Supporting Information for *Acta Phys. -Chim. Sin.* 2016, *32* (7): 1691－1698
doi: 10.3866/PKU.WHXB201604061

取代基效应对二取代二苯基硝酮还原电位的影响

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Effects of Substituents on Reduction Potentials of Disubstituted *N*-Phenyl-*α*-phenylnitrones

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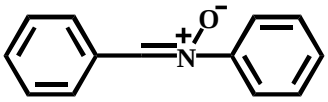
1、数据准备

化合物 XPNYs 的还原电位 $E_{(Red)}$测定均采用三电极体系，工作电极为玻碳电极，参比电极为自制的 $Ag/AgNO_3$ 电极，助电极为铂电极，扫描速度为 100 mV/s。用电子天平称取适量的待测物质，用 0.1 M 的支持电解质溶液定容配制成 0.01 mol/L 左右的溶液，待测。用 CS300 电化学工作站进行测定, 测定时首先用二茂铁校正。

2、化合物 XPNY 的氢谱/碳谱数据

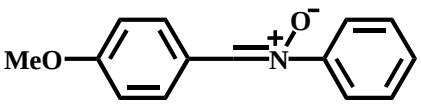
2.1 $C_{13}H_{11}NO$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (m, 2H), 7.92 (s, 1H), 7.77 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.48 (m, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ: 115.77, 115.95, 122.33, 128.80, 131.46, 136.03, 148.04, 160.16, 162.21.

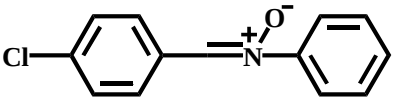
2.2 $C_{14}H_{13}NO_2$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.9 Hz, 2H), 7.85 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.45 (m, 3H), 6.99 (d, *J* = 9.0 Hz, 2H), 3.87 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ:55.48, 114.21, 120.91, 125.60, 129.15, 130.55 ,152.40, 159.77, 162.26.

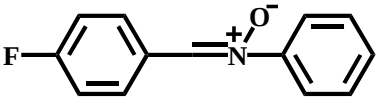
2.3 $C_{13}H_{10}NOCl$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.6 Hz, 2H), 7.91 (s, 1H), 7.76 (m, 2H), 7.47 (m, 5H).

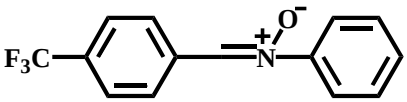
^{13}C NMR (126MHz, $CDCl_3$) δ: 120.83, 126.19, 129.04, 129.18, 129.92, 134.57, 137.31, 151.56, 158.89.

2.4 $C_{13}H_{10}NOF$



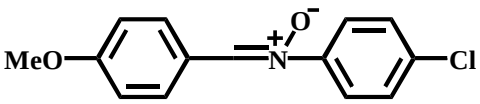
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 8.7, 5.8 Hz, 2H), 7.91 (s, 1H), 7.17 (m, 2H), 7.48 (d, *J* = 7.0 Hz, 3H), 7.17 (t, *J* = 8.7 Hz, 2H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 115.94 (J=22Hz), 120.83, 126.02, 129.18, 130.81, 132.84, 151.80, 158.86, 164.68 (J=252Hz).

2.5 $C_{14}H_{10}NOF_3$



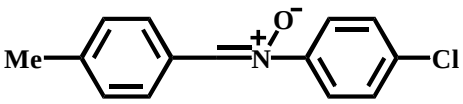
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.3 Hz, 2H), 8.00 (s, 1H), 7.78 (dd, *J* = 6.8, 2.9 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.50 (m, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 101.89, 121.24, 124.78, 128.02, 128.12, 131.78(J=32Hz), 137.95, 137.99, 148.63, 158.05.

2.6 $C_{14}H_{12}NO_2Cl$



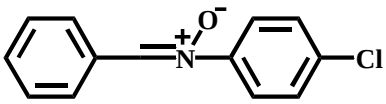
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.9 Hz, 2H), 7.83 (s, 1H), 7.73 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 55.50, 114.27, 122.24, 128.99, 129.22, 130.65, 131.04, 150.84, 160.08, 162.45.

2.7 $C1_4H_{12}NOCl$



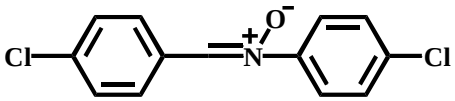
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.1 Hz, 2H), 7.86 (s, 1H), 7.73 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 2.41 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 21.66, 122.19, 128.85, 129.17, 129.55, 131.19, 133.34, 142.17, 150.65, 160.67..

2.8 $C_{13}H_{10}NOCl$



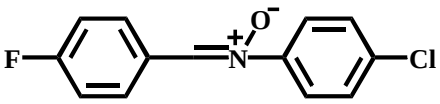
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.90 (s, 1H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.47 (m, 5H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 122.20, 128.83, 128.86, 129.23, 131.44 131.63, 135.90, 150.48, 160.75.

2.9 $C_{13}H_9NOCl_2$



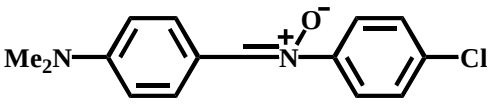
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.4 Hz, 2H), 7.88 (s, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.44 (dd, *J* = 8.5, 2.7 Hz, 4H).
^{13}C NMR (126MHz, $CDCl_3$) δ:122.18, 129.12, 129.27, 129.99, 131.71, 134.38, 137.61, 150.04, 159.12.

2.10 $C_{13}H_9NOFCl$



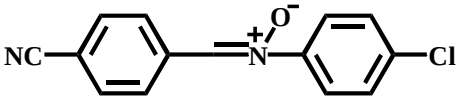
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 8.8, 5.7 Hz, 2H), 7.88 (s, 1H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.17 (t, *J* = 8.7 Hz, 2H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 116.05(J=22Hz), 122.22, 129.31, 130.92, 131.57, 132.32, 150.28, 159.18, 164.84(J=252Hz).

2.11 $C_{15}H_{15}N_2OCl$



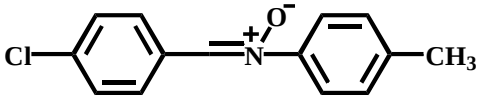
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.9 Hz, 2H), 7.75 (d, *J* = 2.6 Hz, 2H), 7.73 (s, 1H), 7.41 (d, *J* = 8.7 Hz, 2H), 6.72 (d, *J* = 8.8 Hz, 2H), 3.06 (s, 6H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 40.16, 111.50, 122.23, 124.01, 129.05, 130.28, 130.53, 151.42, 152.58, 160.55.

2.12 $C_{14}H_9N_2OCl$



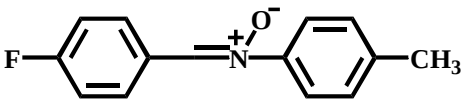
^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.46 (d, *J* = 8.4 Hz, 2H), 7.98 (s, 1H), 7.73 (m, 4H), 7.47 (d, *J* = 8.8 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 147.13, 136.52, 134.12, 132.64, 132.35, 129.45, 128.87, 122.95, 118.39, 113.52.

2.13 $C_{14}H_{12}NOCl$



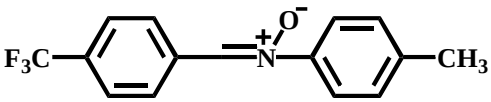
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.4 Hz, 2H), 7.87 (s, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 2.39 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 21.02, 120.79, 129.02, 129.80, 129.83, 134.82, 136.11, 137.12, 149.00, 157.95.

2.14 $C_{14}H_{12}NOF$



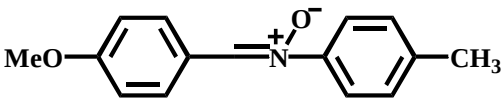
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.90 (dd, *J* = 8.3, 5.7 Hz, 2H), 7.17 (dt, *J* = 15.0, 8.0 Hz, 6H), 2.38 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ:21.01, 115.85(J=22Hz), 120.76, 129.78, 130.60, 132.68, 135.89, 149.17, 157.99, 164.56(J=252Hz)

2.15 $C_{15}H_{12}NOF_3$



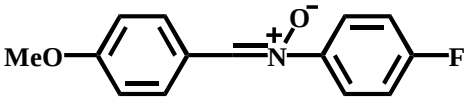
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.2 Hz, 2H), 7.98 (s, 1H), 7.69 (dd, *J* = 24.5, 8.3 Hz, 4H), 7.29 (d, *J* = 8.2 Hz, 2H), 2.43 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 21.07, 120.87,122.81, 125.70, 128.83, 129.87, 132.51(J=32Hz) 136.61, 139.40, 148.68, 157.62.

2.16 $C_{15}H_{15}NO_2$



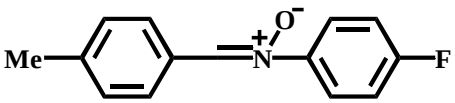
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.84 (d, *J* = 8.6 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H), 2.37 (s, 3H).
^{13}C NMR (126MHz, $CDCl_3$) δ: 2.36 (s, 3H), 3.86(s, 3H), 6.97(d, 2H，J= 10Hz), 7.12(d, 2H, J=10Hz), 7.19(d, 2H, *J* =5Hz),

2.17 $C_{14}H_{12}NO_2F$



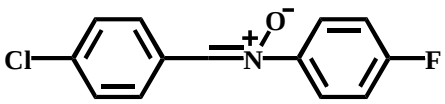
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.8 Hz, 2H), 7.80 (s, 1H), 7.76 (dd, *J* = 8.9, 4.7 Hz, 2H), 7.13 (t, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.79, 161.68, 145.04, 134.12, 131.11, 123.48, 115.99, 115.80, 114.00, 55.36.

2.18 $C_{14}H_{12}NOF$



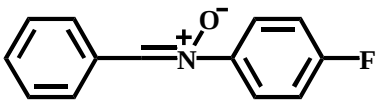
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.2 Hz, 2H), 7.84 (s, 1H), 7.78 (m, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.14 (t, *J* = 8.5 Hz, 2H), 2.41 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.91, 161.92, 145.18, 141.73, 134.56, 129.22, 127.84, 123.59, 115.93, 21.76.

2.19 $C_{13}H_9NOFCl$



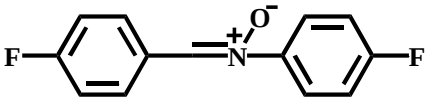
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.5 Hz, 2H), 7.86 (s, 1H), 7.77 (dd, *J* = 8.7, 4.6 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.17 (t, *J* = 8.4 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.14, 145.07, 136.55, 133.35, 130.15, 128.96, 123.64, 116.22, 116.03.

2.20 $C_{13}H_{10}NOF$



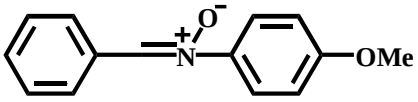
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.88 (s, 1H), 7.78 (dd, *J* = 8.9, 4.7 Hz, 2H), 7.48 (m, 3H), 7.16 (t, *J* = 8.5 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.02, 145.24, 134.54, 131.07, 130.46, 129.00, 128.67, 123.67, 116.02.

2.21 $C_{13}H_9NOF_2$



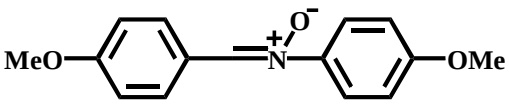
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 8.7, 5.7 Hz, 2H), 7.86 (s, 1H), 7.77 (dd, *J* = 8.9, 4.7 Hz, 2H), 7.17 (t, *J* = 8.2 Hz, 4H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 164.39, 162.37, 145.05, 133.35, 131.30, 126.93, 123.62, 116.17, 115.91.

2.22 $C_{14}H_{13}NO_2$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.7 Hz, 2H), 7.86 (s, 1H), 7.71 (d, *J* = 8.9 Hz, 2H), 7.45 (d, *J* = 6.4 Hz, 3H), 6.94 (d, *J* = 8.9 Hz, 2H), 3.84 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 160.51, 142.32, 133.62, 130.76, 130.62, 128.85, 128.53, 122.87, 113.95, 55.56.

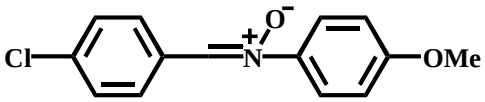
2.23 $C_{15}H_{15}NO_3$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.8 Hz, 2H), 7.80 (s, 1H), 7.71 (d, *J* = 8.9 Hz, 2H), 6.96 (dd, *J* = 17.9, 8.8 Hz, 4H), 3.86 (d, *J* = 10.3 Hz, 6H).

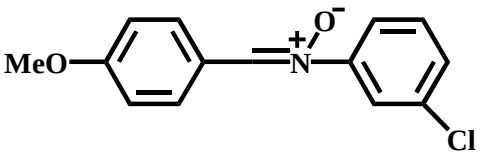
^{13}C NMR (126 MHz, $CDCl_3$) δ: 161.31, 160.34, 142.27, 133.31, 130.97, 123.88, 122.81, 113.97, 55.60, 55.36.

2.24 $C_{14}H_{12}NO_2Cl$



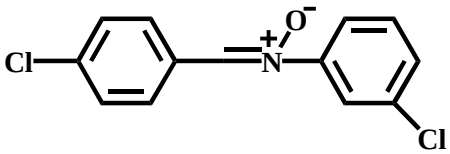
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.4 Hz, 2H), 7.85 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 160.69, 142.14, 136.04, 132.47, 130.01, 129.27, 128.83, 122.85, 114.06, 55.61.

2.25 $C_{14}H_{12}NO_2Cl$



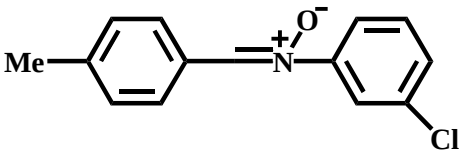
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.8 Hz, 2H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 6.9 Hz, 1H), 7.39 (m, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 161.81, 149.71, 134.91, 134.40, 131.33, 130.10, 129.72, 123.40, 122.23, 119.76, 114.10, 77.25.

2.26 $C_{13}H_9NOCl_2$



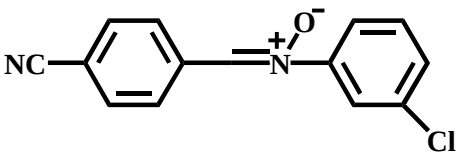
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.4 Hz, 2H), 7.89 (s, 1H), 7.80 (s, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.43 (dd, *J* = 18.9, 8.1 Hz, 4H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 149.59, 136.75, 135.01, 133.70, 130.88, 130.25, 129.42, 128.98, 128.74, 122.27, 119.80.

2.27 $C_{14}H_{12}NOCl$



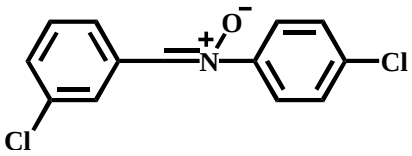
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.0 Hz, 2H), 7.86 (s, 1H), 7.81 (s, 1H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 149.74, 142.03, 134.92, 131.99, 130.13, 129.89, 129.42, 129.25, 127.64, 122.29, 119.83, 21.81.

2.28 $C_{14}H_9N_2OCl$



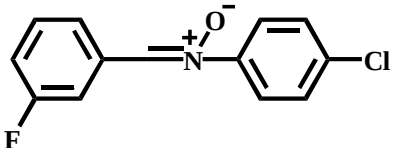
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.3 Hz, 2H), 7.98 (s, 1H), 7.80 (s, 1H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.45 (dt, *J* = 15.9, 8.0 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 149.52, 135.14, 134.03, 132.91, 132.32, 130.70, 130.33, 128.93, 122.27, 119.79, 118.34, 113.61.

2.29 $C_{13}H_9NOCl_2$



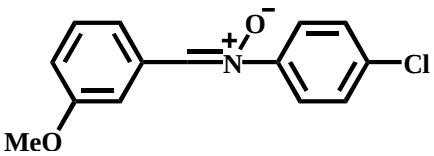
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.88 (s, 1H), 7.72 (d, *J* = 8.8 Hz, 2H), 7.42 (m, 4H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 147.18, 136.08, 134.70, 133.16, 131.89, 131.01, 129.84, 129.35, 128.42, 127.10, 122.94.

2.30 $C_{13}H_9NOFCl$



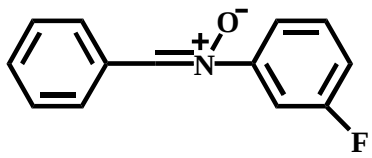
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 10.5 Hz, 1H), 7.91 (s, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.44 (m, 3H), 7.18 (td, *J* = 8.2, 2.3 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.53, 147.21, 136.07, 133.42, 132.18, 130.04, 129.35, 125.06, 122.97, 118.08, 115.20.

2.31 $C_{14}H_{12}NO_2Cl$



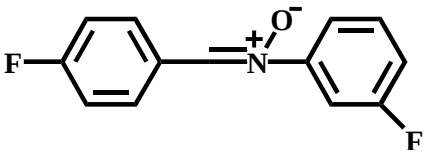
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.89 (s, 1H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 7.1 Hz, 2H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.53, 147.31, 135.75, 134.64, 131.53, 129.47, 129.25, 122.95, 122.28, 118.17, 112.55, 55.31.

2.32 $C_{13}H_{10}NOF$



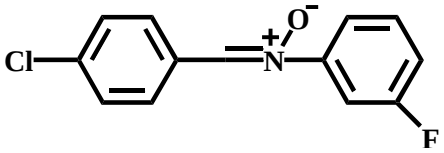
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (s, 2H), 7.92 (s, 1H), 7.57 (t, *J* = 8.6 Hz, 2H), 7.45 (m, 4H), 7.17 (t, *J* = 8.1 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 162.64, 150.26, 134.73, 131.24, 130.38, 129.69, 129.17, 128.68, 117.12, 116.91, 109.92.

2.33 $C_{13}H_9NOF_2$



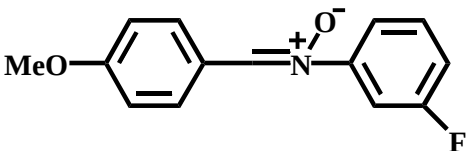
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 8.3, 5.9 Hz, 2H), 7.91 (s, 1H), 7.56 (t, *J* = 8.2 Hz, 2H), 7.45 (dd, *J* = 14.1, 8.2 Hz, 1H), 7.17 (t, *J* = 8.4 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 164.26, 162.25, 150.07, 133.51, 131.48, 130.46, 126.82, 117.17, 117.05, 115.90, 109.88.

2.34 $C_{13}H_9NOFCl$



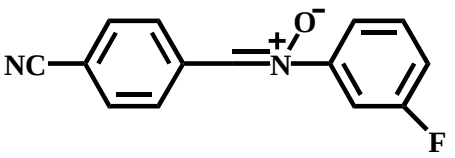
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.8 Hz, 2H), 7.91 (s, 1H), 7.56 (m, 2H), 7.45 (d, *J* = 7.9 Hz, 3H), 7.20 (d, *J* = 7.5 Hz, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 162.61, 149.99, 136.73, 133.61, 130.49, 130.28, 128.99, 128.76, 117.31, 117.09, 109.86.

2.35 $C_{14}H_{12}NO_2F$



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.8 Hz, 2H), 7.86 (s, 1H), 7.56 (m, 2H), 7.42 (dd, *J* = 14.1, 8.0 Hz, 1H), 7.14 (t, *J* = 8.1 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 163.65, 161.73, 150.12, 134.32, 131.94, 131.34, 130.30, 123.39, 116.81, 114.09, 109.75, 55.39.

2.36 $C_{14}H_9N_2OF$

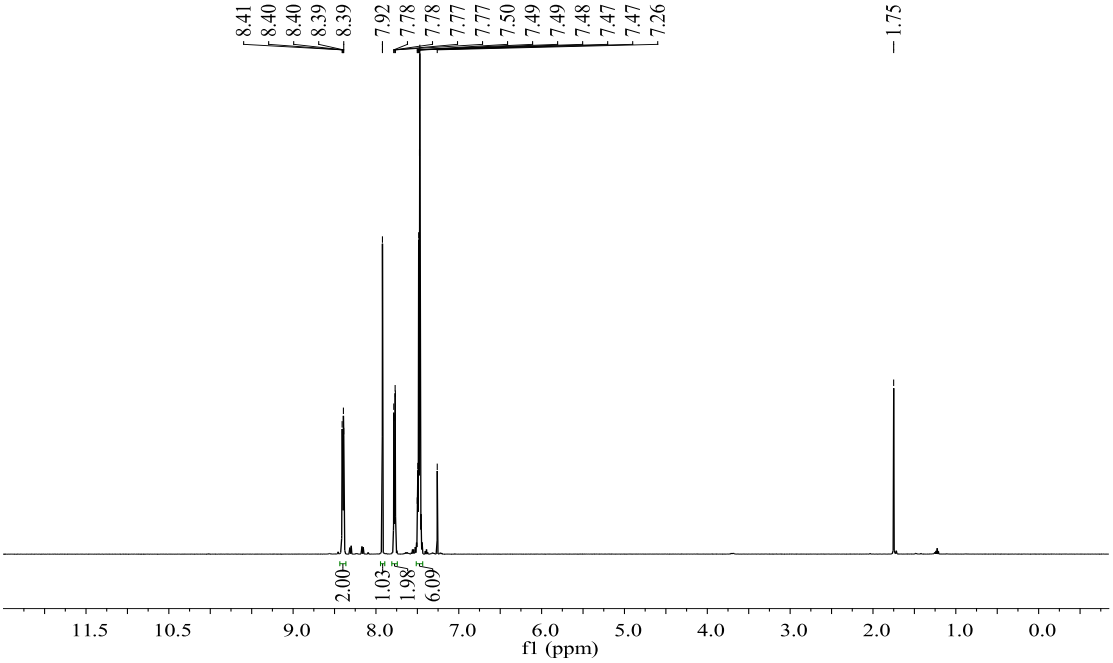


^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.3 Hz, 2H), 8.01 (s, 1H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 7.9 Hz, 2H), 7.48 (d, *J* = 6.4 Hz, 1H), 7.22 (s, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ: 162.58, 149.90, 134.03, 132.86, 132.33, 130.62, 128.95, 118.37, 117.71, 117.08, 113.59, 109.89.

