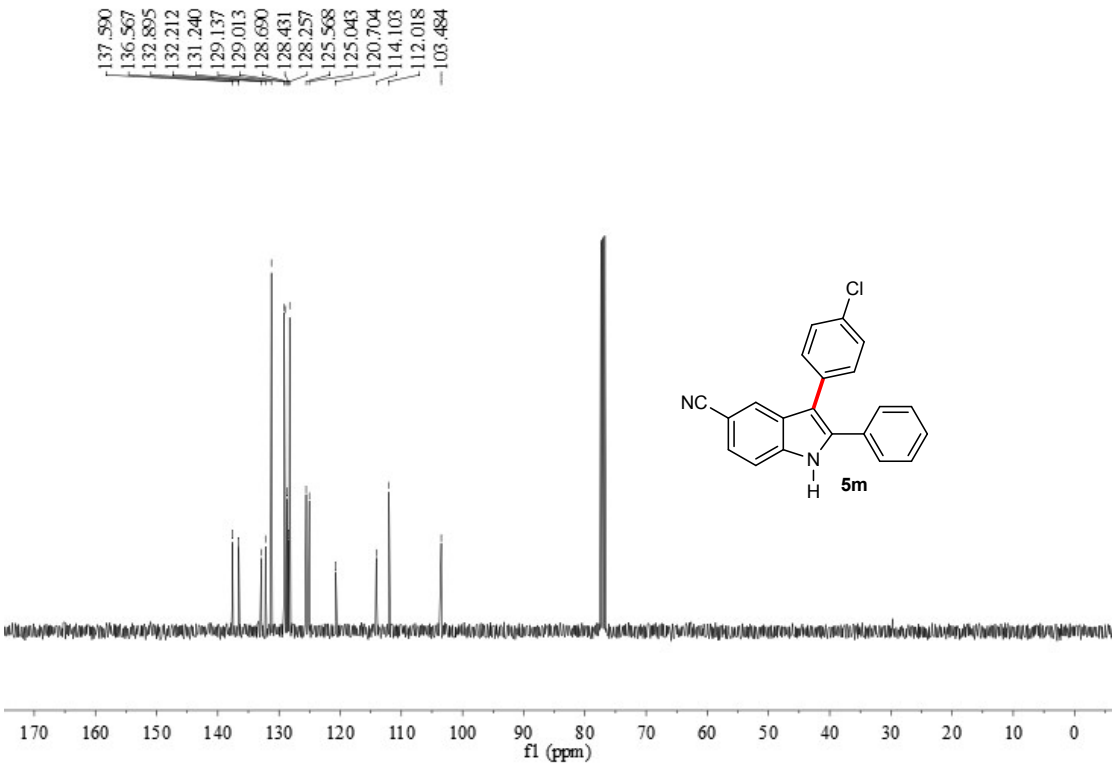
7.309
7.288
Cl
NC
N
H
5m
1.00
1.00
1.07
3.11
5.09
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.043
120.704
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103.484
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N
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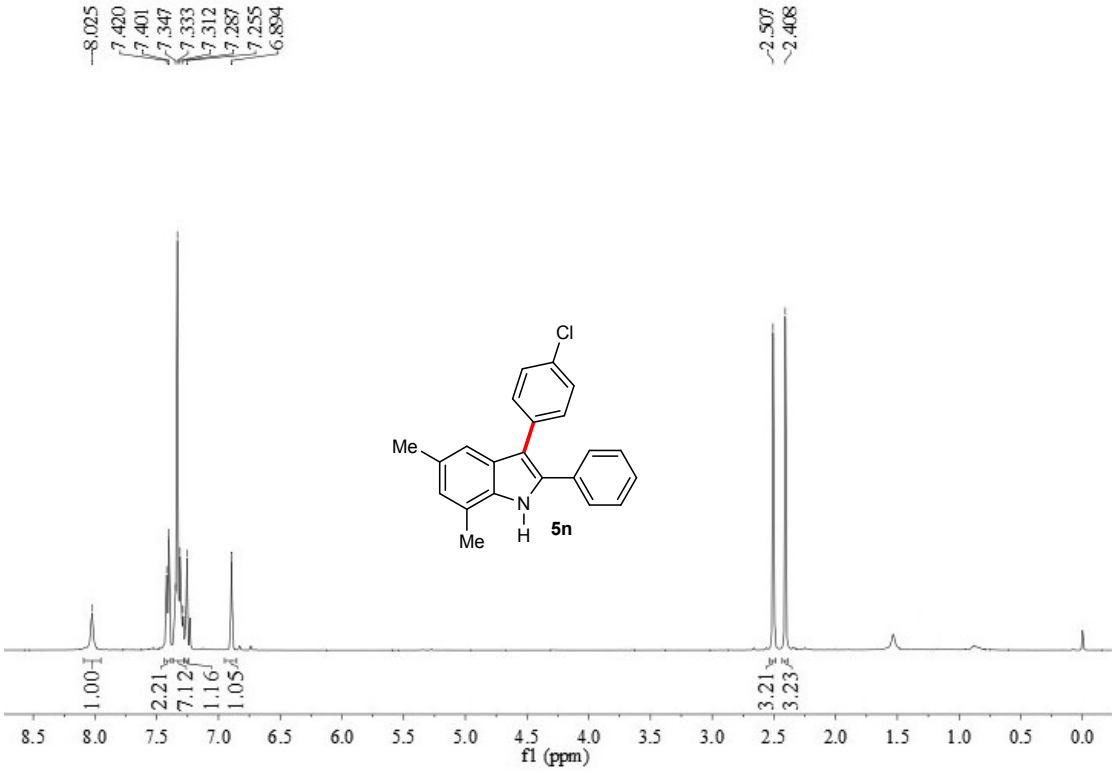
5m
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.025
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7.347
