SUPPORTING INFORMATION

Facile synthesis of 4- and 7-azaindoles from corresponding imines by palladium-catalyzed cascade C-C and C-N coupling

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1. General information

Hexane, ethyl acetate and dichloromethane were dried and distilled using standard methods. Molecular sieves were dried in the oven at 300 °C for 12 hours. Other chemicals and solvents, if not otherwise cited, are commercially available and were used without further purification. Column chromatography was performed using normal silica gel with particle size from 0.006 to 0.043 mm.

NMR measurements were carried out with Bruker AVANCE 250 II (built 2006), Bruker AVANCE 300 III (built 2007) and Bruker AVANCE 500 (built 2001) spectrometers. NMR peaks were adjusted according to the standard ^{1}H- and ^{13}C-NMR signals of $CDCl_3$ at 7.260 and 77.160 ppm, respectively. For multiplicity description, abbreviations s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and dd (doublet doublet) were used.

IR measurements were recorded on a Nicolet 380 FT-IR spectrometer using ATR sampling technique for both liquids and solids. To report peaks, abbreviations w (weak), m (medium) and s (strong) were used.

GC/MS measurements were conducted on a Finnigan MAT 95-XP device with HP-5 capillary column using helium carrier gas and using electron ionization (EI) scan technique.

Yield calculation via ^{1}H-NMR technique was carried out using dimethyl sulfone as internal standard.

2. General synthetic procedure

2.1. Imine synthesis

A mixture of ketone (10.0 mmol), amine (10.0 mmol), $NaHCO_3$ (4.20 g) and molecular sieve 4Å (8.00 g) in dried toluene (10.0 ml) in a flask was heated to 80 °C or refluxed for 12 hours overnight. The reaction was controlled on the next day for completion by TLC. After completion, the mixture was taken up in dichloromethane and filtered through zeolite. The solvents were evaporated under reduced pressure. The products were purified by recrystallization in heptane/ethyl acetate mixture or by Kugelrohr distillation under reduced pressure.

2.2. General procedure for 4-azaindole synthesis

2-Bromo-3-chloropyridine **1b** (0.3 mmol), imine **2a** – **2o** (0.33 mmol), $Pd(OAc)_2$ (0.018 mmol), PCy_3 (0.036 mmol) and NaO*t*Bu (0.84 mmol) were put into a dried pressure tube. The tube was then evacuated and backfilled three times with argon. Dioxane (6 ml) was added to

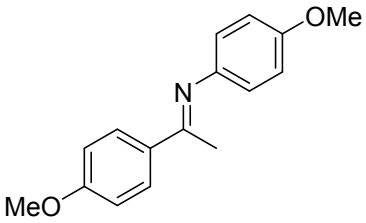
the tube, evacuated and backfilled three times again. The reaction mixture was sealed and stirred in 10 minutes under room temperature and was subsequently heated at 105 °C for 16 – 48 hours. The reaction was controlled by TLC for completion. After that, it was cooled down to room temperature, taken up in dichloromethane and filtered through zeolite. The solvent was removed by evaporation *in vacuo*. The residue was put into column chromatography using the elute mixture heptane/ethyl acetate.

2.3. General procedure for 7-azaindole synthesis

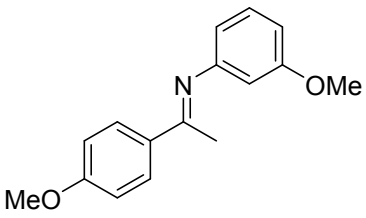
2-Bromo-3-chloropyridine **1c** (0.3 mmol), imine **2a** – **2o** (0.33 mmol), $Pd(OAc)_2$ (0.018 mmol), PCy_3 (0.036 mmol) and NaO*t*Bu (0.84 mmol) were put into a dried pressure tube. The tube was then evacuated and backfilled with argon. Dioxane (6 ml) was added to the tube, evacuated and backfilled again. The reaction mixture was sealed and stirred in 10 minutes under room temperature and subsequently 16 – 48 hours at 105 °C. The reaction was controlled by TLC for completion. After that, it was cooled down to room temperature, taken up in dichloromethane and filtered through zeolite. The solvent was removed by evaporation *in vacuo*. The residue was put into column chromatography using the elute mixture heptane/ethyl acetate.

3. Product characterization

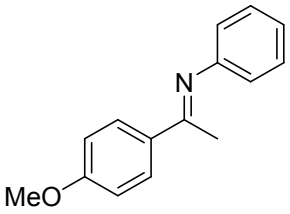
3.1. Imines



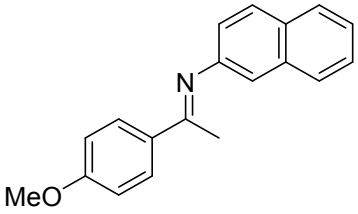
N,1-bis(4-methoxyphenyl)ethan-1-imine (2a): ^{1}H NMR (250 MHz, CDCl3) δ 8.03 – 7.85 (m, 2H), 7.00 – 6.84 (m, 4H), 6.80 – 6.71 (m, 2H), 3.87 (s, 3H), 3.82 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 165.1, 161.7, 156.1, 145.5, 132.7, 129.0 (2C), 121.2 (2C), 114.4 (2C), 113.8 (2C), 55.6, 55.5, 17.3. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[1]



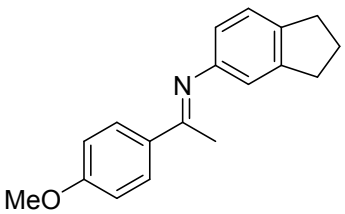
N-(3-methoxyphenyl)-1-(4-methoxyphenyl)ethan-1-imine (2b): ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.04 – 7.85 (m, 2H), 7.34 – 7.17 (m, 1H), 7.00 – 6.89 (m, 2H), 6.69 – 6.58 (m, 1H), 6.48 – 6.33 (m, 2H), 3.87 (s, 3H), 3.80 (d, J = 3.6 Hz, 3H), 2.22 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 165.1, 161.8, 160.4, 153.1, 130.7, 129.9, 129.1 (2C), 113.8 (2C), 112.2, 109.0, 105.5, 55.6, 55.4, 17.4. ^{1}H-NMR spectral data is in accordance with the literature.[2]



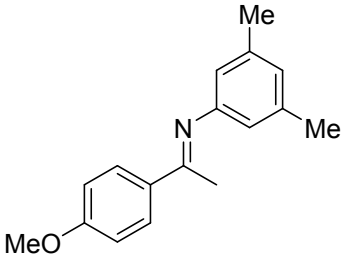
1-(4-methoxyphenyl)-N-phenylethan-1-imine (2c): ^{1}H NMR (250 MHz, CDCl3) δ 7.95 (d, J = 9.0 Hz, 2H), 7.42 – 7.29 (m, 2H), 7.12 – 7.02 (m, 1H), 7.01 – 6.90 (m, 2H), 6.80 (dd, J = 8.4, 1.2 Hz, 2H), 3.87 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 164.7, 161.7, 152.0, 132.3, 129.0 (2C), 129.0 (2C), 123.2, 119.7 (2C), 113.7 (2C), 55.5, 17.3. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[3]



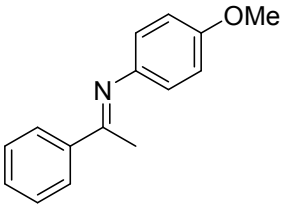
1-(4-methoxyphenyl)-N-(naphthalen-2-yl)ethan-1-imine (2d): Pale yellow crystal, mp. 107 – 108 °C, purified by recrystallization, 61% yield. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.14 – 8.05 (m, 2H), 7.89 – 7.75 (m, 2H), 7.60 (d, J = 8.2 Hz, 1H), 7.53 – 7.35 (m, 3H), 7.06 – 6.97 (m, 2H), 6.79 (dt, J = 4.0, 2.0 Hz, 1H), 3.90 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 166.0, 162.1, 148.3, 134.5, 132.2, 129.4 (2C), 128.3, 126.5, 126.4, 126.2, 125.7, 124.0, 123.4, 114.1, 114.0 (2C), 55.8, 17.8. IR (ATR, cm^{-1}) 3060 (w), 3012 (w), 2975 (w), 2954 (w), 2840 (w), 2050 (w=, 1962 (w), 1913 (w), 1849 (w), 1821 (w), 1788 (w), 1632 (m), 1596 (m), 1504 (m), 1437 (m), 1360 (m), 1307 (m), 1251 (s), 1173 (m), 1024 (m), 960 (m), 838 (s), 777 (s), 572 (m). MS (EI, 70 eV): m/z (%) = 275 (80), $[M]^+$ 276 (16), 261 (20), 260 (100), 217 (20), 127 (64). HRMS (EI): Calculated for $C_{19}H_{17}NO$ $[M]^+$ 275.13047, found 275.13030.



N-(2,3-dihydro-1H-inden-5-yl)-1-(4-methoxyphenyl)ethan-1-imine (2e): Yellow solid, mp. 61 – 62°C, purified by Kugelrohr distillation, 54% yield. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.04 – 7.86 (m, 2H), 7.17 (d, J = 7.9 Hz, 1H), 7.01 – 6.86 (m, 2H), 6.67 (d, J = 1.2 Hz, 1H), 6.61 – 6.48 (m, 1H), 3.87 (s, 3H), 2.90 (t, J = 7.4 Hz, 4H), 2.22 (s, 3H), 2.17 – 2.02 (m, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 161.6, 145.2, 138.9, 132.5, 130.7, 129.0 (2C), 124.6 (2C), 117.7, 115.9, 113.7 (2C), 55.5, 33.2, 32.5, 25.77, 17.3. IR (ATR, cm^{-1}) 3093 (w), 3015 (w), 2967 (w), 2931 (m), 2841 (m), 2062 (w), 2051 (w), 1983 (w), 1923 (w), 1671 (w), 1628 (m), 1598 (s), 1507 (m), 1483 (m), 1444 (m), 1364 (m), 1304 (m), 1255 (s), 1234 (m), 1173 (s), 1118 (m), 1027 (s), 839 (s), 832 (s), 573 (s). MS (EI, 70 eV): m/z (%) = 265 (47), $[M]^+$ 266 (9), 250 (100), 115 (30), 91 (13). HRMS (EI): Calculated for $C_{18}H_{19}ON$ $[M]^+$ 265.14612, found 265.14612.

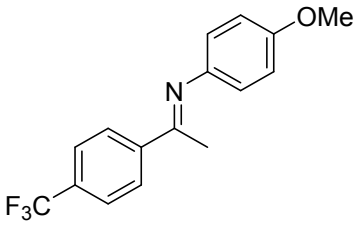


N-(3,5-dimethylphenyl)-1-(4-methoxyphenyl)ethan-1-imine (2f): Yellow solid, mp. 74 – 75 °C, purified by Kugelrohr distillation, 54% yield. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.08 – 7.85 (m, 2H), 7.04 – 6.88 (m, 2H), 6.72 (s, 1H), 6.42 (s, 2H), 3.87 (s, 3H), 2.31 (s, 6H), 2.26 – 2.17 (m, 3H). 13C NMR (63 MHz, CDCl3) δ 164.4, 161.6 (2C), 151.9, 138.6, 132.4, 130.7, 128.9 (2C), 124.8, 117.4 (2C), 113.7 (2C), 55.5, 21.5, 17.31. IR (ATR, cm^{-1}) 3005 (w), 2959 (w), 2913 (m), 2838 (w), 2732 (w), 2052 (w), 1910 (w), 1626 (m), 1590 (s), 1509 (m), 1454 (m), 1366 (m), 1308 (m), 1251 (s), 1171 (m), 1028 (s), 829 (s), 689 (m), 571 (s). MS (EI, 70 eV): m/z (%) = 253 (51), $[M]^+$ 254 (10), 239 (21), 238 (100), 105 (13), 77 (17). HRMS (EI): Calculated for $C_{17}H_{19}ON$ $[M]^+$ 253.14612, found 253.14642.

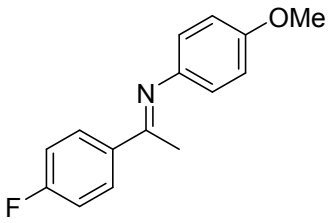


N-(4-methoxyphenyl)-1-phenylethan-1-imine (2g): ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.02 – 7.91 (m, 2H), 7.49 – 7.37 (m, 3H), 6.97 – 6.85 (m, 2H), 6.81 – 6.71 (m, 2H), 3.82 (s, 3H), 2.26 (s, 3H). 13C NMR (63 MHz, $CDCl_3$) δ 166.0, 156.1, 144.9, 139.9, 130.5, 128.5 (2C),

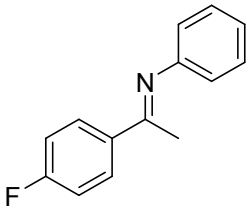
127.3 (2C), 120.9 (2C), 114.4 (2C), 55.9, 17.5. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[4]



N-(4-methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)ethan-1-imine (2h): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, J = 8.1 Hz, 2H), 7.69 (d, J = 8.2 Hz, 2H), 6.93 (dd, J = 9.3, 2.7 Hz, 2H), 6.83 – 6.66 (m, 2H), 3.83 (s, 3H), 2.28 (s, 3H). 19F NMR (282 MHz, $CDCl_3$) δ -62.7. 13C NMR (63 MHz, CDCl3): δ 164.4, 156.3, 144.1, 142.9, 131.9 (q, J = 32.4 Hz), 127.5 (2C), 125.4 (q, J = 3.8 Hz) (2C), 124.1 (q, J = 269.9 Hz), 120.7 (2C), 114.3 (2C), 55.5, 17.4. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[5]

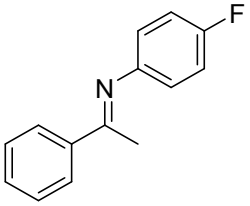


1-(4-fluorophenyl)-N-(4-methoxyphenyl)ethan-1-imine (2i): Orange solid, mp. 66 – 67 °C, purified by Kugelrohr distillation, 51% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.92 (m, 2H), 7.17 – 7.05 (m, 2H), 6.96 – 6.86 (m, 2H), 6.79 – 6.69 (m, 2H), 3.82 (s, 3H), 2.24 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -110.7. 13C NMR (126 MHz, $CDCl_3$) δ 164.5, 164.4 (d, J = 250.4 Hz), 156.2, 144.8, 136.1 (d, J = 3.1 Hz), 129.3 (d, J = 8.6 Hz) (2C), 120.9 (2C), 115.4 (d, J = 21.6 Hz) (2C), 114.4 (2C), 55.7, 17.4. ^{1}H- and ^{19}F-NMR spectral data are in accordance with the literature.[6]

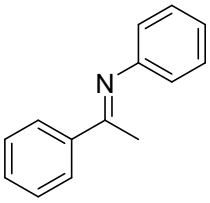


1-(4-fluorophenyl)-N-phenylethan-1-imine (2j): ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.94 (m, 2H), 7.35 (t, J = 7.8 Hz, 2H), 7.21 – 7.05 (m, 3H), 6.84 – 6.76 (m, 2H), 2.22 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -105.34. 13C NMR (75 MHz, $CDCl_3$) δ 164.6 (d, J = 252 Hz),

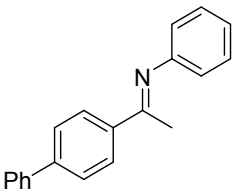
164.5, 152.8, 136.1, 130.2 (d, J = 8.6 Hz), 130.2, 124.6, 120.2, 116.7 (d, J = 21.5 Hz), 17.5. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[7]



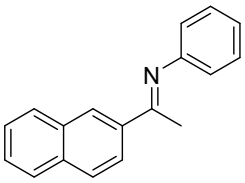
N-(4-fluorophenyl)-1-phenylethan-1-imine (2k): ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.24 (s, 3H), 6.74-6.78 (m, 2H), 7.04-7.08 (m, 2H), 7.43-7.49 (m, 3H), 7.96-7.99 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 159.5 (d, J = 241 Hz), 147.8 (d, J = 2.4 Hz), 139.5, 130.7, 128.4 (2C), 127.3 (2C), 120.8 (d, J = 8.2 Hz) (2C), 115.7 (d, J = 22 Hz) (2C), 17.4. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[3]



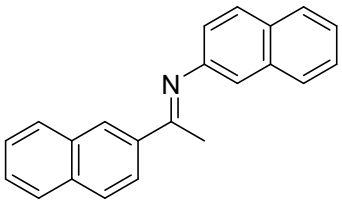
N,1-diphenylethan-1-imine (2l): Yellow solid, mp. 40 – 41 °C, purified by Kugelrohr distillation, 51% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 2H), 7.50 – 7.42 (m, 3H), 7.39 – 7.31 (m, 2H), 7.12 – 7.05 (m, 1H), 6.83 – 6.77 (m, 2H), 2.24 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 165.5, 152.9, 140.3, 131.2, 129.7, 129.0, 128.0, 123.8, 120.0, 17.2. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[4]



1-([1,1'-biphenyl]-4-yl)-N-phenylethan-1-imine (2m): Yellow solid, mp. 136 – 137 °C, purified by recrystallization, 71% yield. ^{1}H NMR (250 MHz, $CDCl_3$, ppm): δ 8.05 (d, J = 8.4 Hz, 2H), 7.68 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.0 Hz, 2H), 7.51-7.42 (m, 2H), 7.40-7.33 (m, 3H), 7.09 (t, J = 7.2 Hz, 1H), 6.81 (d, J = 7.6 Hz, 2H), 2.26 (s, 3H). 13C NMR (63 MHz, $CDCl_3$) δ 165.2, 151.9, 143.3, 140.6, 138.5, 129.1 (2C), 129.0 (2C), 127.9, 127.8 (2C), 127.3 (2C), 127.2 (2C), 123.4, 119.6 (2C), 17.5. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[8]

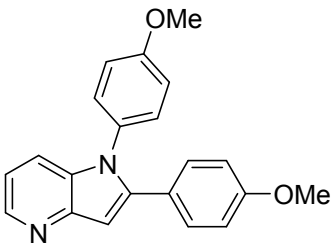


1-(naphthalen-2-yl)-N-phenylethan-1-imine (2n): ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.35 (s, 1H), 8.23 (d, J = 8.8 Hz, 2H), 7.96-7.85 (m, 3H), 7.59-7.48 (m, 2H), 7.38 (dd, J = 7.6 Hz, 7.6 Hz, 2H), 7.12 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 7.6 Hz, 2H), 2.36 (s, 3H). 13C NMR (63 MHz, $CDCl_3$) δ 165.5, 151.8, 137.0, 134.6, 133.1, 129.1 (2C), 129.1, 128.2, 127.8 (2C), 127.3, 126.5, 124.4, 123.5, 119.6 (2C), 17.5. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[7]

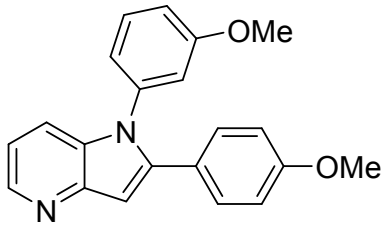


N,1-di(naphthalen-2-yl)ethan-1-imine (2o): Brown crystal, mp. 136 – 137 °C, purified by recrystallization, yield 47%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.41 (dd, J = 8.7, 1.8 Hz, 1H), 8.02 – 7.80 (m, 5H), 7.63 (m, 1H), 7.60 – 7.54 (m, 2H), 7.52 – 7.39 (m, 3H), 6.86 (d, J = 7.2 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.7, 134.8, 134.4, 133.1, 129.7, 129.2, 128.6, 128.3, 128.2, 128.1, 127.9, 127.5, 126.6, 126.3, 126.2, 126.1, 125.6, 124.5, 123.8, 123.6, 113.8, 17.9. IR (ATR, cm^{-1}) 3468 (w), 3397 (w), 3239 (w), 3084 (w), 3050 (m), 3006 (w), 2963 (w), 2852 (w), 2704 (w), 2561 (w), 1938 (w), 1915 (w), 1848 (w), 1690 (w), 1625 (s), 1570 (m), 1504 (m), 1433 (w), 1387 (m), 1366 (m), 1292 (m), 1293 (m), 1223 (m), 1129 (m), 1080 (m), 1014 (m), 858 (m), 802 (m), 777 (s), 747 (m), 868 (m). MS (EI, 70 eV): m/z (%) = 295 (74), $[M]^+$ 296 (17), 281 (23), 280 (100), 153 (15), 127 (67), 126 (29). HRMS (EI): Calculated for $C_{22}H_{17}N$ $[M]^+$ 295.13555, found 295.13563.

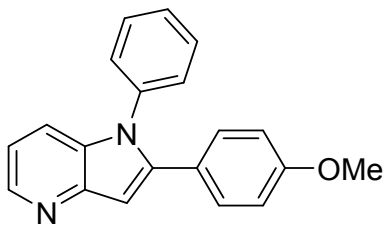
3.2. 4-Azaindoles



1,2-bis(4-methoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (3a): Yellow solid, mp. 188 – 189 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.50 – 7.29 (m, 1H), 7.16 (dt, J = 5.0, 2.8 Hz, 2H), 7.12 – 7.00 (m, 2H), 6.96 (dt, J = 13.7, 6.9 Hz, 1H), 6.87 (dt, J = 5.3, 3.2 Hz, 3H), 6.78 – 6.63 (m, 2H), 3.75 (d, J = 9.0 Hz, 3H), 3.71 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.4, 158.8, 146.5 (2C), 144.2, 143.8, 132.4, 130.3 (2C), 128.9 (2C), 124.2, 117.5, 116.6, 114.6 (2C), 113.8 (2C), 102.9, 55.5, 55.2. IR (ATR, cm^{-1}) 3122 (w), 3076 (w), 2918 (m), 2848 (w), 2045 (w), 1923 (w), 1716 (w), 1608 (m), 1510 (s), 1498 (s), 1458 (m), 1414 (s), 1247 (s), 1186 (m), 1104 (m), 1025 (s), 923 (m), 834 (s), 800 (s), 789 (s), 729 (m), 644 (w), 580 (s). MS (EI, 70 eV): m/z (%) = 330 (100), $[M]^+$ 331 (24), 315 (28), 243 (17). HRMS (EI): Calculated for $C_{21}H_{18}N_2O_2$ $[M+H]^+$ 331.14410, found 331.14419.

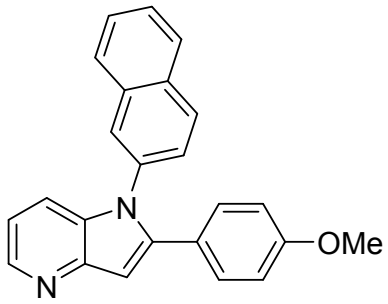


1-(3-methoxyphenyl)-2-(4-methoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (3b): Yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (dd, J = 4.7, 1.3 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.23 (t, J = 8.1 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.97 (dd, J = 8.3, 4.7 Hz, 1H), 6.86 – 6.80 (m, 2H), 6.76 – 6.69 (m, 3H), 6.67 (t, J = 2.2 Hz, 1H), 3.69 (s, 3H), 3.64 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 160.4, 159.6, 146.9, 144.3, 144.0, 138.8, 132.1, 130.4 (2C), 130.2, 124.3, 120.1, 117.6, 116.9, 113.9 (2C), 113.6, 113.4, 103.7, 55.5, 55.3. IR (ATR, cm^{-1}) 3036 (w), 2002 (w), 2933 (w), 2834 (w), 2926 (w), 2034 (w), 1891 (w), 1676 (w), 1588 (s), 1491 (s), 1454 (m), 1411 (s), 1281 (m), 1246 (s), 1172 (s), 1027 (s), 833 (m), 778 (s), 725 (m), 694 (m), 552 (m). MS (EI, 70 eV): m/z (%) = 330 (100), $[M]^+$ 331 (25), 315 (24), 243 (17). HRMS (EI): Calculated for $C_{21}H_{18}O_2N_2$ $[M]^+$ 330.13628, found 330.13602.

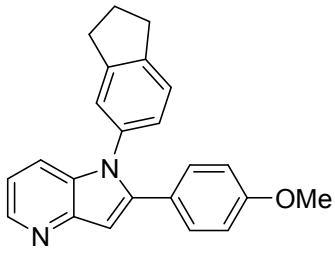


2-(4-methoxyphenyl)-1-phenyl-1H-pyrrolo[3,2-b]pyridine (3c): Yellow solid, mp. 137 – 138 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.43 (d, J = 8.1 Hz, 1H), 7.38 – 7.26 (m, 3H), 7.17 – 7.09 (m, 4H), 6.99 (d, J = 4.6 Hz, 1H), 6.85 (s, 1H), 6.76 – 6.67 (m, 2H), 3.69 (s, 3H). ^{13}C NMR (63 MHz, CDCl3) δ 159.6, 146.8, 144.1, 137.8, 132.2, 130.5 (2C), 129.6 (2C),

127.9 (2C), 127.7, 124.2, 117.6, 116.9, 113.9, 103.6, 55.3. IR (ATR, cm^{-1}) 3117 (w), 3060 (w), 2960 (w), 2834 (w), 1595 (m), 1500 (s), 1414 (s), 1242 (m), 1179 (m), 1023 (m), 834 (m), 782 (s), 700 (s), 598 (m). MS (EI, 70 eV): m/z (%) = 300 (100), $[M]^+$, 301 (23), 285 (39), 255 (27), 128 (10), 77 (10), 51(8). HRMS (EI): Calculated for $C_{20}H_{16}ON_2$ $[M]^+$ 300.12571, found 300.12513

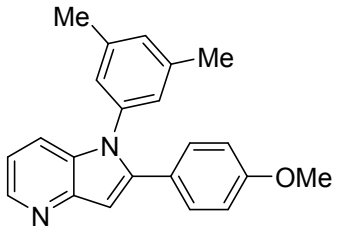


2-(4-methoxyphenyl)-1-(naphthalen-2-yl)-1H-pyrrolo[3,2-b]pyridine (3d): Yellow solid, mp. 140 – 141 °C. ^1H NMR (250 MHz, $CDCl_3$) δ 8.50 (d, J = 3.5 Hz, 1H), 7.94 (d, J = 8.2 Hz, 2H), 7.56 – 7.44 (m, 2H), 7.44 – 7.29 (m, 3H), 7.22 – 7.13 (m, 2H), 7.07 (d, J = 7.2 Hz, 2H), 6.97 (dd, J = 8.3, 4.6 Hz, 1H), 6.66 (d, J = 8.9 Hz, 2H), 3.69 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.6, 146.8, 145.5, 144.1, 134.5, 134.5, 133.4, 131.2, 129.8 (2C), 129.1, 128.6, 127.5, 127.3, 126.88, 125.7, 124.3, 123.2, 118.2, 116.9, 113.9 (2C), 103.1, 55.3. IR (ATR, cm^{-1}) 3048 (w), 2921 (w), 2850 (w), 1607 (m), 1496 (m), 1417 (m), 1251 (s), 1178 (m), 1024 (m), 842 (m), 806 (s), 797 (s), 773 (s), 590 (m), 539 (m). MS (EI, 70 eV): m/z (%) = 350 (100) $[M]^+$ 351 (22), 335 (17), 305 (20), 153 (11). HRMS (EI): Calculated for $C_{24}H_{18}N_2O$ $[M+H]^+$ 351.14919, found 351.14934

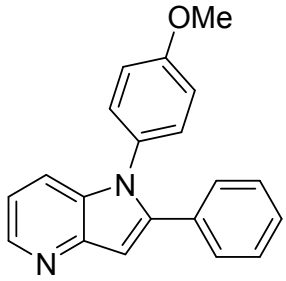


1-(2,3-dihydro-1H-inden-5-yl)-2-(4-methoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (3e): Yellow solid, mp. 51 – 52 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 10.95 – 8.44 (m, 1H), 7.55 – 7.48 (m, 1H), 7.29 (d, J = 1.7 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.10 (s, 1H), 7.06 (dd, J = 8.3, 4.7 Hz, 1H), 6.96 (dd, J = 7.9, 2.0 Hz, 1H), 6.93 (d, J = 0.7 Hz, 1H), 6.86 – 6.80 (m, 2H), 3.81 (s, 3H), 3.05 – 2.86 (m, 4H), 2.20 – 2.08 (m, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.5, 146.8, 145.8, 144.2, 144.1, 144.0, 135.8, 132.5, 130.4 (2C), 125.9, 125.1, 124.5, 123.8, 117.7, 116.7, 113.9 (2C), 103.2, 55.4, 33.0, 32.7, 25.7. IR (ATR, cm^{-1}) 3038 (w), 3005 (w), 2924 (m), 2844

(m), 2197 (w), 2058 (w), 2035 (w), 1889 (w), 1722 (w), 1674 (w), 1068 (m), 1596 (w), 1496 (s), 1412 (s), 1281 (m), 1246 (s), 1174 (s), 1028 (m), 832 (m), 780 (s), 726 (m). MS (EI, 70 eV): m/z (%) = 340 (100), $[M]^+$ 341 (25), 325 (18), 156 (12), 115 (6). HRMS (EI): Calculated for $C_{23}H_{20}ON_2$ $[M]^+$ 340.15701, found 340.15685.

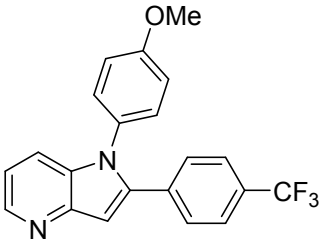


1-(3,5-dimethylphenyl)-2-(4-methoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (3f): Yellow solid, mp. 143 – 144 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (dd, J = 4.7, 1.4 Hz, 1H), 7.41 (dd, J = 8.2, 2.1 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.96 (dd, J = 8.3, 4.7 Hz, 1H), 6.92 (s, 1H), 6.82 (d, J = 0.7 Hz, 1H), 6.76 – 6.72 (m, 3H), 6.72 – 6.69 (m, 1H), 3.70 (s, 3H), 2.22 (s, 6H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.5, 146.9, 144.1, 144.0, 139.3, 137.62, 132.3, 130.4 (2C), 129.5, 125.6 (2C), 124.5, 117.7, 116.7, 113.9 (2C), 103.3, 55.4, 21.4 (2C). IR (ATR, cm^{-1}) 3038 (w), 3008 (w), 2920 (w), 2837 (w), 1610 (m), 1594 (m), 1497 (s), 1413 (s), 1377 (m), 1250 (s), 1177 (m), 1037 (m), 837 (m), 783 (m). MS (EI, 70 eV): m/z (%) = 328 (100), $[M]^+$ 329 (25), 313 (21), 269 (13), 157 (12). HRMS (EI): Calculated for $C_{22}H_{20}ON_2$ $[M]^+$ 328.15701, found 328.15685.

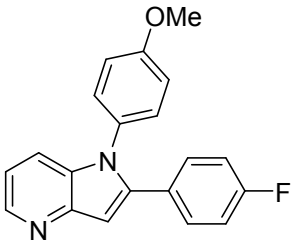


1-(4-methoxyphenyl)-2-phenyl-1H-pyrrolo[3,2-b]pyridine (3g): Yellow solid, mp. 146 – 147 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, J = 4.1 Hz, 1H), 7.50 (d, J = 8.2 Hz, 1H), 7.35 – 7.25 (m, 5H), 7.17 – 7.11 (m, 2H), 7.08 (dd, J = 8.3, 4.6 Hz, 1H), 6.99 (s, 1H), 6.94 (d, J = 8.9 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 158.9, 146.3, 144.2, 143.9, 132.6, 131.7, 130.2, 129.1 (2C), 128.9 (2C), 128.3 (2C), 127.9, 117.8, 116.9, 114.7 (2C), 103.8, 55.5. IR (ATR, cm^{-1}) 3128 (w), 3012 (w), 2921 (w), 2850 (w), 2044 (w), 1891 (w), 1852 (w), 1597 (m), 1510 (s), 1414 (s), 1245 (s), 1176 (m), 1022 (m), 843 (m), 769 (s), 696 (s), 583 (m).

MS (EI, 70 eV): m/z (%) = 300 (100), $[M]^+$ 301 (22), 209 (19), 285 (18), 255 (22), 128 (11). HRMS (EI): Calculated for $C_{20}H_{16}ON_2$ $[M]^+$ 300.12571, found 300.12562.

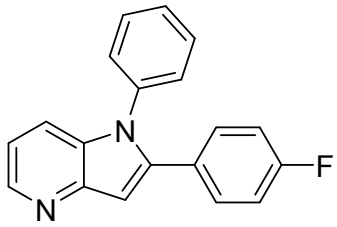


1-(4-methoxyphenyl)-2-(4-(trifluoromethyl)phenyl)-1H-pyrrolo[3,2-b]pyridine (3h): Yellow solid, mp. 143 – 144 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.52 (dd, J = 4.6, 1.4 Hz, 1H), 7.56 – 7.47 (m, 3H), 7.41 (d, J = 8.1 Hz, 2H), 7.16 – 7.06 (m, 3H), 7.04 (d, J = 0.7 Hz, 1H), 6.99 – 6.92 (m, 2H), 3.85 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.7. ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.3, 146.4, 144.7, 142.2, 135.4, 133.0, 130.0, 129.8 (q, J = 32.6 Hz), 129.2 (2C), 129.0 (2C), 125.4 (q, J = 3.7 Hz) (2C), 124.1 (q, J = 272.1 Hz), 118.0, 117.7, 115.0 (2C), 105.2, 55.6. IR (ATR, cm^{-1}) 3044 (w), 3014 (w), 2959 (w), 2932 (w), 2840 (w), 1726 (w), 1616 (w), 1514 (s), 1416 (m), 1322 (s), 1317 (s), 1245 (m), 1167 (s), 1109 (s), 1061 (m), 856 (m), 804 (s), 758 (m), 623 (m). MS (EI, 70 eV): m/z (%) = 368 (100), $[M]^+$ 369 (23), 367 (19), 255 (11), 182 (11), 128 (11). HRMS (EI): Calculated for $C_{21}H_{15}ON_2F_3$ $[M]^+$ 368.11310, found 368.11256.

