Synthesis and Characterization of a Green and Recyclable Arginine-based Palladium/$CoFe_2O_4$ Nanomagnetic Catalyst for Efficient Cyanation of Aryl Halides

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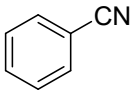
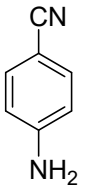
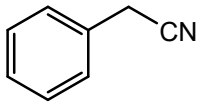
Characterization of aryl nitrile derivatives:



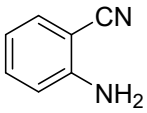
Benzonitrile (2a). Colorless oil; ^{1}H NMR (499 MHz, DMSO-d_6) δ 7.81 (d, J = 7.6 Hz, 2H), 7.72-7.69 (m, 1H), 7.56 (t, J = 7.6 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 132.62, 131.15, 128.77, 118.57, 112.64. HRMS (ESI): Calcd for C_7H_5N $(M+H)^+$ 103.04, found 103.09.



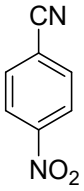
4-Aminobenzonitrile (2b). White solid, mp 83-85 °C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 7.38 (d, J = 8.1 Hz, 2H), 6.58 (d, J = 8.2 Hz, 2H), 6.12 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 151.00, 133.12, 118.44, 114.66, 98.60. HRMS (ESI): Calcd for $C_7H_6N_2$ $(M+H)^+$ 118.05, found 118.11.



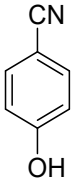
2-Phenylacetonitrile (2c). Colorless oil; ^{1}H NMR (499 MHz, DMSO-d_6) δ 7.39-7.31 (m, 2H), 7.31-7.25 (m, 3H), 3.71 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 129.8, 129.0, 127.9, 127.8, 117.8, 23.4. HRMS (ESI): Calcd for C_8H_7N (M +H) $^{+}$ 117.06, found 117.11.



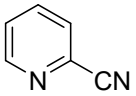
2-Aminobenzonitrile (2d). Beige-brown solid, mp 49-50 ° C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 7.35 (d, J = 7.9 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 6.76 (d, J = 8.5 Hz, 1H), 6.57 (t, J = 7.5 Hz, 1H), 5.98 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 151.10, 133.59, 13.95, 118.01, 116.75, 115.05, 94.31. HRMS (ESI): Calcd for $C_7H_6N_2$ (M +H) $^{+}$ 118.05, found 118.08.



4-Nitrobenzonitrile (2e). Yellow solid, mp 147-149 ° C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 8.37 (d, J = 8.3 Hz, 2H), 8.16 (d, J = 8.3 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 15.01, 133.80, 123.92, 117.93, 117.07. HRMS (ESI): Calcd for $C_7H_4N_2O_2$ (M +H) $^{+}$ 148.03, found 148.08.

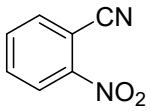


4-Hydroxybenzonitrile (2f). White solid, mp 110-112 ° C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 10.54 (s, 1H), 7.55 (d, J = 8.2 Hz, 2H), 6.85 (d, J = 8.3 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 161.80, 134.22, 118.56, 116.27, 102.33. HRMS (ESI): Calcd for C_7H_5NO (M +H) $^{+}$ 119.04, found 119.18.

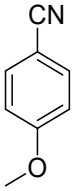


Picolinonitrile (2g). White solid, mp 28-30 ° C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 8.75 (d, J = 4.8 Hz, 1H), 8.07-8.01 (m, 2H), 7.73 (t, J = 6.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO-d_6) δ

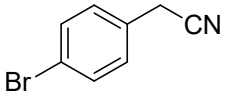
151.37, 138.00, 133.98, 128.20, 127.66,117.32. HRMS (ESI): Calcd for $C_6H_4N_2$ (M +H) $^+$ 104.04, found 104.12.



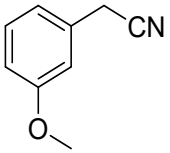
2-Nitrobenzonitrile (2h). Yellow solid, mp 109-110 ^{o} C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 8.42-8.35 (m, 1H), 8.17 (dd, J = 5.7, 3.4 Hz, 1H), 7.98 (dd, J = 6.0, 3.4 Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 149.39, 135.51, 134.36, 133.83, 124.14, 115.13,107.96. HRMS (ESI): Calcd for $C_7H_4N_2O_2$ (M +H) $^+$ 148.03, found 148.11.



4-Methoxybenzonitrile (2i). White solid, mp 60-61 ^{o} C; ^{1}H NMR (499 MHz, DMSO-d_6) δ 7.76 (d, J = 8.6 Hz, 2H), 7.09 (d, J = 8.6 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.10, 133.88, 118.55, 114.22, 104.08, 55.32. HRMS (ESI): Calcd for $C_{13}H_{13}N_2O$ (M +H) $^+$ 133.05, found 133.09.

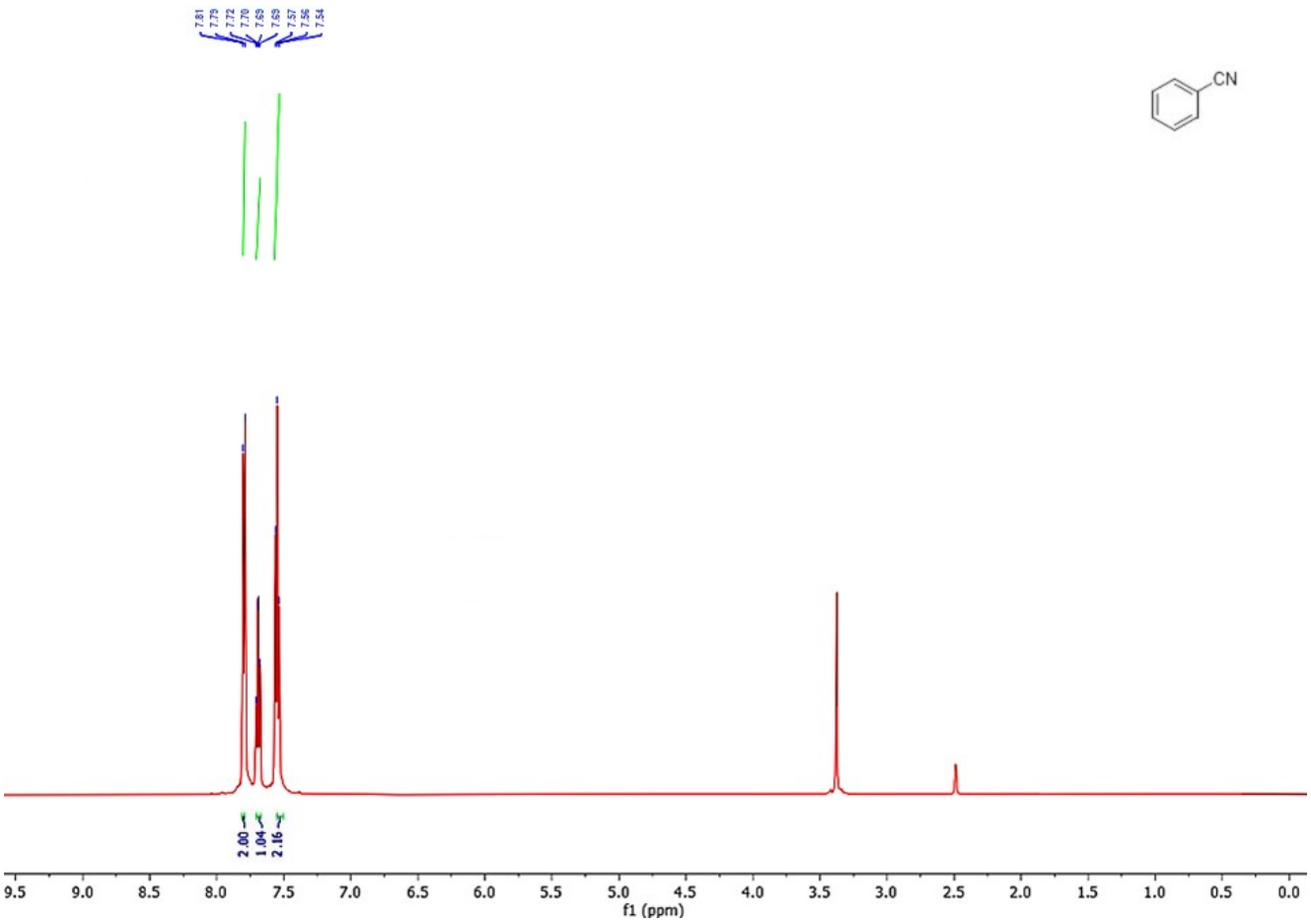


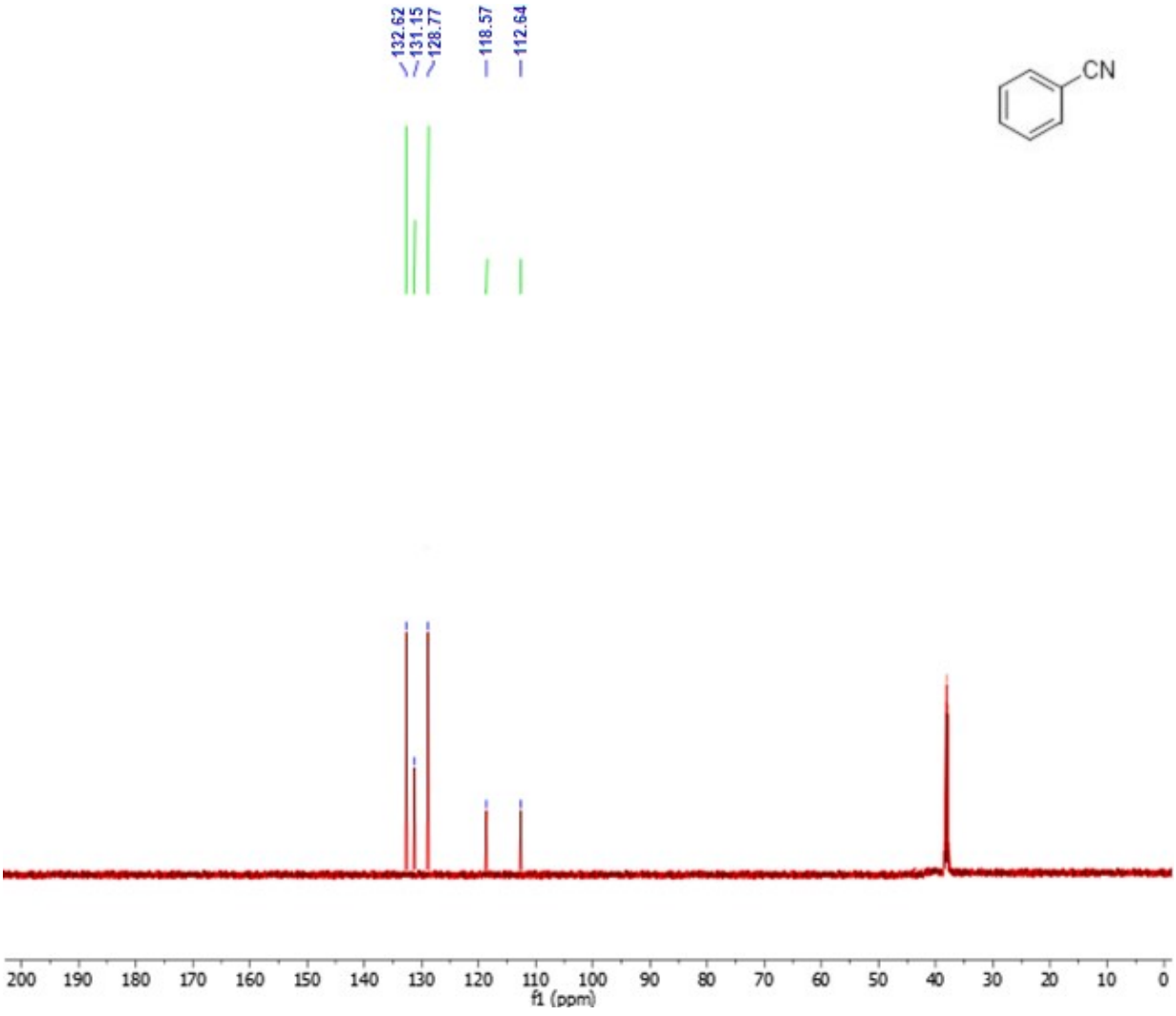
2-(4-bromophenyl)acetonitrile (2j). White solid, mp 48-50 ^{o} C; ^{1}H NMR (499 MHz, $CDCl_3$) δ 7.54-7.47 (m, 2H), 7.21 (d, J = 8.5 Hz, 2H), 3.71 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 132.3, 129.6, 128.9, 122.2, 117.3, 23.2. HRMS (ESI): Calcd for C_8H_6BrN (M +H) $^+$ 194.97, found 195.03.



