

Electronic Supporting Information for:
Evaluating 1,1'-Bisphosphinoferrocene Ancillary Ligand Variants
in the Nickel-Catalyzed C-N Cross-Coupling of (Hetero)aryl
Chlorides

Jillian S. K. Clark,^a Christopher N. Voth,^a Michael J. Ferguson,^b and Mark Stradiotto*,^a

^a Department of Chemistry, Dalhousie University, 6274 Coburg Road, P.O. 15000, Halifax,
Nova Scotia B3H 4R2, Canada

^b X-Ray Crystallography Laboratory, Department of Chemistry, University of Alberta, Edmonton,
Alberta T6G 2G2, Canada

Table of Contents

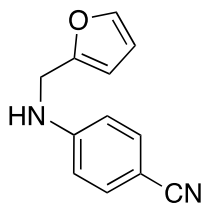
Characterization Data for Isolated Cross-Coupling Products (S2)

NMR Spectra (S9)

SI References (S28)

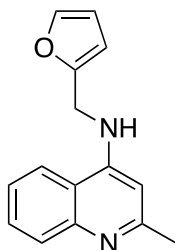
Characterization Data for Isolated Cross-Coupling Products:

4-((furan-2-ylmethyl)amino)benzonitrile (1b)



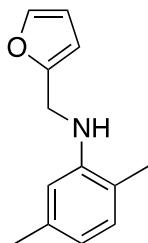
The title compound was synthesized from the corresponding chloride according to **GP1**, conducted at 110 °C using 5 mol% 1,1'-bis(diisopropylphosphino)ferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using 19:1 hexanes/ethyl acetate which afforded the title product in 82% isolated yield (163 mg, 0.82 mmol) as a yellow solid. ¹H NMR (500 MHz; CDCl₃): δ 7.39-7.35 (m, 3H), 6.63-6.61 (m, 2H), 6.32-6.31 (m, 1H), 6.24 (m, 1H), 4.81 (br. s, 1H), 4.33-4.32 (d, *J* = 5.9 Hz, 2H). ¹³C{¹H} NMR (125.8 MHz; CDCl₃): δ 151.3, 150.9, 142.3, 133.6, 120.5, 112.5, 110.5, 107.6, 99.0, 40.4. HRMS *m/z* ESI⁺ found 221.0685 [M + H]⁺ calculated for C₁₂H₁₀N₂NaO 221.0691.

N-(furan-2-ylmethyl)-2-methylquinolin-4-amine (1e)



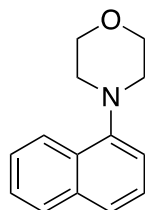
The title compound was synthesized from the corresponding chloride according to **GP1**, conducted at 25 °C using 6.7 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A which afforded the title product in a 73 % yield (175 mg) as a light brown powder. ¹H NMR (300 MHz, CDCl₃): δ 7.94-7.91 (m, 1H), 7.72-7.69 (m, 1H), 7.62-7.57 (m, 1H), 7.42-7.45 (m, 2H), 6.43 (s, 1H), 6.38-6.32 (m, 2H), 5.33 (br. s, 1H), 4.51-4.50 (d, *J* = 5.3 Hz, 2H), 2.62 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 159.7, 151.2, 149.4, 148.4, 142.7, 129.4, 129.3, 124.3, 119.4, 117.6, 110.7, 108.0, 99.7, 40.8, 25.9. HRMS *m/z* ESI⁺ found 239.1179 [M + H]⁺ calculated for C₁₅H₁₅N₂O 239.1184.

N-(furan-2-ylmethyl)-2,5-dimethylaniline (1f)



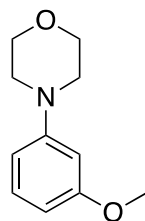
The title compound was synthesized from the corresponding chloride according to **GP1**, conducted at 110 °C using 10 mol% 1,1'-bis(diphenylphosphino)ferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using a gradient of dichloromethane and hexanes which afforded the title product in a 47% isolated yield (45 mg, 0.22 mmol) as a yellow oil. The loss of material due to handling/compound volatility was confirmed on the basis of calibrated NMR experiments: Following Workup Method C the title product was produced in a 68% calculated yield using 20 mol% ferrocene as an internal standard. ¹H NMR (500 MHz, CDCl₃): δ 7.40-7.39 (m, 1H), 6.97-6.94 (m, 1H), 6.54-6.52 (m, 2H), 6.35-6.34 (m, 1H), 6.26-6.25 (m, 1H), 4.36 (s, 1H), 3.81 (br, 1H), 2.30 (s, 3H), 2.13 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 152.9, 145.5, 141.9, 136.7, 130.0, 119.4, 118.2, 111.1, 110.4, 106.9, 41.6, 21.5, 17.0. Spectral data are in agreement with literature. HRMS *m/z* ESI⁺ found 224.1046 [M + Na]⁺ calculated for C₁₃H₁₅NNaO 224.1051.

4-(naphthalen-1-yl)morpholine (2a)



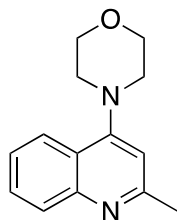
The title compound was synthesized from the corresponding chloride according to **GP2**, conducted at 100 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (19:1) hexanes/ethyl acetate which afforded the title product in 85% isolated yield (181 mg, 0.85 mmol) as a white solid. ¹H NMR (500 MHz, CDCl₃): δ 8.25-8.23 (m, 1H), 7.86-7.84 (m, 1H), 7.60-7.58 (d, *J* = 8.2 Hz, 1H), 7.52-7.47 (m, 2H), 7.44-7.41 (m, 1H), 7.12-7.10 (d, *J* = 7.4 Hz, 1H), 4.01-3.99 (m, 4H), 3.14-3.12 (m, 4H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 149.6, 135.0 (2 signals), 129.0, 128.7, 126.1, 125.7, 124.0, 123.6, 114.9, 67.7, 53.7. Spectral data are in agreement with literature.^{S1}

4-(3-methoxyphenyl)morpholine (2c)



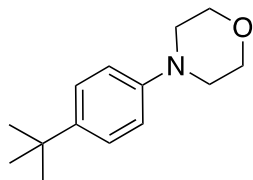
The title compound was synthesized from the corresponding chloride according to **GP2**, conducted at 100 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (9:1) hexanes/ethyl acetate which afforded the title product in 84% isolated yield (162 mg, 0.84 mmol) as a pale brown oil. ¹H NMR (300 MHz, CDCl₃): δ 7.22-7.16 (m, 1H), 6.55-6.52 (m, 1H), 6.46-6.43 (m, 2H), 3.87-3.84 (m, 4H), 3.80 (s, 3H), 3.17-3.14 (m, 4H). ¹³C{¹H} NMR (75.5 MHz, CDCl₃): δ 160.7, 152.7, 129.9, 108.5, 104.8, 102.3, 66.9, 55.2, 49.3. Spectral data are in agreement with literature.^{S2}

4-(2-methylquinolin-4-yl)morpholine (2e)



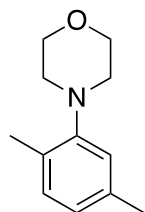
The title compound was synthesized from the corresponding chloride according to **GP2**, conducted at 25 °C using 6.7 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (1:4) hexanes/ethyl acetate which afforded the title product in 91% isolated yield (207 mg, 0.91 mmol) as a light brown solid. ¹H NMR (500 MHz, CDCl₃): δ 7.99-7.95 (m, 2H), 7.64-7.59 (m, 1H), 7.44-7.39 (m, 1H), 6.74 (s, 1H), 3.99-3.96 (m, 4H), 3.22-3.19 (m, 4H), 2.68 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 159.5, 156.7, 149.3, 129.3, 129.1, 124.7, 123.2, 121.7, 109.3, 67.0, 52.6, 25.7. Spectral data are consistent with literature.^{S3}

4-(4-(tert-butyl)phenyl)morpholine (2f)



The title compound was synthesized from the corresponding bromide according to **GP2**, conducted at 100 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (19:1) hexanes/ethyl acetate which afforded the title product in 82% isolated yield (179 mg, 0.82 mmol) as an off-white solid. ¹H NMR (500 MHz, CDCl₃): δ 7.33-7.31 (d, *J* = 8.8 Hz, 2H), 6.89-6.87 (d, *J* = 8.8 Hz, 2H), 3.88-3.86 (m, 4H), 3.16-3.14 (m, 4H), 1.31 (s, 9H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 149.1, 143.0, 126.2, 115.6, 67.2, 49.8, 34.2, 31.7. Spectral data are consistent with literature.^{S4}

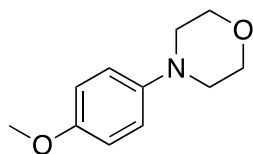
4-(2,5-dimethylphenyl)morpholine (2g)



The title compound was synthesized from the corresponding chloride according to **GP2**, conducted at 100 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using 24:1 hexanes/ethyl acetate which afforded the title product in a 16% yield (45 mg) as a light brown oil. ¹H NMR (300 MHz,

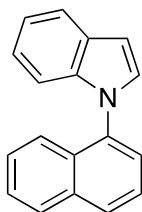
CDCl₃): δ 7.09-7.06 (d, J = 8.8 Hz, 1H), 6.84-6.81 (m, 2H), 3.87-3.84 (m, 4H), 2.92-2.89 (m, 4H), 2.32 (s, 3H), 2.28 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 151.4, 136.4, 131.2, 129.5, 124.2, 119.9, 67.7, 52.5, 21.4, 17.7. Spectral data are consistent with literature.^{S5}

4-(4-methoxyphenyl)morpholine (2h)



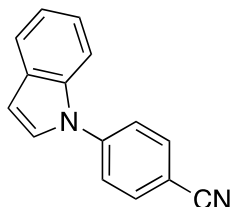
The title compound was synthesized from the corresponding chloride according to **GP2**, conducted at 100 °C using 6.7 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (9:1) hexanes/ethyl acetate which afforded the title product in 65% isolated yield (126 mg, 0.65 mmol) as a white solid. ¹H NMR (300 MHz, CDCl₃): δ 6.91-6.83 (m, 4H), 3.87-3.84 (m, 4H), 3.77 (s, 3H), 3.07-3.04 (m, 4H). ¹³C{¹H} NMR (75.5 MHz, CDCl₃): δ 154.0, 145.7, 117.8, 114.5, 67.0, 55.6, 50.8. Spectral data are in agreement with literature values.^{S1}

1-(naphthalen-1-yl)-1H-indole (3a)



The title compound was synthesized from the corresponding chloride according to **GP3**, conducted at 110 °C using 5 mol% 1,1'-bis(di(bis-3,5-trifluoromethyl)phenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using (19:1) hexanes/ethyl acetate which afforded the title product in an 80% isolated yield (117 mg, 0.48 mmol) as an off-white solid. ¹H NMR (500 MHz, CDCl₃): δ 7.99-7.98 (m, 2H), 7.77-7.75 (d, J = 7.9 Hz, 1H), 7.61-7.53 (m, 3H), 7.48-7.46 (m, 1H), 7.43-7.40 (m, 1H), 7.37 (d, J = 3.2 Hz, 1H), 7.21-7.13 (m, 2H), 7.05-7.04 (m, 1H), 6.79-6.78 (d, J = 3.2 Hz, 1H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 138.2, 136.3, 134.7, 130.8, 130.0, 128.7, 128.5, 127.2, 126.9, 125.7, 125.4, 123.6, 122.4, 121.1, 120.3, 111.1, 103.1. Spectral data are in agreement with literature.^{S6}

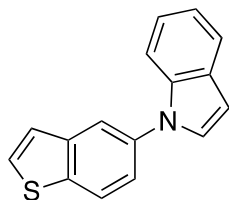
4-(1H-indol-1-yl)benzonitrile (3b)



The title compound was synthesized from the corresponding chloride according to **GP3**, conducted

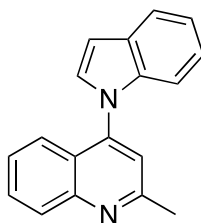
at 110 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using a gradient of 100:0 to 19:1 hexanes/ethyl acetate which afforded the title product in a quantitative isolated yield (213 mg, 0.98 mmol) as a light brown oil. ¹H NMR (500 MHz; CDCl₃): δ 7.82-7.80 (m, 2H), 7.71-7.70 (m, 1H), 7.65-7.61 (m, 3H) 7.35 (d, *J* = 3.4 Hz, 1H), 7.30-7.22 (m, 2H), 6.76 (d, *J* = 3.4 Hz, 1H). ¹³C{¹H} NMR (125.8 MHz; CDCl₃): δ 143.8, 135.4, 134.0, 130.2, 127.3, 124.1, 123.4, 121.8, 121.6, 118.6, 110.6, 109.6, 106.0. Spectral data are consistent with literature.^{S7}

1-(benzo[b]thiophen-5-yl)-1H-indole (3d)



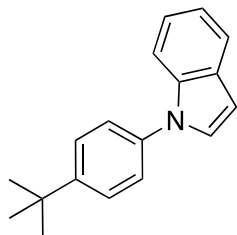
The title compound was synthesized from the corresponding chloride according to **GP3**, conducted at 110°C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using hexanes which afforded the title product in 92 % isolated yield (229 mg, 0.92 mmol) as a yellow oil. ¹H NMR (500 MHz, CDCl₃): δ 8.06-8.04 (d, *J* = 8.5 Hz, 1H), 7.99 (m, 1H), 7.81-7.79 (d, *J* = 7.7 Hz, 1H), 7.66-7.62 (m, 2H), 7.58-7.55 (dd, *J* = 8.5 Hz, 2.0 Hz, 1H), 7.46-7.44 (m, 2H), 7.33-7.26 (m, 2H), 6.80-6.79 (d, *J* = 3.2 Hz, 1H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 140.9, 138.3, 137.1, 136.7, 129.7, 128.8, 124.3, 123.9, 122.8, 121.9, 121.6, 120.8, 119.7, 110.9, 103.9. HRMS *m/z* ESI⁺ found 272.0504 [M + Na]⁺ calculated for C₁₆H₁₁NNaS 272.0510.