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7.312
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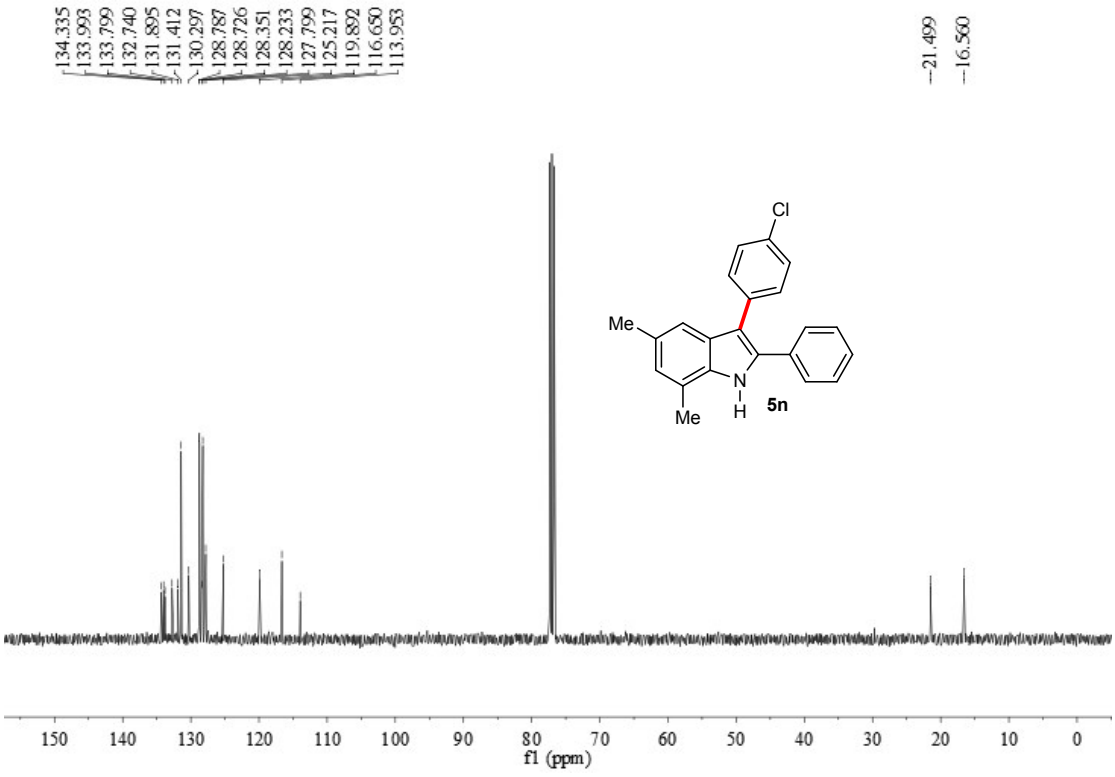
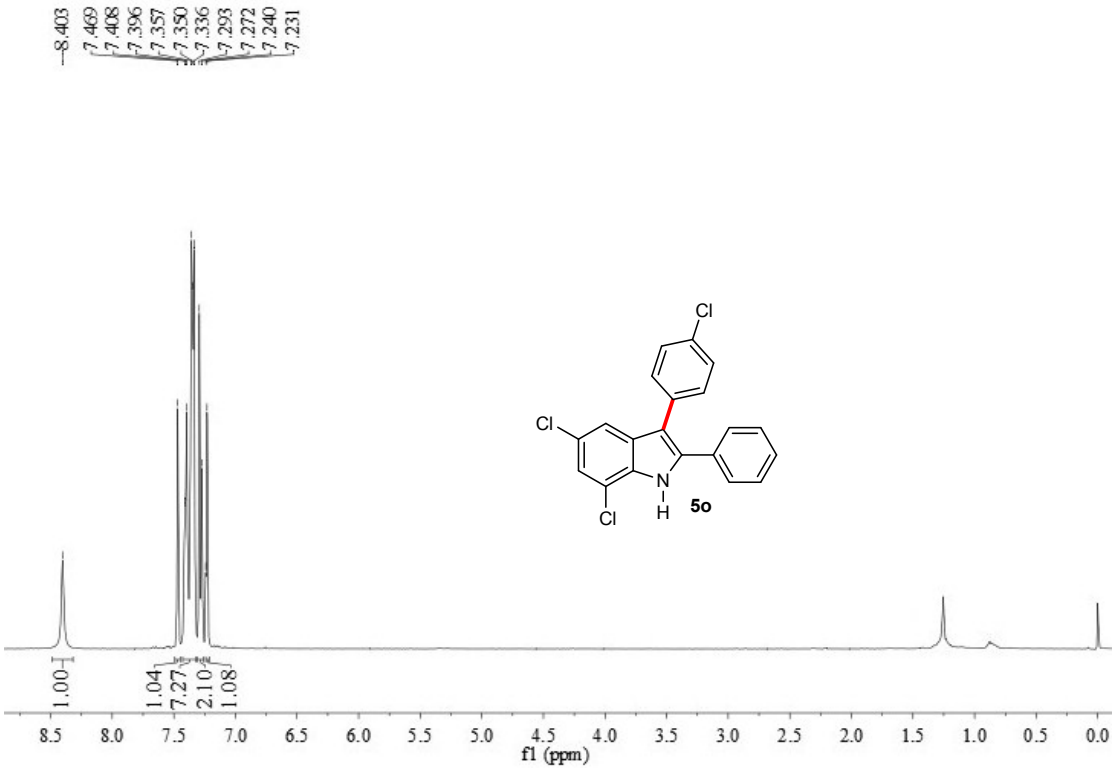
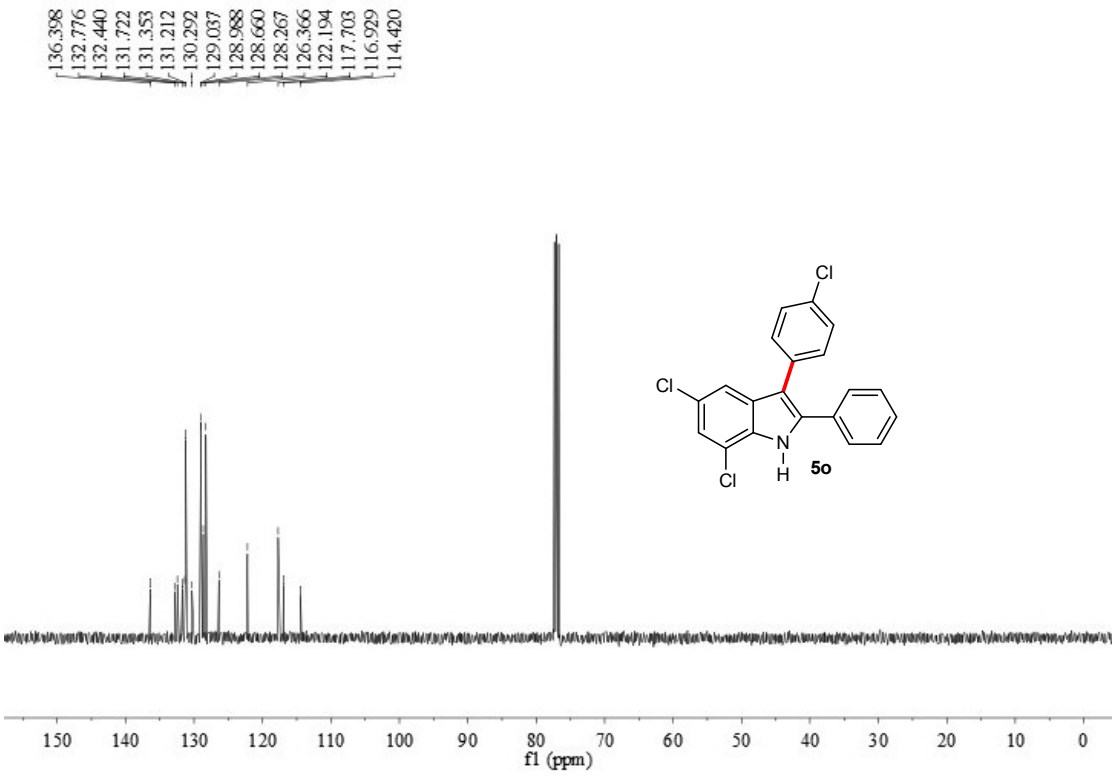
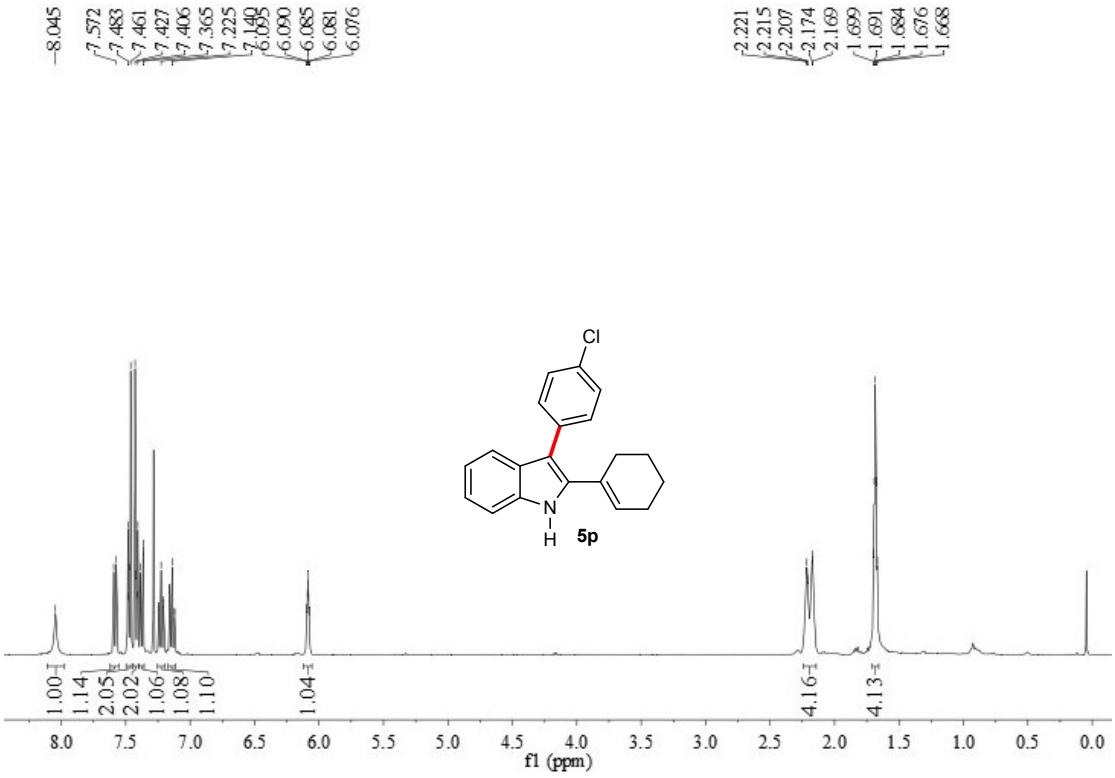
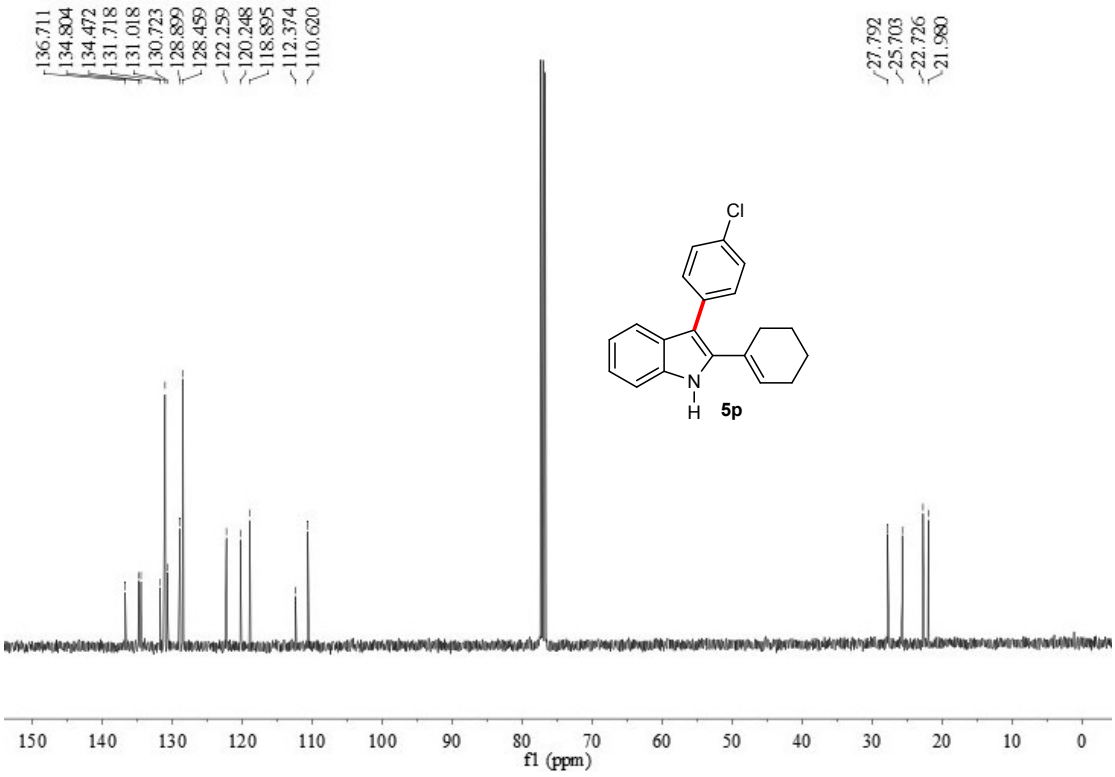
7.255
6.894
2.507
2.408
Cl
Me
N
H
Me
5n
1.00
2.21
7.12
1.16
1.05
3.21
3.23
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

