

Supporting data

Synthesis, Cytotoxicity and Photophysical Investigations of 2-Amino-4,6-diphenylnicotinonitriles: An Experimental and Theoretical Study

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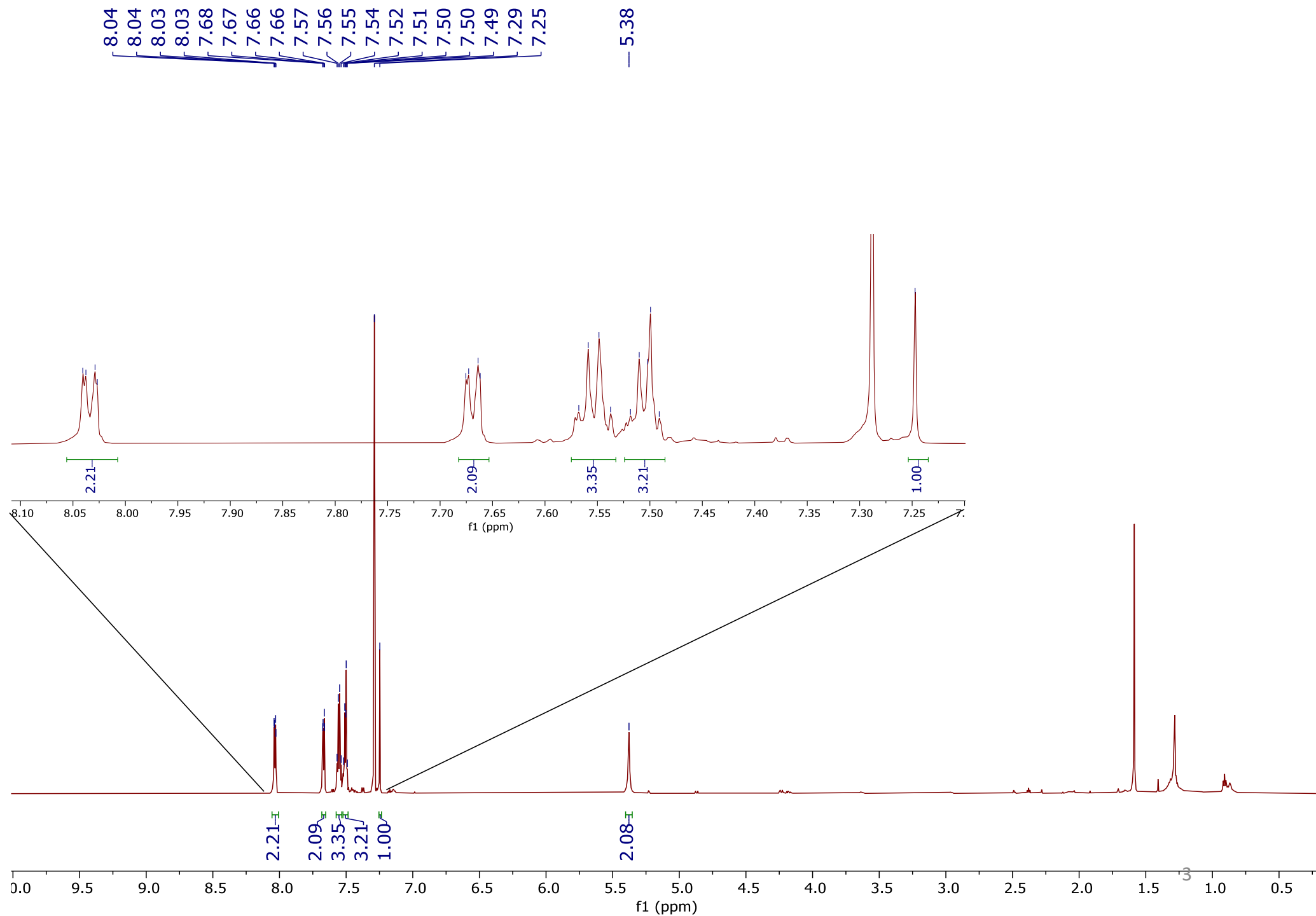