4-(1H-indol-1-yl)-2-methylquinoline (3e)



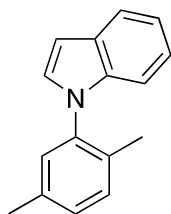
The title compound was synthesized from the corresponding chloride according to **GP3**, conducted at 110 °C using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using a gradient of 19:1 to 5.7:1 hexanes/ethyl acetate which afforded the title product in a 96 % isolated yield (247 mg, 0.96 mmol) as a white solid. ¹H NMR (500 MHz, CDCl₃): δ 8.19-8.18 (d, *J* = 8.5 Hz, 1H), 7.77-7.72 (m, 2H), 7.69-7.67 (d, *J* = 8.3 Hz, 1H), 7.43-7.40 (m, 1H), 7.37-7.36 (d, *J* = 3.3 Hz, 1H), 7.34 (s, 1H), 7.24-7.18 (m, 3H), 6.82-6.81 (d, *J* = 3.3 Hz, 1H), 2.82 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 159.7, 149.8, 144.5, 137.2, 130.3, 129.4, 129.1, 126.5, 123.6, 122.9, 121.4, 121.0, 119.2, 111.0, 104.7, 25.6. HRMS *m/z* ESI⁺ found 259.1230 [M + H]⁺ calculated for C₁₈H₁₅N₂ 259.1235.

1-(4-(tert-butyl)phenyl)-1H-indole (3f)



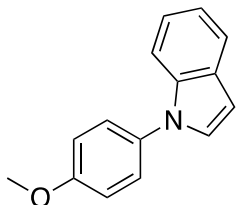
The title compound was synthesized from the corresponding bromide according to **GP3**, conducted at 110°C using using 5 mol% 1,1'-bis(diphenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using a gradient of 99:1 to 49:1 hexanes/ethyl acetate which afforded the title product in a 64 % isolated yield (160 mg, 0.64 mmol) as a white solid. ¹H NMR (500 MHz, CDCl₃): δ 7.83-7.82 (d, *J* = 7.7 Hz, 1H), 7.71-7.70 (d, *J* = 8.2 Hz, 1H), 7.64-7.62 (m, 2H), 7.55-7.53 (m, 2H), 7.44-7.43 (d, *J* = 3.3 Hz, 1H), 7.36-7.28 (m, 2H), 6.80-6.79 (d, *J* = 3.2 Hz, 1H), 1.52 (s, 9H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): δ 149.6, 137.4, 136.2, 129.4, 128.2, 126.6, 124.2, 122.4, 121.3, 120.4, 111.8, 103.4, 34.8, 31.6. Spectral data are consistent with literature.^{S4}

1-(2,5-dimethylphenyl)-1H-indole (3g)^{S8}



The title compound was synthesized from the corresponding bromide according to **GP3**, conducted at 110°C using using 10 mol% 1,1'-bis(3,5-(bis-trifluoromethyl)phenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using 99:1 hexanes/ethyl acetate which afforded the title product in 67% isolated yield (89 mg, 0.40 mmol) as a light brown oil. ¹H NMR (500 MHz, CDCl₃): δ 7.79-7.75 (m, 1H), 7.33-7.31 (d, *J* = 7.8 Hz, 1H), 7.24-7.19 (m, 5H), 7.13-7.11 (m, 1H), 6.73-6.72 (m, 1H), 2.43 (s, 3H), 2.09 (s, 3H). ¹³C{¹H} NMR (125.8 MHz, CDCl₃): 138.3, 137.2, 136.8, 132.7, 131.2, 129.1, 128.9, 128.8, 128.5, 122.2, 121.0, 120.0, 110.8, 102.6, 21.0, 17.4. See footnote in the main text.²⁴

1-(4-methoxyphenyl)-1H-indole (3h)



The title compound was synthesized from the corresponding chloride according to **GP3**, conducted

at 110°C using using 5 mol% 1,1'-bis(3,5-(bis-trifluoromethyl)phenyl)phosphinoferrocene, and purified according to Workup Method A. Purified by flash column chromatography on silica gel using 49:1 hexanes/ethyl acetate which afforded the title product in 91% isolated yield (203 mg, 0.91 mmol) as a yellow oil. ¹H NMR (500 MHz; CDCl₃): δ 7.79-7.77 (d, *J* = 7.7 Hz, 1H), 7.56-7.55 (d, *J* = 8.1 Hz, 1H), 7.50-7.47 (m, 2H), 7.36 (d, *J* = 3.2 Hz, 1H), 7.31-7.24 (m, 2H), 7.12-7.09 (m, 2H), 6.75 (d, *J* = 3.2 Hz, 1H), 3.95 (s, 3H). ¹³C{¹H} NMR (125.8 MHz; CDCl₃): δ 158.6, 136.5, 133.0, 129.2, 128.5, 126.2, 122.3, 121.2, 120.3, 114.9, 110.6, 103.1, 55.8. Spectral data are in agreement with literature.^{S9}

NMR Spectra

Figure S1. ^1H NMR Spectrum of 4-((furan-2-ylmethyl)amino)benzonitrile (**1b**), (CDCl_3 , 500 MHz)

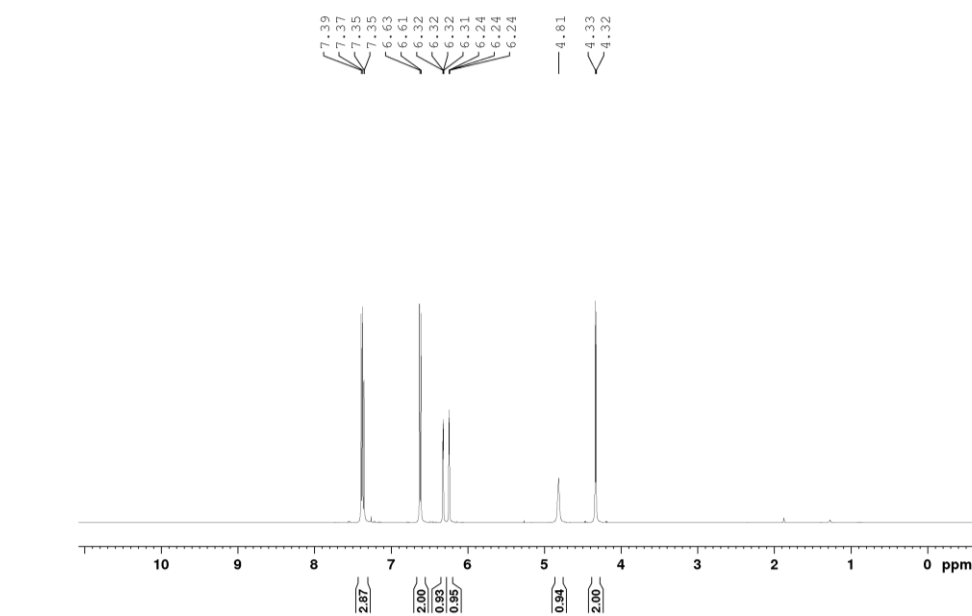


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-((furan-2-ylmethyl)amino)benzonitrile (**1b**), (CDCl_3 , 125.8 MHz)

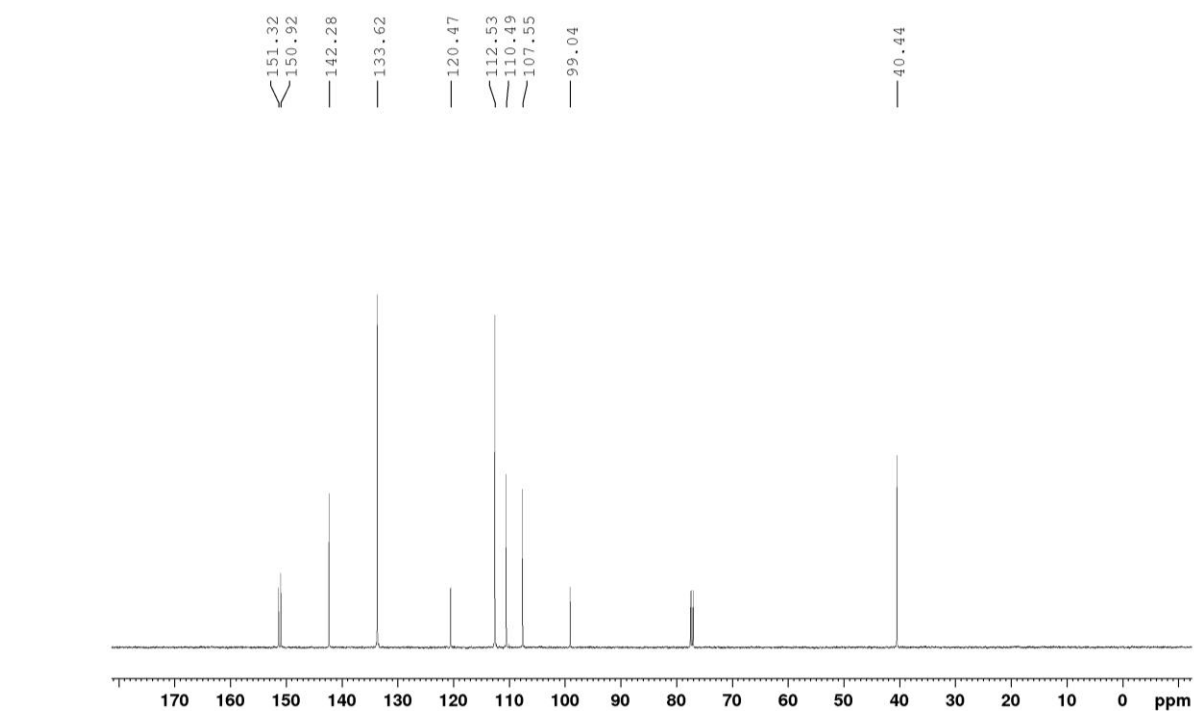


Figure S3. ^1H NMR Spectrum of N-(furan-2-ylmethyl)-2-methylquinolin-4-amine (**1e**), (CDCl_3 , 500 MHz)

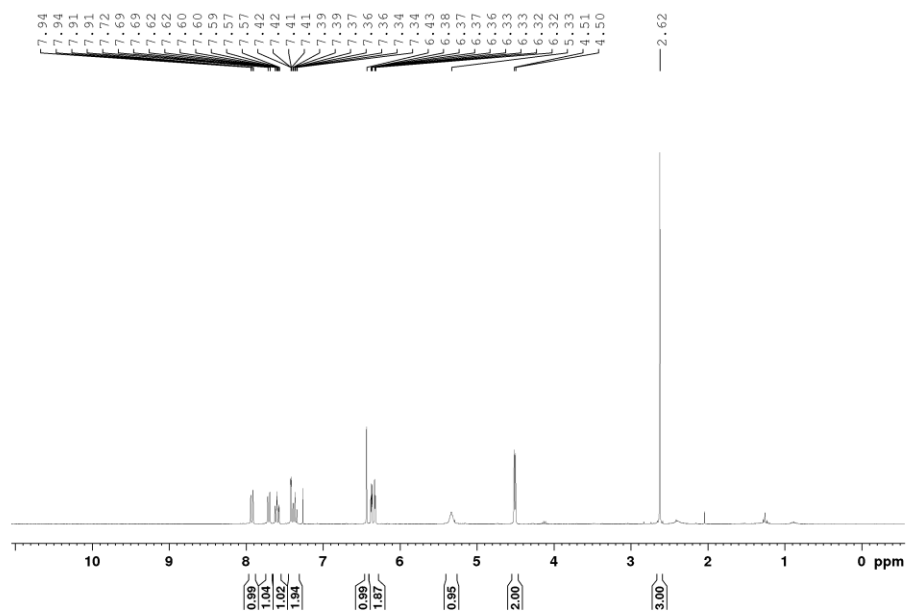


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR N-(furan-2-ylmethyl)-2-methylquinolin-4-amine (**1e**), (CDCl_3 , 125.8 MHz)