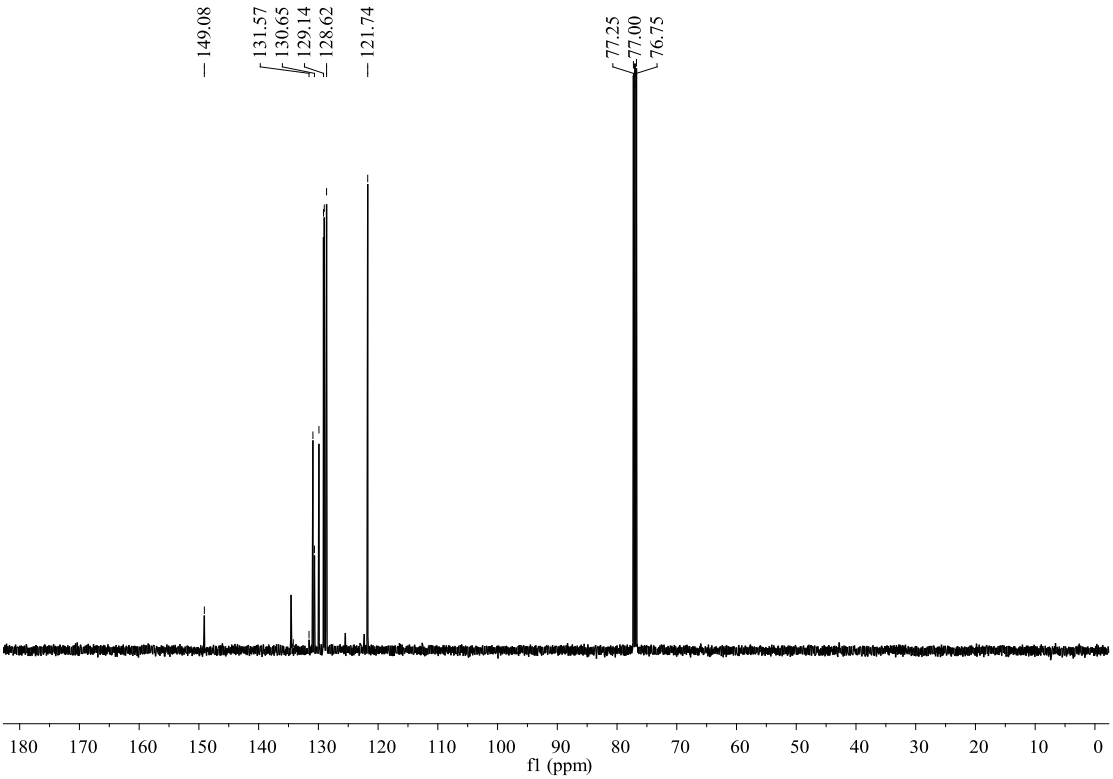
3、化合物 XPNY 的氢谱/碳谱谱图

3.1 Spectrum of ^{1}H NMR of HPNH

$C_{13}H_{11}NO$



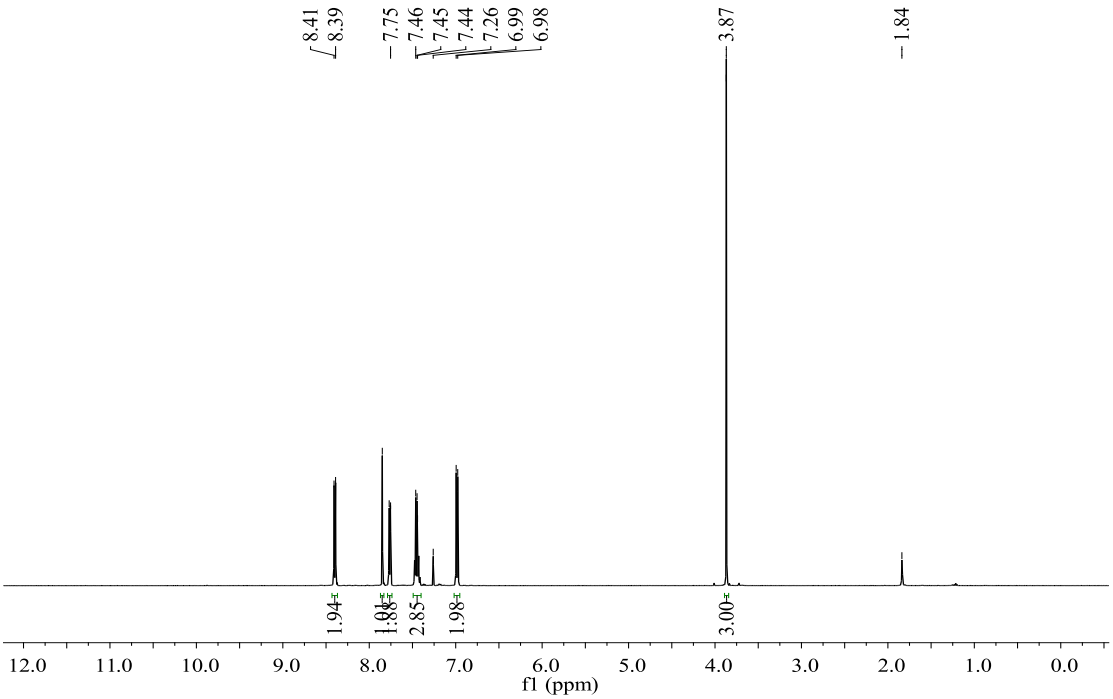
The ^{1}H NMR spectrum of HPNH



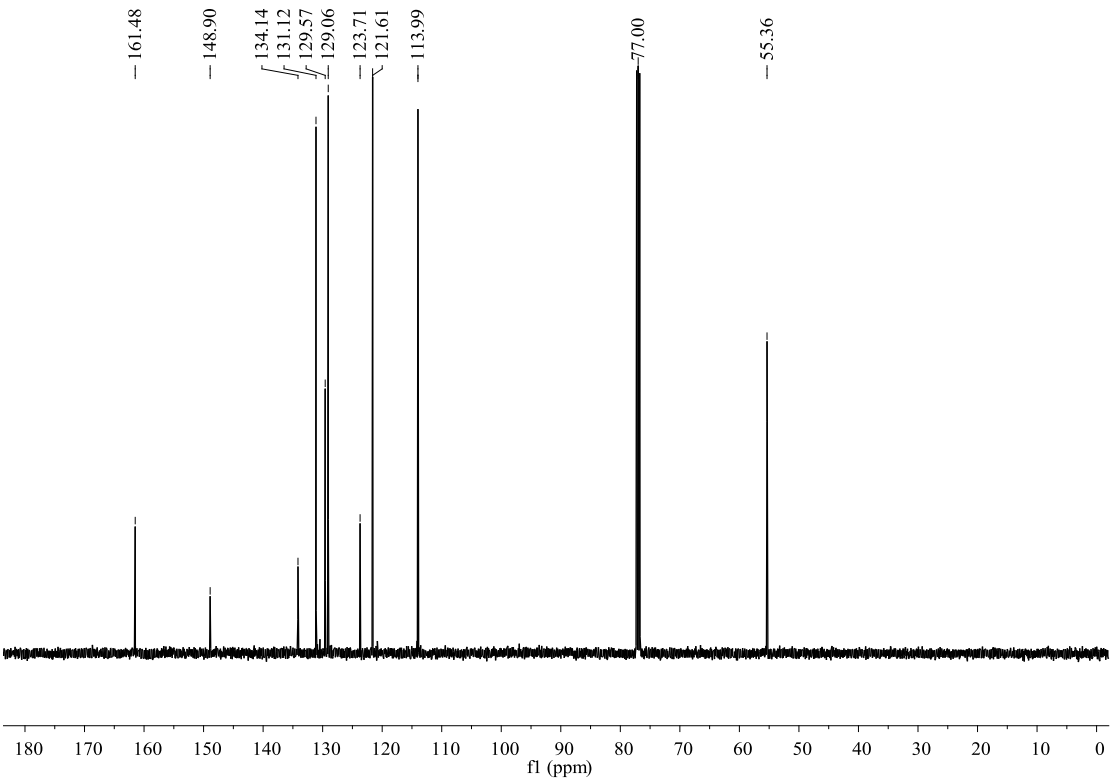
The ^{13}C NMR spectrum of HPNH

3.2 Spectrum of ^{1}H NMR of *p*-MeOPNH

$C_{14}H_{13}NO_2$



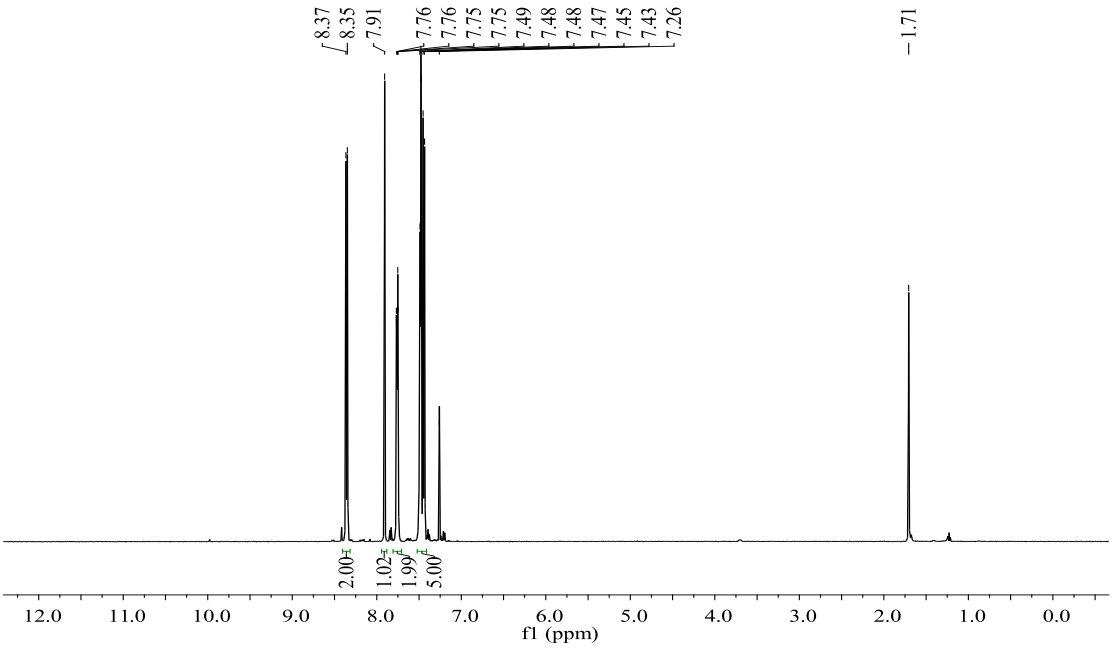
The ^{1}H NMR spectrum of *p*-MeOPNH



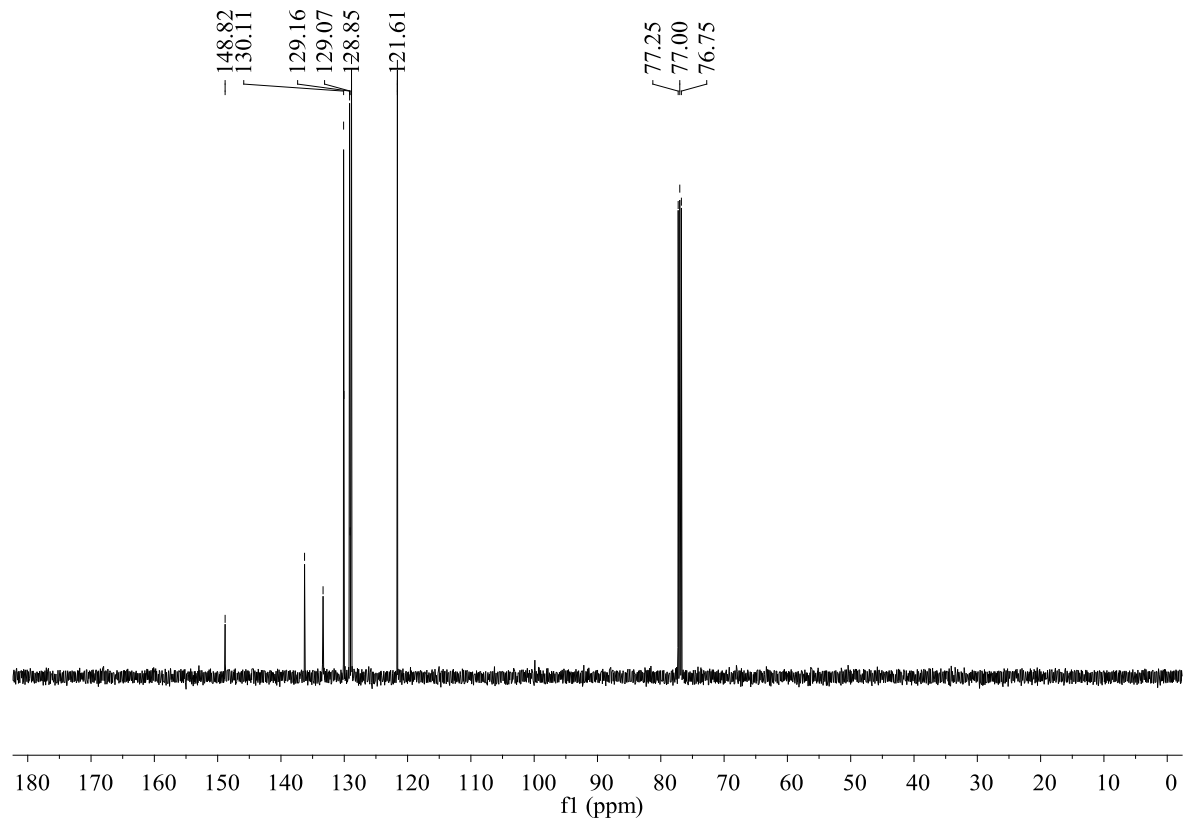
The ^{13}C NMR spectrum of *p*-MeOPNH

3.3 Spectrum of ^{1}H NMR of *p*-ClPNH

$C_{13}H_{10}NOCl$



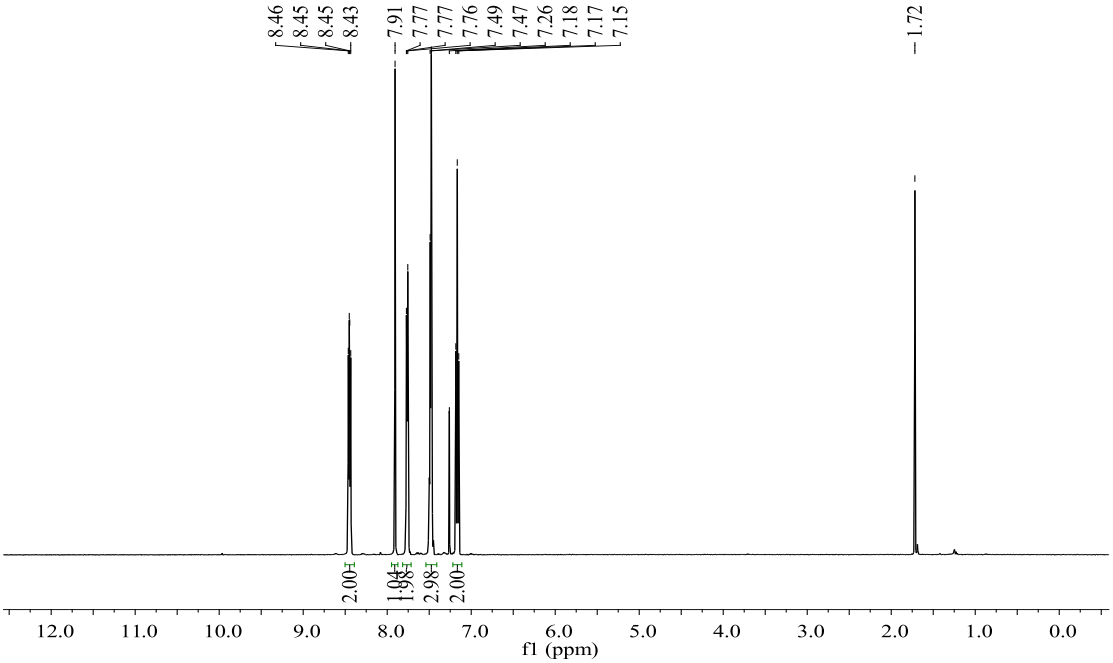
The ^{1}H NMR spectrum of *p*-ClPNH



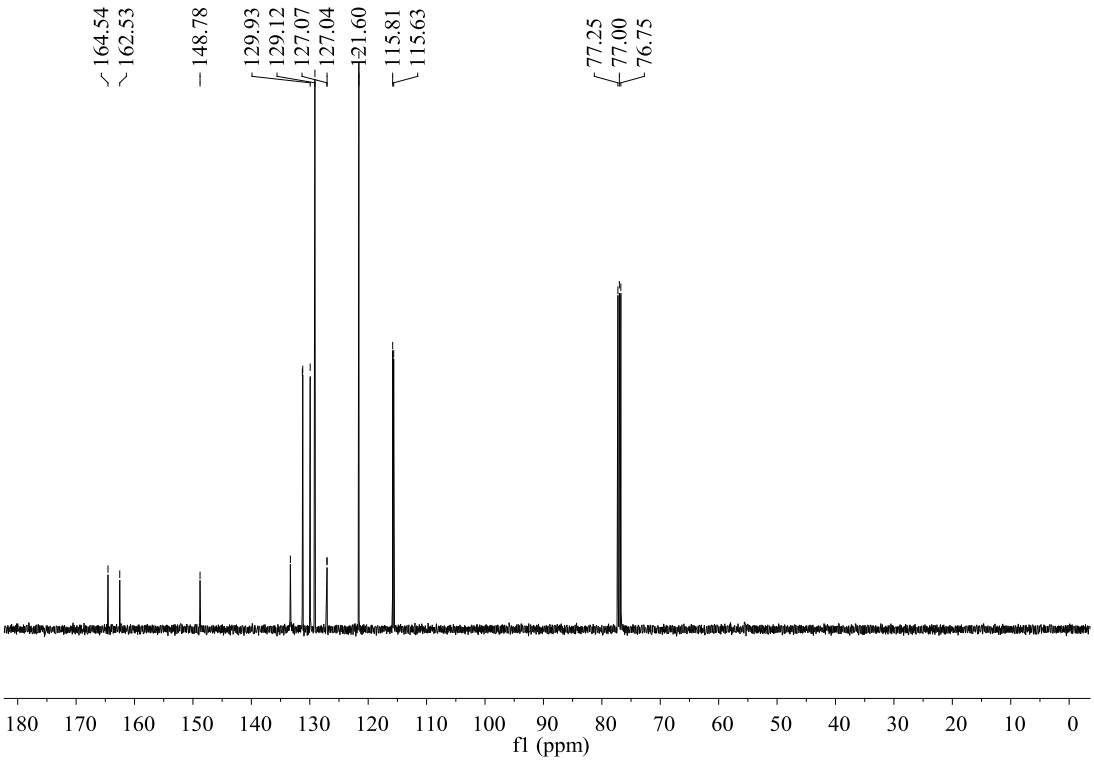
The ^{13}C NMR spectrum of *p*-ClPNH

3.4 Spectrum of ^{1}H NMR of *p*-FPNH

$C_{13}H_{10}NOF$



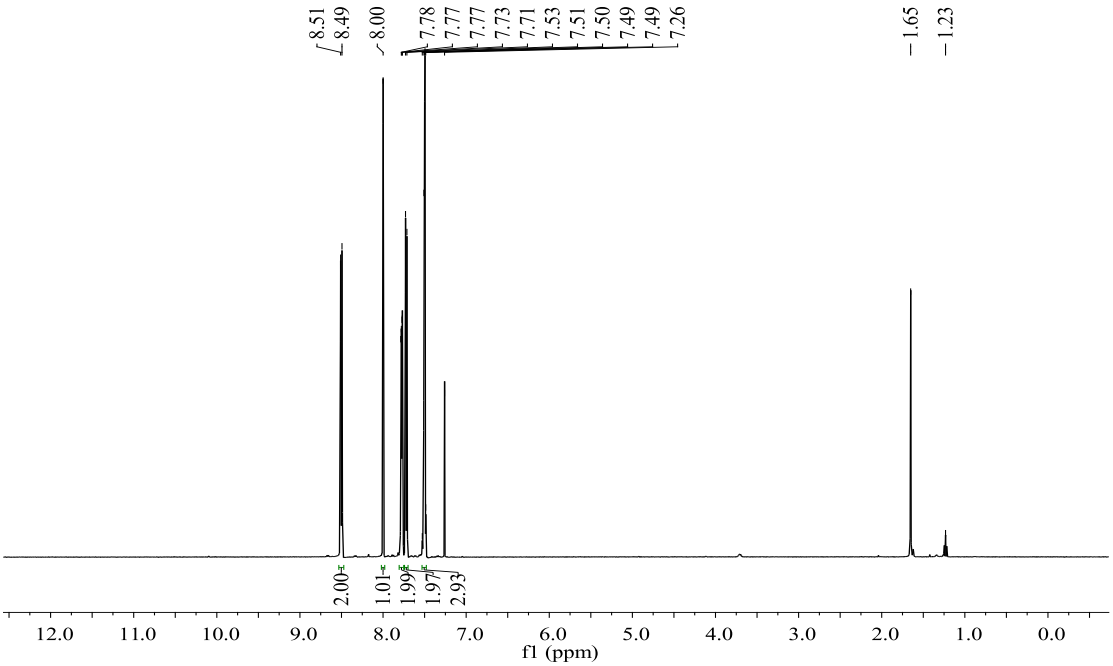
The ^{1}H NMR spectrum of *p*-FPNH



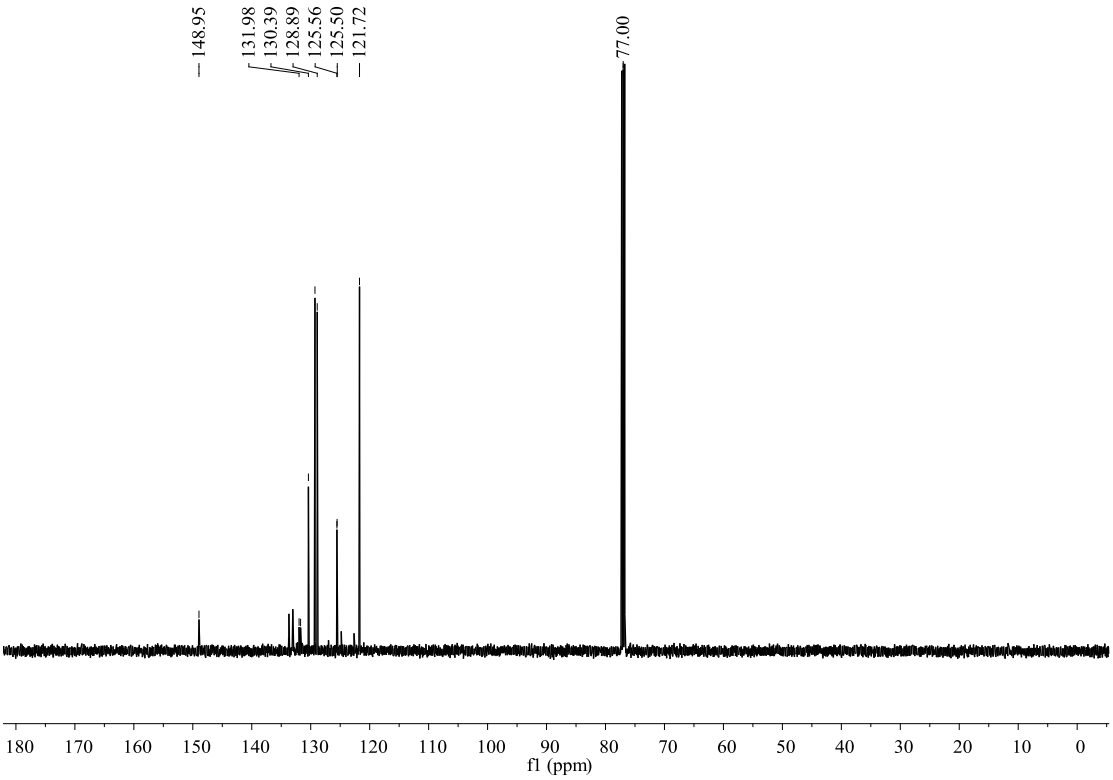
The ^{13}C NMR spectrum of *p*-FPNH

3.5 Spectrum of ^{1}H NMR of *p*-CF_3PNH

$C_{14}H_{10}NOF_3$



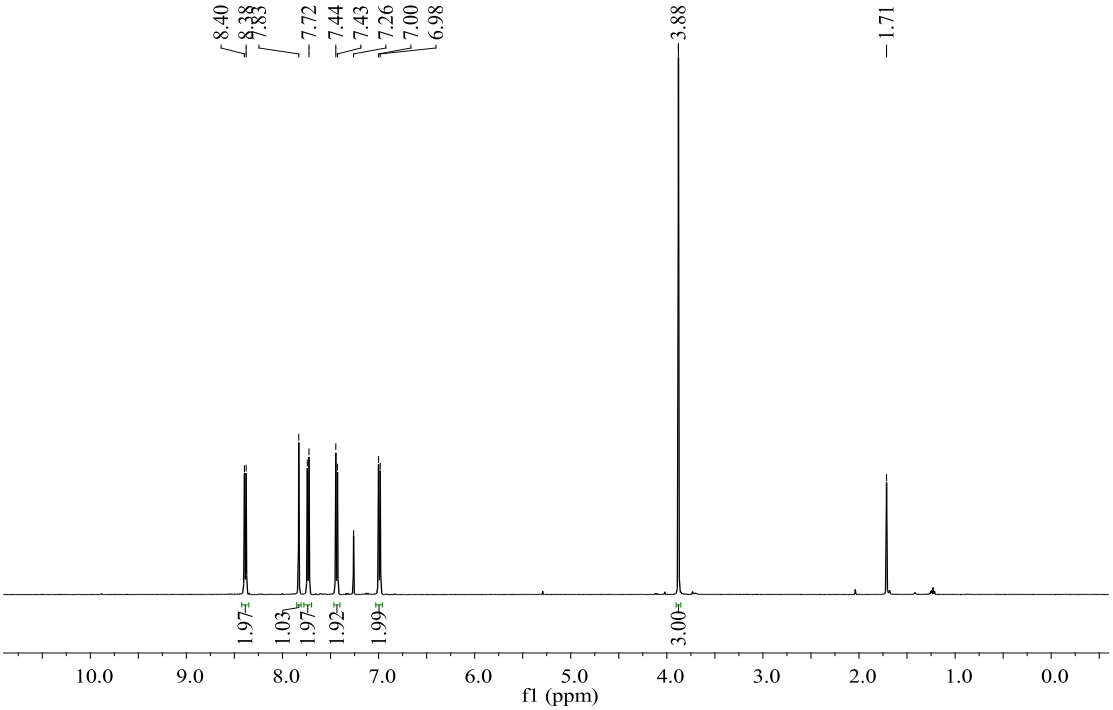
The ^{1}H NMR spectrum of *p*-CF_3PNH



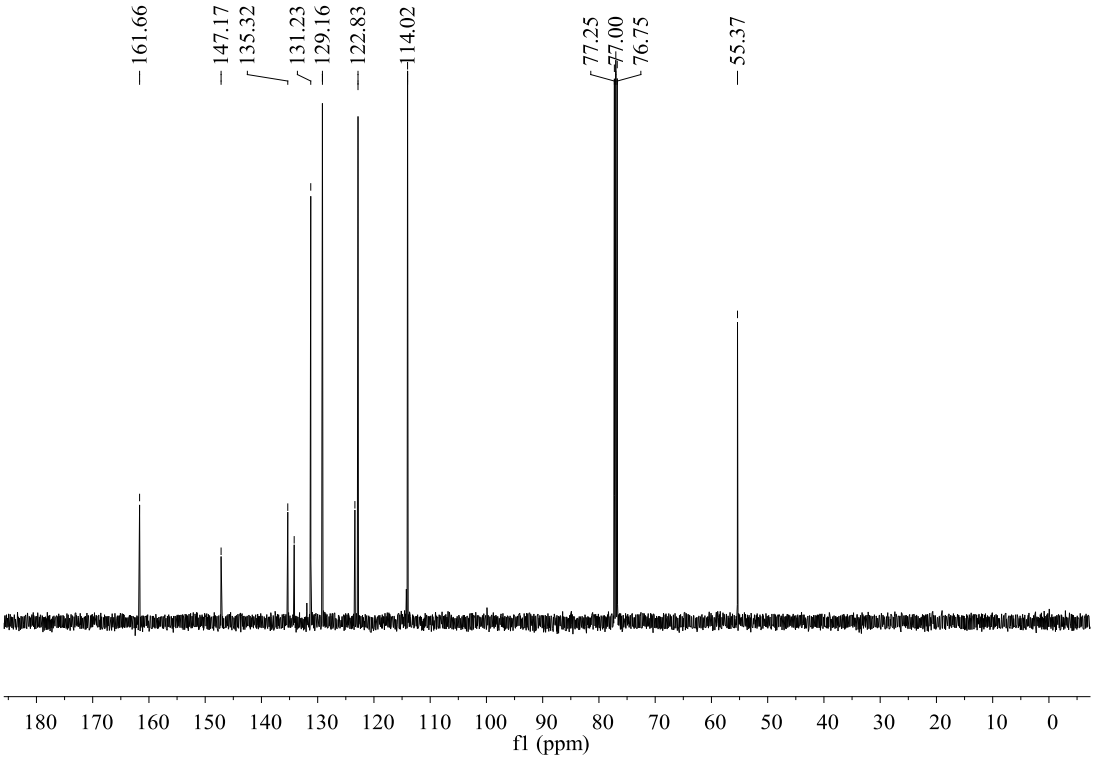
The ^{13}C NMR spectrum of *p*-CF_3PNH

3.6 Spectrum of ^{1}H NMR of *p*-MeOPNCl-*p*

$C_{14}H_{12}NO_2Cl$



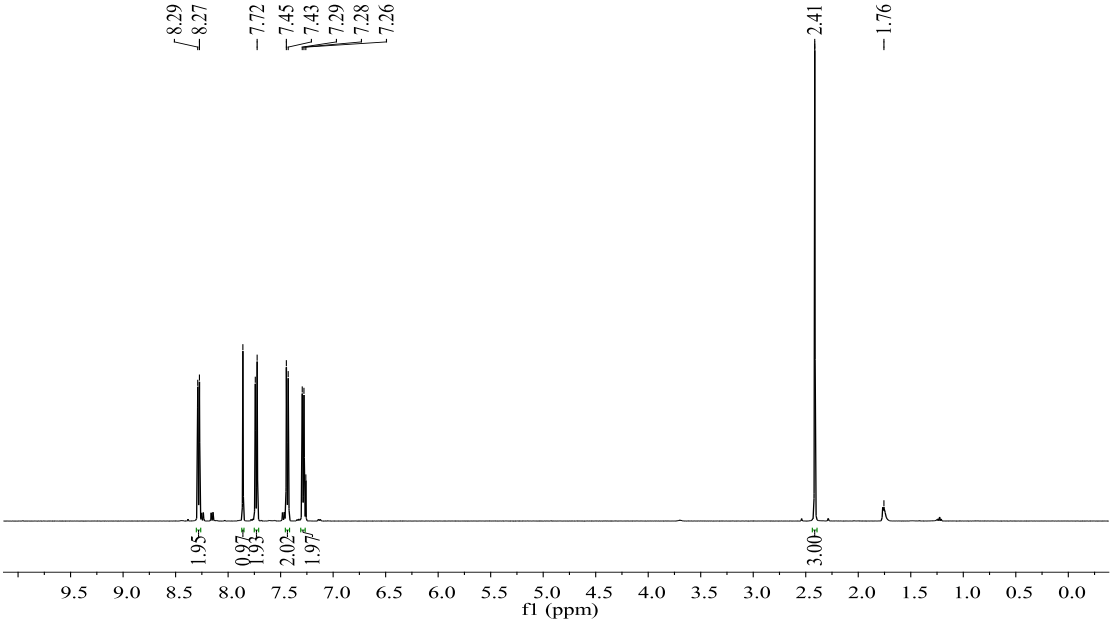
The ^{1}H NMR spectrum of *p*-MeOPNCl-*p*



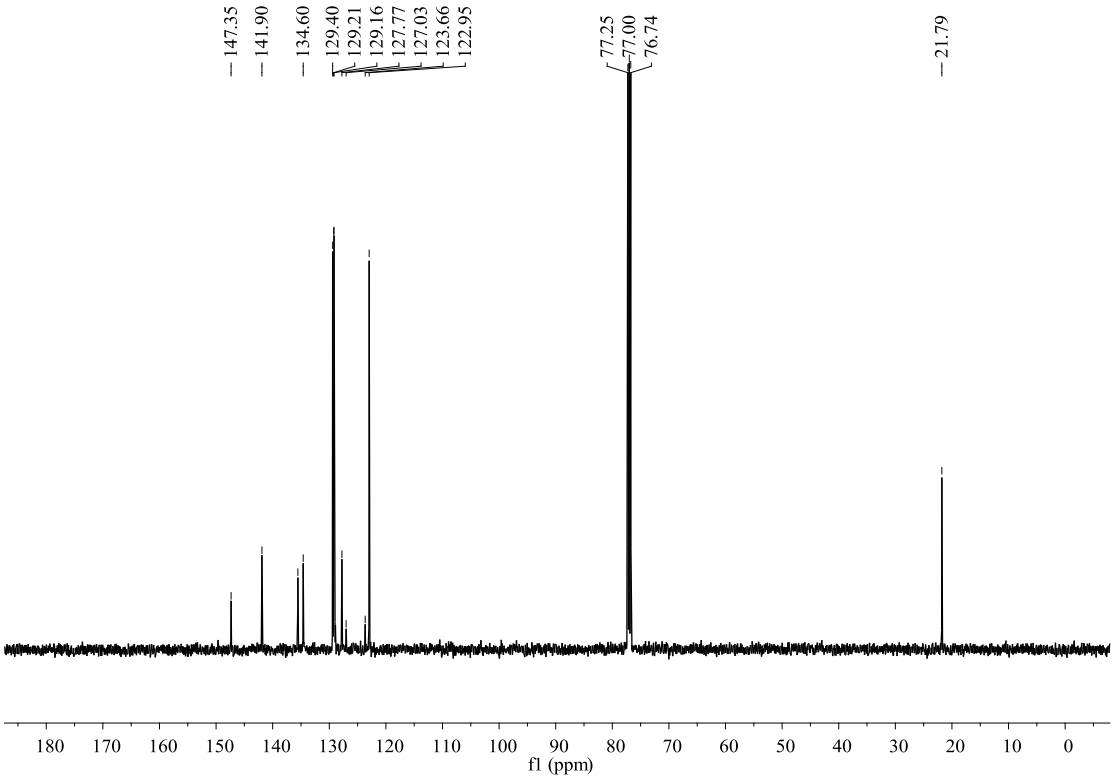
The ^{13}C NMR spectrum of *p*-MeOPNCl-

3.7 Spectrum of ^{1}H NMR of *p*-MePNCl-*p*

$C_{14}H_{12}NOCl$



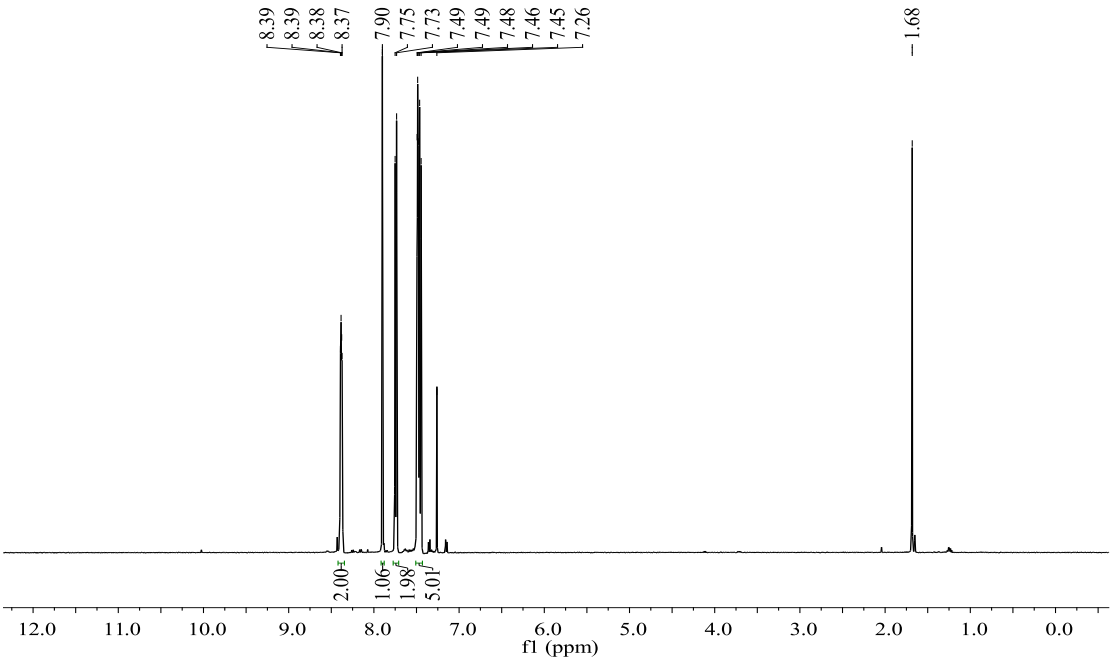
The ^{1}H NMR spectrum of *p*-MePNCl-*p*



