

Supporting Information

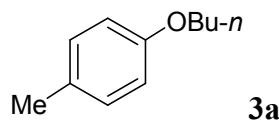
MCM-41-immobilized 1,10-phenanthroline-copper(I) complex: A highly efficient and recyclable catalyst for the coupling of aryl iodides with aliphatic alcohols

Yang Lin^a, Mingzhong Cai^{b*}, Zhiqiang Fang^a and Hong Zhao^{a*}

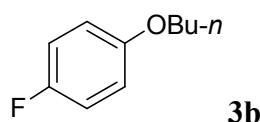
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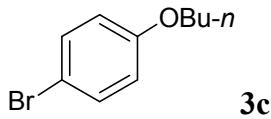
The spectral data of aryl alkyl ethers 3a-3f':



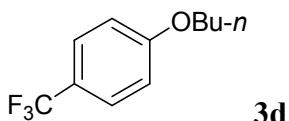
4-Butoxytoluene.¹ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.07 (d, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 3.93 (t, *J* = 6.6 Hz, 2H), 2.28 (s, 3H), 1.7-1.71 (m, 2H), 1.53-1.43 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 157.0, 129.9, 129.6, 114.4, 67.8, 31.4, 20.5, 19.3, 13.9.



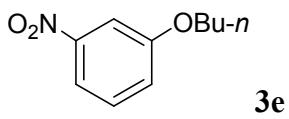
1-Butoxy-4-fluorobenzene.² Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 6.96 (t, *J* = 8.8 Hz, 2H), 6.84-6.80 (m, 2H), 3.91 (t, *J* = 6.6 Hz, 2H), 1.78-1.71 (m, 2H), 1.53-1.43 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 157.1 (d, *J* = 237.2 Hz), 155.3 (d, *J* = 2.0 Hz), 115.7 (d, *J* = 23.0 Hz), 115.4 (d, *J* = 7.9 Hz), 68.3, 31.4, 19.3, 13.9.



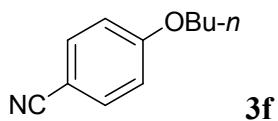
1-Bromo-4-butoxybenzene.³ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.26 (d, *J* = 9.2 Hz, 2H), 6.68 (d, *J* = 9.2 Hz, 2H), 3.82 (t, *J* = 6.4 Hz, 2H), 1.70-1.61 (m, 2H), 1.44-1.34 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 158.3, 132.2, 116.3, 112.6, 67.9, 31.3, 19.3, 13.9.



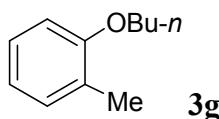
1-Butoxy-4-(trifluoromethyl)benzene.⁴ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.52 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 3.98 (t, *J* = 6.4 Hz, 2H), 1.81-1.74 (m, 2H), 1.54-1.44 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 161.7, 126.8 (q, ³*J* = 3.7 Hz), 124.5 (q, ¹*J* = 269.3 Hz), 122.6 (q, ²*J* = 32.4 Hz), 114.4, 67.9, 31.1, 19.2, 13.7.



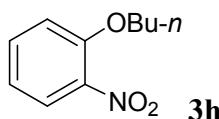
1-Butoxy-3-nitrobenzene.⁵ pale yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ = 7.81-7.77 (m, 1H), 7.71 (t, *J* = 2.4 Hz, 1H), 7.41 (t, *J* = 8.2 Hz, 1H), 7.23-7.19 (m, 1H), 4.03 (t, *J* = 6.4 Hz, 2H), 1.84-1.77 (m, 2H), 1.57-1.46 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 159.7, 149.2, 129.9, 121.6, 115.5, 108.7, 68.4, 31.0, 19.2, 13.8.



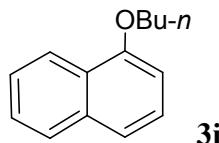
4-Butoxybenzonitrile.⁴ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.57 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.00 (t, *J* = 6.6 Hz, 2H), 1.83-1.74 (m, 2H), 1.55-1.44 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 162.5, 134.0, 119.4, 115.2, 103.6, 68.1, 31.0, 19.1, 13.8.



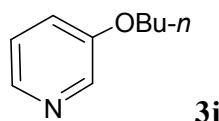
2-Butoxytoluene.⁶ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.09-7.03 (m, 2H), 6.78-6.71 (m, 2H), 3.88 (t, *J* = 6.4 Hz, 2H), 2.15 (s, 3H), 1.73-1.68 (m, 2H), 1.47-1.41 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 157.3, 130.6, 126.9, 126.7, 120.0, 110.9, 67.6, 31.5, 19.4, 16.2, 13.9.



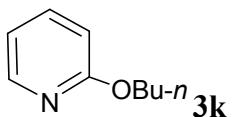
1-Butoxy-2-nitrobenzene.⁴ Yellow oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.73 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.45-7.40 (m, 1H), 7.00-6.90 (m, 2H), 4.03 (t, *J* = 6.2 Hz, 2H), 1.78-1.70 (m, 2H), 1.49-1.39 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 152.5, 140.0, 134.0, 125.5, 120.0, 114.4, 69.3, 31.0, 19.1, 13.7.



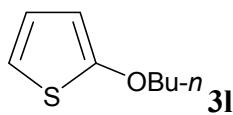
1-Butoxynaphthalene.⁵ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 8.30-8.27 (m, 1H), 7.76-7.74 (m, 1H), 7.46-7.32 (m, 4H), 6.74 (d, *J* = 7.6 Hz, 1H), 4.07 (t, *J* = 6.4 Hz, 2H), 1.88-1.83 (m, 2H), 1.59-1.53 (m, 2H), 0.99 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 155.1, 134.7, 127.5, 126.4, 126.0, 125.9, 125.1, 122.2, 120.1, 104.7, 67.9, 31.5, 19.6, 14.0.



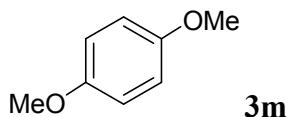
3-Butoxypyridine.⁷ Light yellow oil. ¹H NMR (400 MHz, CDCl₃) δ = 8.24 (s, 1H), 8.13 (s, 1H), 7.16-7.08 (m, 2H), 3.93 (t, *J* = 6.4 Hz, 2H), 1.75-1.67 (m, 2H), 1.46-1.37 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 155.3, 141.8, 138.0, 123.8, 121.1, 68.0, 31.2, 19.1, 13.8.



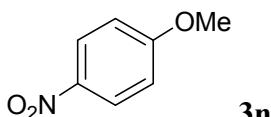
2-Butoxypyridine.¹ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 8.08 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.51-7.46 (m, 1H), 6.79-6.75 (m, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 4.21 (t, *J* = 6.8 Hz, 2H), 1.73-1.65 (m, 2H), 1.46-1.36 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 164.1, 146.9, 138.5, 116.5, 111.1, 65.7, 31.2, 19.3, 13.9.



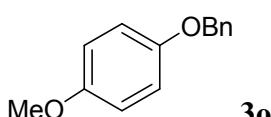
2-Butoxythiophene.¹ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 6.65-6.62 (m, 1H), 6.46-6.44 (m, 1H), 6.13-6.11 (m, 1H), 3.95 (t, *J* = 6.4 Hz, 2H), 1.72-1.65 (m, 2H), 1.45-1.35 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ = 165.9, 124.7, 111.7, 104.5, 73.7, 31.2, 19.1, 13.8.



1,4-Dimethoxybenzene.⁸ White solid. Mp: 48-49 °C. ¹H NMR (400 MHz, CDCl₃) δ = 6.83 (s, 4H), 3.75 (s, 6H). ¹³C NMR (100 MHz, CDCl₃) δ = 153.8, 114.7, 55.7.

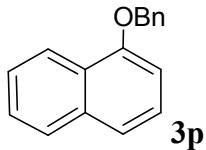


4-Nitroanisole.⁹ Light yellow solid, Mp: 50.8 °C. ¹H NMR (400 MHz, CDCl₃) δ = 8.20 (d, *J* = 9.2 Hz, 2H), 6.96 (d, *J* = 9.2 Hz, 2H), 3.92 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 164.6, 141.5, 125.9, 114.0, 56.0.

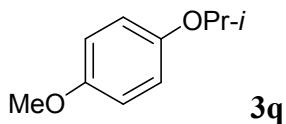


4-Benzylxyanisole.¹⁰ White solid. Mp: 63 °C. ¹H NMR (400 MHz, CDCl₃) δ = 7.43-

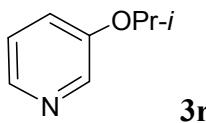
7.28 (m, 5H), 6.90 (d, J = 9.2 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H), 4.99 (s, 2H), 3.74 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ = 154.0, 153.0, 137.4, 128.6, 127.9, 127.5, 115.9, 114.7, 70.8, 55.7.



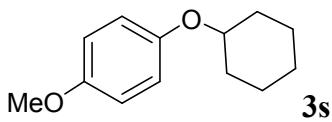
1-Benzylloxynaphthalene.¹¹ Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ = 8.36-8.33 (m, 1H), 7.76-7.73 (m, 1H), 7.49 (d, J = 7.2 Hz, 2H), 7.46-7.32 (m, 7H), 6.83 (d, J = 7.6 Hz, 1H), 5.19 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ = 154.6, 137.3, 134.7, 128.7, 128.0, 127.6, 127.5, 126.6, 126.0, 125.4, 122.3, 120.6, 105.3, 70.2.



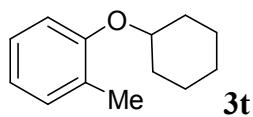
4-*iso*-Propoxyanisole.¹⁰ Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ = 6.84 (d, J = 9.2 Hz, 2H), 6.81 (d, J = 9.2 Hz, 2H), 4.44-4.37 (m, 1H), 3.76 (s, 3H), 1.30 (d, J = 6.0 Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ = 153.9, 151.9, 117.5, 114.7, 71.0, 55.7, 22.1.



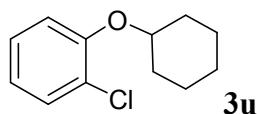
3-*iso*-Propoxypyridine.¹² Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ = 8.29 (s, 1H), 8.18 (s, 1H), 7.23-7.16 (m, 2H), 4.62-4.54 (m, 1H), 1.36 (d, J = 6.0 Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ = 154.1, 141.8, 139.3, 123.9, 122.5, 70.6, 21.9.



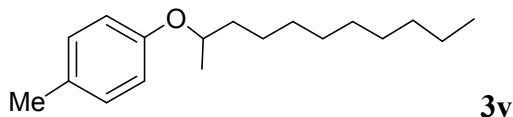
(p-Methoxyphenoxy)cyclohexane.¹³ Colorless oil. ^1H NMR (400 MHz, CDCl_3) δ = 6.86-6.79 (m, 4H), 4.12-4.05 (m, 1H), 3.75 (s, 3H), 1.96-1.92 (m, 2H), 1.79-1.74 (m, 2H), 1.53-1.42 (m, 3H), 1.36-1.27 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ = 153.9, 151.8, 117.7, 114.6, 76.6, 55.7, 32.0, 25.7, 23.9.



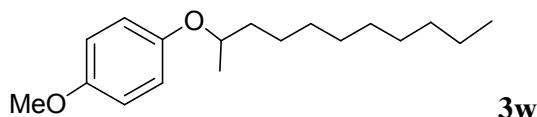
1-Cyclohexyloxy-2-methylbenzene.¹⁴ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.14-7.08 (m, 2H), 6.84-6.79 (m, 2H), 4.27-4.21 (m, 1H), 2.22 (s, 3H), 1.96-1.89 (m, 2H), 1.83-1.74 (m, 2H), 1.63-1.51 (m, 3H), 1.41-1.30 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 156.0, 130.9, 128.0, 126.6, 120.2, 113.3, 75.3, 31.9, 25.8, 23.7, 16.5.



1-Chloro-2-cyclohexyloxybenzene.¹⁵ Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.34 (dd, *J* = 8.0, 1.6, 1H), 7.18-7.13 (m, 1H), 6.94 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.88-6.83 (m, 1H), 4.31-4.25 (m, 1H), 1.97-1.91 (m, 2H), 1.86-1.78 (m, 2H), 1.67-1.52 (m, 3H), 1.40-1.30 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 153.5, 130.4, 127.5, 124.5, 121.4, 116.3, 77.1, 31.7, 25.6, 23.5.

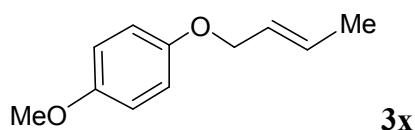


1-Methyl-4-(1-methyldecyloxy)benzene. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.06 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 2H), 4.32-4.24 (m, 1H), 2.27 (s, 3H), 1.76-1.67 (m, 1H), 1.58-1.49 (m, 1H), 1.42-1.24 (m, 17H), 0.88 (t, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 156.1, 129.9, 129.7, 116.0, 74.1, 36.6, 31.9, 29.7, 29.6, 29.4, 25.6, 22.7, 20.5, 19.8, 14.1. Anal. Calcd. for C₁₈H₃₀O: C, 82.38; H, 11.52. Found: C, 82.14; H, 11.33.

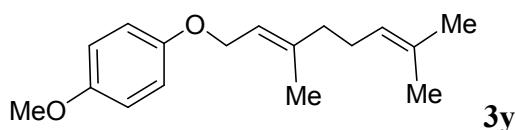


1-Methoxy-4-(1-methyldecyloxy)benzene. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 6.86-6.79 (m, 4H), 4.23-4.18 (m, 1H), 3.76 (s, 3H), 1.74-1.67 (m, 1H), 1.55-1.48 (m, 1H), 1.43-1.23 (m, 17H), 0.88 (t, *J* = 6.8 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 153.8, 152.3, 117.5, 114.6, 75.1, 55.7, 36.6, 31.9, 29.7, 29.6, 29.3, 25.6, 22.7, 19.8,

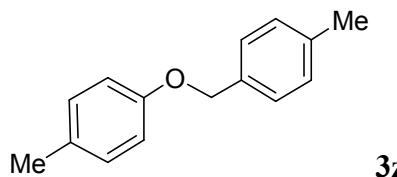
14.1. Anal. Calcd. for C₁₈H₃₀O₂: C, 77.65; H, 10.86. Found: C, 77.39; H, 10.57.



1-(But-2-enyloxy)-4-methoxybenzene.¹² Light yellow oil. ¹H NMR (400 MHz, CDCl₃) δ = 6.86-6.80 (m, 4H), 5.84-5.79 (m, 1H), 5.76-5.71 (m, 1H), 4.39 (d, *J* = 6.0 Hz, 2H), 3.75 (s, 3H), 1.74 (dd, *J* = 6.0, 1.2 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 153.9, 152.9, 130.3, 126.4, 115.7, 114.6, 69.4, 55.7, 17.9.

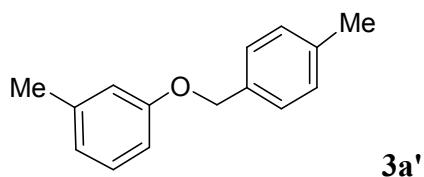


1-(3,7-Dimethyl-octa-2,6-dienyloxy)-4-methoxybenzene.¹⁶ Light yellow oil. ¹H NMR (400 MHz, CDCl₃) δ = 6.78-6.71 (m, 4H), 5.39 (t, *J* = 1.2 Hz, 1H), 5.01 (t, *J* = 1.2 Hz, 1H), 4.39 (d, *J* = 6.8 Hz, 2H), 3.66 (s, 3H), 2.07-1.95 (m, 4H), 1.63 (s, 3H), 1.59 (s, 3H), 1.52 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 153.8, 153.1, 140.8, 131.7, 123.9, 120.0, 115.7, 114.6, 65.5, 55.7, 39.6, 26.4, 25.7, 17.7, 16.6.



3z

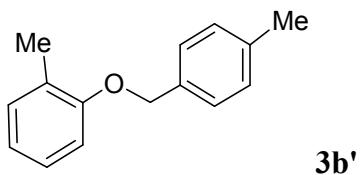
1-(4-Methylbenzyloxy)-4-methylbenzene.¹⁷ White solid, Mp: 71 °C. ¹H NMR (400 MHz, CDCl₃) δ = 7.30 (d, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 7.6 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 4.98 (s, 2H), 2.34 (s, 3H), 2.27 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 156.8, 137.7, 134.3, 130.1, 129.9, 129.3, 127.6, 114.8, 70.1, 21.3, 20.5.



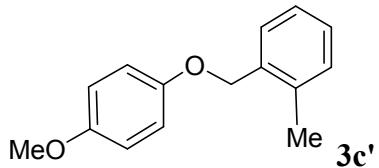
3a'

1-(4-Methylbenzyloxy)-3-methylbenzene. White solid, Mp: 38-39 °C. ¹H NMR (400

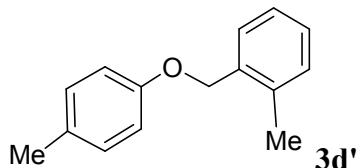
MHz, CDCl₃) δ = 7.20 (d, *J* = 7.6 Hz, 2H), 7.09-7.02 (m, 3H), 6.70-6.64 (m, 3H), 4.87 (s, 2H), 2.24 (s, 3H), 2.21 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 159.1, 139.6, 137.7, 134.3, 129.4, 129.3, 127.7, 121.8, 115.9, 111.8, 69.9, 21.7, 21.3. Anal. Calcd. for C₁₅H₁₆O: C, 84.87; H, 7.60. Found: C, 84.63; H, 7.46.



1-(4-Methylbenzyloxy)-2-methylbenzene.¹⁸ White solid, Mp: 62 °C. ¹H NMR (400 MHz, CDCl₃) δ = 7.24 (d, *J* = 6.8 Hz, 2H), 7.12-7.02 (m, 4H), 6.78 (d, *J* = 7.6 Hz, 2H), 4.93 (s, 2H), 2.27 (s, 3H), 2.19 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 157.1, 137.5, 134.6, 130.8, 129.3, 127.3, 127.2, 126.8, 120.6, 111.5, 69.8, 21.3, 16.5.