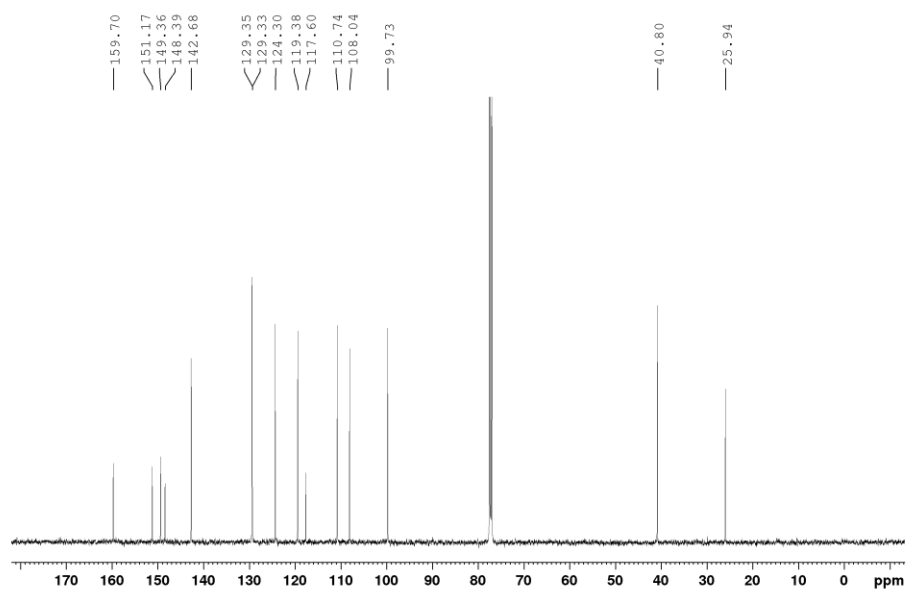


Figure S5. ^1H NMR Spectrum of N-(furan-2-ylmethyl)-2,5-dimethylaniline (**1f**) (CDCl_3 , 300 MHz)

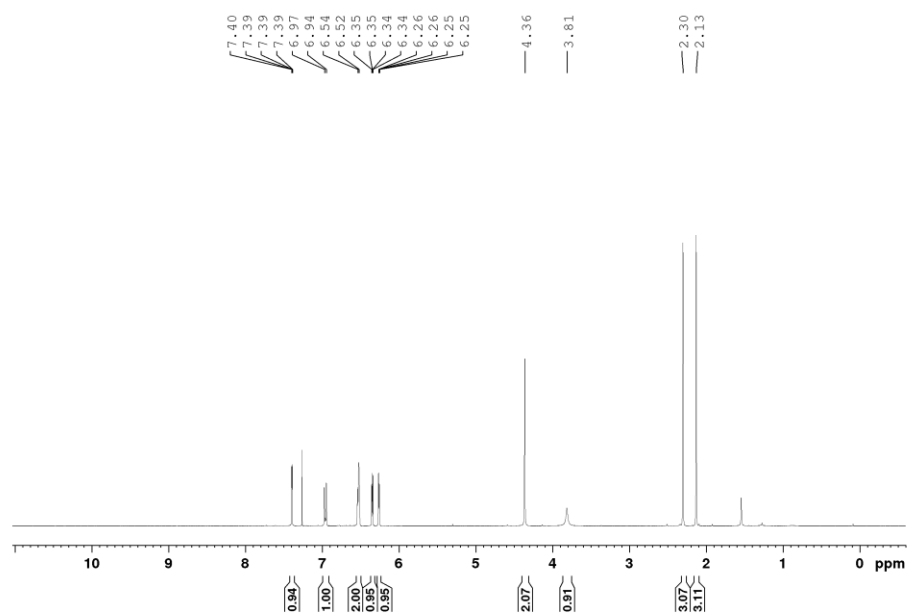


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of N-(furan-2-ylmethyl)-2,5-dimethylaniline (**1f**), (CDCl_3 , 125.8 MHz)

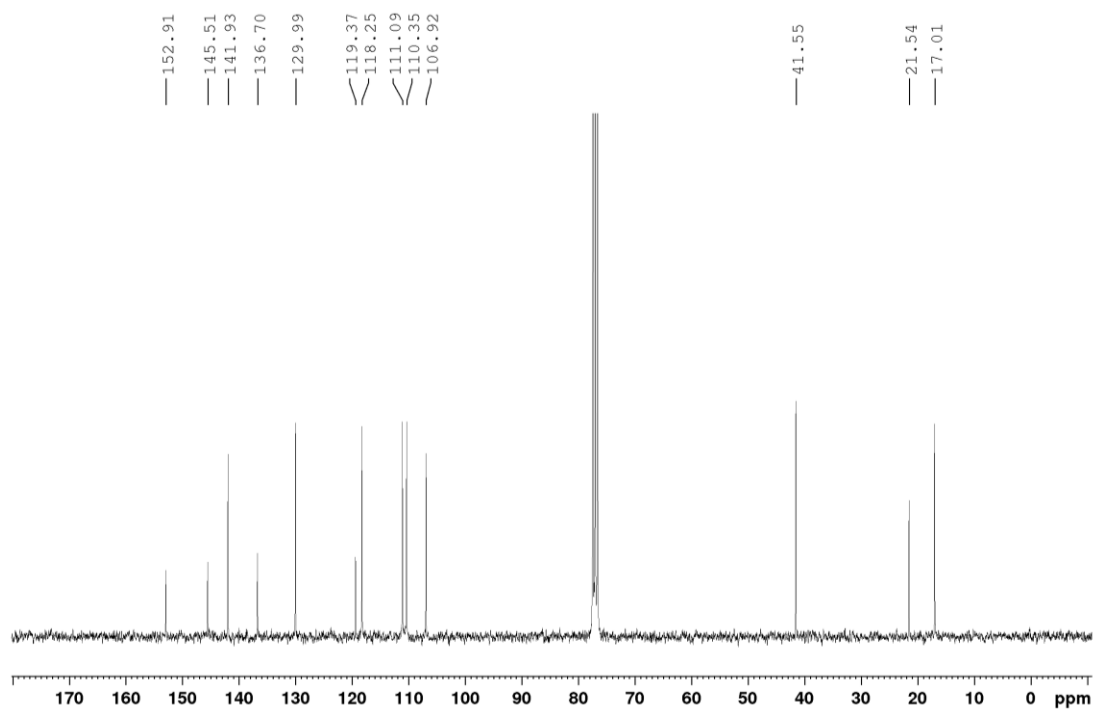


Figure S7. ^1H NMR Spectrum of 4-(naphthalen-1-yl)morpholine (**2a**), (CDCl_3 , 500 MHz)

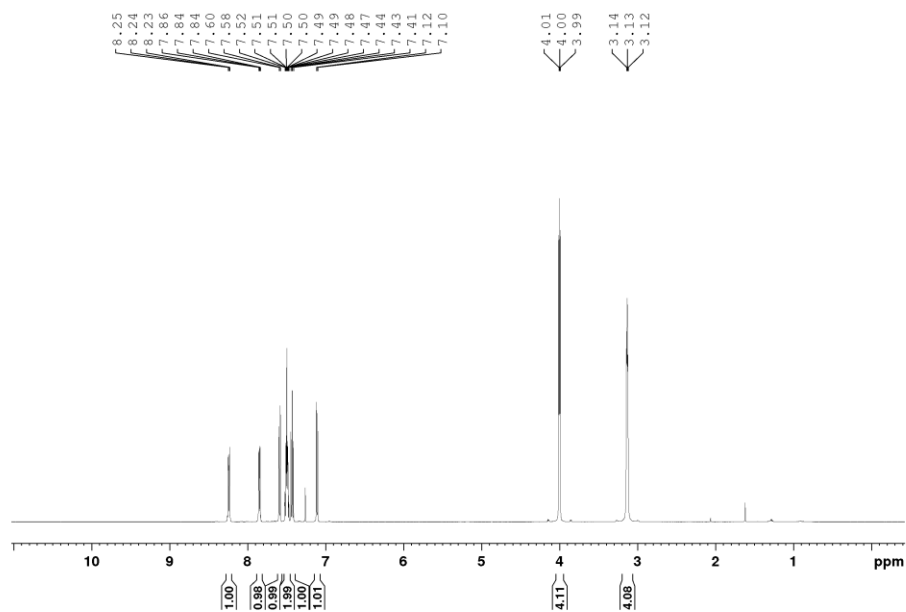


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(naphthalen-1-yl)morpholine (**2a**), (CDCl_3 , 500 MHz)

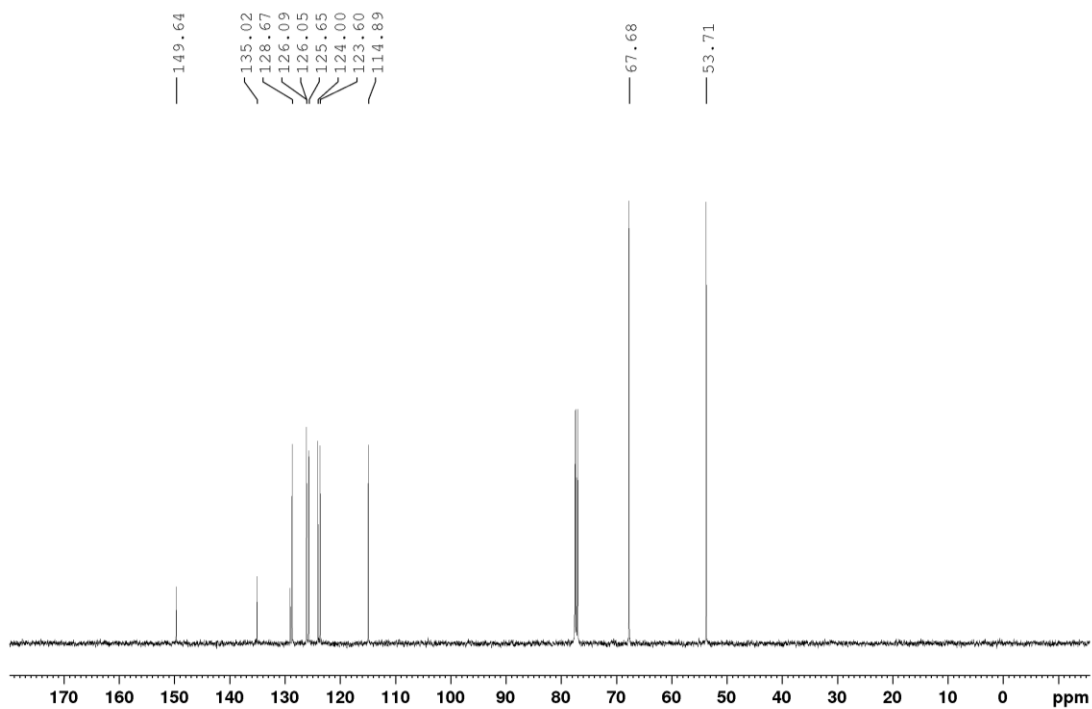


Figure S9. ^1H NMR Spectrum 4-(3-methoxyphenyl)morpholine (**2c**), (CDCl_3 , 300 MHz)

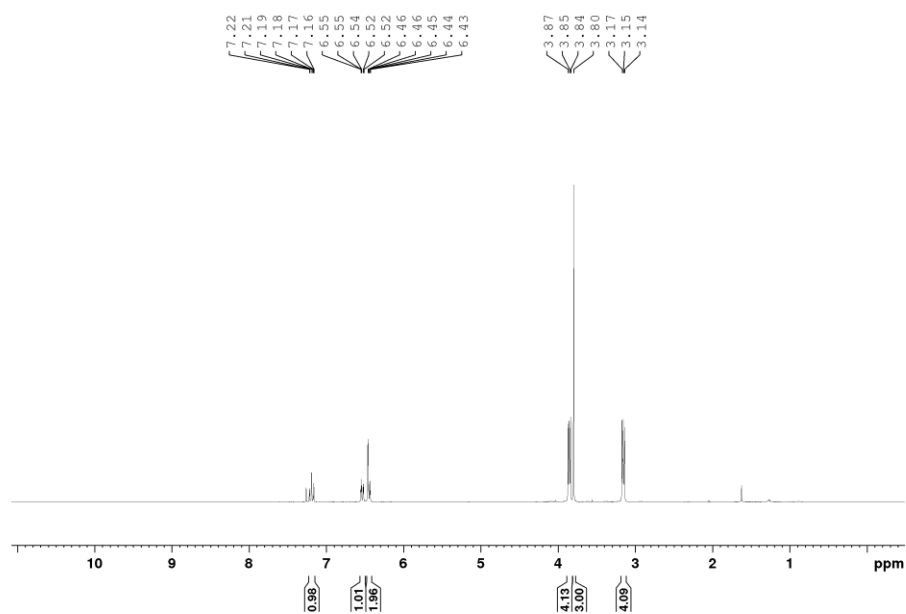


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum 4-(3-methoxyphenyl)morpholine (**2c**), (CDCl_3 , 75.5 MHz)