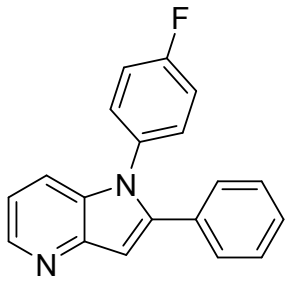


2-(4-fluorophenyl)-1-(4-methoxyphenyl)-1H-pyrrolo[3,2-b]pyridine (3i): Yellow solid, mp. 143 – 144 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (d, J = 4.0 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.23 – 7.15 (m, 2H), 7.07 – 7.02 (m, 2H), 6.99 (dd, J = 8.3, 4.6 Hz, 1H), 6.92 (m, 1H), 6.90 – 6.83 (m, 4H), 3.76 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.25. ^{13}C NMR (63 MHz, $CDCl_3$) δ 162.6 (d, J = 248.6 Hz), 159.1, 146.5, 144.4, 143.1, 132.6, 131.0 (d, J = 8.2 Hz) (2C), 130.1, 129.0 (2C), 128.1 (d, J = 3.4 Hz), 117.8, 117.2, 115.6 (d, J = 21.7 Hz) (2C), 114.8 (2C), 103.9, 55.6. IR (ATR, cm^{-1}) 3117 (w), 3050 (w=, 3014 (w), 2916 (w), 2835 (w), 1600 (m), 1558 (w), 1515 (s), 1496 (s), 1419 (m), 1359 (m), 1248 (s), 1221 (m), 1158 (m), 1108 (m), 1024 (s), 840 (s), 681 (s), 577 (s). MS (EI, 70 eV): m/z (%) = 318 (100), $[M]^+$ 319

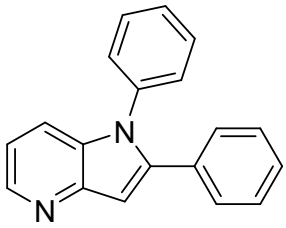
(23), 317 (17), 275 (18), 137 (9). HRMS (EI): Calculated for $C_{20}H_{15}ON_2F$ $[M]^+$ 318.11629, found 318.11615.



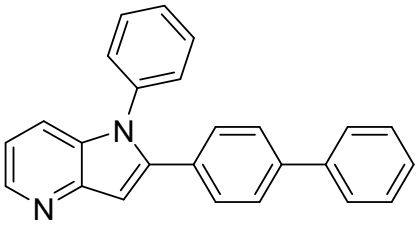
2-(4-fluorophenyl)-1-phenyl-1H-pyrrolo[3,2-b]pyridine (3j): Yellow solid, mp. 128 – 129 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.48 (d, J = 8.2 Hz, 1H), 7.42 – 7.28 (m, 3H), 7.26 – 7.08 (m, 4H), 7.08 – 6.97 (m, 1H), 6.95 – 6.82 (m, 3H). 19F NMR (282 MHz, $CDCl_3$) δ -112.85. ^{13}C NMR (63 MHz, $CDCl_3$) δ 162.7 (d, J = 249.0 Hz), 146.1, 143.8, 143.4, 137.3, 131.0 (d, J = 8.2 Hz) (2C), 129.8 (2C), 128.1, 127.9 (2C), 127.8 (d, J = 3.4 Hz), 118.3, 117.3, 115.6 (d, J = 21.7 Hz) (2C), 104.1. IR (ATR, cm^{-1}) 3046 (w), 2920 (w), 2851 (w), 1893 (w), 1596 (m), 1495 (s), 1412 (s), 1359 (m), 1219 (m), 1156 (m), 1013 (m), 835 (s), 798 (s), 782 (s), 696 (s), 594 (s). MS (EI, 70 eV): m/z (%) = 288 (100), $[M]^+$ 289 (20), 287 (47), 286 (15), 120 (7), 77 (12), 51 (12). HRMS (EI): Calculated for $C_{19}H_{13}FN_2$ $[M]^+$ 288.10573, found 288.10600.



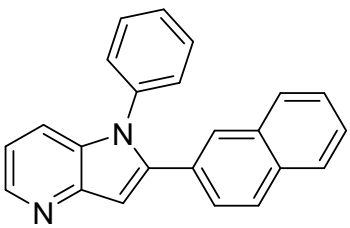
1-(4-fluorophenyl)-2-phenyl-1H-pyrrolo[3,2-b]pyridine (3k): Yellow solid, mp. 120 – 121 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (dd, J = 4.6, 1.2 Hz, 1H), 7.49 (d, J = 8.2 Hz, 1H), 7.28 (s, 5H), 7.22 – 7.17 (m, 2H), 7.15 – 7.07 (m, 3H), 6.99 (s, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.2. ^{13}C NMR (63 MHz, $CDCl_3$) δ 161.8 (d, J = 248.2 Hz), 146.8, 144.6, 144.1, 133.7 (d, J = 3.0 Hz), 131.6, 129.5 (d, J = 8.5 Hz) (2C), 129.2 (2C), 128.5 (2C), 128.3, 117.6, 117.3, 116.6 (d, J = 22.8 Hz) (2C), 104.7. IR (ATR, cm^{-1}) 3054 (w), 2924 (w), 2853 (w), 1888 (w), 1599 (w), 1560 (w), 1507 (s), 1415 (s), 1221 (s), 1153 (m), 965 (m), 850 (m), 763 (s), 693 (s), 581 (s). MS (EI, 70 eV): m/z (%) = 288 (100), $[M]^+$ 289 (21), 287 (45), 286 (14), 143 (8), 75 (7). HRMS (EI): Calculated for $C_{19}H_{13}NF$ $[M]^+$ 288.10573, found 288.10531.



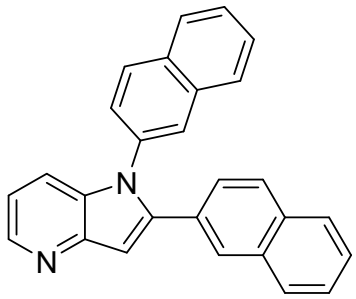
1,2-diphenyl-1H-pyrrolo[3,2-b]pyridine (3l): Yellow solid, mp. 117 – 118 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.49 (d, J = 4.3 Hz, 1H), 7.54 (d, J = 8.2 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.28 – 7.25 (m, 4H), 7.24 – 7.20 (m, 2H), 7.20 – 7.17 (m, 1H), 7.07 (dd, J = 8.3, 4.6 Hz, 1H), 6.99 (d, J = 0.5 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 146.7, 144.3, 144.1, 137.8, 132.4, 131.8, 129.6 (2C), 129.2 (2C), 128.4 (2C), 128.2, 127.9 (2C), 127.8, 117.9, 117.2, 104.5. IR (ATR, cm^{-1}) 3046 (w), 2920 (w), 2850 (w), 1595 (m), 1558 (w), 1598 (m), 1454 (w), 1412 (s), 1382 (m), 1327 (m), 1290 (m), 1178 (m), 1113 (m), 963 (m), 769 (s), 690 (s), 604 (s). MS (EI, 70 eV): m/z (%) = 270 (100), $[M]^+$ 271 (21), 269 (52), 268 (18), 77 (12), 51 (14). HRMS (EI): Calculated for $C_{19}H_{14}N_2$ $[M+H]^+$ 271.12297, found 271.12302. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[9]



2-([1,1'-biphenyl]-4-yl)-1-phenyl-1H-pyrrolo[3,2-b]pyridine (3m): Yellow solid, mp. 169 – 170 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.45 (d, J = 4.5 Hz, 1H), 7.55 – 7.25 (m, 13H), 7.24 – 7.15 (m, 2H), 7.07 – 6.97 (m, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 146.7, 144.4, 143.7, 140.8, 140.3, 137.7, 132.5, 130.7, 129.7 (2C), 129.5 (2C), 128.9 (2C), 127.92 (2C), 127.9, 127.7, 127.1 (4C), 117.8, 117.2, 104.6. IR (ATR, cm^{-1}) 3113 (w), 3061 (w), 2921 (w), 2851 (w), 1920 (w), 1681 (w), 1596 (m), 1494 (m), 1411 (s), 1353 (m), 844 (m), 805 (m), 785 (m), 769 (s), 698 (s), 605 (m). MS (EI, 70 eV): m/z (%) = 346 (100), $[M]^+$ 347 (27), 345 (32), 269 (8), 77 (11), 51 (7). HRMS (EI): Calculated for $C_{25}H_{18}N_2$ $[M]^+$ 346.14645, found 346.14578.

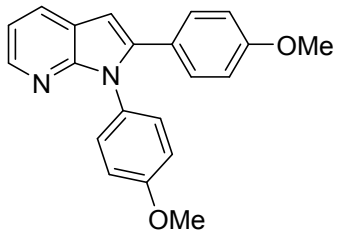


2-(naphthalen-2-yl)-1-phenyl-1H-pyrrolo[3,2-b]pyridine (3n): Brownish solid, mp. 130 – 131 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.80 – 7.57 (m, 4H), 7.51 (d, J = 8.2 Hz, 1H), 7.44 – 7.13 (m, 8H), 7.11 – 6.97 (m, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 146.6, 144.2, 137.7, 133.2, 132.8, 129.7 (2C), 129.2, 128.6, 128.4, 128.0, 127.9 (2C), 127.8, 126.7, 126.60, 126.6, 118.0, 117.3, 104.8. IR (ATR, cm^{-1}) 3053 (w), 2923 (w), 2851 (w), 1592 (m), 1497 (s), 1414 (s), 1288 (m), 865 (m), 827 (m), 781 (s), 759 (m), 693 (s). MS (EI, 70 eV): m/z (%) = 320 (100), $[M]^+$ 321 (26), 319 (49), 318 (16), 159 (7). HRMS (EI): Calculated for $C_{23}H_{16}N_2$ $[M+H]^+$ 320.13080, found 320.13045.



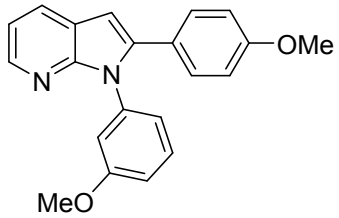
1,2-di(naphthalen-2-yl)-1H-pyrrolo[3,2-b]pyridine (3o): yellow solid, mp. 157 – 158 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.46 (dd, J = 4.6, 1.4 Hz, 1H), 7.85 (dd, J = 8.2, 3.4 Hz, 2H), 7.69 (d, J = 1.3 Hz, 1H), 7.63 – 7.54 (m, 1H), 7.52 – 7.44 (m, 2H), 7.43 – 7.38 (m, 1H), 7.38 – 7.33 (m, 2H), 7.32 – 7.25 (m, 4H), 7.23 (dd, J = 8.6, 1.8 Hz, 1H), 7.19 – 7.15 (m, 1H), 7.04 (ddd, J = 8.2, 1.4, 0.9 Hz, 1H), 6.92 (dd, J = 8.3, 4.6 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.7, 145.3, 144.4, 134.4, 134.3, 133.6, 133.0, 132.7, 131.1, 129.2, 129.1, 128.5, 128.2, 127.9, 127.8, 127.5, 127.5, 127.2, 126.8, 126.4, 126.3, 125.9, 125.5, 123.1, 118.2, 117.2, 104.4. IR (ATR, cm^{-1}) 3050 (w), 2923 (w), 2850 (w), 1595 (m), 1505 (m), 1465 (m), 1415 (m), 1399 (m), 1284 (m), 1016 (m), 863 (m), 798 (m), 770 (s), 755 (m), 663 (m), 589 (m). MS (EI, 70 eV): m/z (%) = 370 (100), $[M]^+$, 371 (31), 369 (36), 368 (13), 367 (15), 184 (13). HRMS (EI): Calculated for $C_{27}H_{18}N_2$ $[M]^+$ 370.14645, found 370.14572.

3.3. 7-Azaindoles

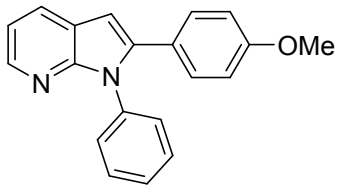


1,2-bis(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4a): White solid, mp. 145 – 146 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.22 (dd, J = 4.7, 1.5 Hz, 1H), 7.85 (dd, J = 7.8, 1.5 Hz, 1H),

7.22 – 7.09 (m, 4H), 7.02 (dd, J = 7.8, 4.8 Hz, 1H), 6.92 – 6.82 (m, 2H), 6.78 – 6.69 (m, 2H), 6.56 (s, 1H), 3.75 (s, 3H), 3.71 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.3, 158.6, 150.0, 143.2, 141.2, 130.2, 129.9, 129.5, 128.0, 124.6, 120.9, 116.8, 114.4, 113.8, 99.9, 77.5, 77.2, 77.0, 76.5, 55.4, 55.2. IR (ATR, cm^{-1}) 3114 (w), 3049 (w), 3018 (w), 2929 (w), 2835 (w), 2037 (w), 1905 (w), 1833 (w), 1610 (m), 1567 (w), 1515 (s), 1500 (s), 1454 (m), 1371 (m), 1301 (m), 1242 (s), 1184 (m), 1024 (m), 833 (s), 798 (s), 766 (s), 584 (m). MS (EI, 70 eV): m/z (%) = 330 (83), $[M]^+$ 331 (18), 329 (100), 286 (11), 243 (17), 121 (7). HRMS (EI): Calculated for $C_{21}H_{18}N_2O_2$ $[M+H]^+$ 331.14410, found 331.14454.

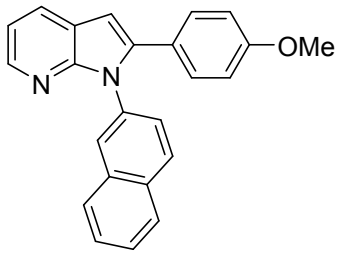


1-(3-methoxyphenyl)-2-(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4b): Yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 – 8.04 (m, 1H), 7.83 (t, J = 8.0 Hz, 1H), 7.32 – 7.06 (m, 3H), 7.06 – 6.93 (m, 1H), 6.92 – 6.62 (m, 5H), 6.55 (d, J = 9.6 Hz, 1H), 3.69 (d, J = 9.7 Hz, 3H), 3.63 (d, J = 9.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 159.5, 150.0, 143.4, 141.2, 138.3, 130.2 (2C), 129.8, 128.1, 124.8, 121.1, 121.0, 117.07, 114.3, 113.9 (2C), 113.5, 100.6, 55.5, 55.4. IR (ATR, cm^{-1}) 3041 (w), 3001 (w), 2933 (w), 2834 (w), 2222 8w), 2032 (w), 1920 (w), 1731 (w), 1604 (m), 1588 (m), 1498 (s), 1455 (m), 1406 (s), 1368 (m), 1283 (m), 1247 (s), 1173 (m), 1028 (m), 833 (m), 802 (m), 767 (m), 692 (m), 612 (m). MS (EI, 70 eV): m/z (%) = 330 (98), $[M]^+$ 331 (20), 329 (100), 243 (16), 121 (13). HRMS (EI): Calculated for $C_{21}H_{18}O_2N_2$ $[M]^+$ 330.13628, found 330.13539.

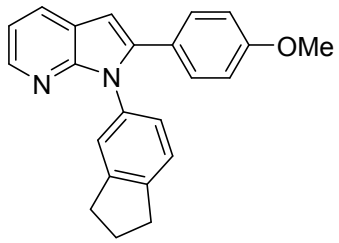


2-(4-methoxyphenyl)-1-phenyl-1H-pyrrolo[2,3-b]pyridine (4c): Yellow solid, mp. 138 – 139 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (dd, J = 4.8, 1.6 Hz, 1H), 7.90 – 7.75 (m, 1H), 7.37 – 7.28 (m, 2H), 7.28 – 7.19 (m, 3H), 7.14 – 7.07 (m, 2H), 7.02 (dd, J = 7.8, 4.8 Hz, 1H), 6.75 – 6.63 (m, 2H), 6.56 (s, 1H), 3.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.8, 163.5, 159.3, 149.9, 143.3, 141.1, 137.2, 130.6, 130.2, 129.1, 128.5, 128.1, 127.3, 124.6, 121.0, 117.0, 113.8, 113.7, 100.5, 55.2. IR (ATR, cm^{-1}) 3044 (w), 3008 (w), 2953 (m), 2833 (m),

1674 (w), 1608 (m), 1500 (s), 1408 (s), 1368 (m), 1242 (s), 1182 (m), 1024 (s), 836 (m), 799 (s), 766 (s), 696 (s), 597 (s). MS (EI, 70 eV): m/z (%) = 300 (91), $[M]^+$, 301 (18), 299 (100), 285 (8), 255 (31), 128 (18), 51 (9). HRMS (EI): Calculated for $C_{20}H_{16}ON_2$ $[M]^+$ 300.12571, found 300.12482.

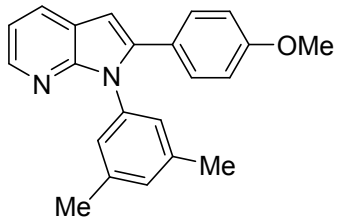


2-(4-methoxyphenyl)-1-(naphthalen-2-yl)-1H-pyrrolo[2,3-b]pyridine (4d): Yellow solid, mp. 123 – 124 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.13 (dd, J = 4.8, 1.6 Hz, 1H), 7.91 (dd, J = 7.8, 1.6 Hz, 1H), 7.87 – 7.77 (m, 2H), 7.48 – 7.30 (m, 3H), 7.29 – 7.18 (m, 2H), 7.10 – 6.97 (m, 3H), 6.69 (s, 1H), 6.62 – 6.47 (m, 2H), 3.58 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.3, 150.9, 143.4, 142.5, 134.4, 134.2, 131.7, 129.5 (2C), 129.0, 128.5, 128.3, 128.1, 127.6, 127.0, 126.4, 125.5, 124.6, 123.5, 120.9, 116.9, 113.7 (2C), 100.0. IR (ATR, cm^{-1}) 3604 (w), 3388 (w), 3044 (w), 2961 (w), 2835 (w), 1609 (m), 1497 (s), 1469 (m), 1425 (m), 1298 (m), 1245 (s), 1176 (m), 1024 (m), 833 (m), 798 (s), 761 (s). MS (EI, 70 eV): m/z (%) = 350 (100) $[M]^+$, 351 (23), 349 (87), 305 (29), 243 (25), 153 (13). HRMS (EI): Calculated for $C_{24}H_{18}N_2O$ $[M+H]^+$ 351.14919, found 351.14934.

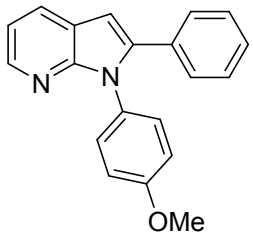


1-(2,3-dihydro-1H-inden-5-yl)-2-(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4e): Yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (dd, J = 4.7, 1.6 Hz, 1H), 7.83 (dd, J = 7.7, 1.7 Hz, 1H), 7.19 – 7.12 (m, 3H), 7.11 (s, 1H), 7.00 (dd, J = 7.8, 4.8 Hz, 1H), 6.94 (d, J = 7.8 Hz, 1H), 6.76 – 6.68 (m, 2H), 6.55 (s, 1H), 3.70 (s, 1H), 2.84 (t, J = 7.0 Hz, 4H), 2.09 – 1.93 (m, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.3, 150.3, 145.3, 143.8, 143.3, 141.4, 135.3, 130.3 (2C), 128.0, 126.5, 125.0, 124.8, 124.6, 121.0, 116.8, 113.9 (2C), 100.0, 55.4, 33.1, 32.8, 25.7. IR (ATR, cm^{-1}) 3042 (w), 2944 (m), 2839 (w), 1675 (w), 1609 (m), 1499 (s), 1407 (m), 1248 (s), 1176 (m), 1030 (m), 834 (m), 803 (m), 769 (m). MS (EI, 70 eV): m/z (%) = 340

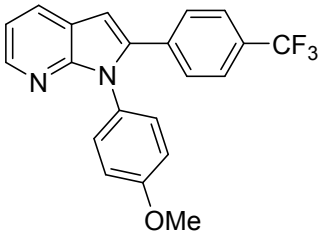
(79), $[M]^+$ 341 (17), 339 (100), 296 (10), 115 (12). HRMS (EI): Calculated for $C_{23}H_{19}ON_2$ $[M]^+$ 339.14919, found 339.14923.



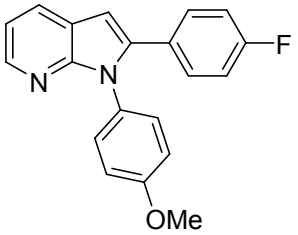
1-(3,5-dimethylphenyl)-2-(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4f): Yellow solid, mp. 95 – 96 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 – 8.14 (m, 1H), 7.86 – 7.80 (m, 1H), 7.17 (d, J = 3.6 Hz, 1H), 7.13 (s, 1H), 7.01 (dd, J = 7.8, 4.8 Hz, 1H), 6.90 (s, 1H), 6.85 (s, 2H), 6.72 (d, J = 8.8 Hz, 2H), 6.55 (s, 1H), 3.71 (s, 3H), 2.22 (s, 6H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.3, 150.2, 143.3, 141.3, 138.7, 137.1, 130.7, 130.2 (2C), 129.6, 128.0, 126.5 (2C), 124.9, 121.0, 116.8, 113.8 (2C), 113.2, 100.1, 55.3, 21.5. IR (ATR, cm^{-1}) 3040 (w), 3006 (w), 2917 (w), 2836 (w), 1609 (m), 1546 (w), 1498 (s), 1473 (m), 1405 (s), 1369 (m), 1247 (s), 1175 (m), 1026 (m), 836 (m), 801 (m), 767 (m), 696 (m). MS (EI, 70 eV): m/z (%) = 328 (99), $[M]^+$ 329 (21), 327 (100), 313 (12), 312 (14), 269 (17), 157 (12), 135 (10). HRMS (EI): Calculated for $C_{22}H_{19}ON_2$ $[M-H]^+$ 327.14919, found 327.14906.



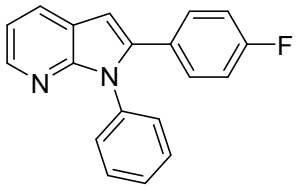
1-(4-methoxyphenyl)-2-phenyl-1H-pyrrolo[2,3-b]pyridine (4g): Yellow solid, mp. 188 – 189 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.24 (dd, J = 4.7, 1.6 Hz, 1H), 7.87 (dd, J = 7.8, 1.6 Hz, 1H), 7.28 – 7.11 (m, 7H), 7.03 (dd, J = 7.8, 4.7 Hz, 1H), 6.90 – 6.82 (m, 1H), 6.63 (s, 1H), 3.74 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 158.7, 150.1, 143.5, 141.2, 132.2, 129.8, 129.4 (2C), 128.9 (2C), 128.3, 128.3 (2C), 127.7, 120.8, 116.9, 114.4 (2C), 100.9, 55.4. IR (ATR, cm^{-1}) 3067 (w), 3043 (w), 3010 (w), 2840 (w), 1901 (w), 1856 (w), 1604 (w), 1510 (m), 1419 (m), 1236 (s), 1025 (s), 842 (m), 806 (m), 752 (s), 693 (s), 556 (s). MS (EI, 70 eV): m/z (%) = 300 (68), $[M]^+$ 301 (13), 299 (100), 256 (27), 128 (9). HRMS (EI): Calculated for $C_{20}H_{15}ON_2$ $[M]^+$ 299.11789, found 299.11775.



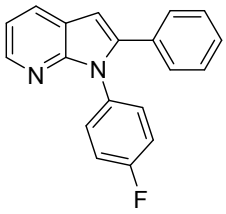
1-(4-methoxyphenyl)-2-(4-(trifluoromethyl)phenyl)-1H-pyrrolo[2,3-b]pyridine (4h): Yellow solid, mp. 158 – 159 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (dd, J = 4.7, 1.6 Hz, 1H), 7.89 (dd, J = 7.8, 1.6 Hz, 1H), 7.45 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 8.1 Hz, 2H), 7.23 – 7.11 (m, 2H), 7.05 (dd, J = 7.8, 4.7 Hz, 1H), 6.94 – 6.83 (m, 2H), 6.70 (s, 1H), 3.75 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.0, 150.5, 144.5, 139.5, 135.8, 129.7 (q, J = 32.6 Hz), 129.6, 129.5 (2C), 129.0 (2C), 128.9, 125.4 (q, J = 3.8 Hz) (2C), 124.2 (q, J = 272.1 Hz), 120.6, 117.3, 114.7 (2C), 102.3, 55.6. IR (ATR, cm^{-1}) 3020 (w), 2971 (w), 2843 (w), 2549 (w), 2315 (w), 2051 (w), 1934 (w), 1869 (w), 1613 (m), 1567 (w), 1515 (s), 1468 (m), 1442 (m), 1323 (s), 1300 (m), 1250 (s), 1162 (s), 1115 (s), 1028 (m), 918 (m), 844 (s), 800 (s), 764 (s), 591 (m), 561 (m). MS (EI, 70 eV): m/z (%) = 368 (69), $[M]^+$ 369 (13), 367 (100), 324 (22), 323 (10), 255 (7). HRMS (EI): Calculated for $C_{21}H_{14}ON_2F_3$ $[M]^+$ 367.10527, found 367.10514.



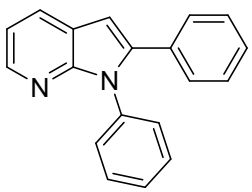
2-(4-fluorophenyl)-1-(4-methoxyphenyl)-1H-pyrrolo[2,3-b]pyridine (4i): Yellow solid, mp. 173 – 174 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (dd, J = 4.7, 1.6 Hz, 1H), 7.86 (dd, J = 7.8, 1.6 Hz, 1H), 7.23 – 7.10 (m, 4H), 7.04 (dd, J = 7.8, 4.7 Hz, 1H), 6.94 – 6.83 (m, 4H), 6.59 (s, 1H), 3.75 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.6. ^{13}C NMR (63 MHz, $CDCl_3$) δ 162.5 (d, J = 248.2 Hz), 158.9, 150.2, 143.9, 140.3, 130.8 (d, J = 8.1 Hz) (2C), 129.8, 129.6 (2C), 128.5, 128.4, 120.8, 117.1, 115.5 (d, J = 21.7 Hz) (2C), 114.6 (2C), 100.9, 55.6. IR (ATR, cm^{-1}) 3103 (w), 3014 (w), 2969 (w), 2841 (w), 2050 (w), 1893 (w), 1602 (w), 1511 (s), 1496 (s), 1297 (m), 1245 (s), 1152 (m), 1106 (m), 1029 (m), 834 (s), 813 (s), 773 (s), 581 (s). MS (EI, 70 eV): m/z (%) = 318 (67), $[M]^+$ 319 (12), 317 (100), 274 (29), 273 (21), 137 (7), 63 (8). HRMS (EI): Calculated for $C_{20}H_{14}ON_2F$ $[M-H]^+$ 317.10847, found 317.10836.



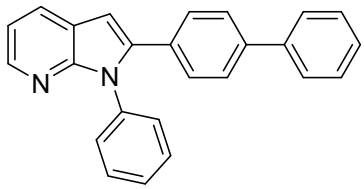
2-(4-fluorophenyl)-1-phenyl-1H-pyrrolo[2,3-b]pyridine (4j): White solid, mp. 141 – 142 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (d, J = 3.7 Hz, 1H), 8.03 – 7.91 (m, 1H), 7.48 – 7.23 (m, 7H), 7.15 (dd, J = 7.8, 4.7 Hz, 1H), 7.02 – 6.90 (m, 2H), 6.70 (s, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.4. ^{13}C NMR (63 MHz, $CDCl_3$) δ 162.6 (d, J = 248.4 Hz), 149.8, 143.8, 140.3, 136.9, 130.8 (d, J = 8.2 Hz) (2C), 129.3 (2C), 128.6, 128.5 (2C), 128.4 (d, J = 3.4 Hz), 127.7, 121.0, 117.3, 115.5 (d, J = 21.7 Hz) (2C), 101.5. IR (ATR, cm^{-1}) 3064 (w), 3043 (w), 2921 (w), 1589 (m), 1543 (m), 1496 (s), 1424 (m), 1402 (m), 1220 (s), 1157 (m), 840 (s), 802 (s), 768 (s), 691 (s), 592 (s), 539 (m). MS (EI, 70 eV): m/z (%) = 288 (62), $[M]^+$ 289 (10), 287 (100), 286 (21), 143 (6), 51 (7). HRMS (EI): Calculated for $C_{19}H_{13}FN_2$ $[M+H]^+$ 289.11355, found 289.11359.



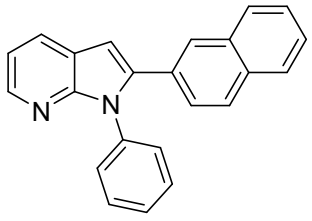
1-(4-fluorophenyl)-2-phenyl-1H-pyrrolo[2,3-b]pyridine (4k): Yellow solid, mp. 164 – 165 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (dd, J = 4.7, 1.6 Hz, 1H), 7.95 (dd, J = 7.8, 1.6 Hz, 1H), 7.35 – 7.20 (m, 7H), 7.16 – 7.04 (m, 3H), 6.71 (d, J = 3.6 Hz, 1H). ^{19}F NMR (282 MHz, CDCl3) δ -114.4. ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.7 (d, J = 247.1 Hz), 150.1, 143.8, 141.2, 133.1 (d, J = 3.2 Hz), 132.0, 130.1 (d, J = 8.6 Hz) (2C), 129.1 (2C), 128.6, 128.5 (2C), 128.1, 121.0, 117.3, 116.1 (d, J = 22.8 Hz) (2C), 101.6. IR (ATR, cm^{-1}) 3110 (w), 3059 (w), 3008 (w), 2924 (w), 1907 (w), 1858 (w), 1675 (w), 1568 (w), 1508 (m), 1420 (m), 1208 (m), 1096 (w), 852 (m), 804 (s), 747 (s). 698 (s), 552 (m). MS (EI, 70 eV): m/z (%) = 288 (60), $[M]^+$ 289 (10), 287 (100), 286 (21), 75 (11). HRMS (EI): Calculated for $C_{19}H_{12}FN_2$ $[M-H]^+$ 287.09790, found 287.09747.



1,2-diphenyl-1H-pyrrolo[2,3-b]pyridine (4l): White solid, mp. 130 – 132 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.33 (dd, J = 4.7, 1.6 Hz, 1H), 7.97 (dd, J = 7.8, 1.6 Hz, 1H), 7.48 – 7.26 (m, 10H), 7.14 (dd, J = 7.8, 4.7 Hz, 1H), 6.74 (s, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 150.1, 143.8, 141.3, 137.2, 132.3, 129.2 (2C), 129.1 (2C), 128.5 (3C), 128.4 (2C), 127.9, 127.5, 121.0, 117.2, 101.6. IR (ATR, cm^{-1}) 3116 (w), 3064 (w), 2925 (w), 1852 (w), 1594 (m), 1540 (m), 1496 (s), 1474 (m), 1425 (m), 1401 (m), 1370 (m), 1224 (s), 1158 (m), 841 (m), 799 (s), 767 (s), 692 (s), 593 (s). MS (EI, 70 eV): m/z (%) = 270 (59), $[M]^+$ 271 (11), 269 (100), 268 (21), 135 (8). HRMS (EI): Calculated for $C_{19}H_{14}N_2$ $[M+H]^+$ 271.12297, found 271.12322. ^{1}H- and ^{13}C-NMR spectral data are in accordance with the literature.[10]

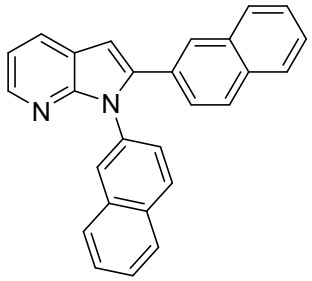


2-([1,1'-biphenyl]-4-yl)-1-phenyl-1H-pyrrolo[2,3-b]pyridine (4m): White solid, mp. 182 – 183 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.36 (dd, J = 4.7, 1.5 Hz, 1H), 7.99 (dd, J = 7.8, 1.5 Hz, 1H), 7.63 – 7.33 (m, 14H), 7.15 (dd, J = 7.8, 4.7 Hz, 1H), 6.80 (s, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 150.2, 143.8, 140.9, 140.5, 140.4, 137.2, 131.1, 129.3 (2C), 129.3 (2C), 128.9 (2C), 128.6 (2C), 128.5, 127.6, 127.5 (2C), 127.1 (2C), 127.0, 121.0, 117.2, 101.6. IR (ATR, cm^{-1}) 3110 (w), 3050 (w), 3034 (w), 3001 (w), 1591 (w), 1500 (m), 1421 (m), 1293 (w), 1247 (w), 997 (w), 842 (m), 807 (m), 760 (s), 694 (s), 610 (w). MS (EI, 70 eV): m/z (%) = 345 (100), $[M]^+$, 347 (19), 346 (84), 268 (8), 173 (6), 77 (9). HRMS (EI): Calculated for $C_{25}H_{18}N_2$ $[M+H]^+$ 347.15419, found 347.15428.