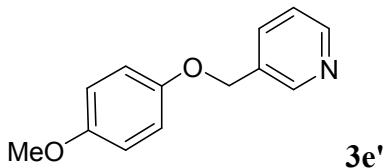


1-(2-Methylbenzyloxy)-4-methoxybenzene. White solid, Mp: 53-54 °C. ¹H NMR (400 MHz, CDCl₃) δ = 7.38 (d, *J* = 7.2 Hz, 1H), 7.25-7.16 (m, 3H), 6.91 (d, *J* = 9.2 Hz, 2H), 6.82 (d, *J* = 9.2 Hz, 2H), 4.95 (s, 2H), 3.73 (s, 3H), 2.35 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 154.1, 153.2, 136.7, 135.2, 130.5, 128.7, 128.3, 126.1, 115.9, 114.8, 69.4, 55.8, 19.0. Anal. Calcd. for C₁₅H₁₆O₂: C, 78.92; H, 7.06. Found: C, 78.64; H, 6.87.

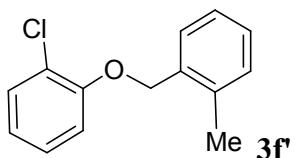


1-(2-Methylbenzyloxy)-4-methylbenzene. White solid, Mp: 42-43 °C. ¹H NMR (400 MHz, CDCl₃) δ = 7.40 (d, *J* = 6.8 Hz, 1H), 7.27-7.20 (m, 3H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 5.00 (s, 2H), 2.37 (s, 3H), 2.29 (s, 3H). ¹³C NMR (100

MHz, CDCl₃) δ = 156.9, 136.7, 135.1, 130.4, 130.2, 129.9, 128.6, 128.2, 126.0, 114.7, 68.7, 20.5, 18.9. Anal. Calcd. for C₁₅H₁₆O: C, 84.87; H, 7.60. Found: C, 84.66; H, 7.43.



3-[(4-methoxyphenoxy)methyl]pyridine. Light yellow solid. Mp: 35 °C. ¹H NMR (400 MHz, CDCl₃) δ = 8.66 (s, 1H), 8.57 (d, *J* = 4.8 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.33-7.28 (m, 1H), 6.90 (d, *J* = 9.2 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 5.02 (s, 2H), 3.76 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 154.3, 152.5, 149.3, 149.0, 135.3, 132.8, 123.5, 115.9, 114.8, 68.3, 55.7. Anal. Calcd. for C₁₃H₁₃NO₂: C, 72.54; H, 6.09; N, 6.51. Found: C, 72.28; H, 6.23; N, 6.31.



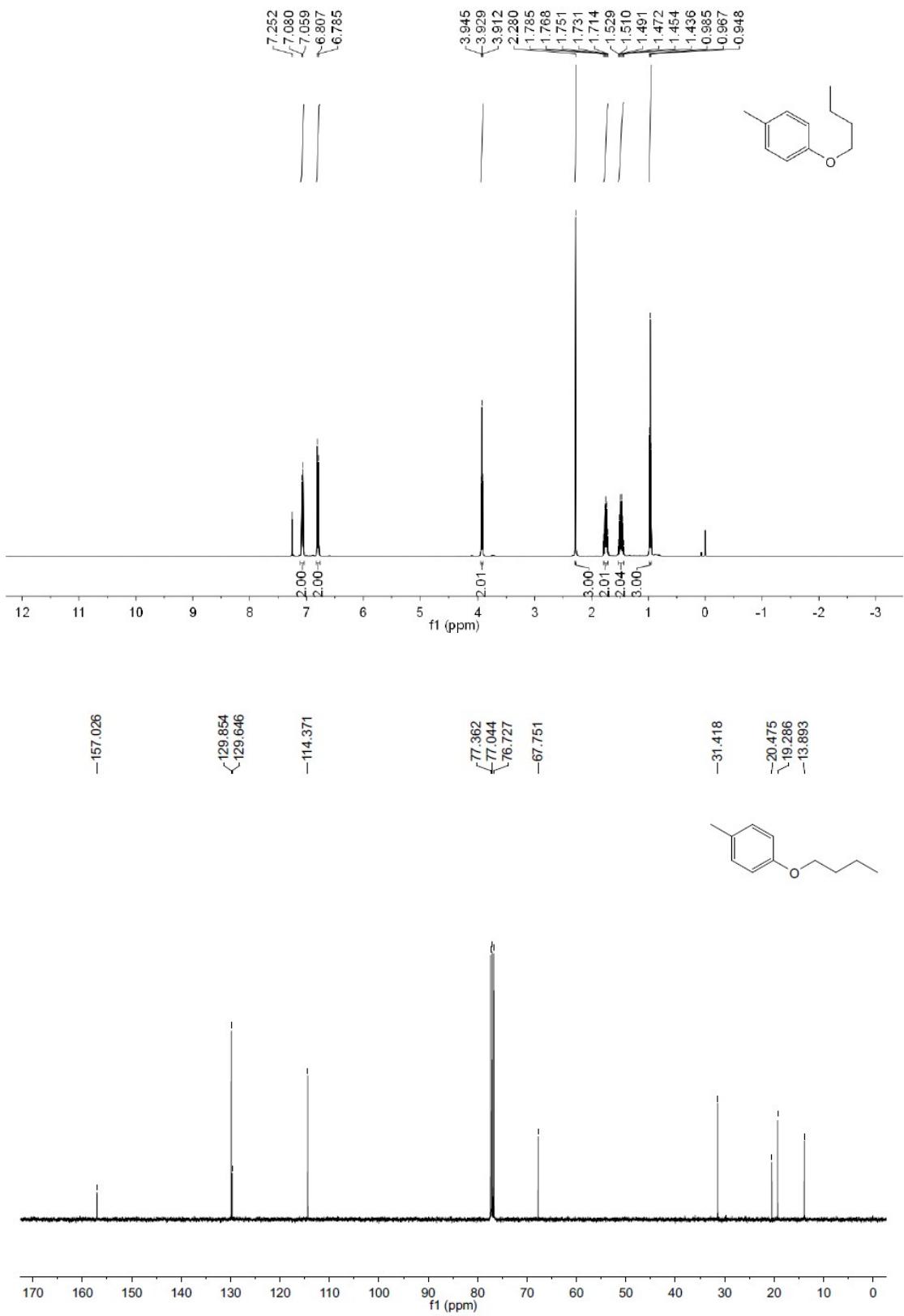
1-(2-Methylbenzyloxy)-2-chlorobenzene. Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ = 7.38 (d, *J* = 6.8 Hz, 1H), 7.29 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.17-7.09 (m, 4H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 1H), 5.02 (s, 2H), 2.31 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ = 154.3, 136.5, 134.4, 130.4, 128.3, 127.7, 126.1, 123.4, 121.7, 114.0, 69.5, 19.0. Anal. Calcd. for C₁₄H₁₃ClO: C, 72.26; H, 5.63. Found: C, 72.38; H, 5.39.

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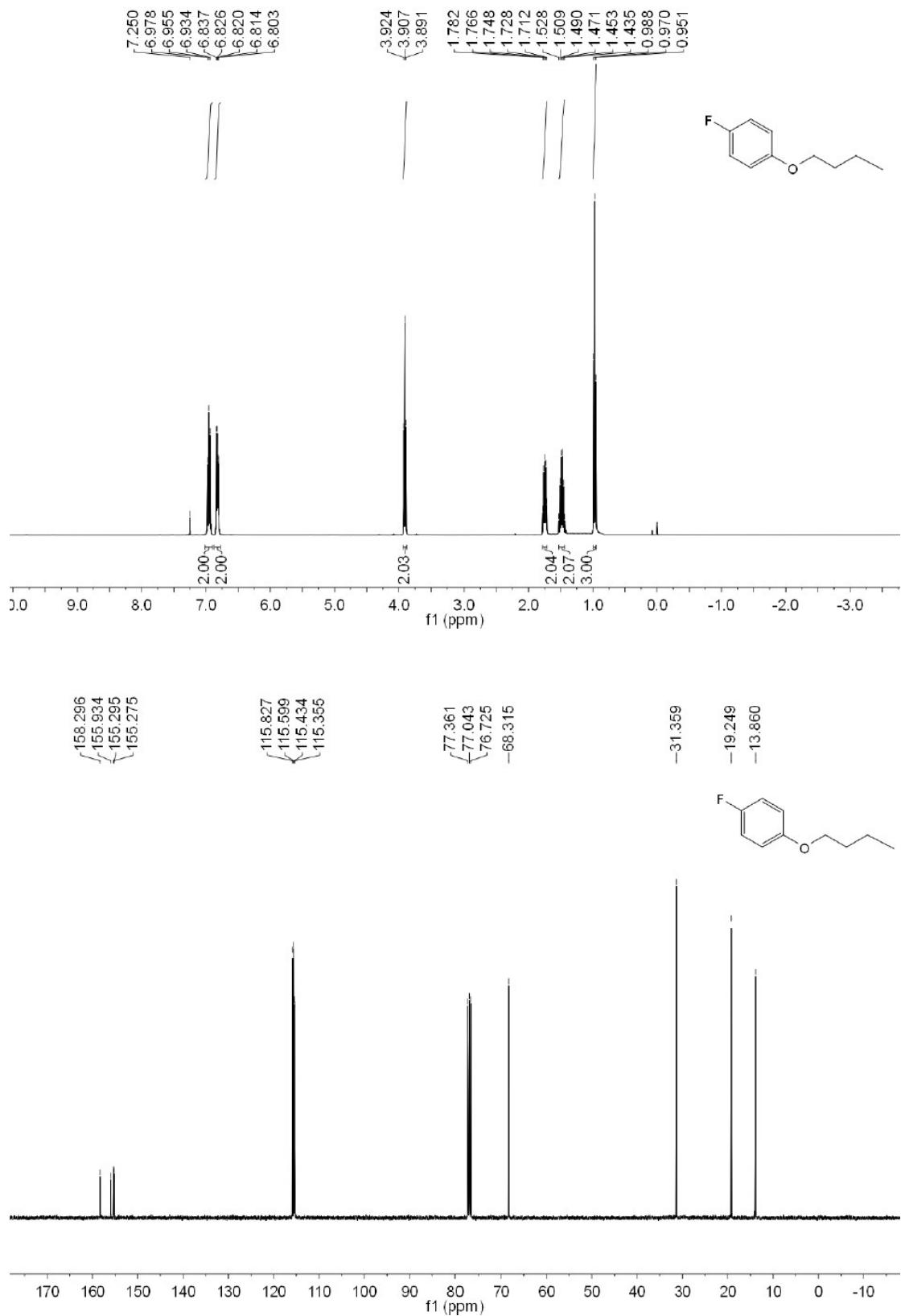
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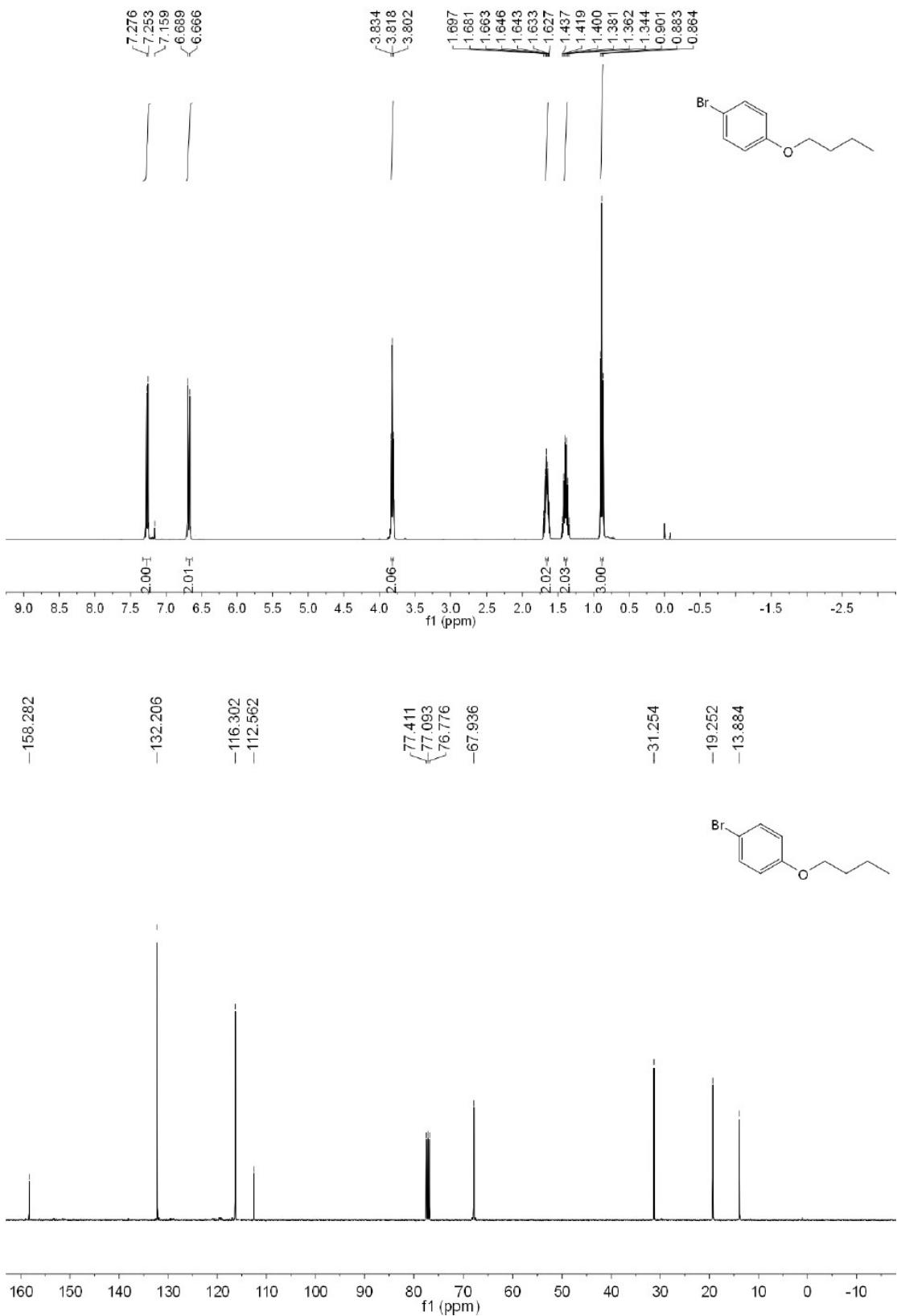
¹H NMR and ¹³C NMR spectra of compounds 3a-3f'



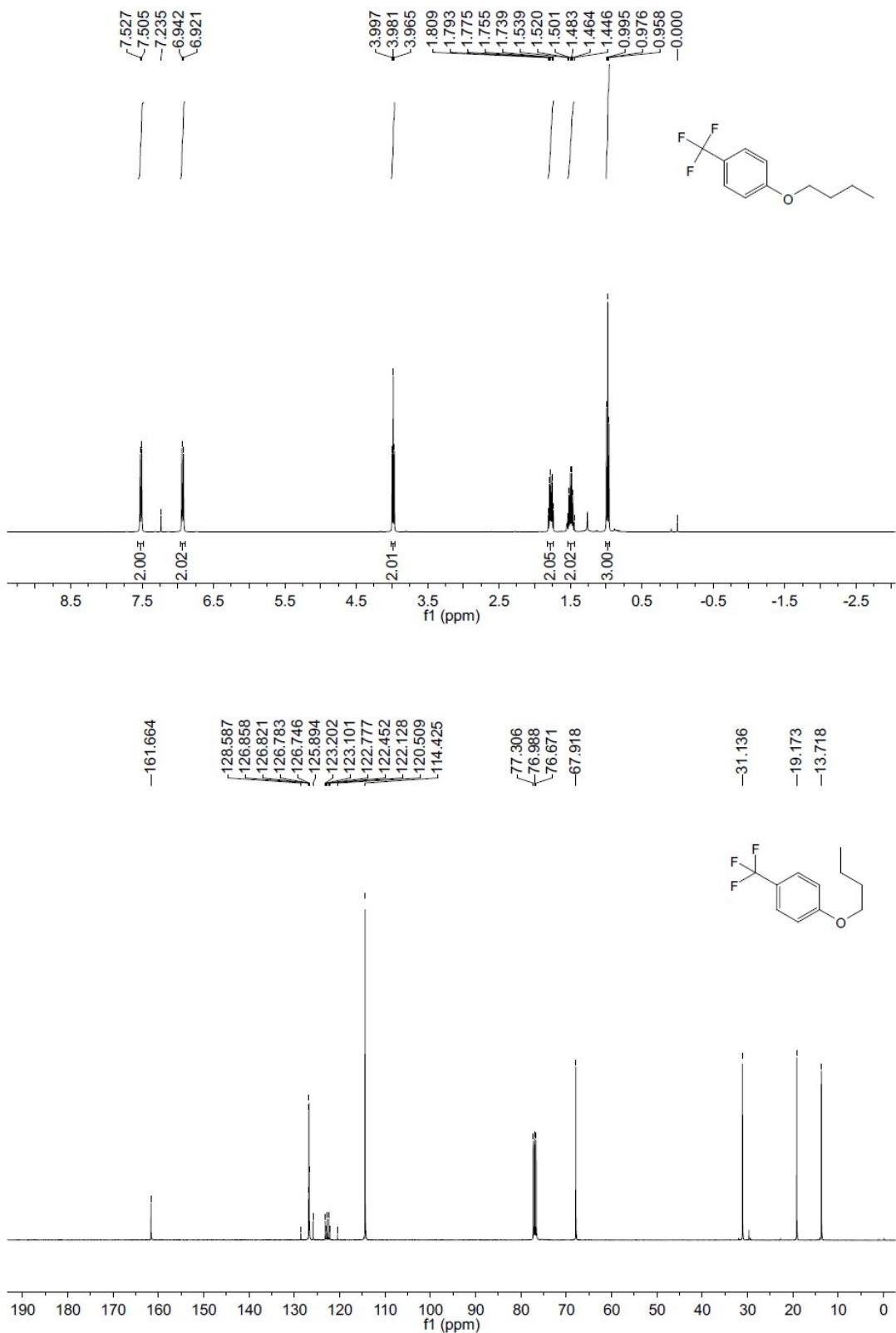
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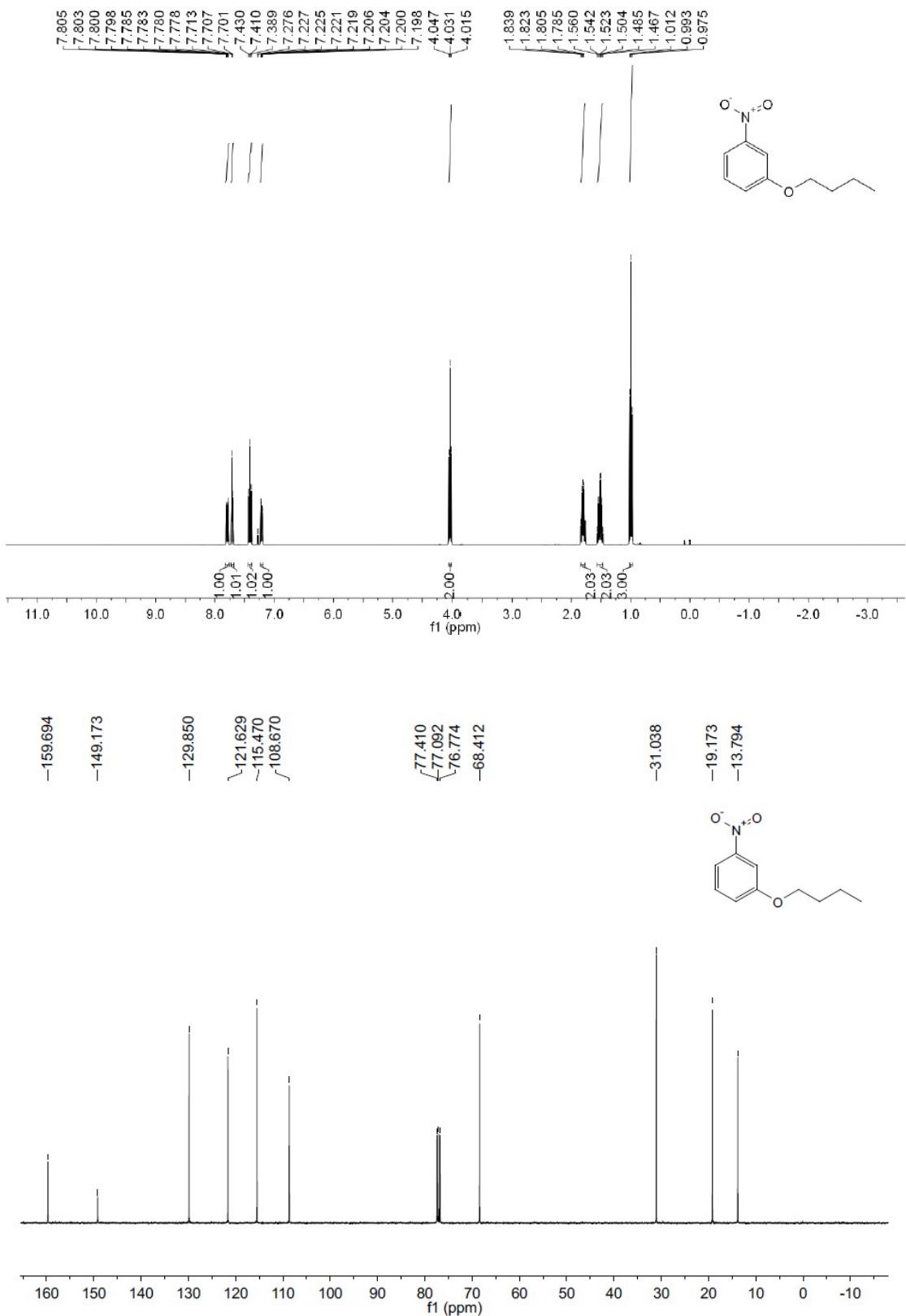
¹H NMR and ¹³C NMR spectra of compound 3b