2-(3-methoxyphenyl)acetonitrile (2k). Yellow oil; ^{1}H NMR (499 MHz, $CDCl_3$) δ 7.30-7.24 (m, 1H), 6.90-6.84 (m, 3H), 3.80 (s, 3H), 3.71 (s, 2H); ^{13}C NMR (126 MHz, DMSO-d_6) δ 160.26, 131.40, 130.32, 120.28, 117.89, 113.74, 113.70, 55.47, 23.76. HRMS (ESI): Calcd for C_9H_9NO (M +H) $^+$ 147.07, found 147.13.

^{1}H NMR and ^{13}CNMR spectra of aryl nitrile derivatives:

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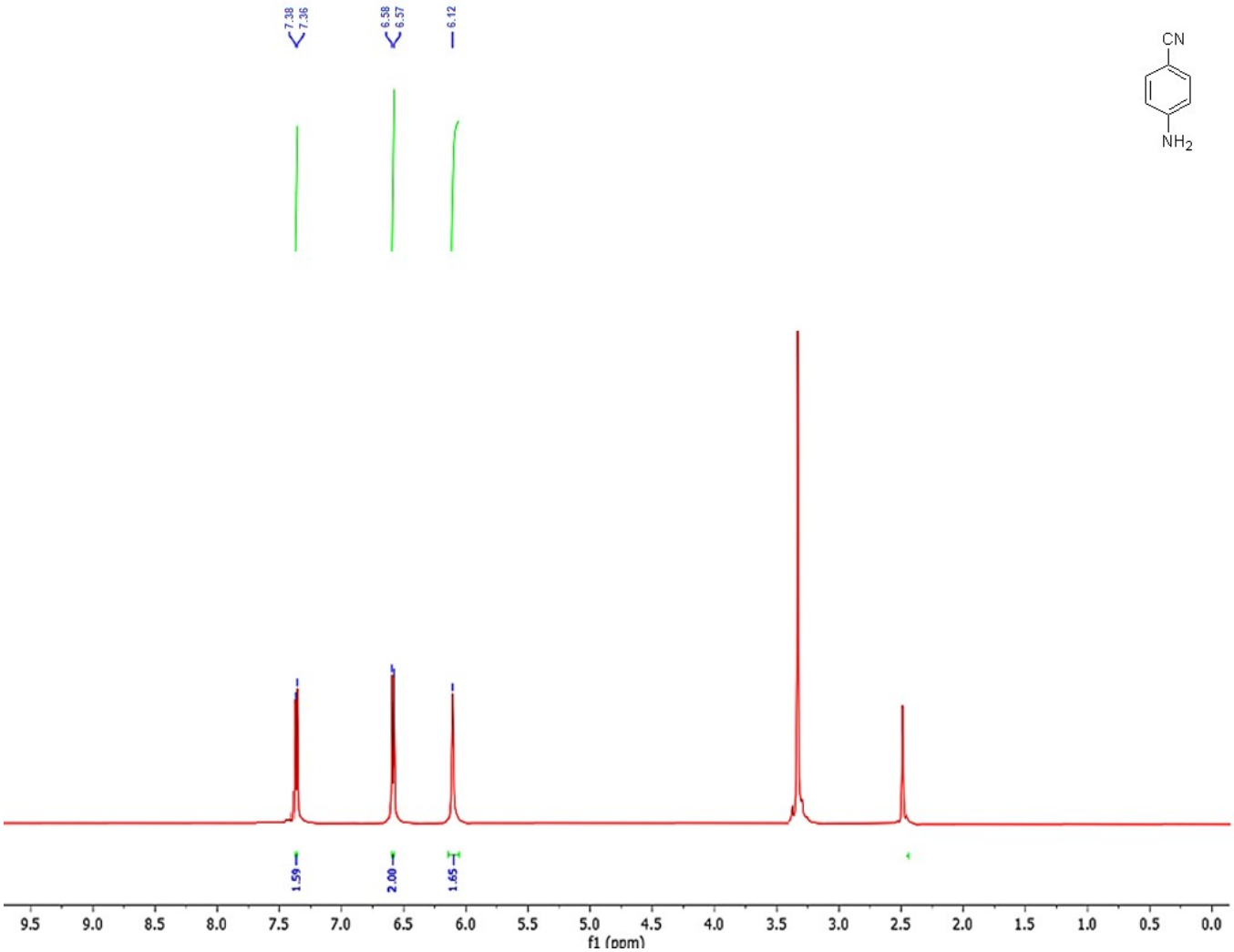
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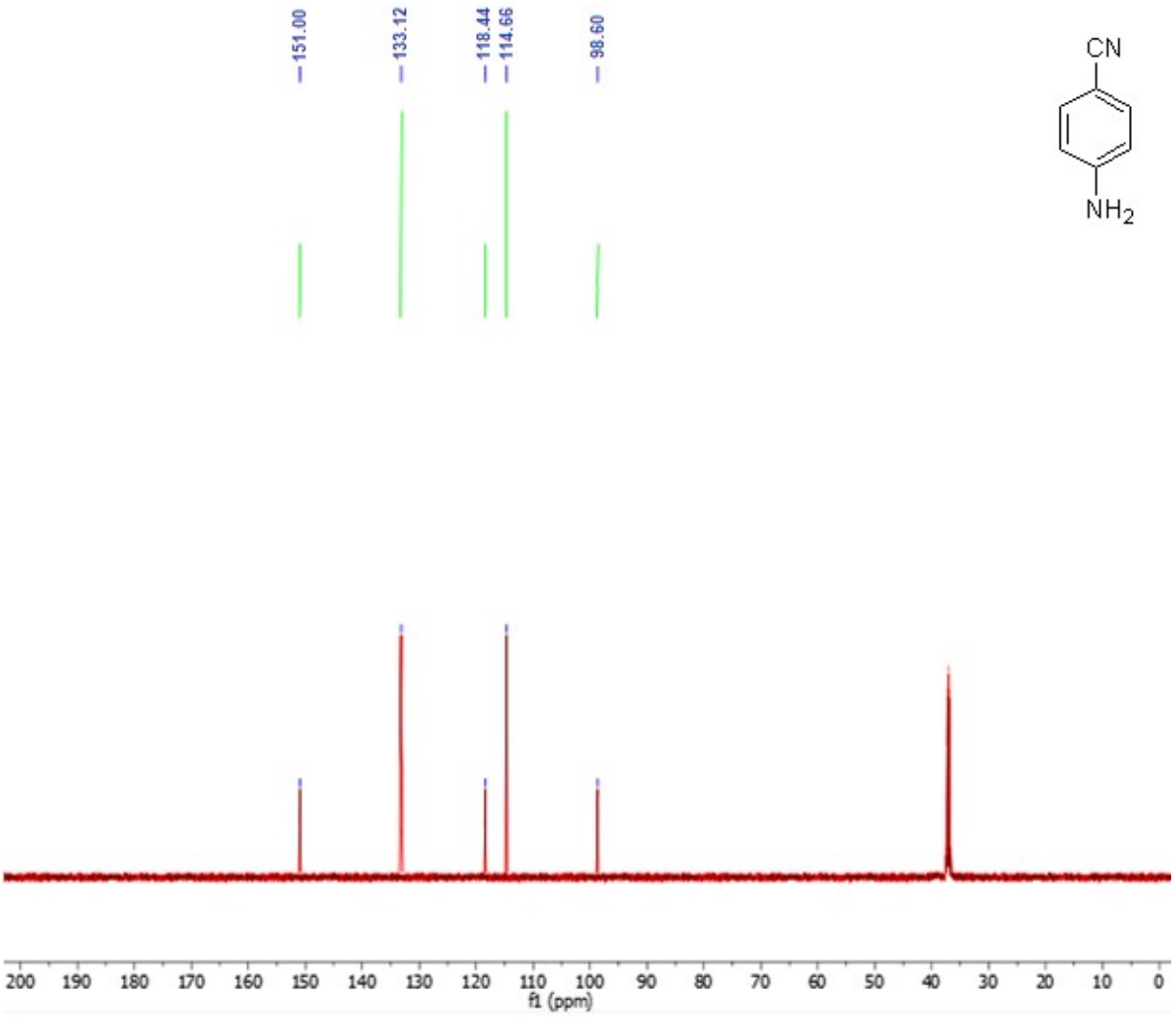
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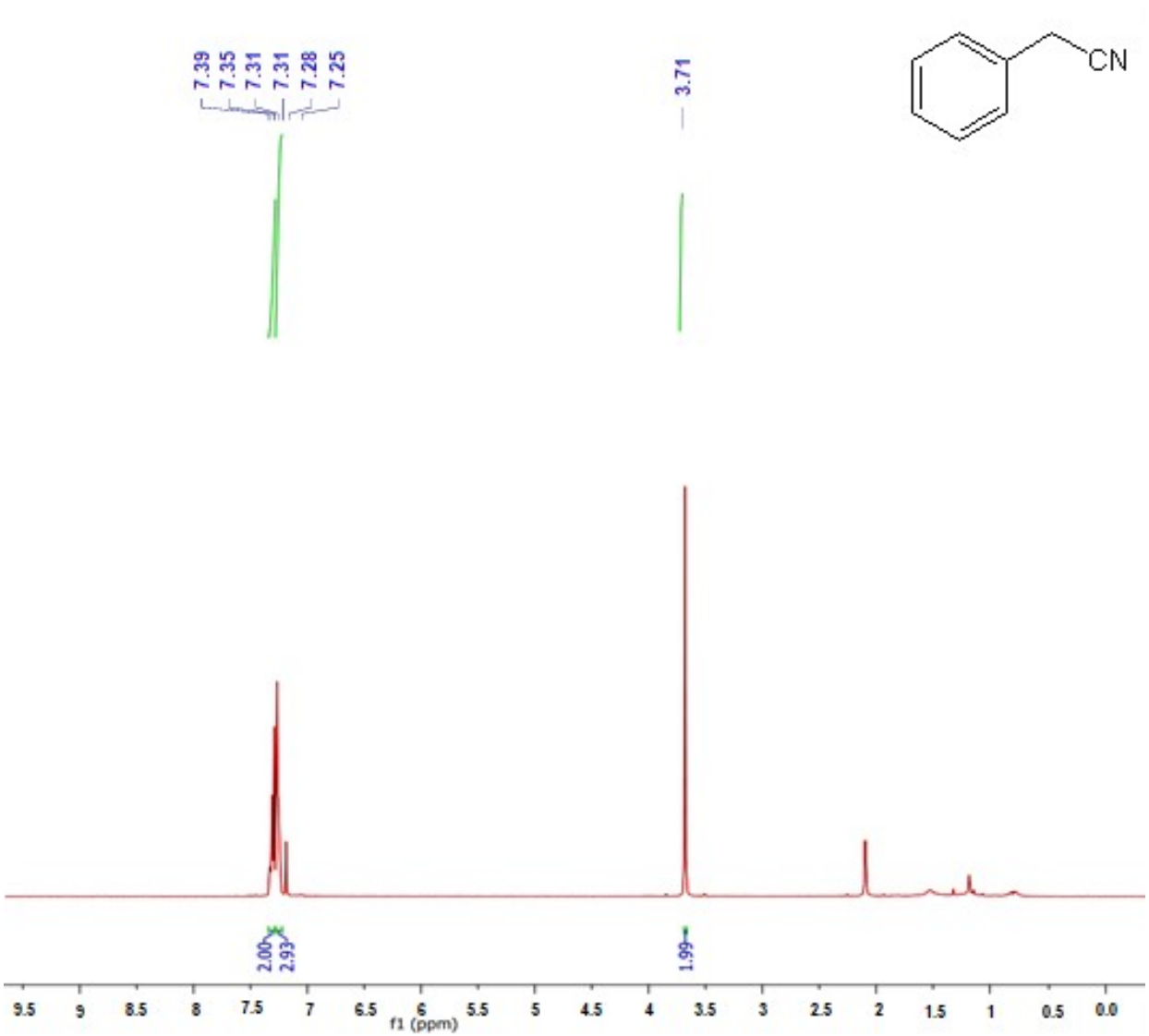
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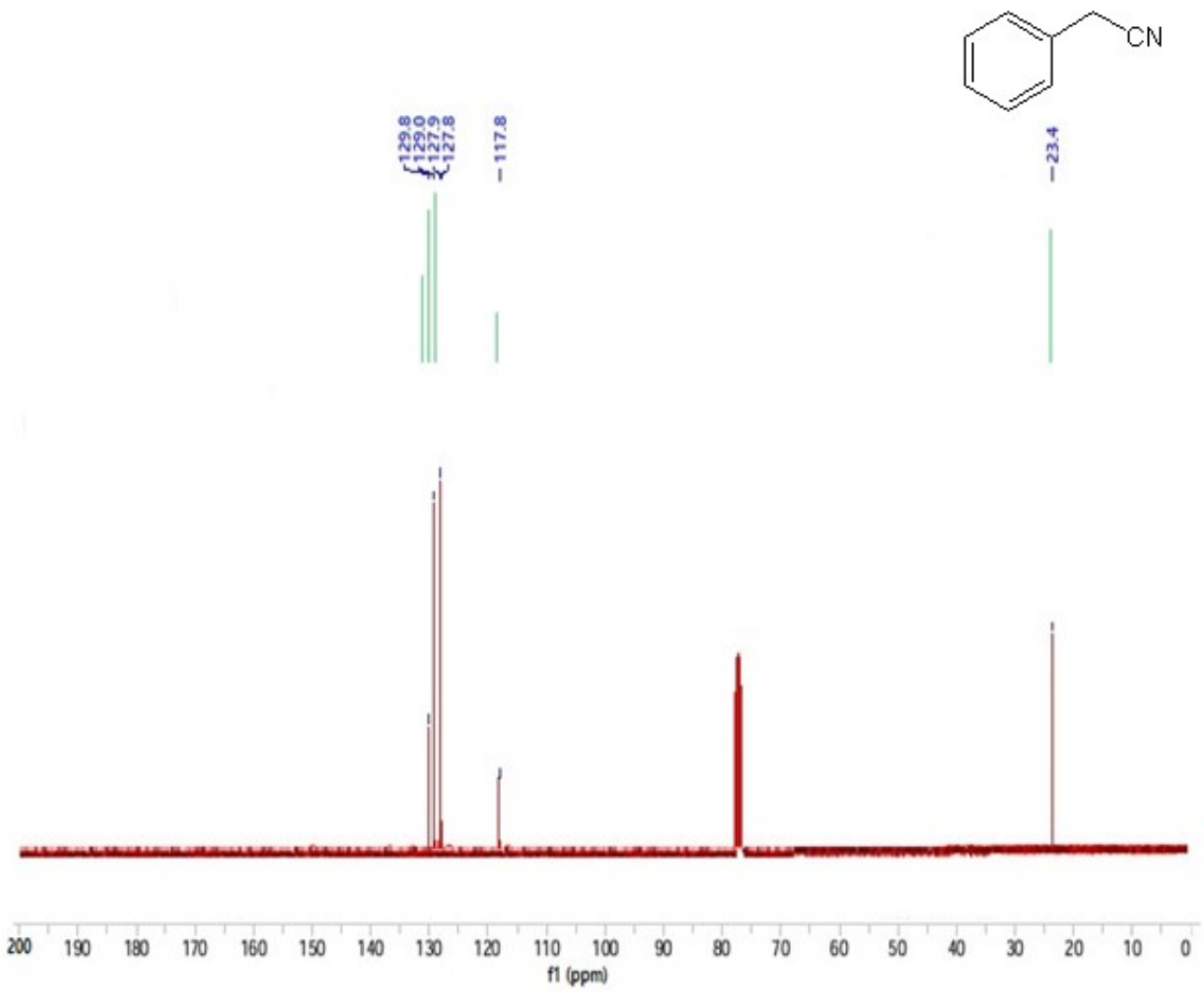