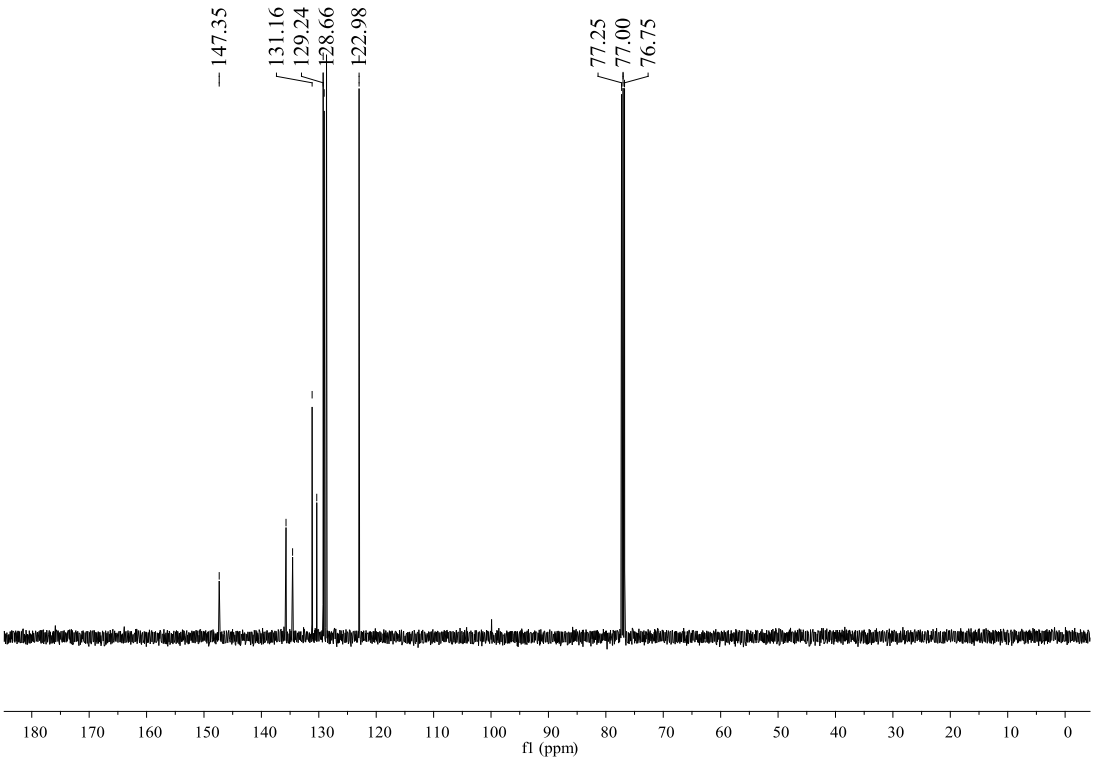
The ^{13}C NMR spectrum of *p*-MePNCl-*p*

3.8 Spectrum of ^{1}H NMR HPNCl-*p*

$C_{13}H_{10}NOCl$



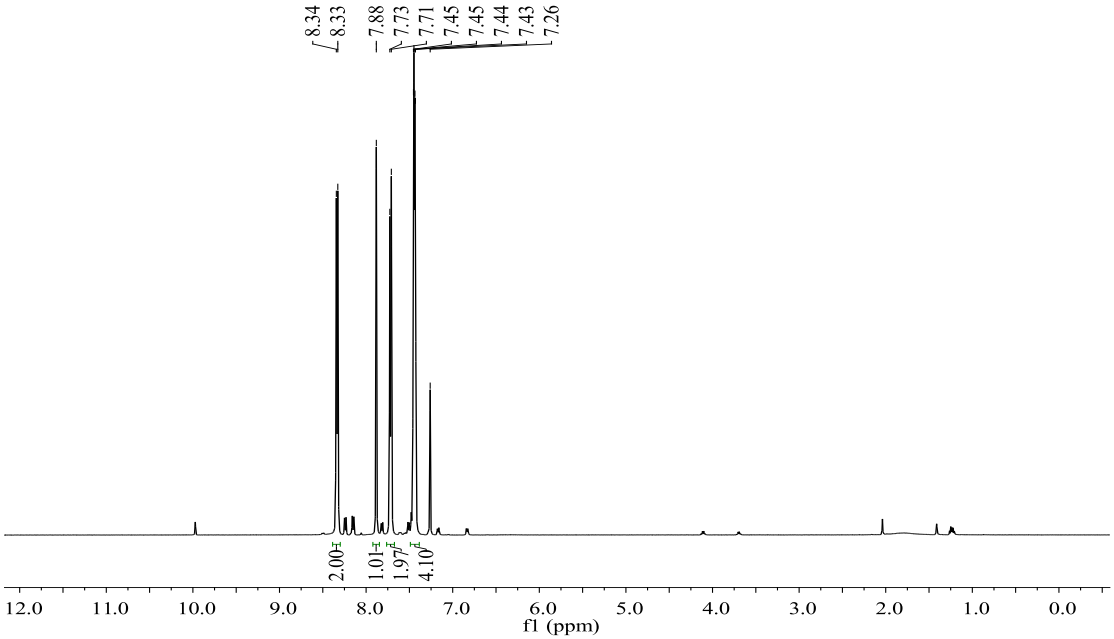
The ^{1}H NMR spectrum of HPNCl-*p*



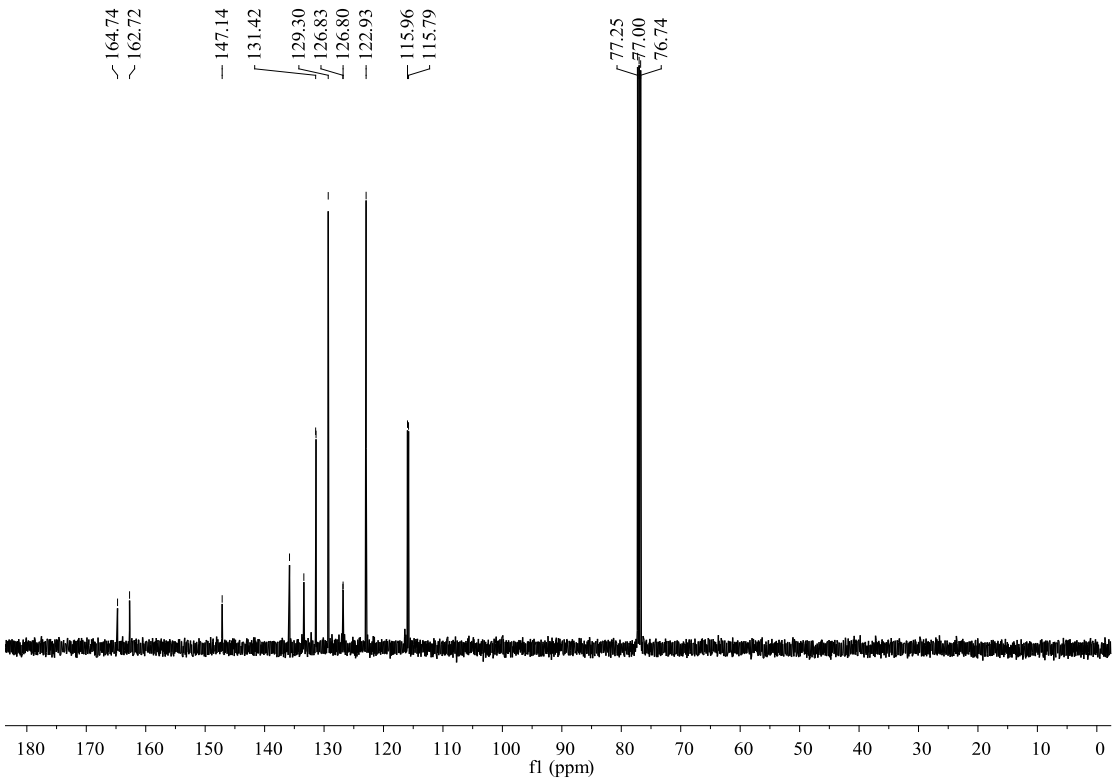
The ^{13}C NMR spectrum of HPNCl-*p*

3.9 Spectrum of ^{1}H NMR *p*-ClPNCl-*p*

$C_{13}H_9NOCl_2$



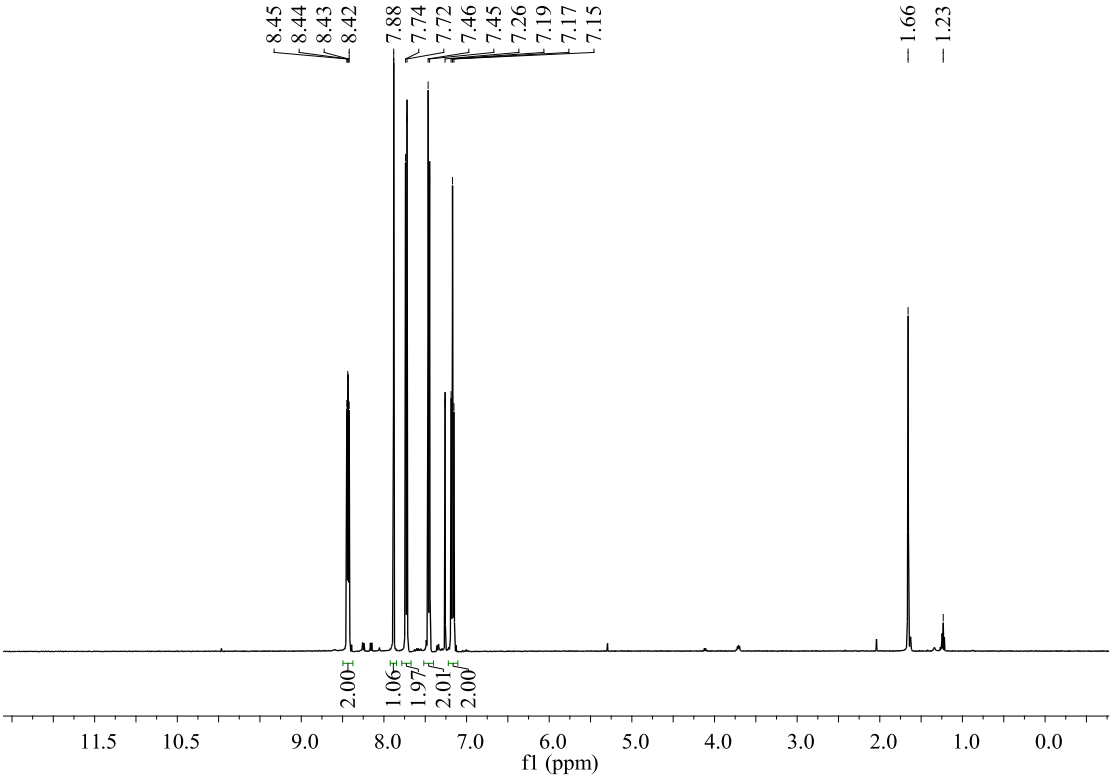
The ^{1}H NMR spectrum of *p*-ClPNCl-*p*



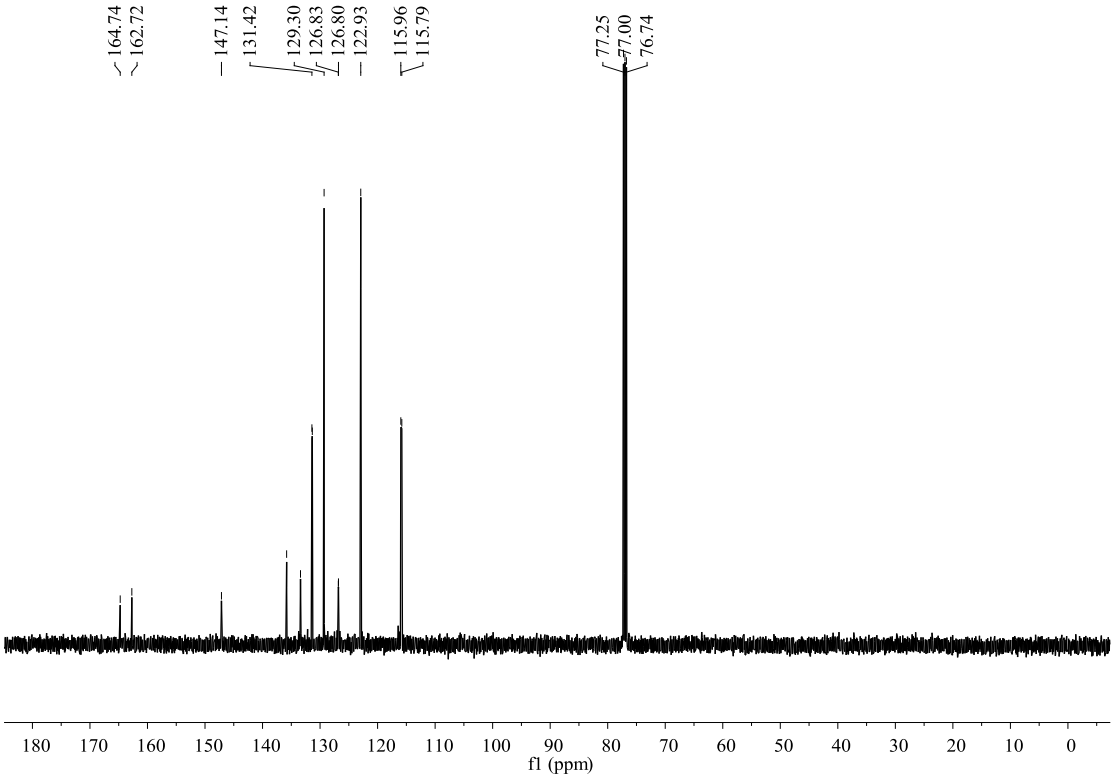
The ^{13}C NMR spectrum of *p*-ClPNCl-*p*

3.10 Spectrum of ^{1}H NMR of *p*-FPNCl-*p*

$C_{13}H_9NOFCl$



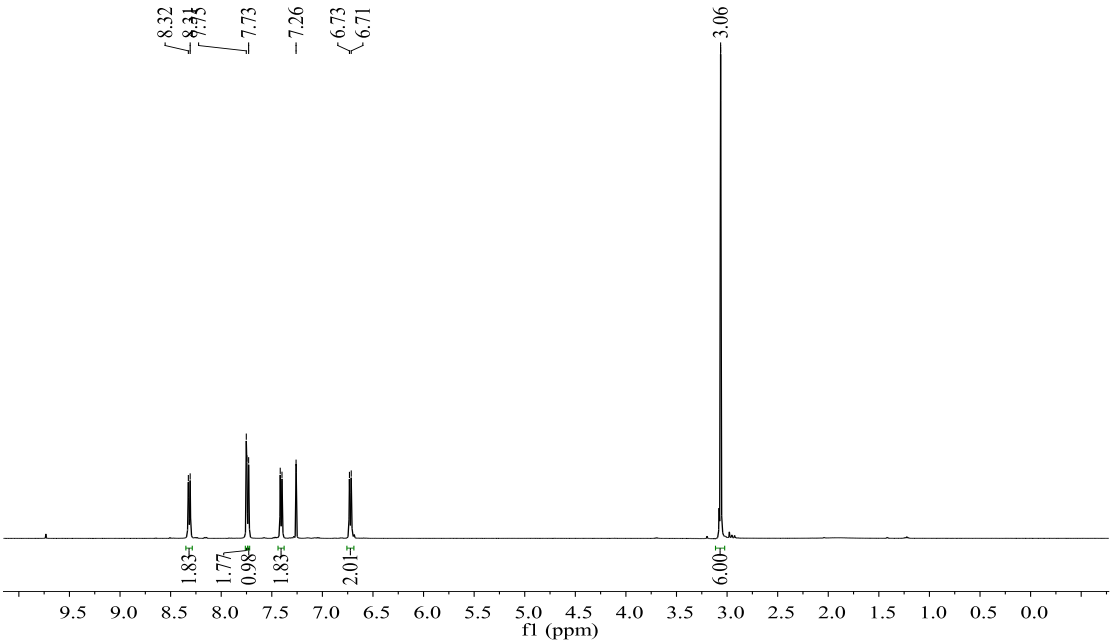
The ^{1}H NMR spectrum of *p*-FPNCl-*p*



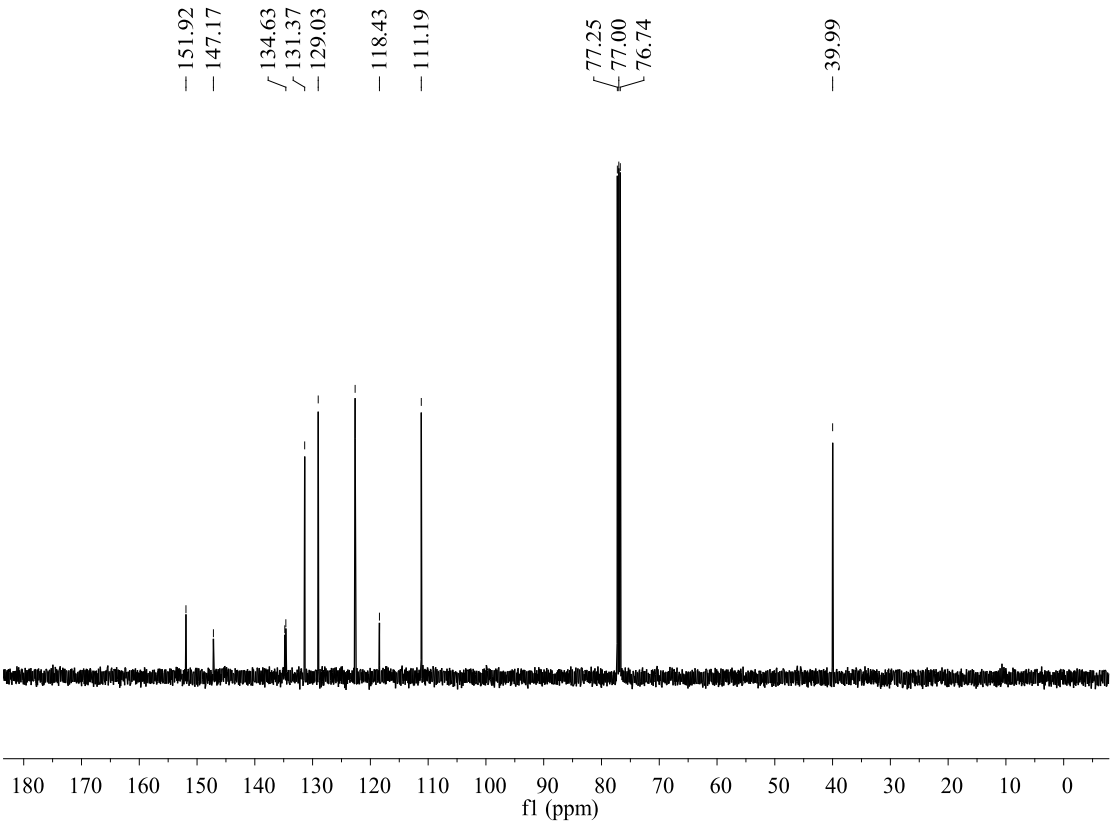
The ^{13}C NMR spectrum of *p*-FPNCl-*p*

3.11 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-Me_2NPNCl-*p*

$C_{15}H_{15}N_2OCl$



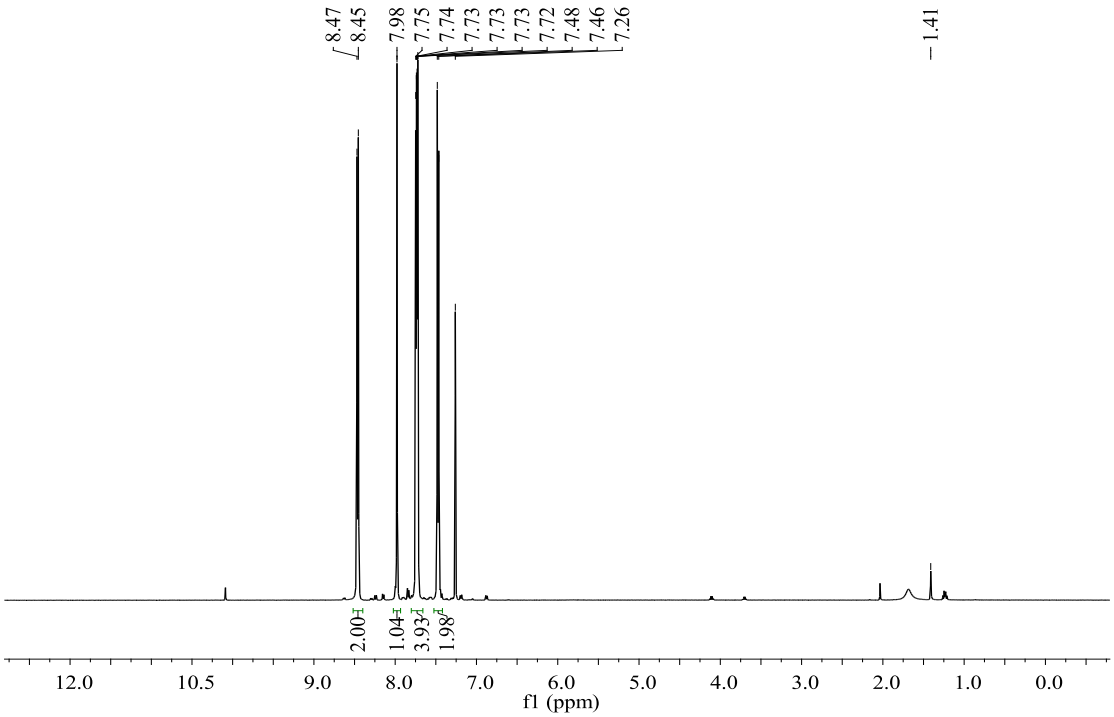
The ^{1}H NMR spectrum of *p*-Me_2NPNCl-*p*



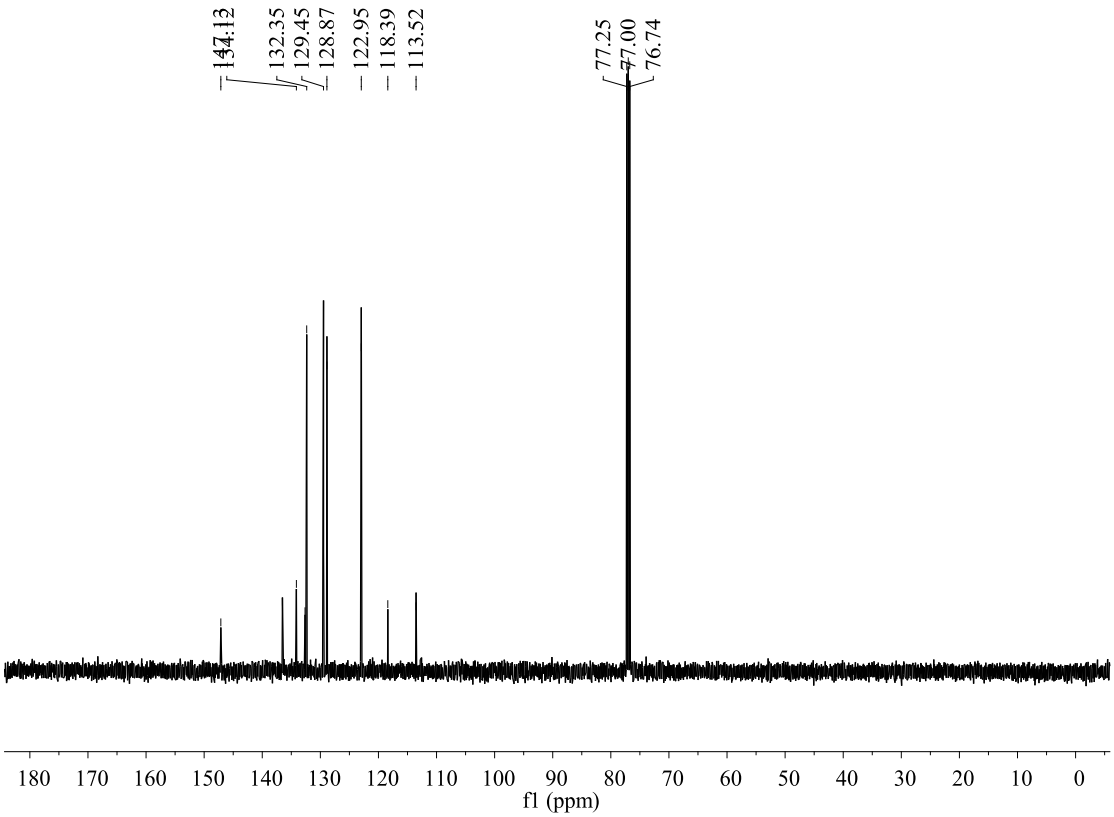
The ^{13}C NMR spectrum of *p*-Me_2NPNCl-*p*

3.12 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-CNPNCl-*p*

$C_{14}H_9N_2OCl$



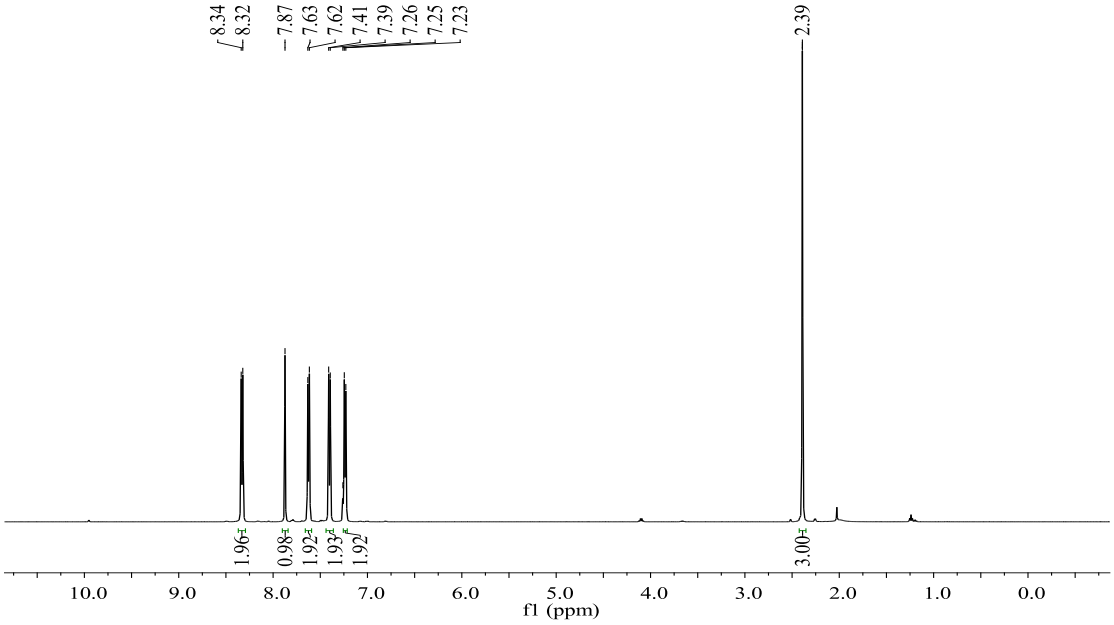
The ^{1}H NMR spectrum of *p*-CNPNCl-*p*