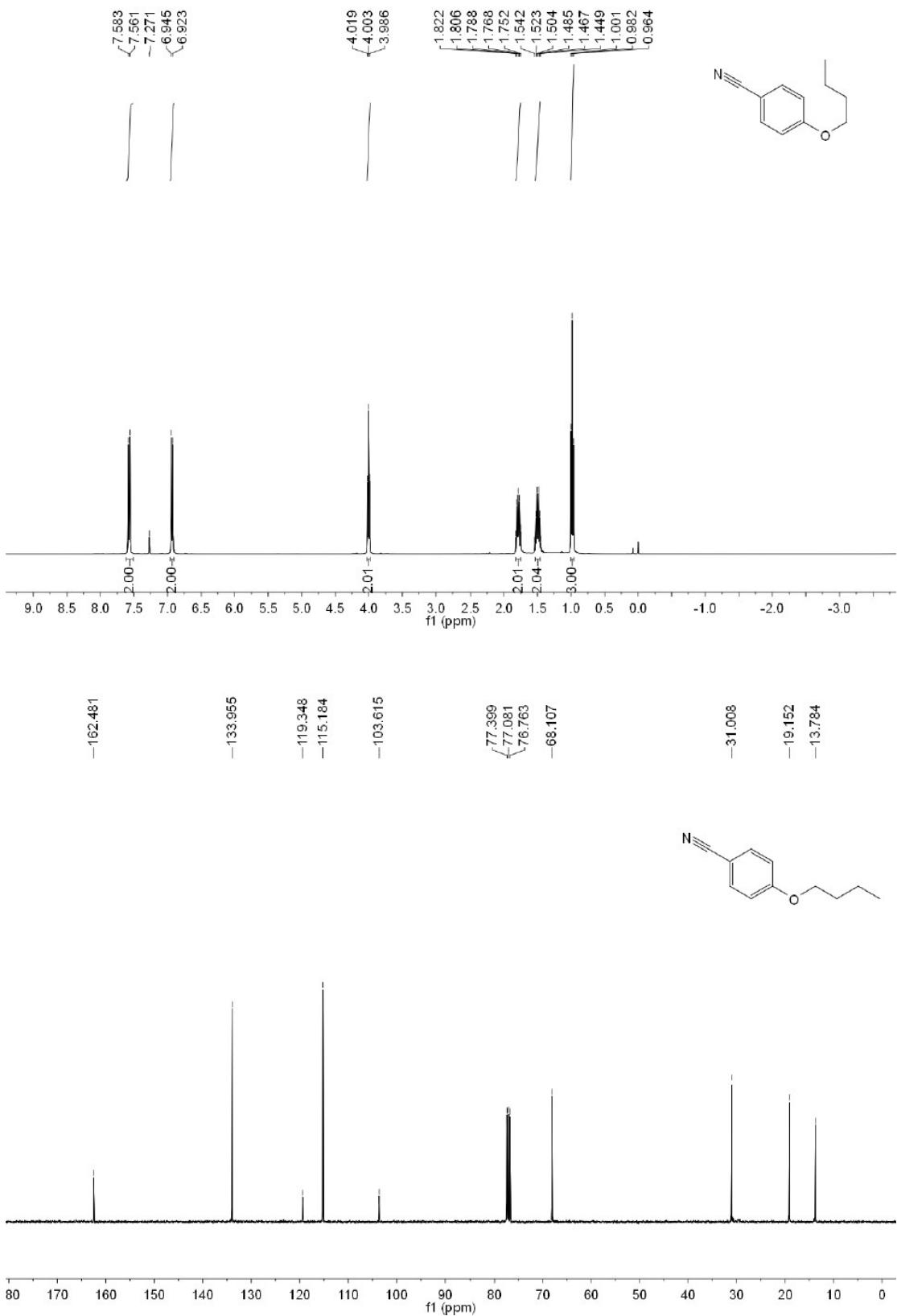
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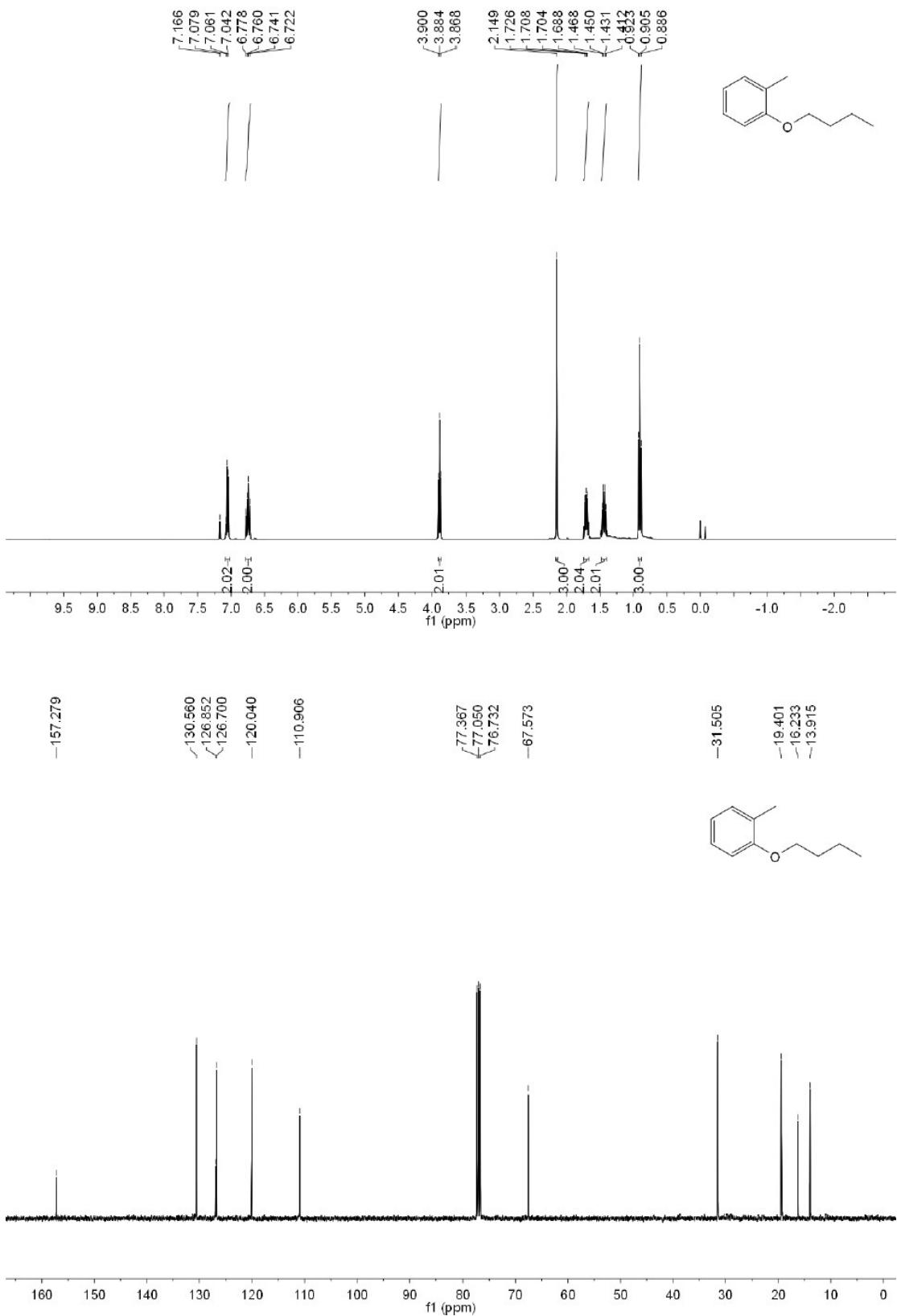
¹H NMR and ¹³C NMR spectra of compound 3d



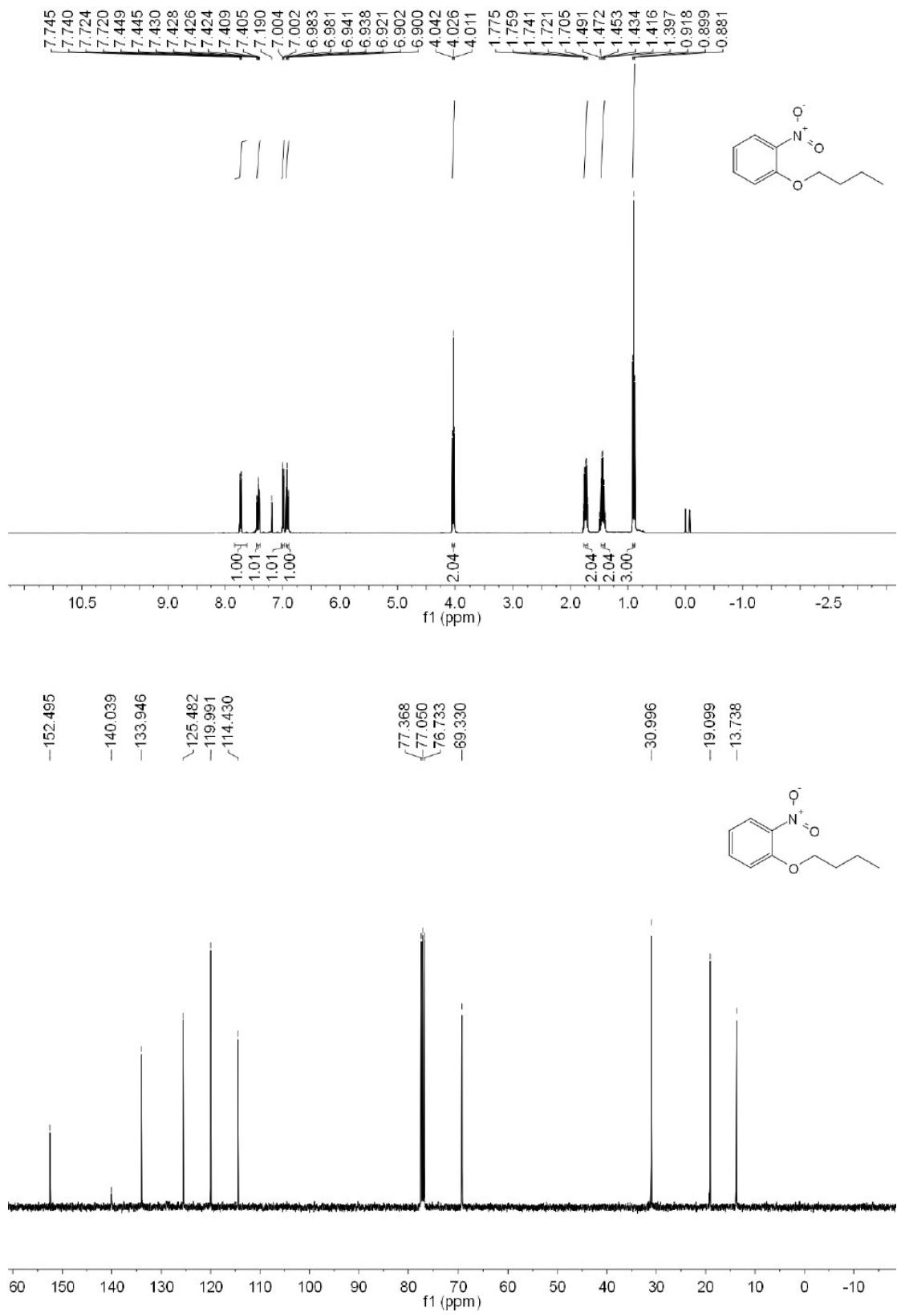
¹H NMR and ¹³C NMR spectra of compound 3e