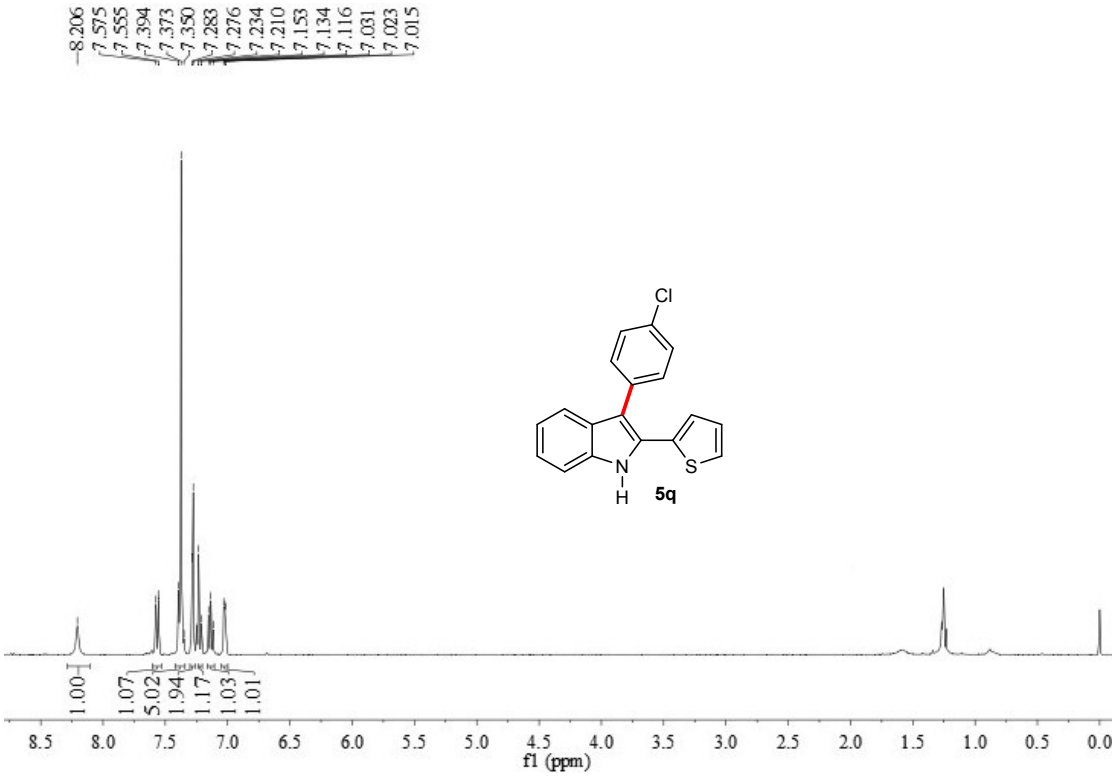

134.335
133.993
133.799
132.740
131.895
131.412
130.297
128.787
128.726
128.351
128.233
127.799
125.217
119.892
116.650
113.953
21.499
16.560
Cl
Me
N
H
Me
5n
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