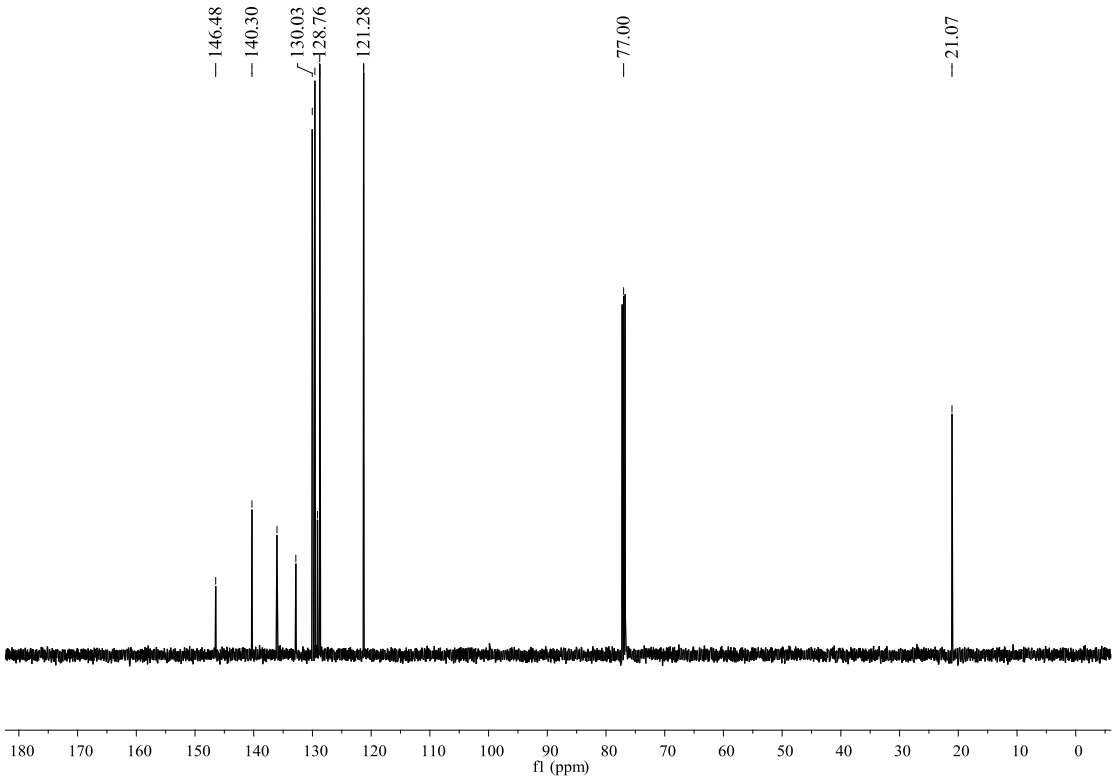
The ^{13}C NMR spectrum of *p*-CNPNCl-*p*

3.13 Spectrum of ^{1}H NMR of *p*-ClPNMe-*p*

$C_{14}H_{12}NOCl$



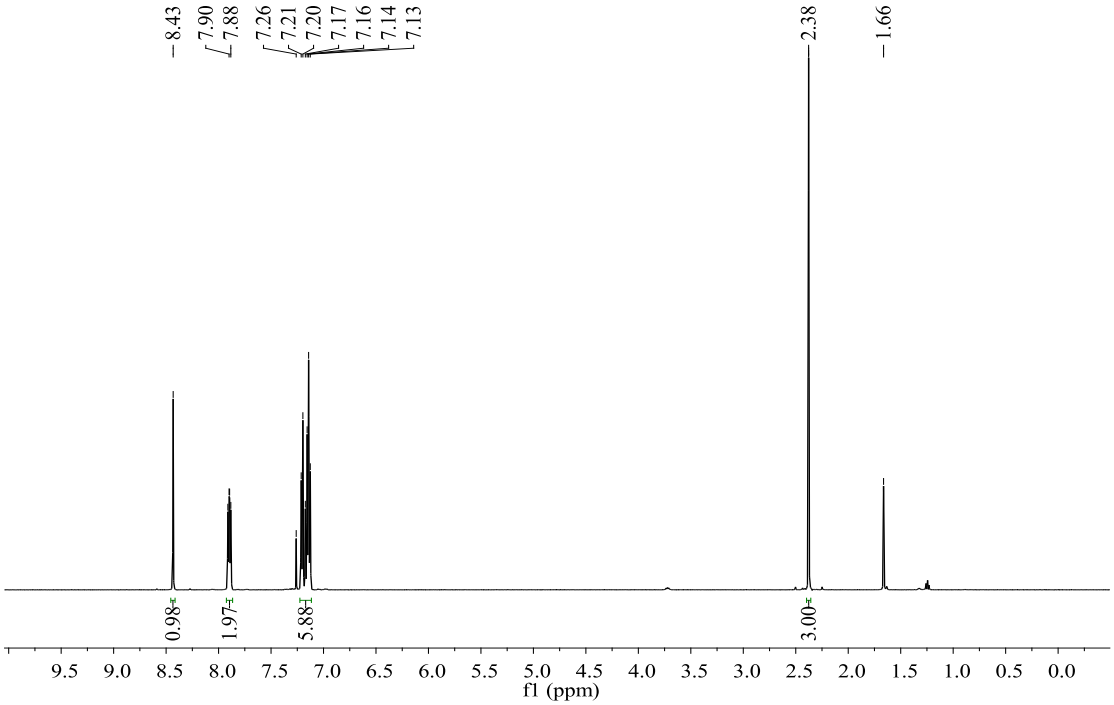
The ^{1}H NMR spectrum of *p*-ClPNMe-*p*



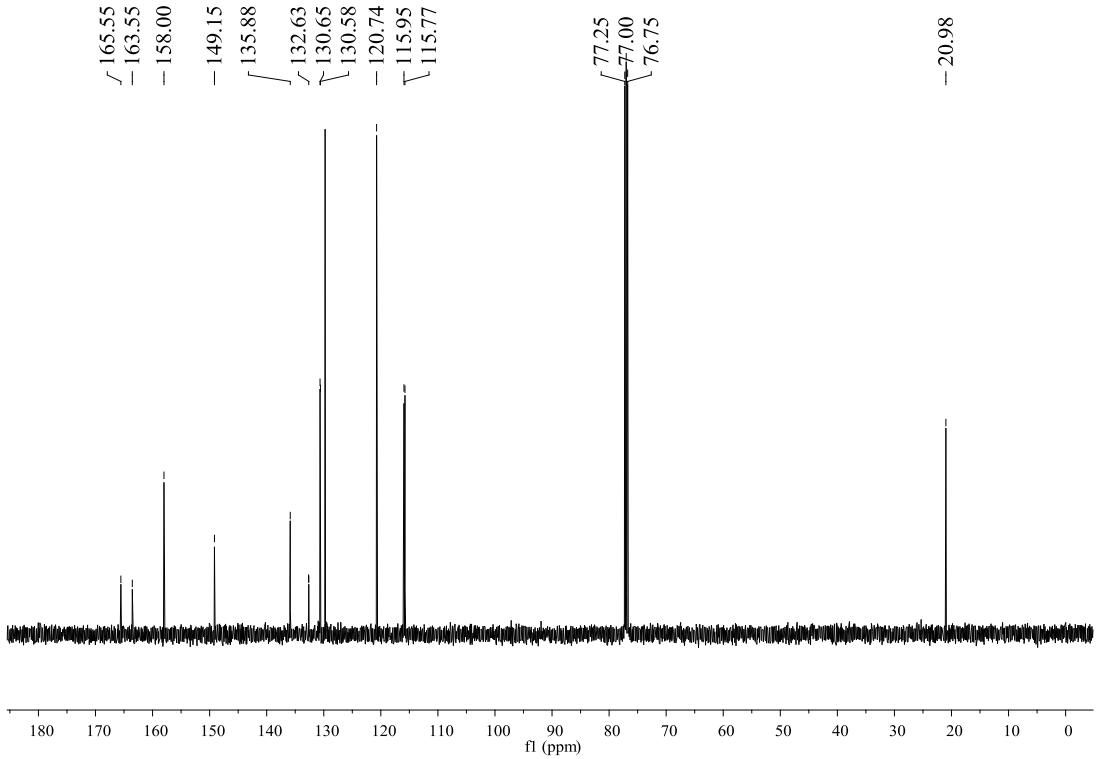
The ^{13}C NMR spectrum of *p*-ClPNMe-*p*

3.14 Spectrum of ^{1}H NMR of *p*-FPNMe-*p*

$C_{14}H_{12}NOF$



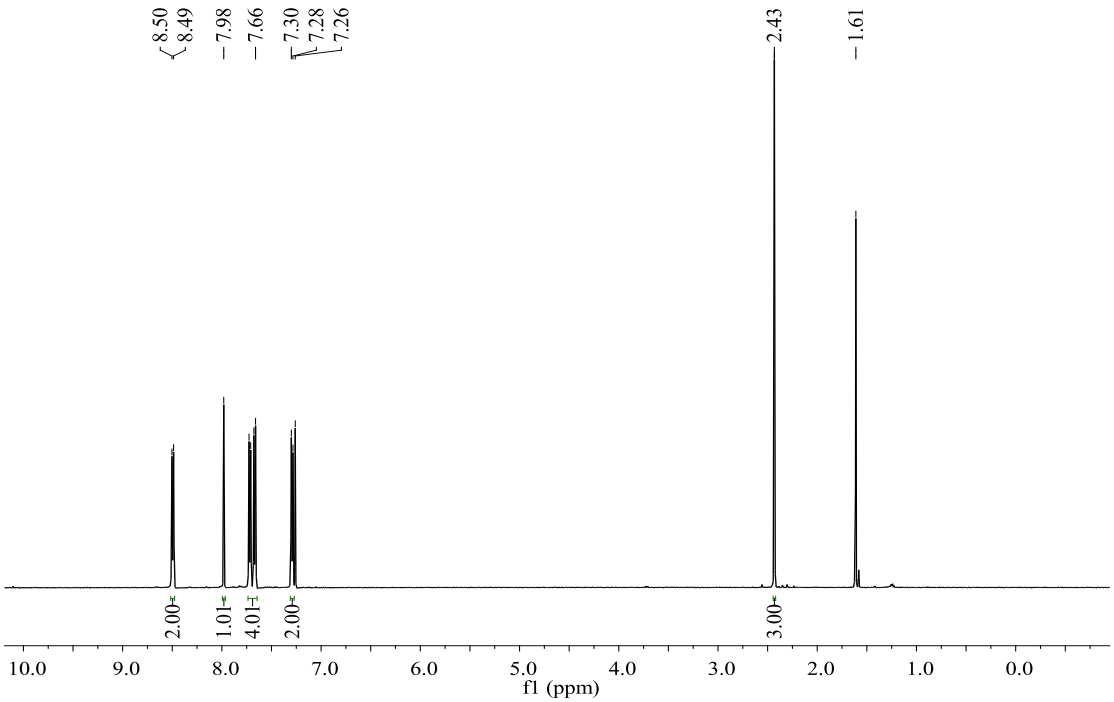
The ^{1}H NMR spectrum of *p*-FPNMe-*p*



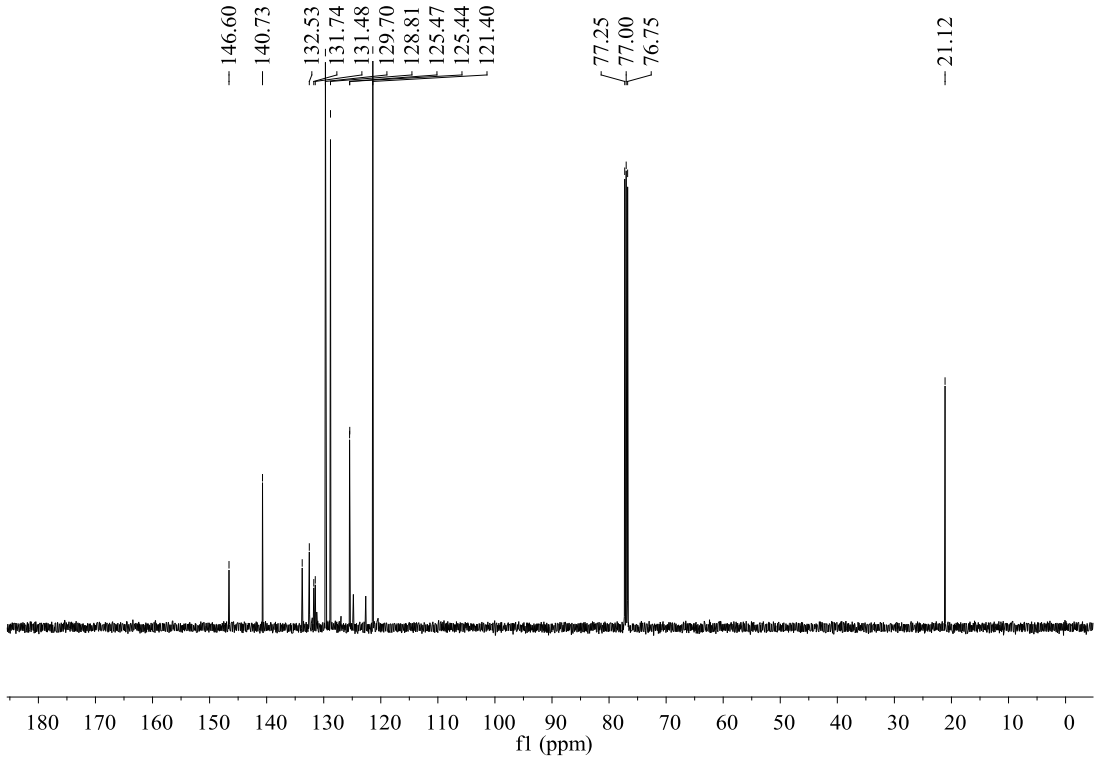
The ^{13}C NMR spectrum of *p*-FPNMe-*p*

3.15 Spectrum of ^{1}H NMR of *p*-CF_3PNMe-*p*

$C_{15}H_{12}NOF_3$



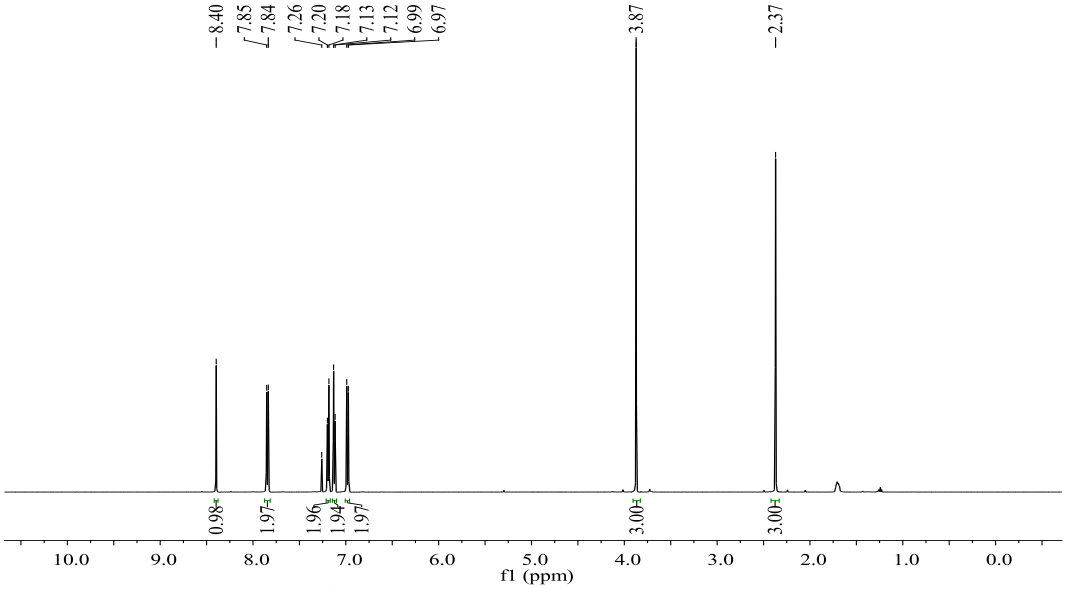
The ^{1}H NMR spectrum of *p*-CF_3PNMe-*p*



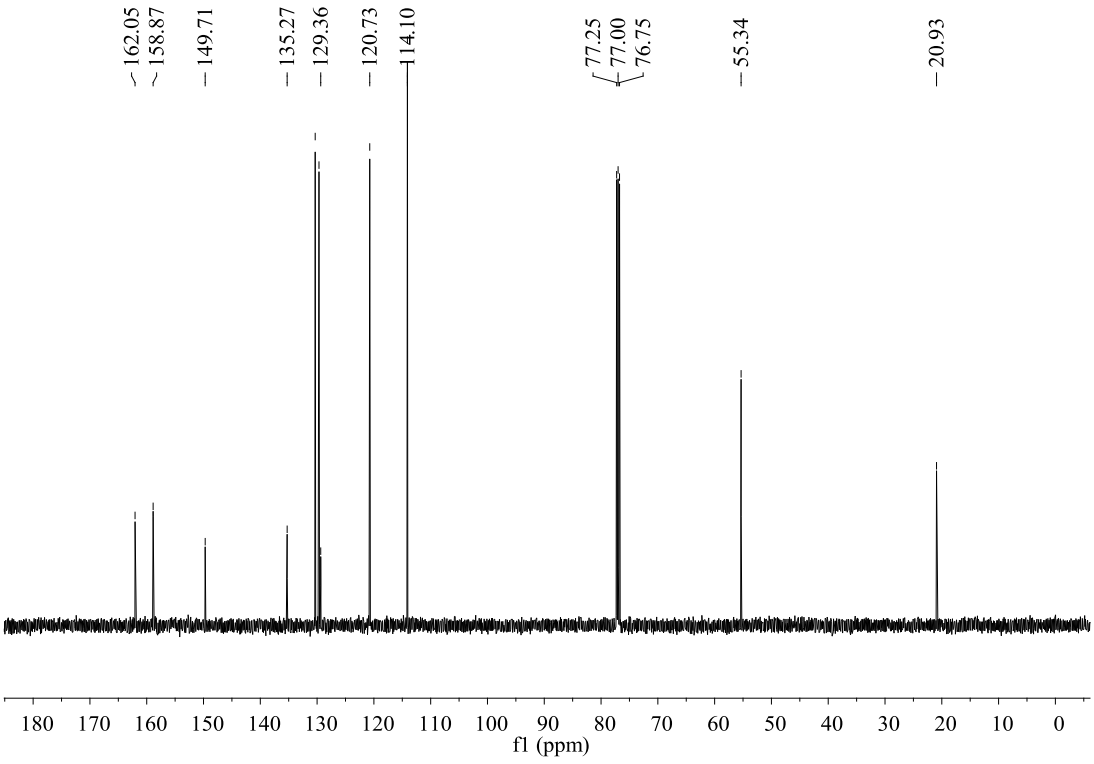
The ^{13}C NMR spectrum of *p*-CF_3PNMe-*p*

3.16 Spectrum of ^{1}H NMR of *p*-OMePNMe-*p*

$C_{15}H_{15}NO_2$



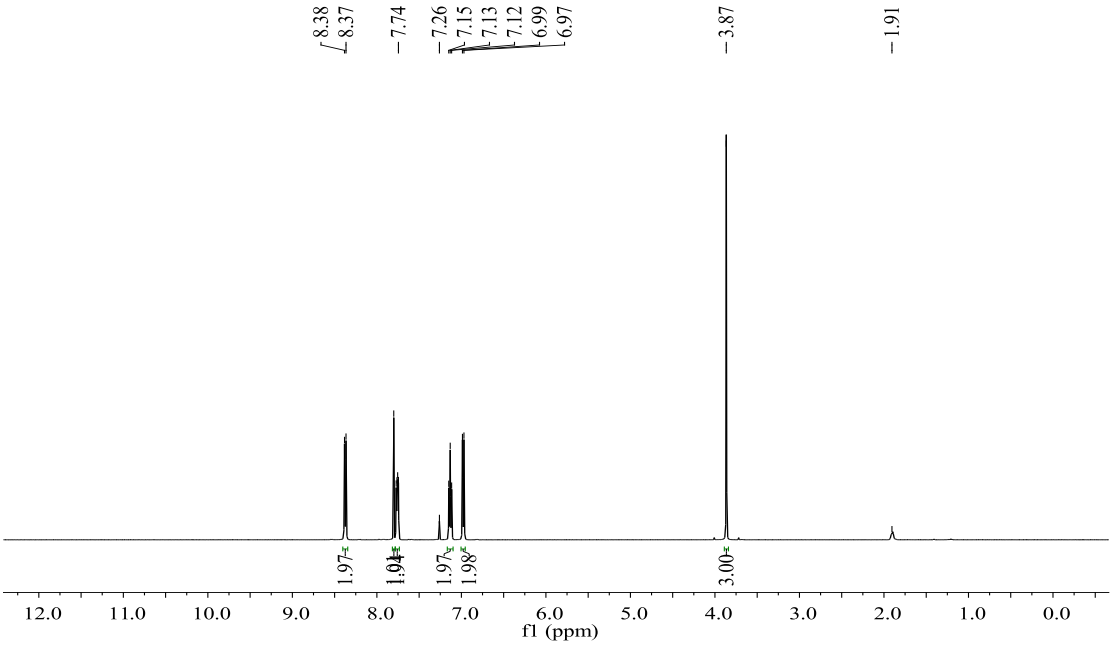
The ^{1}H NMR spectrum of *p*-OMePNMe-*p*



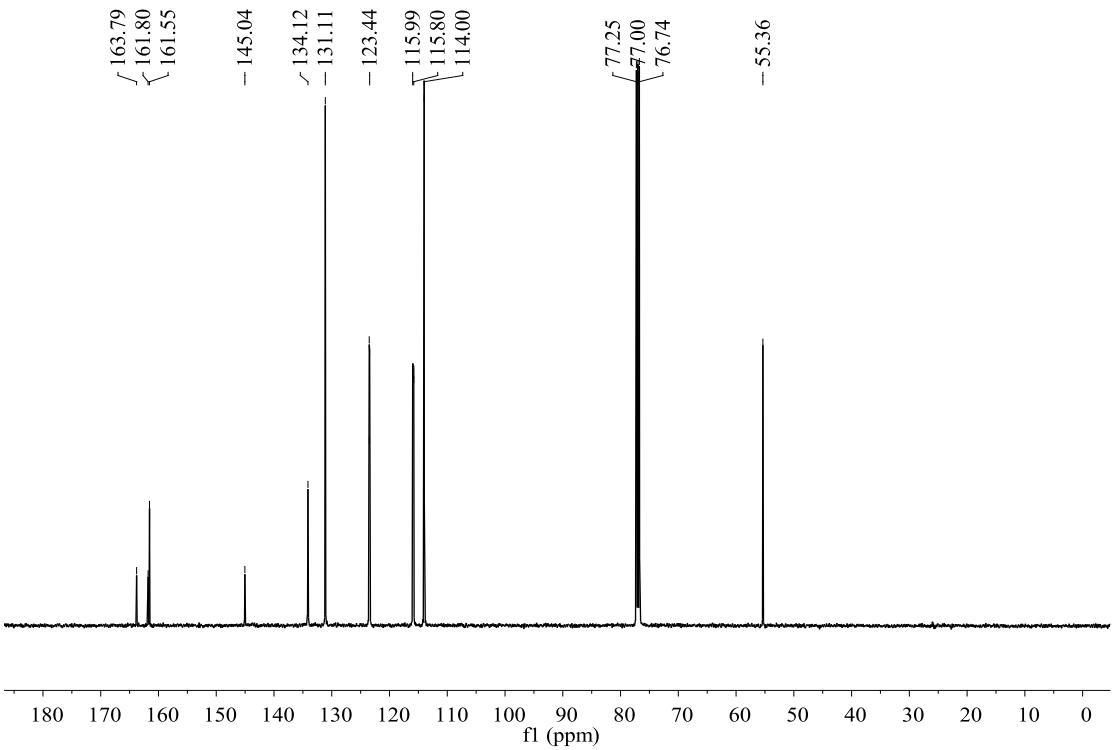
The ^{13}C NMR spectrum of *p*-OMePNMe-*p*

3.17 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-MeOPNF-*p*

$C_{14}H_{12}NO_2F$



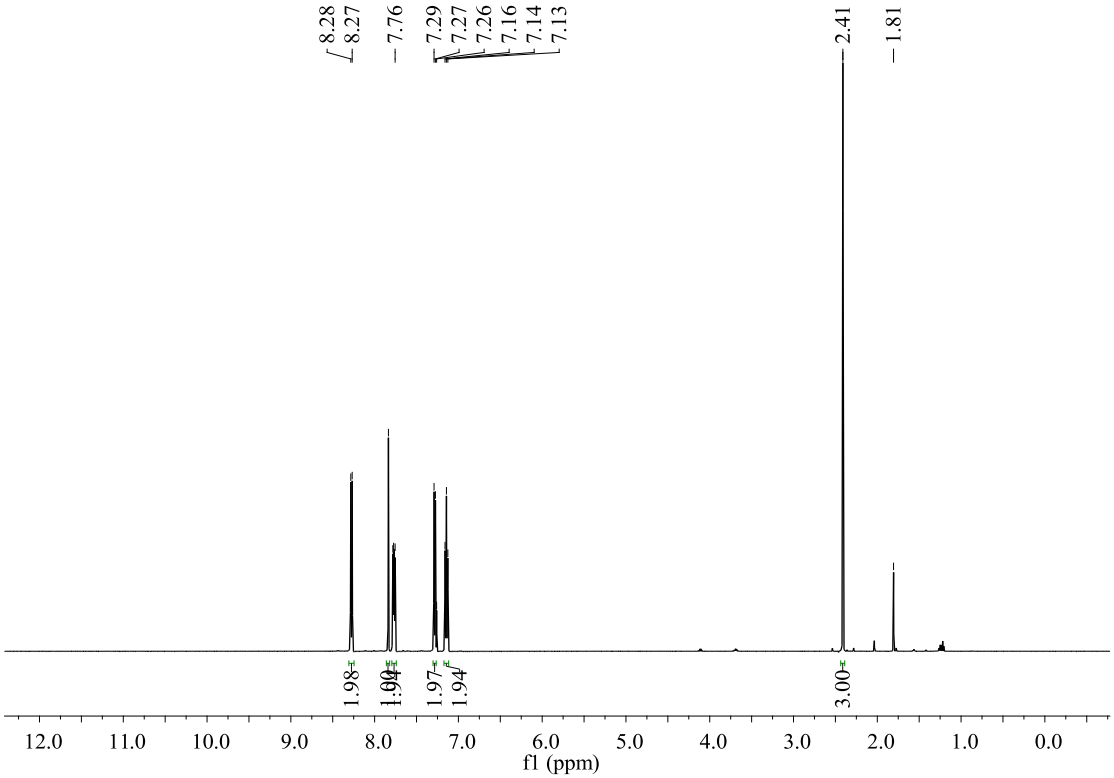
The ^{1}H NMR spectrum of *p*-MeOPNF-*p*