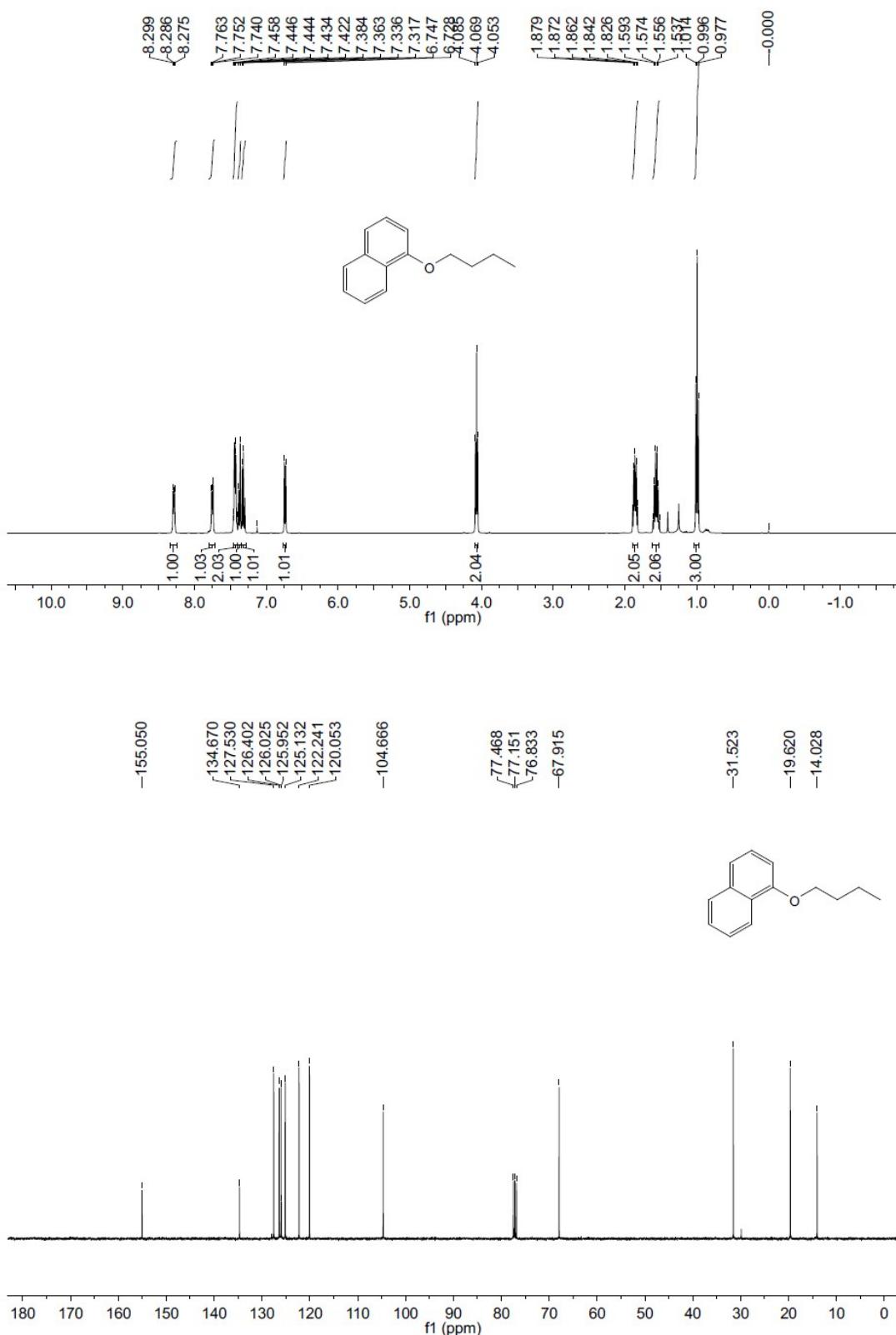
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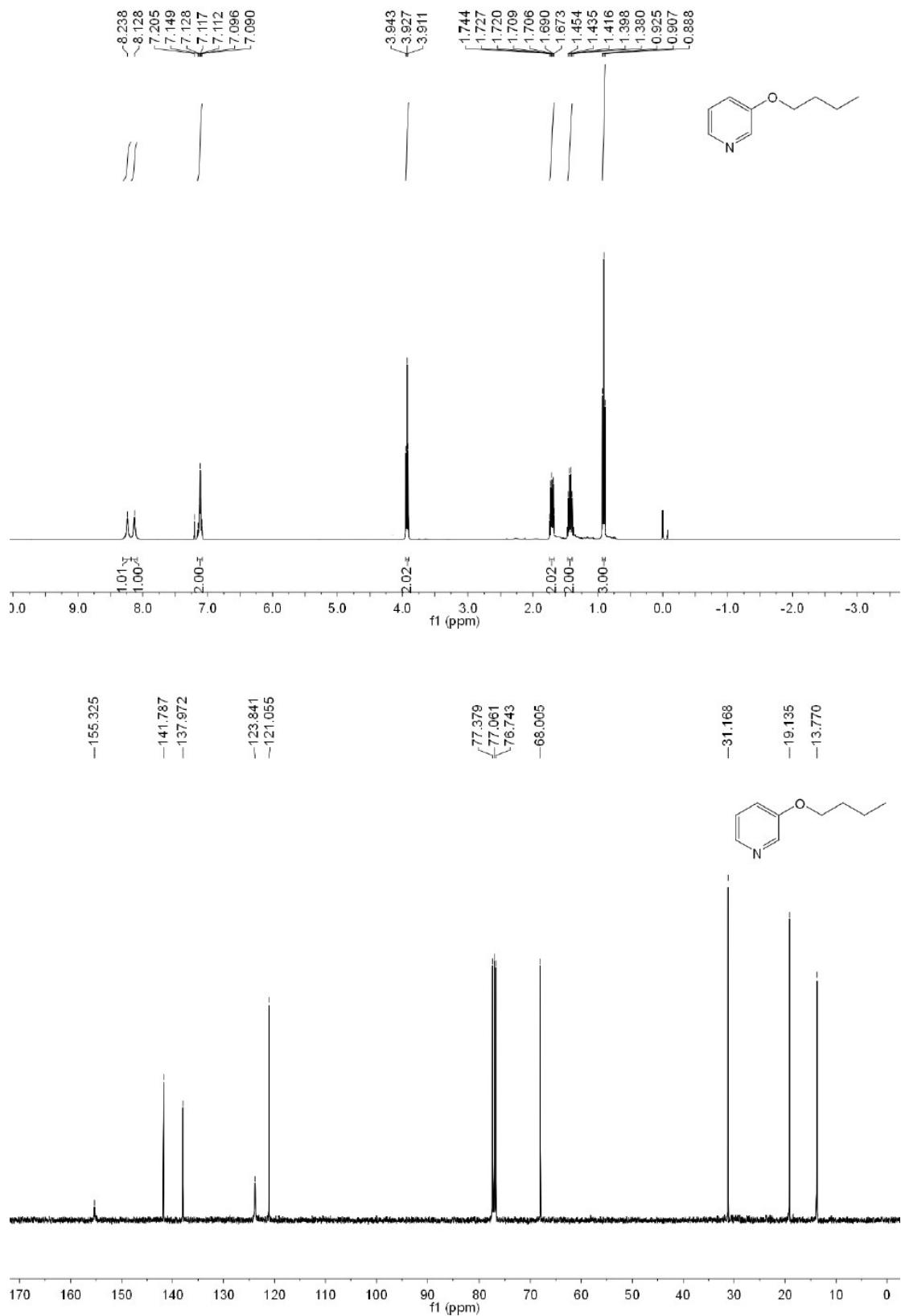
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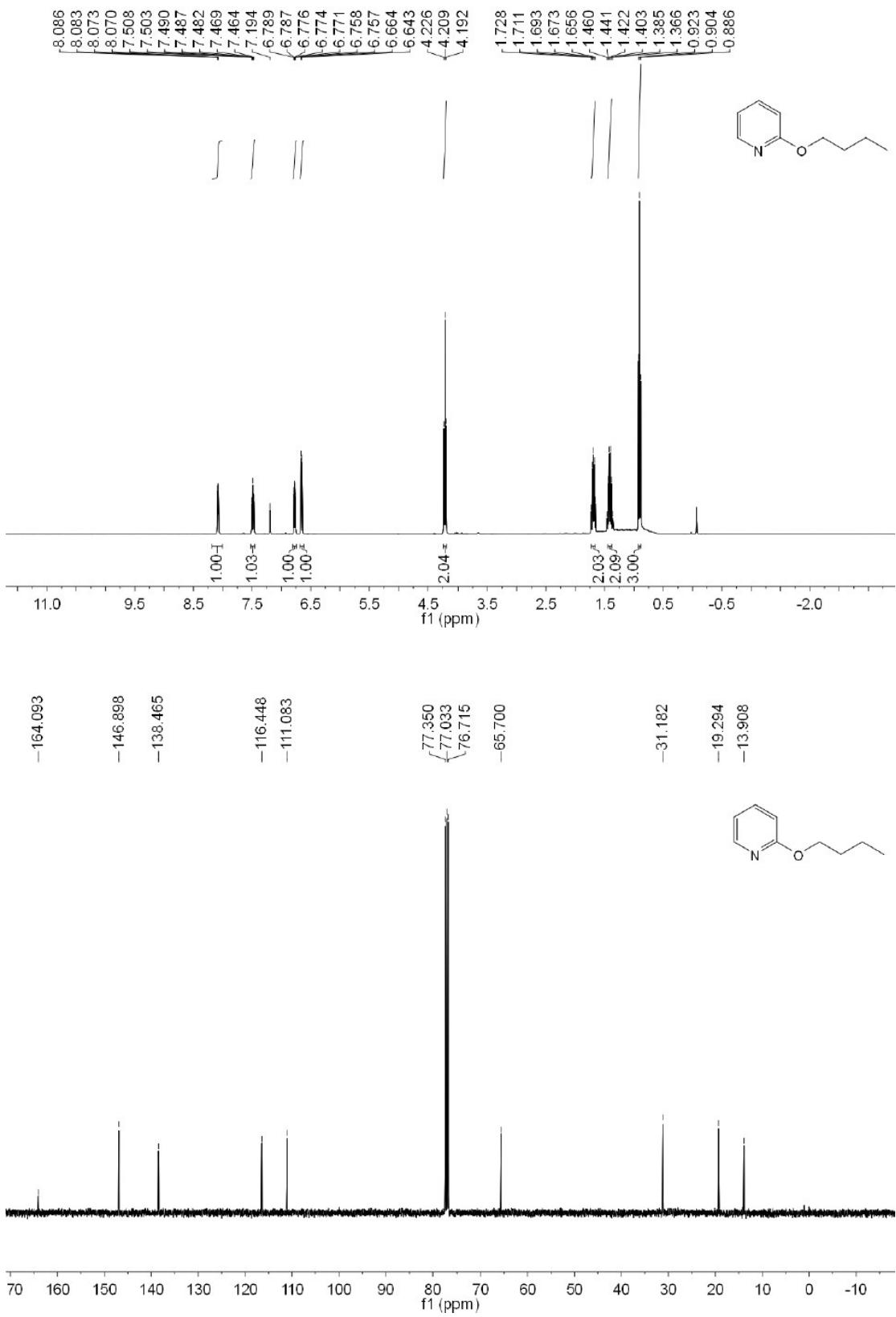
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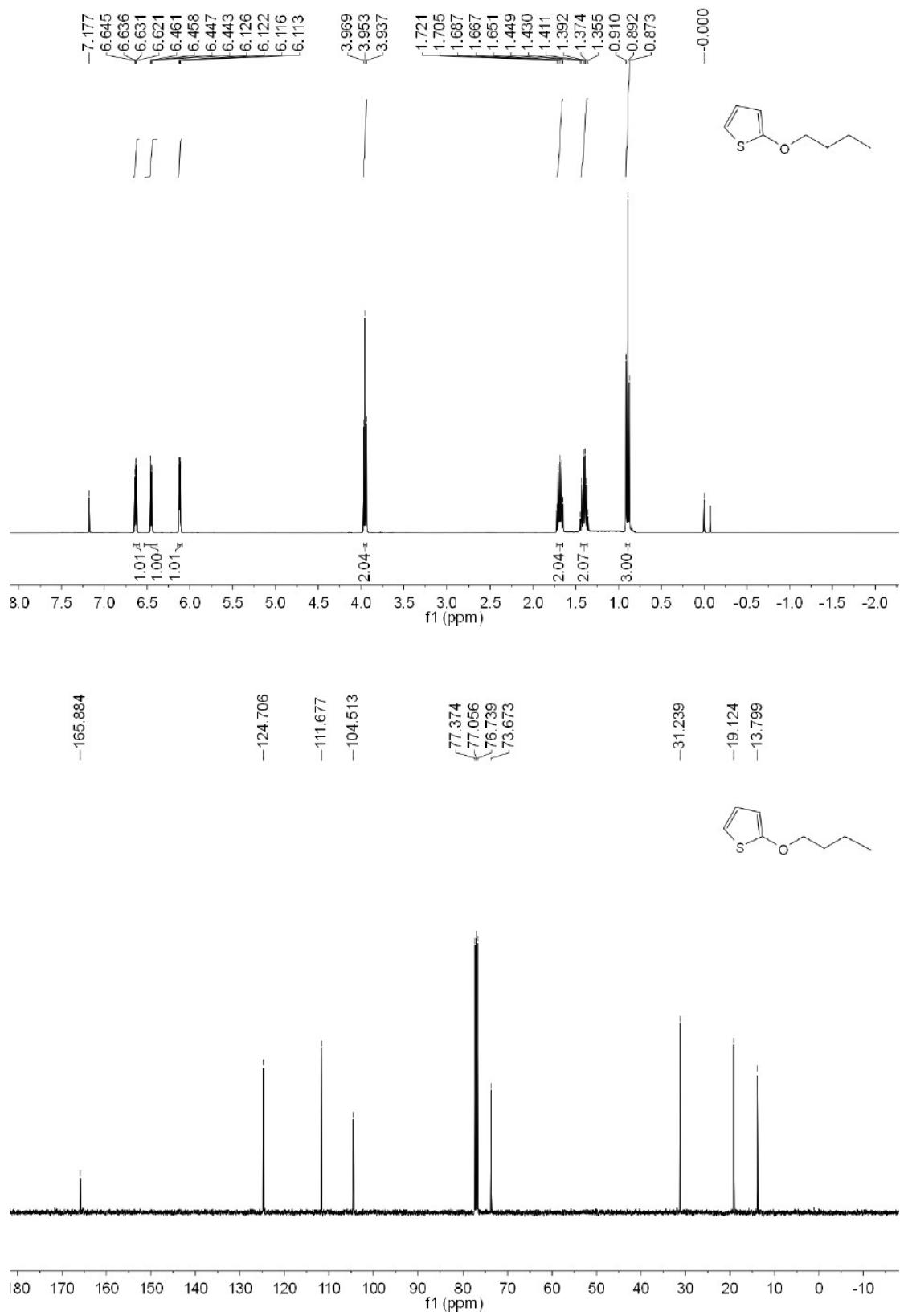
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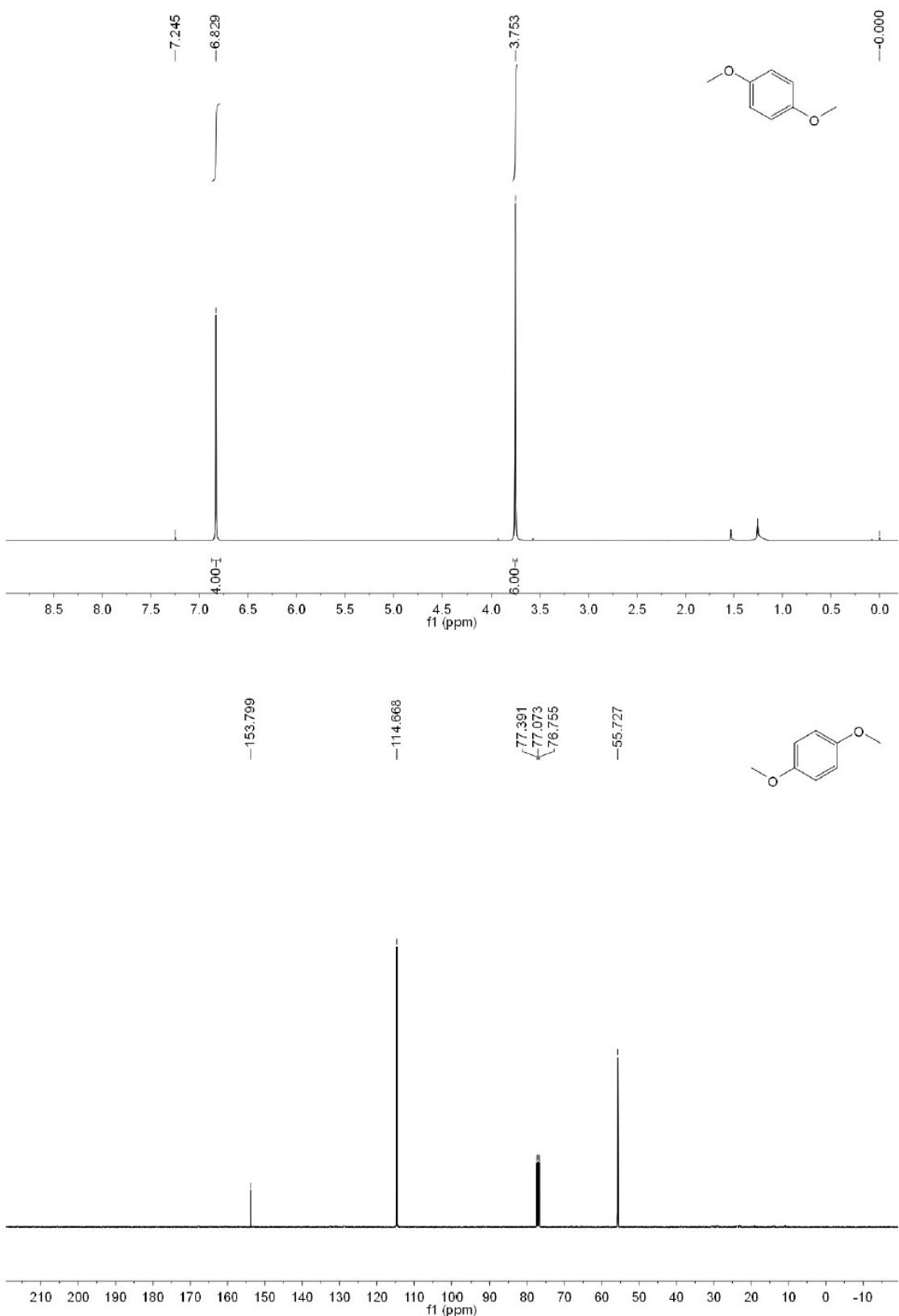