2-(naphthalen-2-yl)-1-phenyl-1H-pyrrolo[2,3-b]pyridine (4n): Yellow solid, mp. 180 – 181 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.37 (dd, J = 4.7, 1.5 Hz, 1H), 8.01 (dd, J = 7.8, 1.5 Hz, 1H), 7.90 – 7.65 (m, 4H), 7.54 – 7.43 (m, 2H), 7.43 – 7.30 (m, 6H), 7.17 (dd, J = 7.8, 4.7 Hz, 1H), 6.87 (s, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 150.1, 143.8, 141.2, 137.2, 133.3, 132.8, 129.7, 129.3 (2C), 128.6, 128.5 (2C), 128.3, 128.3, 127.9, 127.8, 127.5, 126.6, 126.6, 126.5, 121.1, 117.3, 102.0. IR (ATR, cm^{-1}) 3053 (w), 2923 (w), 2851 (w), 1957 (w), 1930 (w), 1879

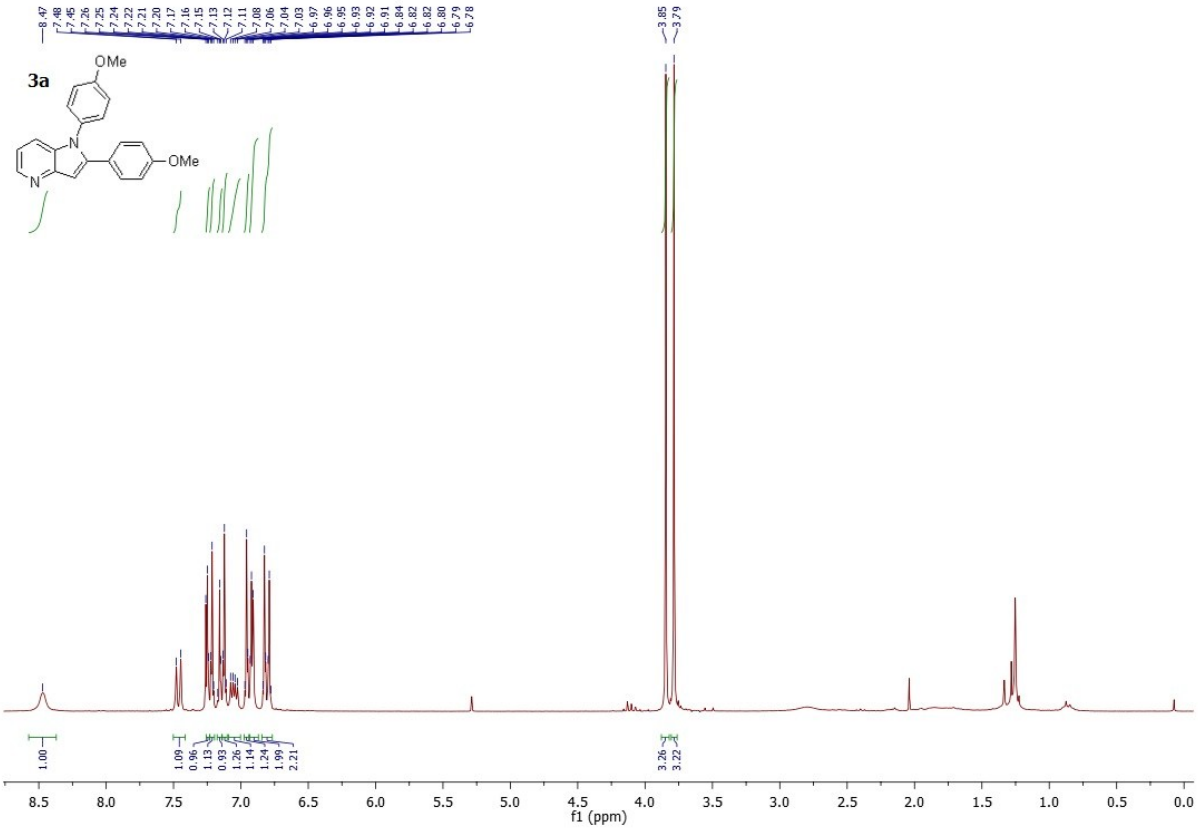
(w), 1865 (w), 1674 (w), 1592 (m), 1499 (m), 1416 (s), 1293 (m), 827 (m), 802 (s), 772 (s), 755 (s), 596 (s), 578 (m). MS (EI, 70 eV): m/z (%) = 320 (68), $[M]^+$ 321 (15), 319 (100), 318 (22), 317 (10), 159 (13). HRMS (EI): Calculated for $C_{23}H_{16}N_2$ $[M+H]^+$ 321.13862, found 321.13885.

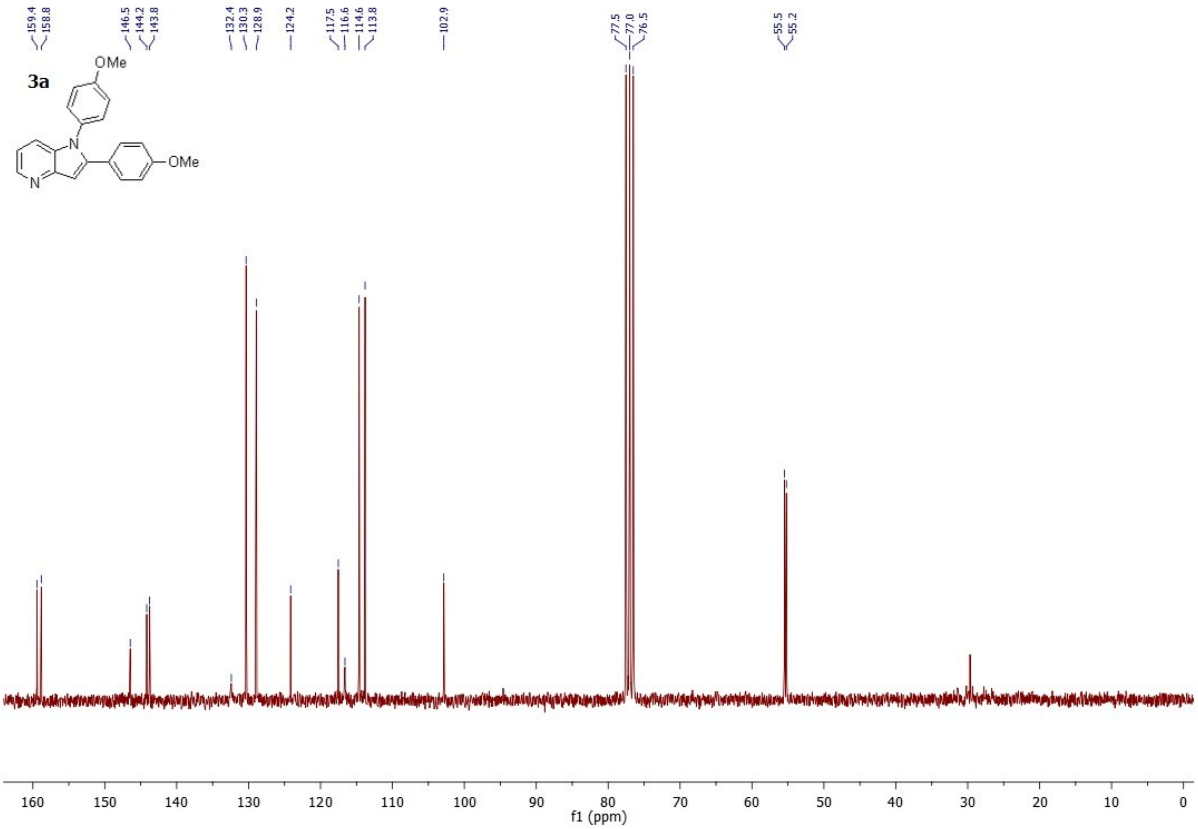


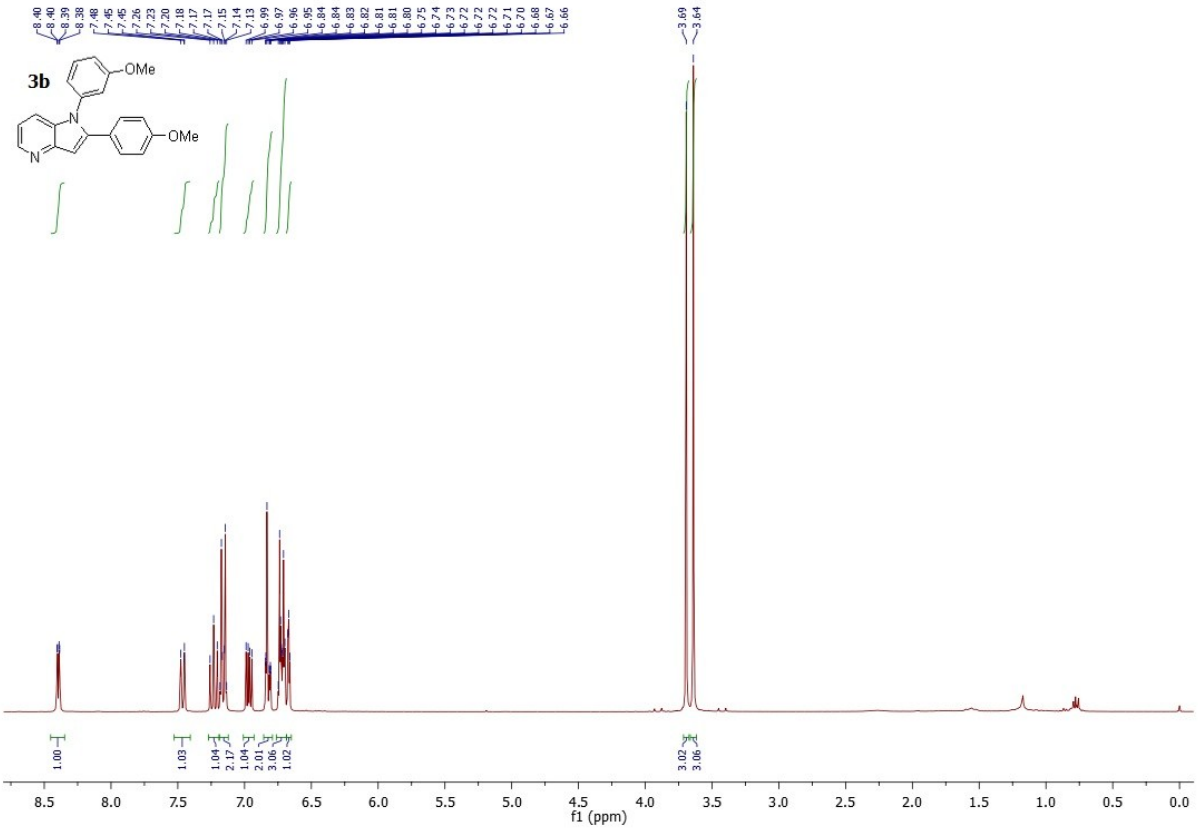
1,2-di(naphthalen-2-yl)-1H-pyrrolo[2,3-b]pyridine (4o): Yellow solid, mp. 168 – 169 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 (dd, J = 4.7, 1.6 Hz, 1H), 8.07 (dd, J = 7.8, 1.6 Hz, 1H), 7.96 – 7.87 (m, 2H), 7.75 (d, J = 1.3 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.60 – 7.51 (m, 2H), 7.51 – 7.45 (m, 2H), 7.45 – 7.42 (m, 1H), 7.42 – 7.34 (m, 4H), 7.31 (dd, J = 8.6, 1.8 Hz, 1H), 7.17 (dd, J = 7.8, 4.7 Hz, 1H), 7.00 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.2, 144.0, 142.5, 134.4, 134.2, 133.0, 132.6, 131.7, 129.5, 129.1, 128.5, 128.4, 128.2, 127.7, 127.7, 127.5 (2C), 127.1, 126.5, 126.3, 126.2, 125.8, 125.5, 123.4, 120.8, 117.1, 101.4. IR (ATR, cm^{-1}) 3052 (w), 2922 (w), 2851 (w), 1929 (w), 1595 (m), 1415 (m), 1297 (m), 958 (w), 786 (m), 768 (s), 758 (s). MS (EI, 70 eV): m/z (%) = 370 (99), $[M]^+$ 371 (28), 369 (100), 367 (16), 243 (25), 184 (10), 127 (11), 77 (6). HRMS (EI): Calculated for $C_{27}H_{18}N_2$ $[M]^+$ 370.14645, found 370.14531.