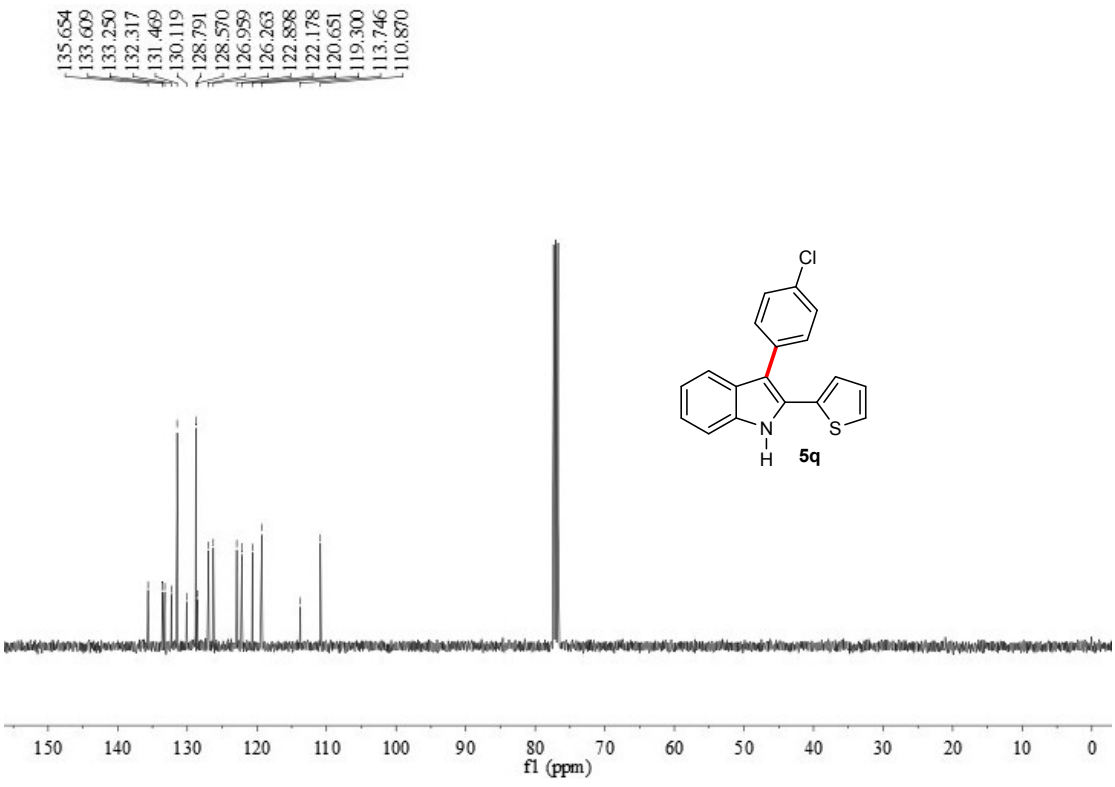

8.403
7.469
7.408
7.396
7.357
7.350
7.336
7.293
7.272
7.240
7.231
Cl
Cl
N
H
Cl
5o
1.00
1.04
7.27
2.10
1.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

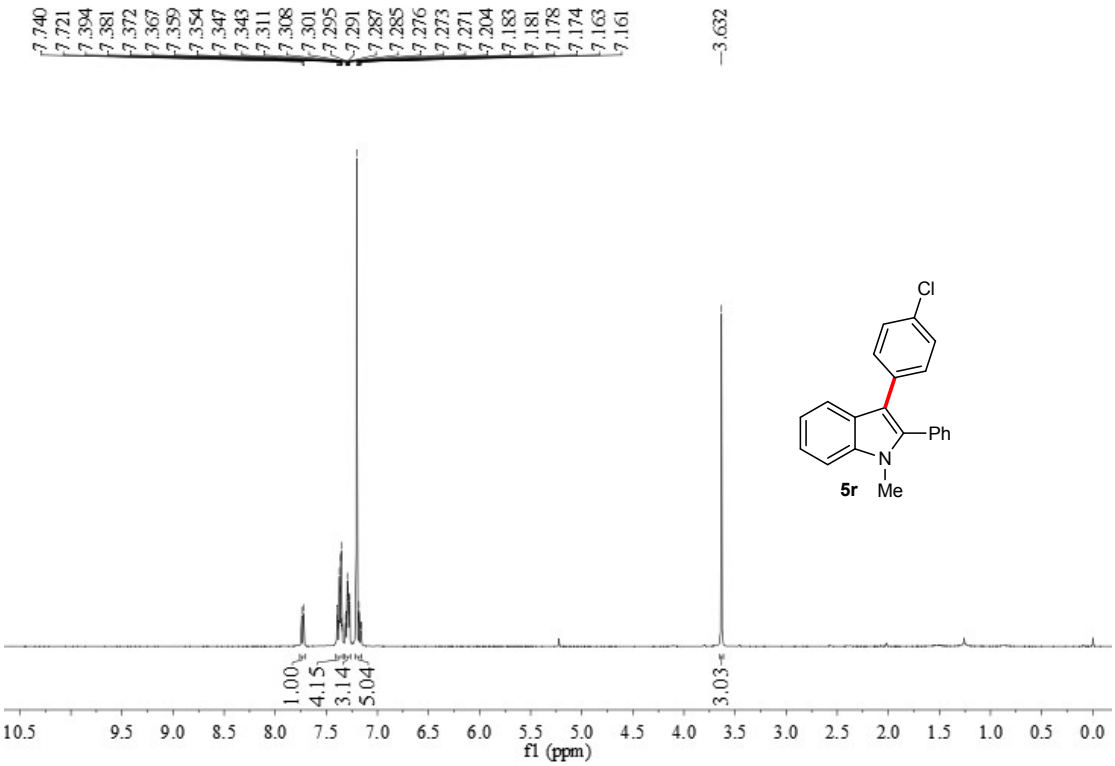

136.398
132.776
132.440
131.722
131.353
131.212
130.292
129.037
128.988
128.660
128.267
126.366
122.194
117.703
116.929
114.420
Cl
Cl
N
H
Cl
5o
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

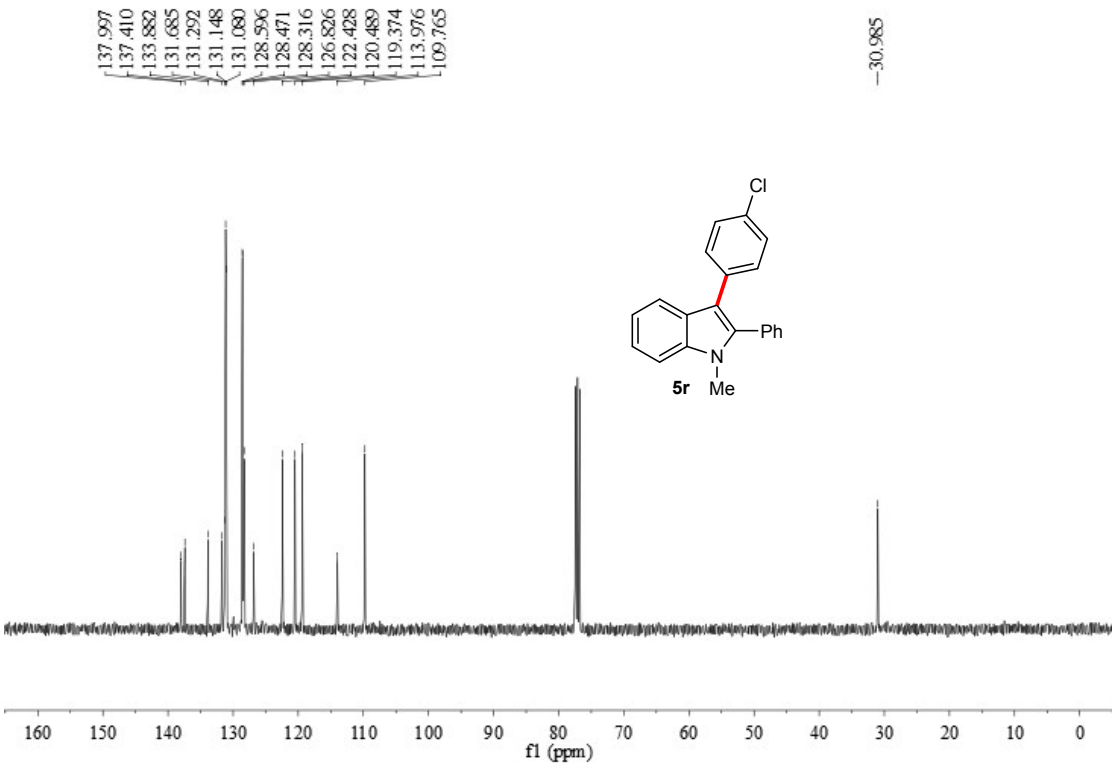

8.045
7.572
7.483
7.461
7.427
7.406
7.365
7.225
7.140
6.095
6.090
6.085
6.081
6.076
2.221
2.215
2.207
2.174
2.169
1.699
1.691
1.684
1.676
1.668
Cl
N
H
5p
1.00
1.14
2.05
2.02
1.06
1.08
1.10
1.04
4.16
4.13
f1 (ppm)