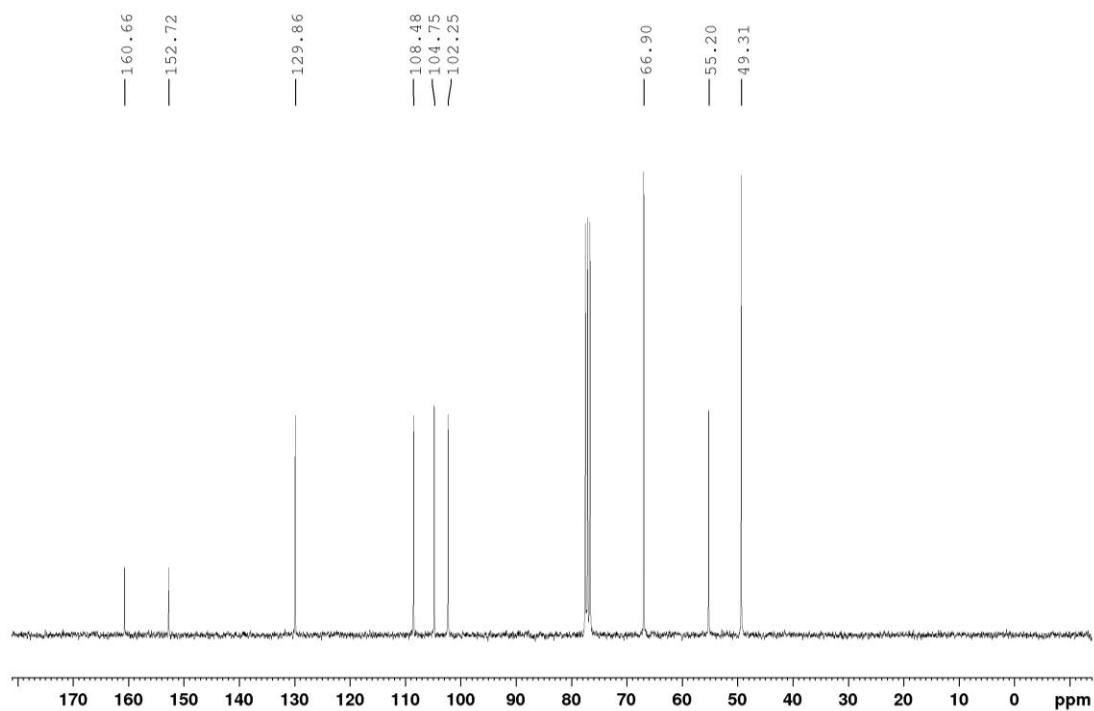


Figure S11. ^1H NMR Spectrum of 4-(2-methylquinolin-4-yl)morpholine (**2e**), (CDCl_3 , 300 MHz)

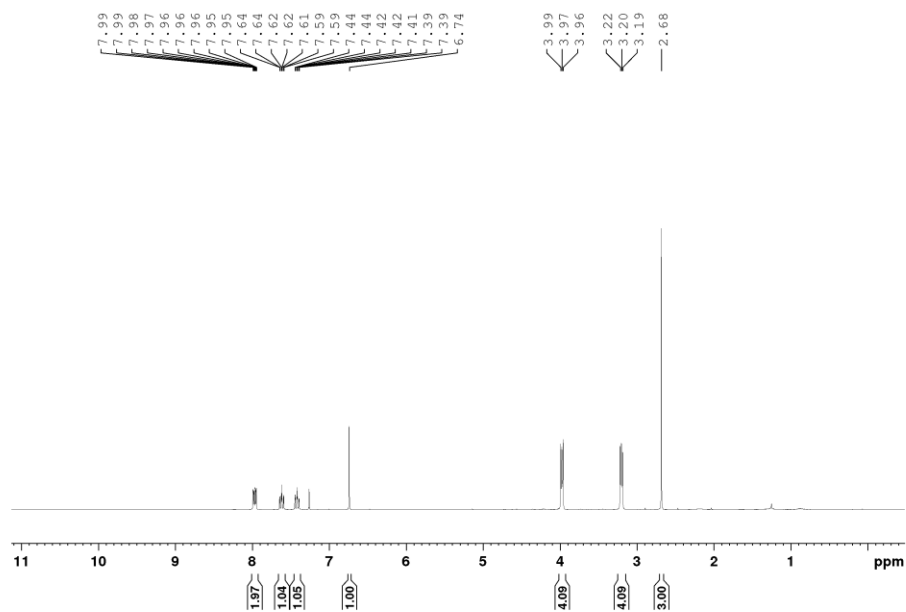


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(2-methylquinolin-4-yl)morpholine (**2e**), (CDCl_3 , 75.5 MHz)

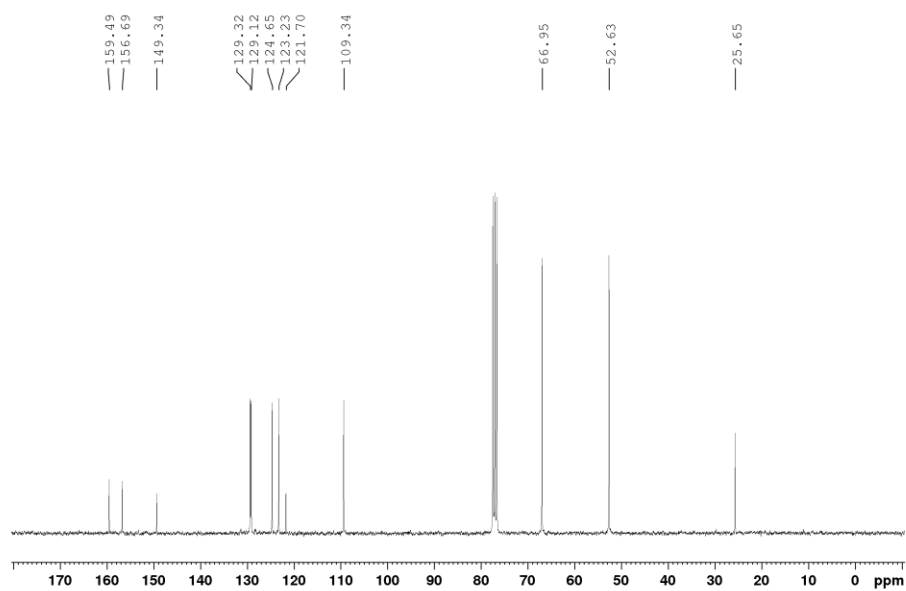


Figure S13. ^1H NMR Spectrum of 4-(4-(tert-butyl)phenyl)morpholine (**2f**), (CDCl_3 , 500 MHz)

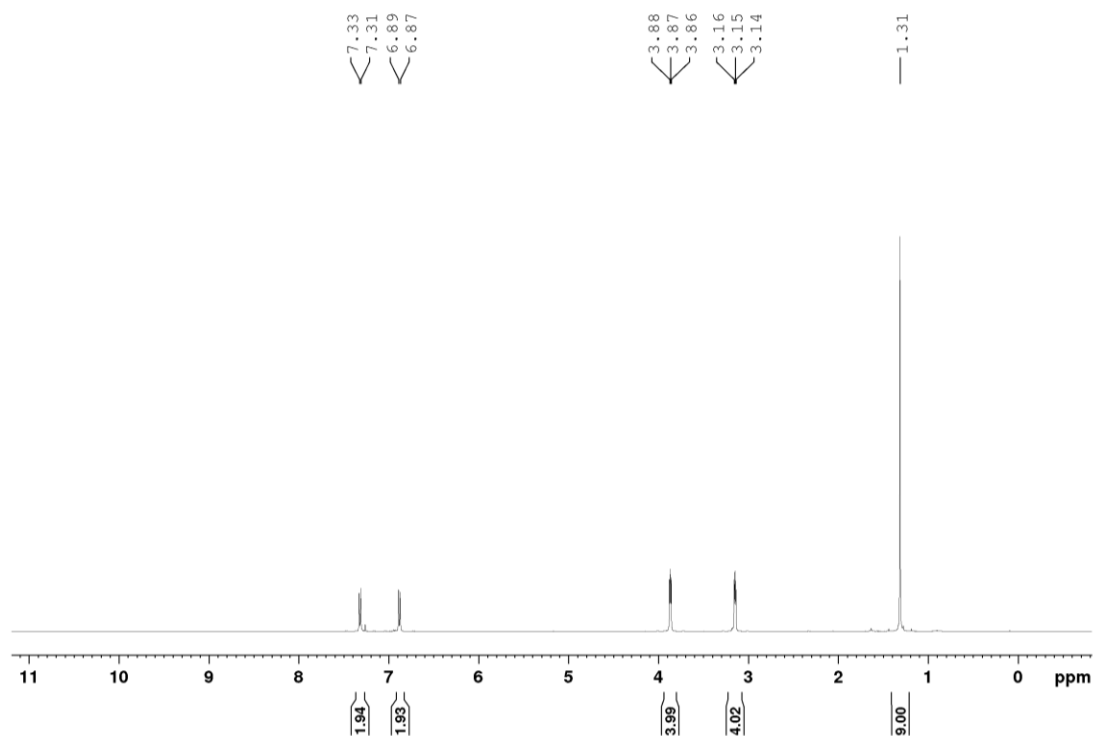


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(4-(tert-butyl)phenyl)morpholine (**2f**), (CDCl_3 , 125.8 MHz)

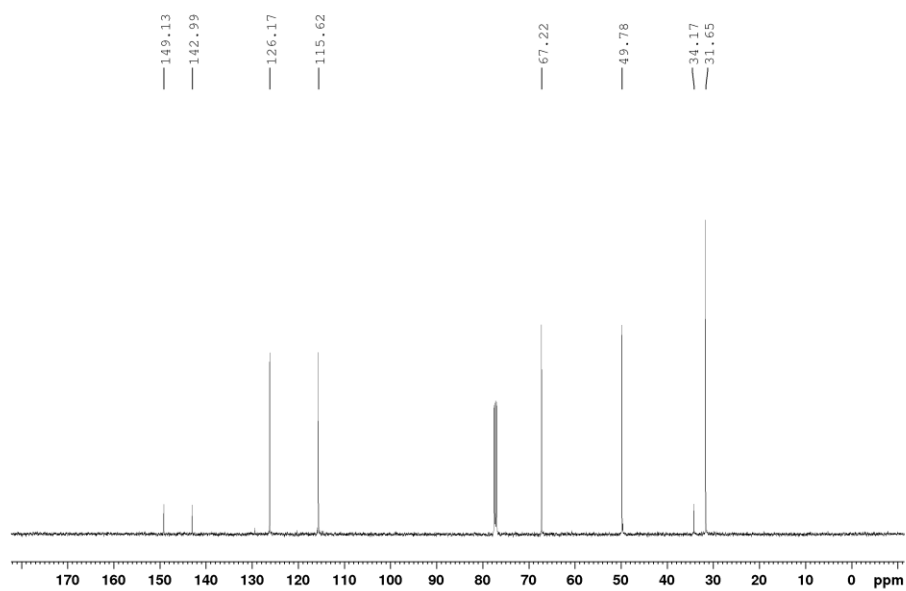


Figure S15. ^1H NMR Spectrum of 4-(2,5-dimethylphenyl)morpholine (**2g**), (CDCl_3 , 300 MHz)