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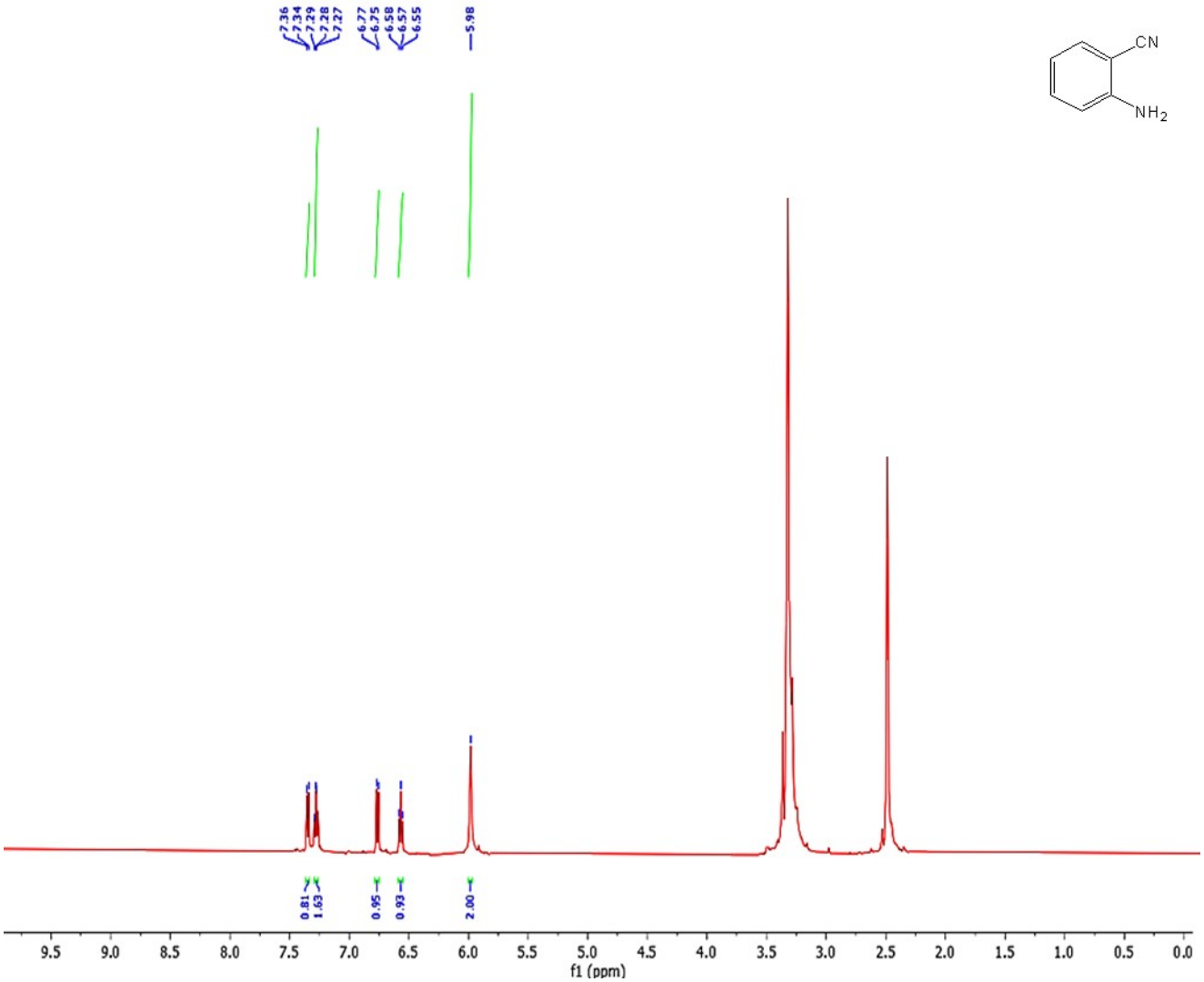
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0.93
2.00
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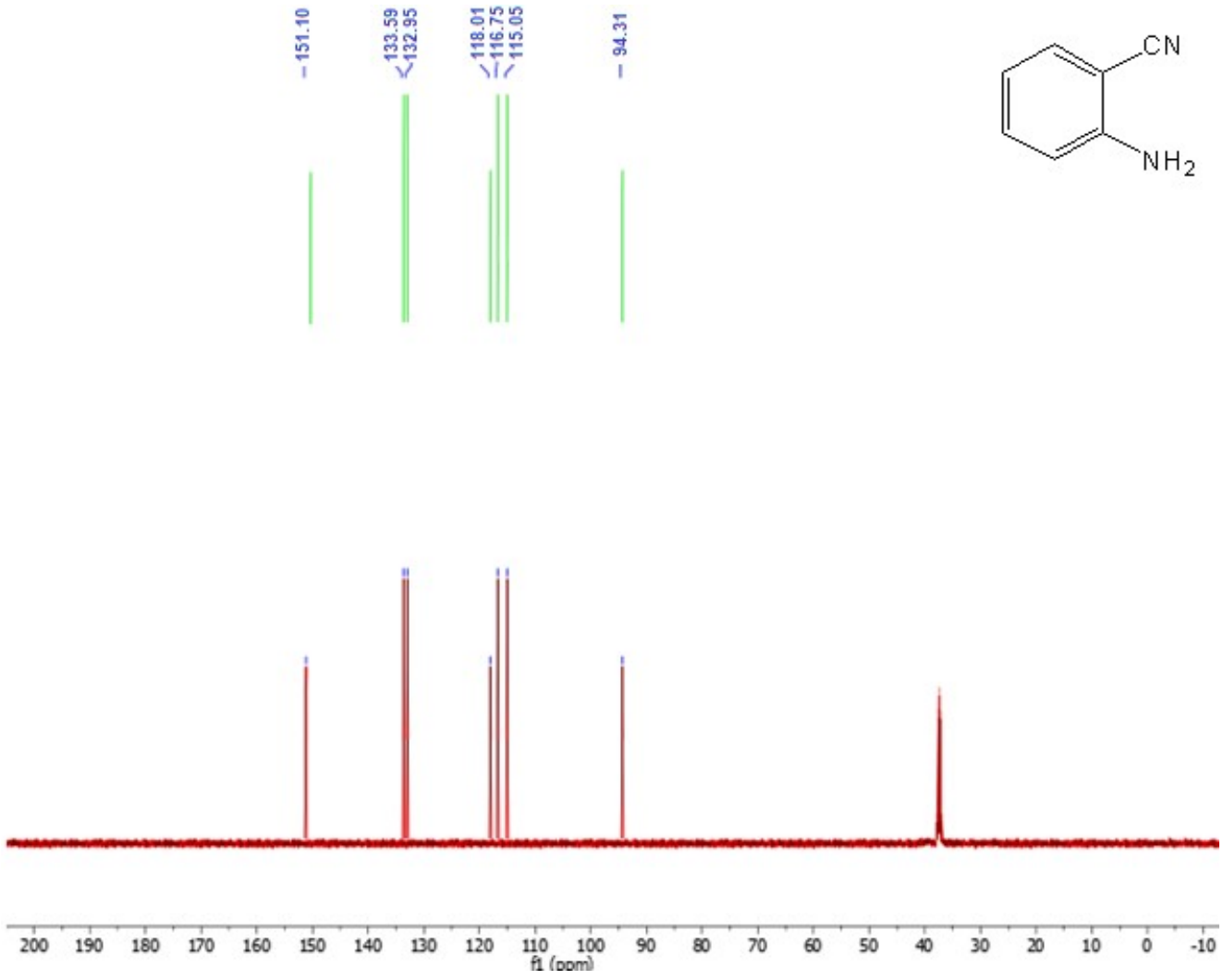
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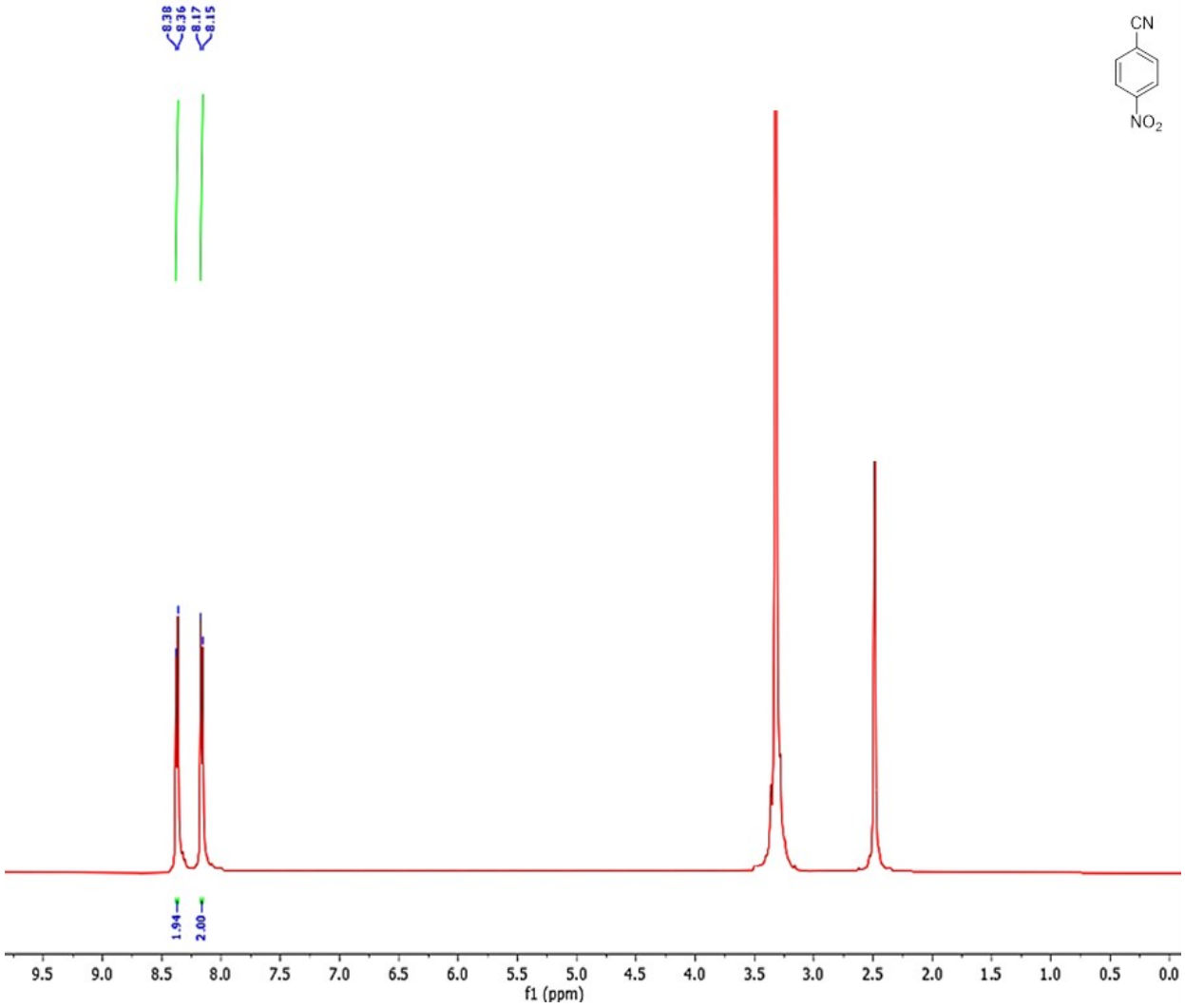