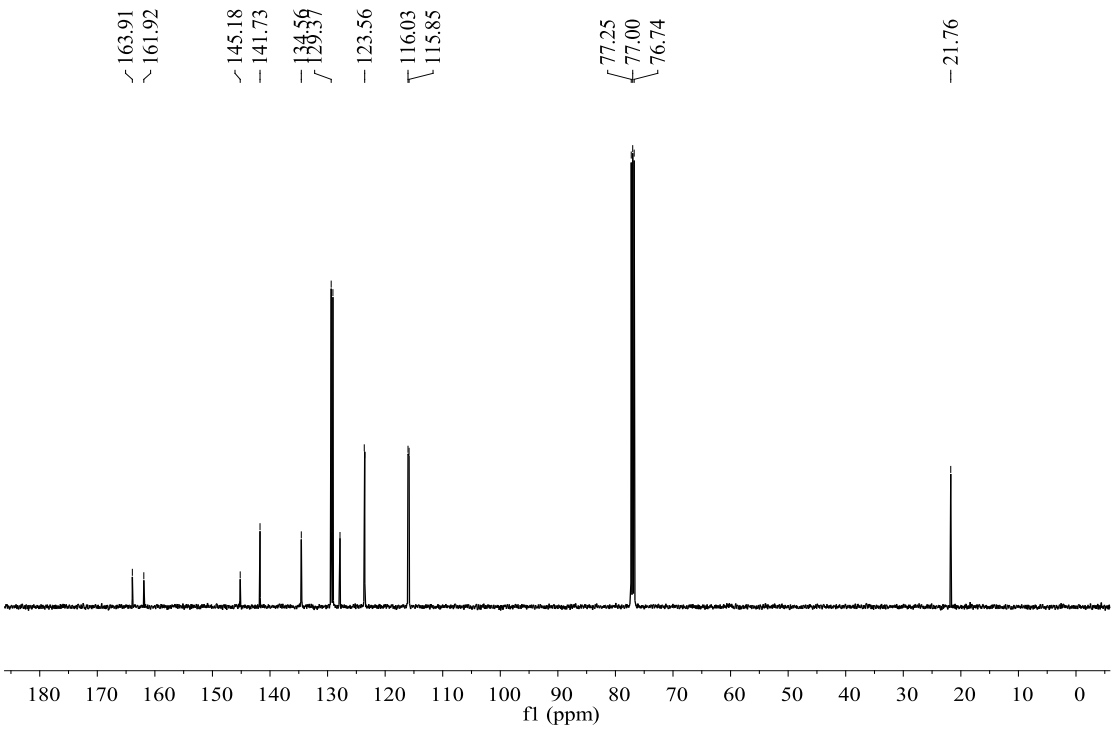
The ^{13}C NMR spectrum of *p*-MeOPNF-*p*

3.18 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-MePNF-*p*

$C_{14}H_{12}NOF$



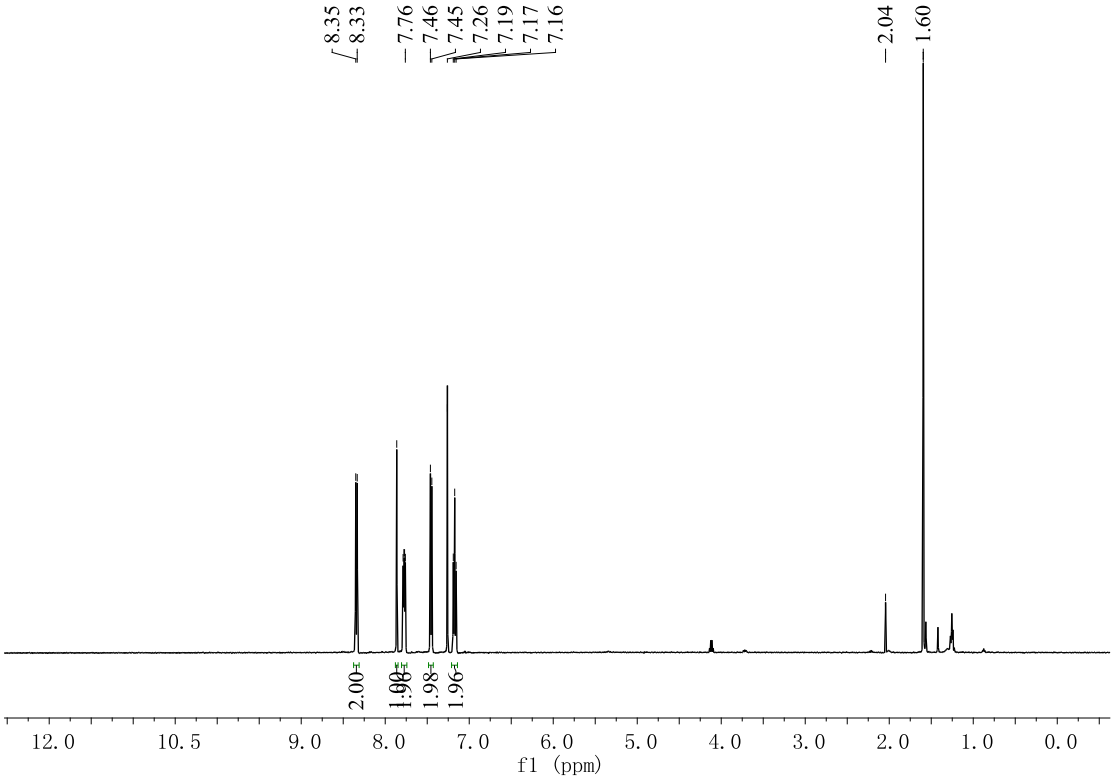
The ^{1}H NMR spectrum of *p*-MePNF-*p*



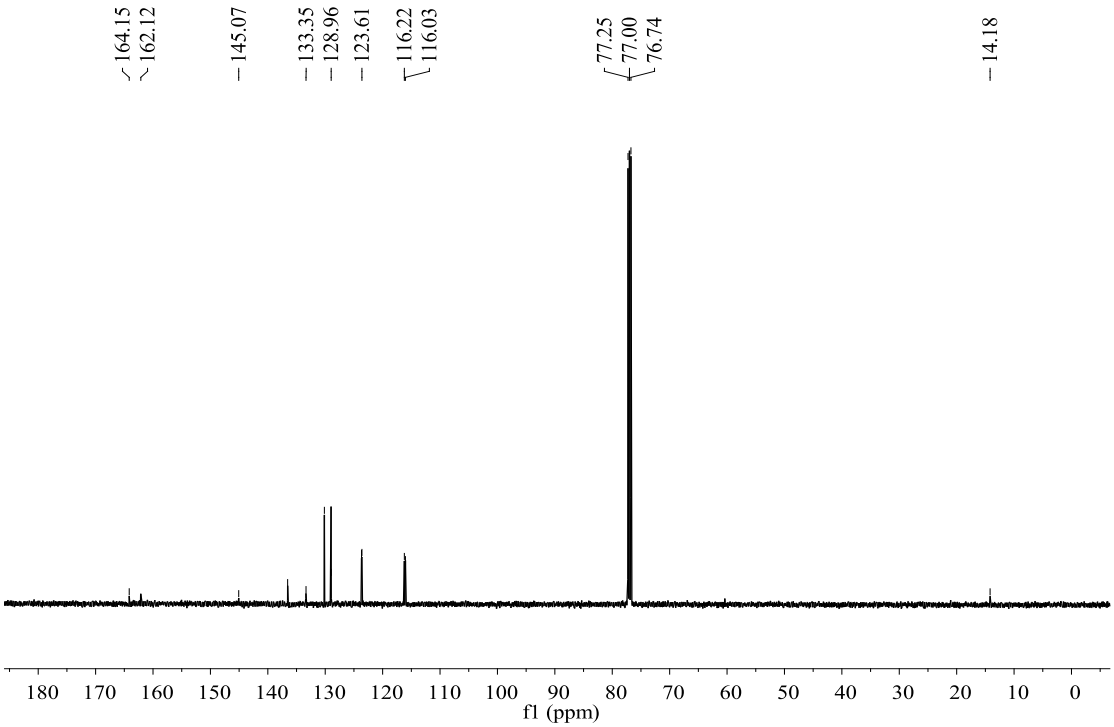
The ^{13}C NMR spectrum of *p*-MePNF-*p*

3.19 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-ClPNF-*p*

$C_{13}H_9NOFCl$



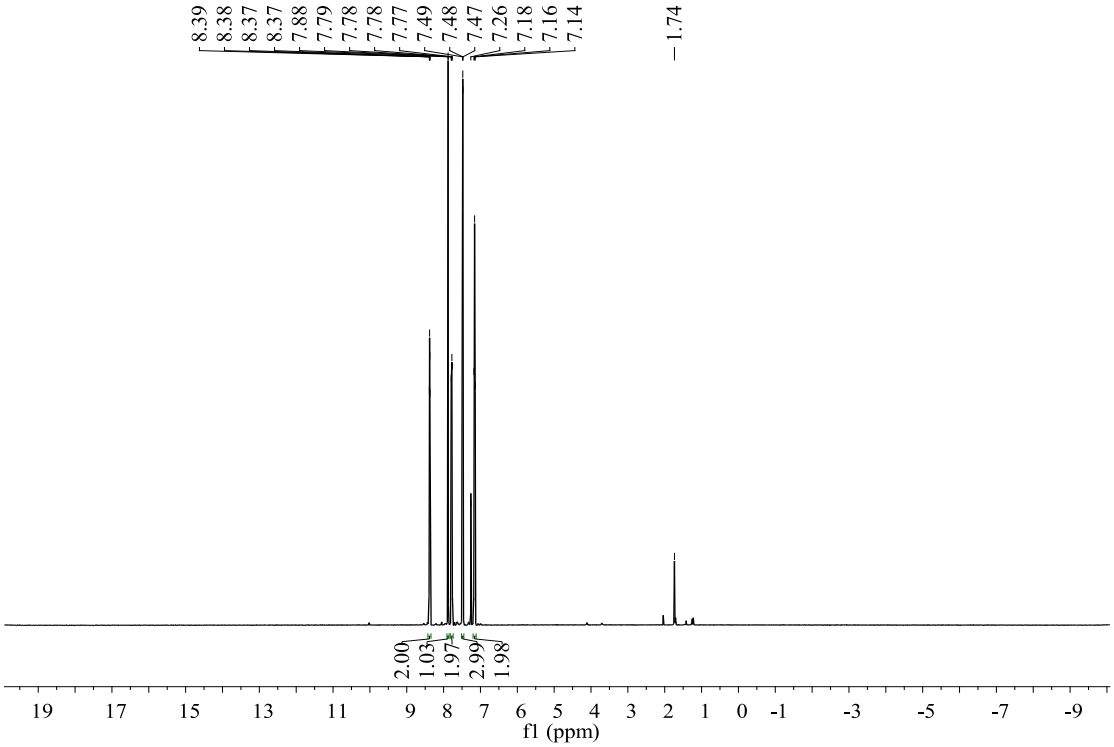
The ^{1}H NMR spectrum of *p*-ClPNF-*p*



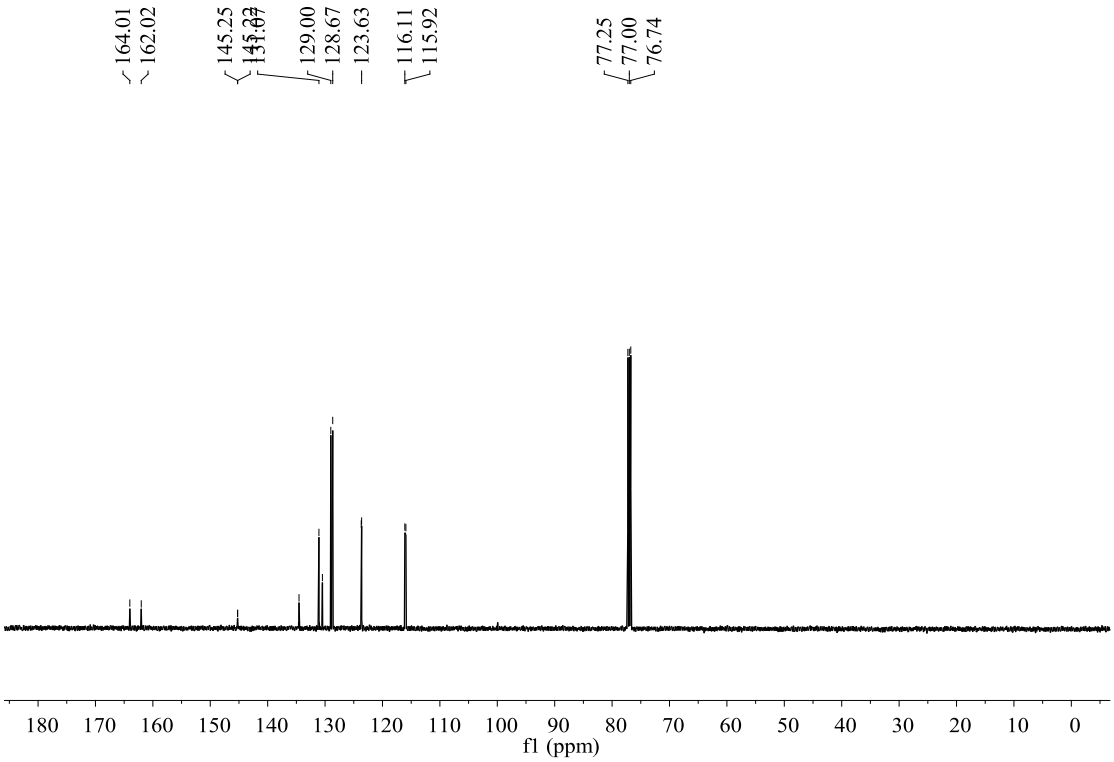
The ^{13}C NMR spectrum of *p*-ClPNF-*p*

3.20 Spectrum of ^{1}H NMR and ^{13}C NMR of HPNF-*p*

$C_{13}H_{10}NOF$



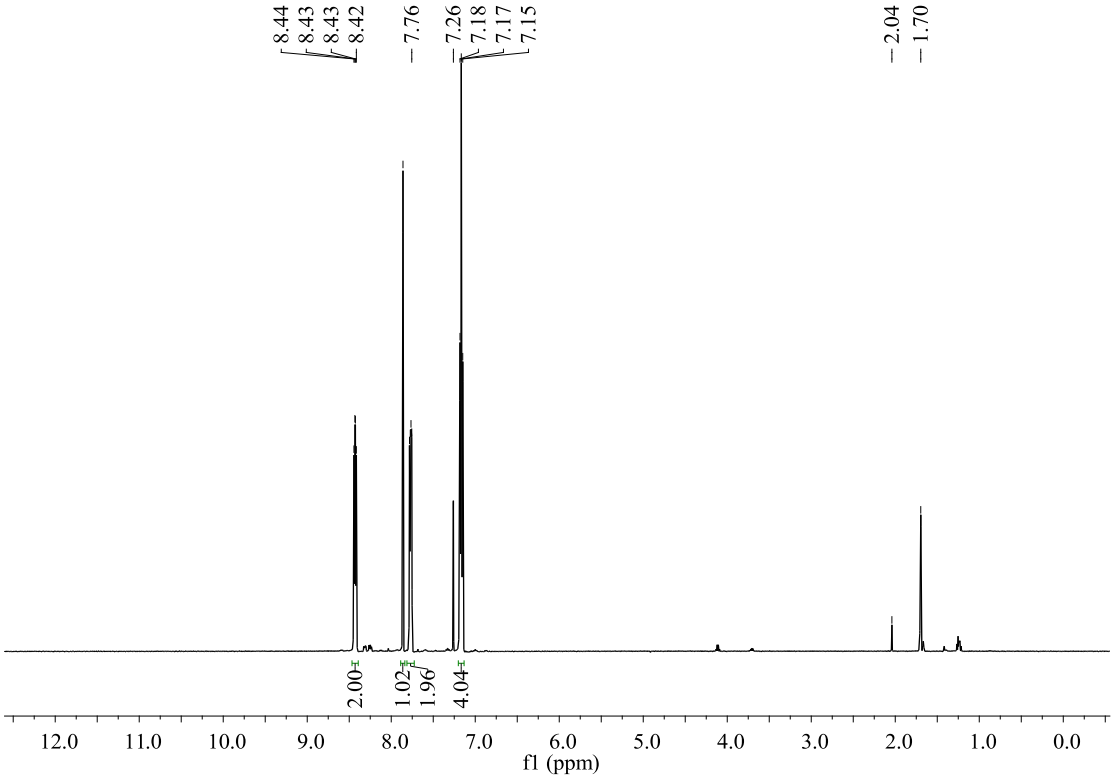
The ^{1}H NMR spectrum of HPNF-*p*



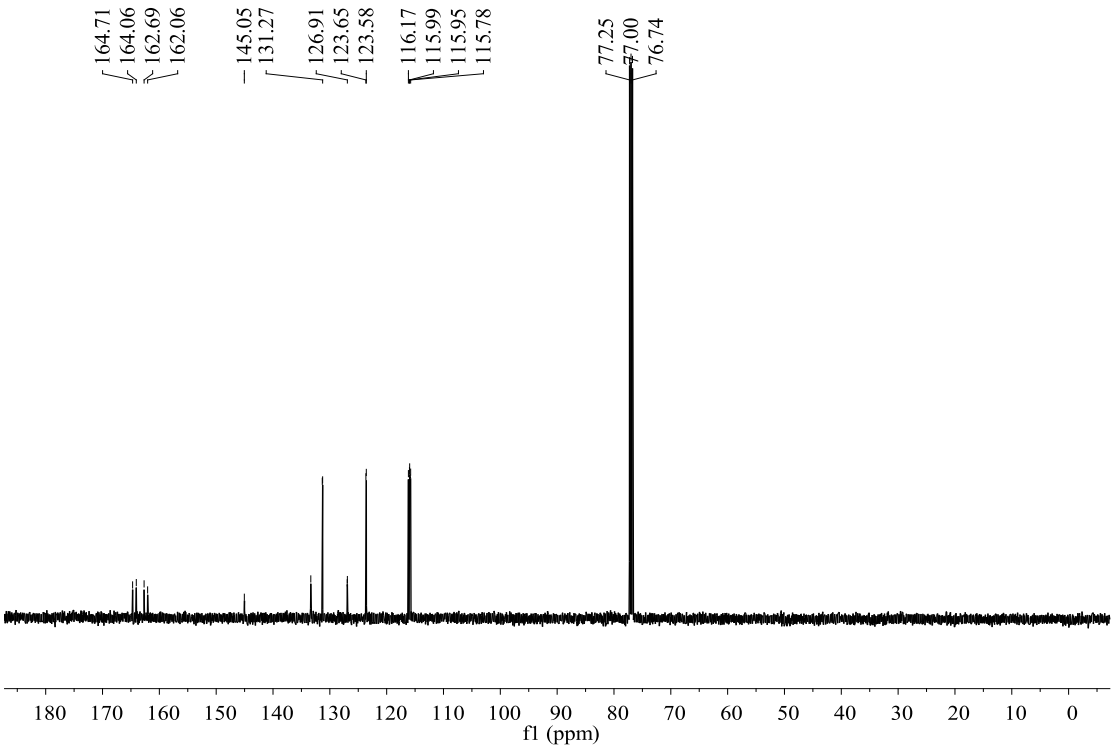
The ^{13}C NMR spectrum of HPNF-*p*

3.21 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-FPNF-*p*

$C_{13}H_9NOF_2$



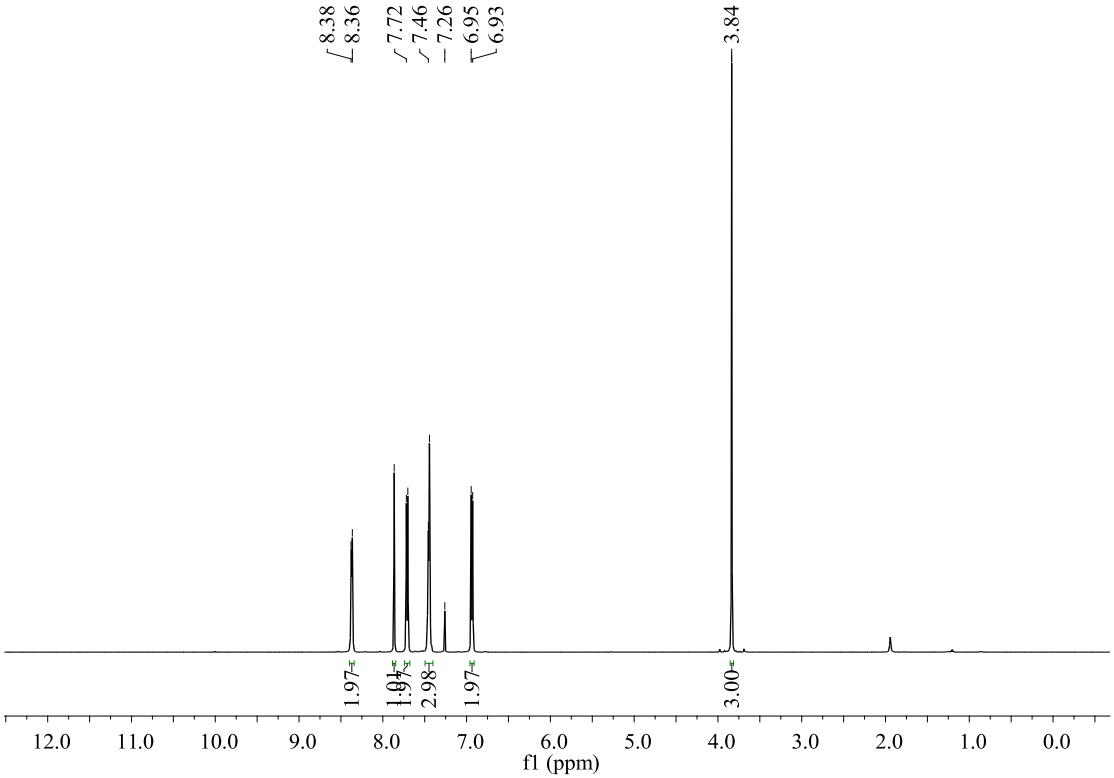
The ^{1}H NMR spectrum of *p*-FPNF-*p*



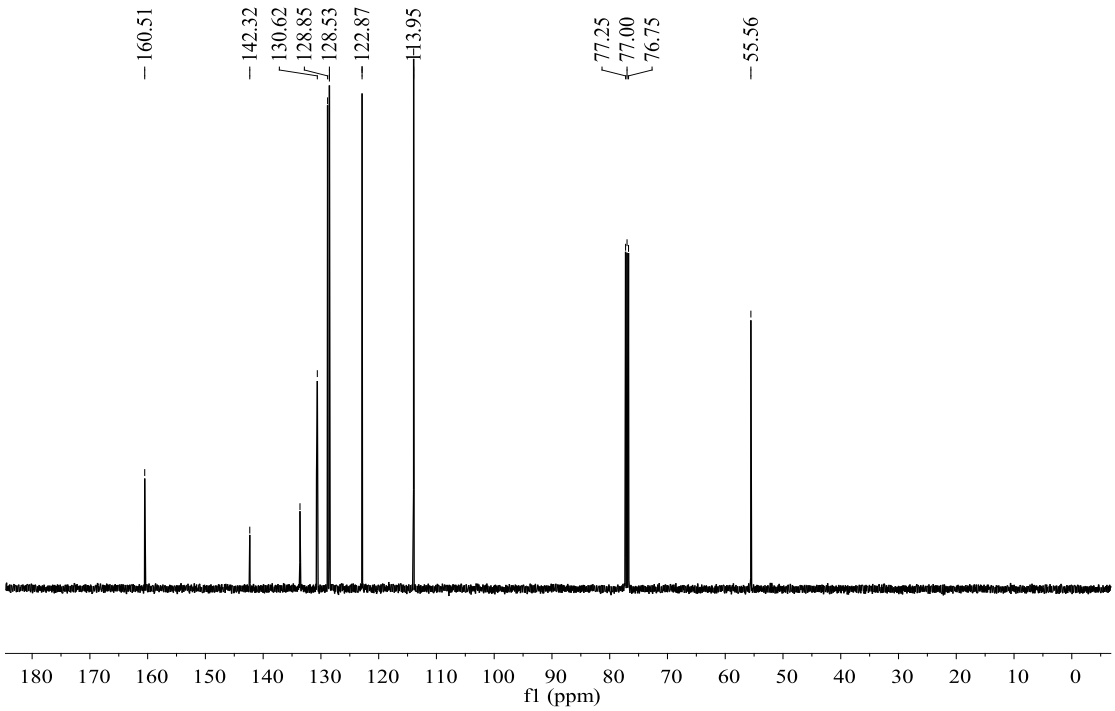
The ^{13}C NMR spectrum of *p*-FPNF-*p*

3.22 Spectrum of ^{1}H NMR and ^{13}C NMR of HPNMeO-*p*

$C_{14}H_{13}NO_2$



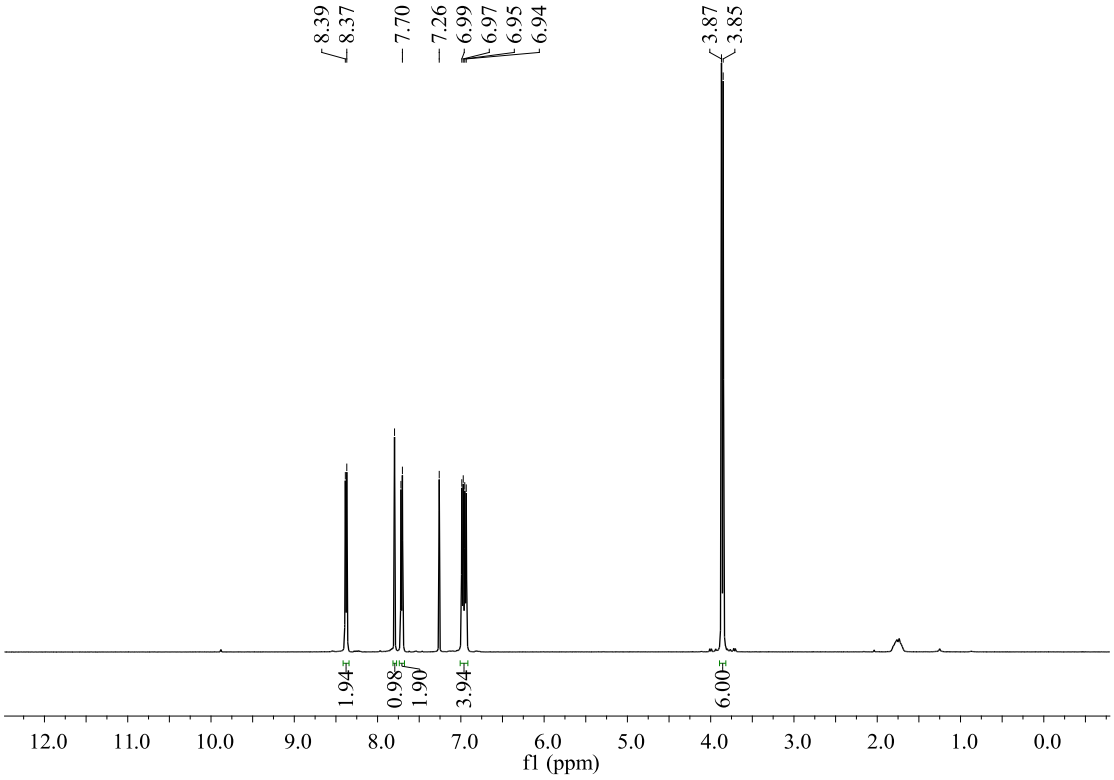
The ^{1}H NMR spectrum of HPNMeO-*p*



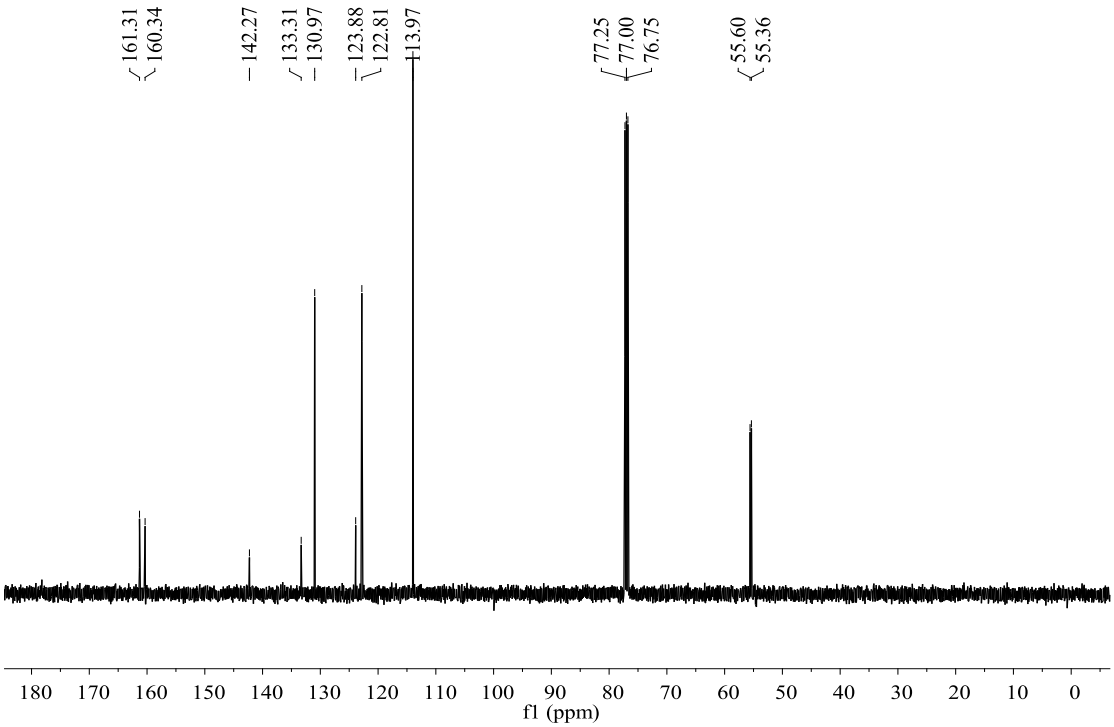
The ^{13}C NMR spectrum of HPNMeO-*p*

3.23 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-OMePNMeO-*p*

$C_{15}H_{15}NO_3$



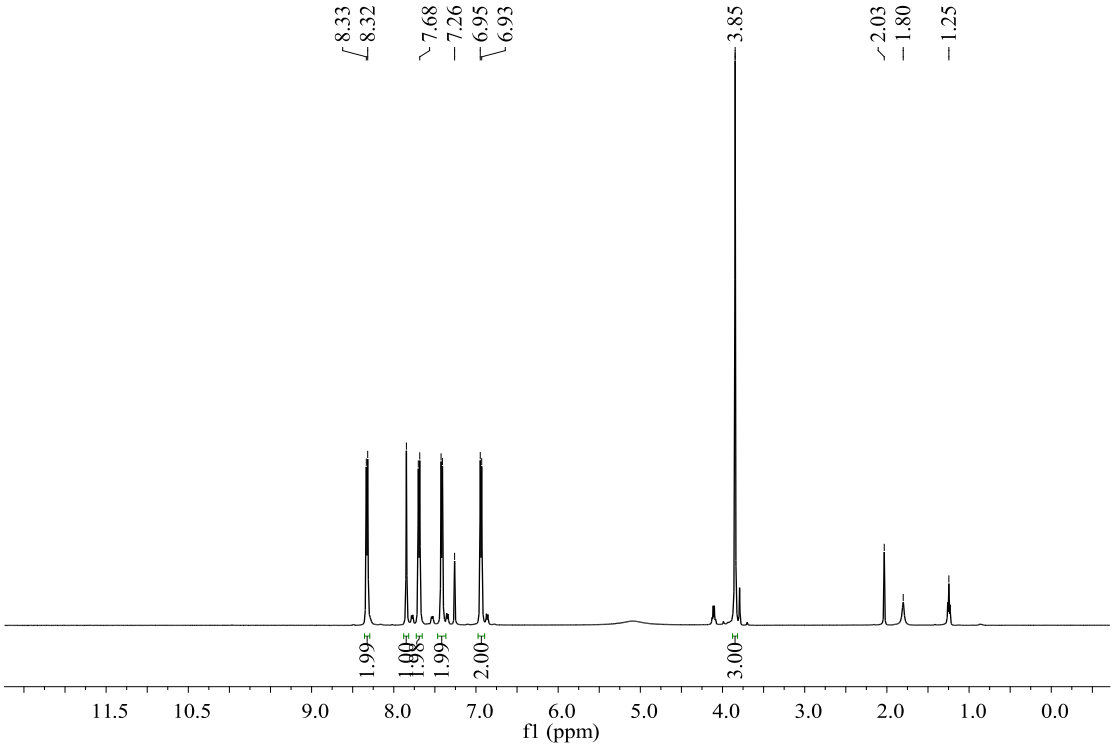
The ^{1}H NMR spectrum of *p*-OMePNMeO-*p*