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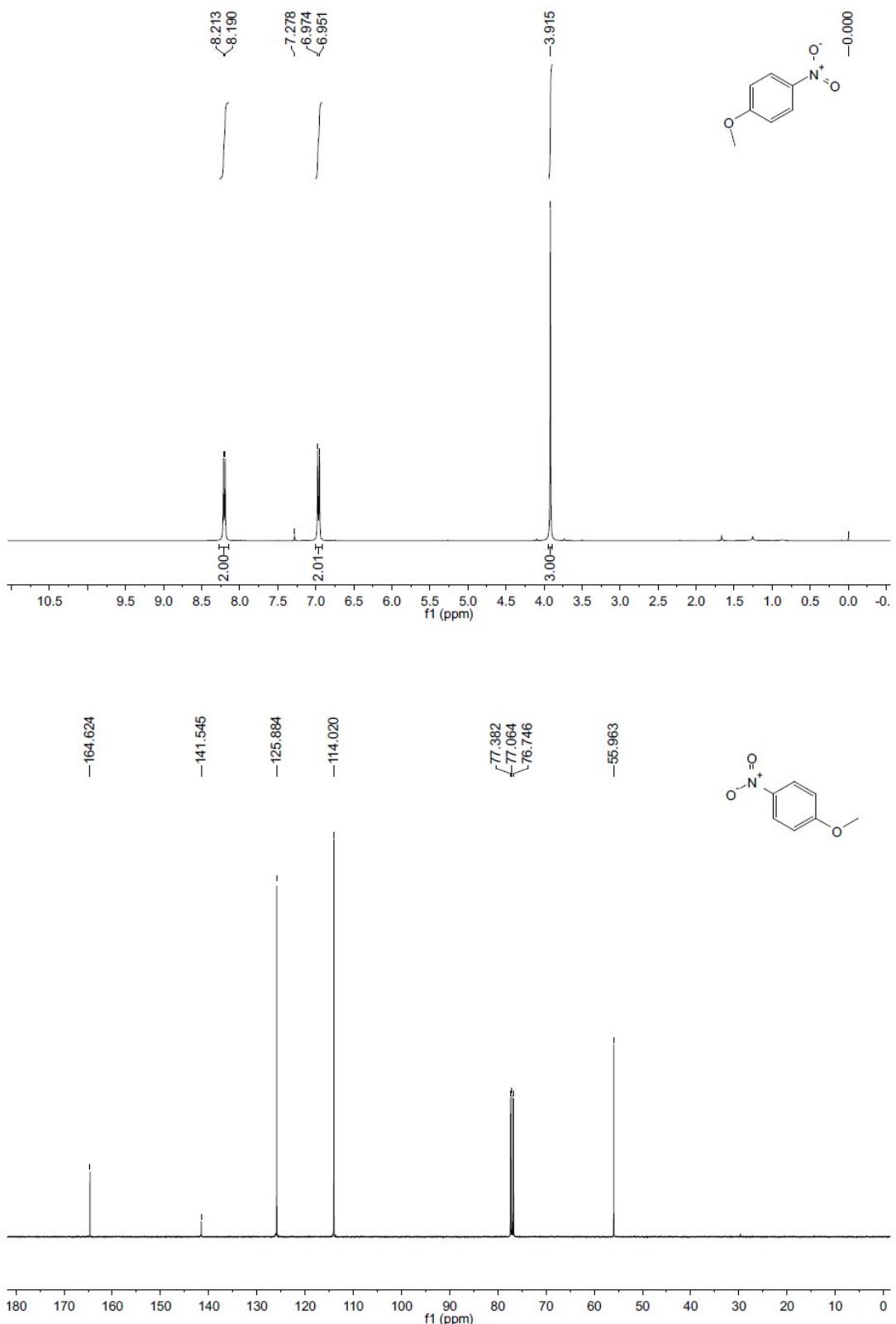
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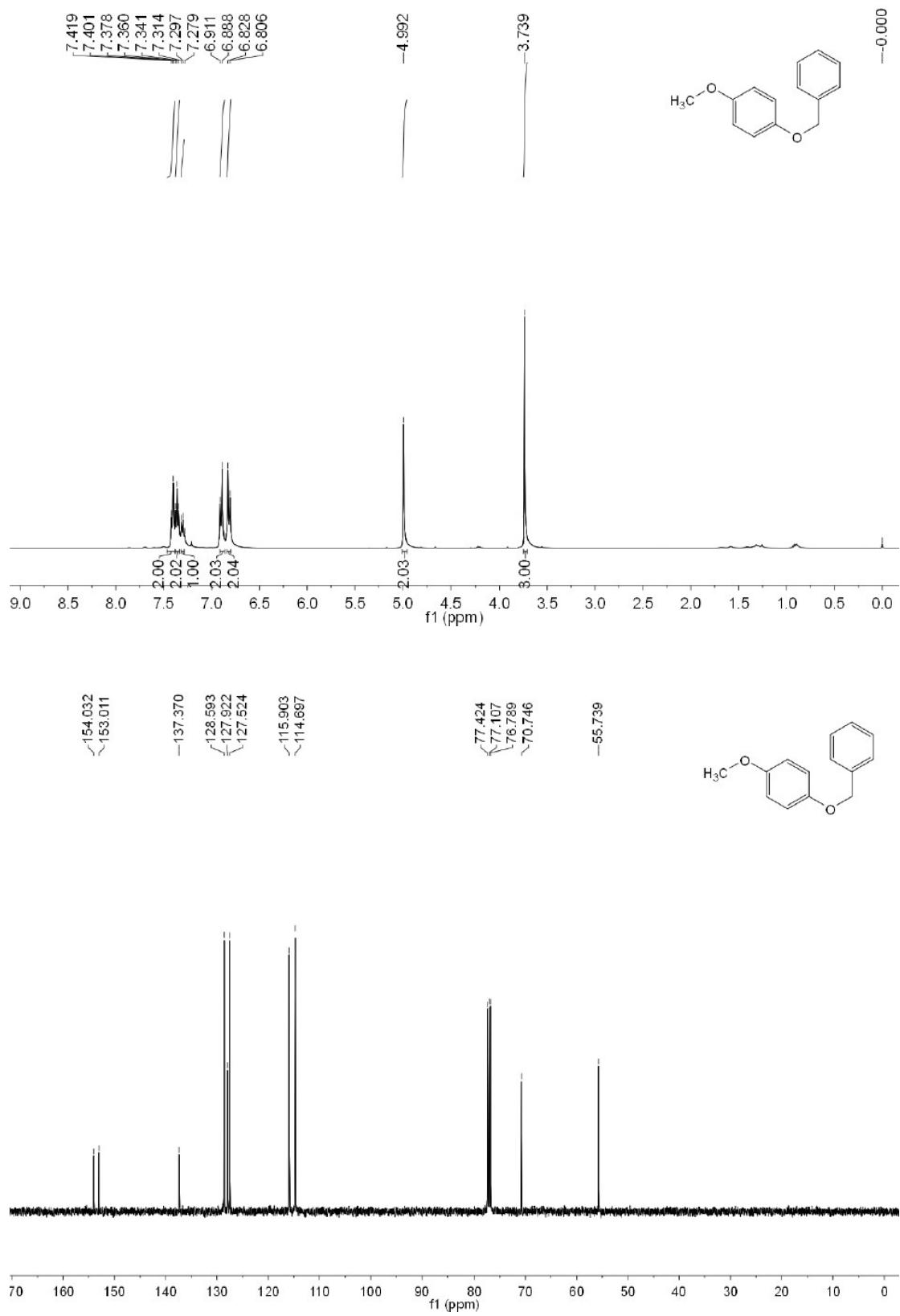
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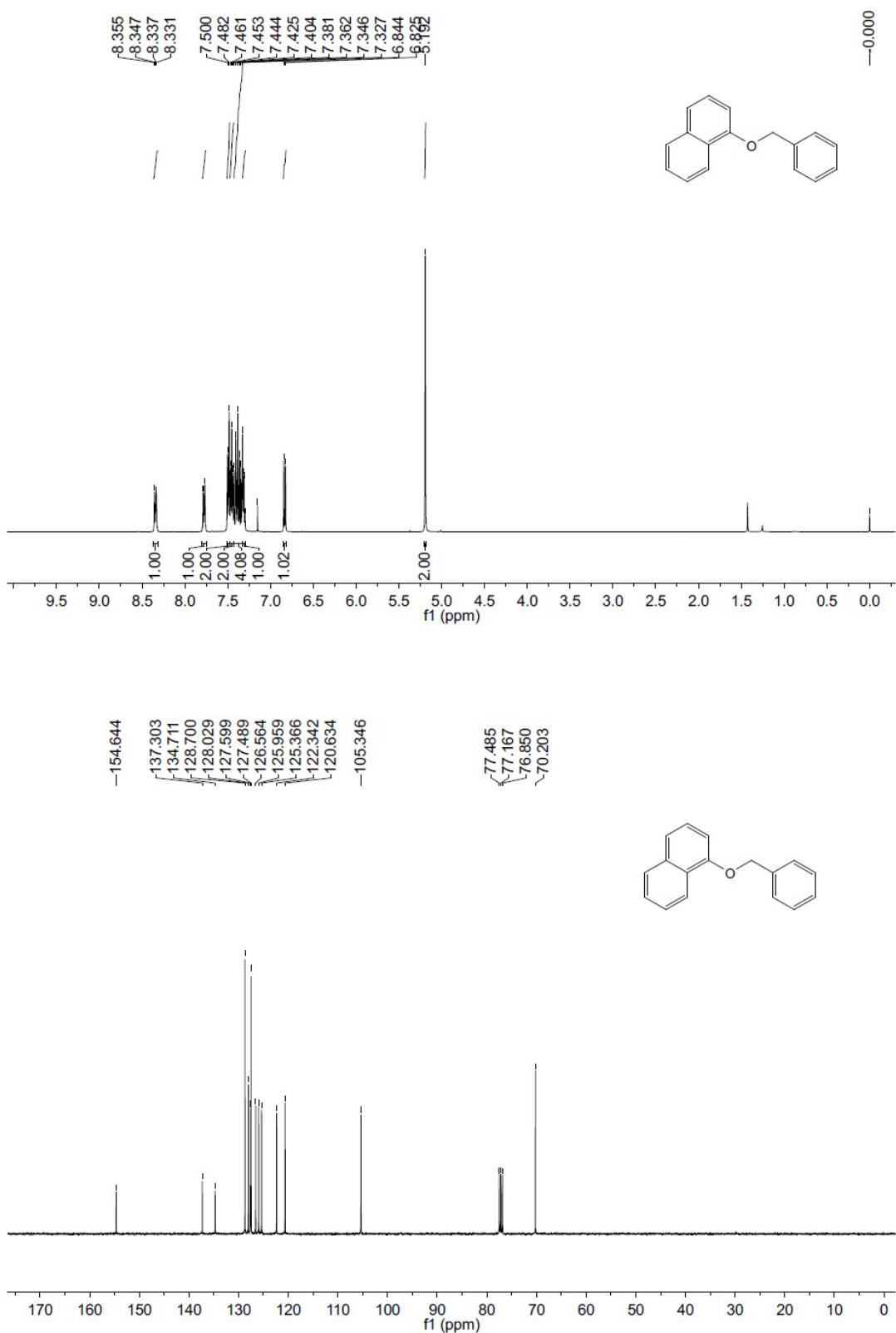
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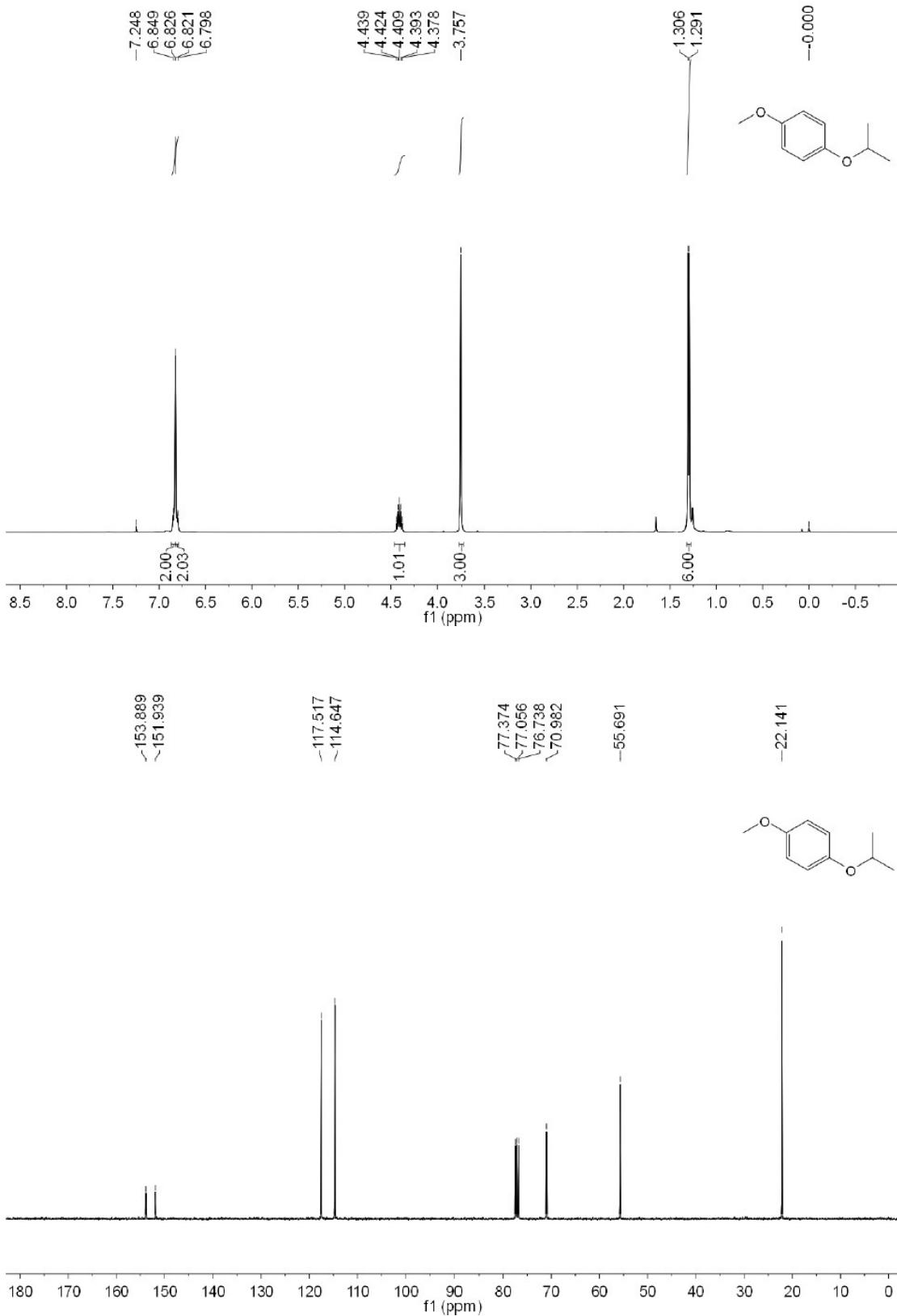
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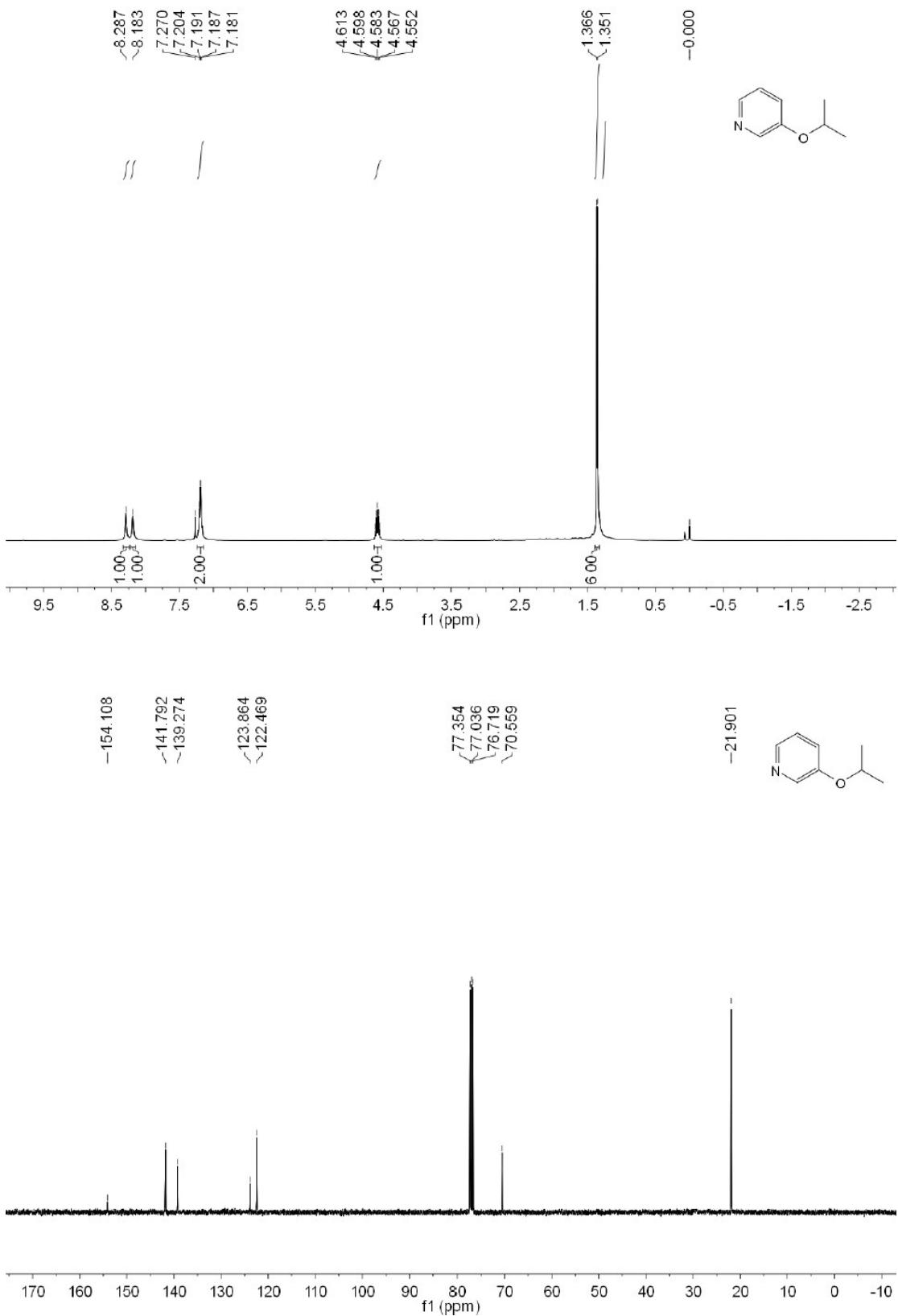