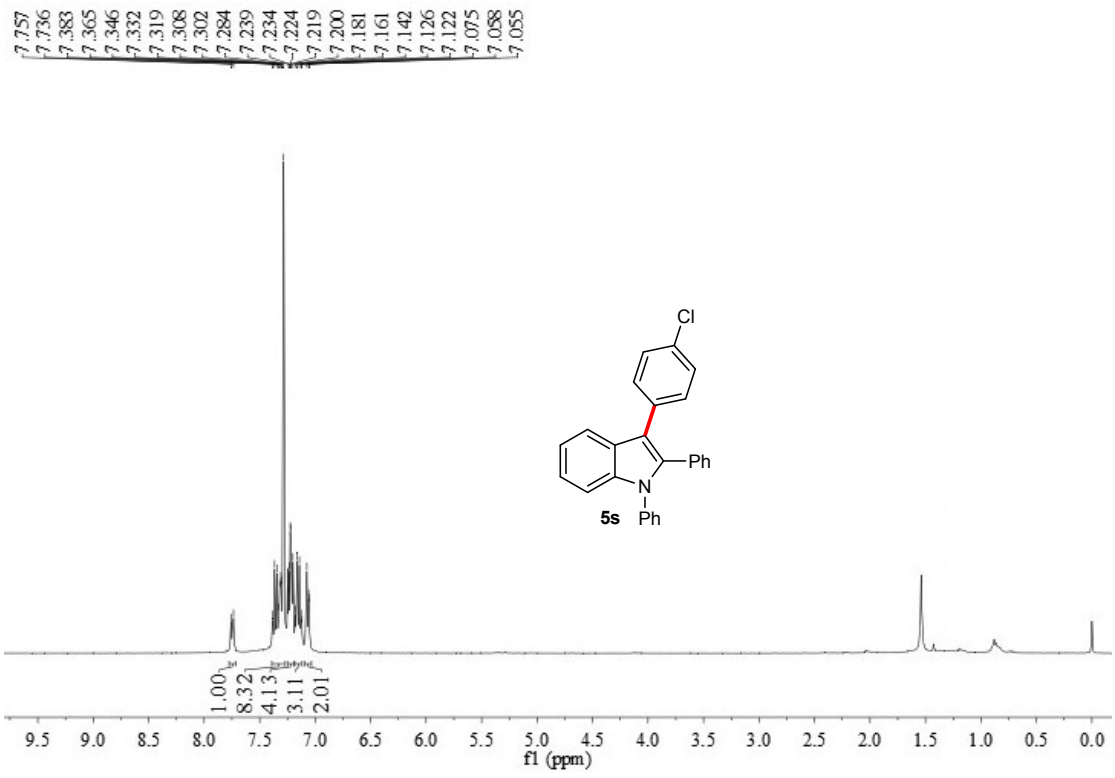

136.711
134.804
134.472
131.718
131.018
130.723
128.899
128.459
122.259
120.248
118.895
112.374
110.620
27.792
25.703
22.726
21.980
Cl
N
H
5p
f1 (ppm)

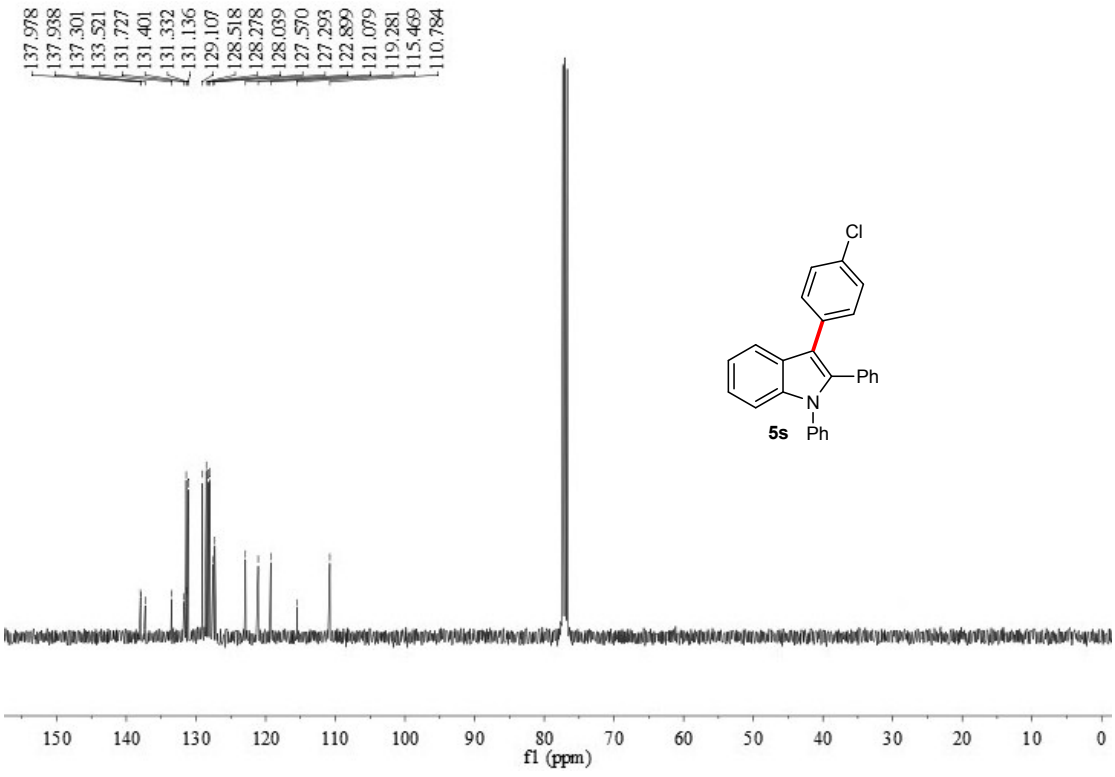

8.206
7.575
7.555
7.394
7.373
7.350
7.283
7.276
7.234
7.210
7.153
7.134
7.116
7.031
7.023
7.015
Cl
N
H
S
5q
1.00
1.07
5.02
1.94
1.17
1.03
1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