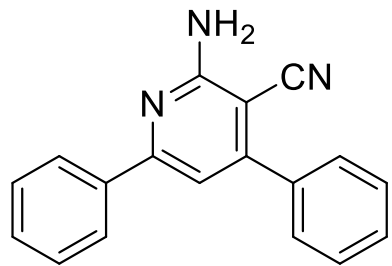
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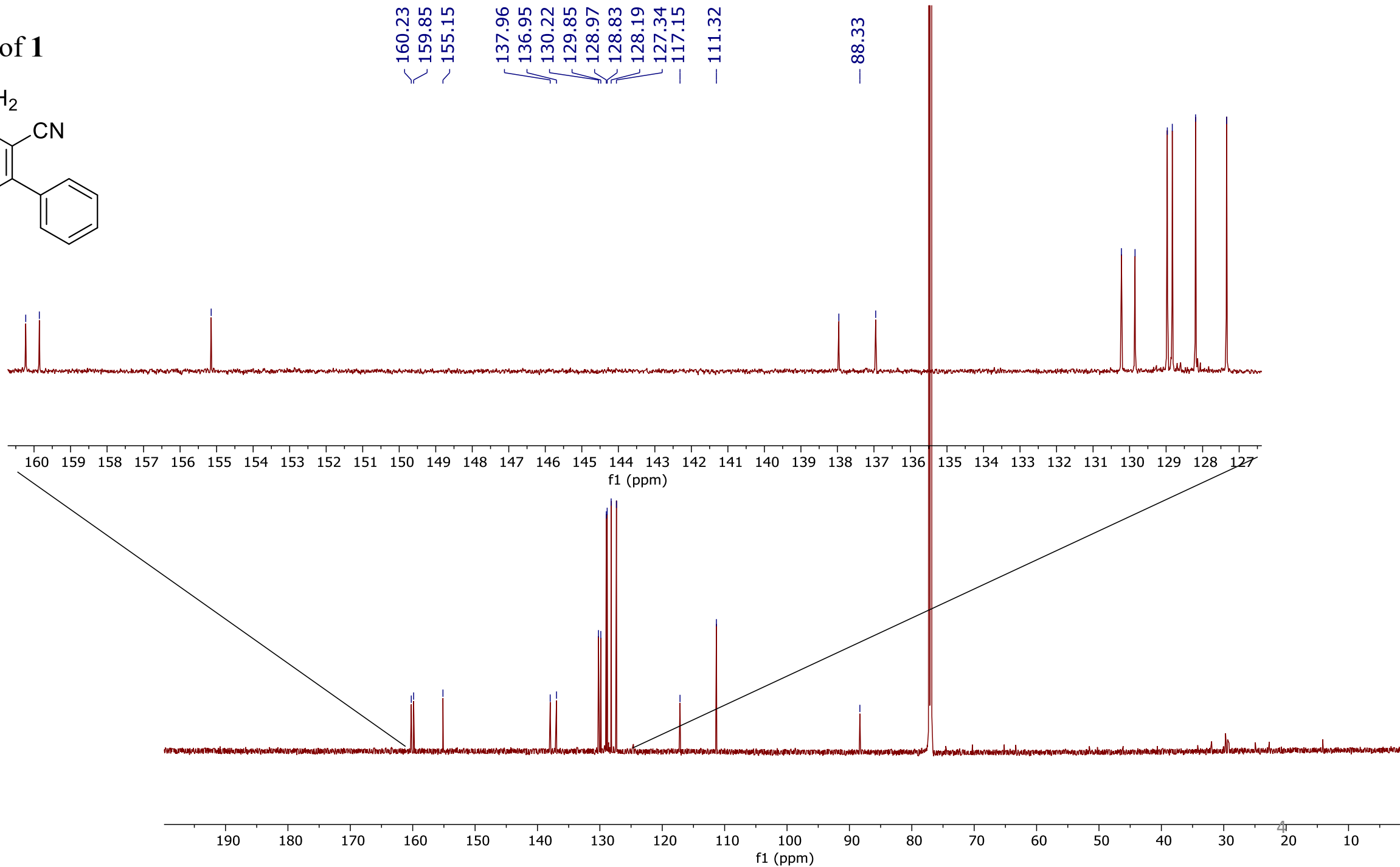
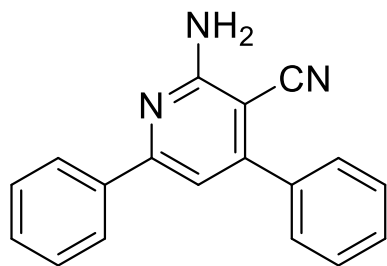
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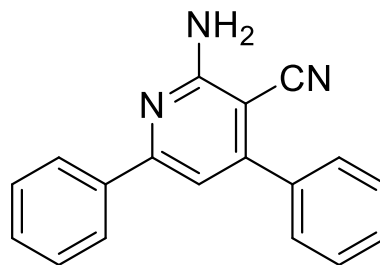
^1H -NMR of **1**