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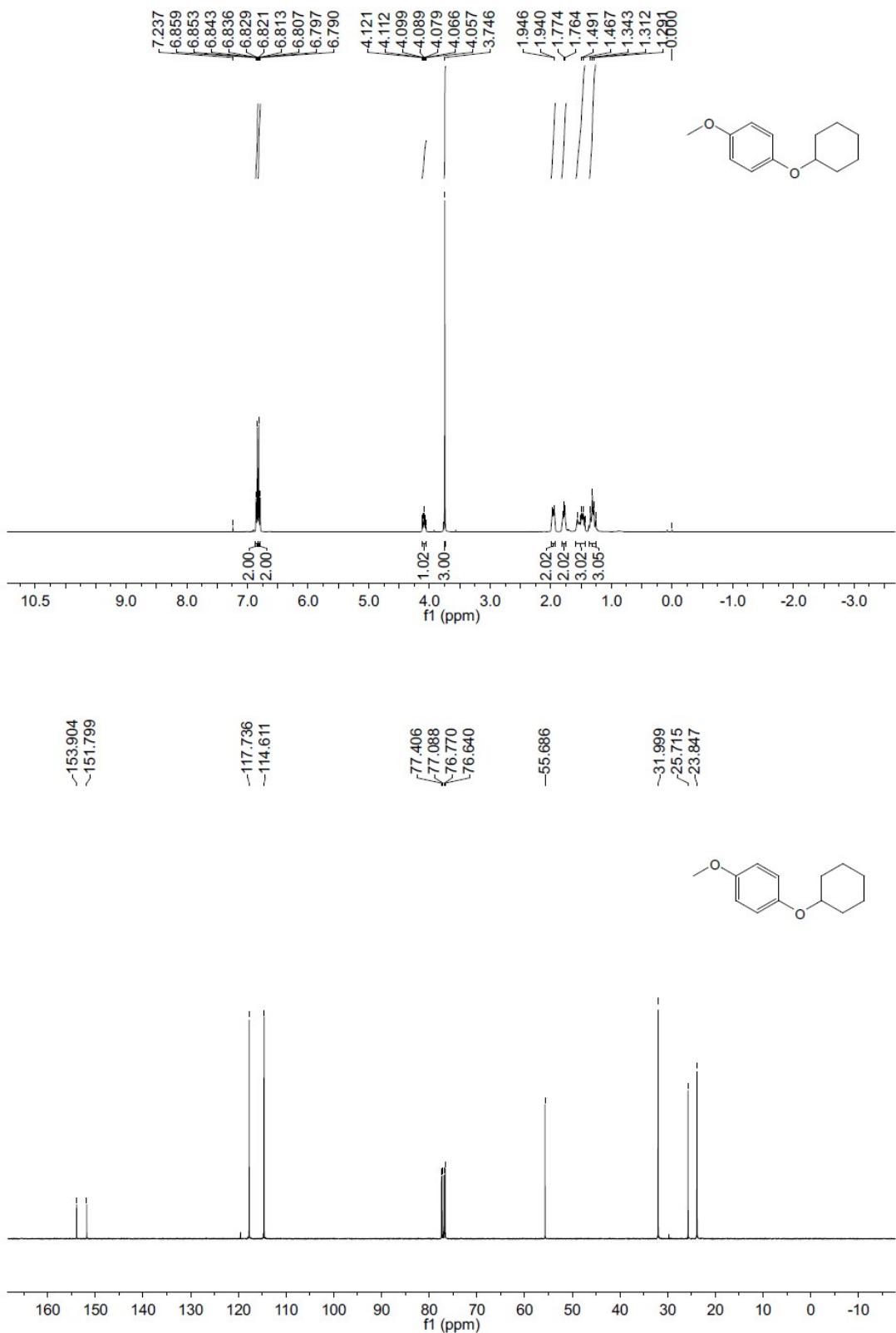
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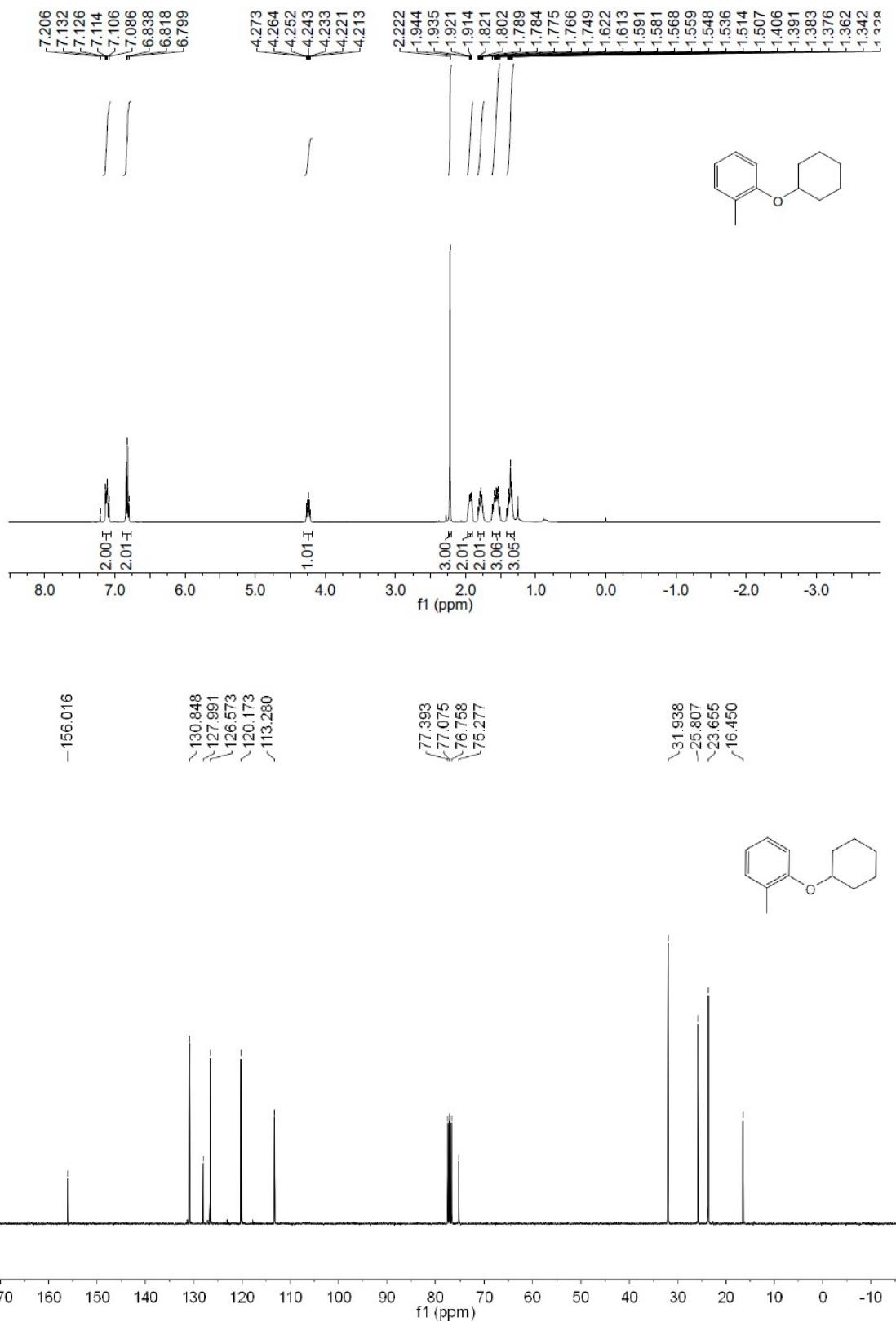
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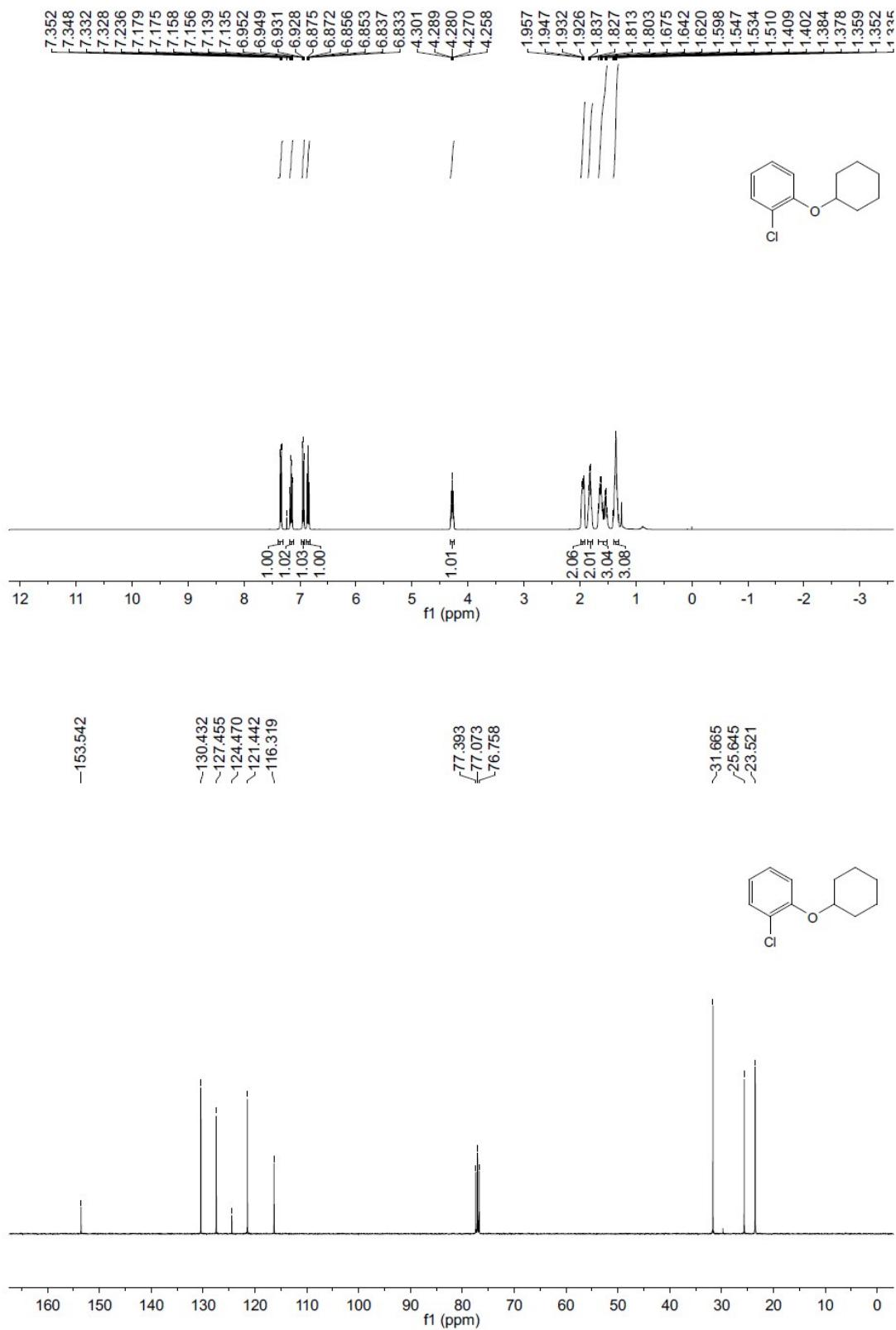
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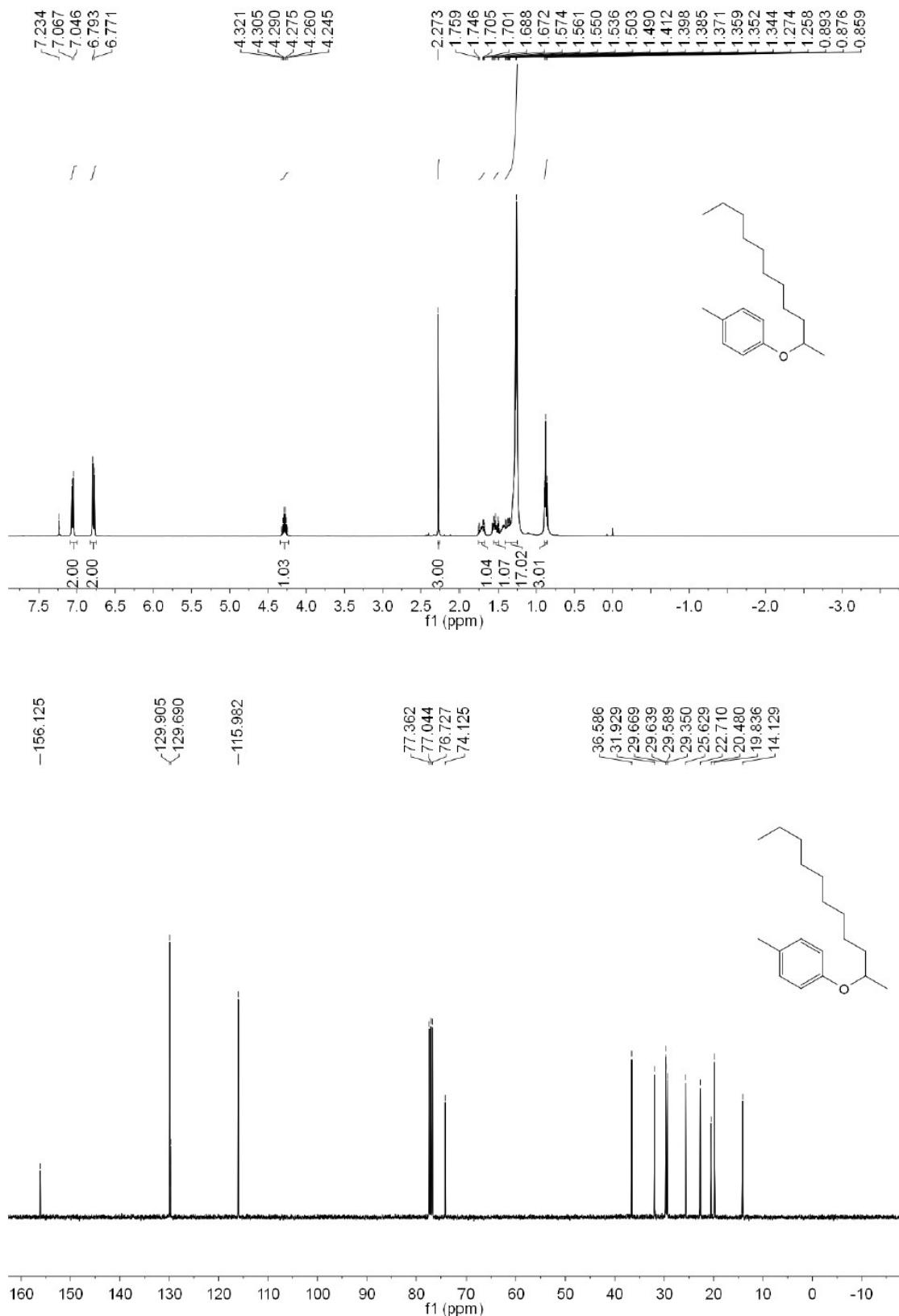