4. Spectral appendix

4.1. 4-Azaindoles



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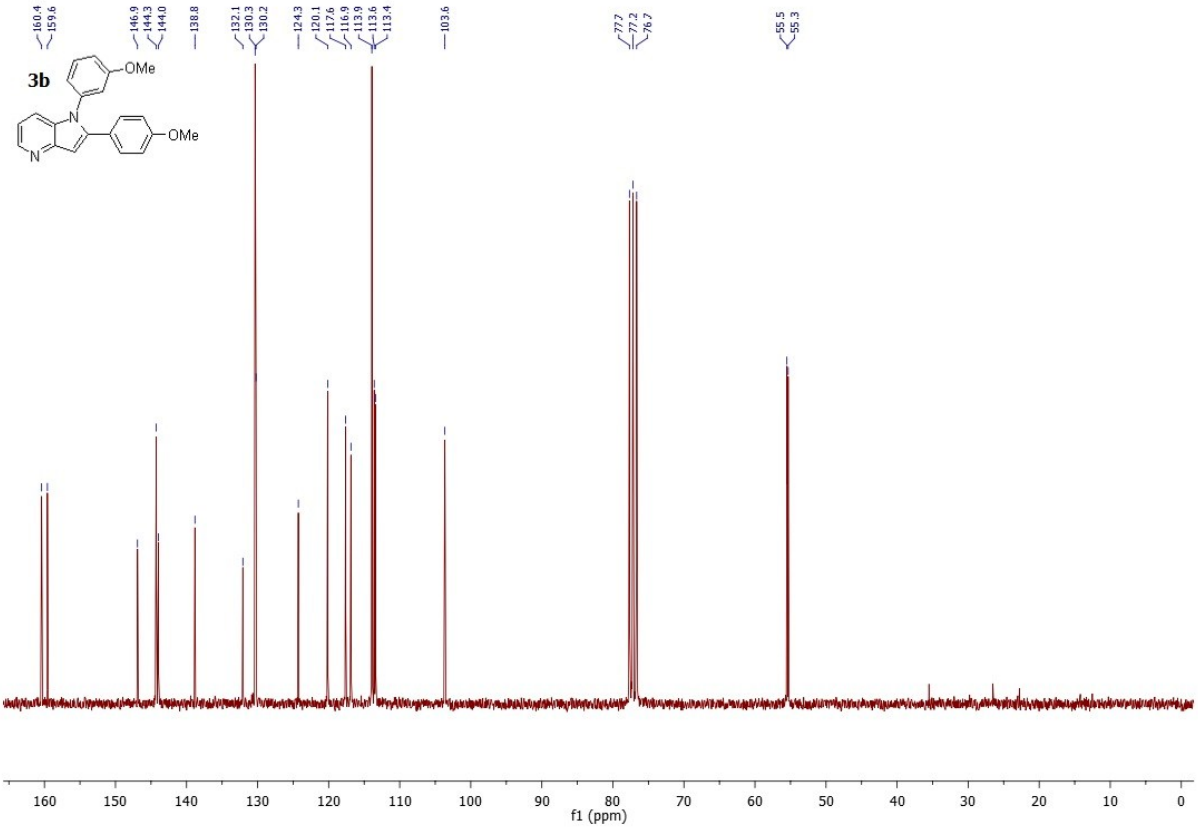
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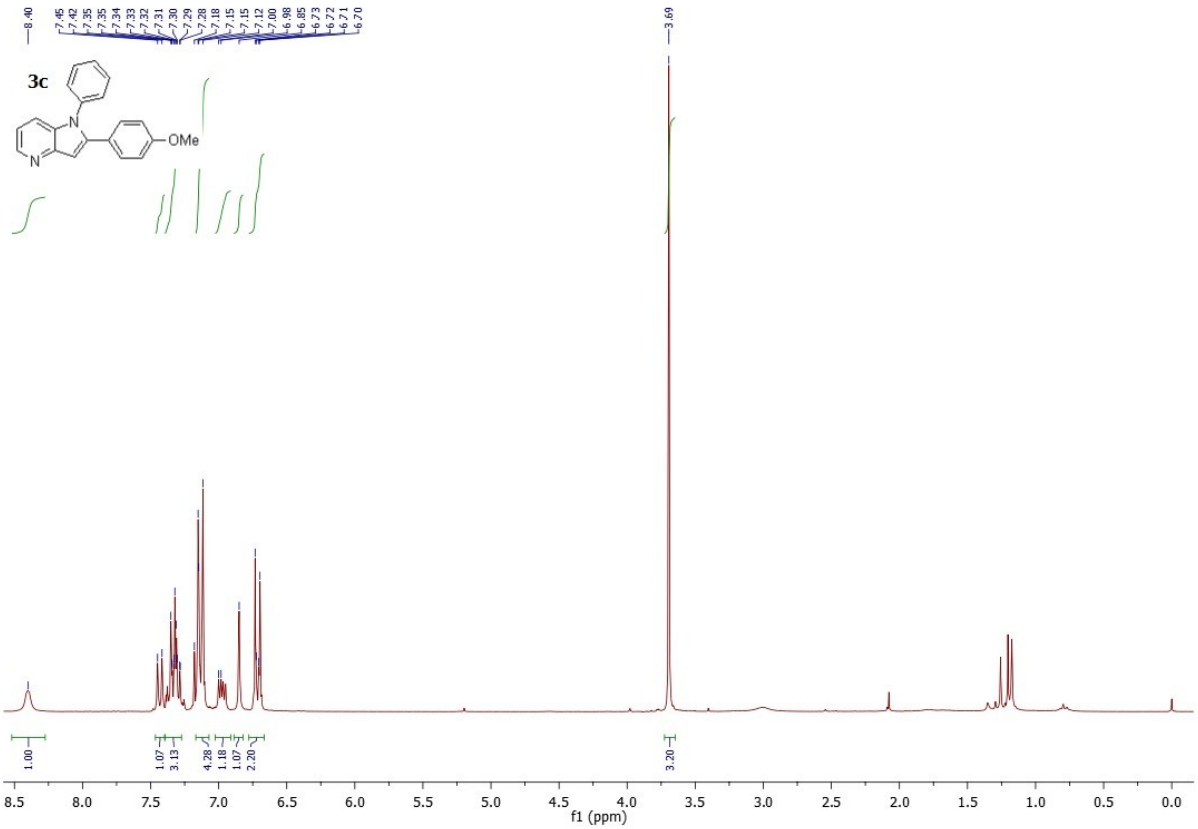
f1 (ppm)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7.15
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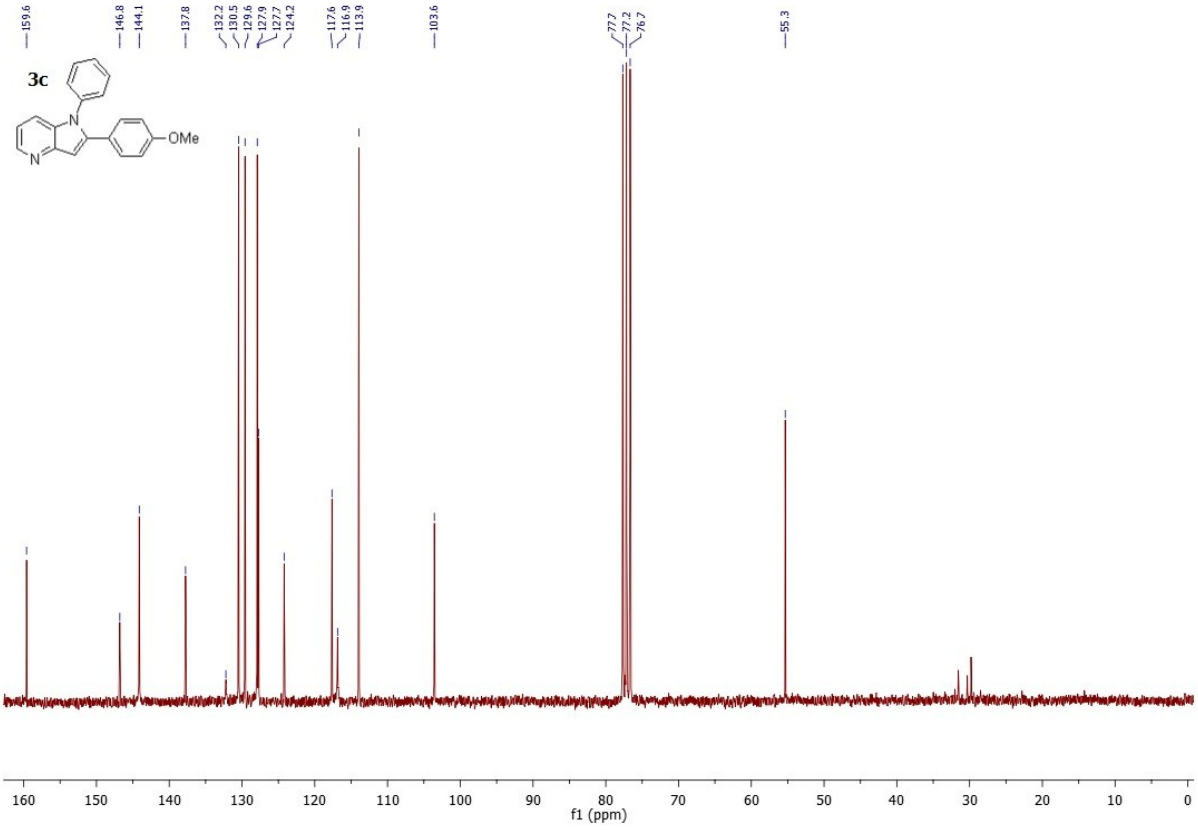
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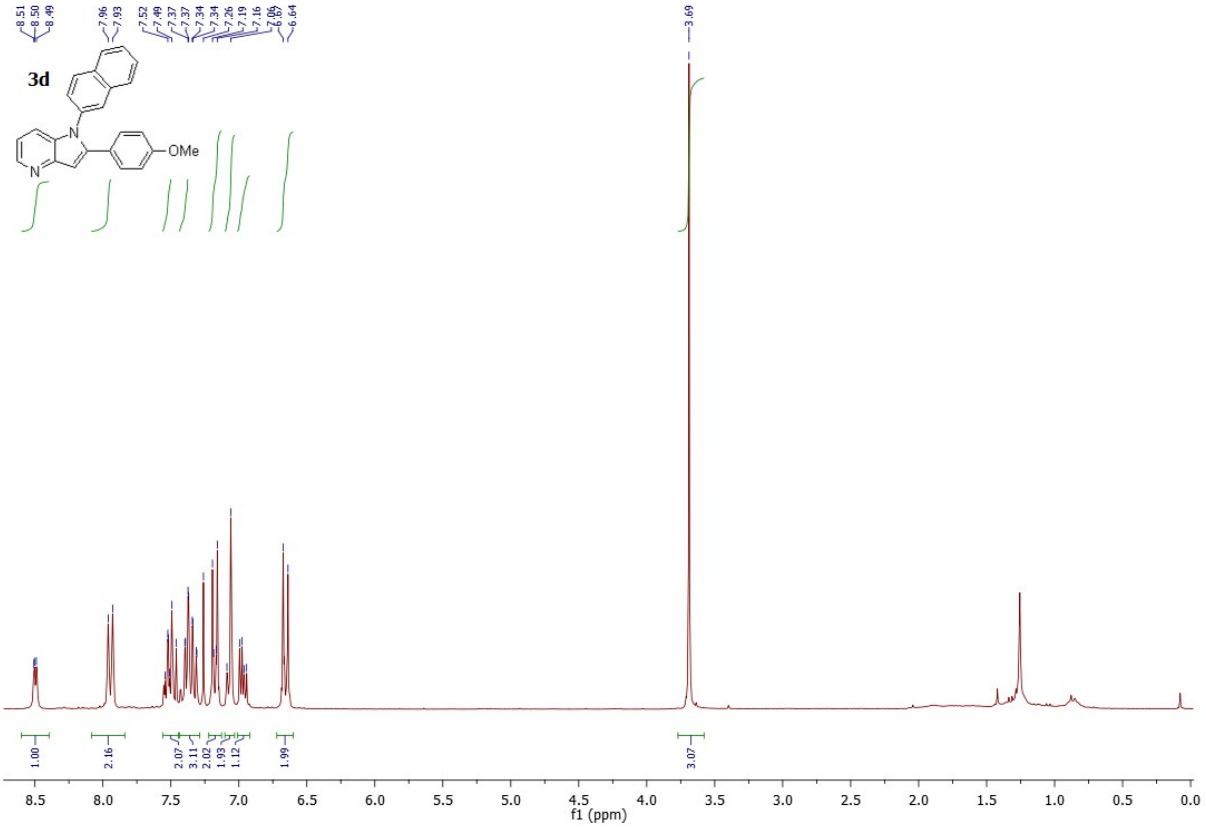
76.7
55.3
f1 (ppm)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3d
OMe
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2.02
1.93
1.12
1.99
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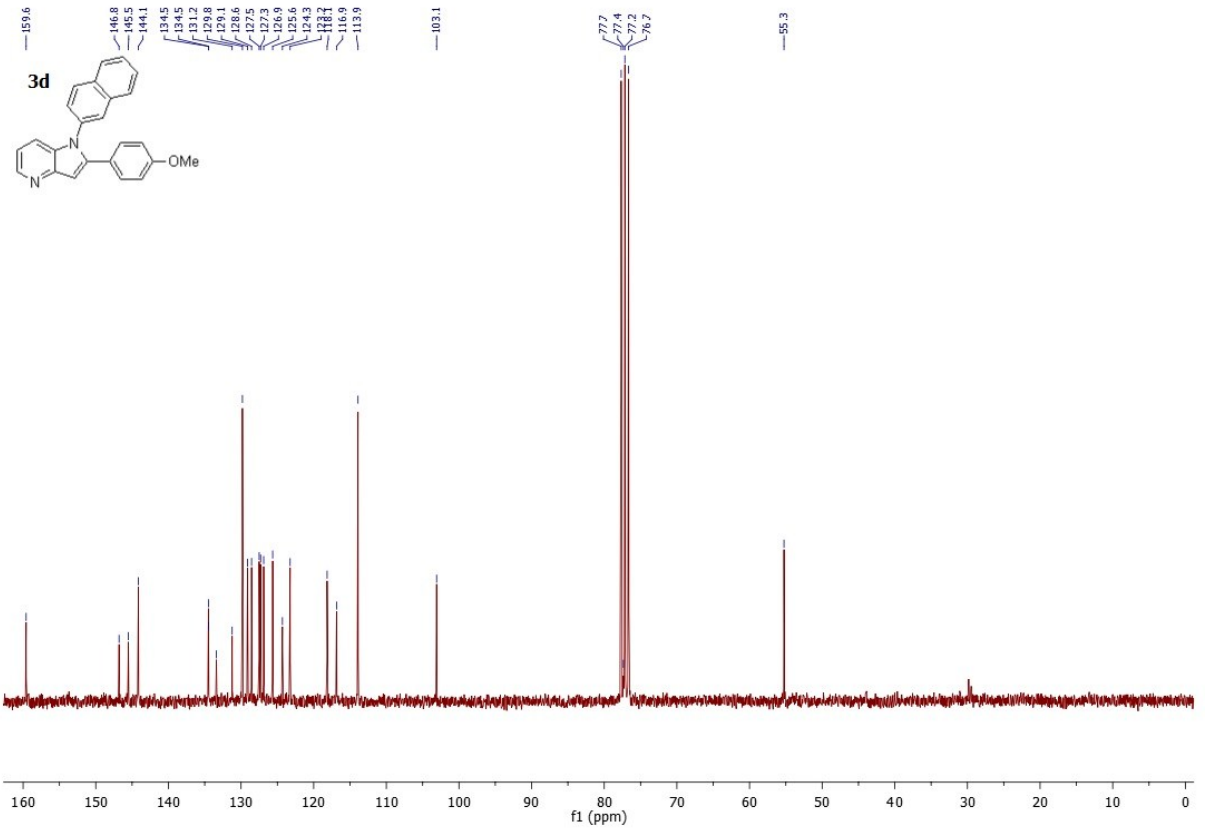
f1 (ppm)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103.1
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77.4
77.2
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55.3
3d
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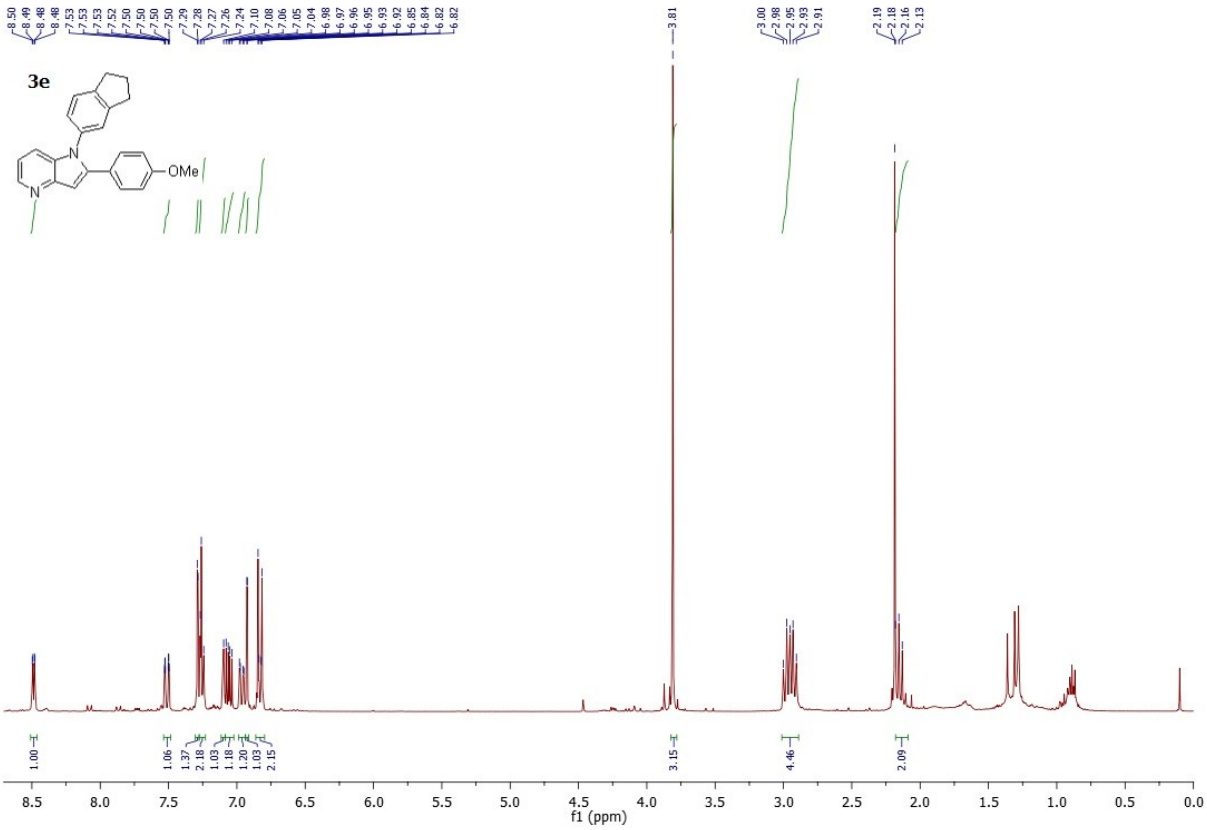
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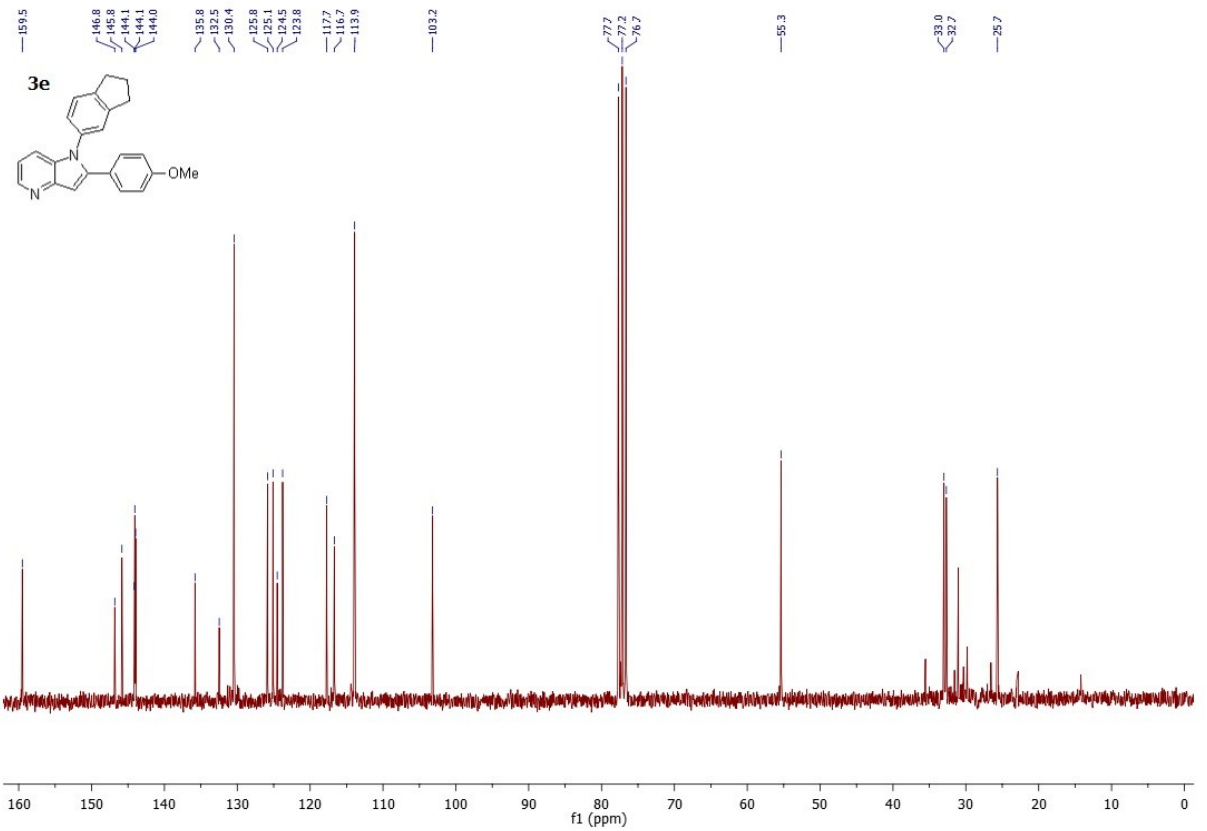
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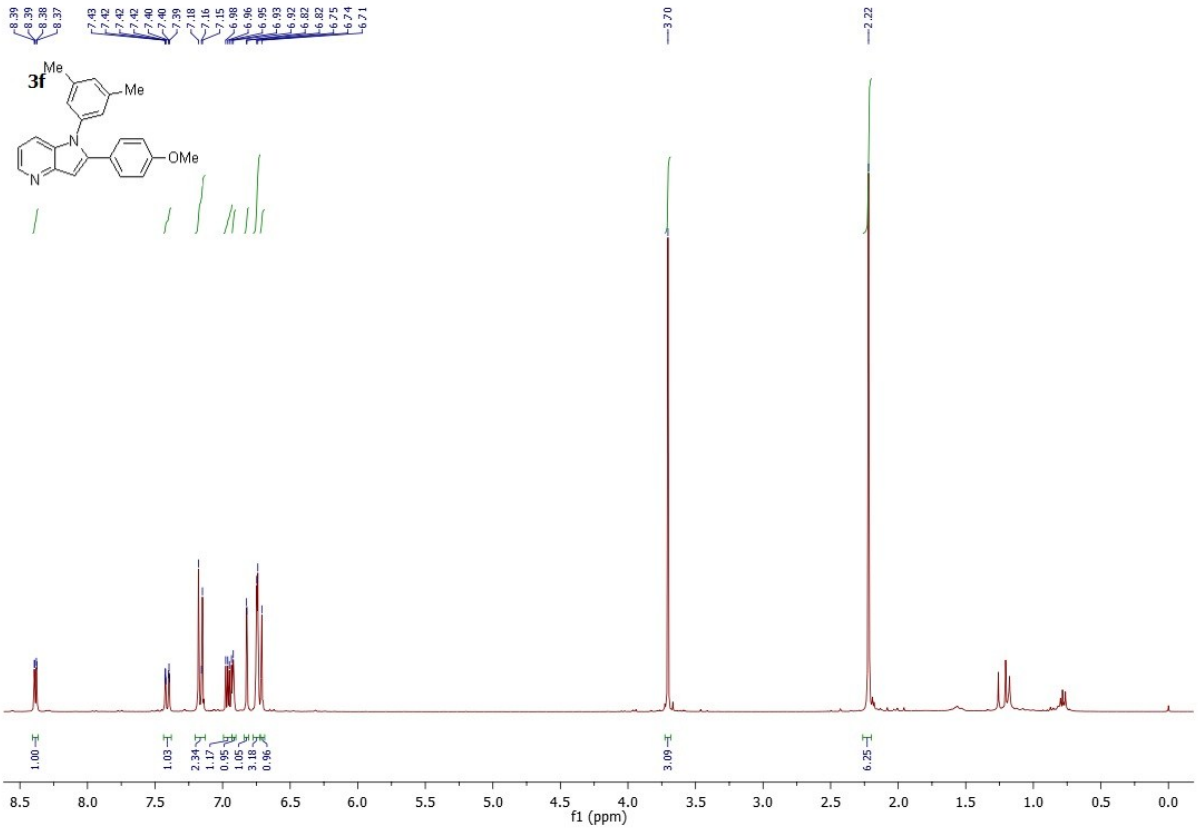
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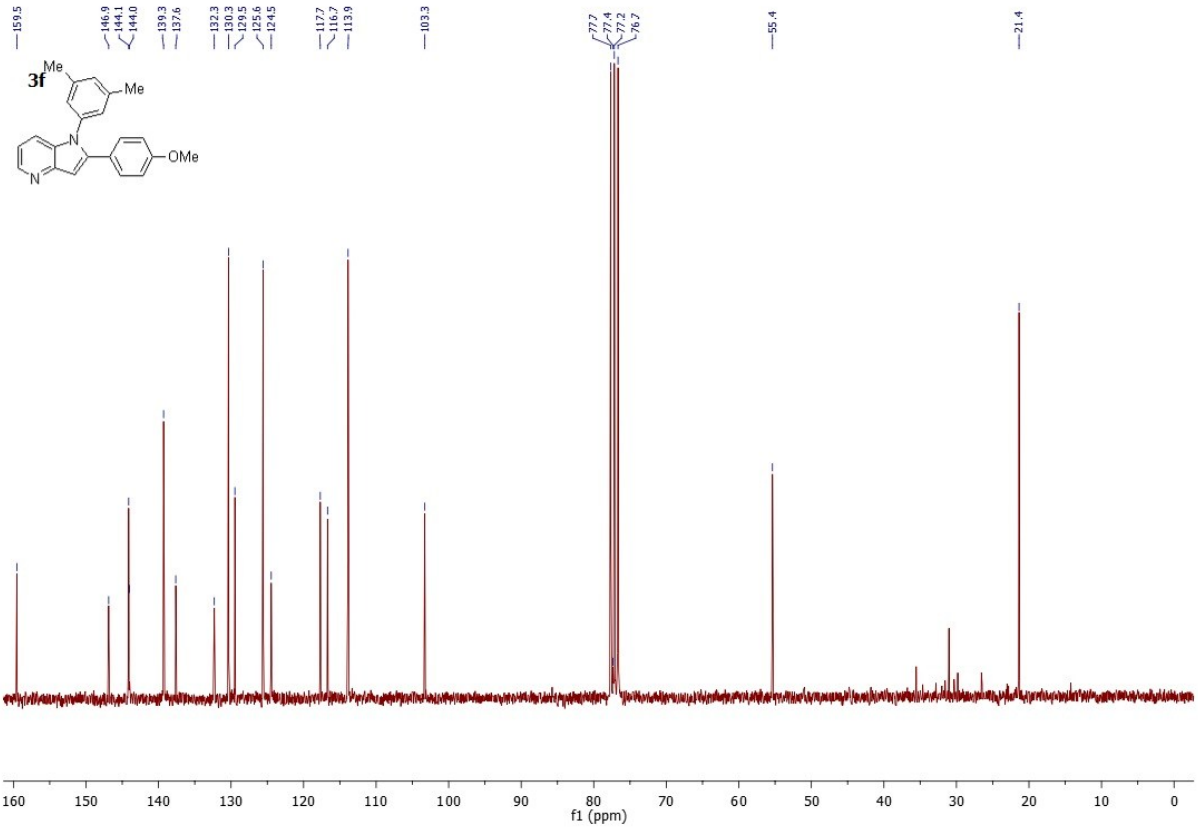
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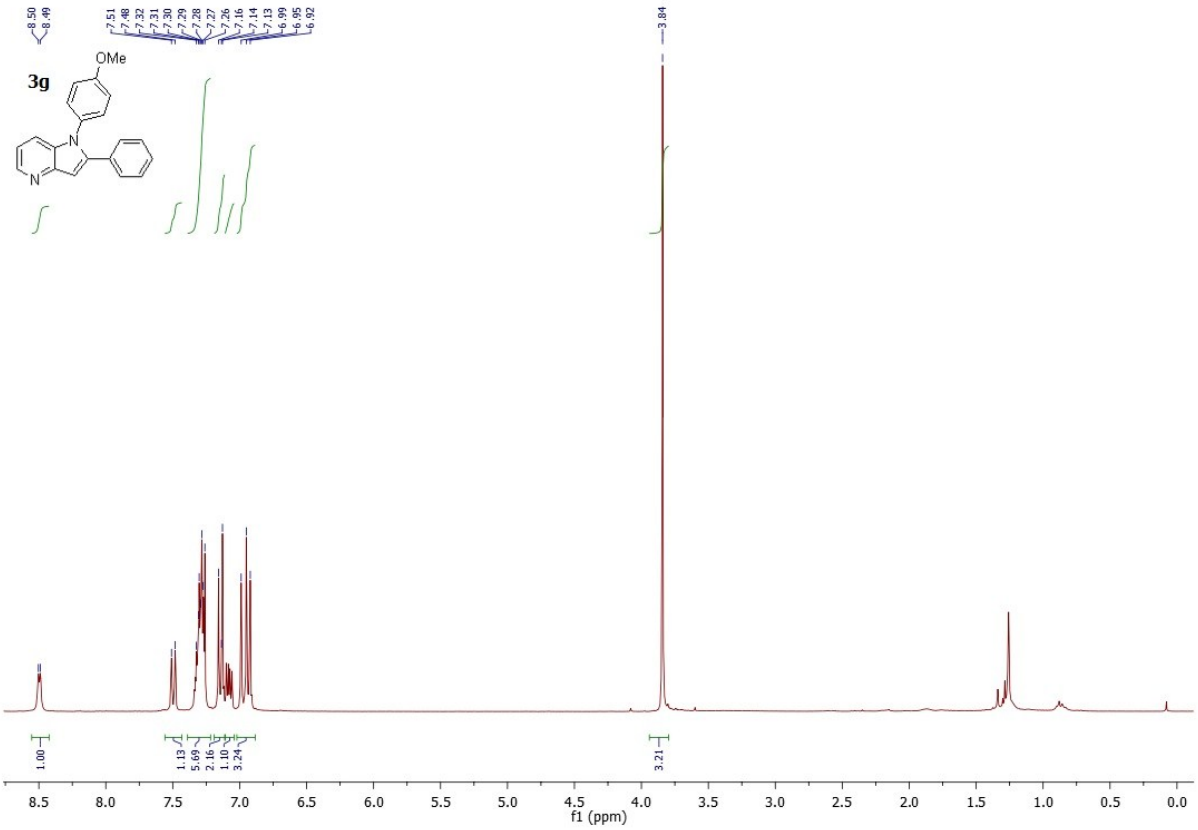
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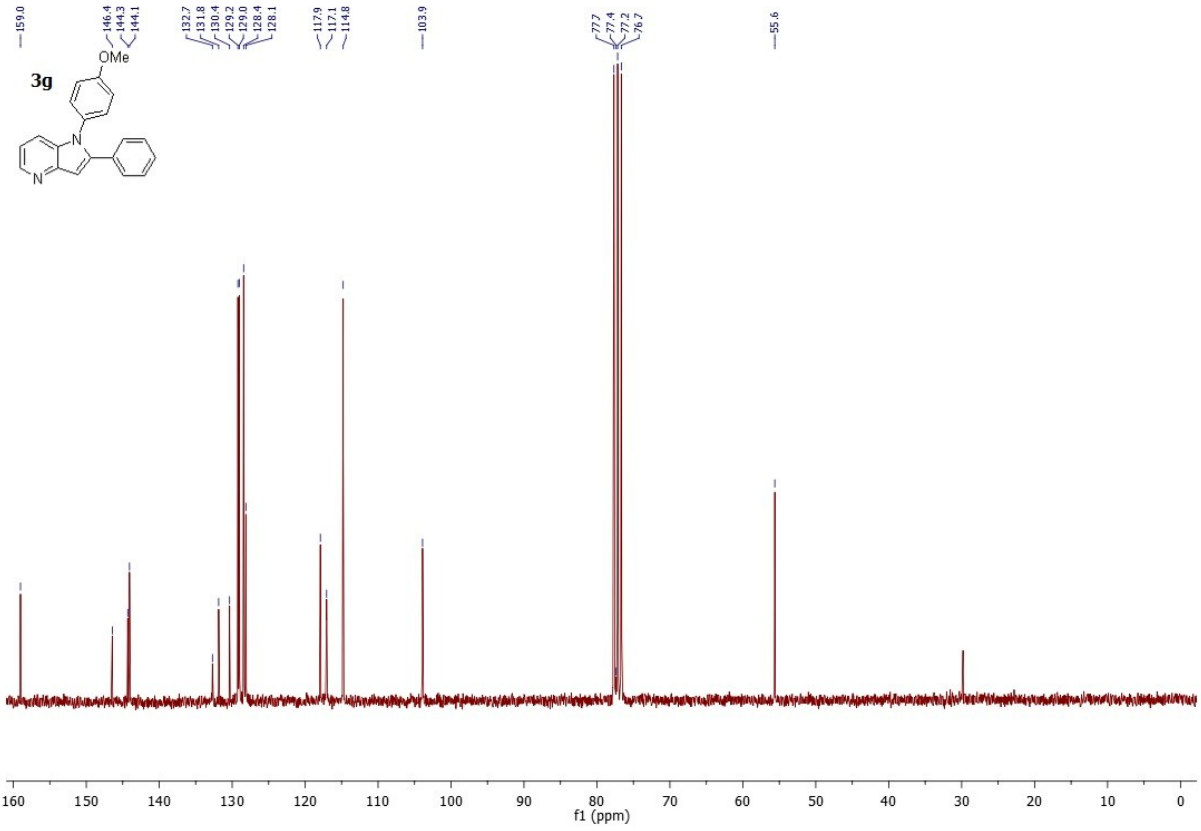
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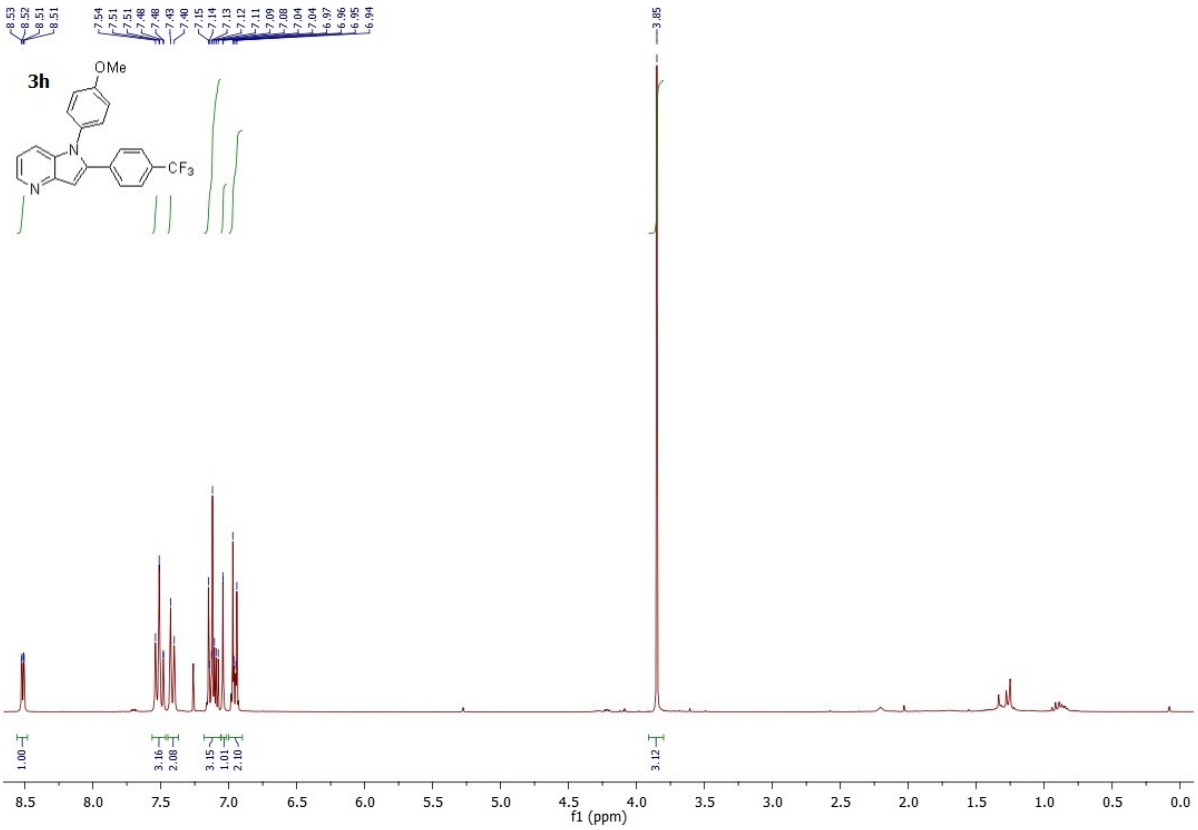
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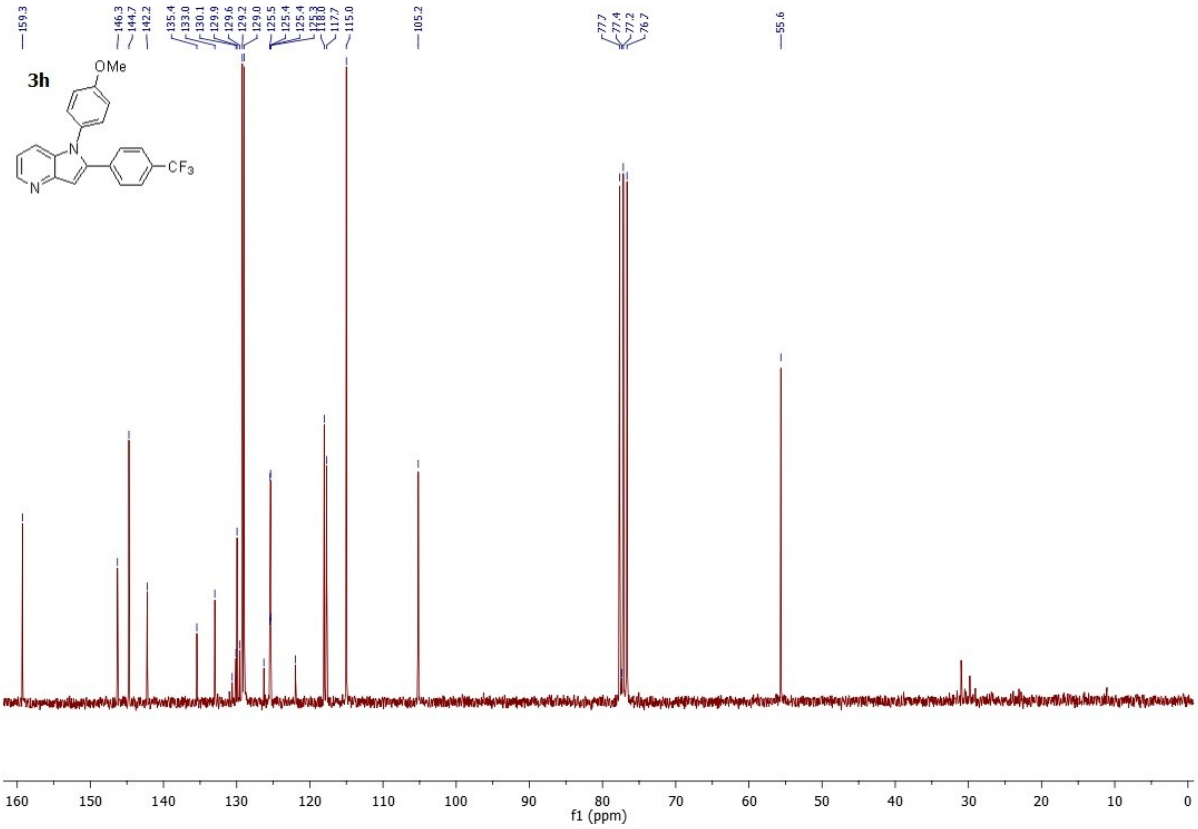
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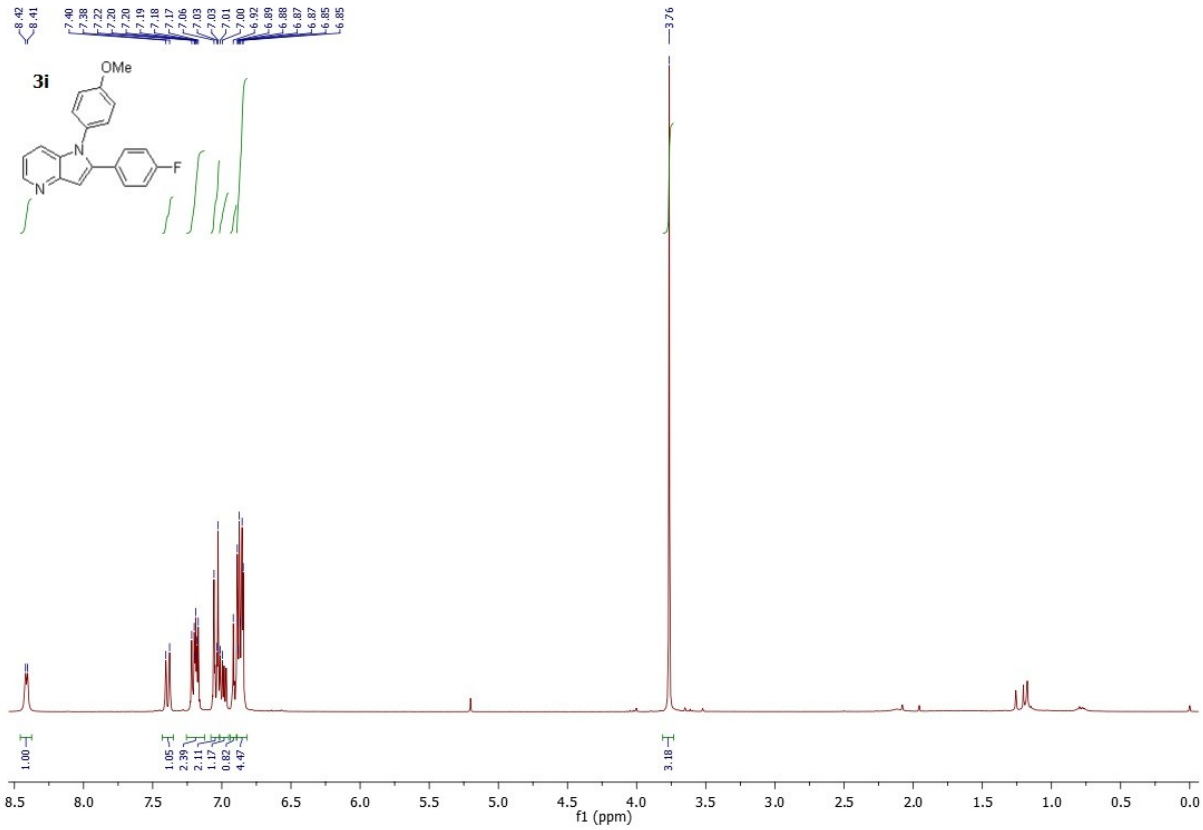
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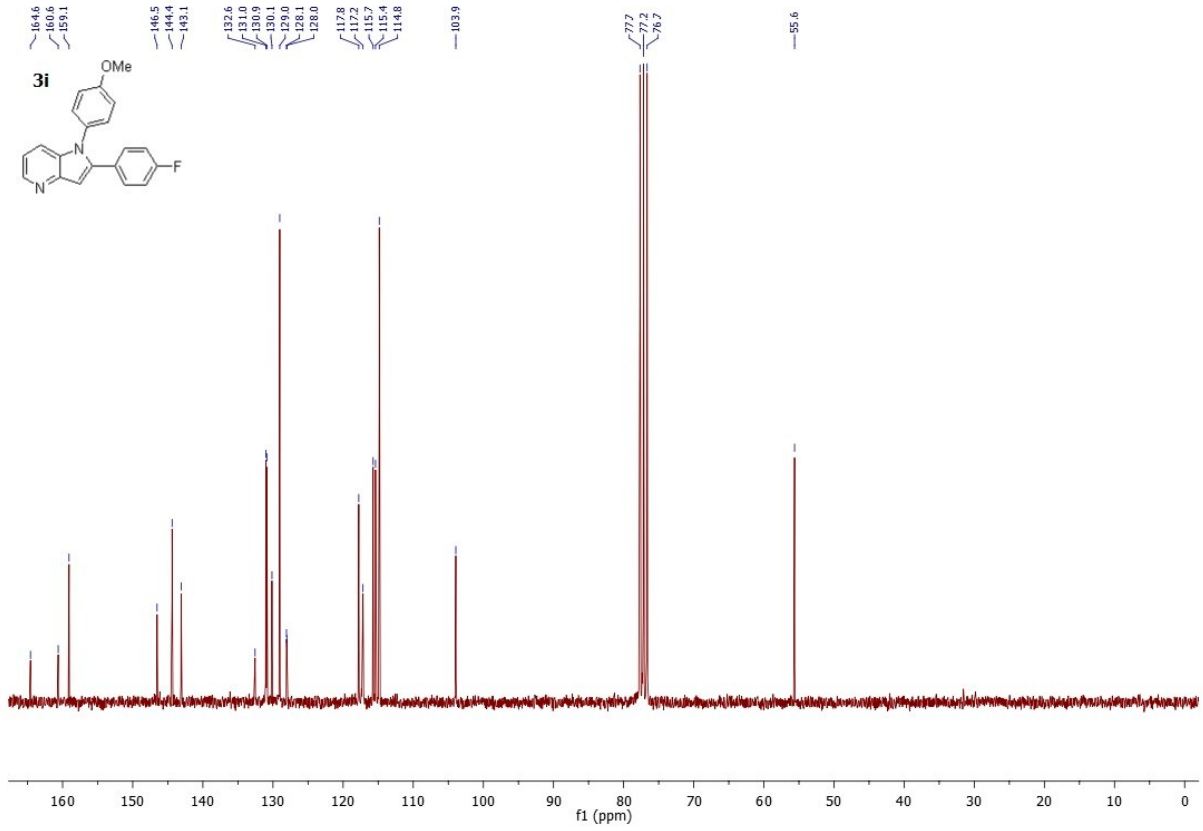
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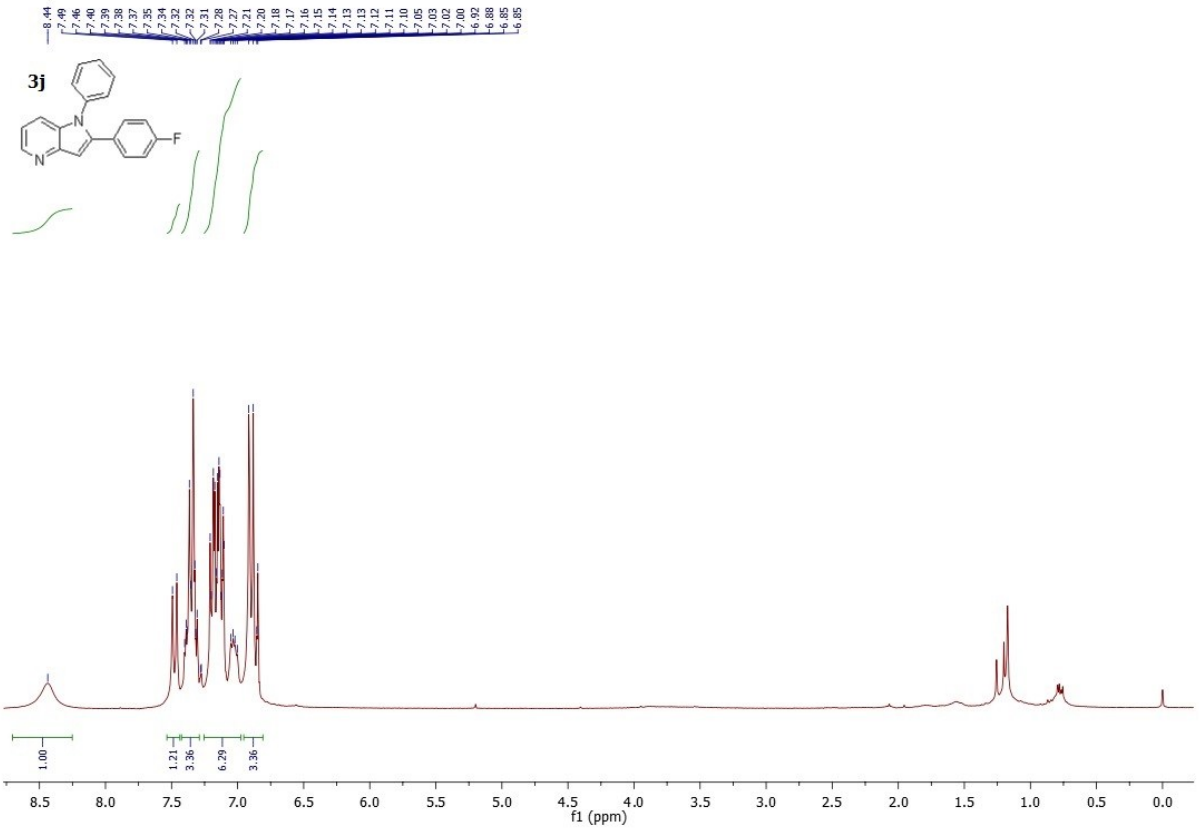
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1.0
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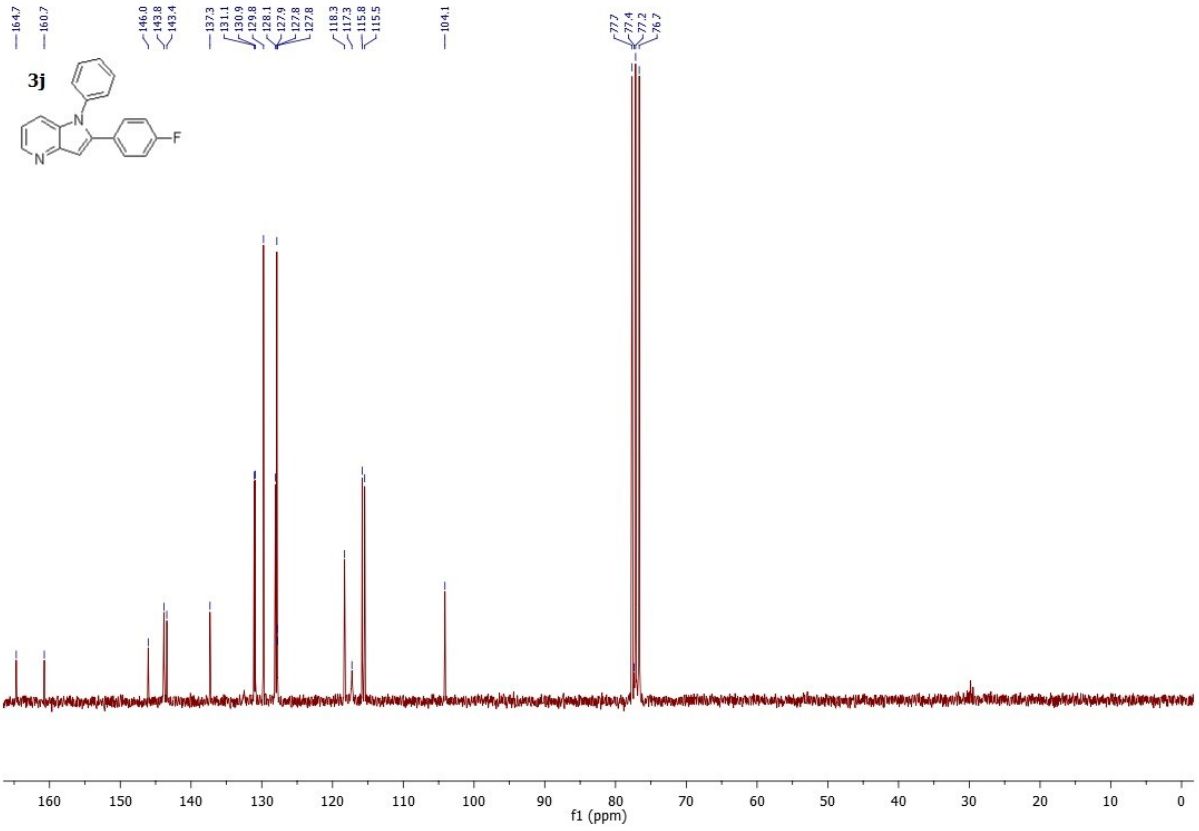
0.0
f1 (ppm)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143.4
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131.1
130.0
129.8
128.1
127.9
127.8
127.8
118.3
117.3
115.8
115.5
104.1
77.7
77.4
77.2
76.7
3j
F
N
160
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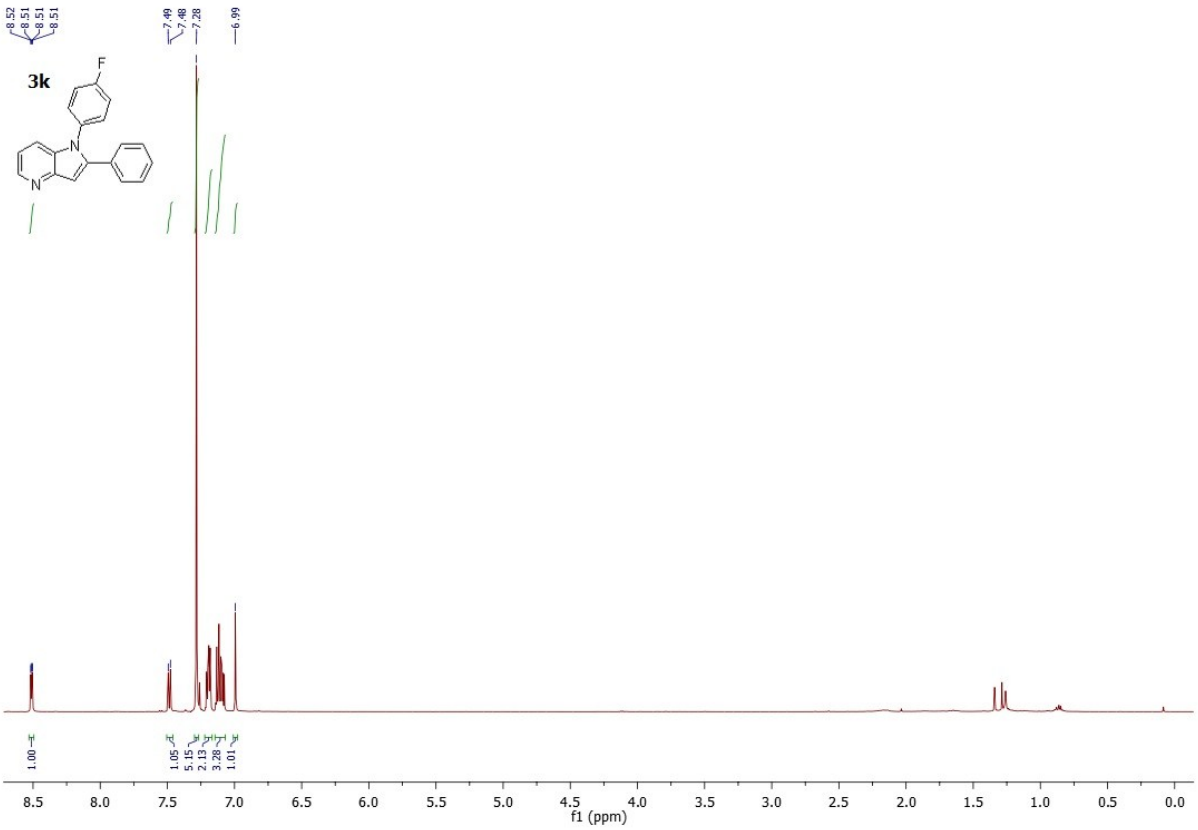
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.51
8.51
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7.48
7.28
6.99
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F
N
N
1.00
1.05
5.15
2.13
3.28
1.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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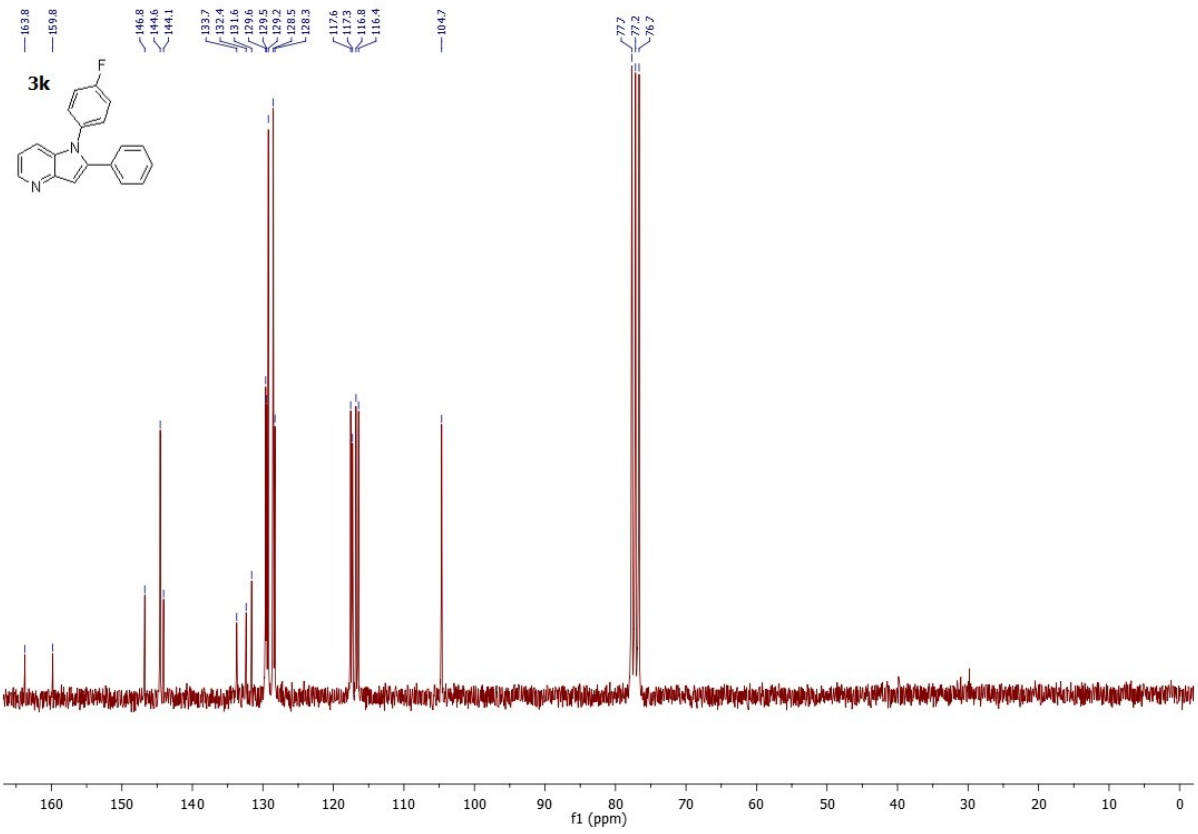
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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144.1
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132.4
131.6
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129.2
128.5
128.3
117.6
117.3
116.8
116.4
104.7
77.7
77.2
76.7
3k
F
N
N
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120
110
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90
80
70
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50
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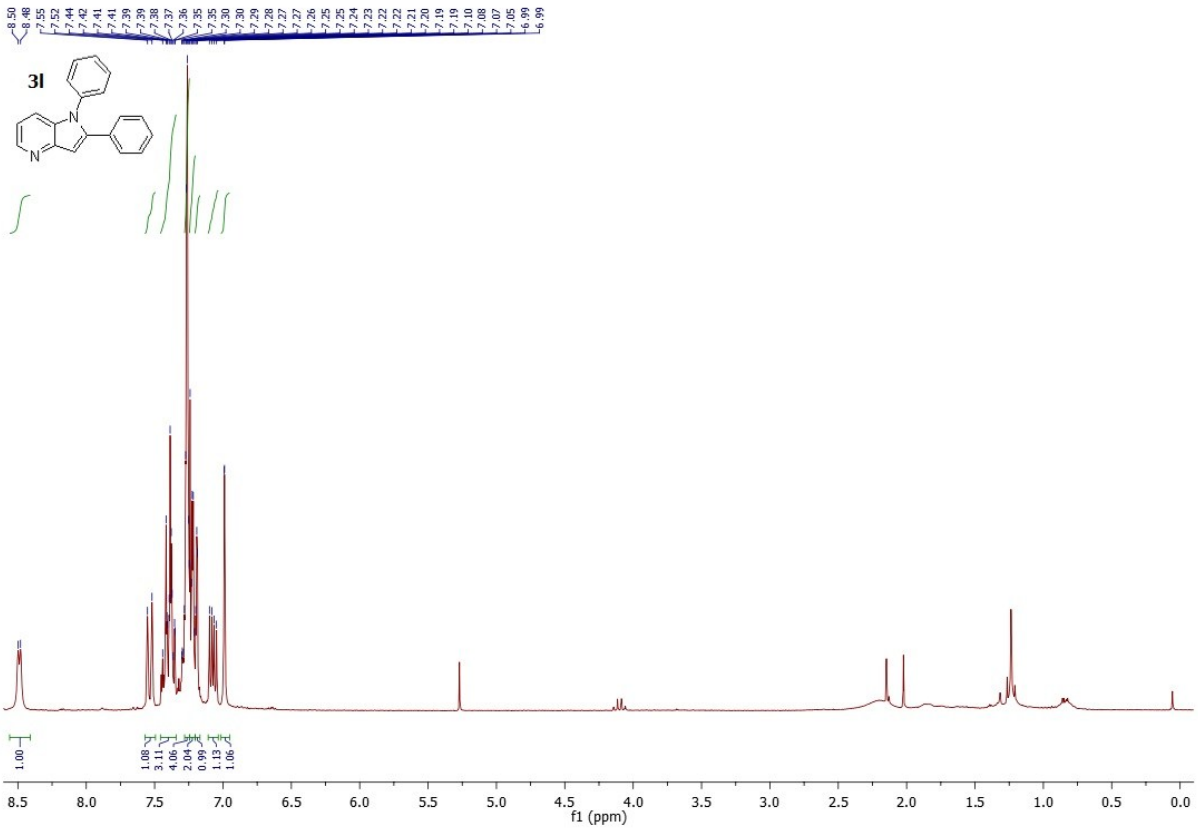
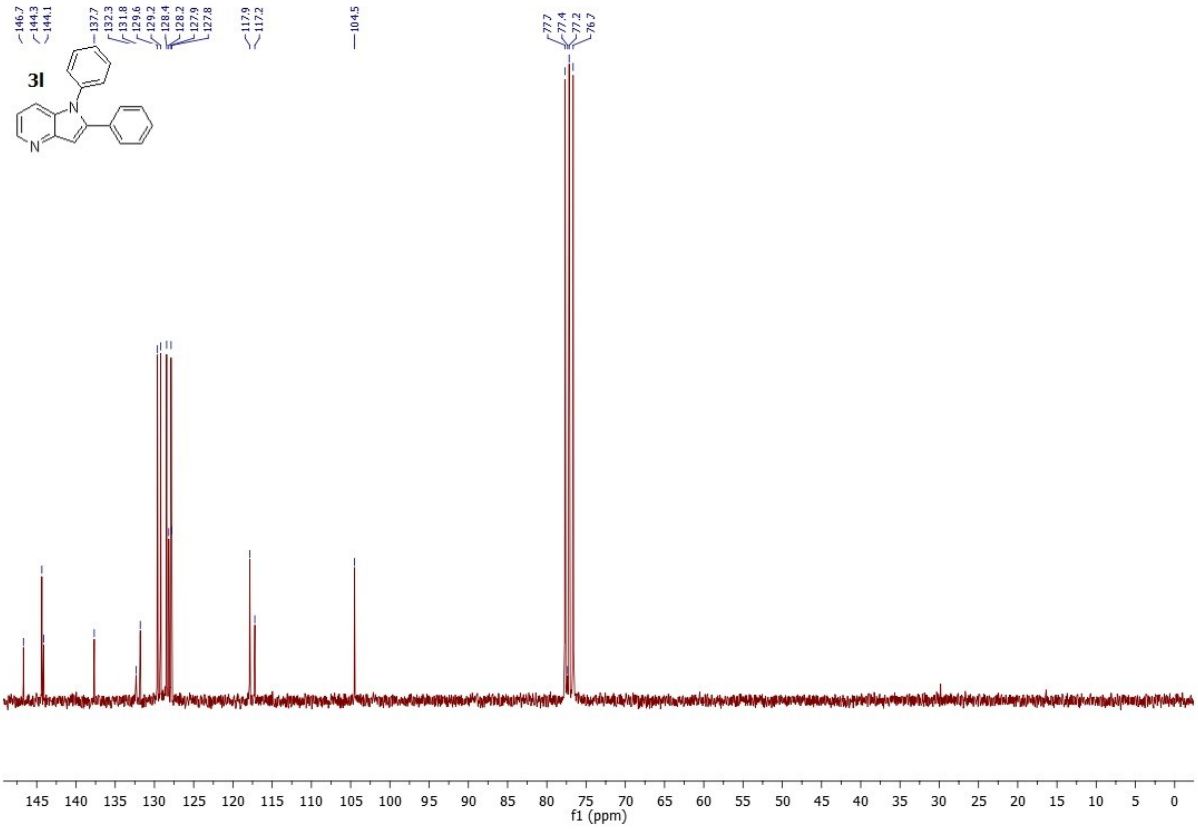
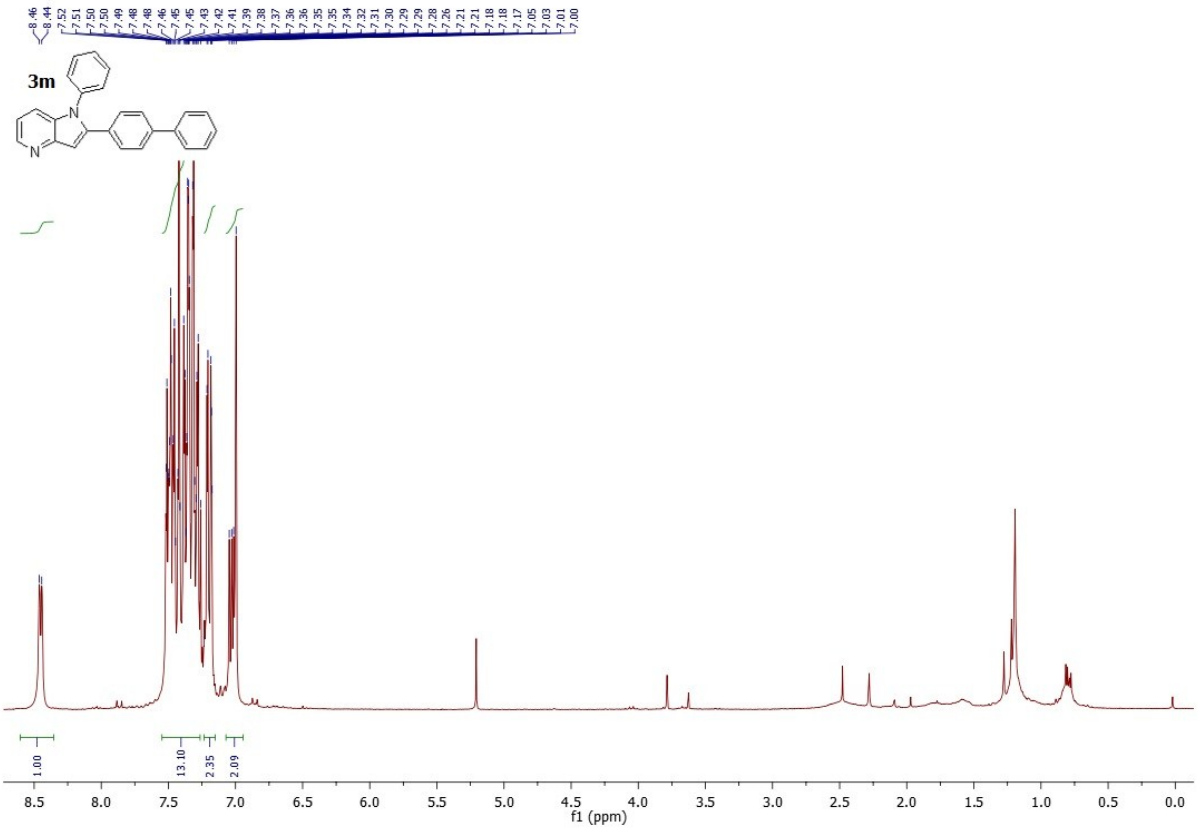
f1 (ppm)