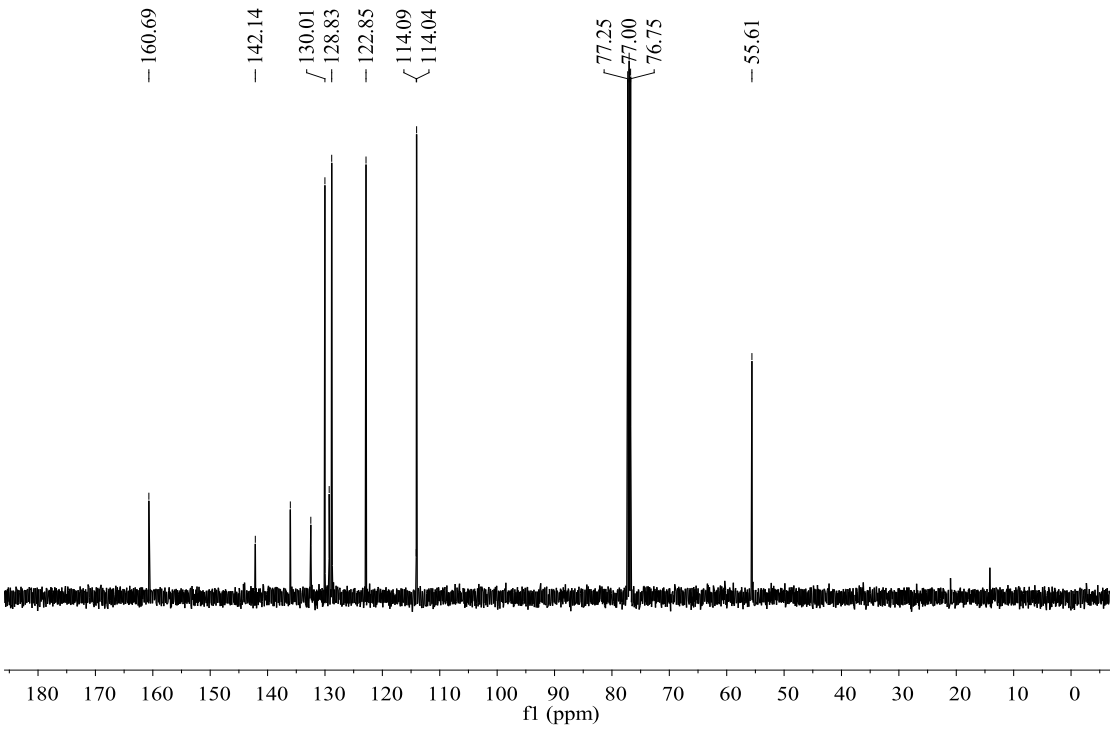
The ^{13}C NMR spectrum of *p*-OMePNMeO-*p*

3.24 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-ClPNMeO-*p*

$C_{14}H_{12}NO_2Cl$



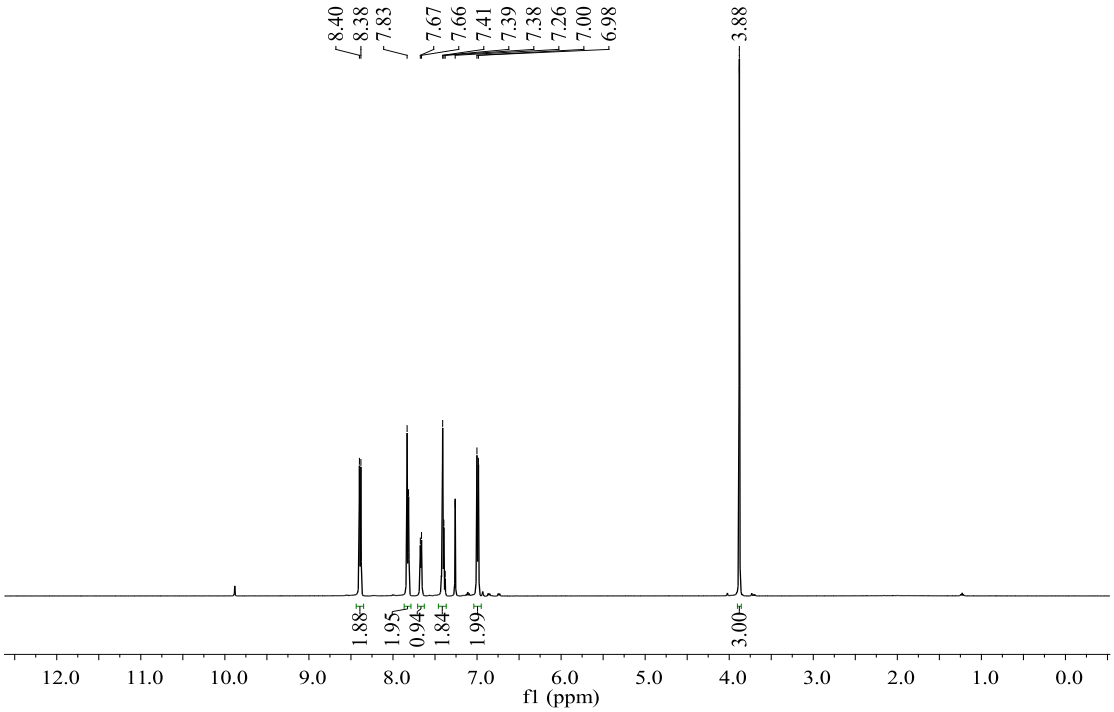
The ^{1}H NMR spectrum of *p*-ClPNMeO-*p*



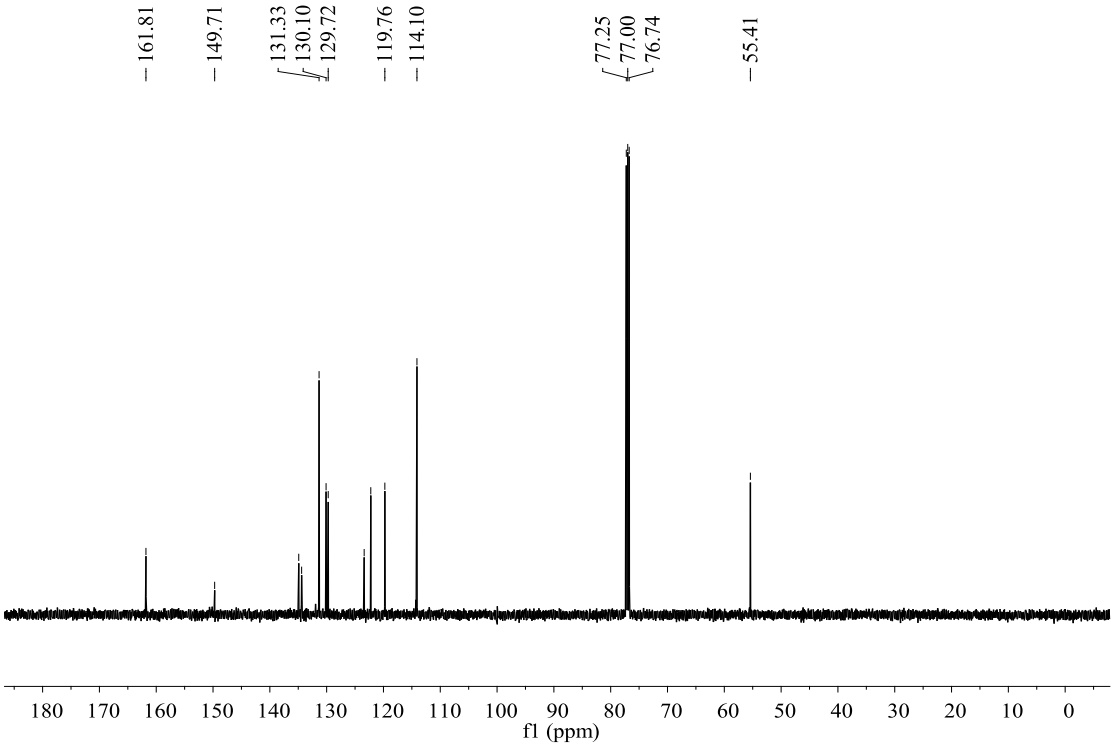
The ^{13}C NMR spectrum of *p*-ClPNMeO-*p*

3.25 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-OMePNCl-*m*

$C_{14}H_{12}NO_2Cl$



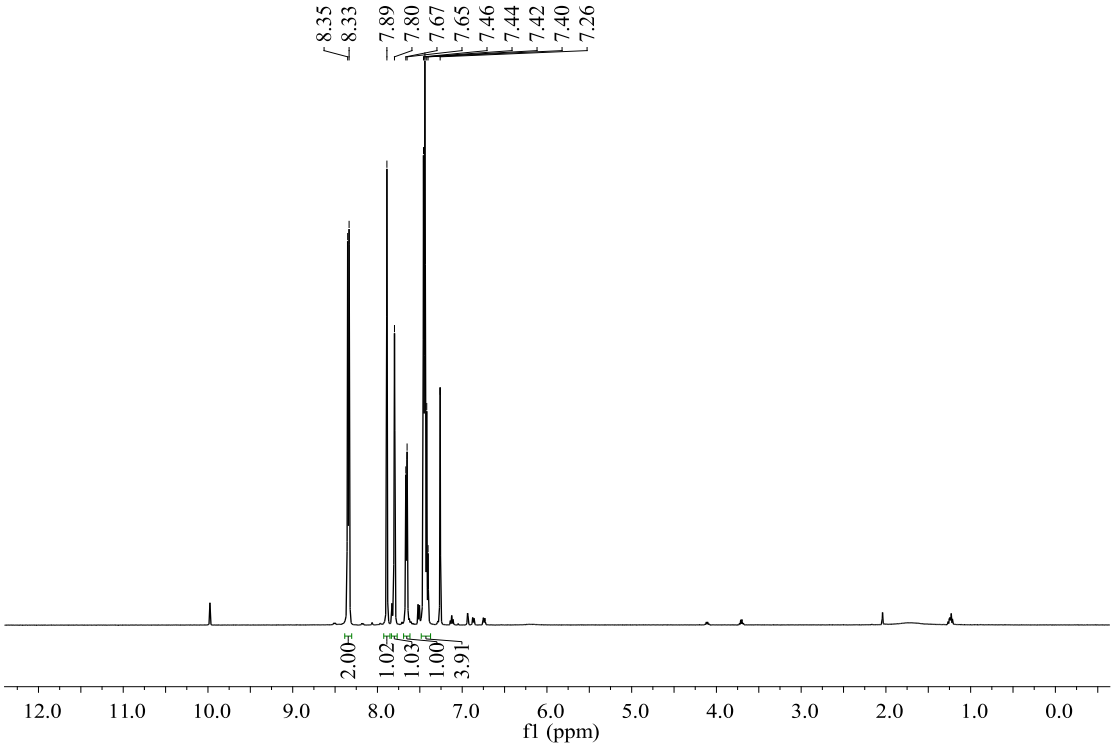
The ^{1}H NMR spectrum of *p*-OMePNCl-*m*



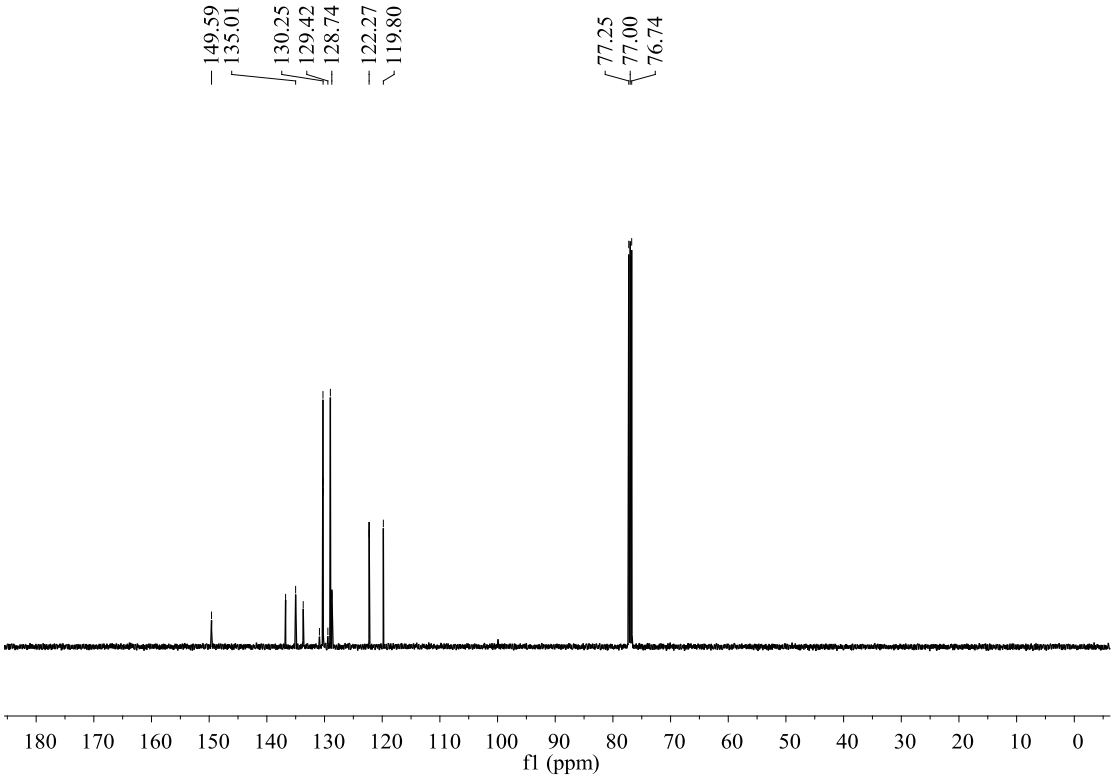
The ^{13}C NMR spectrum of *p*-OMePNCl-*m*

3.26 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-ClPNCl-*m*

$C_{13}H_9NOCl_2$



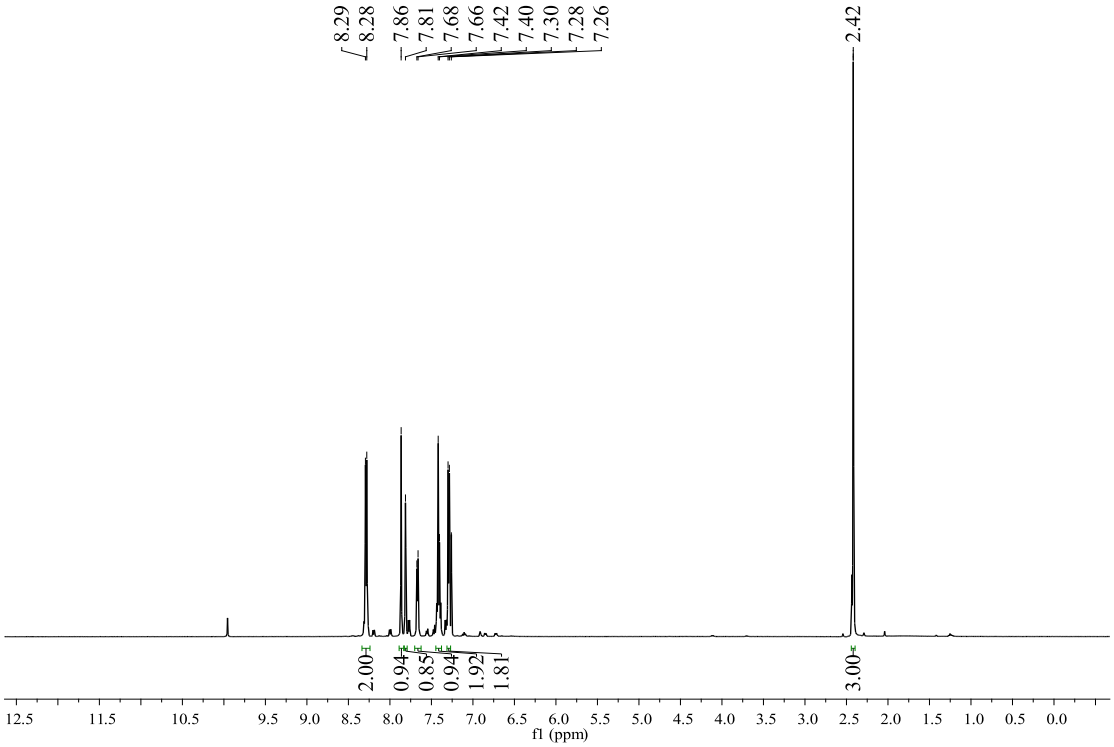
The ^{1}H NMR spectrum of *p*-ClPNCl-*m*



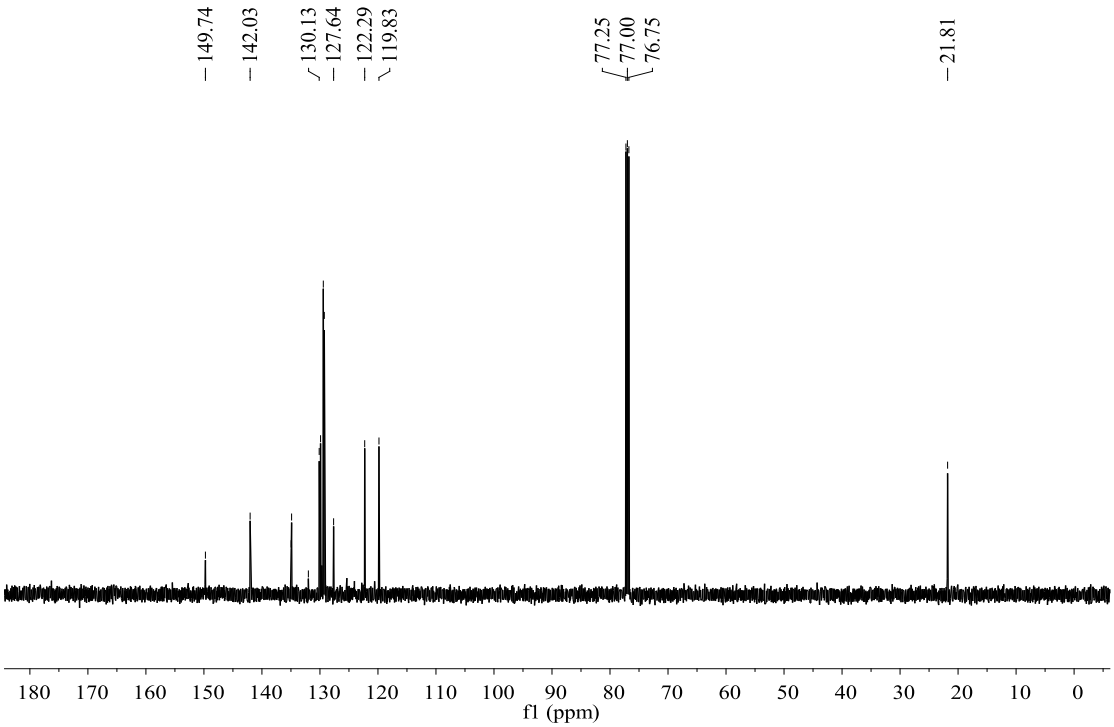
The ^{13}C NMR spectrum of *p*-ClPNCl-*m*

3.27 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-MePNCl-*m*

$C_{14}H_{12}NOCl$



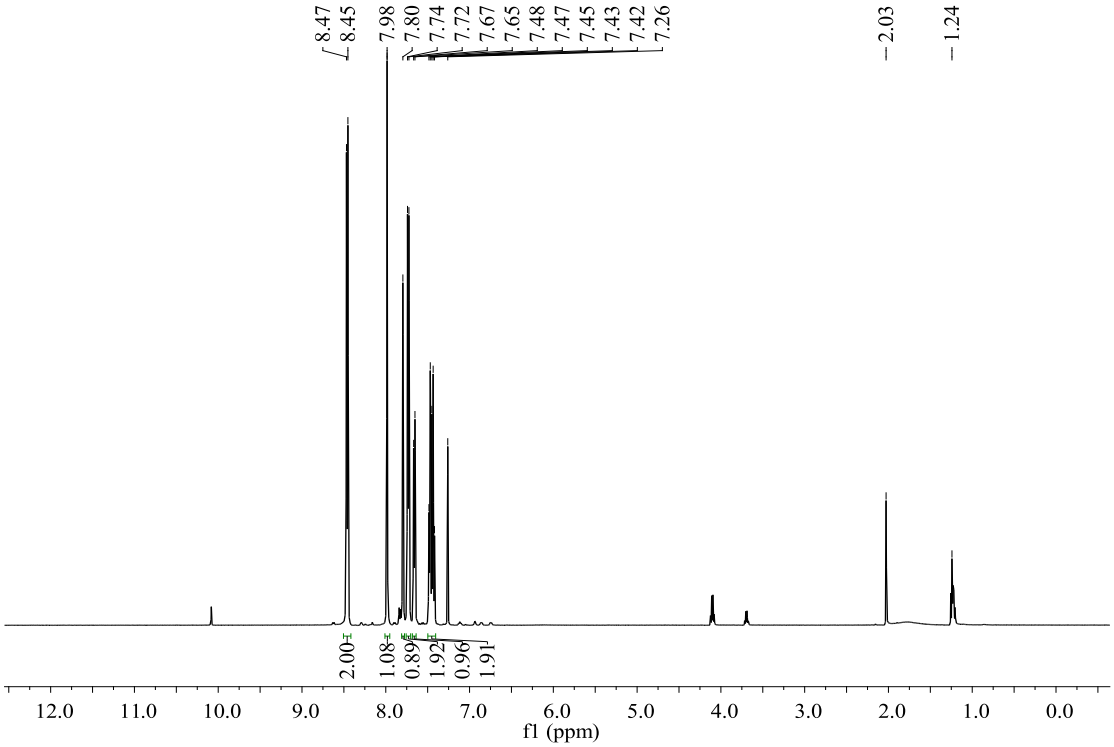
The ^{1}H NMR spectrum of *p*-MePNCl-*m*



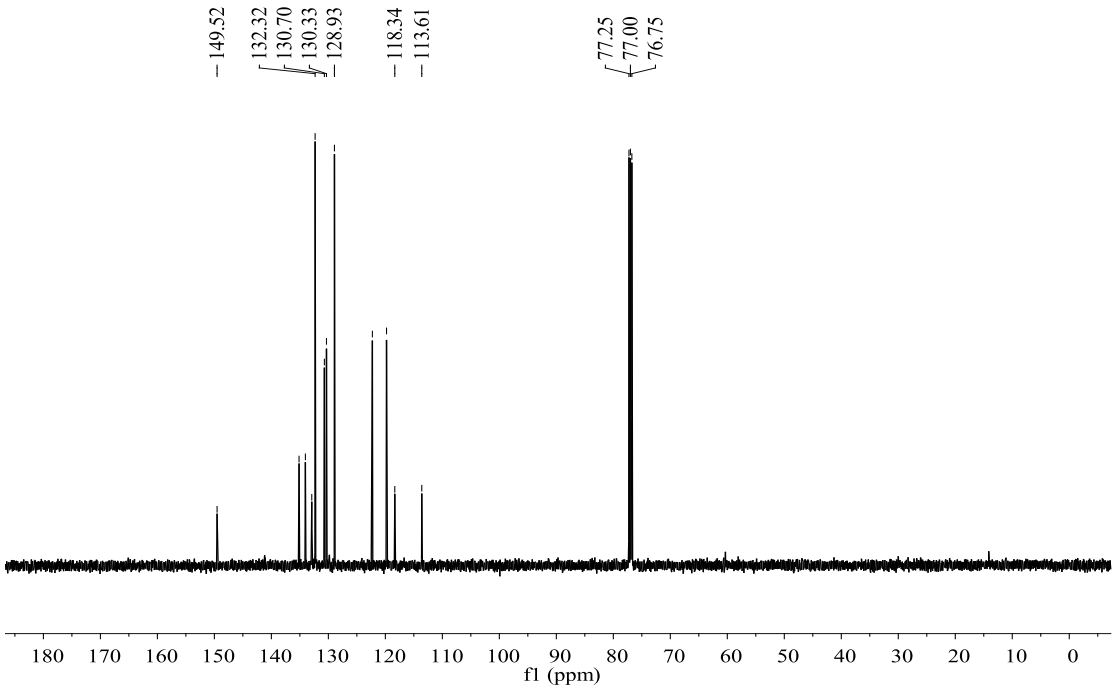
The ^{13}C NMR spectrum of *p*-MePNCl-*m*