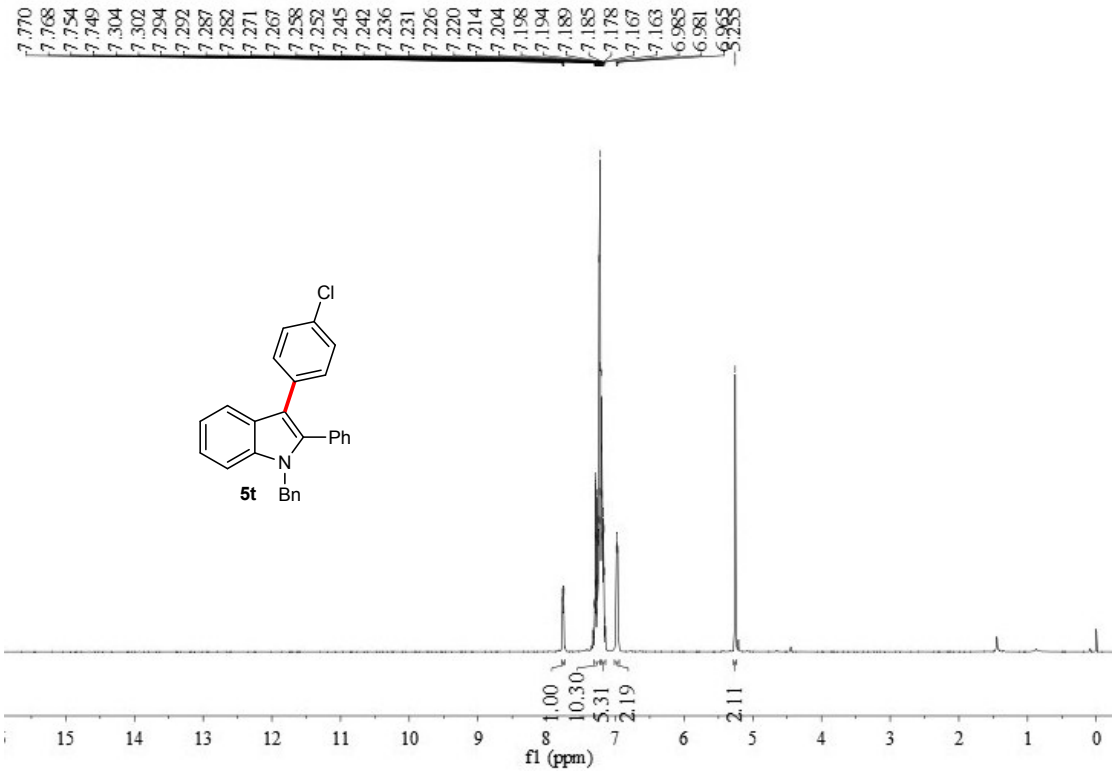

135.654
133.609
133.250
132.317
131.469
130.119
128.791
128.570
126.959
126.263
122.898
122.178
120.651
119.300
113.746
110.870
Cl
N
H
S
5q
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

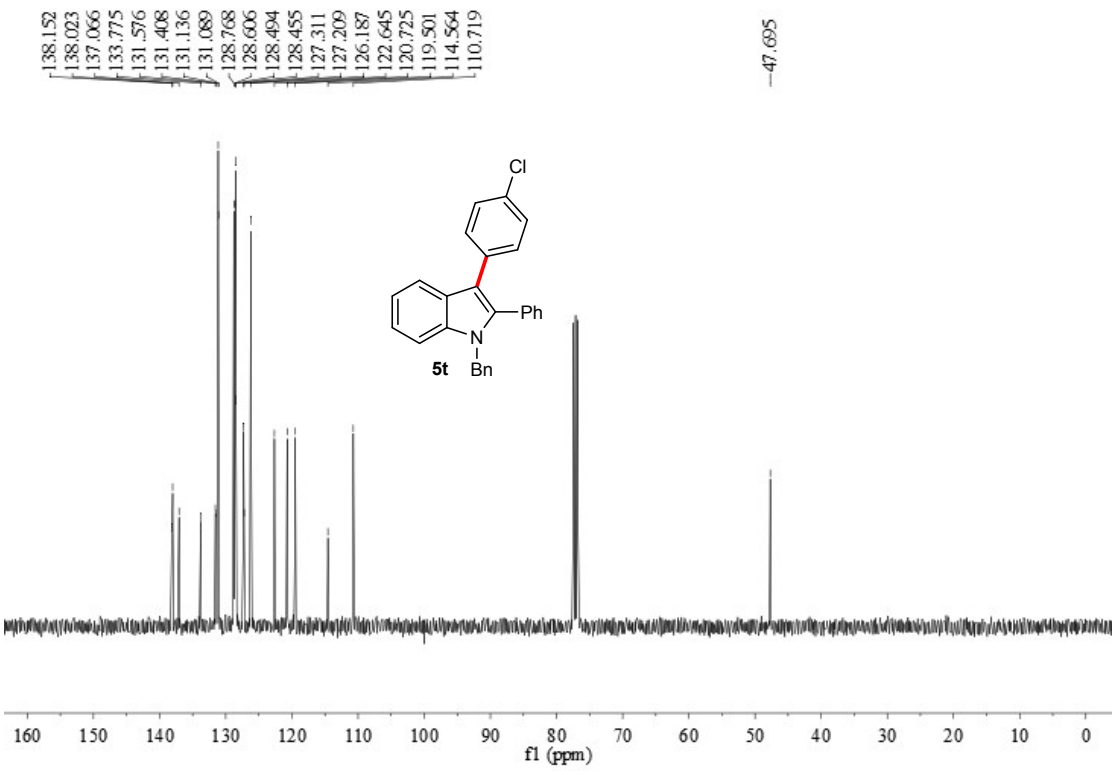

7.740
7.721
7.394
7.381
7.372
7.367
7.359
7.354
7.347
7.343
7.311
7.308
7.301
7.295
7.291
7.287
7.285
7.276
7.273
7.271
7.204
7.183
7.181
7.178
7.174
7.163
7.161
3.632
Cl
Ph
N
Me
5r
1.00
4.15
3.14
5.04
3.03
f1 (ppm)

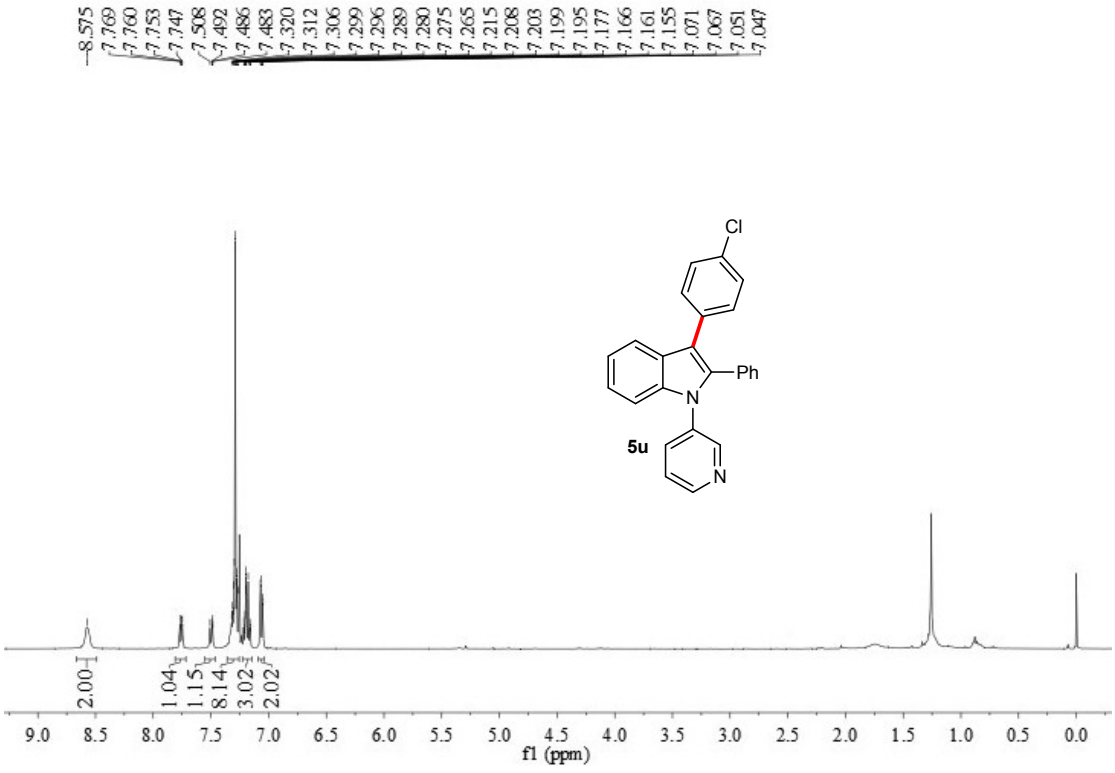

137.997
137.410
133.882
131.685
131.292
131.148
131.080
128.596
128.471
128.316
126.826
122.428
120.489
119.374
113.976
109.765
30.985
Cl
Ph
N
Me
5r
f1 (ppm)