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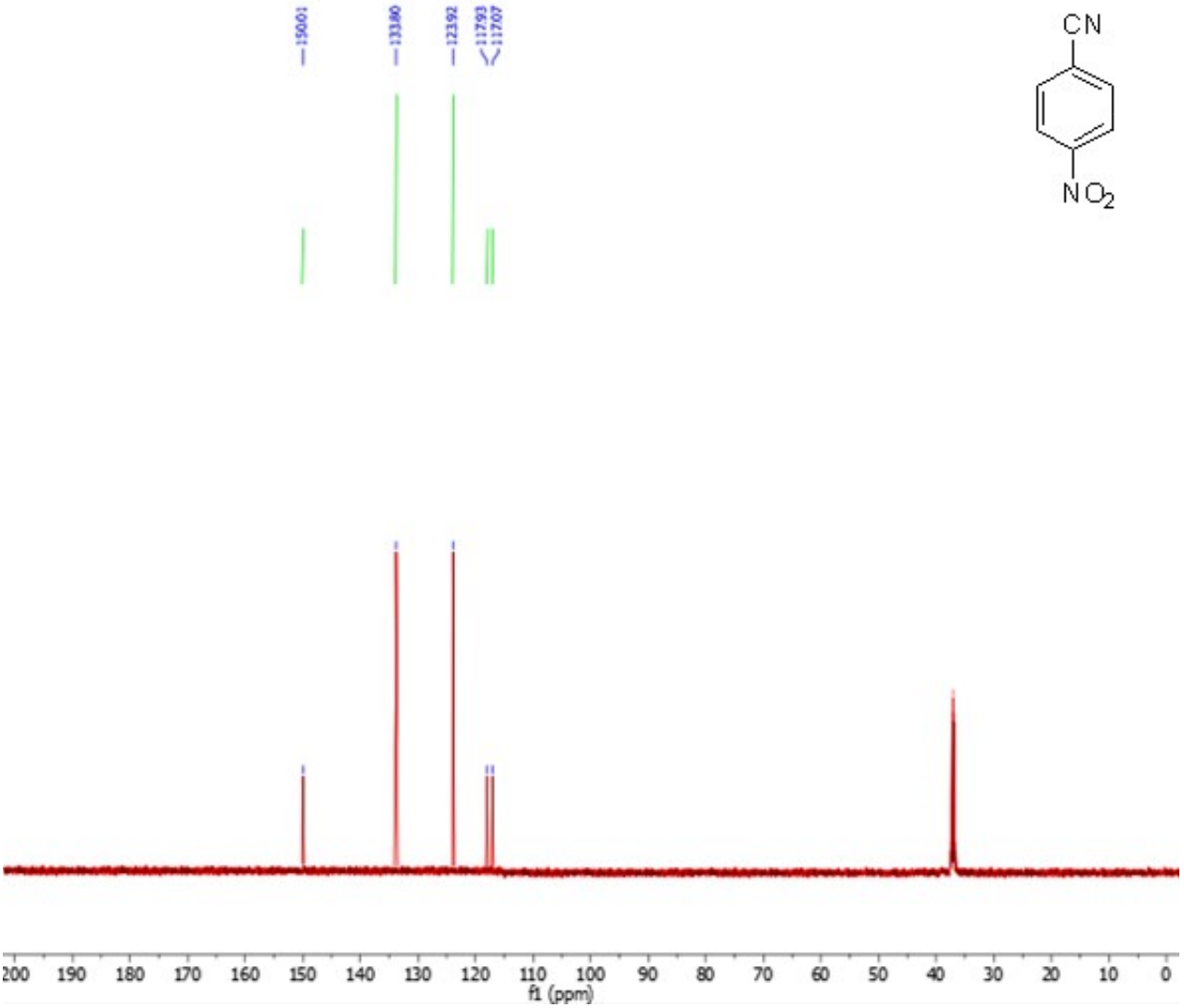
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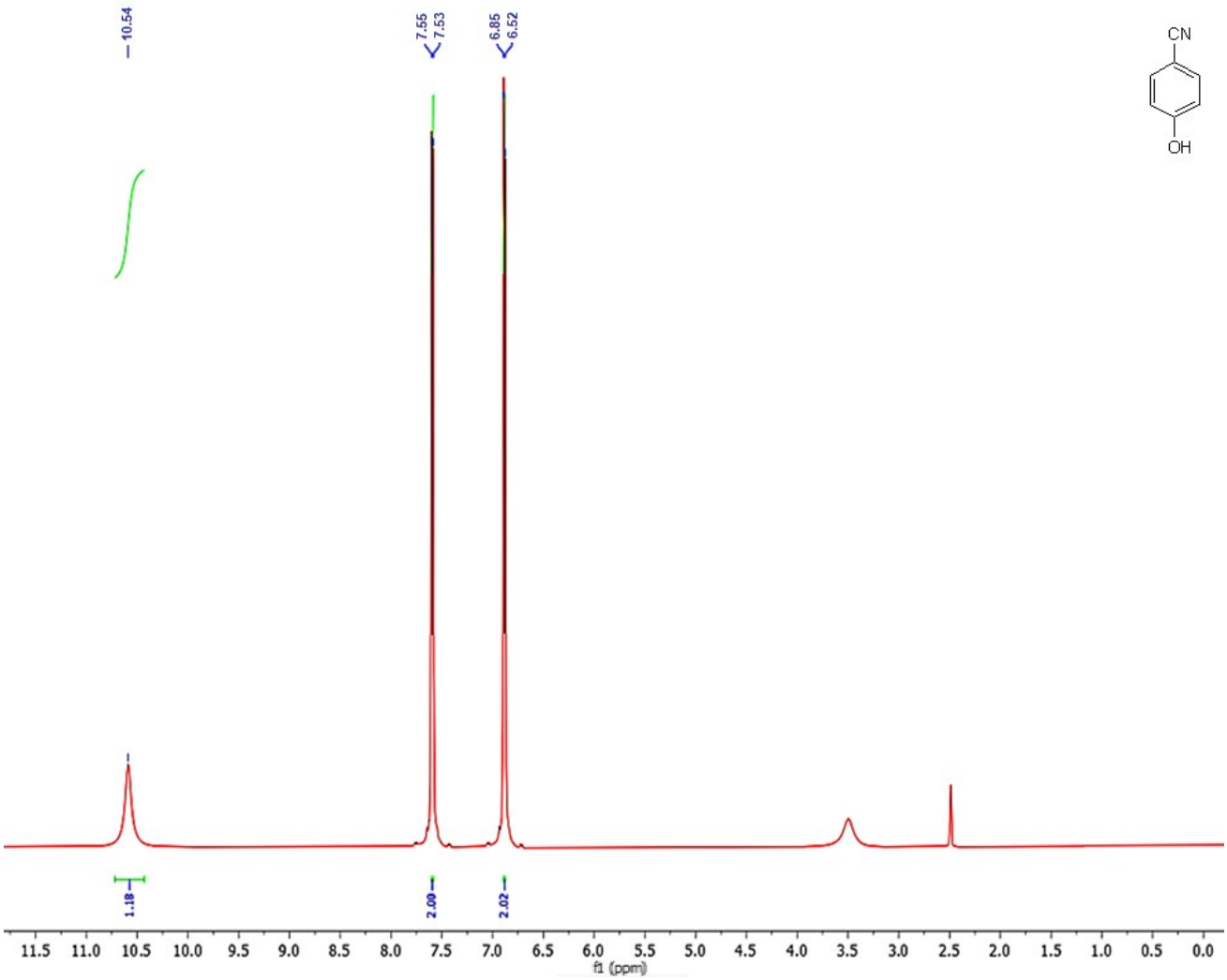
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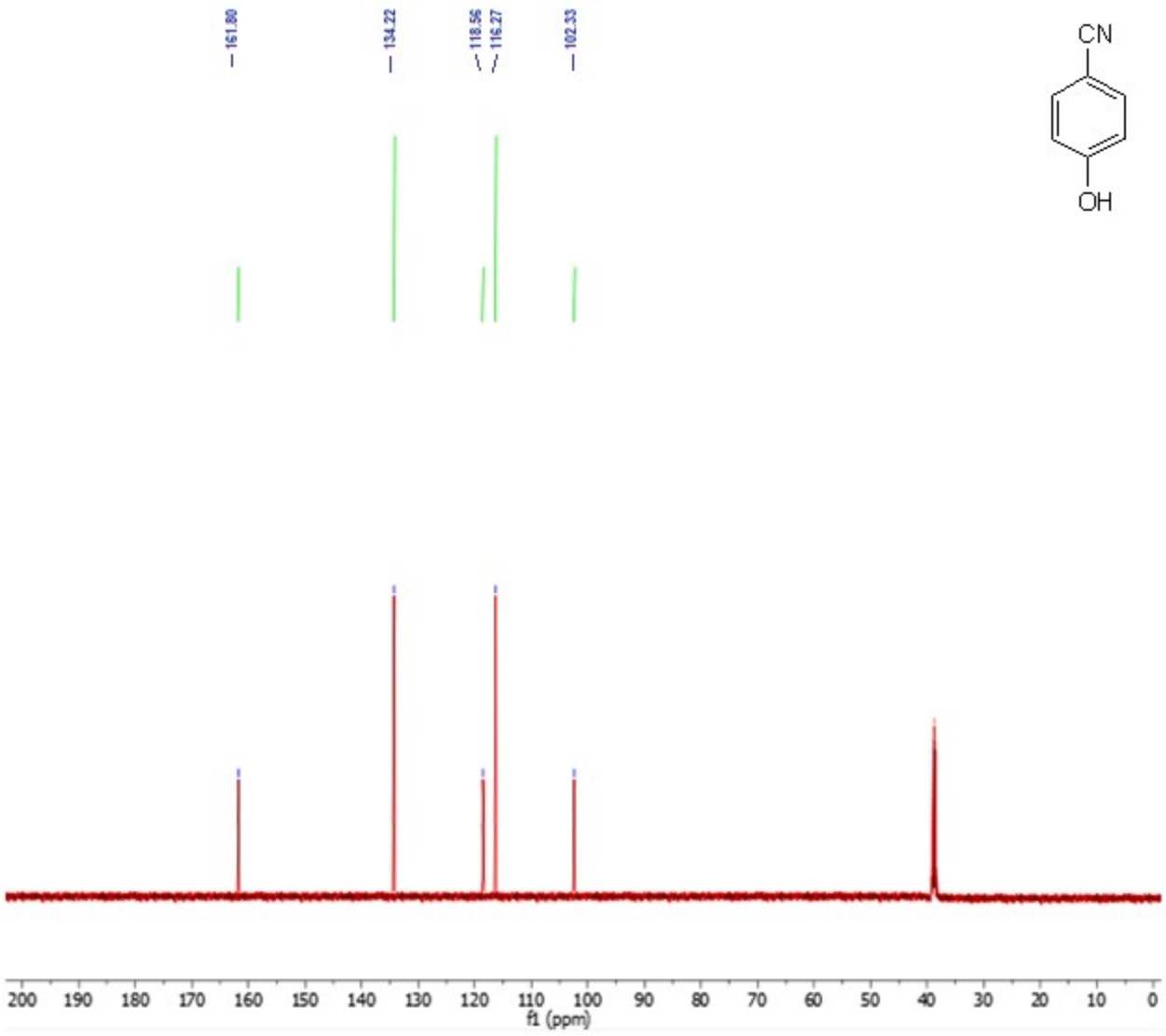
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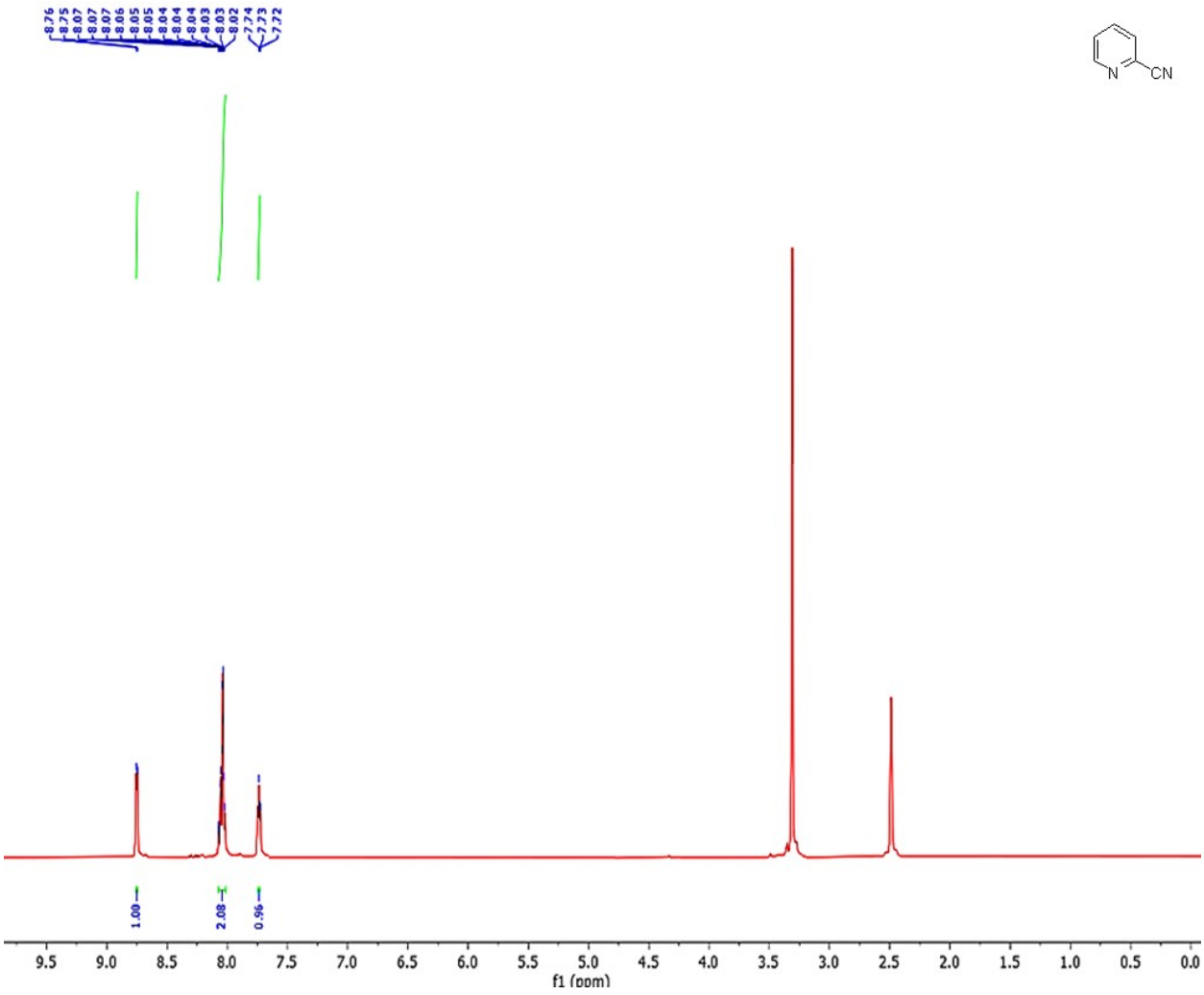