3l
f1 (ppm)


3l
f1 (ppm)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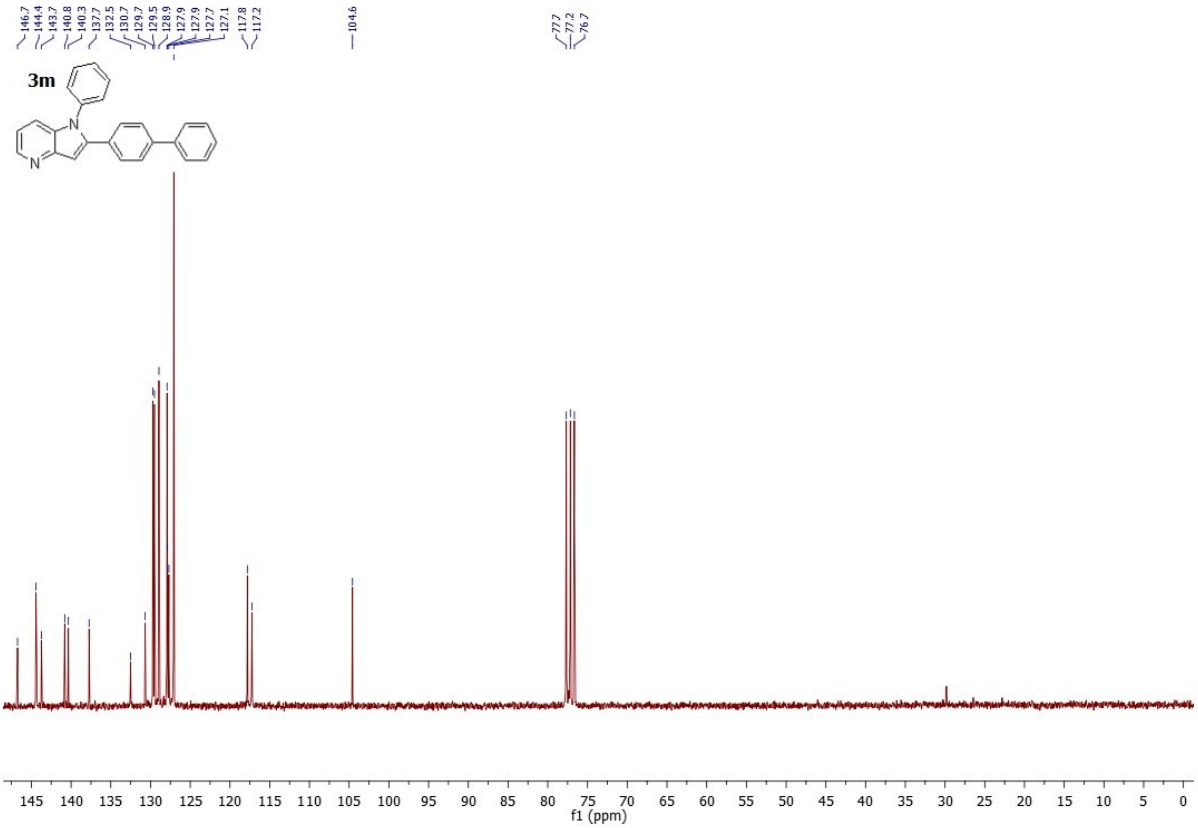
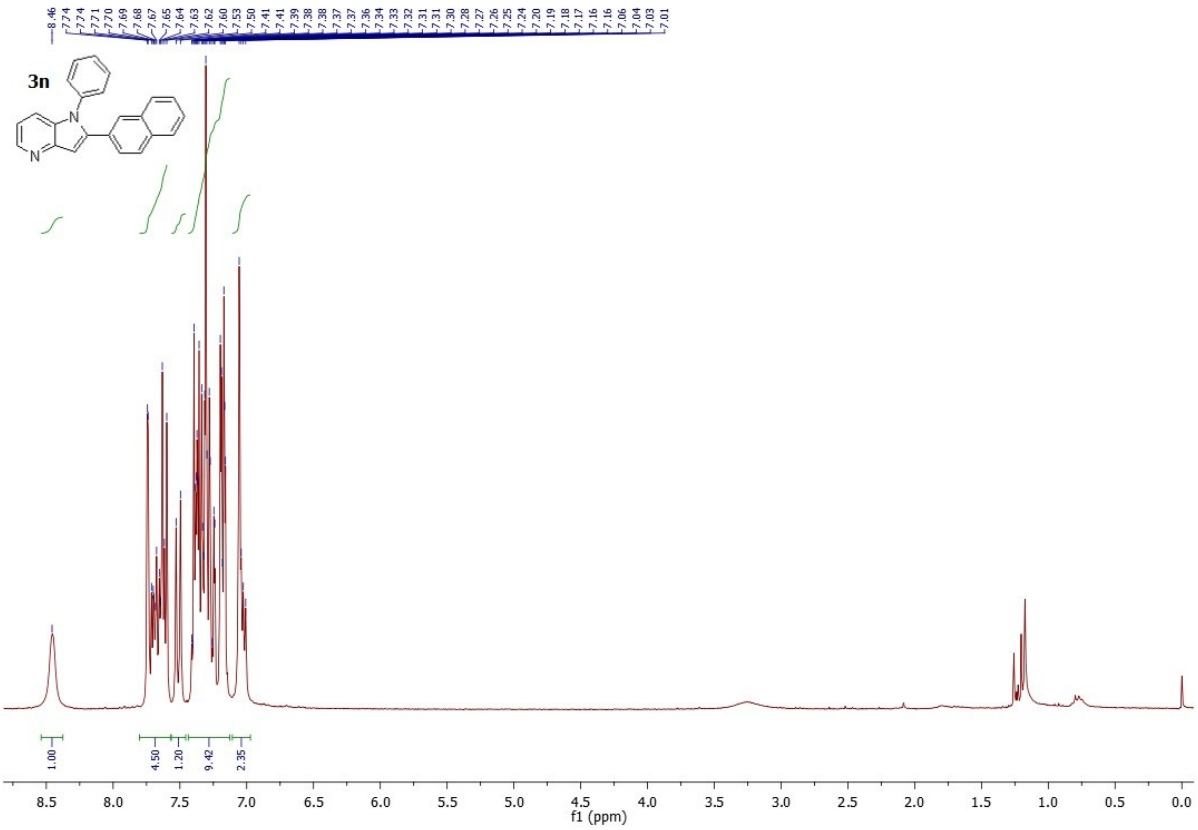
f1 (ppm)


3m
f1 (ppm)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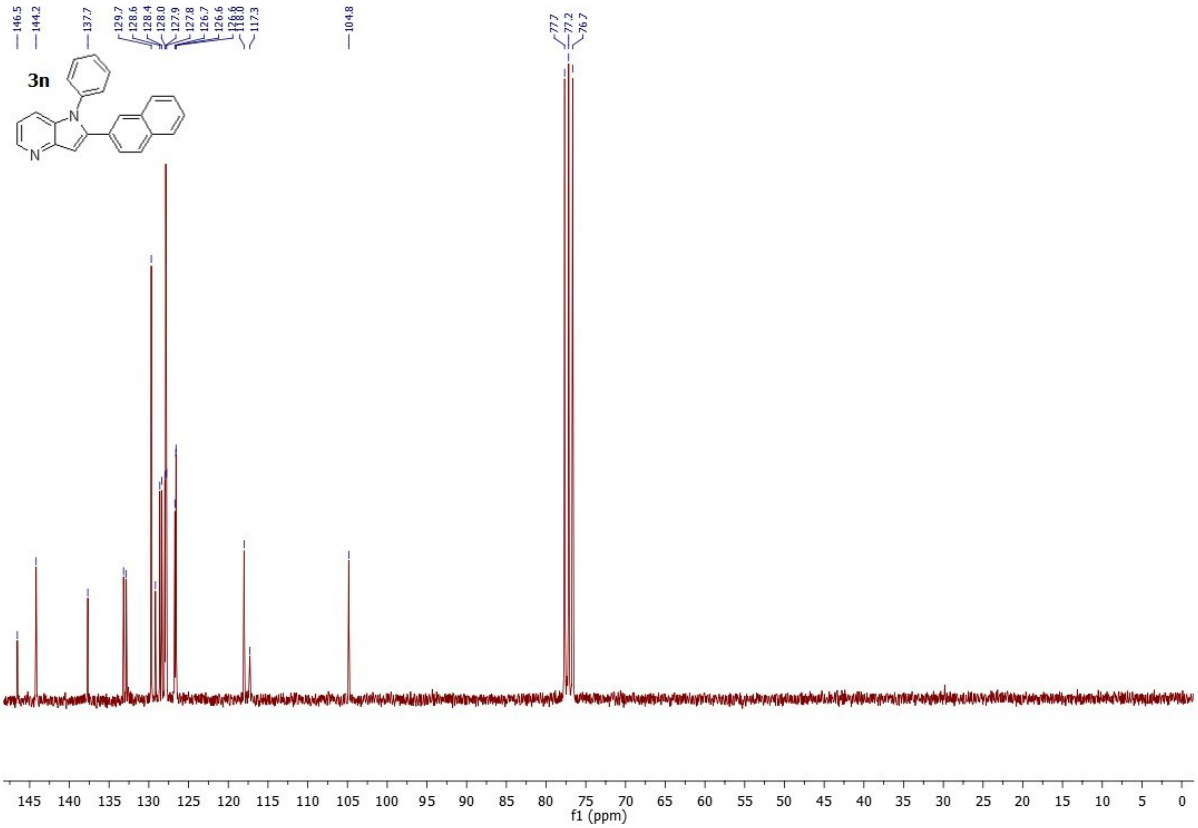
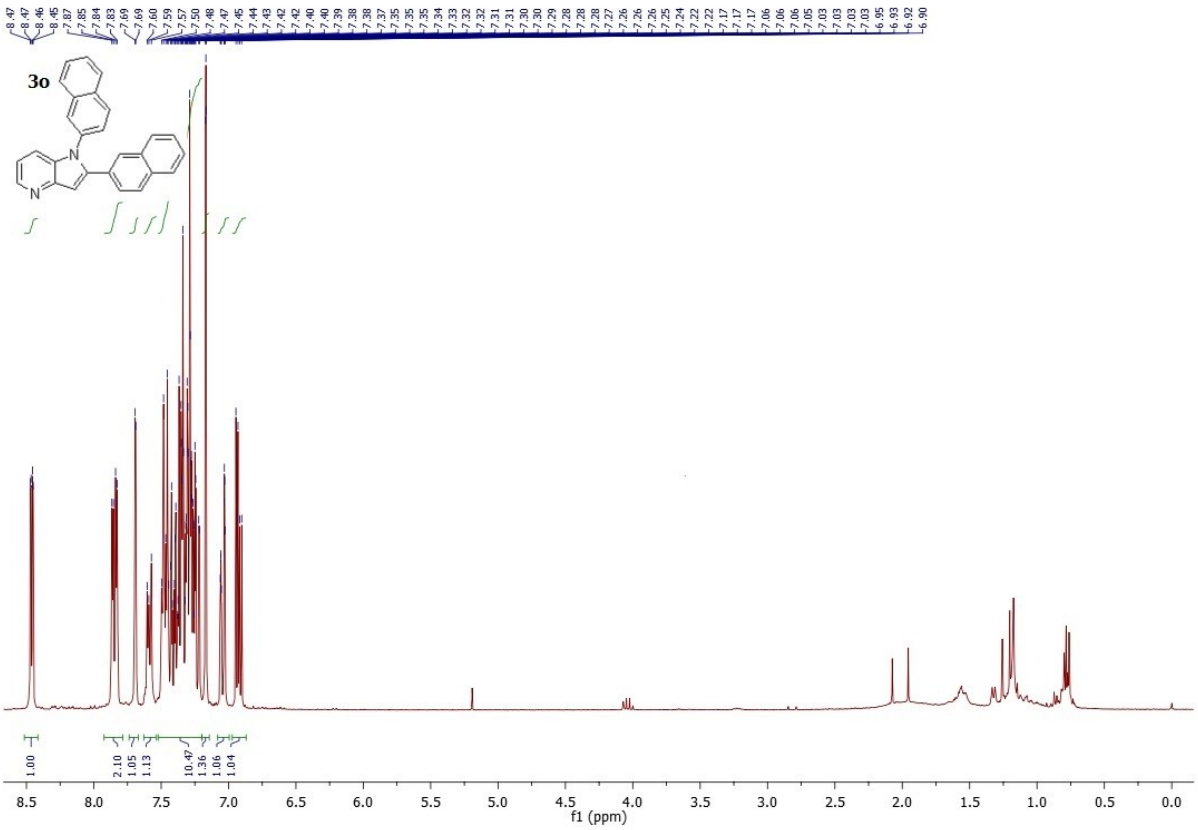
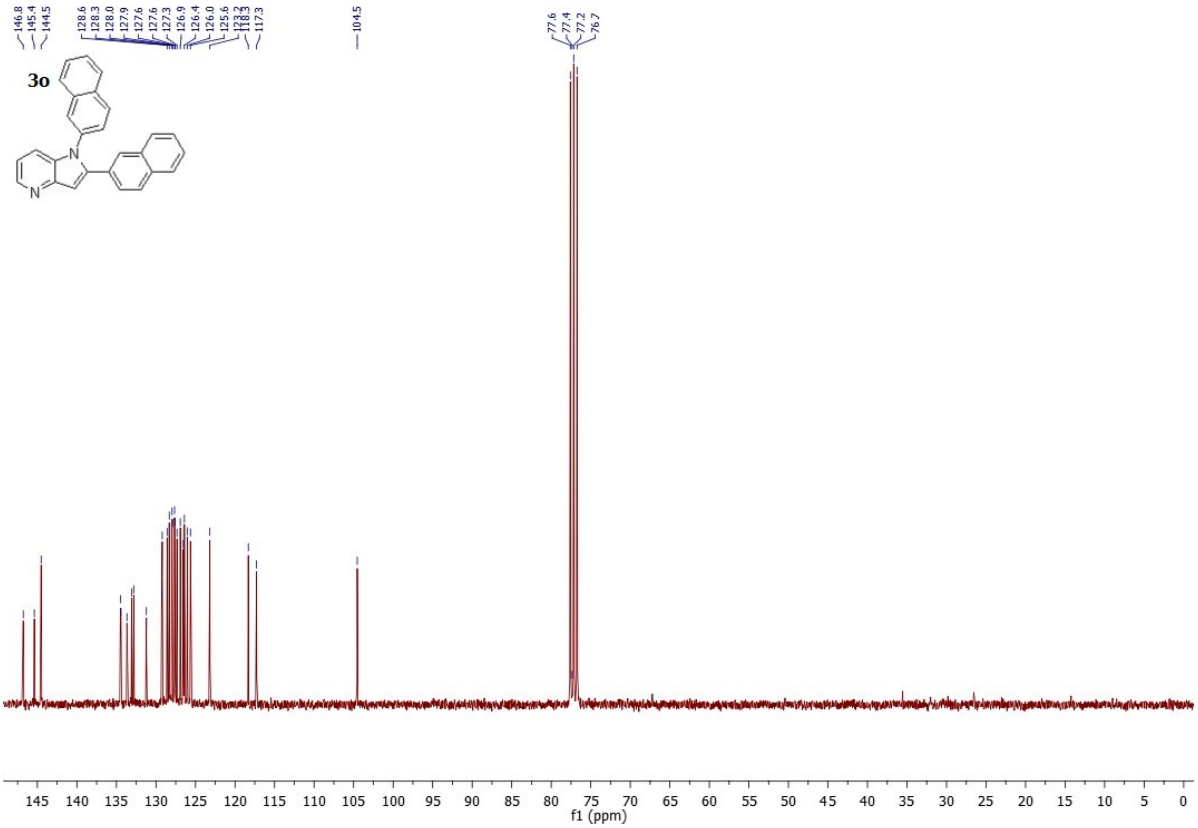
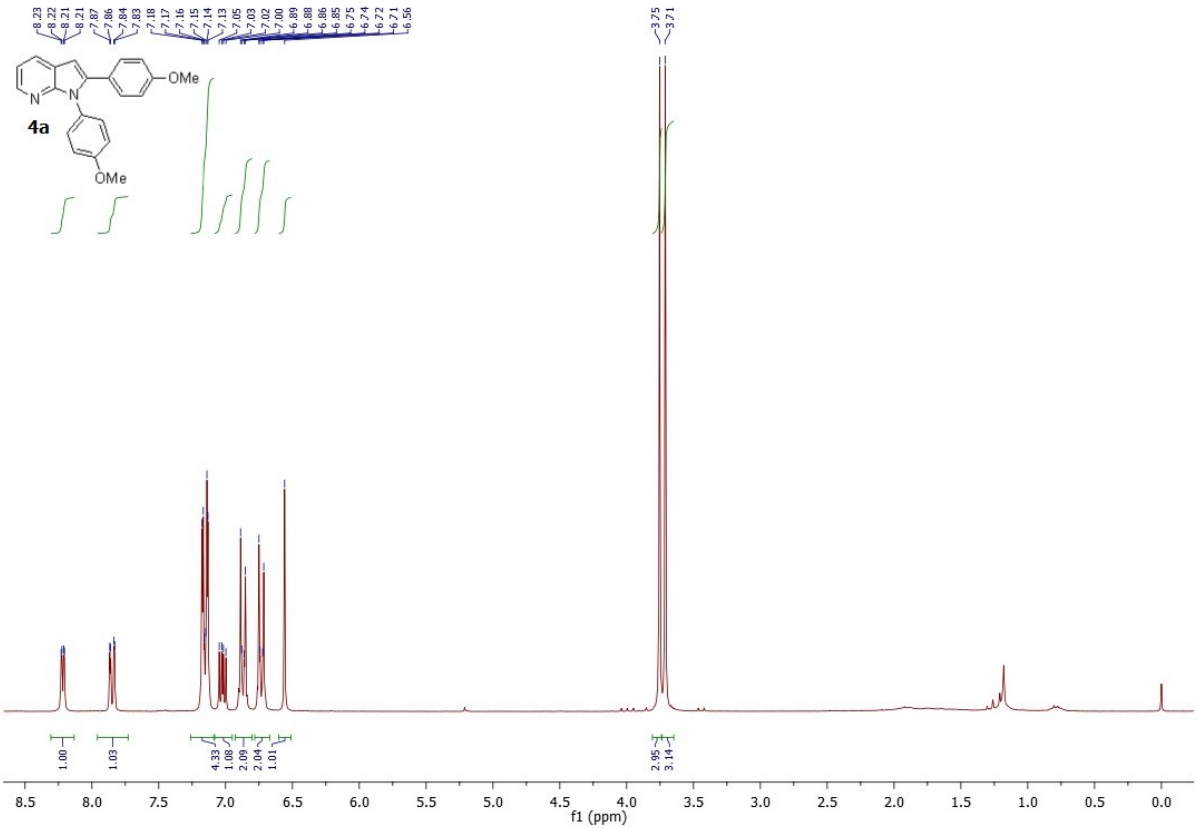
7.70
7.69
7.68
7.67
7.65
7.64
7.63
7.62
7.60
7.53
7.50
7.41
7.39
7.38
7.37
7.36
7.34
7.33
7.32
7.31
7.30
7.28
7.27
7.26
7.25
7.24
7.20
7.19
7.18
7.17
7.16
7.06
7.04
7.03
7.01
1.00
4.50
1.20
9.42
2.35
f1 (ppm)