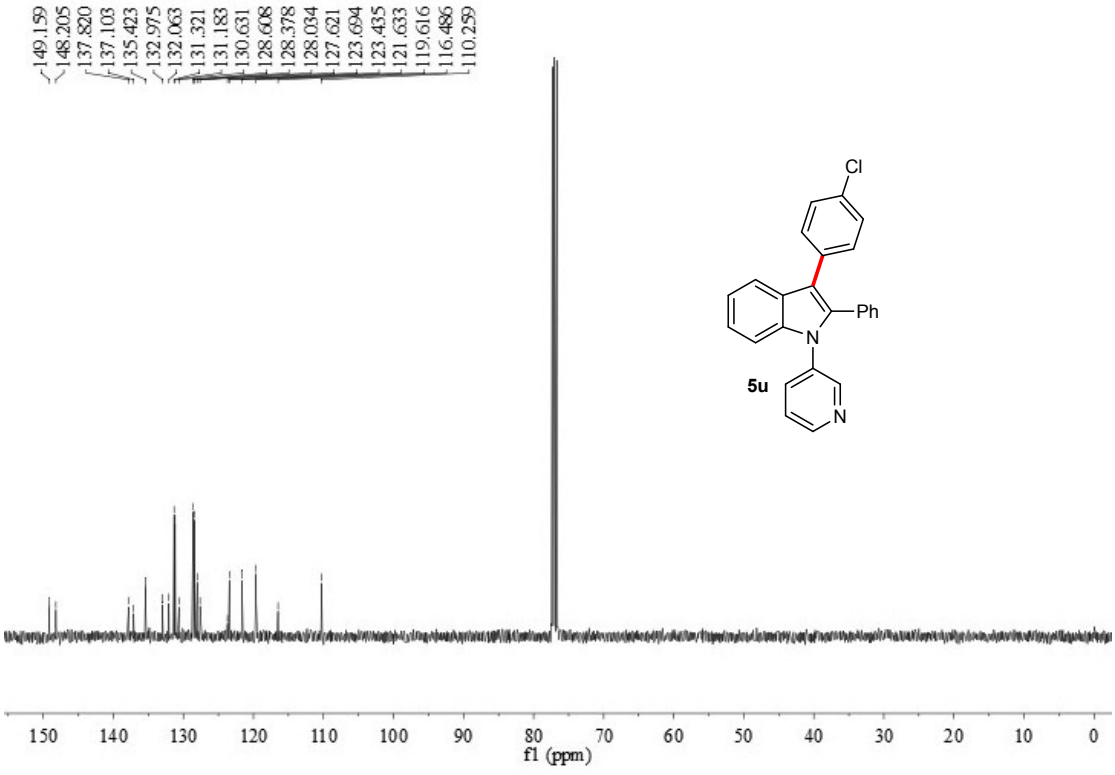

7.757
7.736
7.383
7.365
7.346
7.332
7.319
7.308
7.302
7.284
7.239
7.234
7.224
7.219
7.200
7.181
7.161
7.142
7.126
7.122
7.075
7.058
7.055
Cl
Ph
N
Ph
5s
1.00
8.32
4.13
3.11
2.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.978
137.938
137.301
133.521
131.727
131.401
131.332
131.136
129.107
128.518
128.278
128.039
127.570
127.293
122.899
121.079
119.281
115.469
110.784
Cl
Ph
N
Ph
5s
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

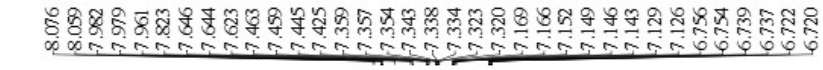

7.770
7.768
7.754
7.749
7.304
7.302
7.294
7.292
7.287
7.282
7.271
7.267
7.258
7.252
7.245
7.242
7.236
7.231
7.226
7.220
7.214
7.204
7.198
7.194
7.189
7.185
7.178
7.167
7.163
6.985
6.981
6.965
5.255
Cl
Ph
N
Bn
5t
1.00
10.30
5.31
2.19
2.11
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

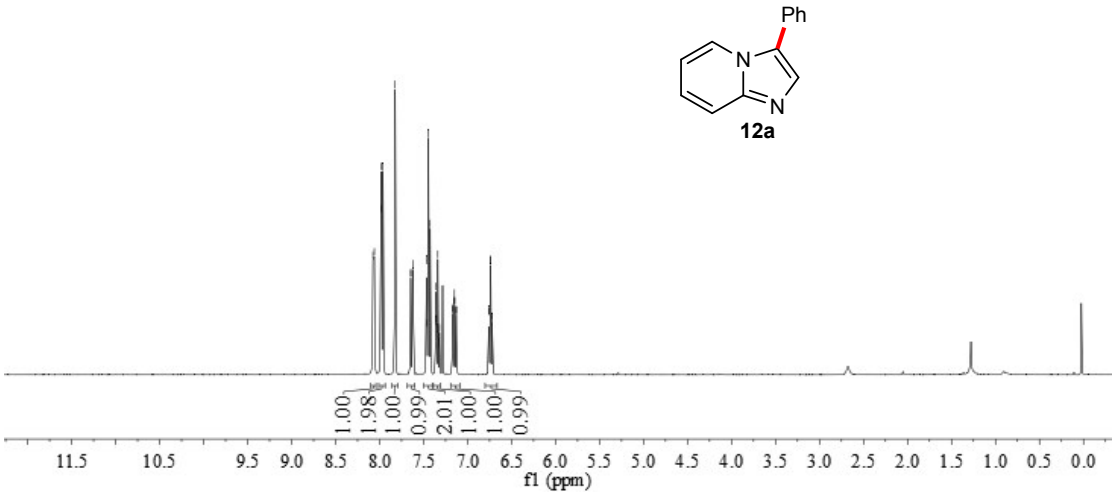

138.152
138.023
137.066
133.775
131.576
131.408
131.136
131.089
128.768
128.606
128.494
128.455
127.311
127.209
126.187
122.645
120.725
119.501
114.564
110.719
47.695
Cl
Ph
N
Bn
5t
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