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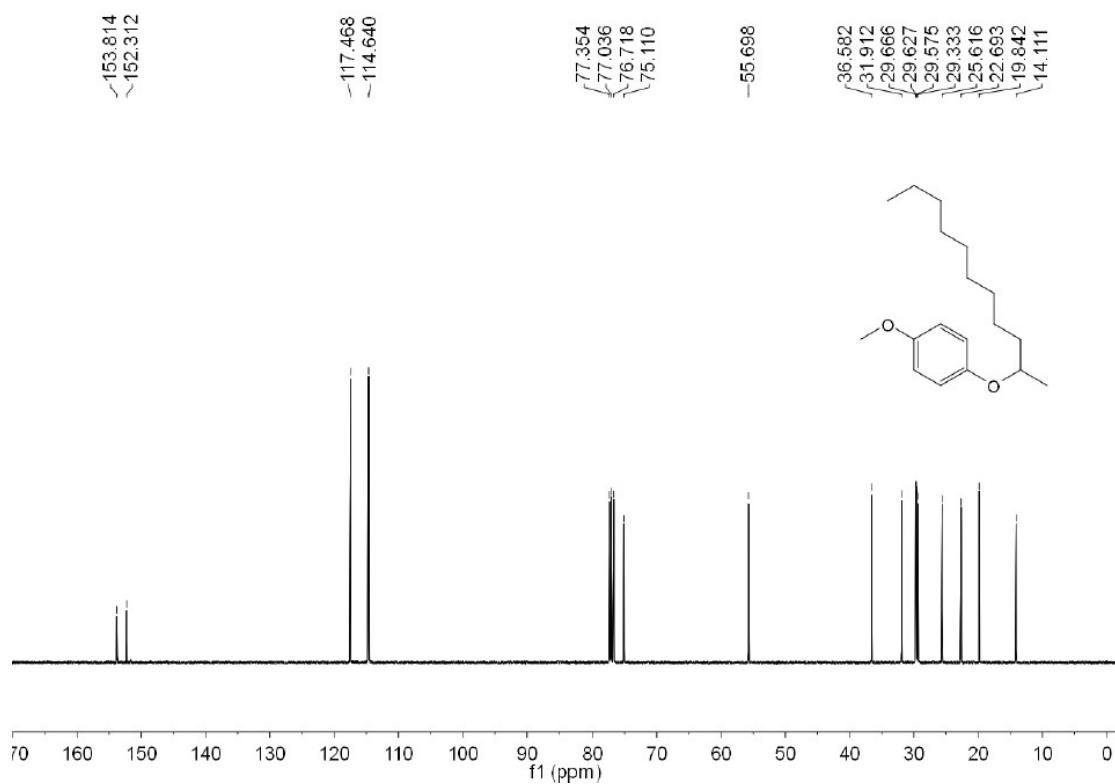
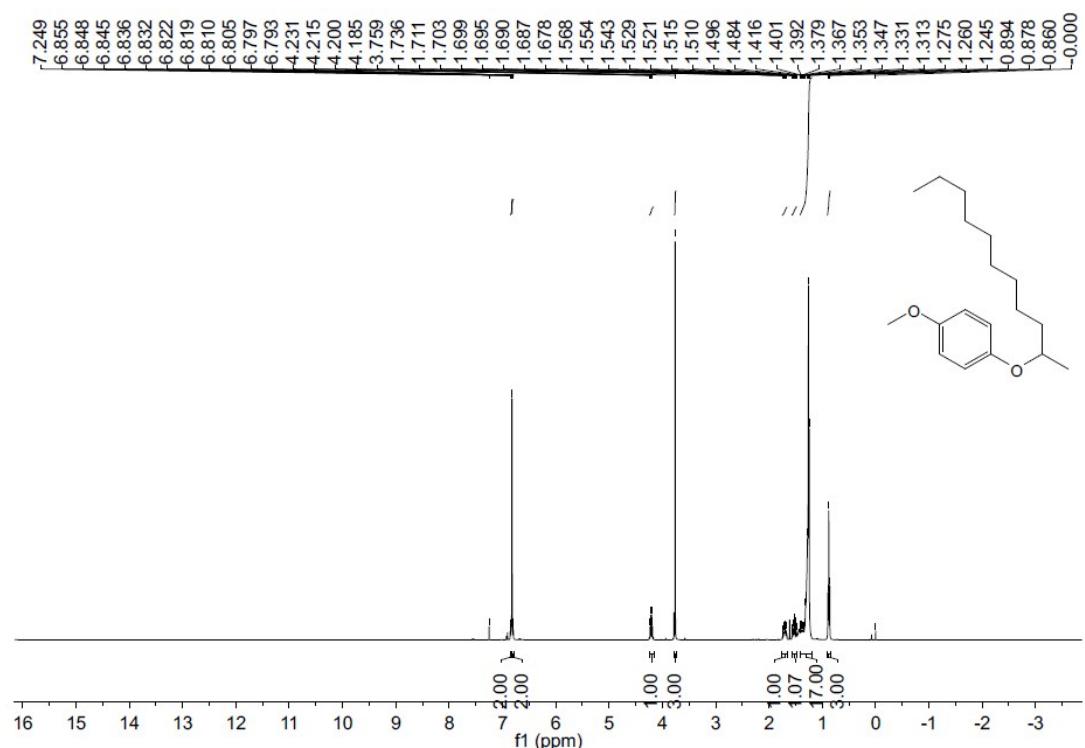
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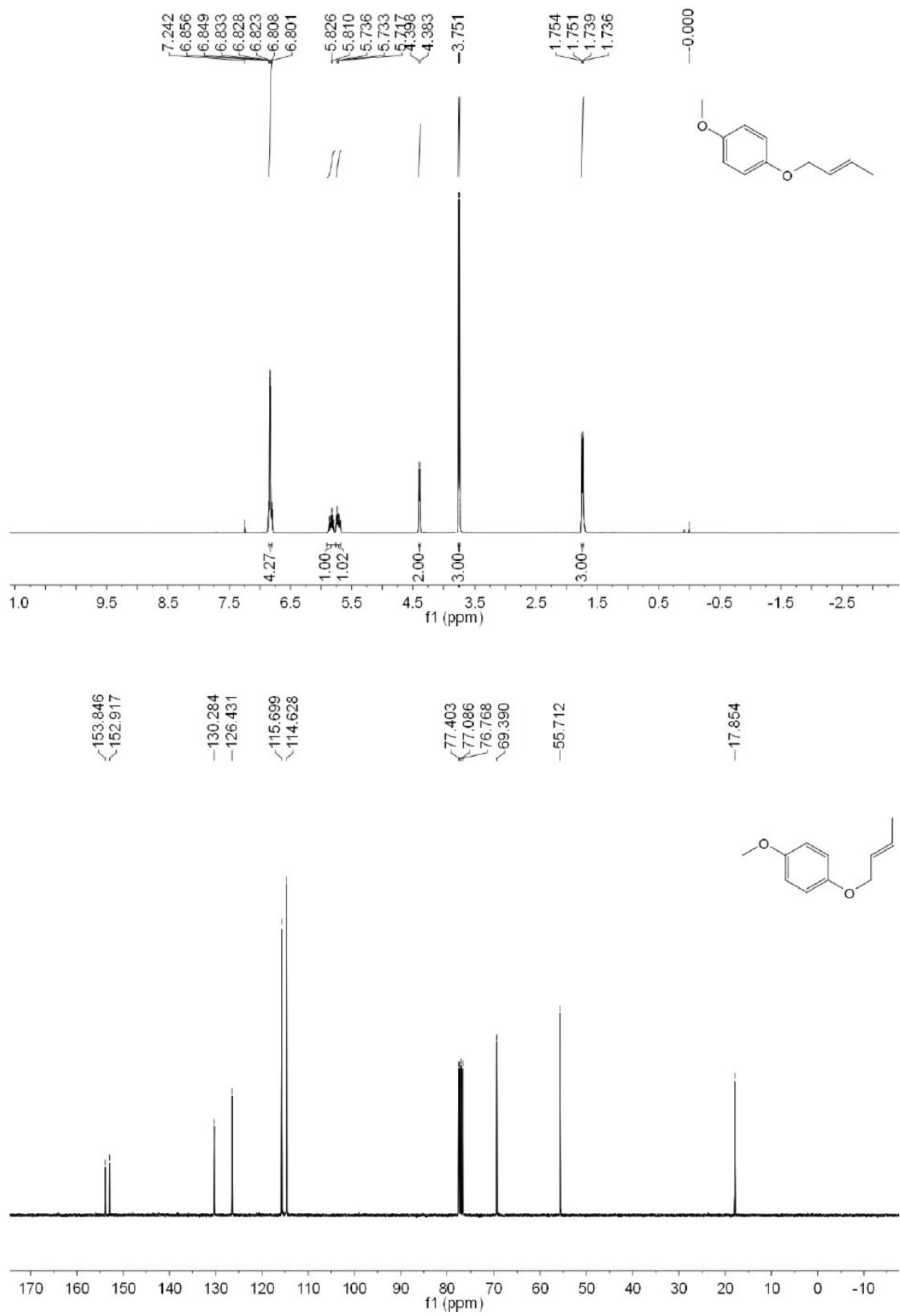
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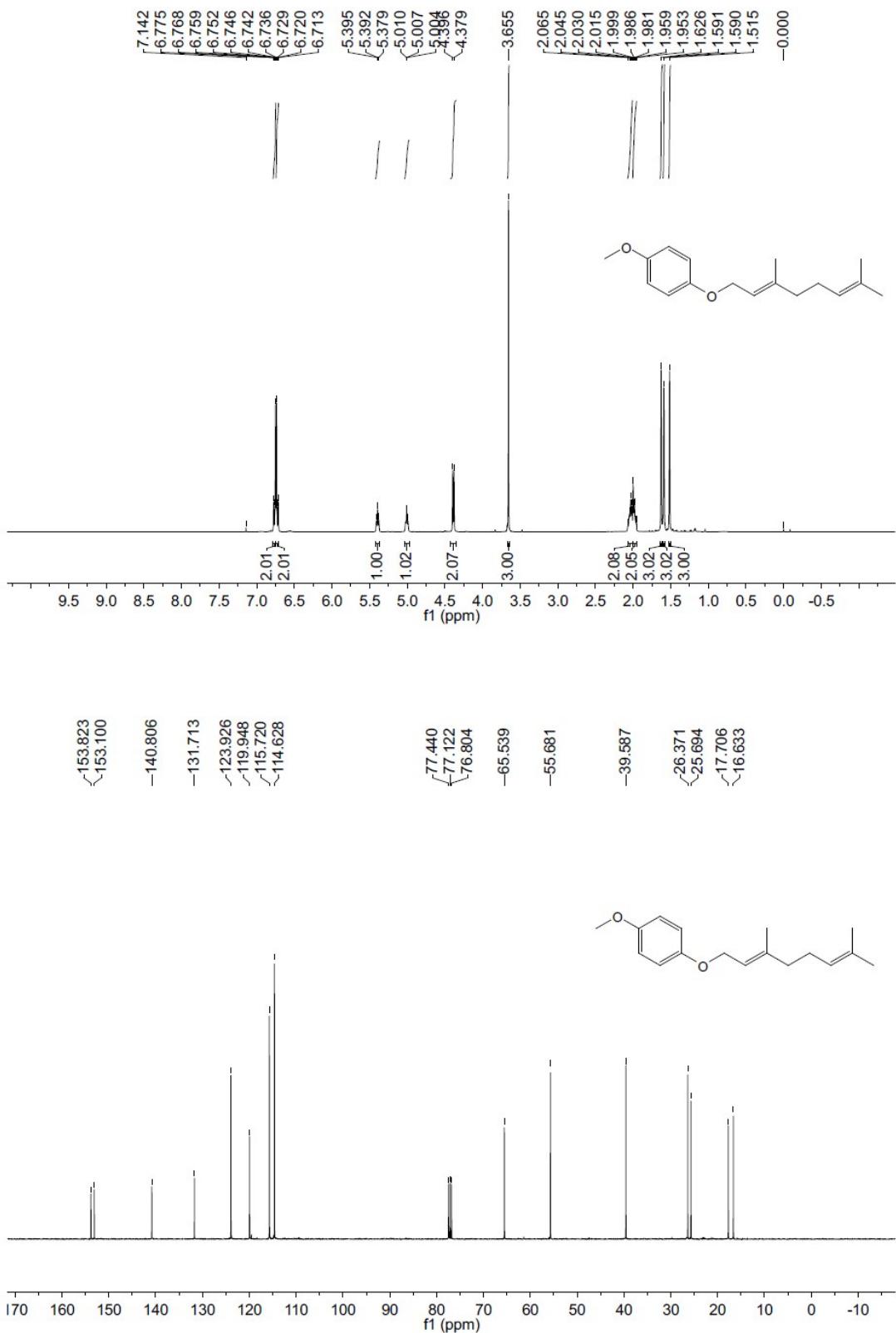
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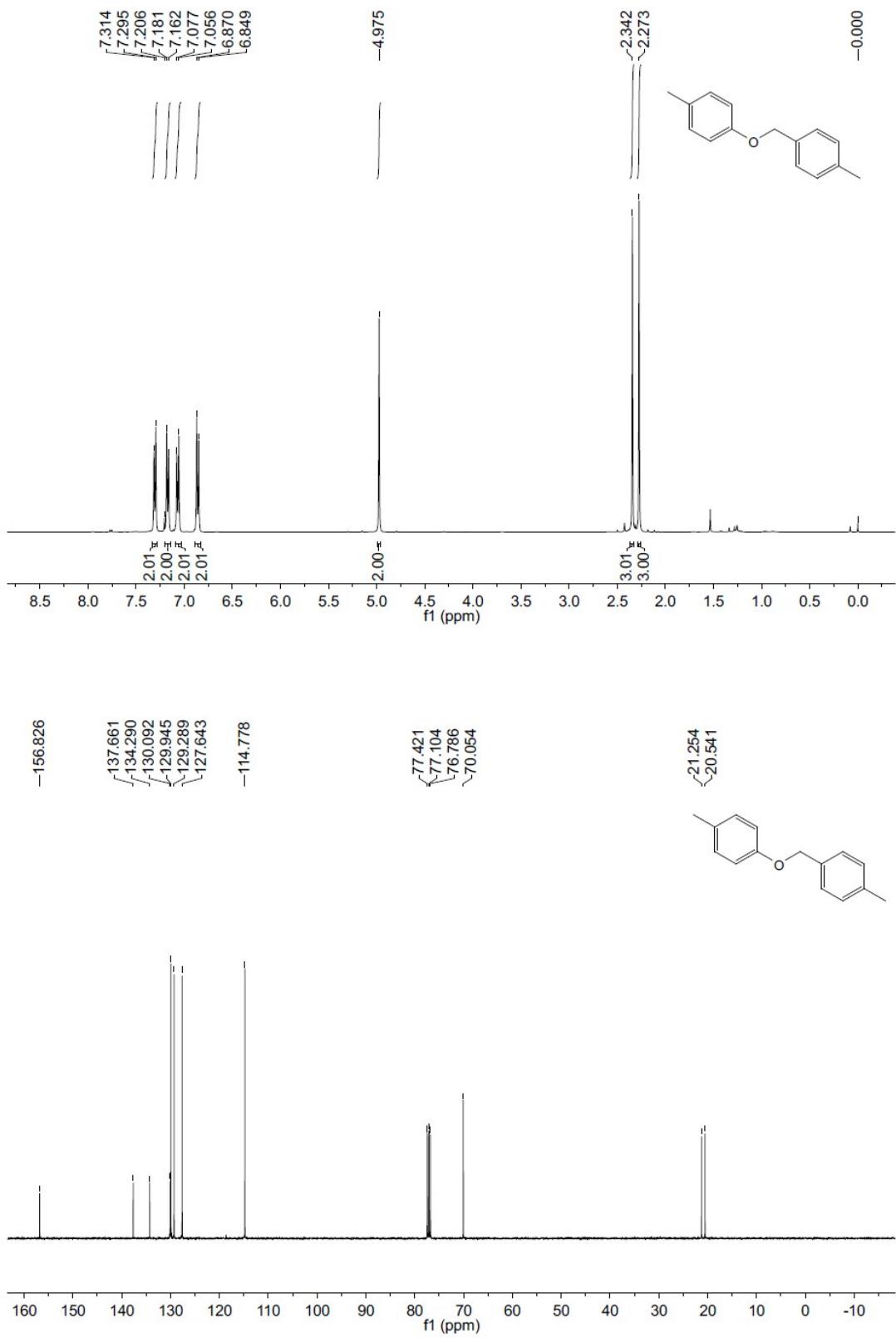
¹H NMR and ¹³C NMR spectra of compound 3w