3.28 Spectrum of ^{1}H NMR and ^{13}C NMR of p-CNPNCl-m

$C_{14}H_9N_2OCl$



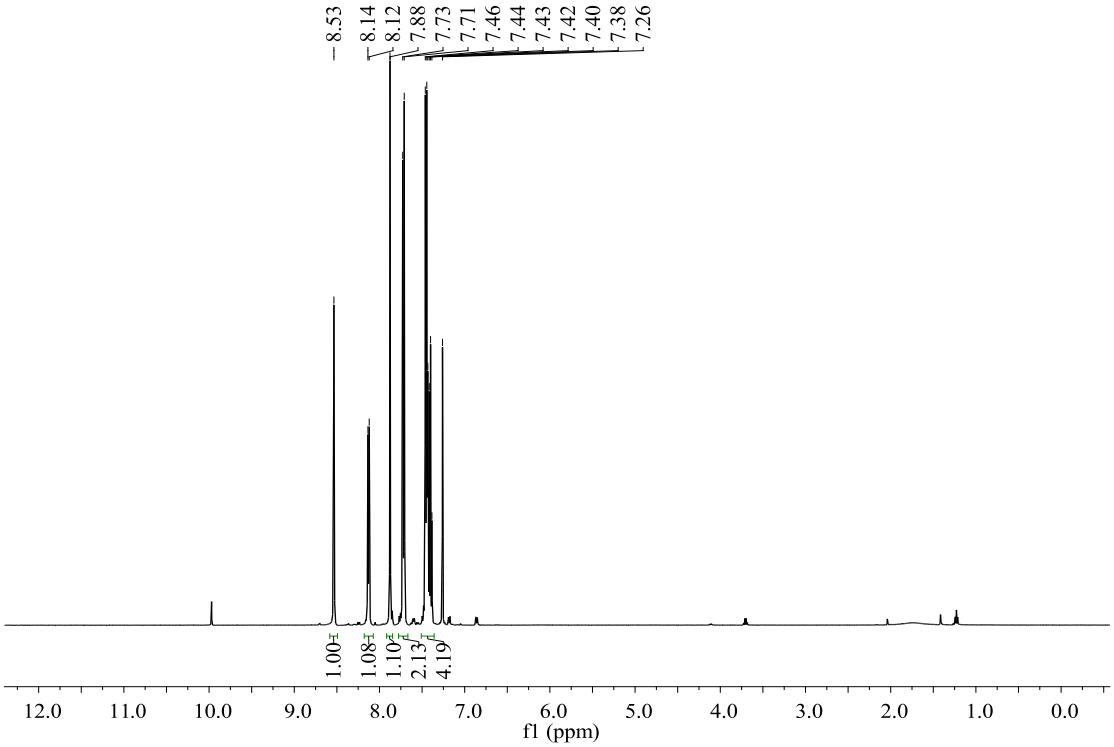
The ^{1}H NMR spectrum of *p*-CNPNCl-*m*



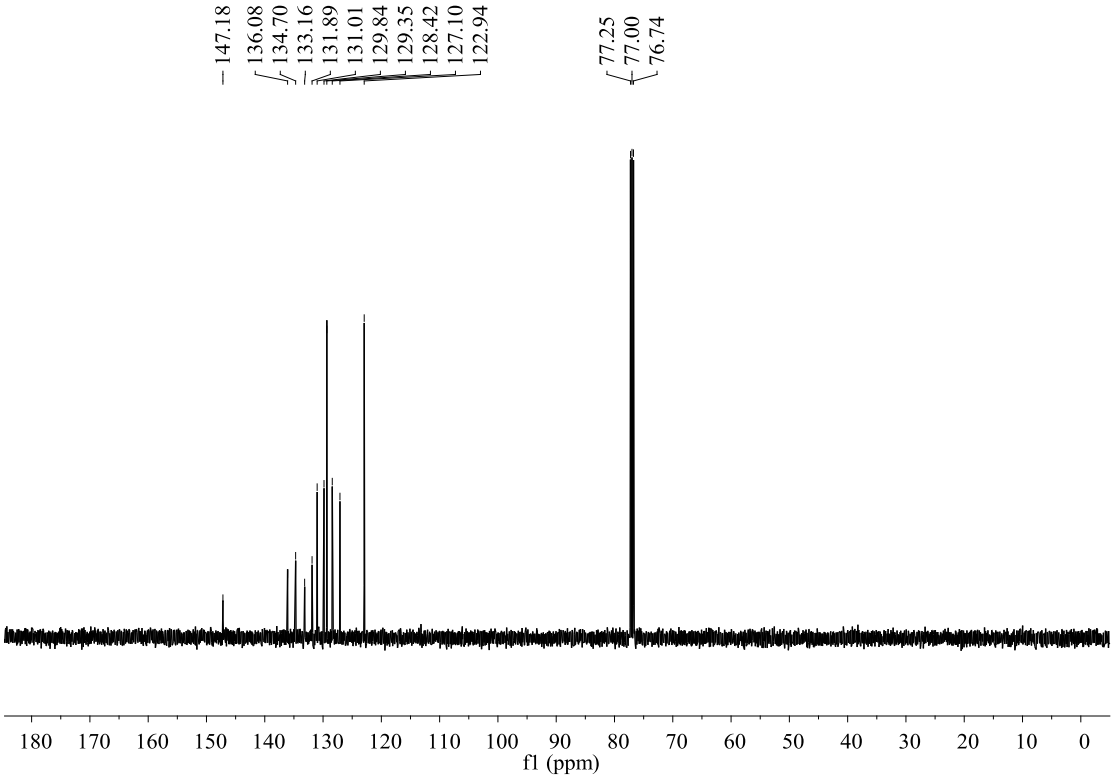
The ^{13}C NMR spectrum of *p*-CNPNCl-*m*

3.29 Spectrum of ^{1}H NMR and ^{13}C NMR of *m*-ClPNCl-*p*

$C_{13}H_9NOCl_2$



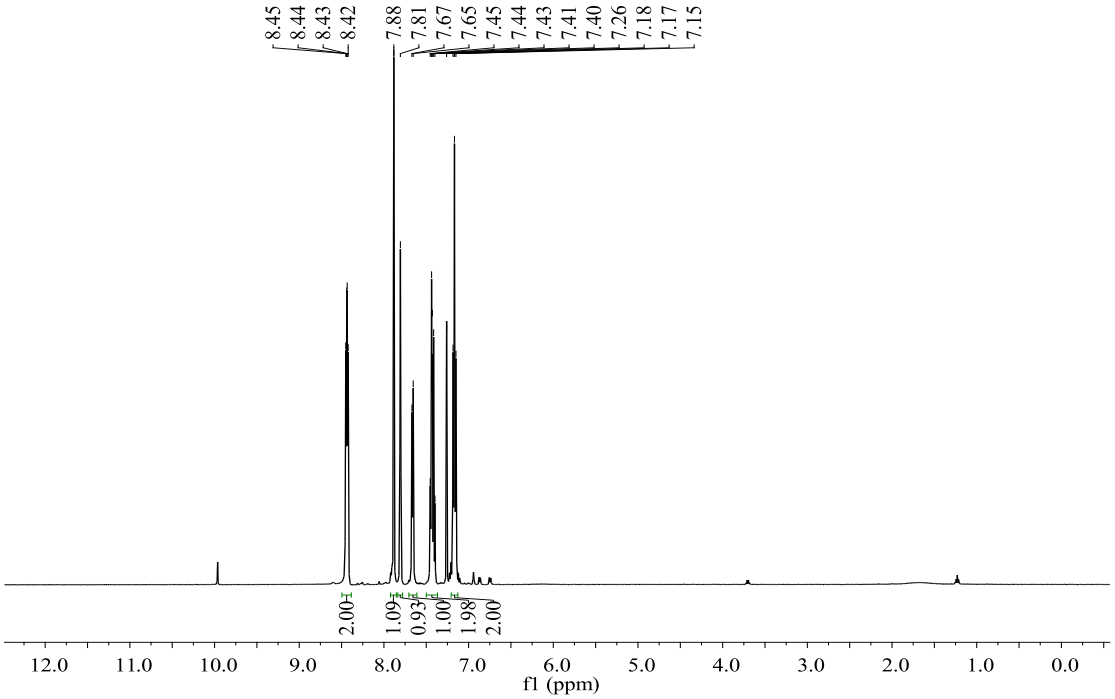
The ^{1}H NMR spectrum of *m*-ClPNCl-*p*



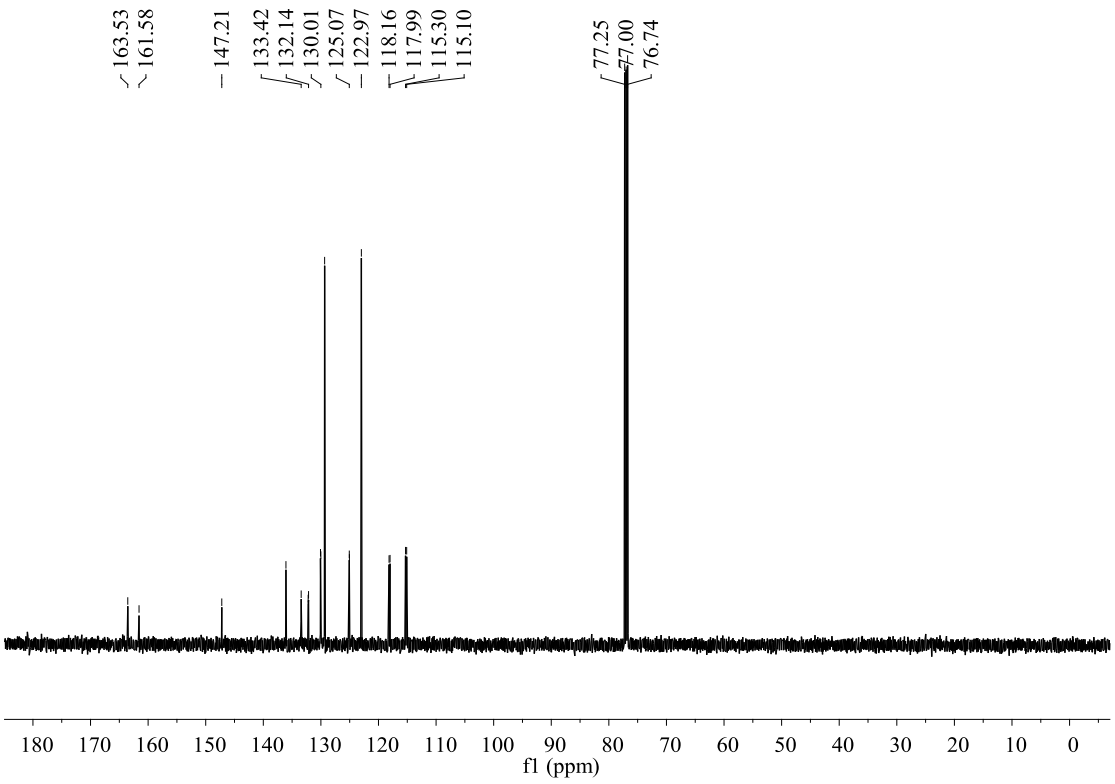
The ^{13}C NMR spectrum of *m*-ClPNCl-*p*

3.30 Spectrum of ^{1}H NMR and ^{13}C NMR of *m*-FPNCl-*p*

$C_{13}H_9NOFCl$



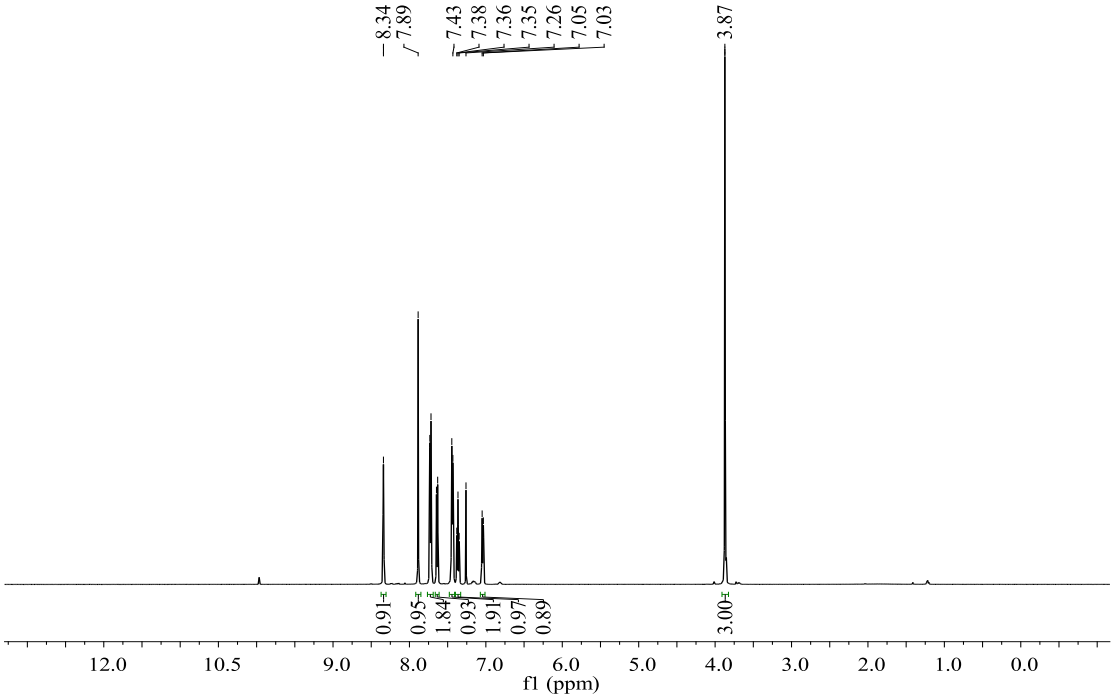
The ^{1}H NMR spectrum of *m*-FPNCl-*p*



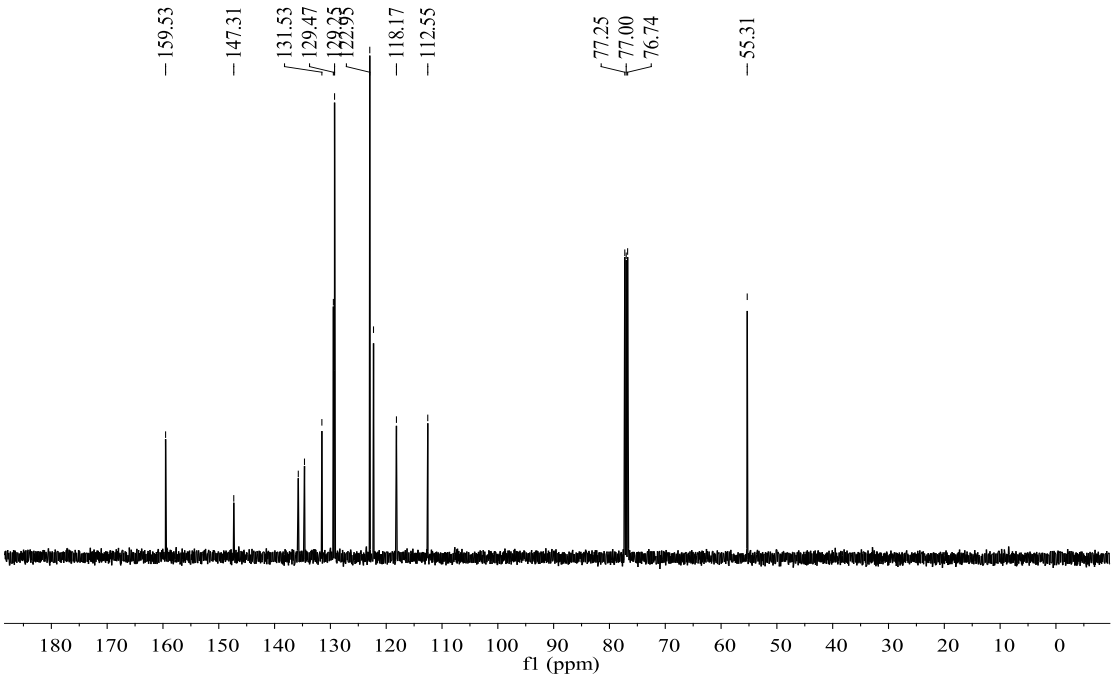
The ^{13}C NMR spectrum of *m*-FPNCl-*p*

3.31 Spectrum of ^{1}H NMR and ^{13}C NMR of *m*-OMePNCl-*p*

$C_{14}H_{12}NO_2Cl$



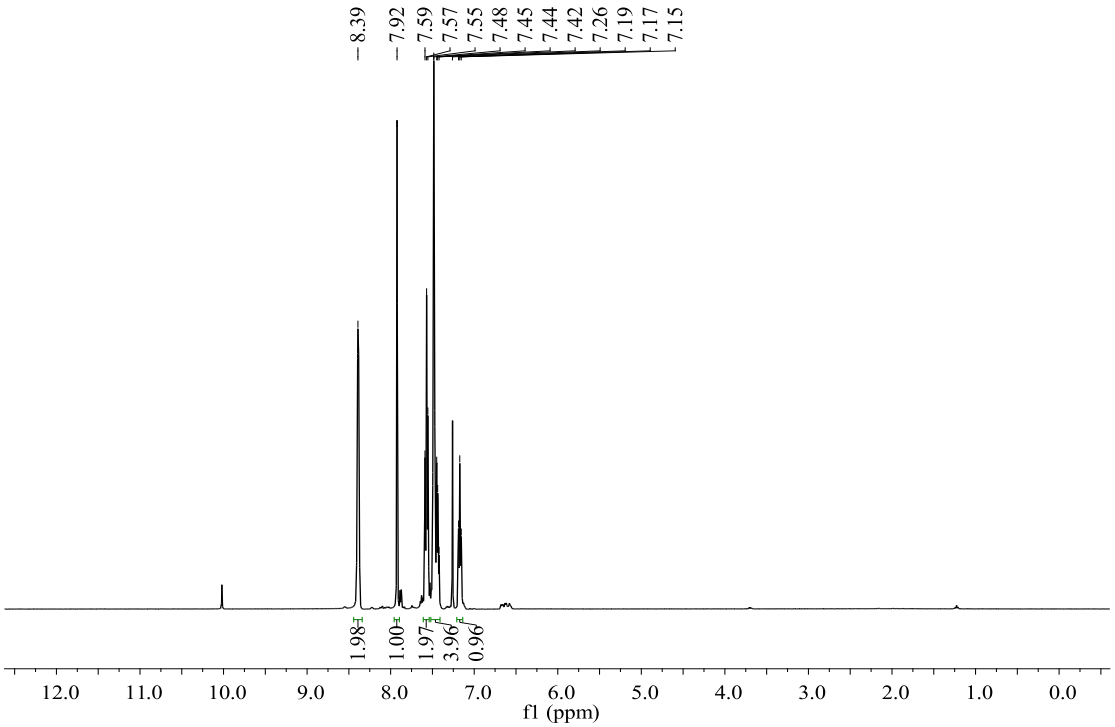
The ^{1}H NMR spectrum of *m*-OMePNCl-*p*



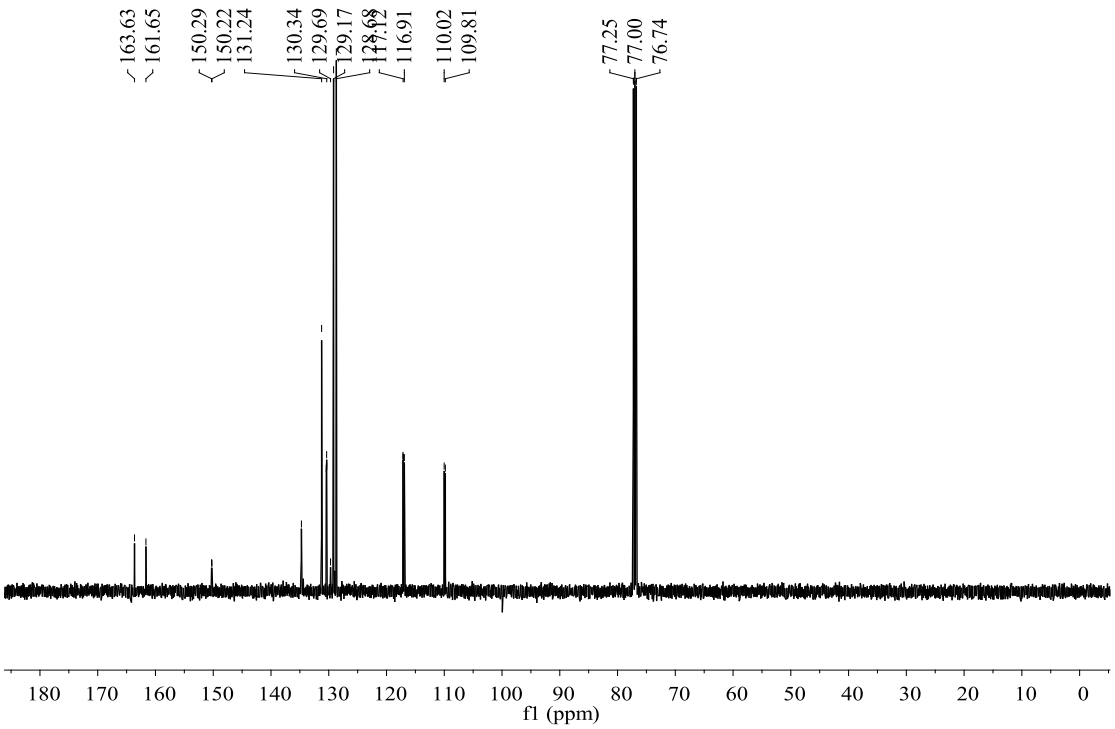
The ^{13}C NMR spectrum of *m*-OMePNCl-*p*