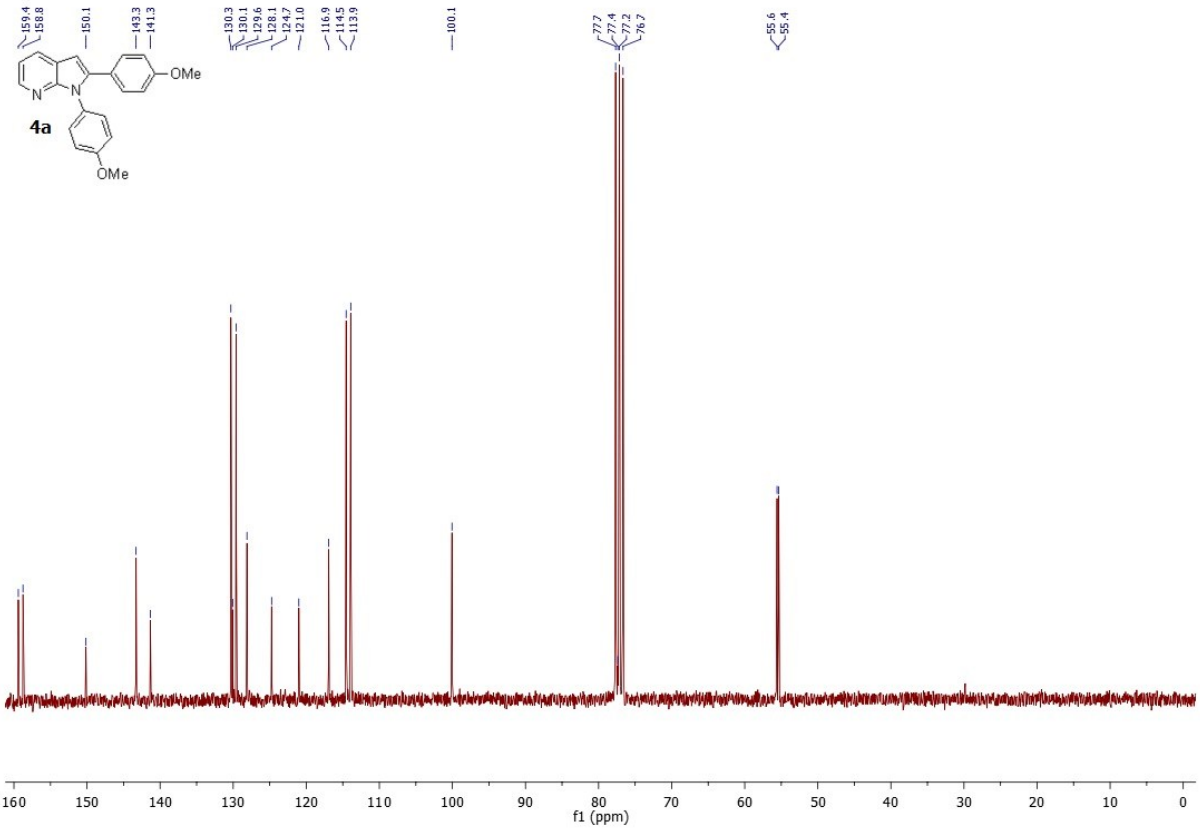

3n
146.5
144.2
137.7
129.7
128.6
128.4
128.0
127.9
127.8
126.7
126.6
118.0
117.3
104.8
77.7
77.2
76.7
f1 (ppm)

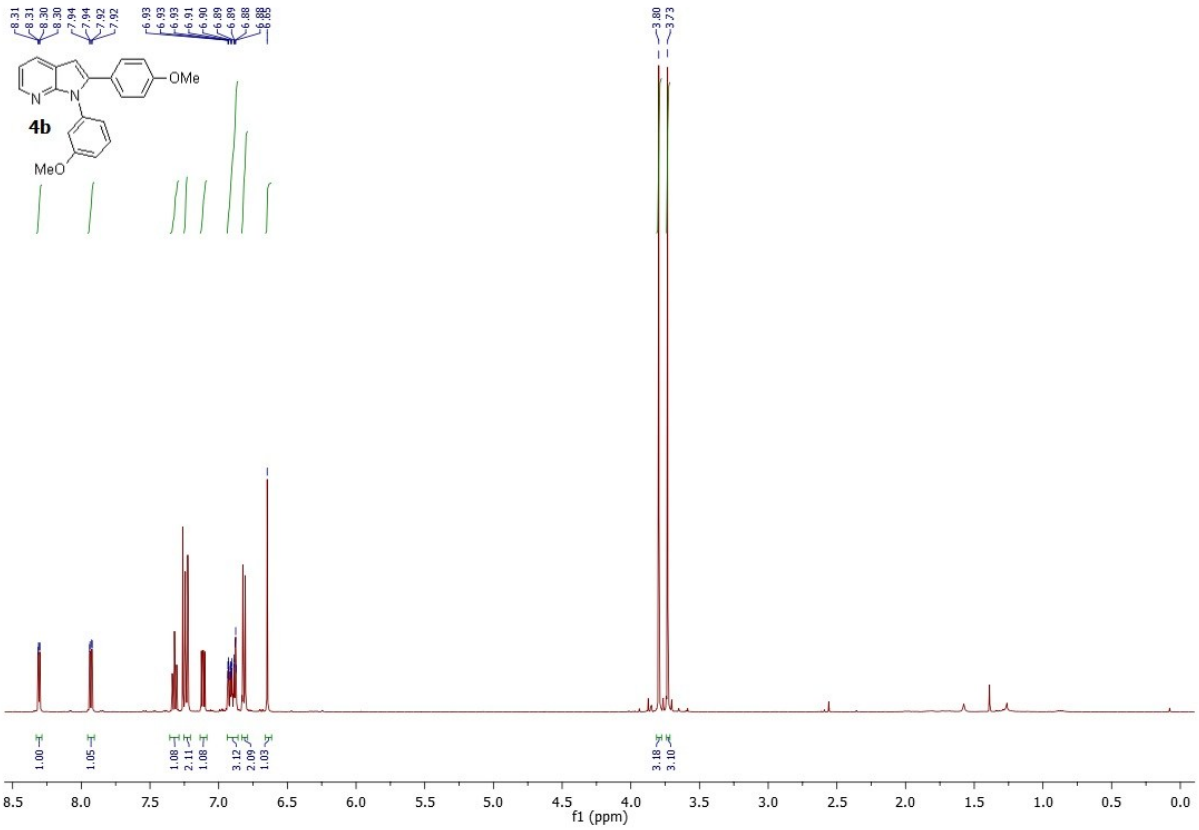

3o
f1 (ppm)


3o
f1 (ppm)

4.2. 7-Azaindoles



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8.30
8.30
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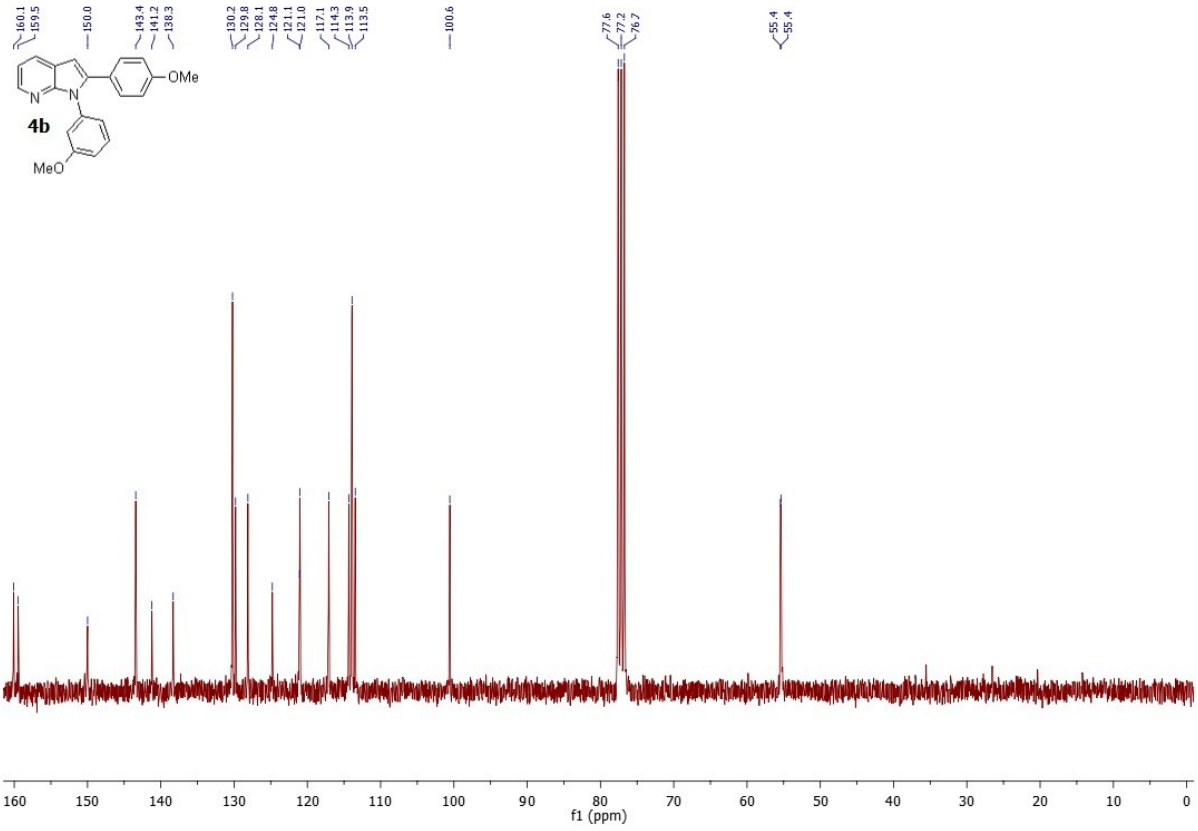
7.94
7.92
7.92
6.93
6.93
6.93
6.91
6.90
6.89
6.89
6.88
6.88
6.85
3.80
3.73
OMe
4b
MeO
1.00
1.05
1.08
2.11
1.08
3.12
2.09
1.03
3.18
3.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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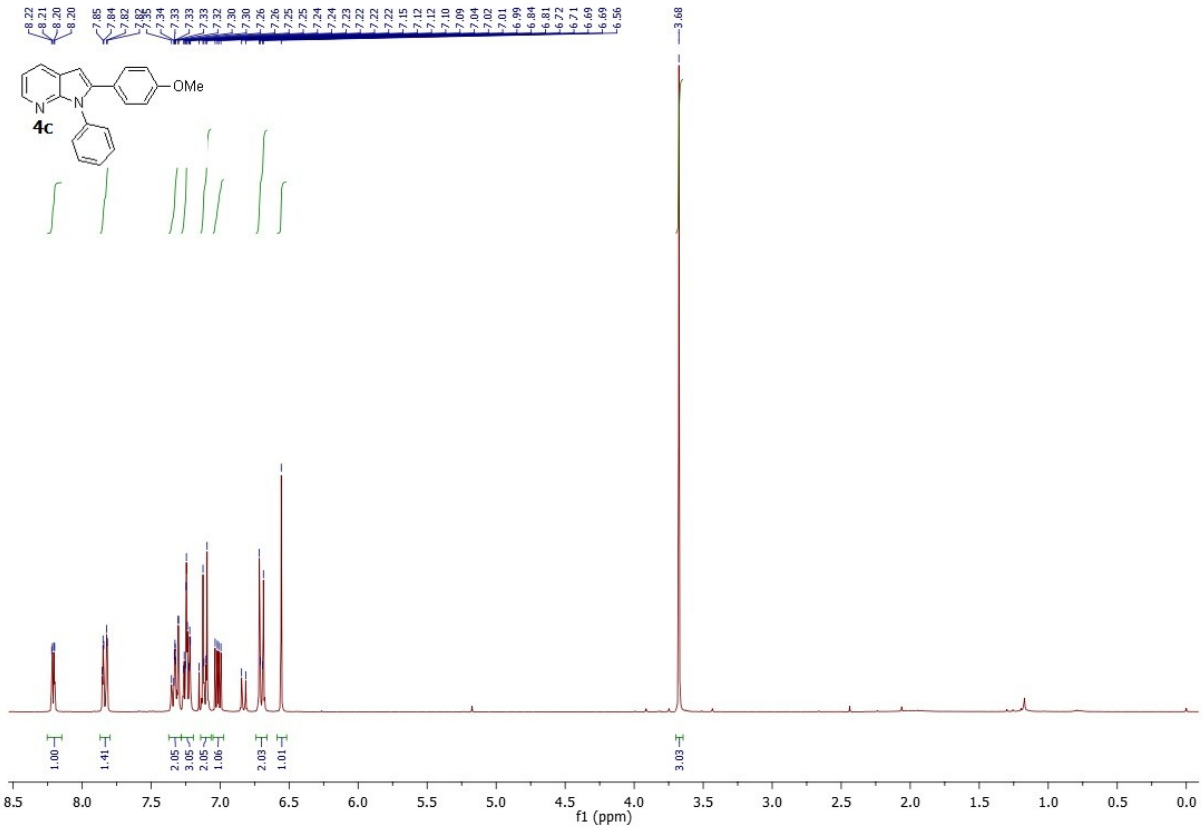
159.5
150.0
143.4
141.2
138.3
130.2
129.8
128.1
124.8
121.1
121.0
117.1
114.3
113.9
113.5
100.6
77.6
77.2
76.7
55.4
55.4
OMe
4b
MeO
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.82
7.82
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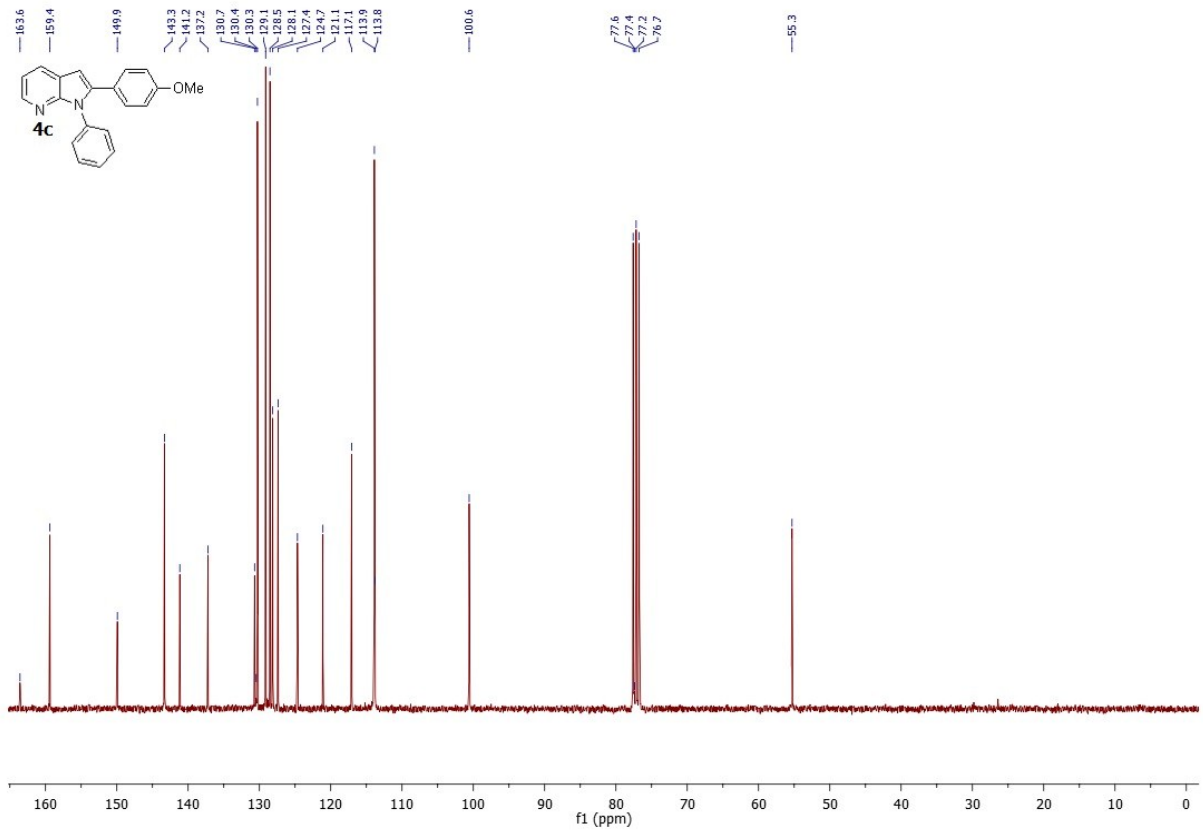
7.34
7.33
7.33
7.33
7.32
7.30
7.30
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.22
7.22
7.15
7.12
7.12
7.10
7.09
7.04
7.02
7.01
6.99
6.84
6.81
6.72
6.71
6.69
6.69
6.56
3.68
OMe
4c
1.00
1.41
2.05
3.05
2.05
1.06
2.03
1.01
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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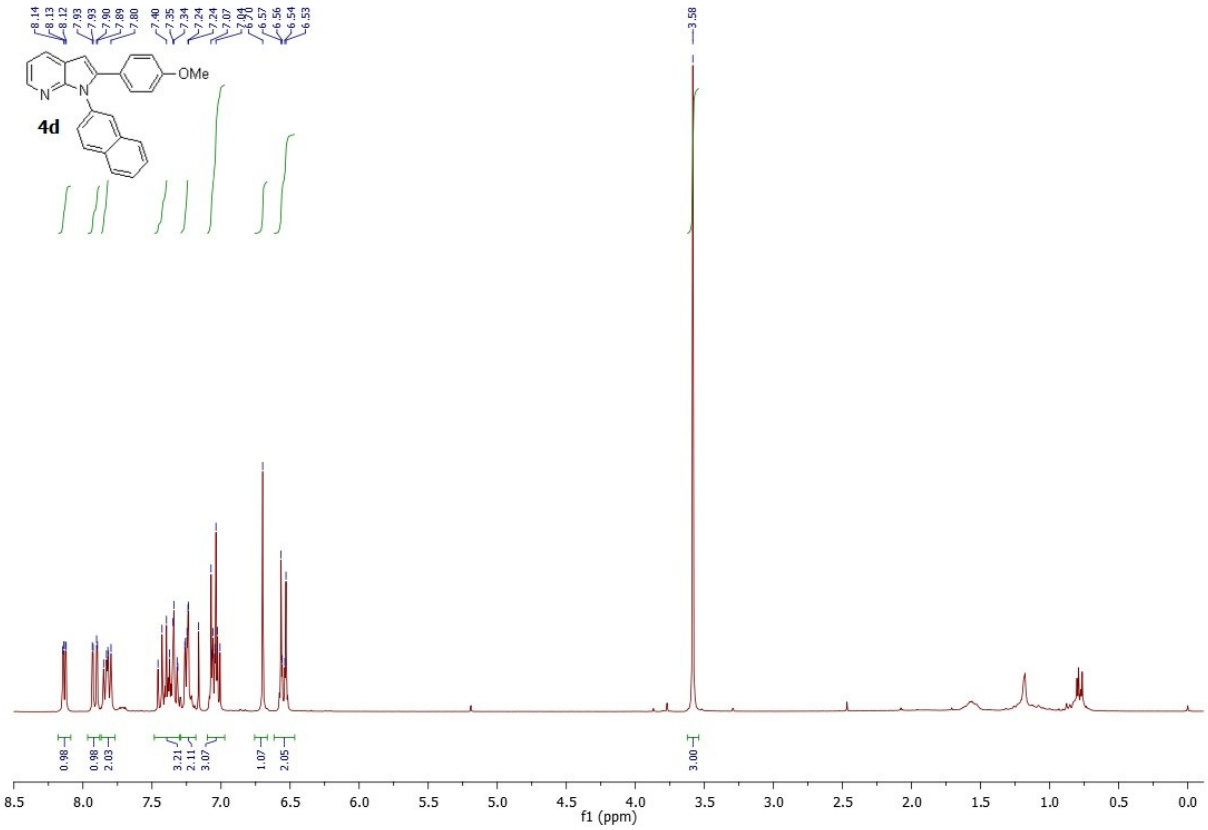
130.4
130.3
129.1
128.5
128.1
127.4
124.7
121.1
117.1
113.9
113.8
100.6
77.6
77.4
77.2
76.7
55.3
OMe
4c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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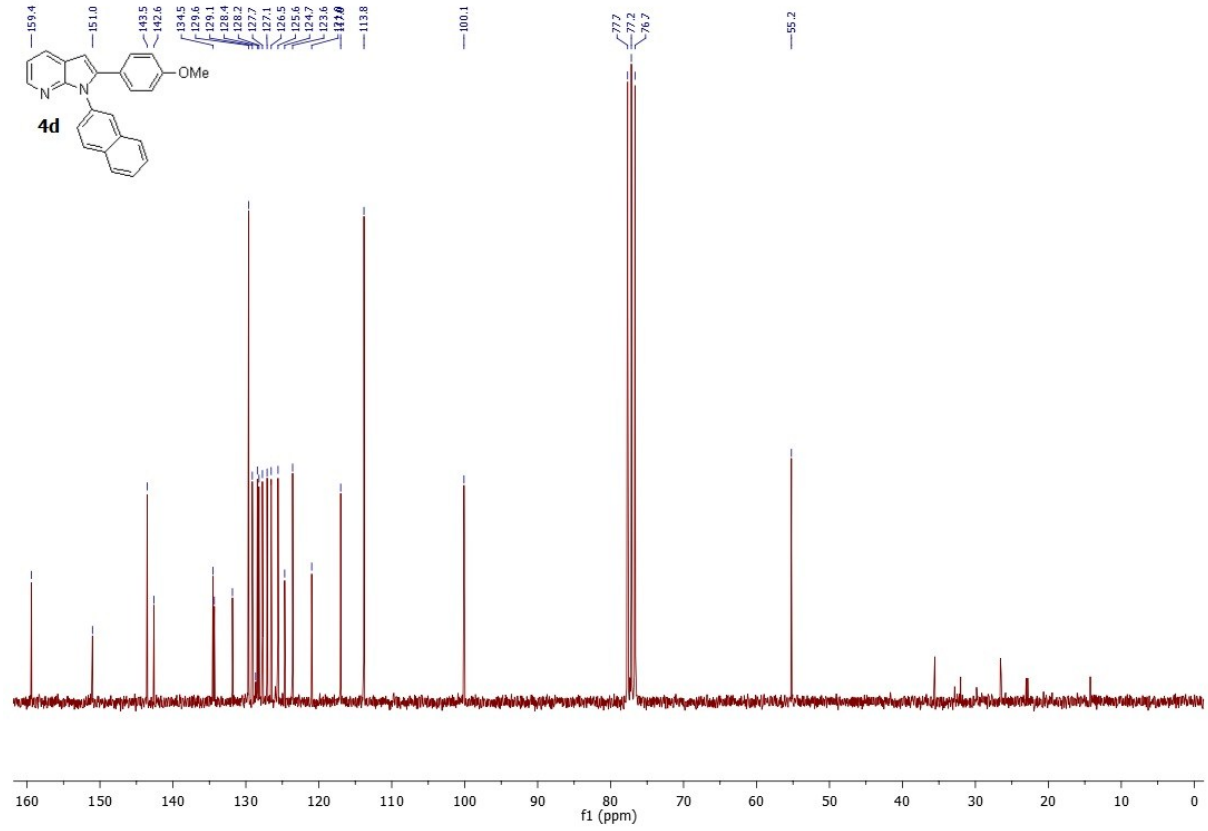
7.35
7.34
7.24
7.24
7.07
6.57
6.56
6.54
6.53
3.58
OMe
4d
0.98
0.98
2.03
3.21
2.11
3.07
1.07
2.05
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.1
128.4
128.2
127.7
127.1
126.5
125.6
124.7
123.6
113.8
100.1
77.7
77.2
76.7
55.2
OMe
4d
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150
140
130
120
110
100
90
80
70
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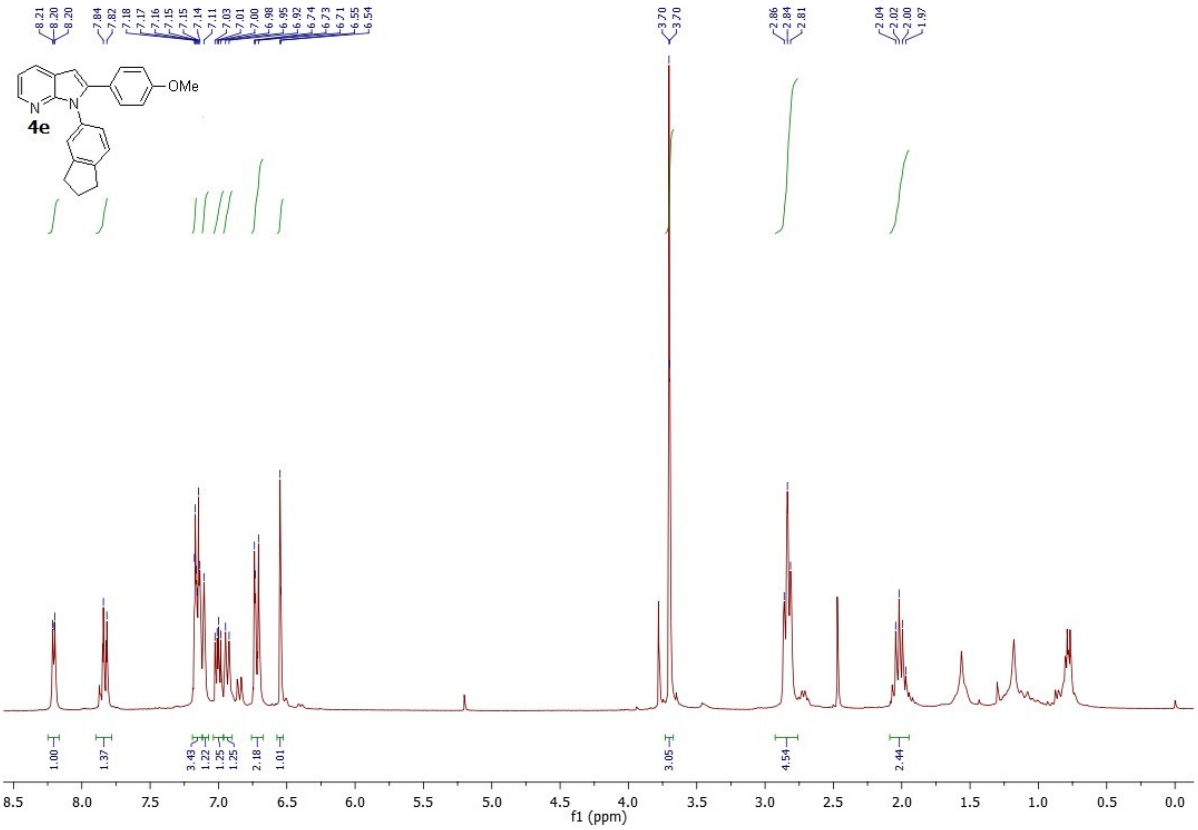
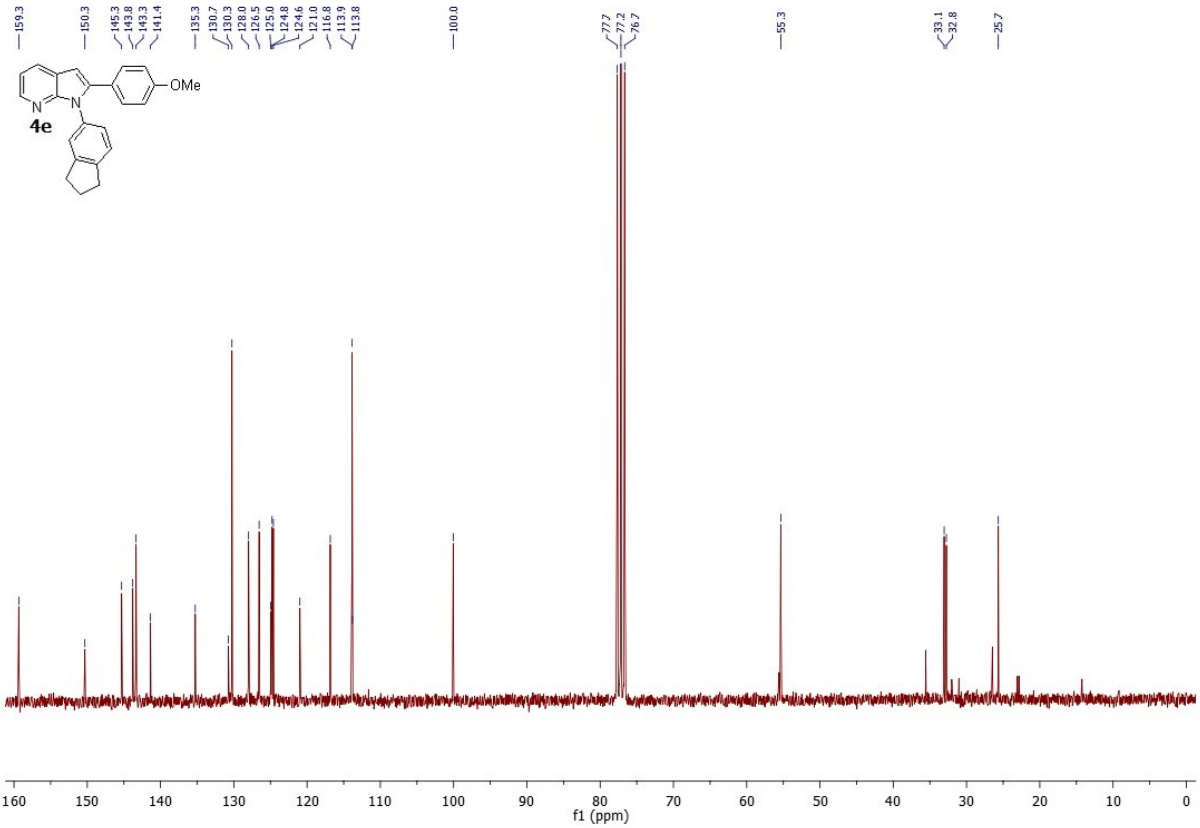
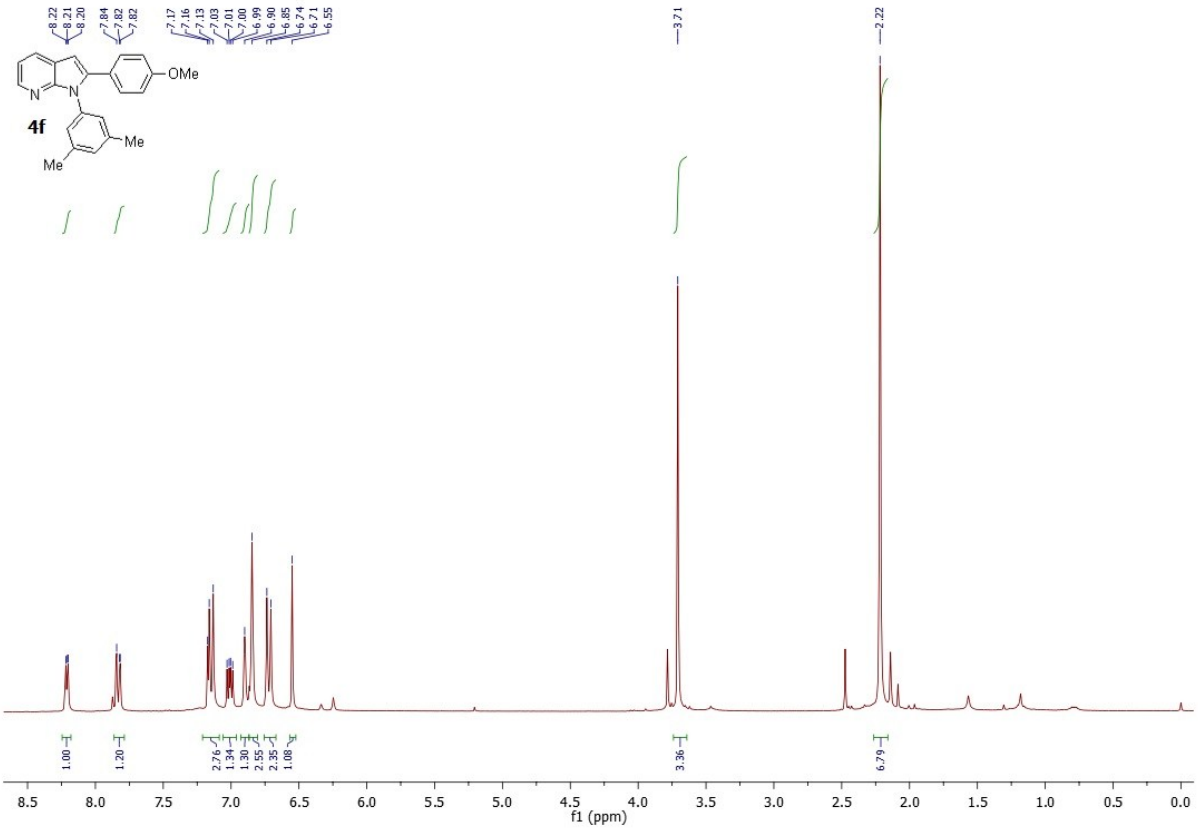
50
40
30
20
10
0
f1 (ppm)