¹³C-NMR of **1**

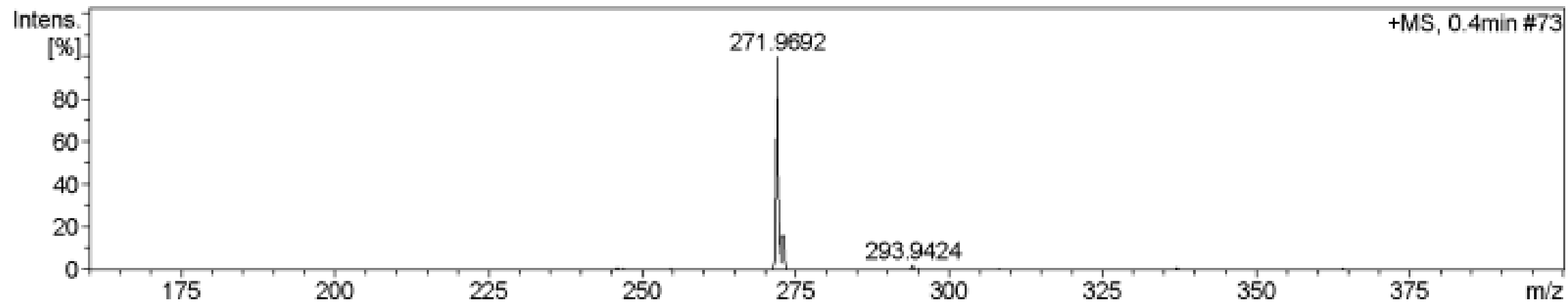


Mass Spectra of **1**

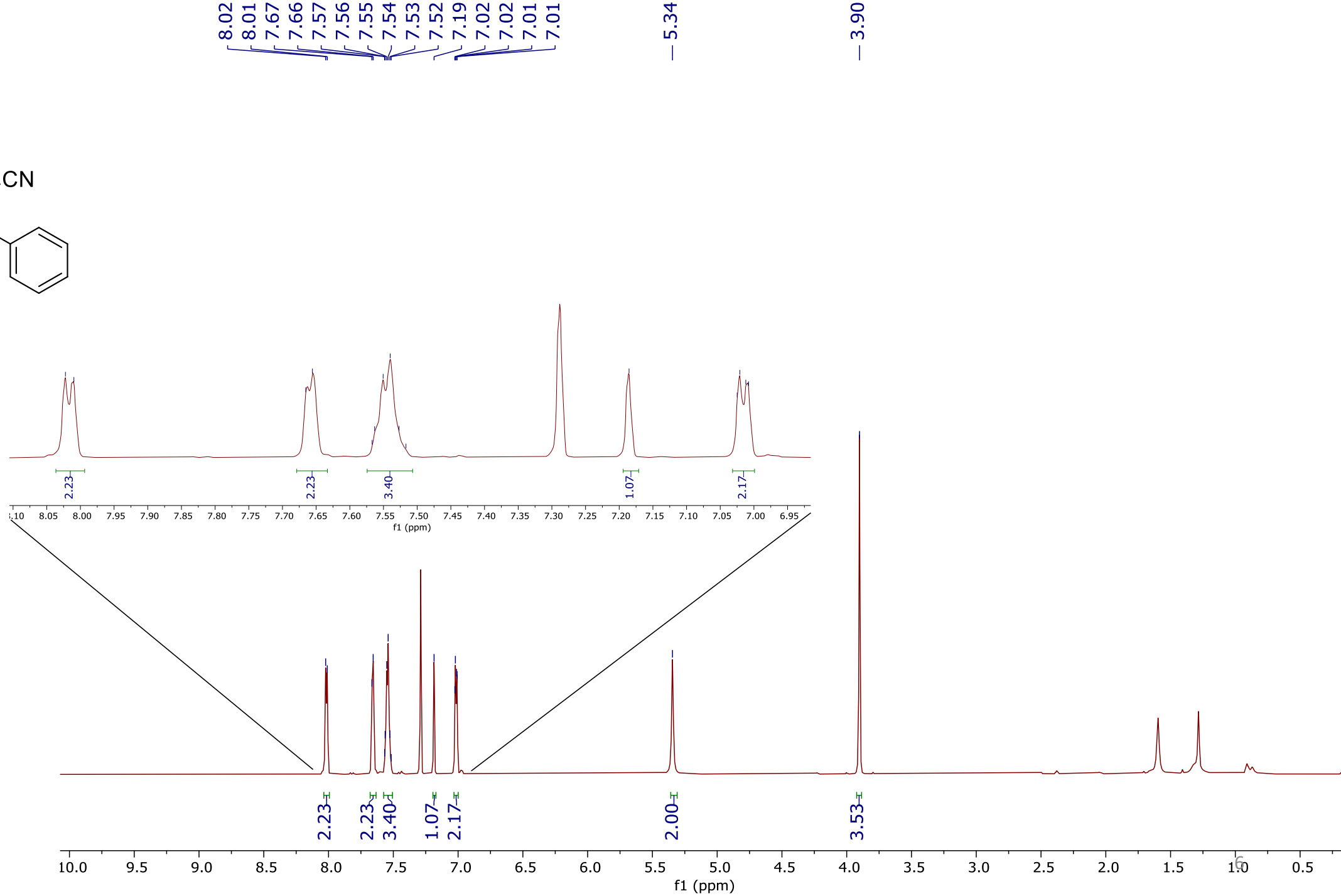
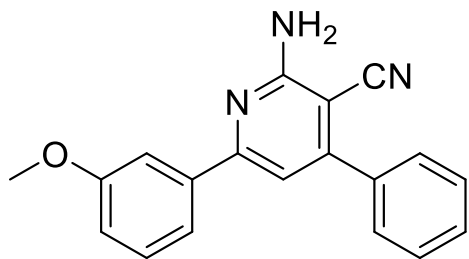