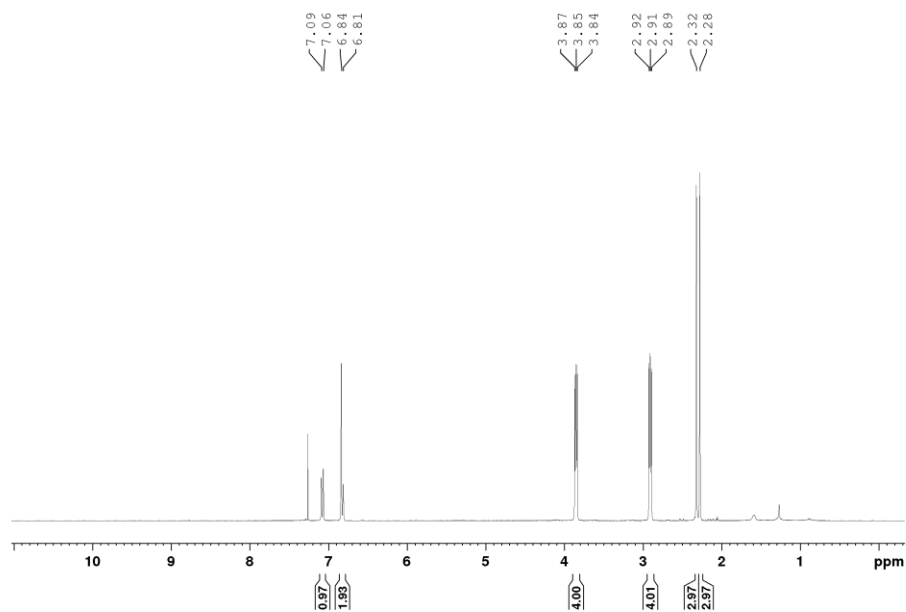


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(2,5-dimethylphenyl)morpholine (**2g**), (CDCl_3 , 125.8 MHz)

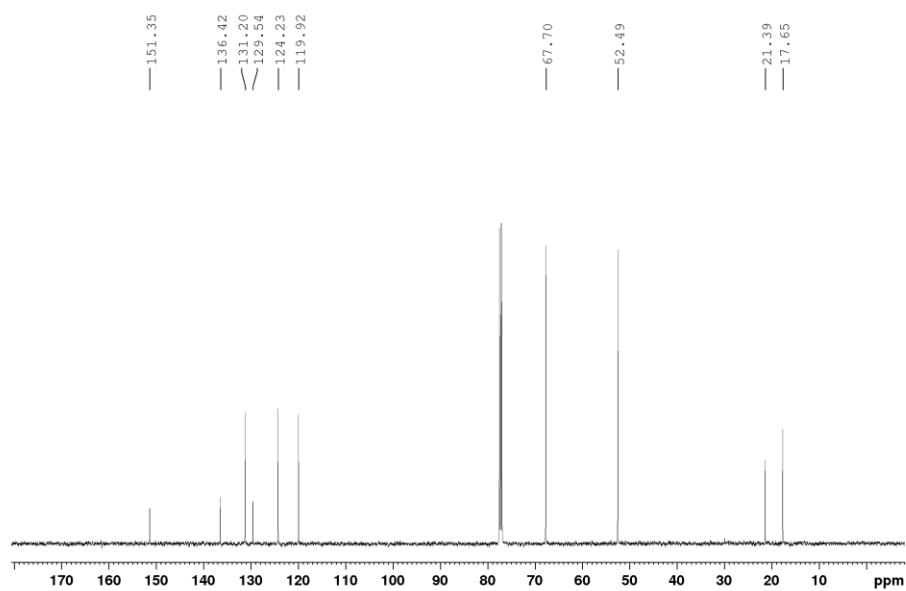


Figure S17. ^1H NMR Spectrum of 4-(4-methoxyphenyl)morpholine (**2h**), (CDCl_3 , 300 MHz)

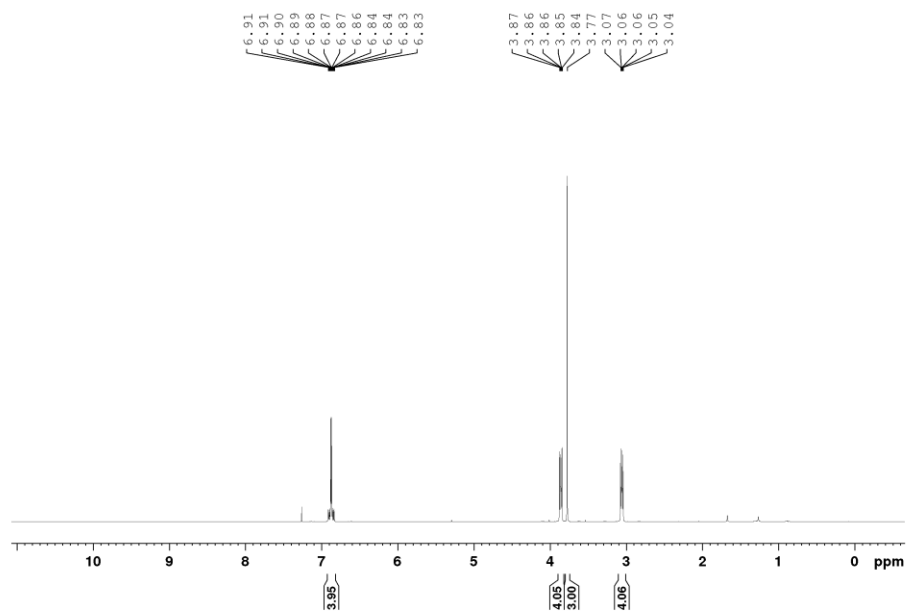


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(4-methoxyphenyl)morpholine (**2h**), (CDCl_3 , 75.5 MHz)

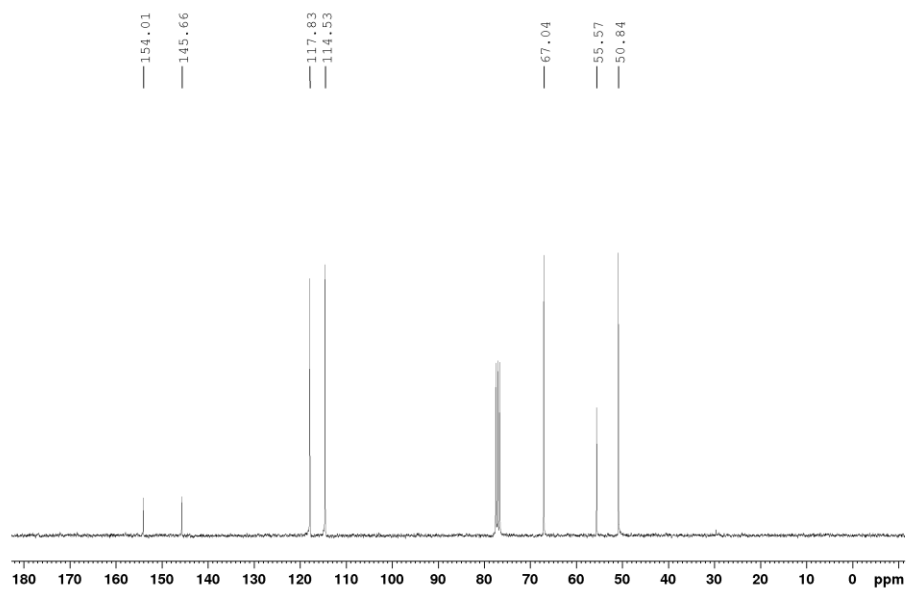


Figure S19. ^1H NMR Spectrum of 1-(naphthalen-1-yl)-1H-indole (**3a**), (CDCl_3 , 500 MHz)

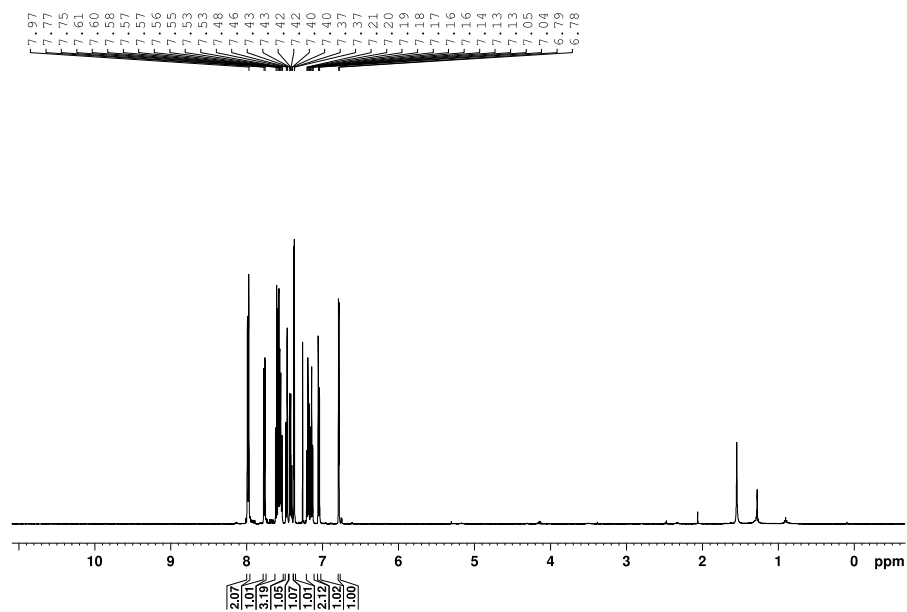


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1-(naphthalen-1-yl)-1H-indole (**3a**), (CDCl_3 , 125.8 MHz)

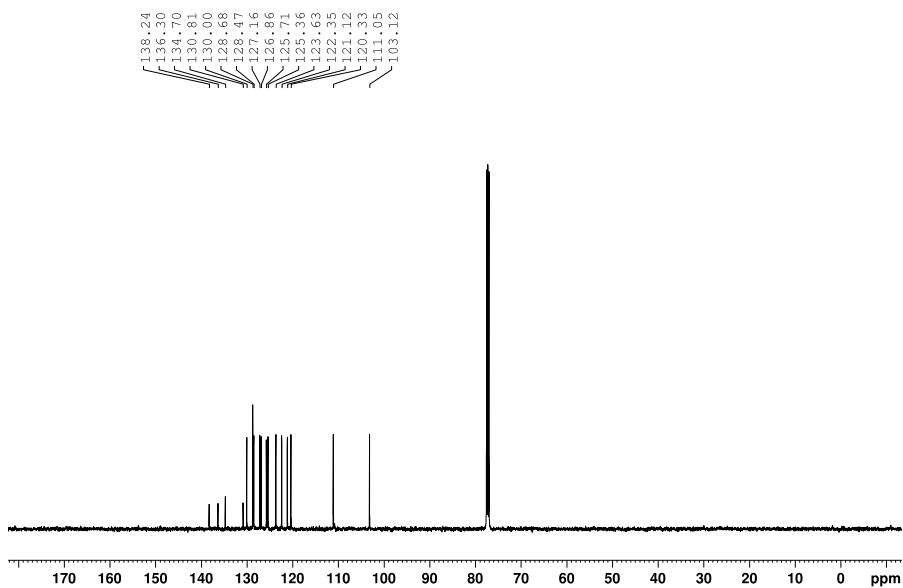


Figure S21. ^1H NMR Spectrum of 4-(1H-indol-1-yl)benzonitrile (**3b**), (CDCl_3 , 500 MHz)

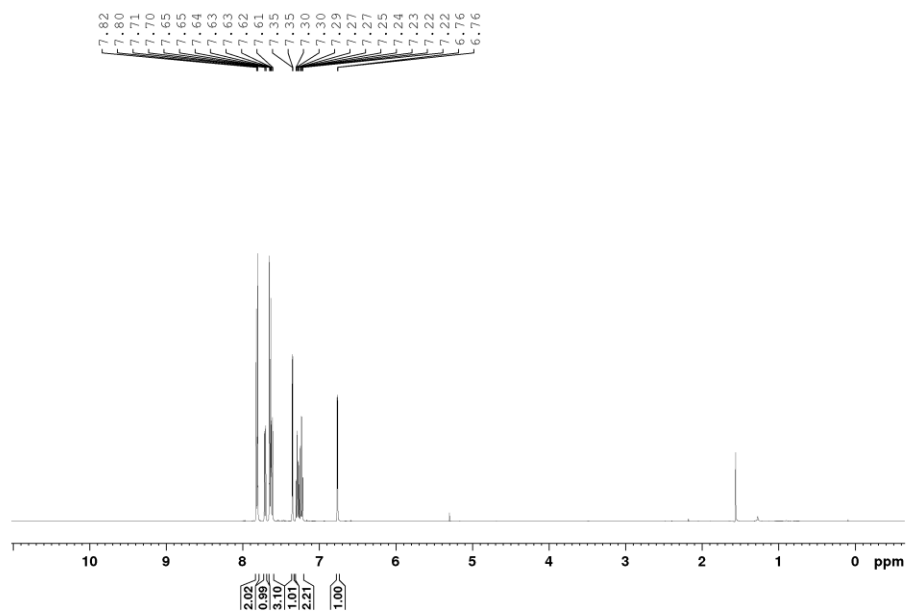


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(1H-indol-1-yl)benzonitrile (**3b**), (CDCl_3 , 125.8 MHz)