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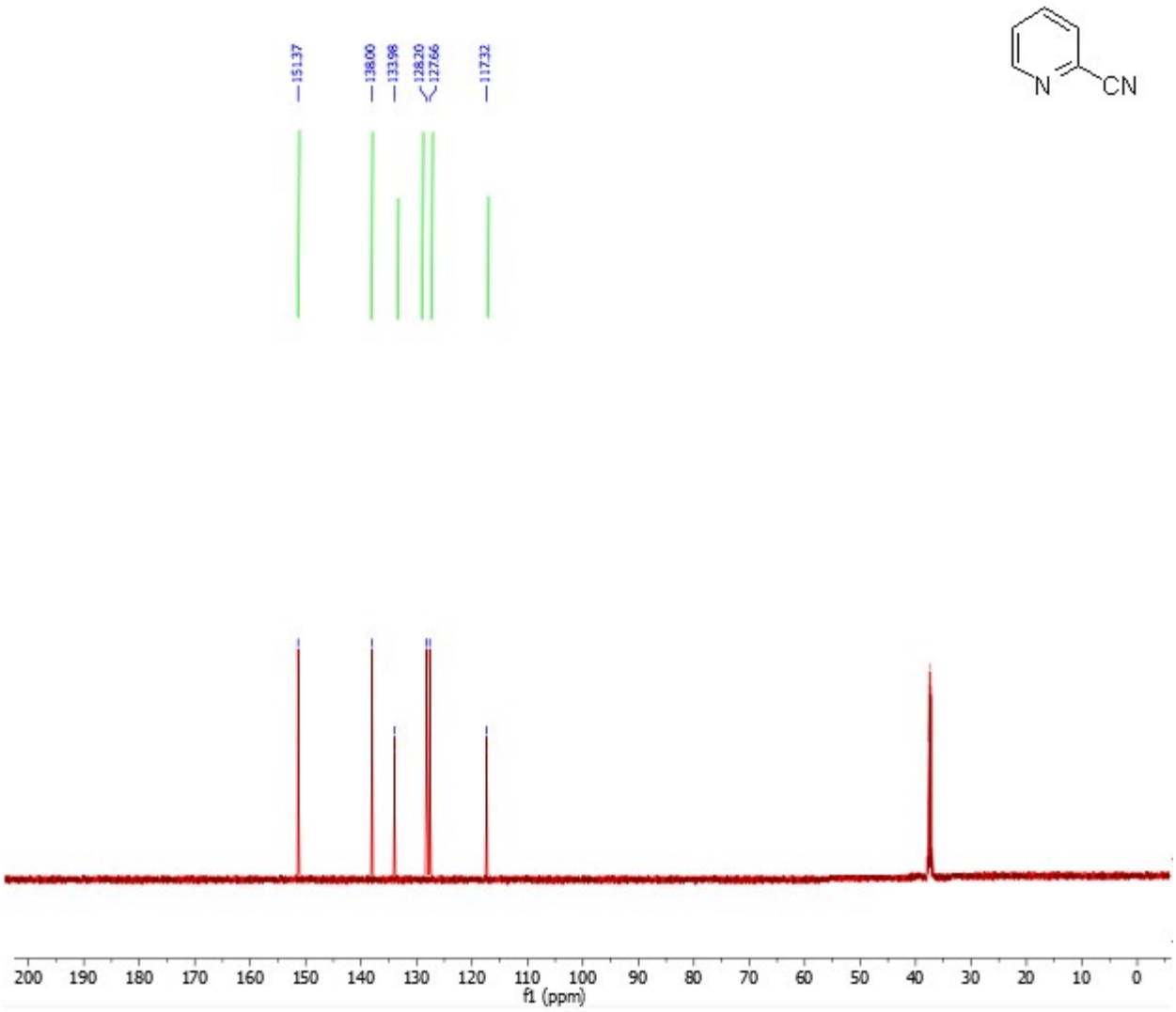
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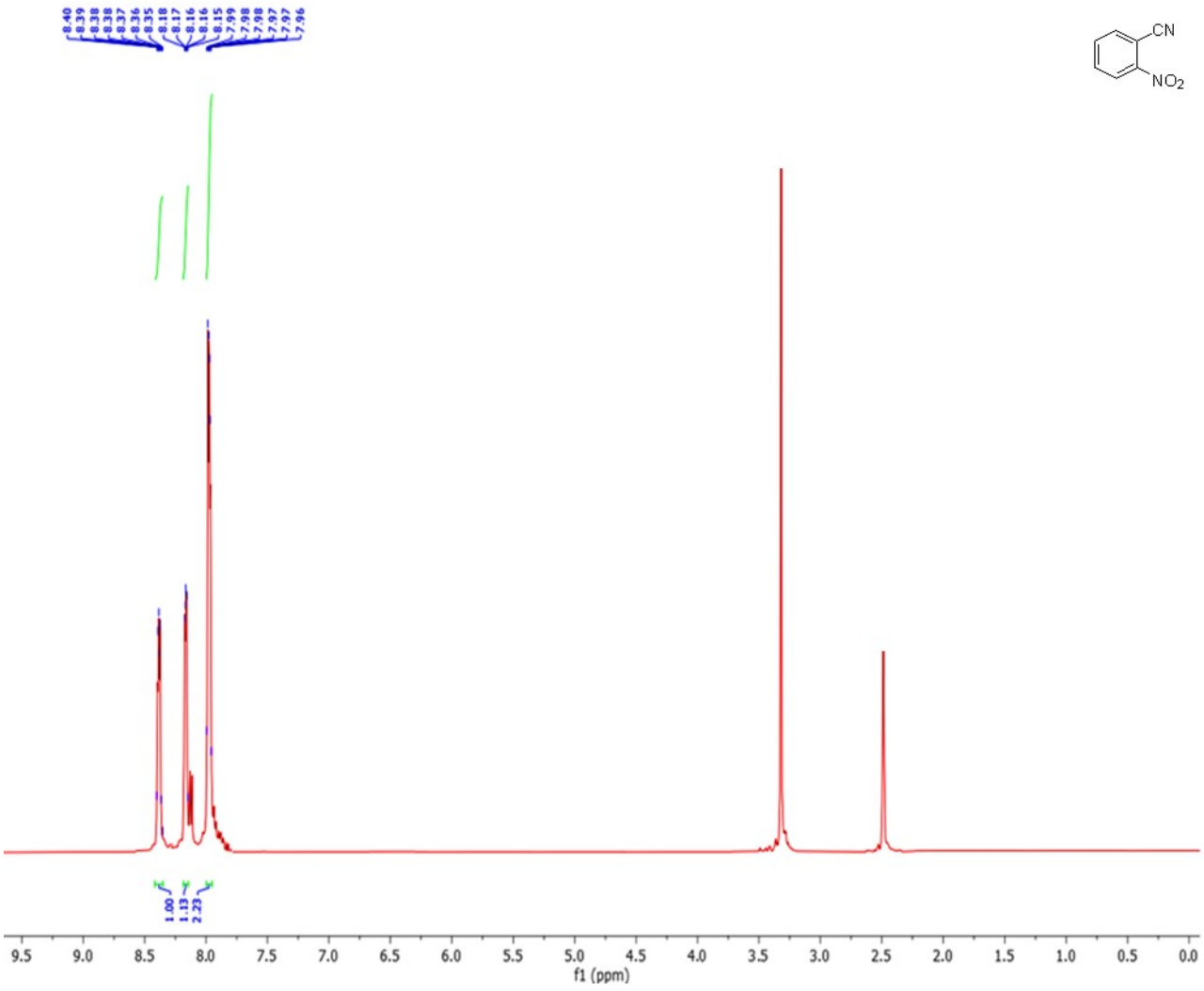
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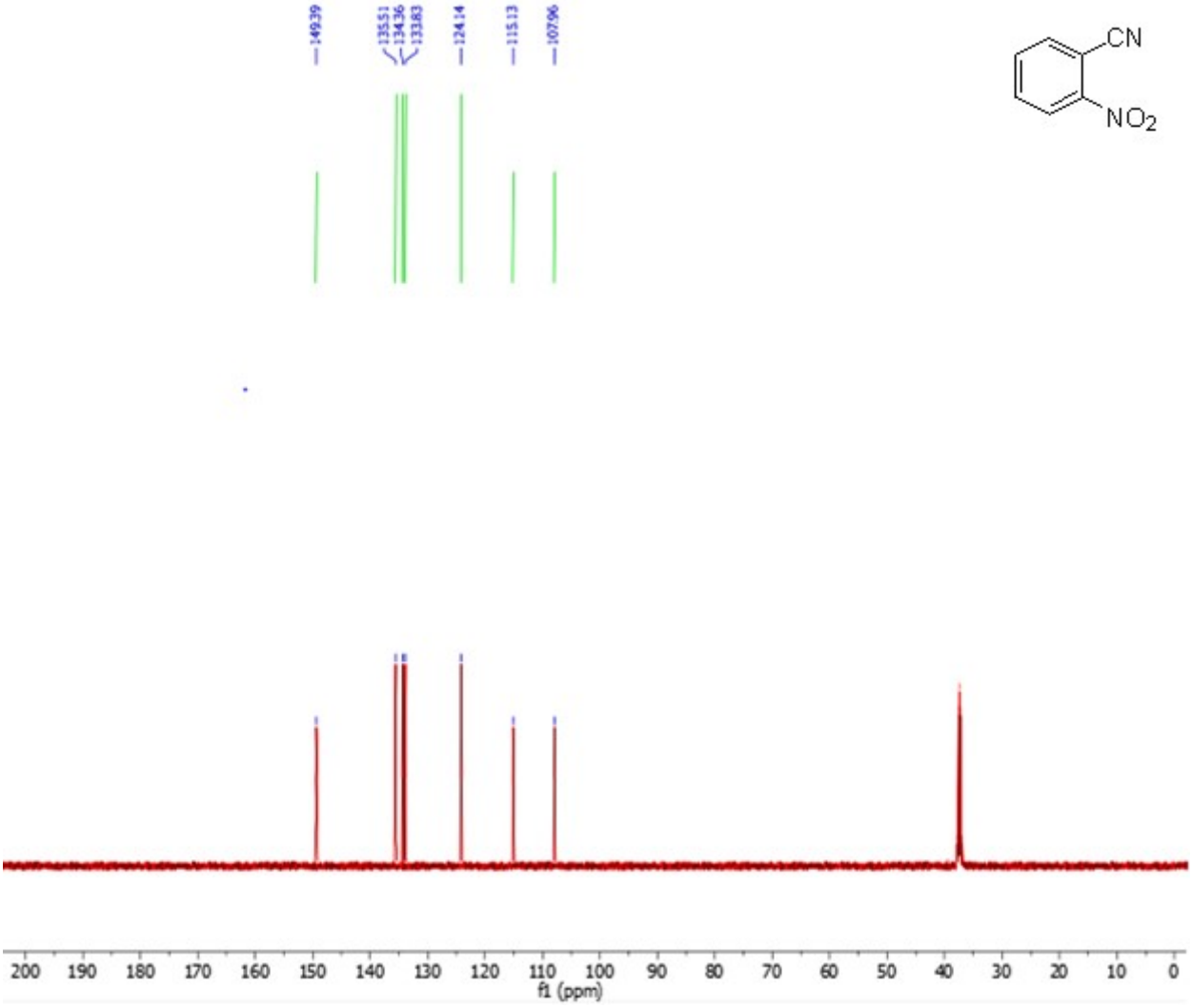
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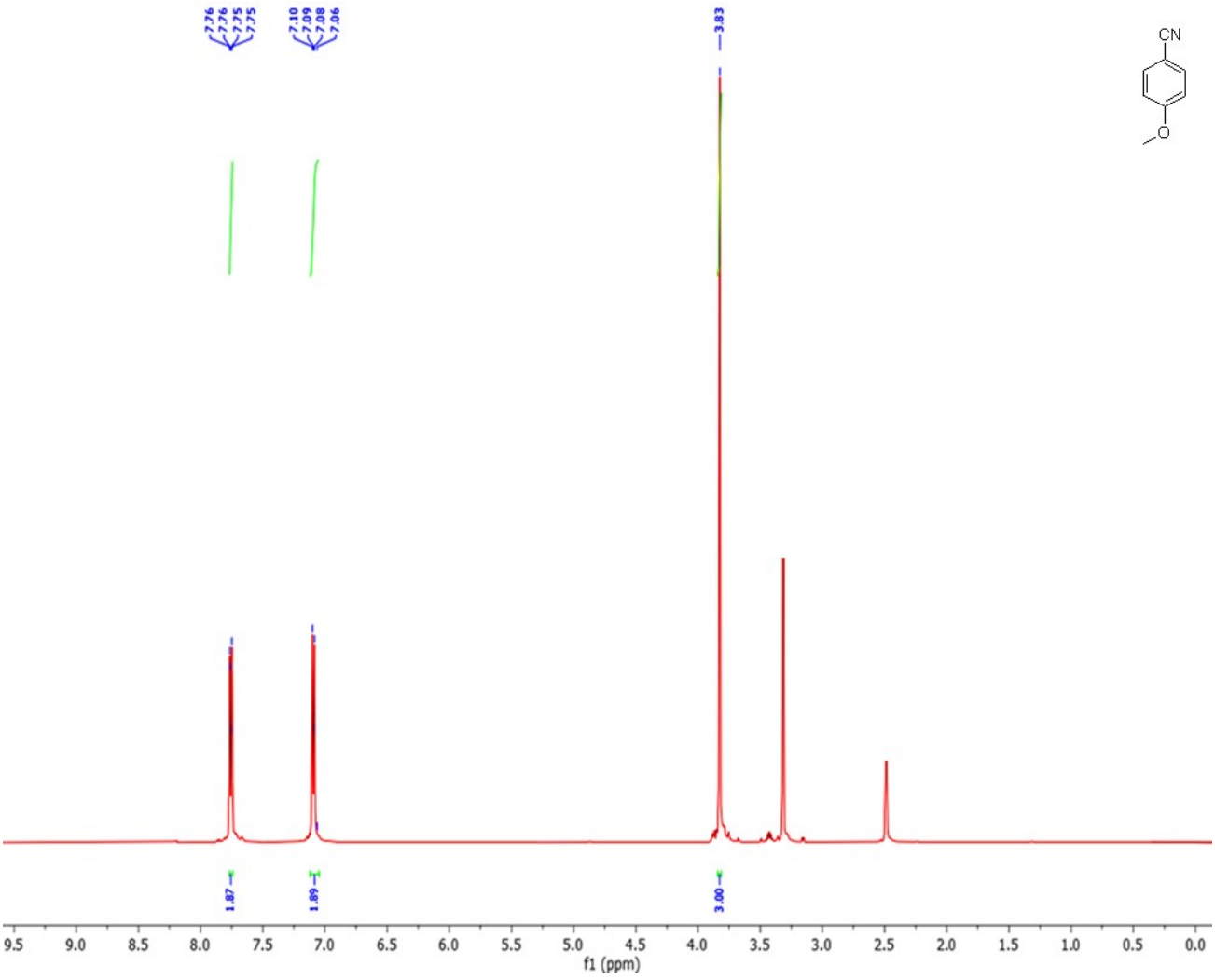