Exact Mass = 271.1109

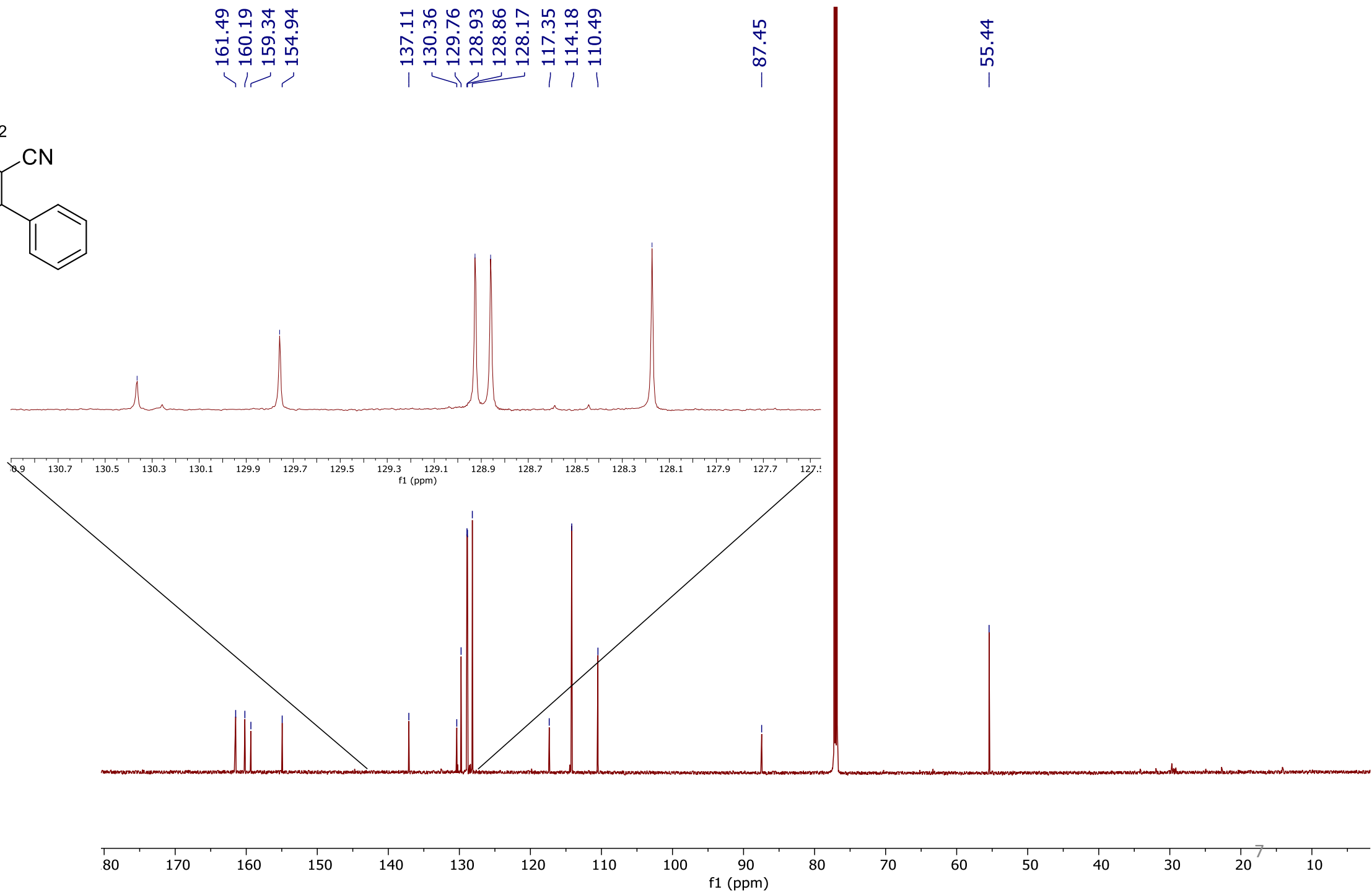
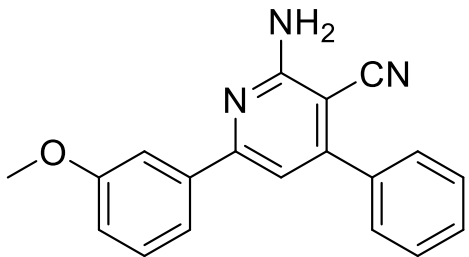
$m/z = 271.9693$ $[M+H]^+$; 293.9424 $[M+Na]^+$