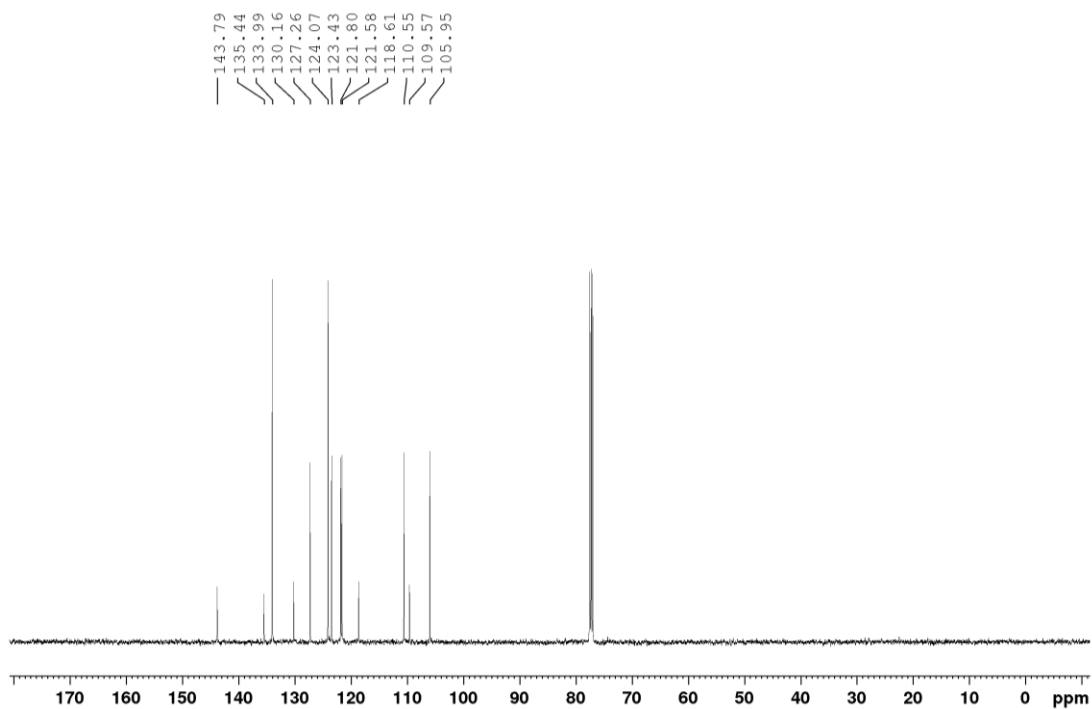


Figure S23. ^1H NMR Spectrum of 1-(benzo[b]thiophen-5-yl)-1H-indole (**3d**), (CDCl_3 , 500 MHz)

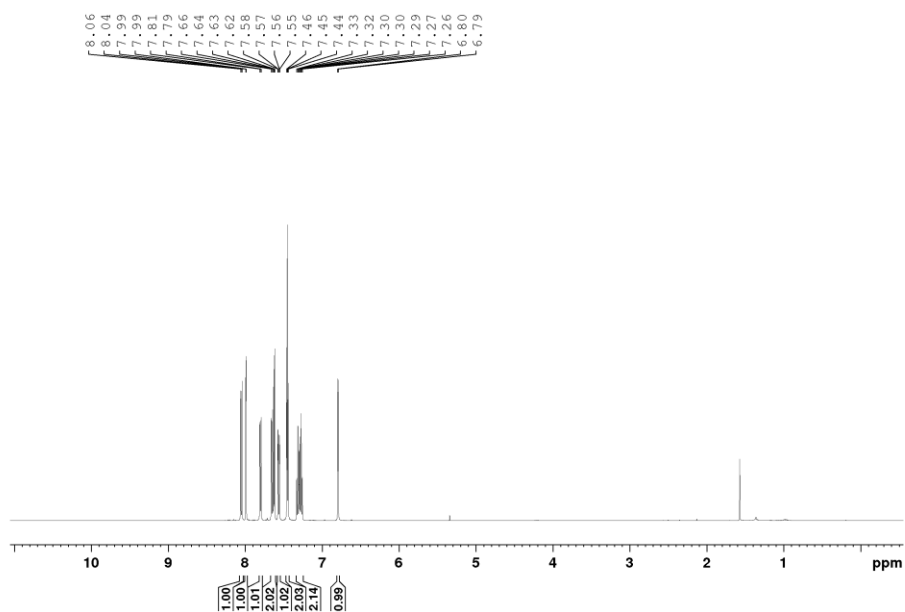


Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1-(benzo[b]thiophen-5-yl)-1H-indole (**3d**), (CDCl_3 , 125.8 MHz)

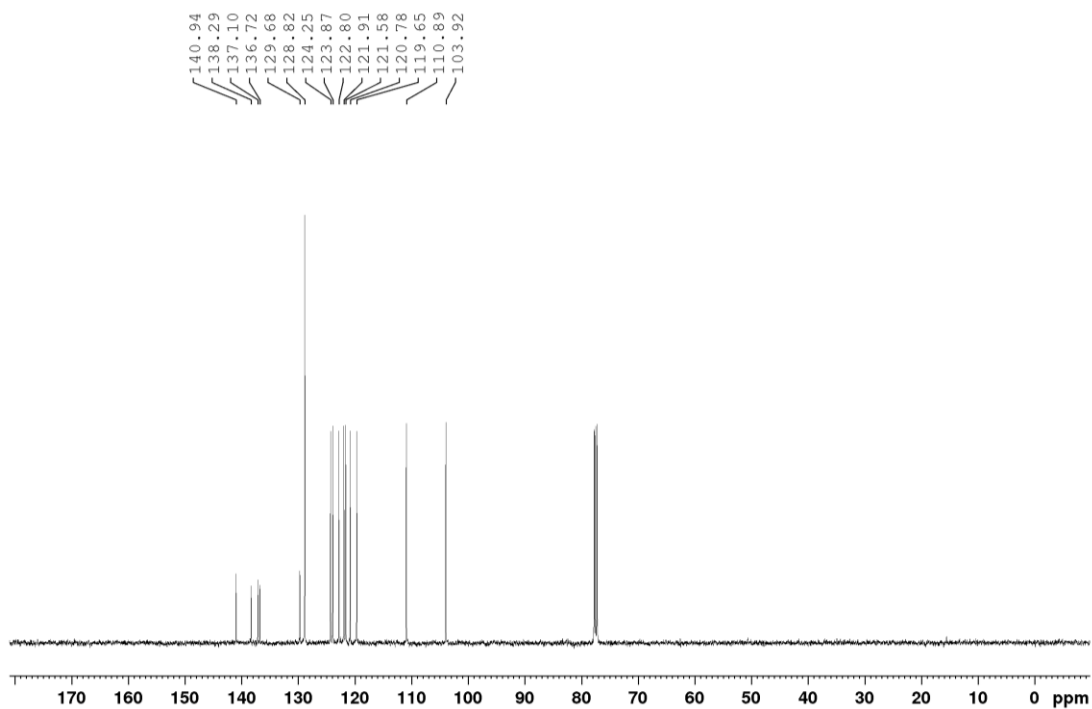


Figure S25. ^1H NMR Spectrum of 4-(1H-indol-1-yl)-2-methylquinoline (**3e**), (CDCl_3 , 500 MHz)

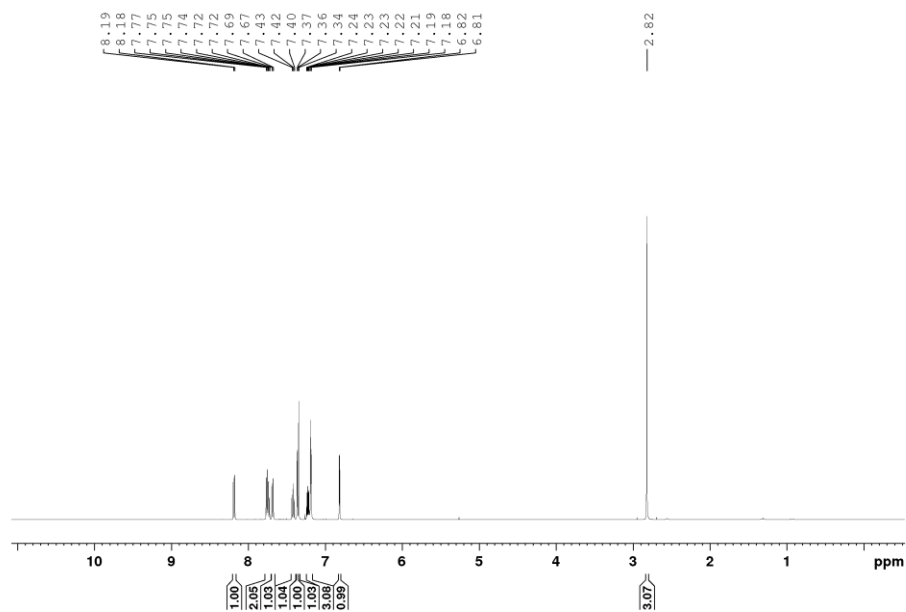


Figure S26. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 4-(1H-indol-1-yl)-2-methylquinoline (**3e**), (CDCl_3 , 125.8 MHz)

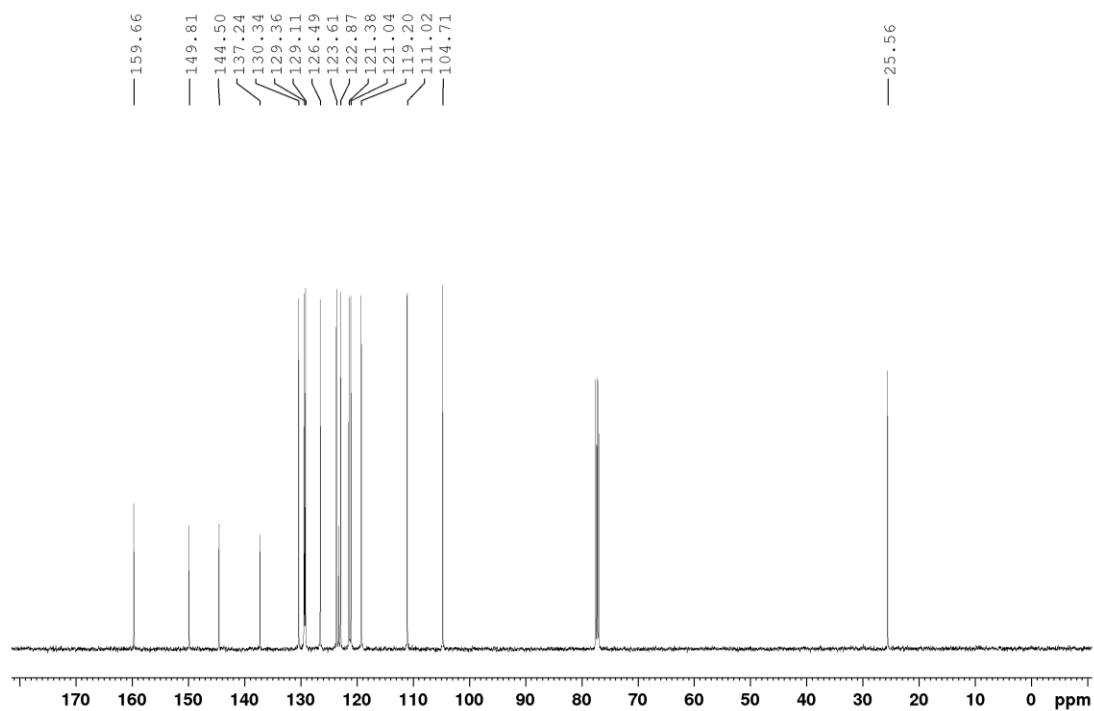


Figure S27. ^1H NMR Spectrum of 1-(4-(tert-butyl)phenyl)-1H-indole (**3f**), (CDCl_3 , 500 MHz)

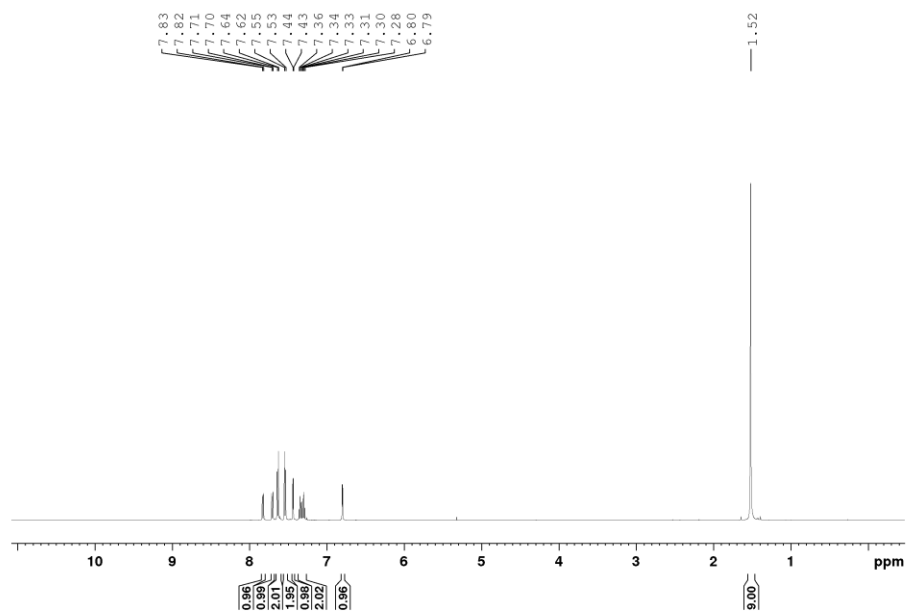


Figure S28. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1-(4-(tert-butyl)phenyl)-1H-indole (**3f**), (CDCl_3 , 125.8 MHz)