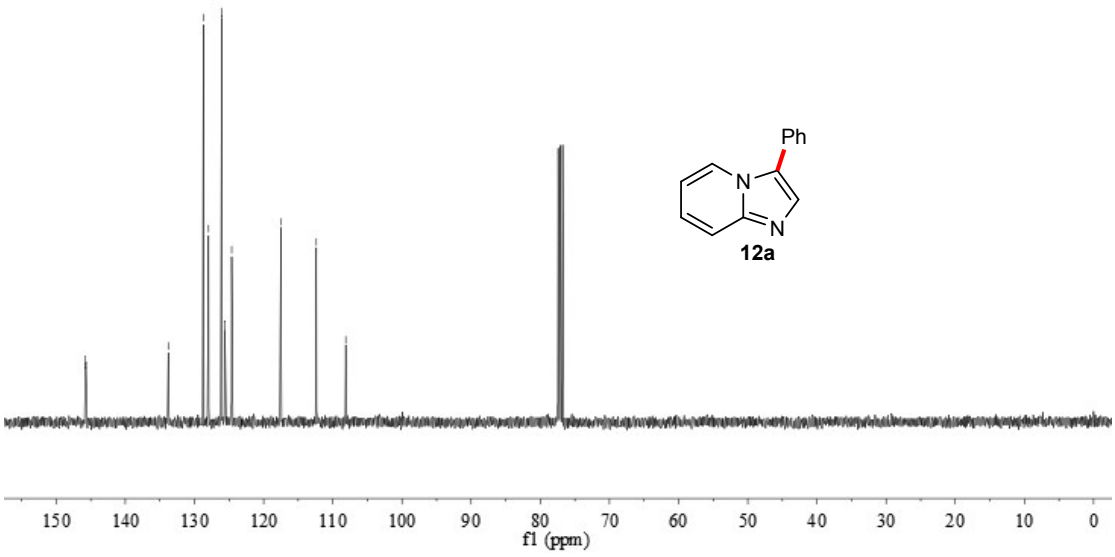

8.575
7.769
7.760
7.753
7.747
7.508
7.492
7.486
7.483
7.320
7.312
7.306
7.299
7.296
7.289
7.280
7.275
7.265
7.215
7.208
7.203
7.199
7.195
7.177
7.166
7.161
7.155
7.071
7.067
7.051
7.047
Cl
Ph
N
5u
N
2.00
1.04
1.15
8.14
3.02
2.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

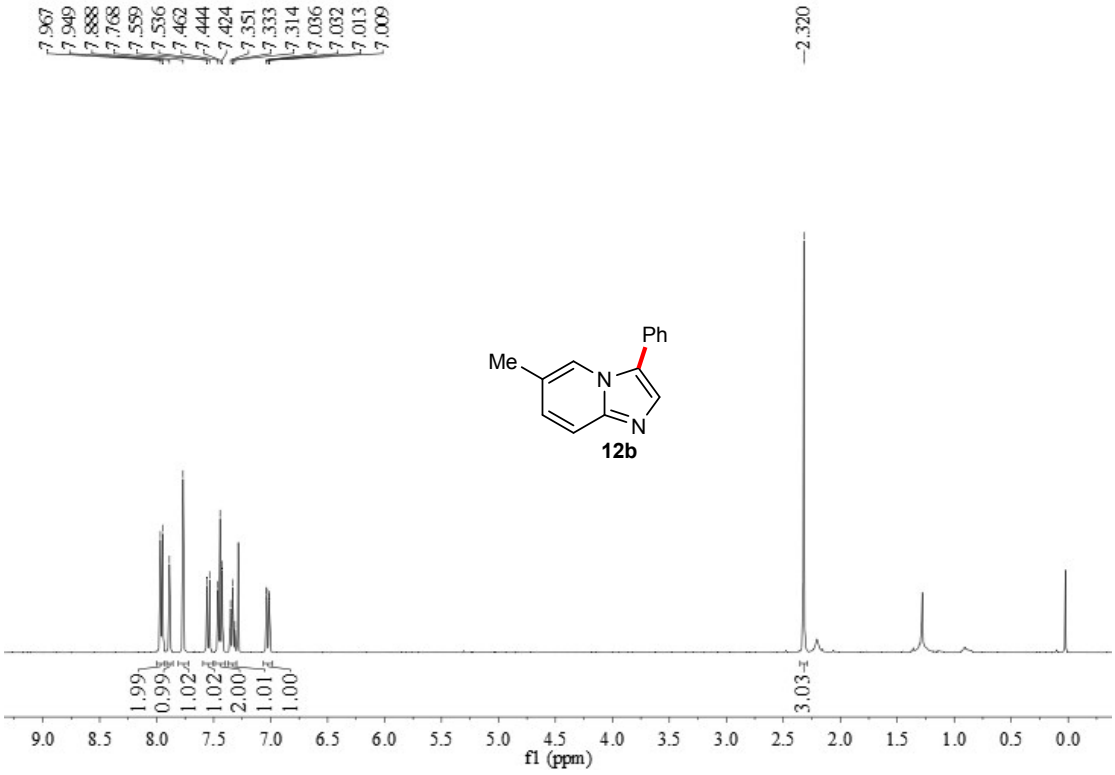

149.159
148.205
137.820
137.103
135.423
132.975
132.063
131.321
131.183
130.631
128.608
128.378
128.034
127.621
123.694
123.435
121.633
119.616
116.486
110.259
Cl
Ph
N
5u
N
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

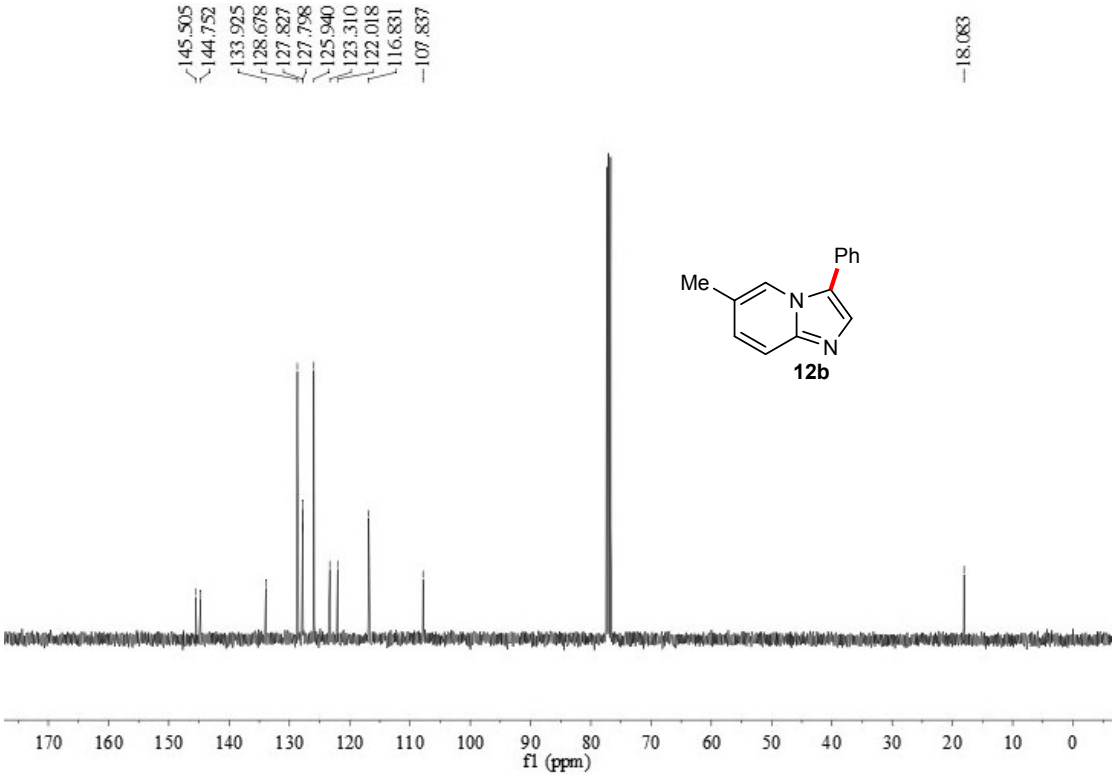
^{1}H and ^{13}C NMR spectra of compounds 12








7.967
7.949
7.888
7.768
7.559
7.536
7.462
7.444
7.424
7.351
7.333
7.314
7.036
7.032
7.013
7.009
2.320
Me
Ph
N
N
12b
1.99
0.99
1.02
1.02
2.00
1.01
1.00
3.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


145.505
144.752
133.925
128.678
127.827
127.798
125.940
123.310
122.018
116.831
107.837
18.083
Me
Ph
N
N
12b
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)