OMe
4e
f1 (ppm)


OMe
4e
f1 (ppm)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7.82
7.17
7.16
7.13
7.03
7.01
7.00
6.99
6.90
6.85
6.74
6.71
6.55
3.71
2.22
OMe
4f
Me
Me
1.00
1.20
2.76
1.34
1.30
2.55
2.35
1.08
3.36
6.79
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
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1.0
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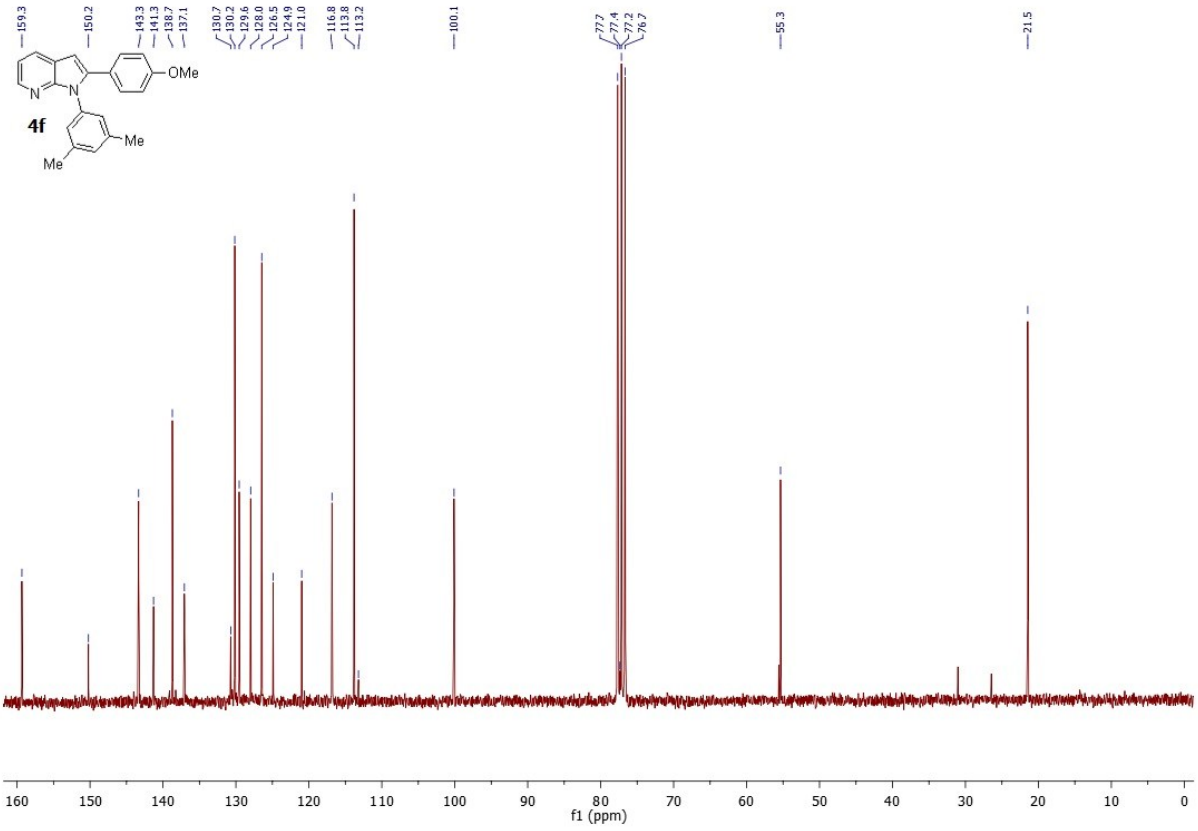
0.0
f1 (ppm)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137.1
130.7
130.2
129.6
128.0
126.5
124.9
121.0
116.8
113.8
113.2
100.1
77.7
77.4
77.2
76.7
55.3
21.5
OMe
4f
Me
Me
160
150
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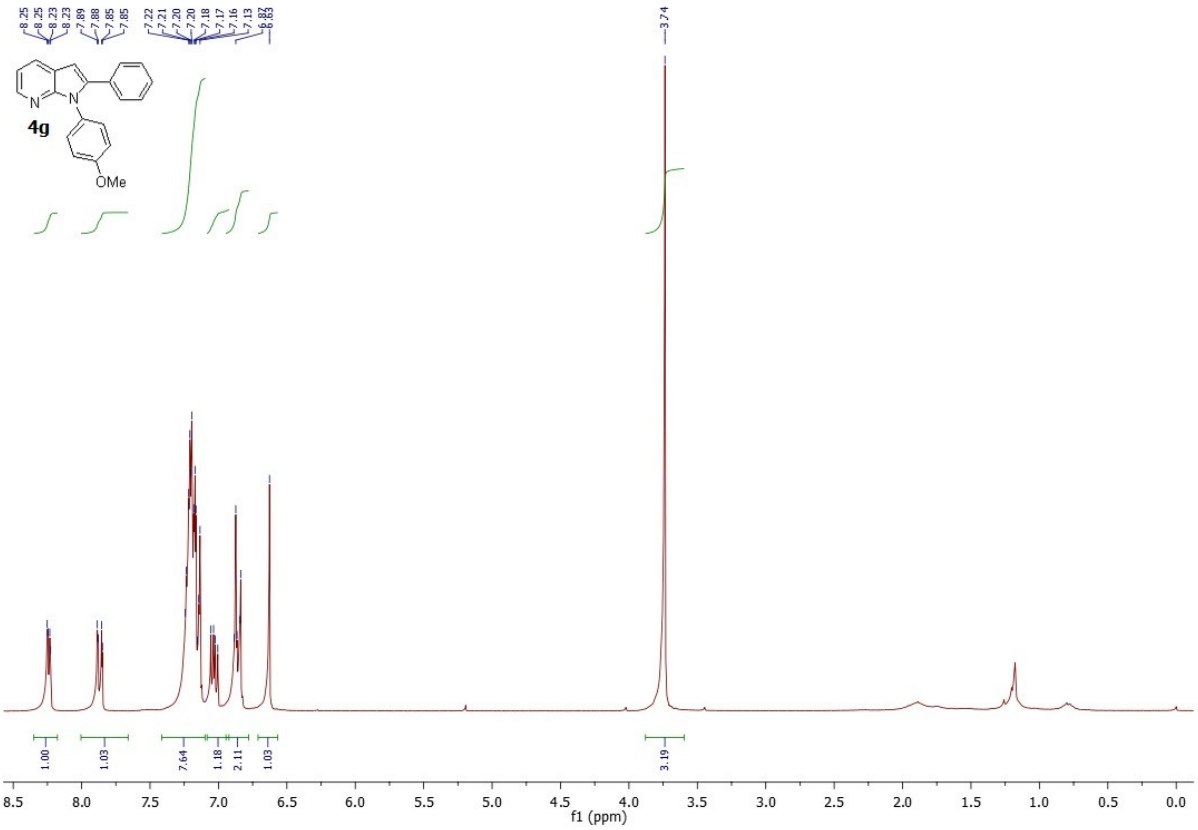
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.85
7.22
7.21
7.20
7.20
7.18
7.17
7.16
7.13
6.87
6.83
3.74
4g
OMe
1.00
1.03
7.64
1.18
2.11
1.03
3.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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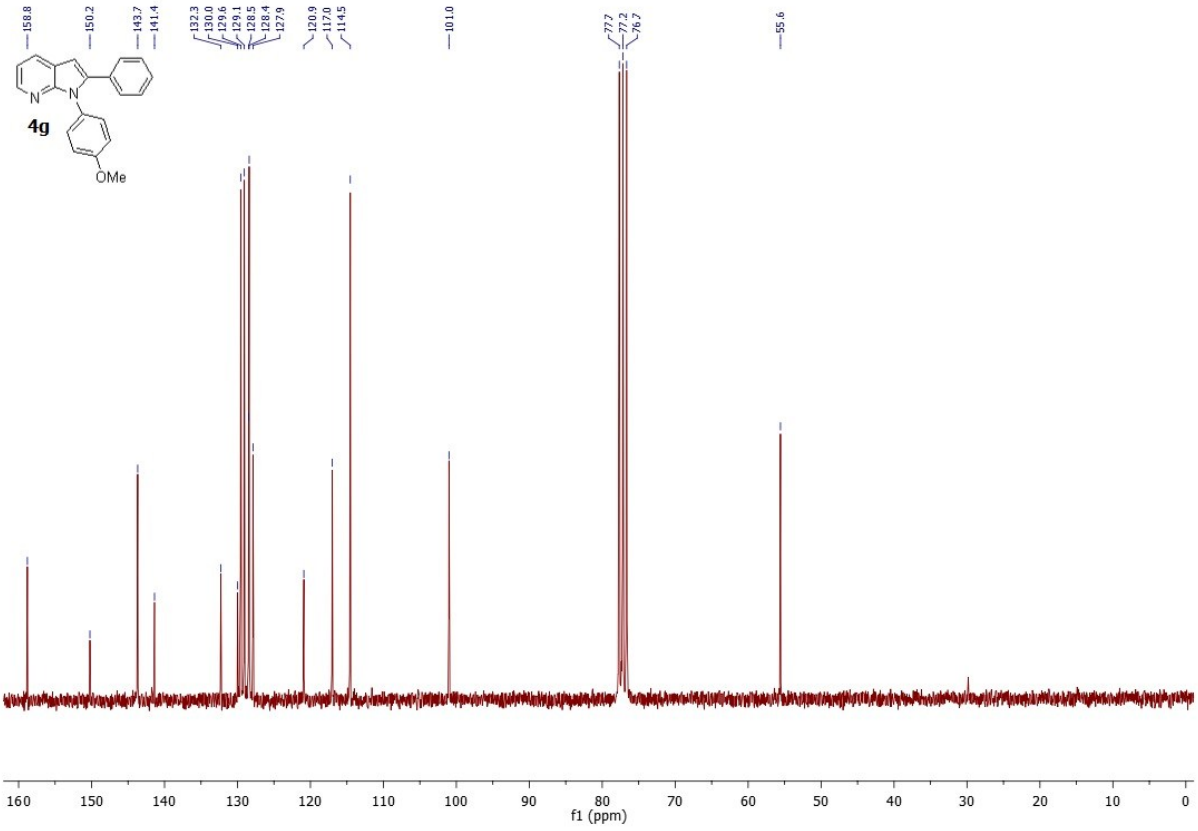
0.0
f1 (ppm)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129.6
129.1
128.5
128.4
127.9
120.9
117.0
114.5
101.0
77.7
77.2
76.7
55.6
4g
OMe
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150
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130
120
110
100
90
80
70
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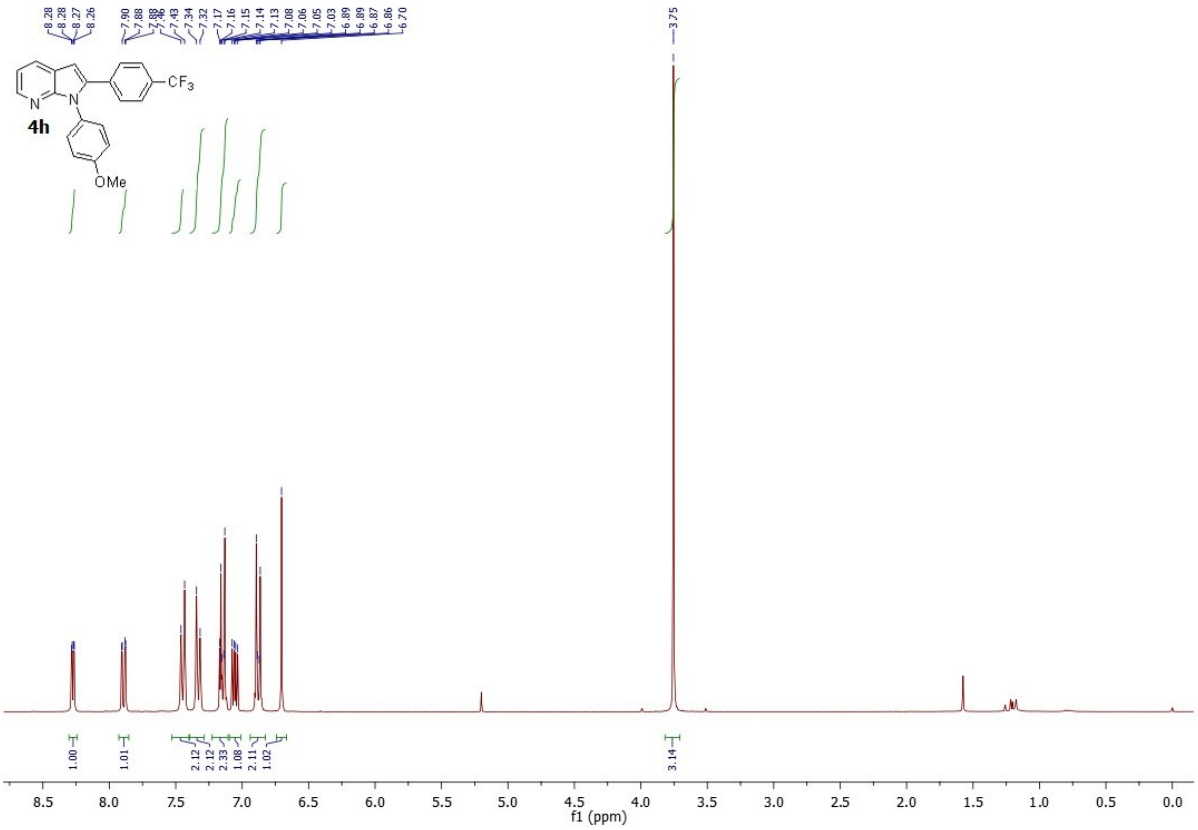
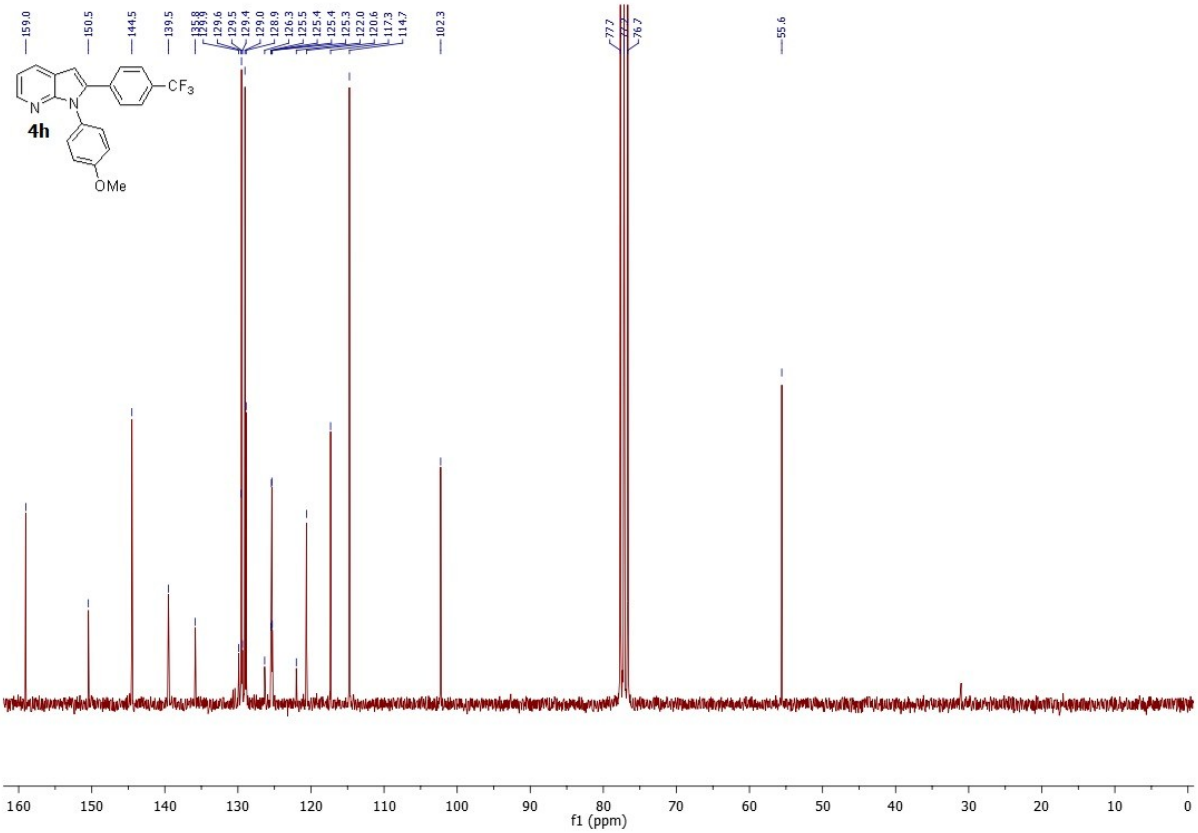
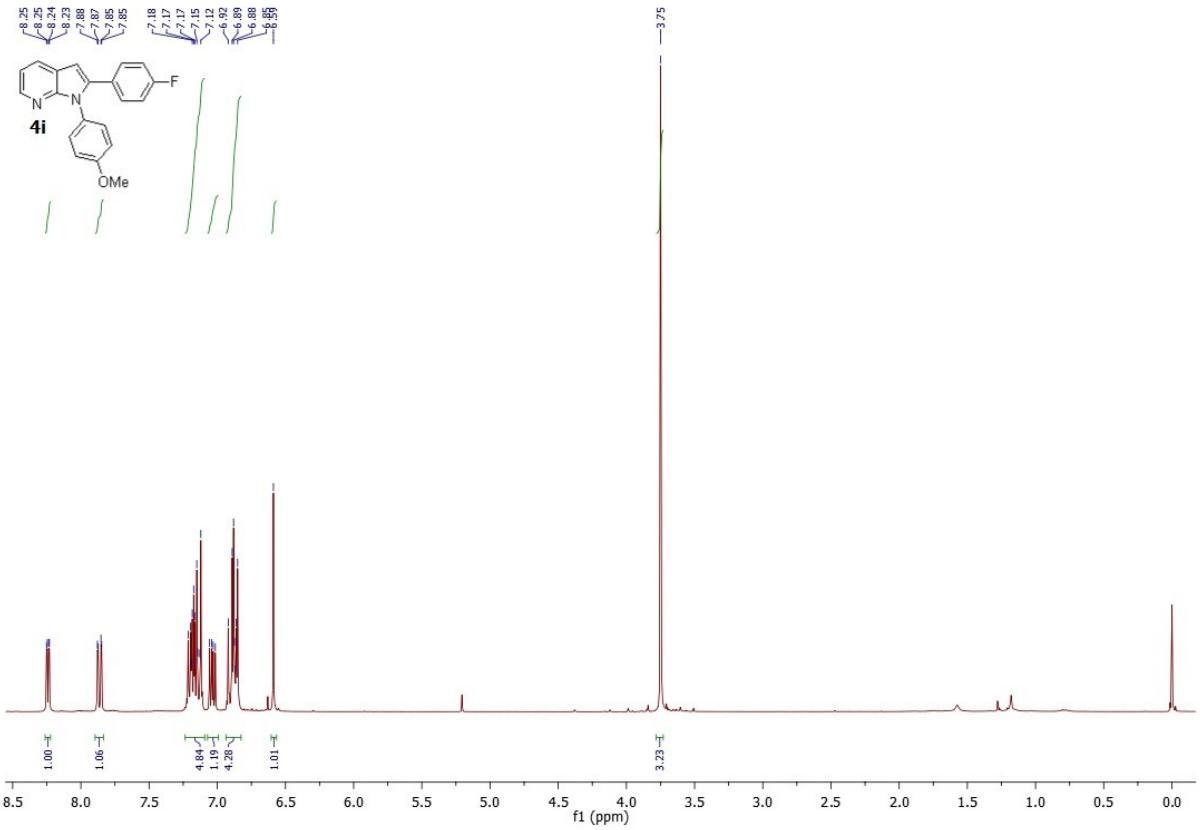
50
40
30
20
10
0
f1 (ppm)


4h
CF3
OMe
f1 (ppm)


4h
CF3
OMe
f1 (ppm)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7.85
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7.17
7.17
7.15
7.12
6.92
6.89
6.88
6.85
6.85
3.75
F
N
N
4i
OMe
1.00
1.06
4.84
1.19
4.28
1.01
3.23
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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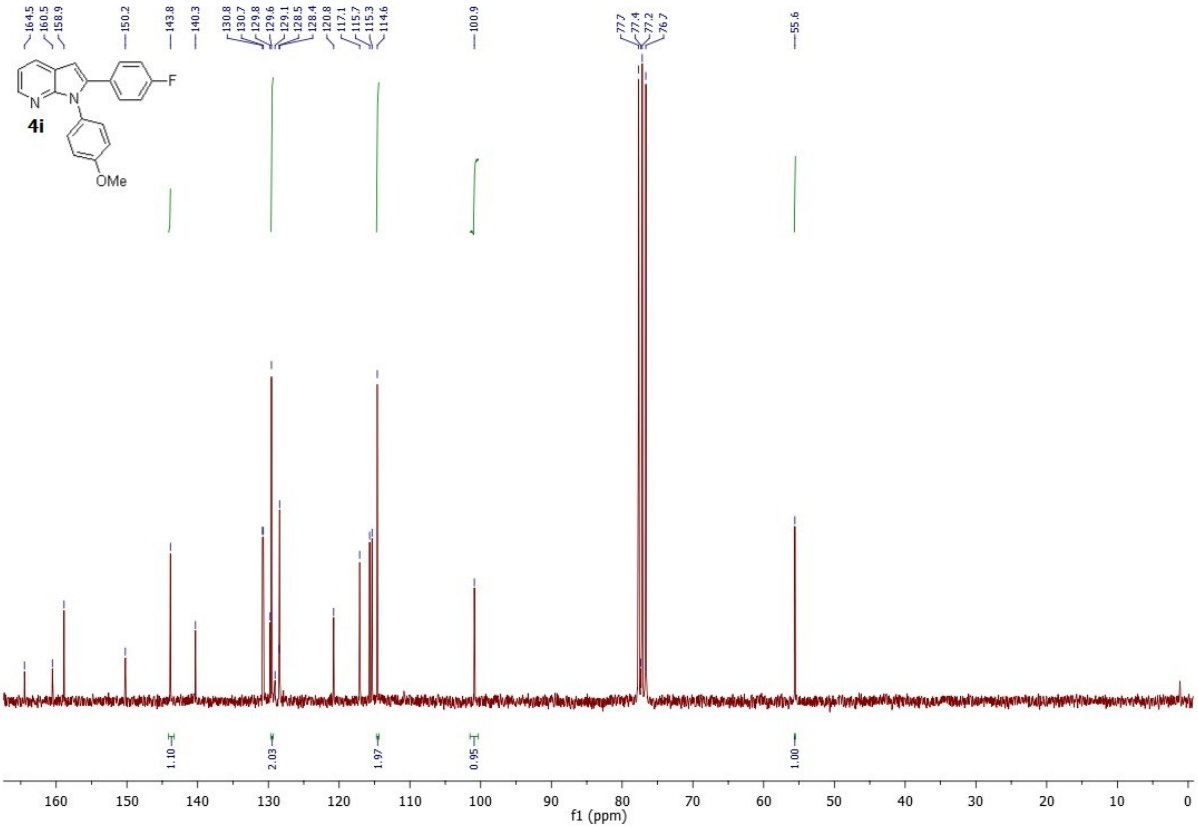
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.7
129.8
129.6
129.1
128.5
128.4
120.8
117.1
115.7
115.3
114.6
100.9
77.7
77.4
77.2
76.7
55.6
F
N
N
4i
OMe
1.10
2.03
1.97
0.95
1.00
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150
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110
100
90
80
70
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50
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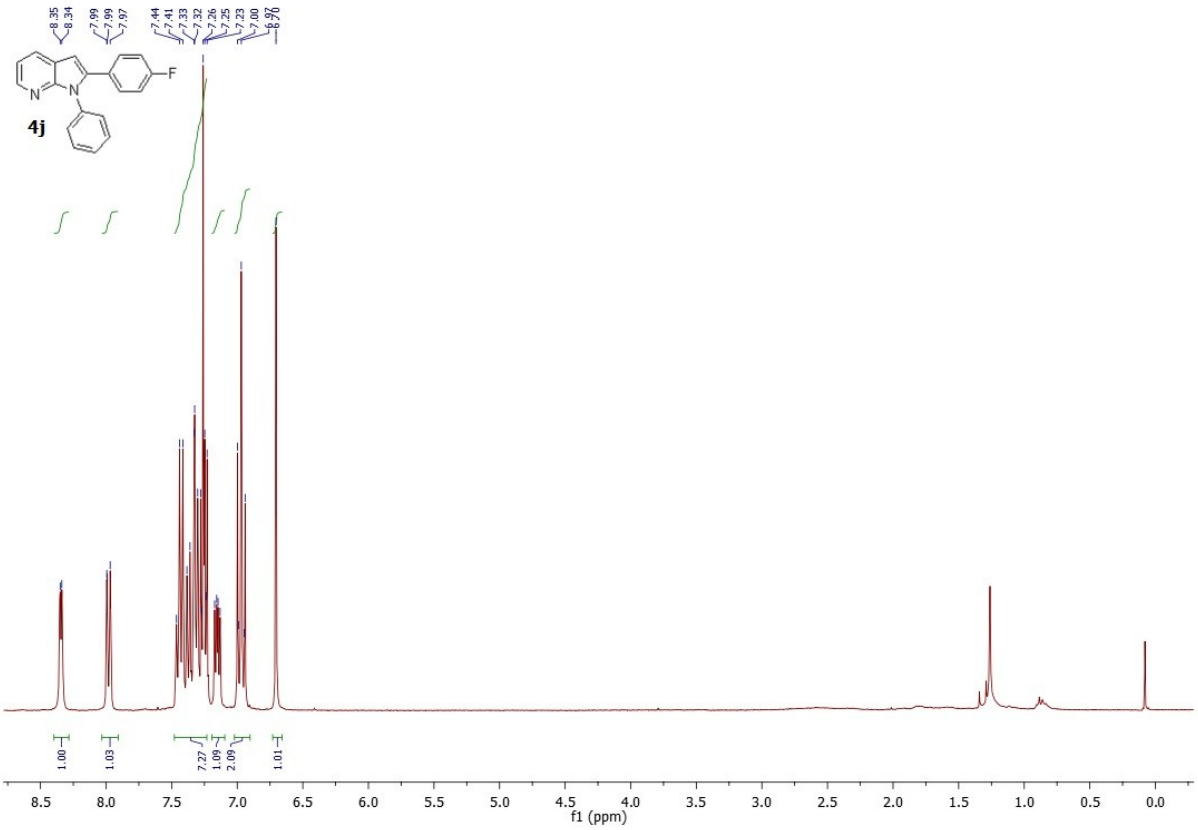
30
20
10
0
f1 (ppm)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7.26
7.25
7.23
7.00
6.97
6.96
F
N
4j
1.00
1.03
7.27
1.09
2.09
1.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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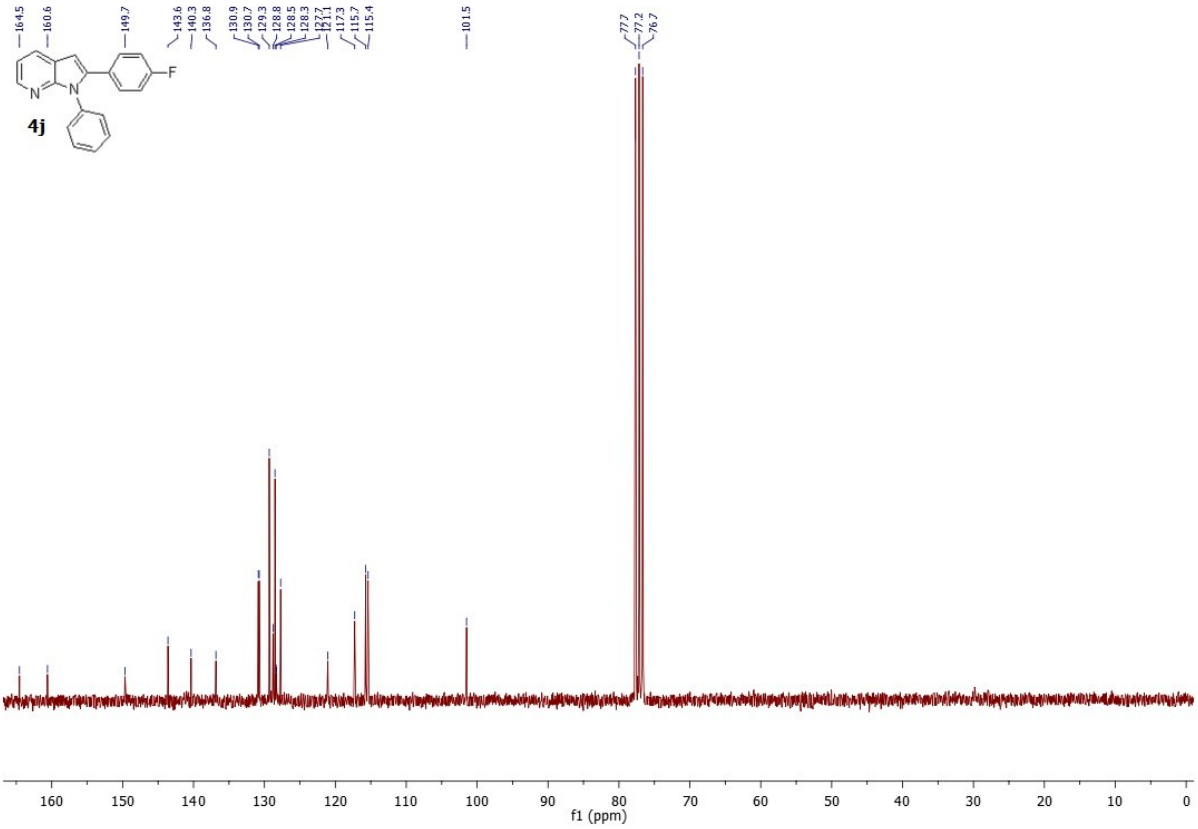
0.0
f1 (ppm)