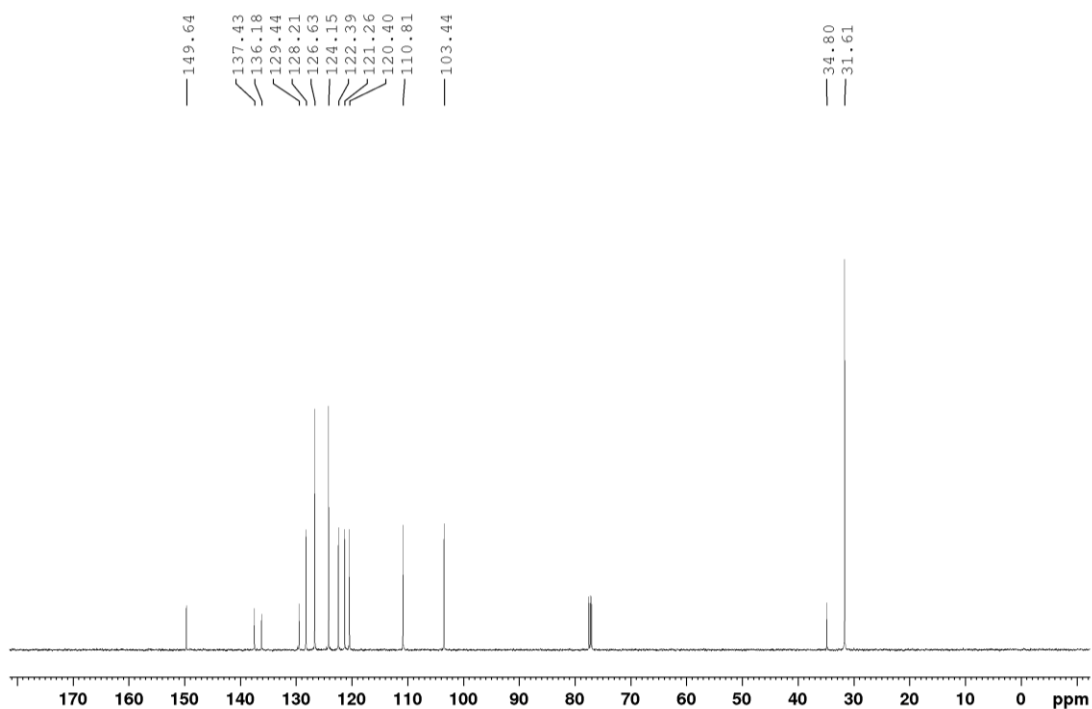


Figure S29. ^1H NMR Spectrum of 1-(2,5-dimethylphenyl)-1H-indole (**3g**), (CDCl_3 , 500 MHz)

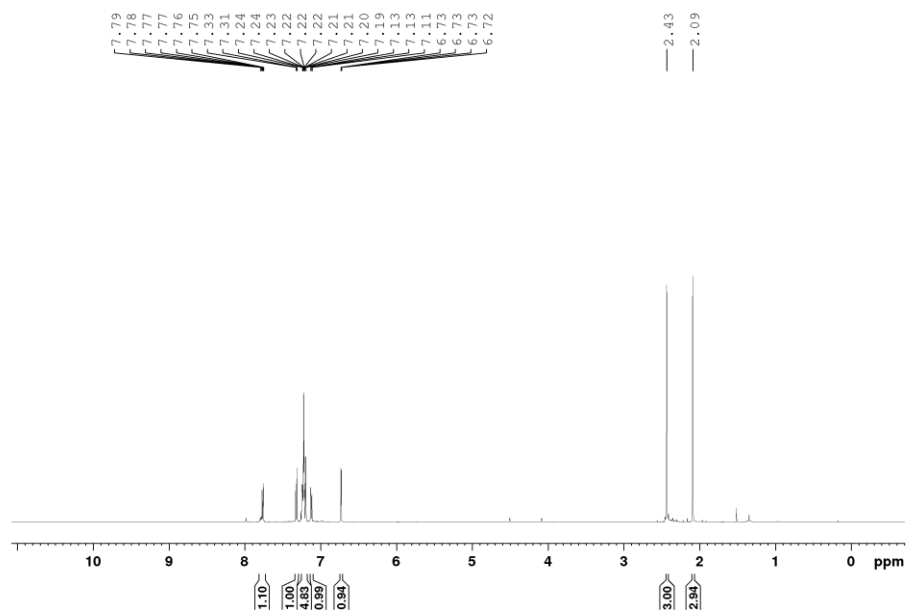


Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1-(2,5-dimethylphenyl)-1H-indole (**3g**), (CDCl_3 , 125.8 MHz)

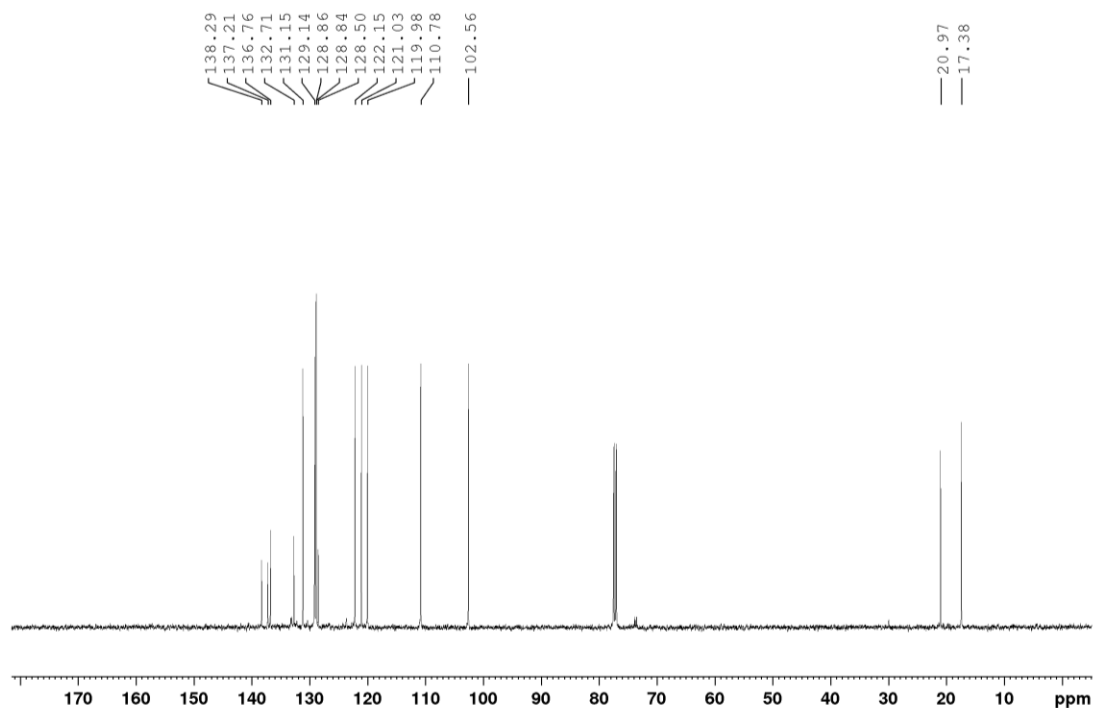


Figure S31. ^1H NMR of Spectrum 1-(4-methoxyphenyl)-1H-indole (**3h**), (CDCl_3 , 500 MHz)

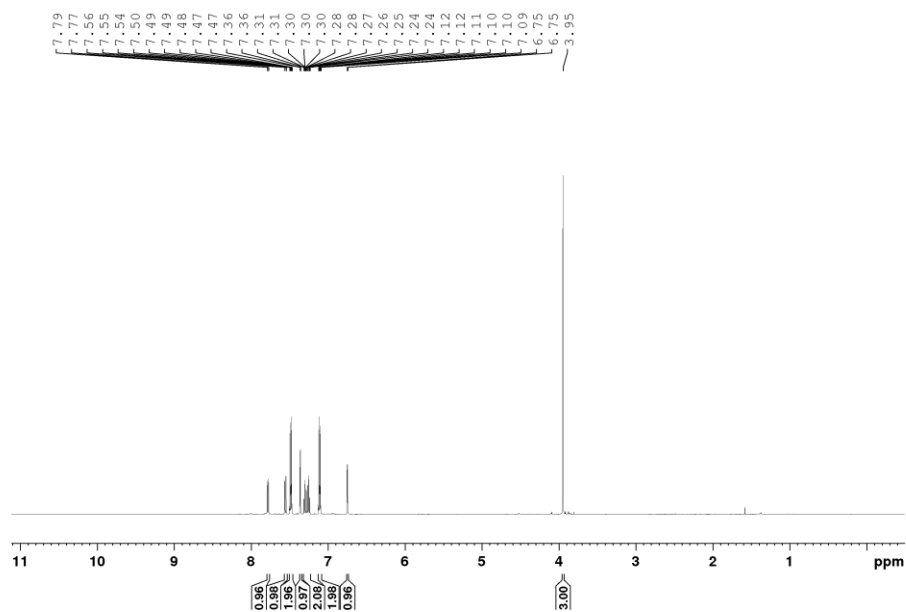


Figure S32. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1-(4-methoxyphenyl)-1H-indole (**3h**), (CDCl_3 , 125.8 MHz)

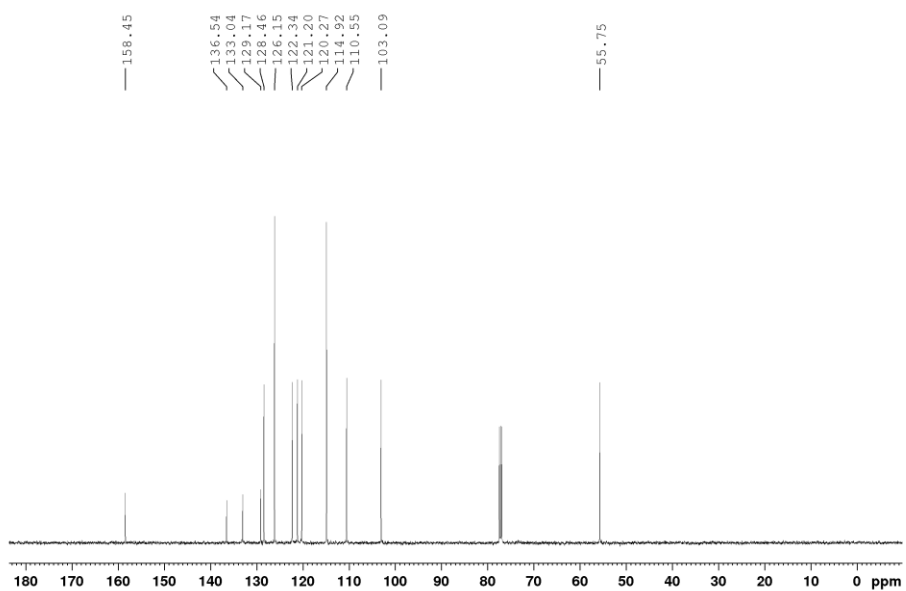


Figure S33. ^1H NMR Spectrum of 1,1'-(bis(di-(3,5-dimethyl-4-methoxyphenyl))phosphino)ferrocene (L^{OMe}) (CDCl_3 , 500 MHz)