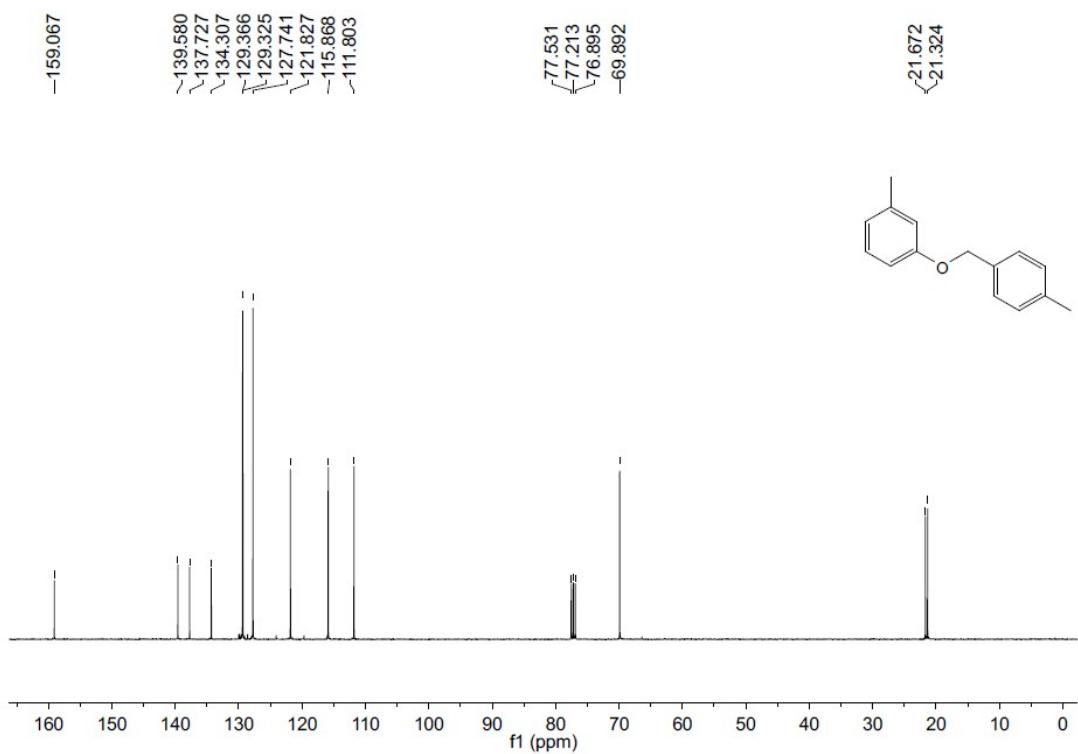
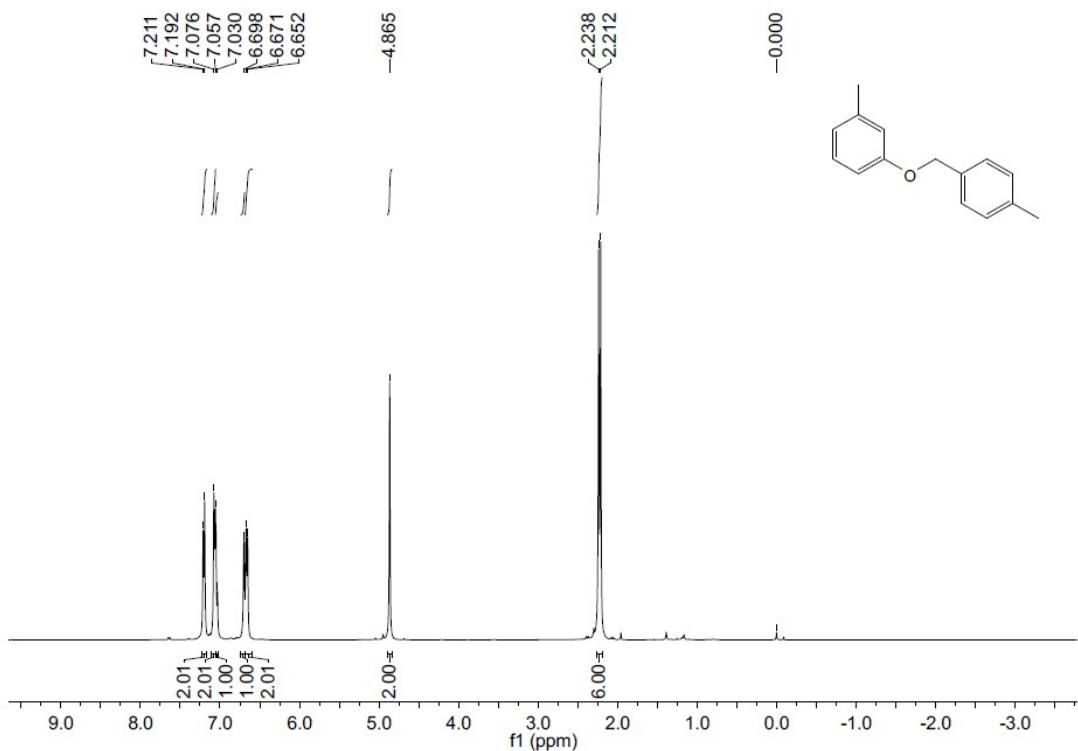
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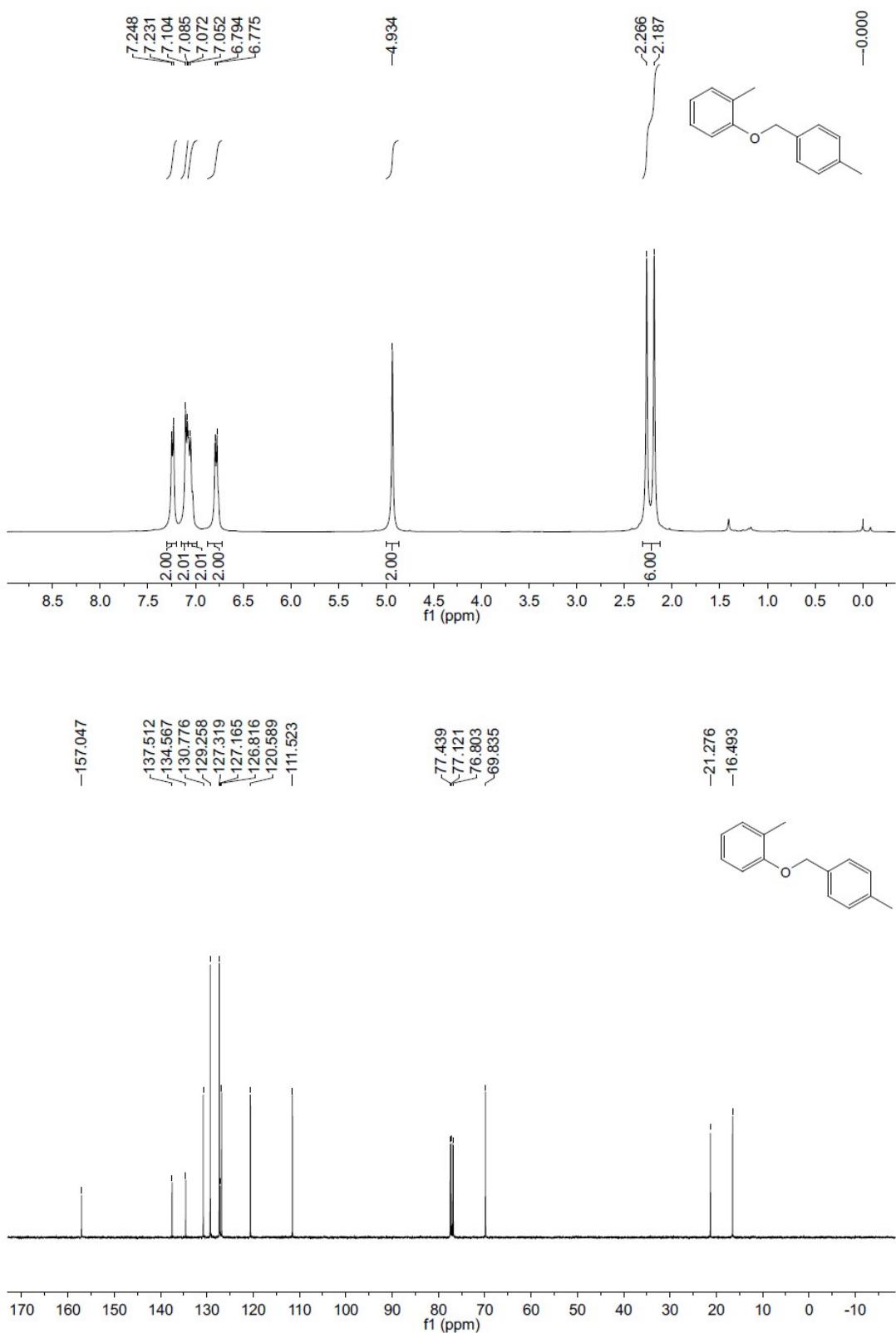
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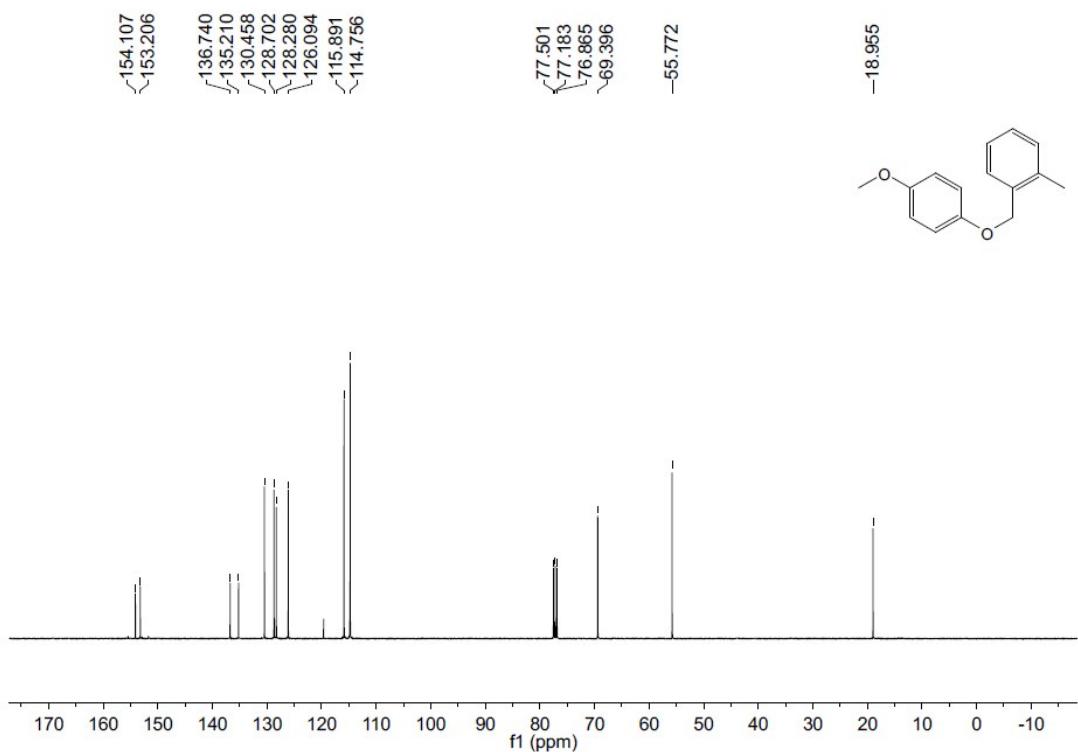
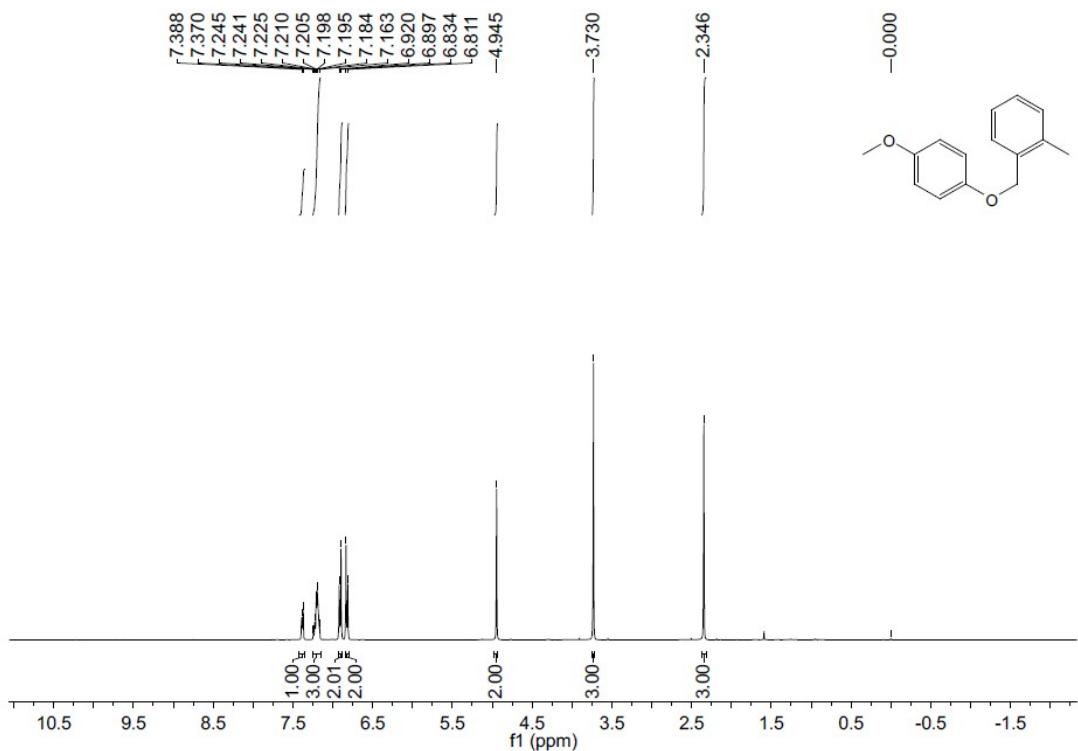
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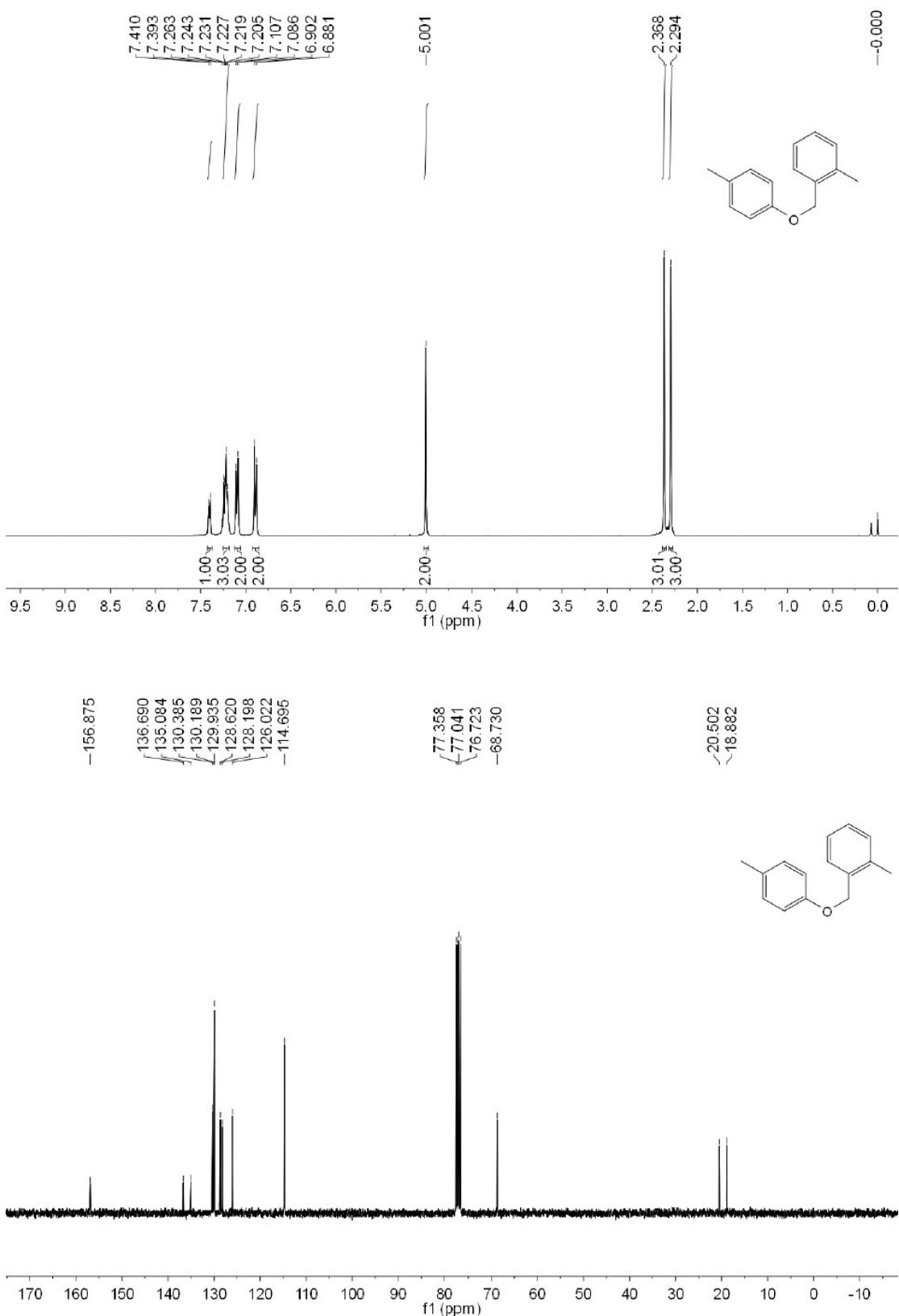
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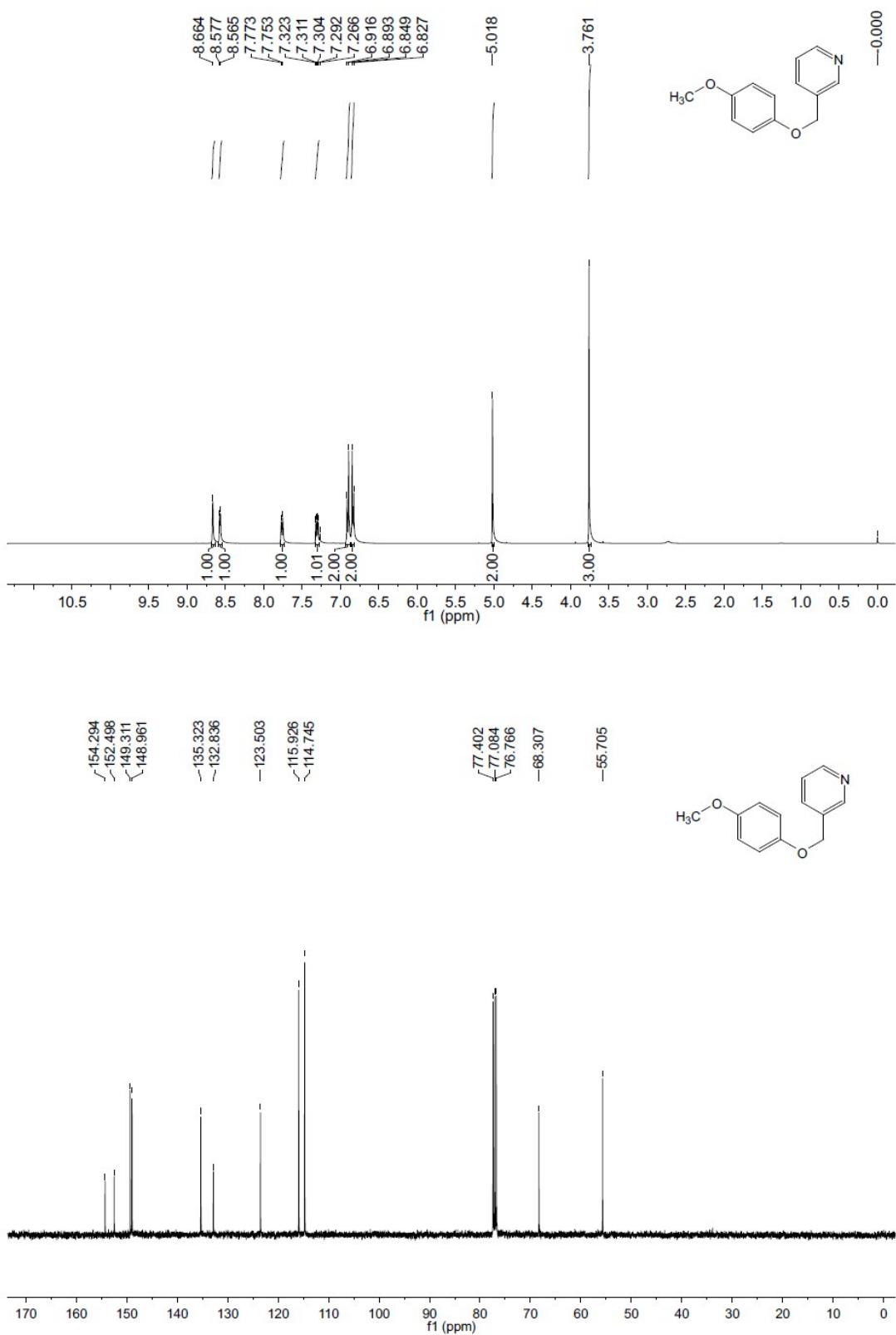
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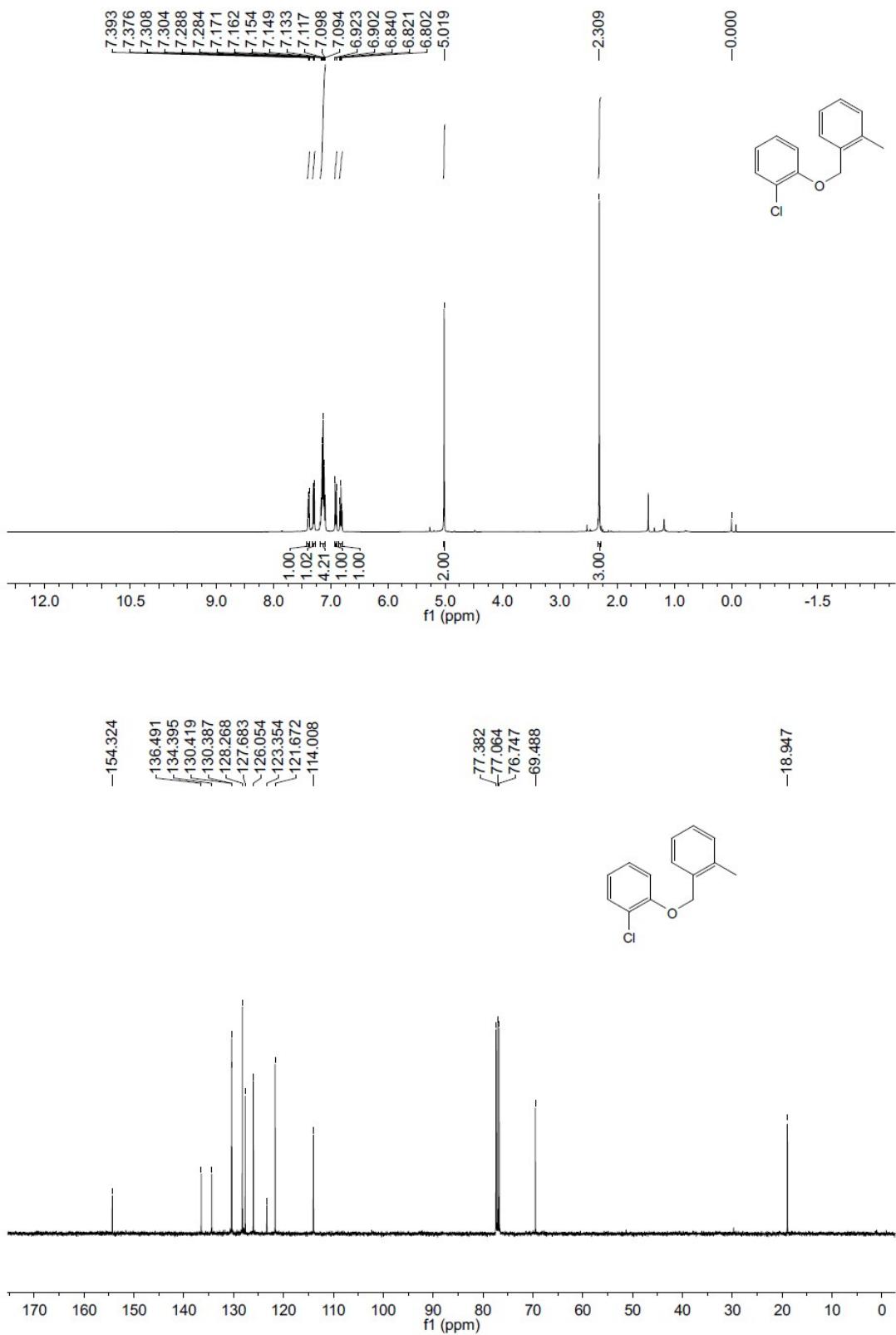
¹H NMR and ¹³C NMR spectra of compound 3c'



¹H NMR and ¹³C NMR spectra of compound **3d'**



¹H NMR and ¹³C NMR spectra of compound 3e'



¹H NMR and ¹³C NMR spectra of compound 3f