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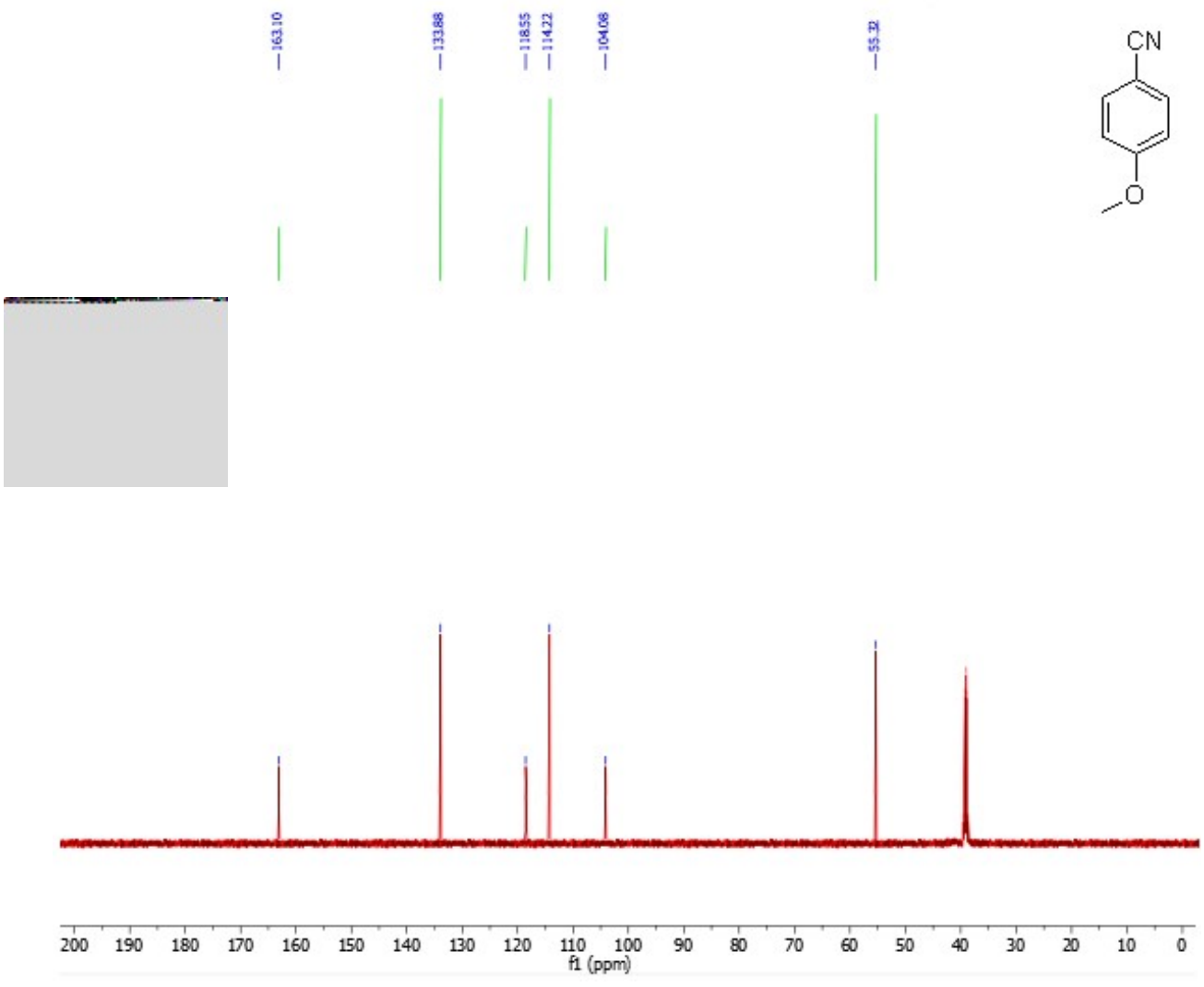
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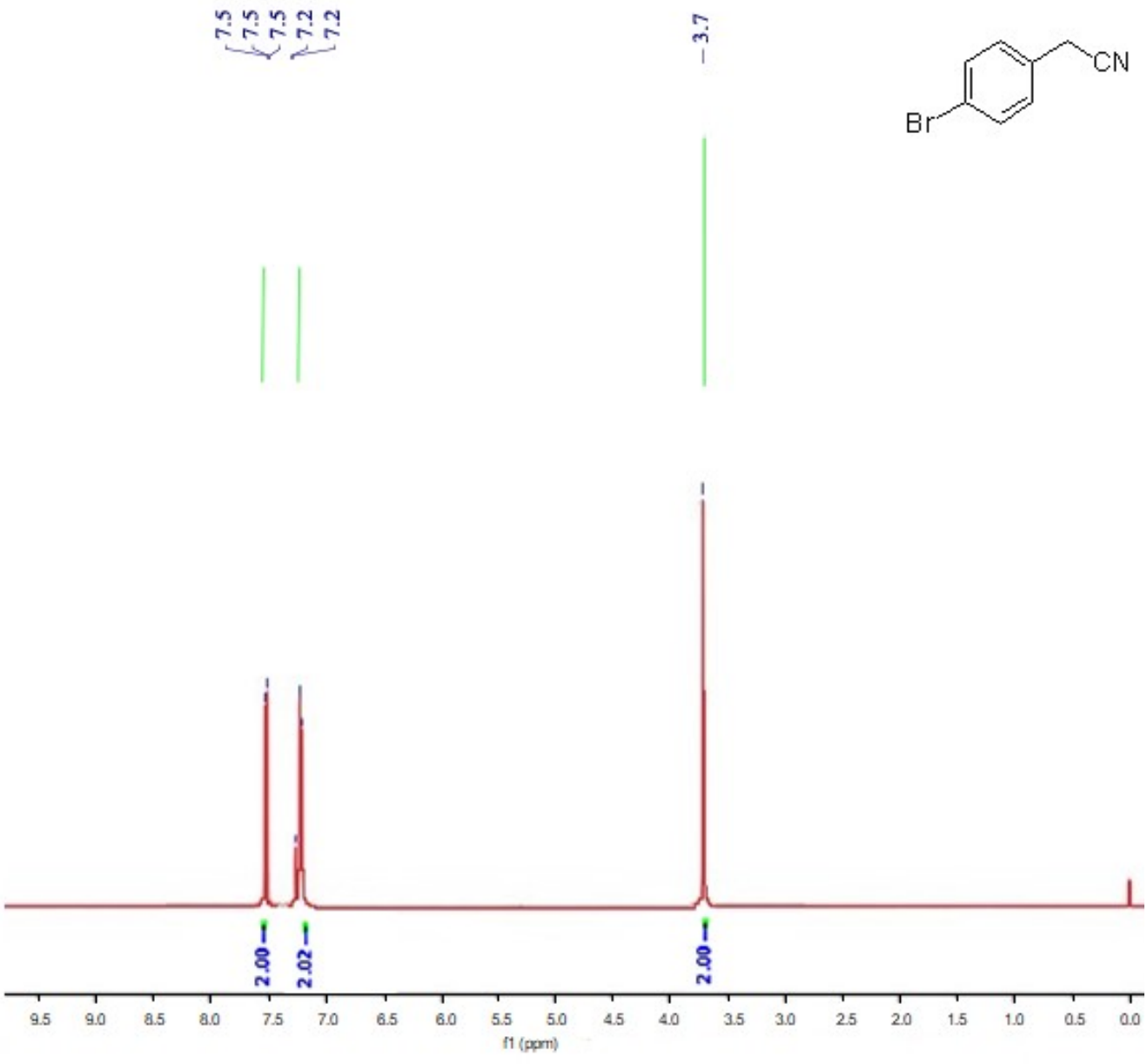
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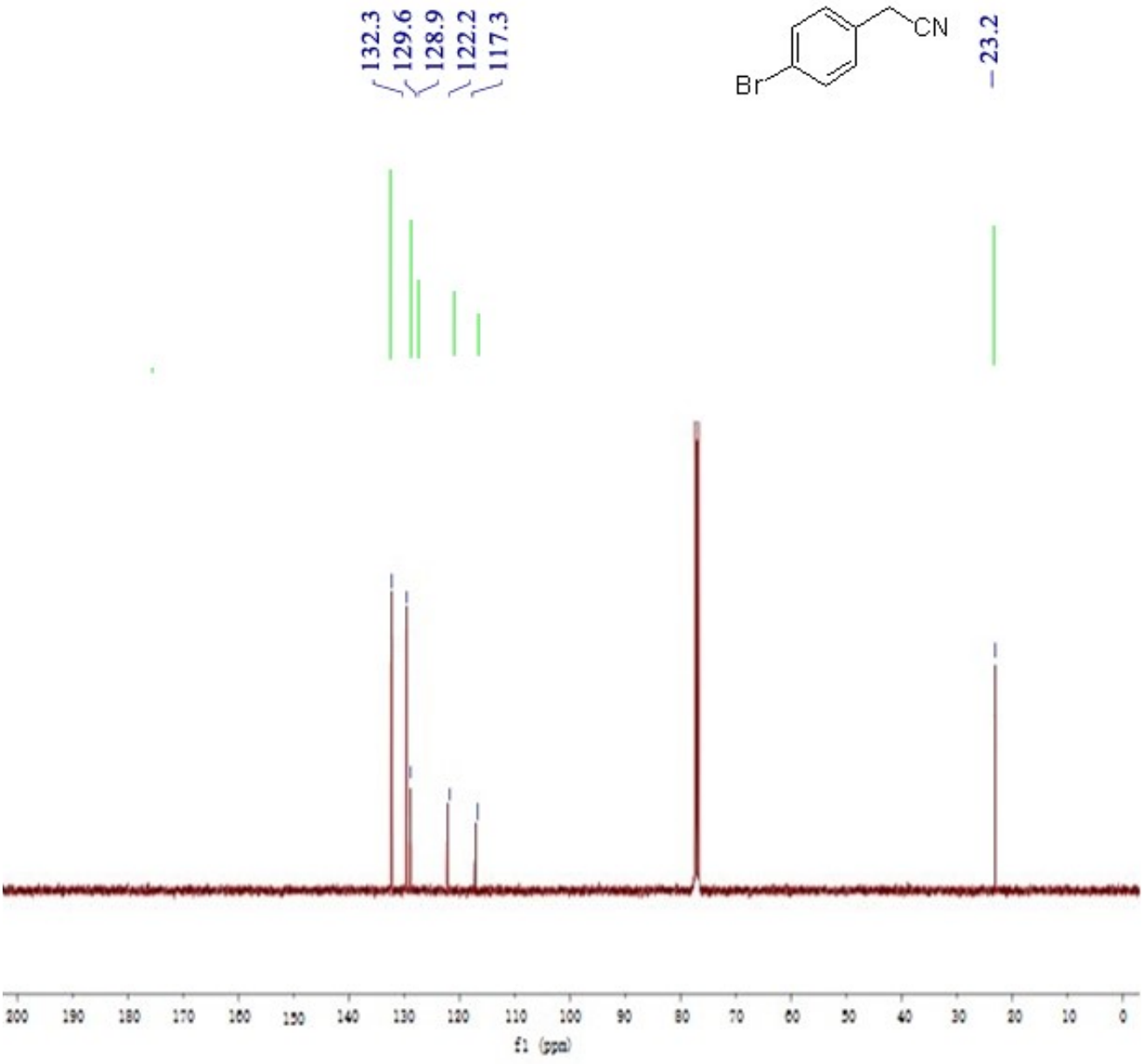
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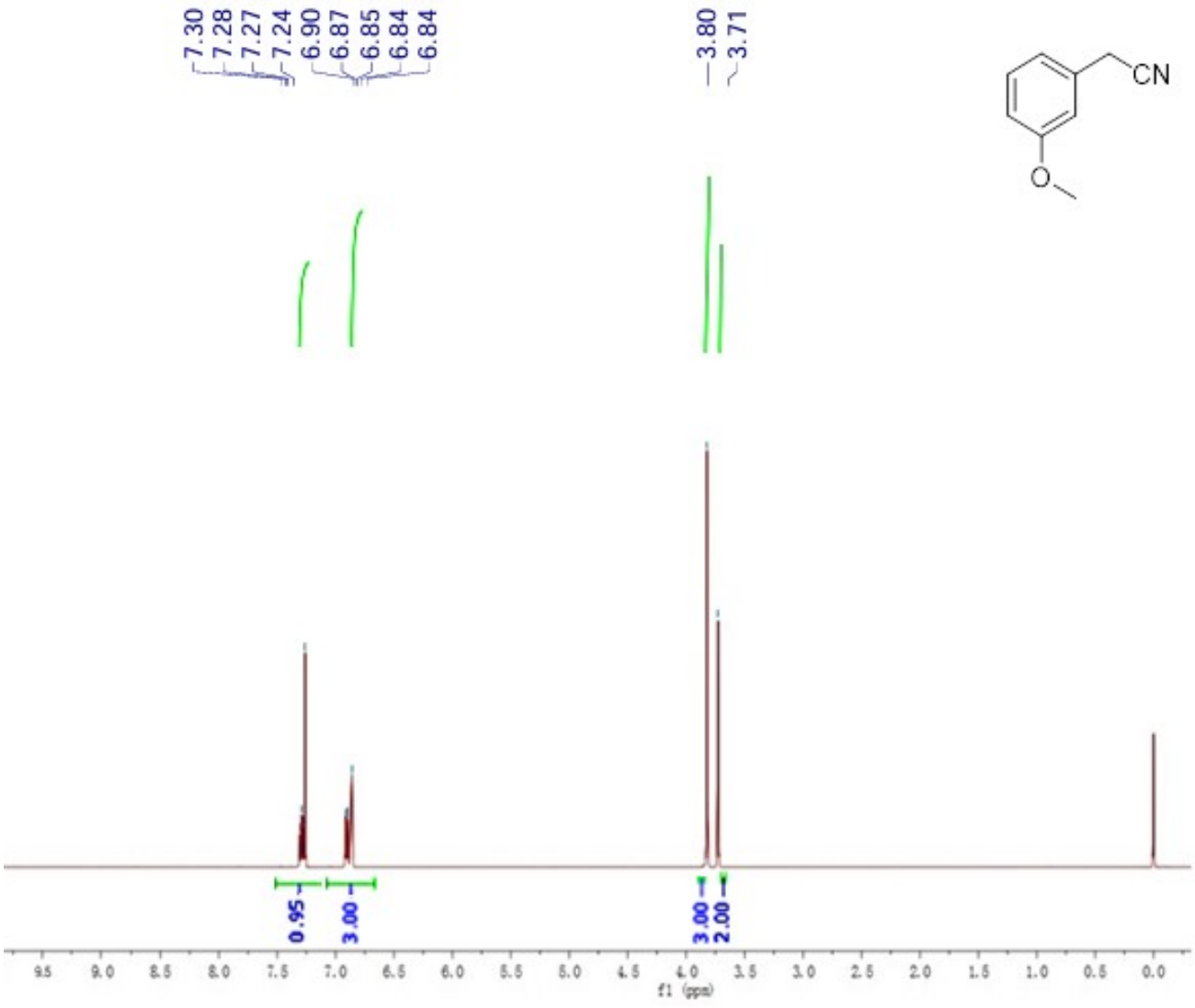