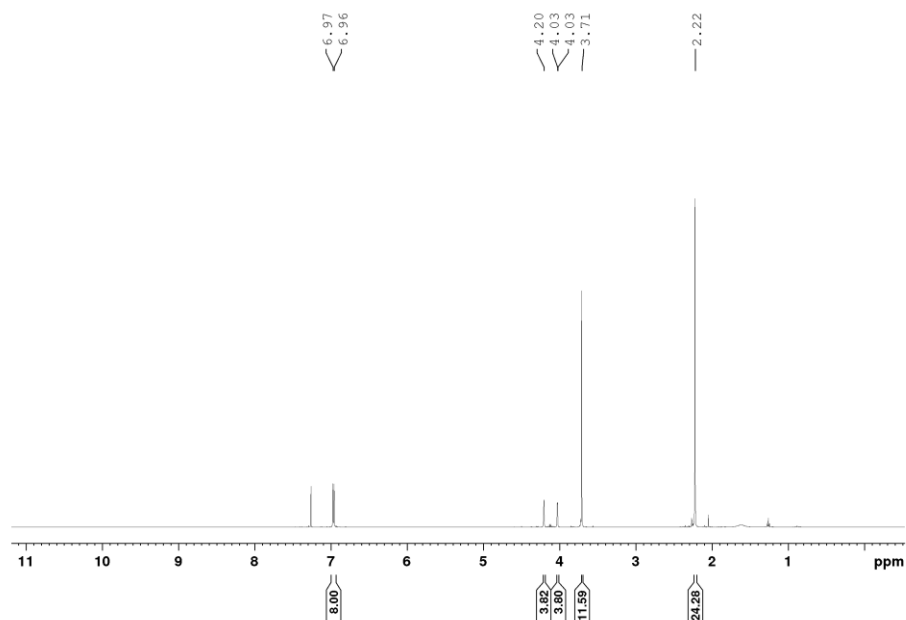


Figure S34. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1,1'-(bis(di-(3,5-dimethyl-4-methoxyphenyl))phosphino)ferrocene (L^{OMe}) (CDCl_3 , 125.8 MHz)

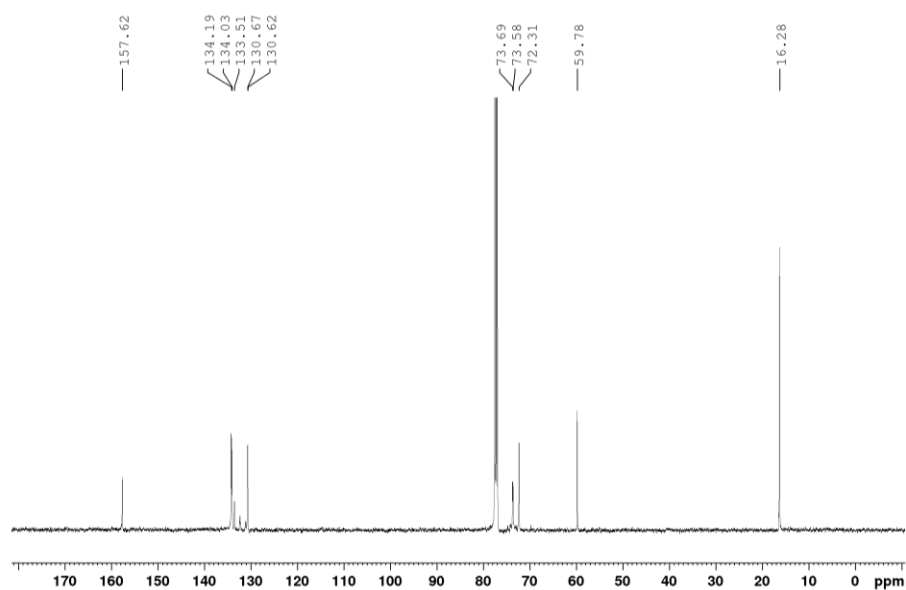


Figure S35. $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of 1,1'-(bis(di-(3,5-dimethyl-4-methoxyphenyl))phosphino)ferrocene (L^{OMe}) (CDCl_3 , 202.5 MHz)

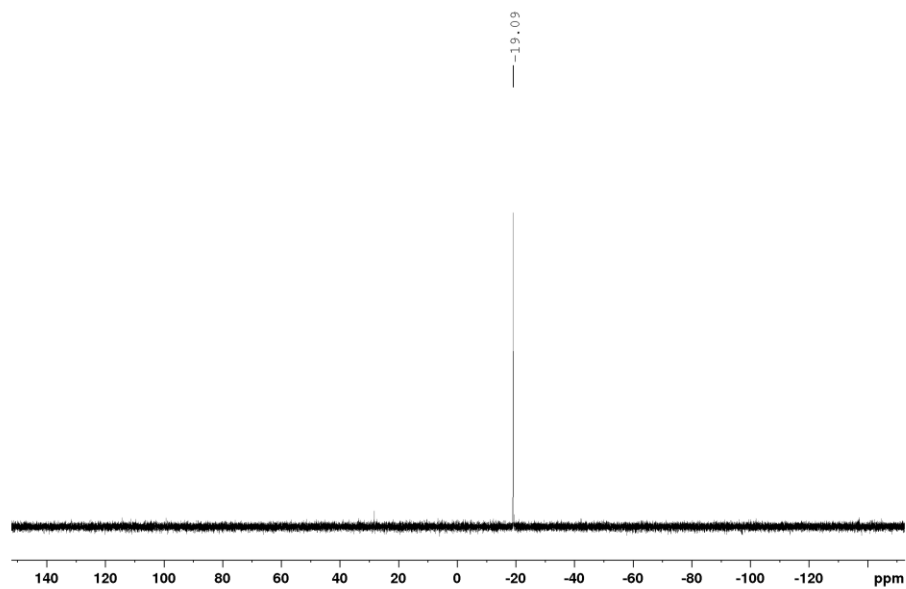


Figure S36. ^1H NMR Spectrum of 1,1'-(bis(3,5-dimethylphenyl)phosphino)ferrocene (L^{Me}) (CDCl_3 , 500 MHz)

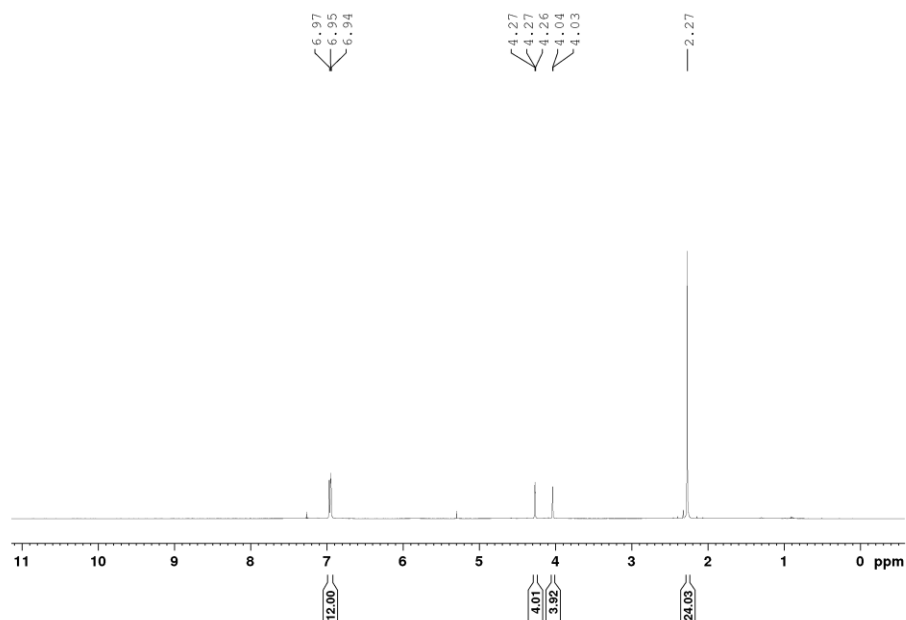


Figure S37. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of 1,1'-(bis(3,5-dimethylphenyl)phosphino)ferrocene (L^{Me}) (CDCl_3 , 125.8 MHz)

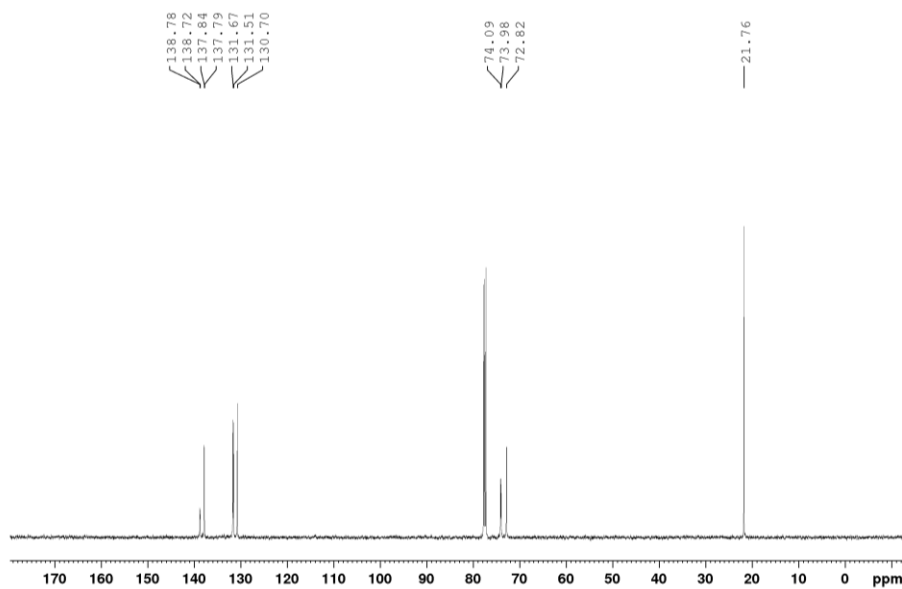
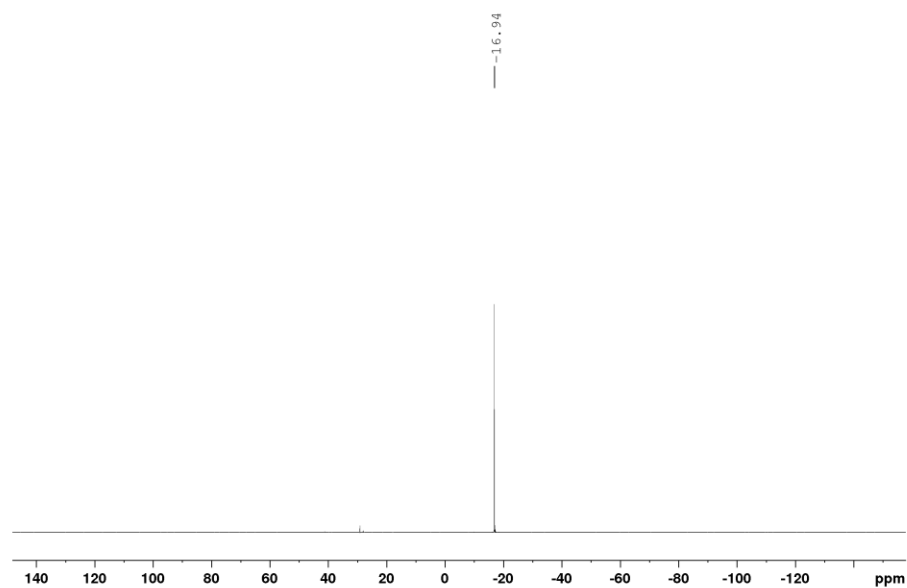


Figure S38. $^{31}\text{P}\{^1\text{H}\}$ NMR Spectrum of 1,1'-(bis(3,5-dimethylphenyl)phosphino)ferrocene (L^{Me}) (CDCl_3 , 202.5 MHz)



SI References

- [S1] M. A. Topchiy, P. B. Dzhevakov, M. S. Rubina, O. S. Morozov, A. F. Asachenko, M. S. Nechaev. *Chem. Eur. J.* **2016**, 22, 1908-1914.
- [S2] S. Zhou, Z. Yang, X. Chen, Y. Li, L. Zhang, H. Fang, W. Wang, X. Zhu, S. Wang. *J. Org. Chem.*, **2015**, 80, 6323-6328.
- [S3] L. Strekowski, S. E. Patterson, L. Janda, R. L. Wydra, D. B. Harden, M. Lipowska, M. T. Cegla. *J. Org. Chem.*, **1992**, 57, 196-201.
- [S4] C. M. So, Z. Zhou, C. P. Lau, F. Y. Kwong. *Angew. Chem. Int. Ed.*, **2008**, 47, 6402-6406.
- [S5] S. Doherty, J. G. Knight, A. M. Ferguson, N. A. B. Ward, R. W. Harrington, W. Clegg. *Adv. Synth. Cat.* **2010**, 352, 201-211.
- [S6] S. M. Crawford, C. B. Lavery, M. Stradiotto. *Chem. Eur. J.* **2013**, 19, 16760-16771.
- [S7] B. S. Lane, D. Sames. *Org. Lett.* **2004**, 6, 2897-2900.
- [S8] Old, D. W., Harris, M. C., Buchwald, S. L. *Org. Lett.*, **2000**, 2, 1403-1406.
- [S9] C. M. Lavoie, P. M. MacQueen, N. L. Rotta-Loria, R. S. Sawatzky, A. Borzenko, A. J. Chisholm, B. K. V. Hargreaves, R. McDonald, M. J. Ferguson, M. Stradiotto. *Nat. Commun.* **2016**, 7, 11073.