3.32 Spectrum of ^{1}H NMR and ^{13}C NMR of HPNF-*m*

$C_{13}H_{10}NOF$



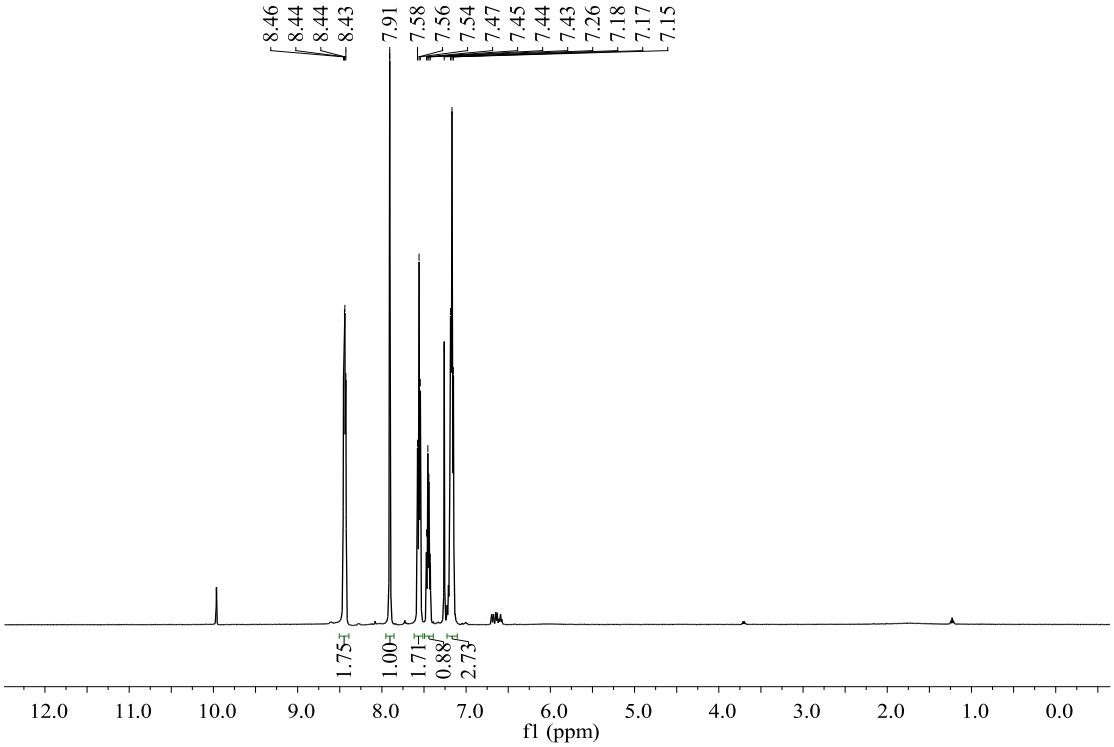
The ^{1}H NMR spectrum of HPNF-*m*



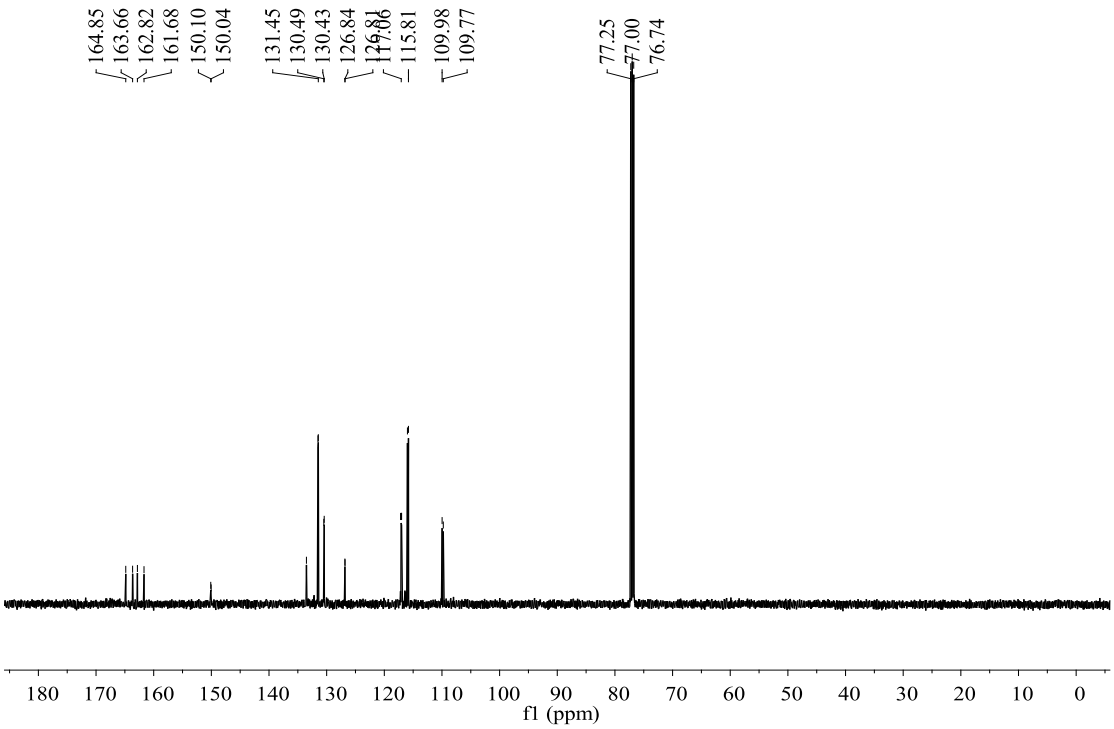
The ^{13}C NMR spectrum of HPNF-*m*

3.33 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-FPNF-*m*

$C_{13}H_9NOF_2$



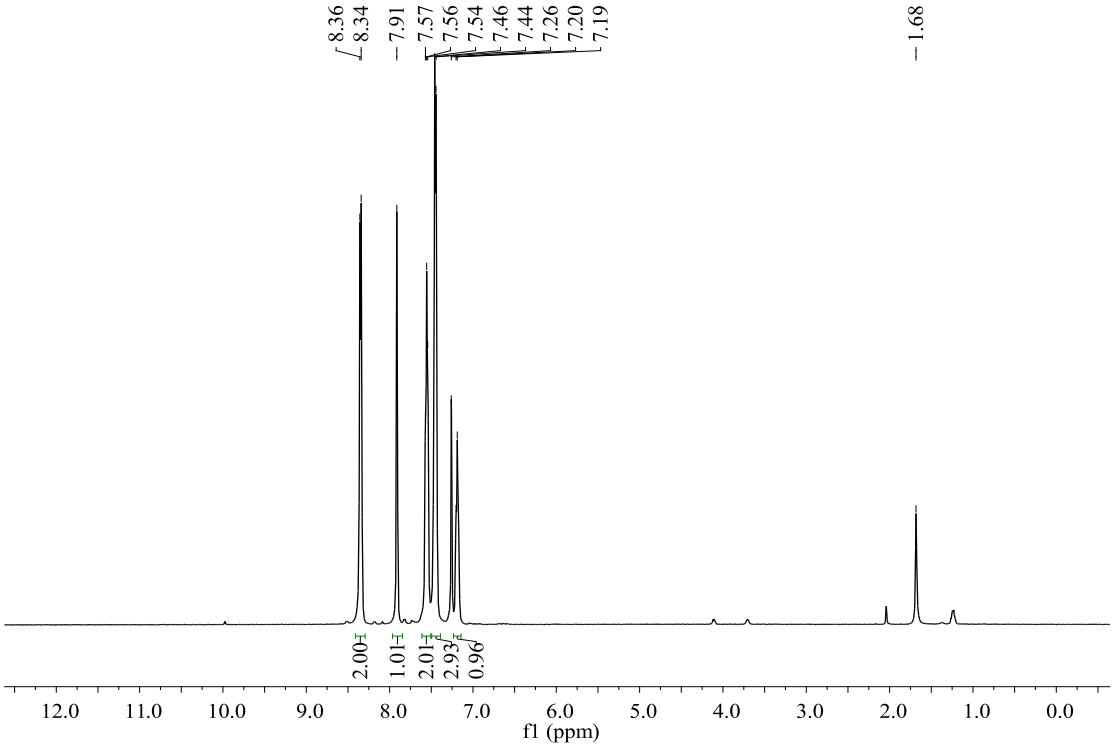
The ^{1}H NMR spectrum of *p*-FPNF-*m*



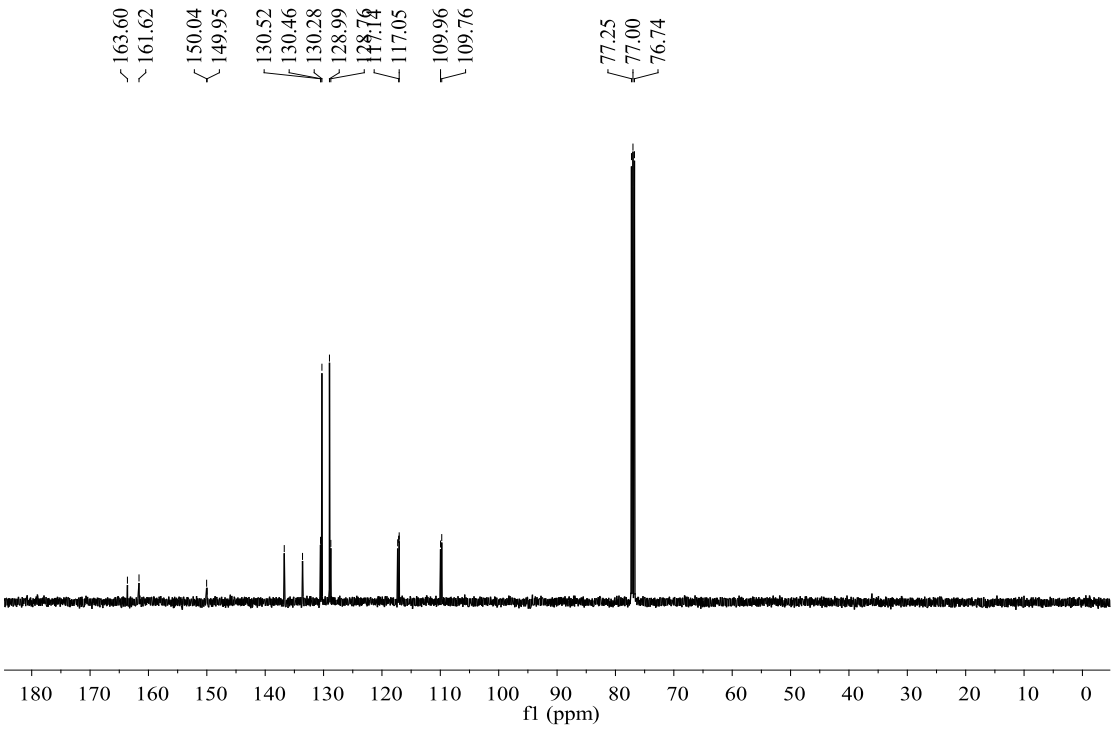
The ^{13}C NMR spectrum of *p*-FPNF-*m*

3.34 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-ClPNF-*m*

$C_{13}H_9NOFCl$



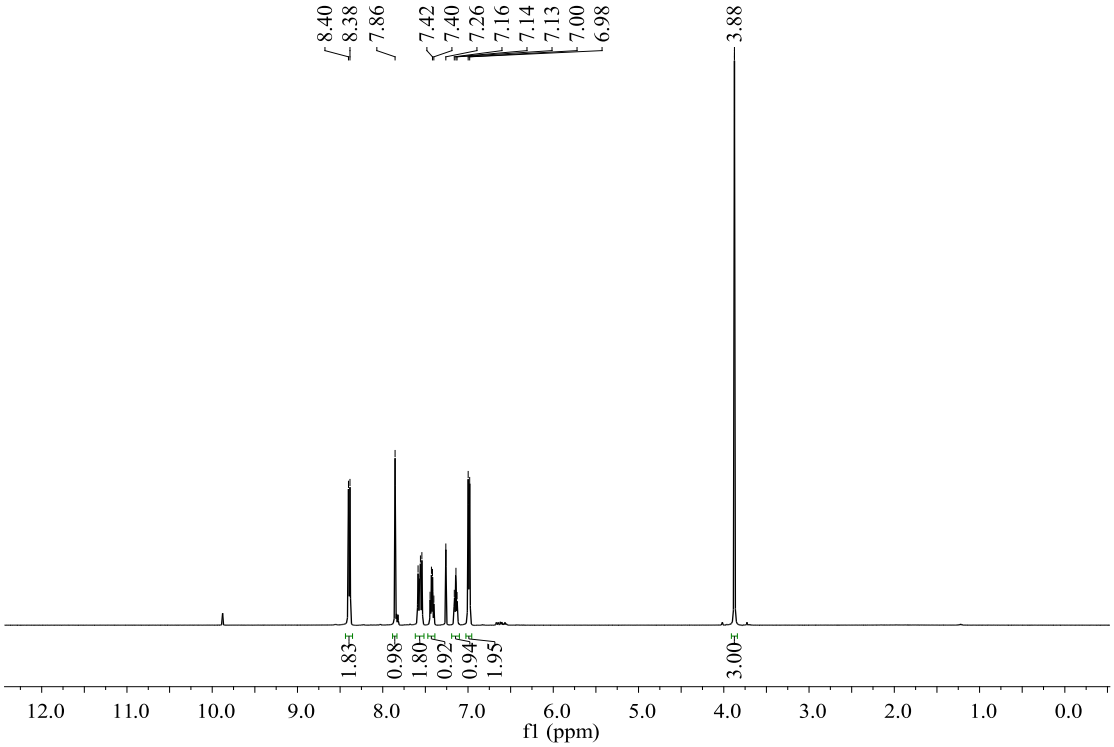
The ^{1}H NMR spectrum of *p*-ClPNF-*m*



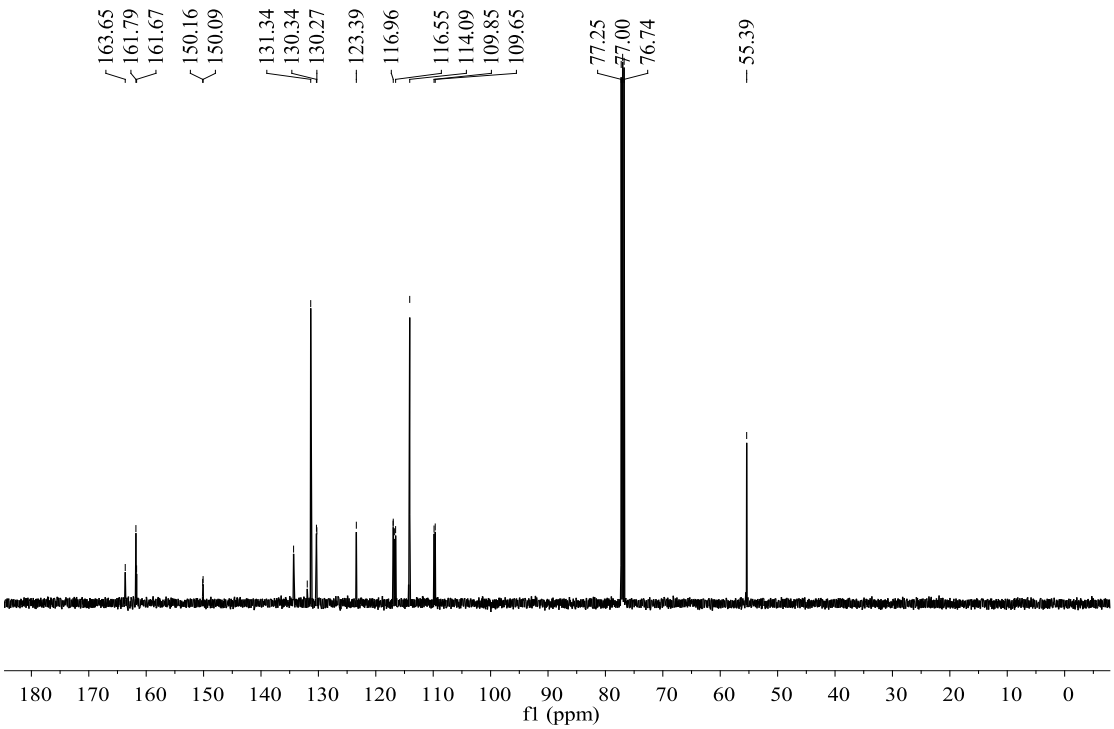
The ^{13}C NMR spectrum of *p*-ClPNF-*m*

3.35 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-OMePNF-*m*

$C_{14}H_{12}NO_2F$



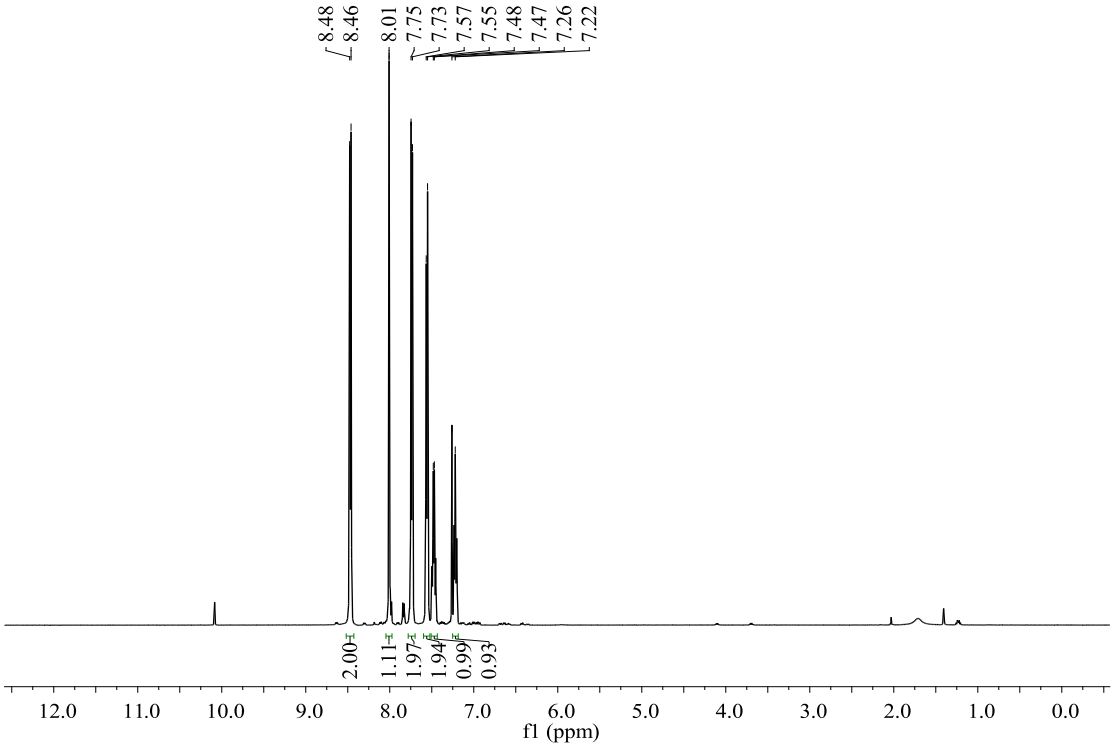
The ^{1}H NMR spectrum of *p*-OMePNF-*m*



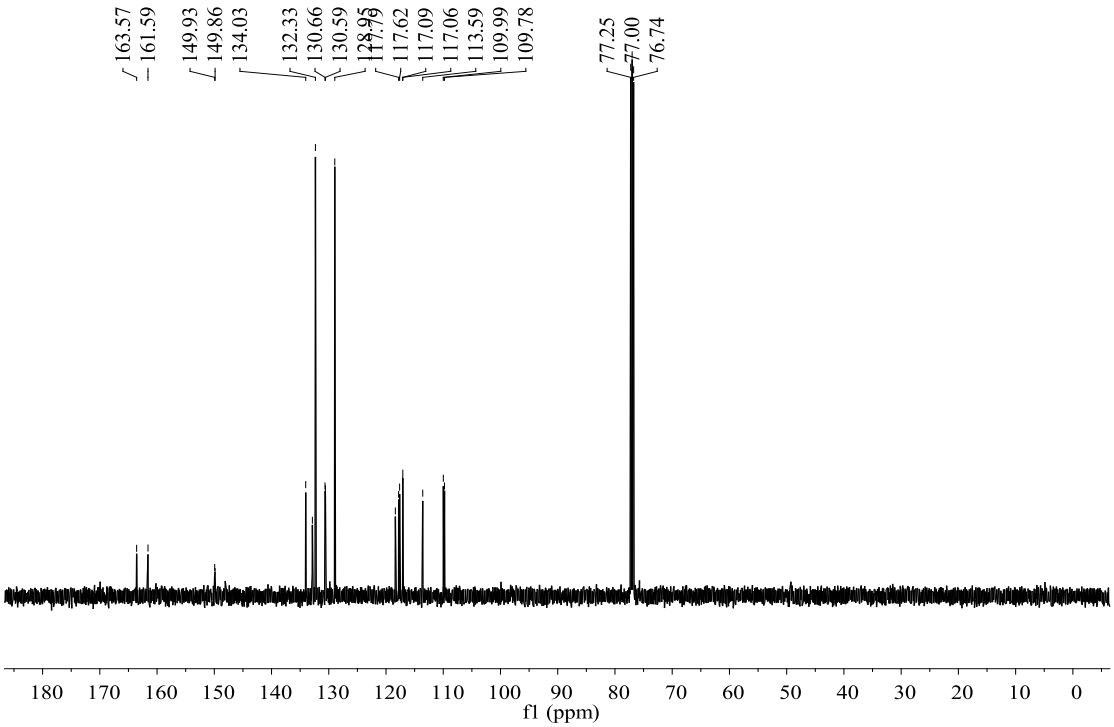
The ^{13}C NMR spectrum of *p*-OMePNF-*m*

3.36 Spectrum of ^{1}H NMR and ^{13}C NMR of *p*-CNPNF-*m*

$C_{14}H_9N_2OF$



The ^{1}H NMR spectrum of *p*-CNPNF-*m*



The ^{13}C NMR spectrum of *p*-CNPNF-*m*

4、化合物 4’4/3,4’/4,3’/3,3’-二取代 XBAY 的 E_{red} 数据

表 3 XBAYs 的 $E_{(Red)}$/V 及取代基 X 和 Y 的 σ_F，σ_R 和 σ_{cc}^{ex} 值

Table 3 The reduction potentials ($E_{(Red)}$) of XBAY and substituent constant values of σ_F，σ_R and σ_{cc}^{ex} for groups X and Y

No	X	Y	$\sigma_F(X)^a$	$\sigma_F(Y)^a$	$\sigma_R(X)^a$	$\sigma_R(Y)^a$	$\sigma_{cc}^{ex}(X)^b$	$\sigma_{cc}^{ex}(Y)^b$	I_m^c	$E_{(Red)exp}^d$
1	*p*-NMe_2	*p*-NMe_2	0.15	0.15	-0.98	-0.98	-1.81	-1.81	0.00	-2.23
2	*p*-OMe	*p*-NMe_2	0.29	0.15	-0.56	-0.98	-0.50	-1.81	0.00	-2.23
3	*p*-Me	*p*-NMe_2	0.01	0.15	-0.18	-0.98	-0.17	-1.81	0.00	-2.17
4	*p*-H	*p*-NMe_2	0.00	0.15	0.00	-0.98	0.00	-1.81	0.00	-2.01
5	*p*-Cl	*p*-NMe_2	0.42	0.15	-0.19	-0.98	-0.22	-1.81	0.00	-1.96
6	*p*-F	*p*-NMe_2	0.45	0.15	-0.39	-0.98	0.06	-1.81	0.00	-2.14
7	*p*-CN	*p*-NMe_2	0.51	0.15	0.15	-0.98	-0.70	-1.81	0.00	-1.70
8	*p*-NO_2	*p*-NMe_2	0.65	0.15	0.13	-0.98	-1.17	-1.81	0.00	-1.60
9	*p*-NMe_2	*p*-OMe	0.15	0.29	-0.98	-0.56	-1.81	-0.50	0.00	-2.23
10	*p*-OMe	*p*-OMe	0.29	0.29	-0.56	-0.56	-0.50	-0.50	0.00	-2.20
11	*p*-Me	*p*-OMe	0.01	0.29	-0.18	-0.56	-0.17	-0.50	0.00	-2.14
12	*p*-H	*p*-OMe	0.00	0.29	0.00	-0.56	0.00	-0.50	0.00	-2.06
13	*p*-Cl	*p*-OMe	0.42	0.29	-0.19	-0.56	-0.22	-0.50	0.00	-1.94
14	*p*-F	*p*-OMe	0.45	0.29	-0.39	-0.56	0.06	-0.50	0.00	-2.10
15	*p*-CN	*p*-OMe	0.51	0.29	0.15	-0.56	-0.70	-0.50	0.00	-1.63
16	*p*-NO_2	*p*-OMe	0.65	0.29	0.13	-0.56	-1.17	-0.50	0.00	-1.57
17	*p*-NMe_2	*p*-Me	0.15	0.01	-0.98	-0.18	-1.81	-0.17	0.00	-2.23
18	*p*-OMe	*p*-Me	0.29	0.01	-0.56	-0.18	-0.50	-0.17	0.00	-2.14
19	*p*-Me	*p*-Me	0.01	0.01	-0.18	-0.18	-0.17	-0.17	0.00	-2.10
20	*p*-Cl	*p*-Me	0.42	0.01	-0.19	-0.18	-0.22	-0.17	0.00	-1.91
21	*p*-F	*p*-Me	0.45	0.01	-0.39	-0.18	0.06	-0.17	0.00	-2.05
22	*p*-CN	*p*-Me	0.51	0.01	0.15	-0.18	-0.70	-0.17	0.00	-1.63
23	*p*-NMe_2	H	0.15	0.00	-0.98	0.00	-1.81	0.00	0.00	-2.11
24	*p*-OMe	H	0.29	0.00	-0.56	0.00	-0.50	0.00	0.00	-1.98
25	*p*-Me	H	0.01	0.00	-0.18	0.00	-0.17	0.00	0.00	-2.05
26	*p*-Cl	H	0.42	0.00	-0.19	0.00	-0.22	0.00	0.00	-1.96
27	*p*-F	H	0.45	0.00	-0.39	0.00	0.06	0.00	0.00	-2.03
28	*p*-CN	H	0.51	0.00	0.15	0.00	-0.70	0.00	0.00	-1.59
29	*p*-NO_2	H	0.65	0.00	0.13	0.00	-1.17	0.00	0.00	-1.53
30	*p*-NMe_2	*p*-Cl	0.15	0.42	-0.98	-0.19	-1.81	-0.22	0.00	-2.17
31	*p*-OMe	*p*-Cl	0.29	0.42	-0.56	-0.19	-0.50	-0.22	0.00	-2.04
32	*p*-Me	*p*-Cl	0.01	0.42	-0.18	-0.19	-0.17	-0.22	0.00	-1.98
33	*p*-H	*p*-Cl	0.00	0.42	0.00	-0.19	0.00	-0.22	0.00	-1.91
34	*p*-Cl	*p*-Cl	0.42	0.42	-0.19	-0.19	-0.22	-0.22	0.00	-1.81
35	*p*-CN	*p*-Cl	0.51	0.42	0.15	-0.19	-0.70	-0.22	0.00	-1.72
36	*p*-NO_2	*p*-Cl	0.65	0.42	0.13	-0.19	-1.17	-0.22	0.00	-1.63
37	*p*-NMe_2	*p*-F	0.15	0.45	-0.98	-0.39	-1.81	0.06	0.00	-2.14

38	*p*-OMe	*p*-F	0.29	0.45	-0.56	-0.39	-0.50	0.06	0.00	-2.14
39	*p*-Me	*p*-F	0.01	0.45	-0.18	-0.39	-0.17	0.06	0.00	-2.07
40	*p*-H	*p*-F	0.00	0.45	0.00	-0.39	0.00	0.06	0.00	-2.04
41	*p*-Cl	*p*-F	0.42	0.45	-0.19	-0.39	-0.22	0.06	0.00	-2.02
42	*p*-F	*p*-F	0.45	0.45	-0.39	-0.39	0.06	0.06	0.00	-2.01
43	*p*-CN	*p*-F	0.51	0.45	0.15	-0.39	-0.70	0.06	0.00	-1.58
44	*p*-NMe_2	*p*-CN	0.15	0.51	-0.98	0.15	-1.81	-0.70	0.00	-2.20
45	*p*-Me	*p*-CN	0.01	0.51	-0.18	0.15	-0.17	-0.70	0.00	-1.97
46	*p*-CN	*p*-CN	0.51	0.51	0.15	0.15	-0.70	-0.70	0.00	-1.59
47	*p*-NO_2	*p*-CN	0.65	0.51	0.13	0.15	-1.17	-0.70	0.00	-1.43
48	*p*-NMe_2	*p*-NO_2	0.15	0.65	-0.98	0.13	-1.81	-1.17	0.00	-2.14
49	*p*-OMe	*p*-NO_2	0.29	0.65	-0.56	0.13	-0.50	-1.17	0.00	-2.06
50	*p*-Me	*p*-NO_2	0.01	0.65	-0.18	0.13	-0.17	-1.17	0.00	-2.10
51	*p*-F	*p*-NO_2	0.45	0.65	-0.39	0.13	0.06	-1.17	0.00	-2.01
52	*p*-CN	*p*-NO_2	0.51	0.65	0.15	0.13	-0.70	-1.17	0.00	-1.54
53	*m*-F	*p*-NMe_2	0.34	0.15	0.00	-0.98	0.02	-1.81	1.00	-2.22
54	*m*-F	*p*-OMe	0.34	0.29	0.00	-0.56	0.02	-0.50	1.00	-2.16
55	*m*-F	*p*-Me	0.34	0.01	0.00	-0.18	0.02	-0.17	1.00	-2.14
56	*m*-F	*p*-Cl	0.34	0.42	0.00	-0.19	0.02	-0.22	1.00	-1.99
57	*m*-Br	*p*-NMe_2	0.39	0.15	0.00	-0.98	-0.03	-1.81	1.00	-2.31
58	*m*-Br	*p*-OMe	0.39	0.29	0.00	-0.56	-0.03	-0.50	1.00	-2.09
59	*m*-Br	*p*-Me	0.39	0.01	0.00	-0.18	-0.03	-0.17	1.00	-2.07
60	*m*-Br	*p*-F	0.39	0.45	0.00	-0.39	-0.03	0.06	1.00	-2.15
61	*m*-Br	*p*-Cl	0.39	0.42	0.00	-0.19	-0.03	-0.22	1.00	-2.14
62	*m*-CN	*p*-NMe_2	0.56	0.15	0.00	-0.98	0.56	-1.81	1.00	-2.13
63	*m*-CN	*p*-OMe	0.56	0.29	0.00	-0.56	0.56	-0.50	1.00	-2.01
64	*m*-CN	*p*-Me	0.56	0.01	0.00	-0.18	0.56	-0.17	1.00	-2.04
65	*m*-CN	*p*-Cl	0.56	0.42	0.00	-0.19	0.56	-0.22	1.00	-1.94
66	*m*-CN	*p*-CN	0.56	0.51	0.00	0.15	0.56	-0.70	1.00	-1.76
67	*m*-OMe	*p*-NMe_2	0.12	0.15	0.00	-0.98	0.10	-1.81	1.00	-2.27
68	*p*-NMe_2	*m*-Me	0.15	-0.07	-0.98	0.00	-1.81	-0.03	1.00	-2.44
69	*p*-OMe	*m*-Me	0.29	-0.07	-0.56	0.00	-0.50	-0.03	1.00	-2.37
70	*p*-Cl	*m*-Me	0.42	-0.07	-0.19	0.00	-0.22	-0.03	1.00	-2.16
71	*p*-CF_3	*m*-Me	0.38	-0.07	0.16	0.00	-0.12	-0.03	1.00	-1.99
72	*p*-CN	*m*-Me	0.51	-0.07	0.15	0.00	-0.70	-0.03	1.00	-1.81
73	*p*-NO_2	*m*-Me	0.65	-0.07	0.13	0.00	-1.17	-0.03	1.00	-1.86
74	*p*-NMe_2	*m*-F	0.15	0.34	-0.98	0.00	-1.81	0.02	1.00	-2.28
75	*p*-OMe	*m*-F	0.29	0.34	-0.56	0.00	-0.50	0.02	1.00	-2.21
76	*p*-Me	*m*-F	0.01	0.34	-0.18	0.00	-0.17	0.02	1.00	-2.17
77	*p*-Cl	*m*-F	0.42	0.34	-0.19	0.00	-0.22	0.02	1.00	-2.04
78	*p*-NMe_2	*m*-Br	0.15	0.39	-0.98	0.00	-1.81	-0.03	1.00	-2.32
79	*p*-OMe	*m*-Br	0.29	0.39	-0.56	0.00	-0.50	-0.03	1.00	-2.37
80	*p*-Me	*m*-Br	0.01	0.39	-0.18	0.00	-0.17	-0.03	1.00	-2.20

81	*p*-Cl	*m*-Br	0.42	0.39	-0.19	0.00	-0.22	-0.03	1.00	-1.99
82	*p*-CN	*m*-Br	0.51	0.39	0.15	0.00	-0.70	-0.03	1.00	-1.71
83	*p*-NMe_2	*m*-OMe	0.15	0.12	-0.98	0.00	-1.81	0.10	1.00	-2.41
84	*p*-CN	*m*-OMe	0.51	0.12	0.15	0.00	-0.70	0.10	1.00	-1.81
85	*p*-NO_2	*m*-OMe	0.65	0.12	0.13	0.00	-1.17	0.10	1.00	-1.75
86	*p*-Cl	*m*-CN	0.42	0.56	-0.19	0.00	-0.22	0.56	1.00	-1.81
87	*p*-CN	*m*-CN	0.51	0.56	0.15	0.00	-0.70	0.56	1.00	-1.78
88	*m*-OMe	*m*-CN	0.12	0.56	0.00	0.00	0.10	0.56	1.00	-1.87
89	*m*-Me	*m*-OMe	-0.07	0.12	0.00	0.00	-0.03	0.10	1.00	-2.24
90	*m*-Me	*m*-Me	-0.07	-0.07	0.00	0.00	-0.03	-0.03	1.00	-2.27
91	*m*-Me	*m*-F	-0.07	0.34	0.00	0.00	-0.03	0.02	1.00	-2.26
92	*m*-F	*m*-Me	0.34	-0.07	0.00	0.00	0.02	-0.03	1.00	-2.12
93	*m*-F	*m*-F	0.34	0.34	0.00	0.00	0.02	0.02	1.00	-2.02
94	*m*-F	*m*-Br	0.34	0.39	0.00	0.00	0.02	-0.03	1.00	-2.04
95	*m*-CN	*m*-OMe	0.56	0.12	0.00	0.00	0.56	0.10	1.00	-1.94
96	*m*-CN	*m*-Me	0.56	-0.07	0.00	0.00	0.56	-0.03	1.00	-2.00
97	*m*-CN	*m*-F	0.56	0.34	0.00	0.00	0.56	0.02	1.00	-1.90
98	*m*-CN	*m*-CN	0.56	0.56	0.00	0.00	0.56	0.56	1.00	-1.89
99	*m*-Br	*m*-Me	0.39	-0.07	0.00	0.00	-0.03	-0.03	1.00	-2.14
100	*m*-Br	*m*-CN	0.39	0.56	0.00	0.00	-0.03	0.56	1.00	-1.97
101	*m*-Br	*m*-Br	0.39	0.39	0.00	0.00	-0.03	-0.03	1.00	-1.96

[a] The values were taken from Reference[22]. [b] The values were taken from Reference[24]. [c] The $E_{(Red)}$ values of 4,4'-substituted XBAYs (No 1~52) were taken from Reference[23], and were adjusted by Ferrocene, in this work, that is, 0.27V was added to the $E_{(Red)}$ values of ref.[23]. For example, the $E_{(Red).exp}$ of *p*-Me_2NBANMe_2-*p* is -2.50+0.27 = -2.23V. [d] The $E_{(Red)}$ values of 4,3'/3,4'/3,3'- substituted XBAYs (No 53~101) were taken from Reference[25].