164.5
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149.7
143.6
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128.8
128.5
128.3
127.7
121.1
117.3
115.7
115.4
101.5
77.7
77.2
76.7
F
N
4j
160
150
140
130
120
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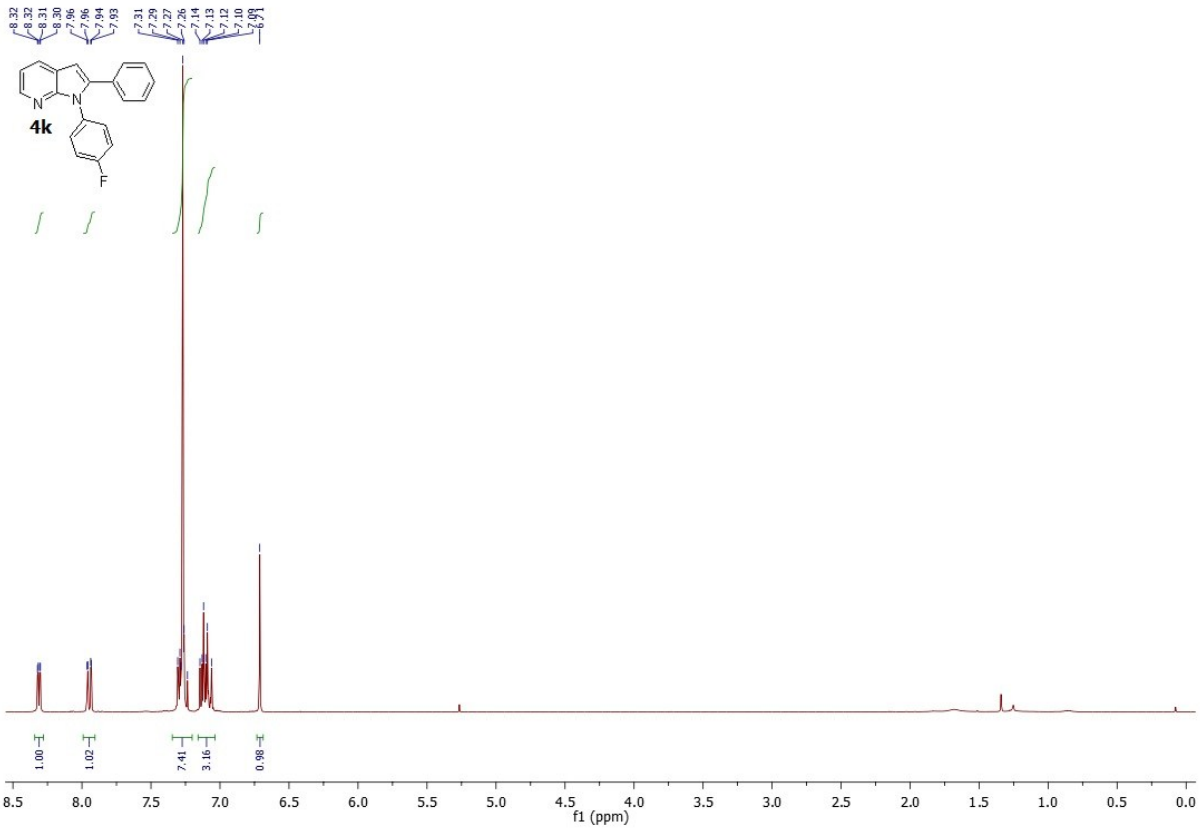
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8.31
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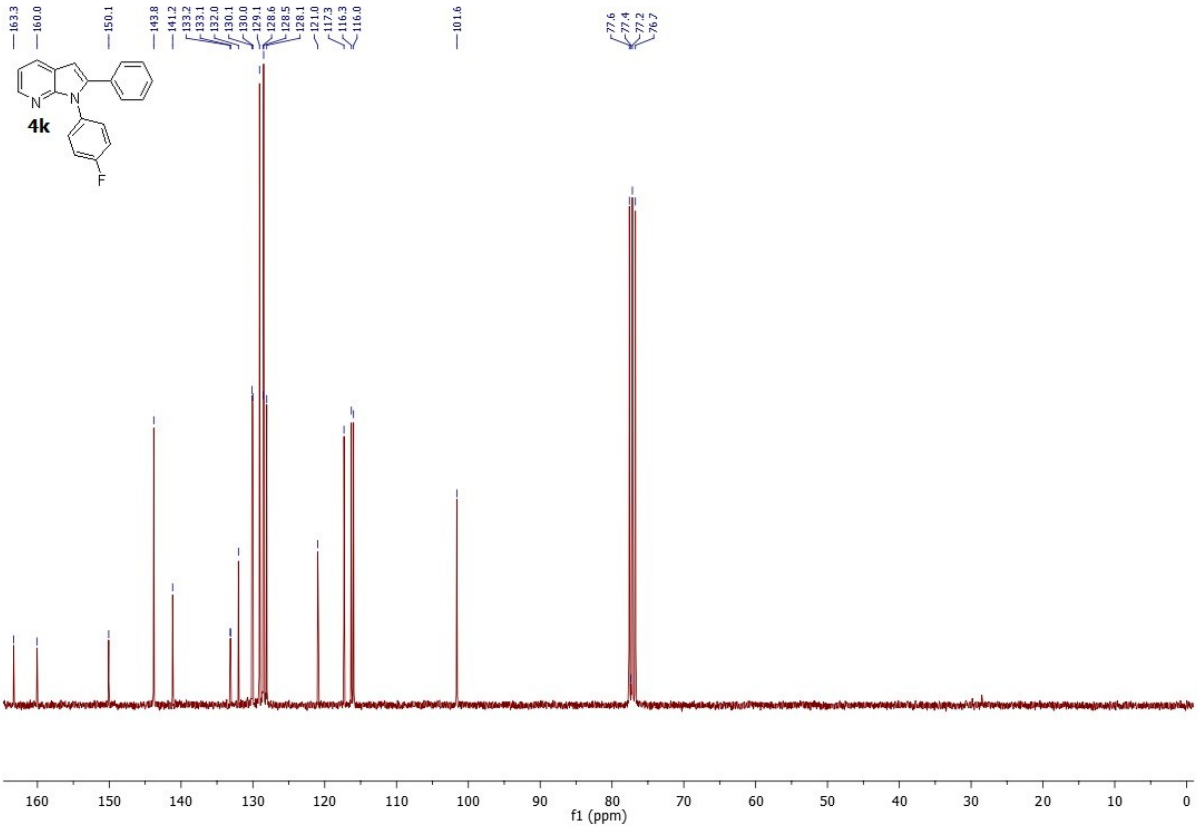
7.96
7.94
7.93
7.31
7.29
7.27
7.26
7.14
7.13
7.12
7.10
7.09
6.97
4k
F
1.00
1.02
7.41
3.16
0.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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141.2
133.2
133.1
132.0
130.1
130.0
129.1
128.6
128.5
128.1
121.0
117.3
116.3
116.0
101.6
77.6
77.4
77.2
76.7
4k
F
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150
140
130
120
110
100
90
80
70
60
50
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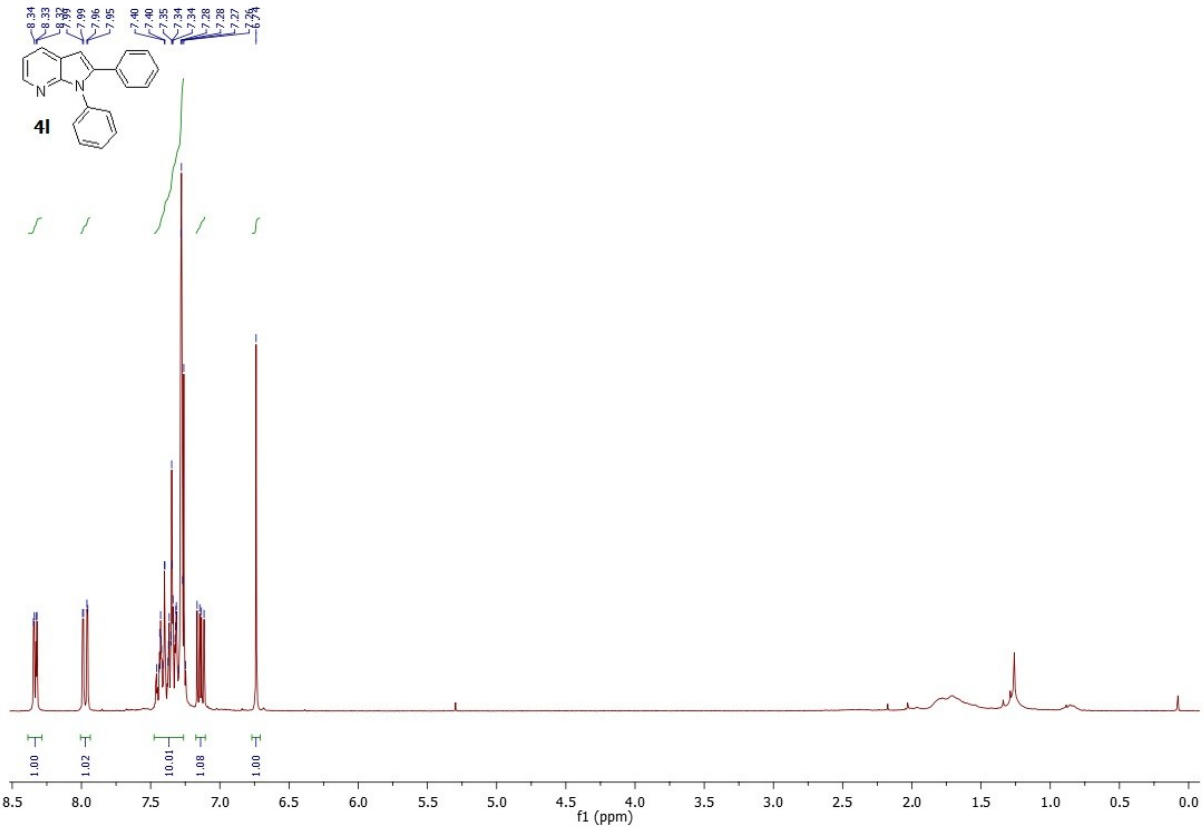
30
20
10
0
f1 (ppm)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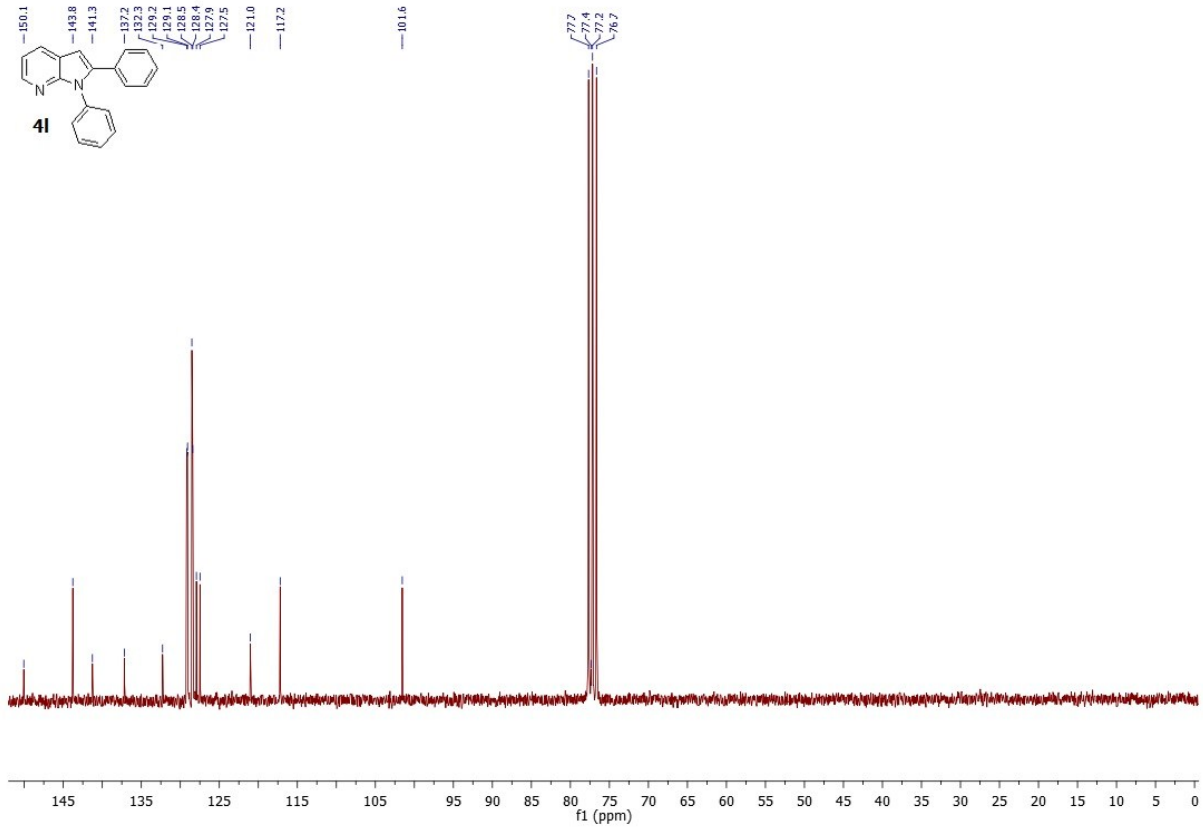
7.28
7.27
4l
1.00
1.02
10.01
1.08
1.00
f1 (ppm)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137.2
132.3
129.2
129.1
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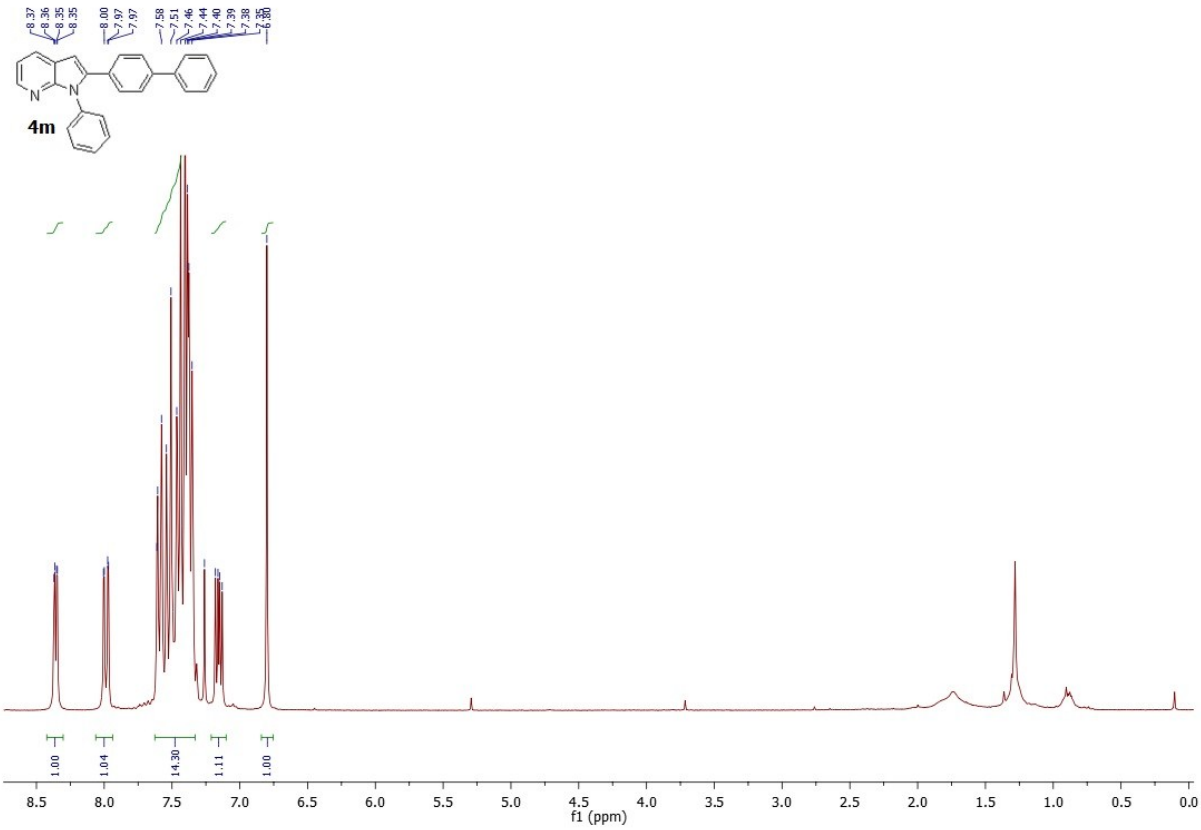
117.2
101.6
77.7
77.4
77.2
76.7
4l
f1 (ppm)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7.46
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7.39
7.38
7.35
7.30
4m
1.00
1.04
14.30
1.11
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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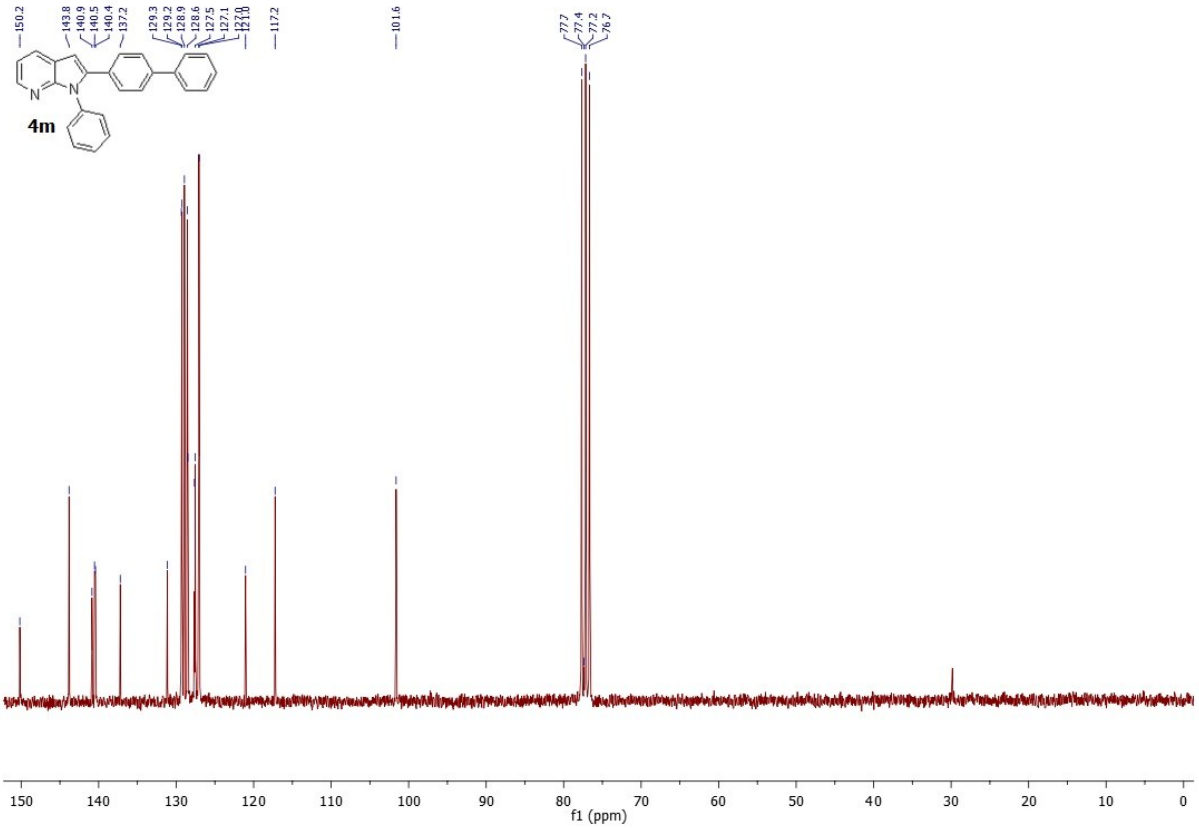
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.2
129.3
129.2
128.9
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127.5
127.1
121.0
117.2
101.6
77.7
77.4
77.2
76.7
4m
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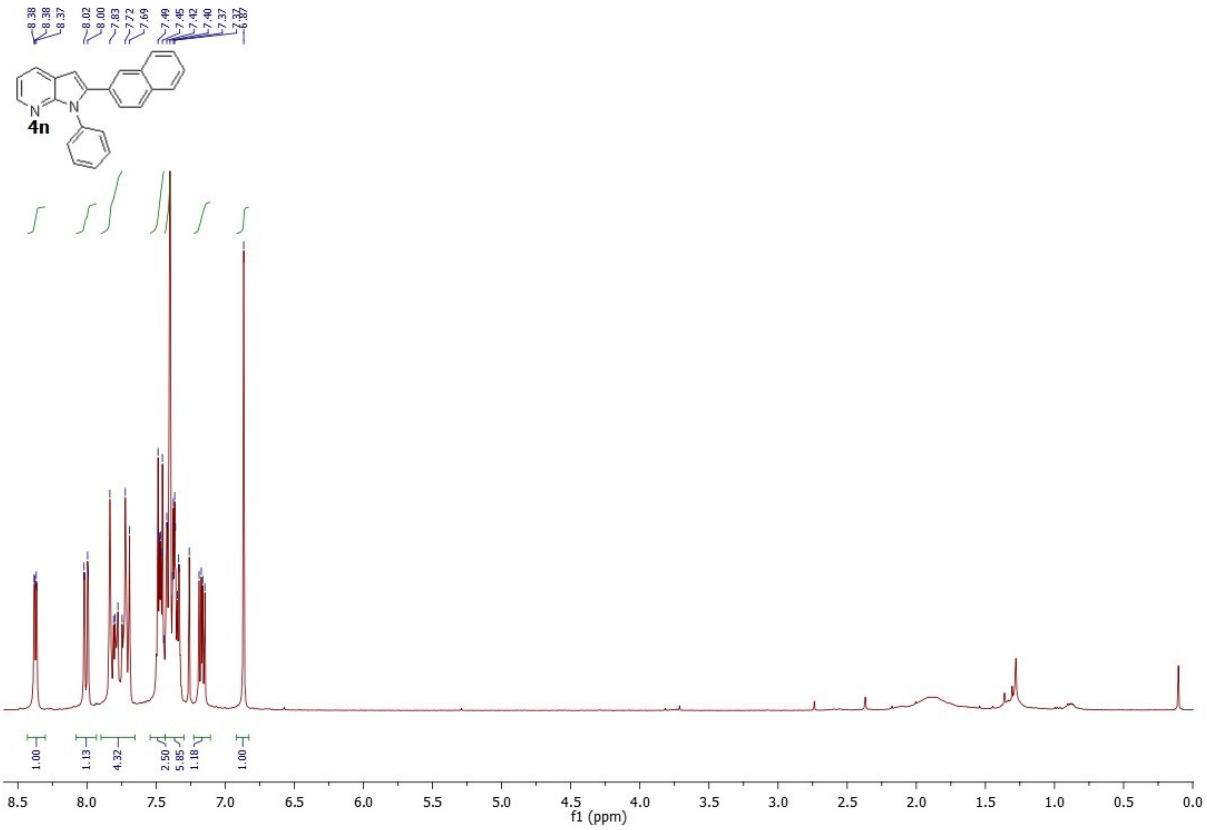
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.83
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7.69
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7.42
7.40
7.37
6.87
4n
1.00
1.13
4.32
2.50
5.85
1.18
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
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1.0
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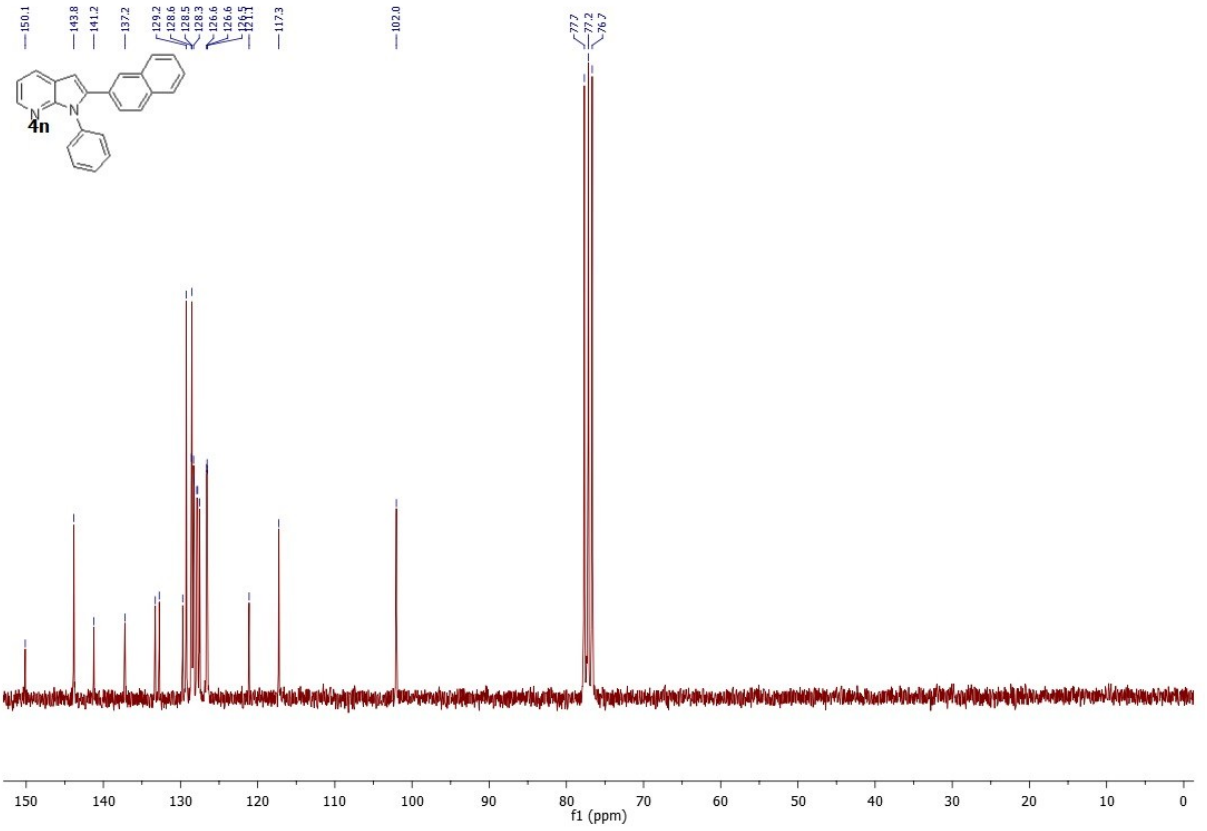
f1 (ppm)


150.1
143.8
141.2
137.2
129.2
128.6
128.5
128.3
126.6
126.6
117.3
102.0
77.7
77.2
76.7
4n
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120
110
100
90
80
70
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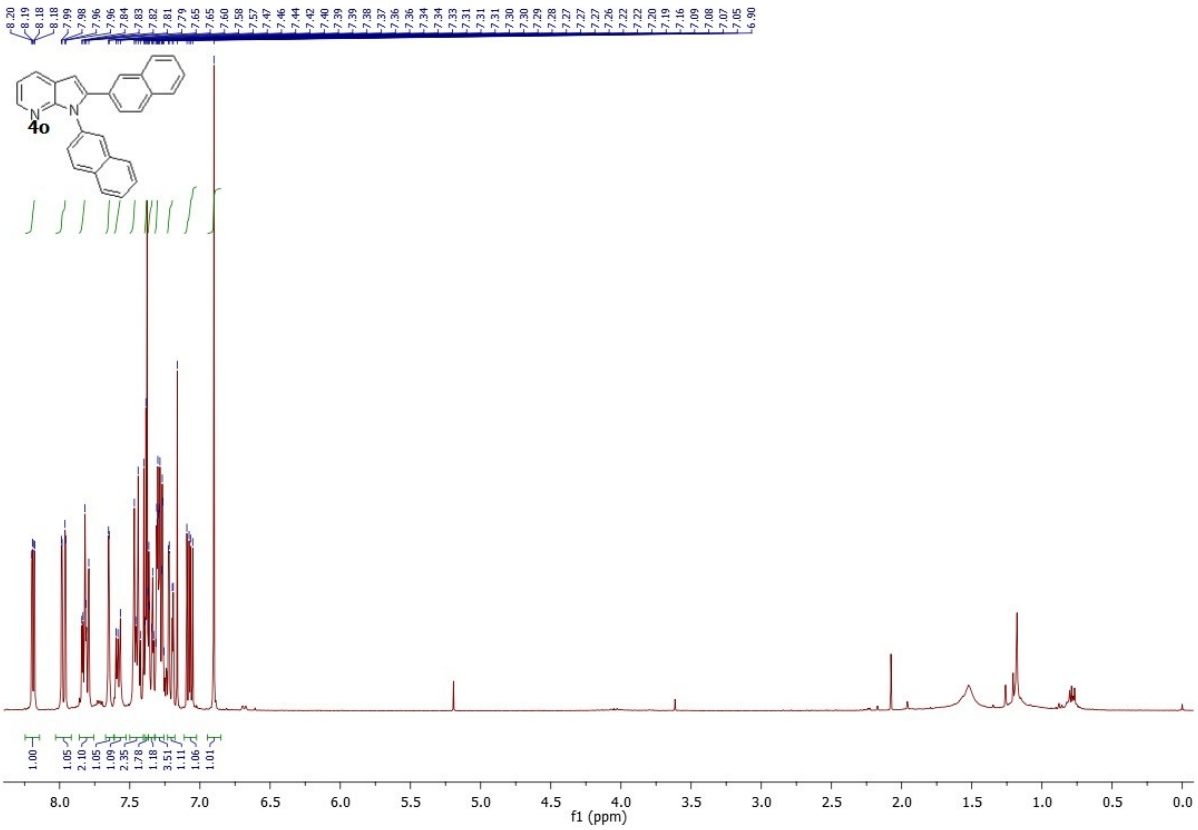
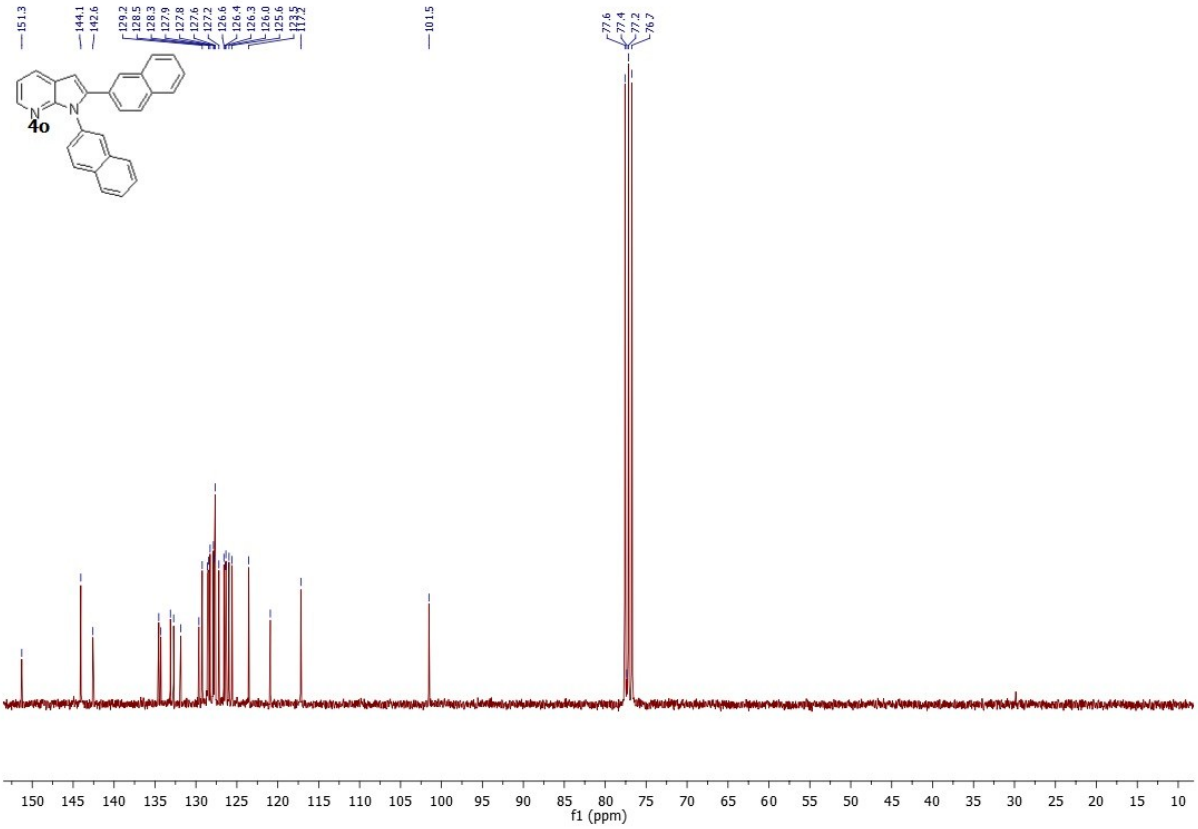
50
40
30
20
10
0
f1 (ppm)


4o
f1 (ppm)


4o
f1 (ppm)

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