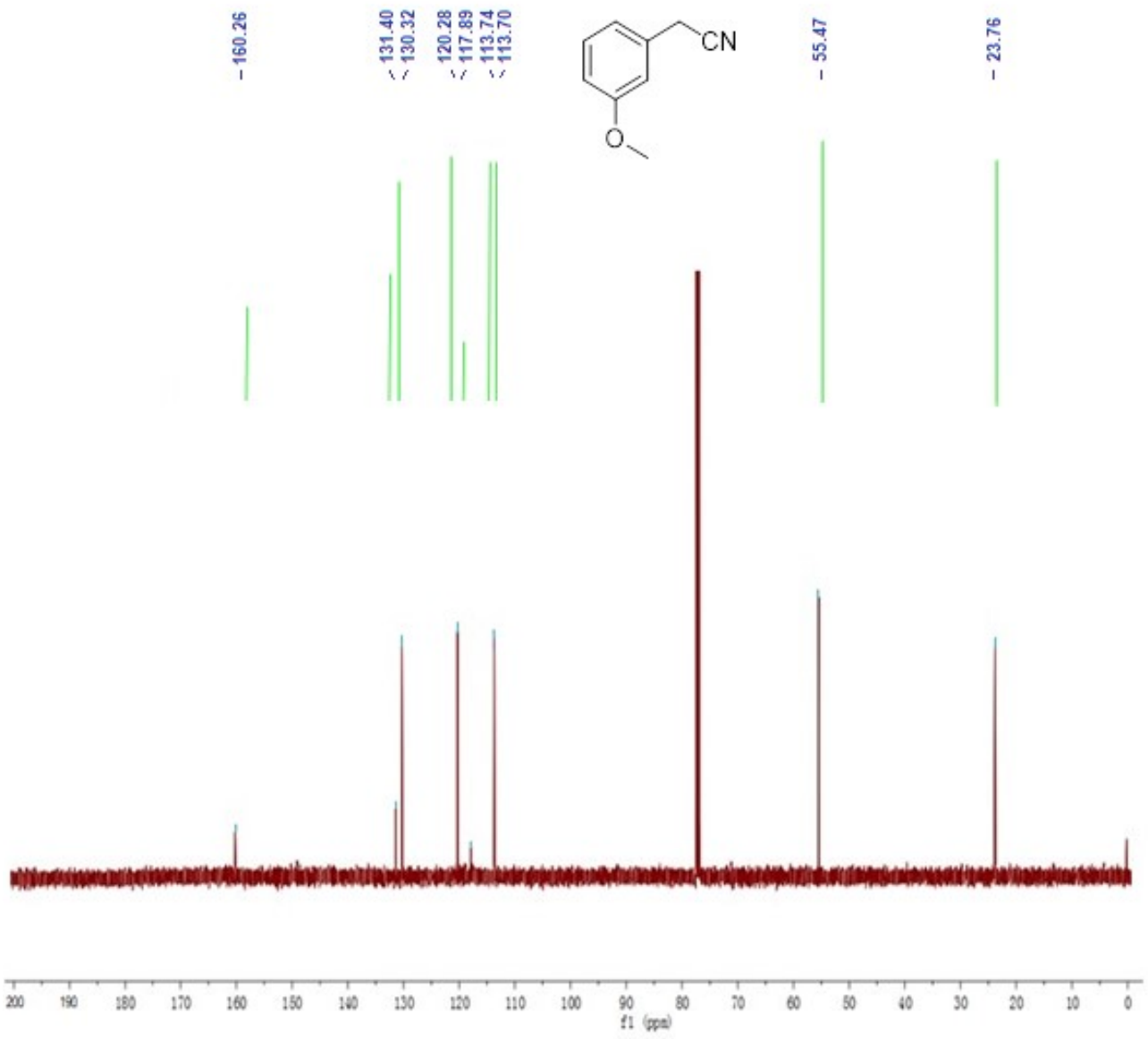
10
0
f1 (ppm)


7.30
7.28
7.27
7.24
6.90
6.87
6.85
6.84
6.84
3.80
3.71
CN
O
0.95
3.00
3.00
2.00
f1 (ppm)


160.26
131.40
130.32
120.28
117.89
113.74
113.70
55.47
23.76
CN
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

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