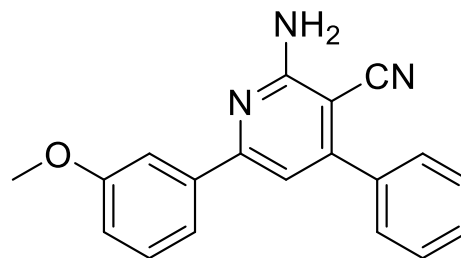
¹H-NMR of 2



¹³C-NMR of **2**

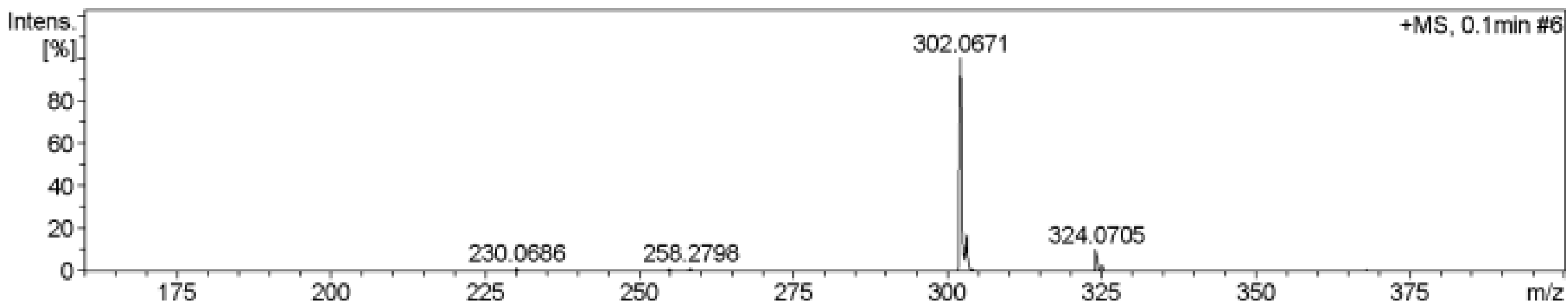


Mass Spectra of **2**

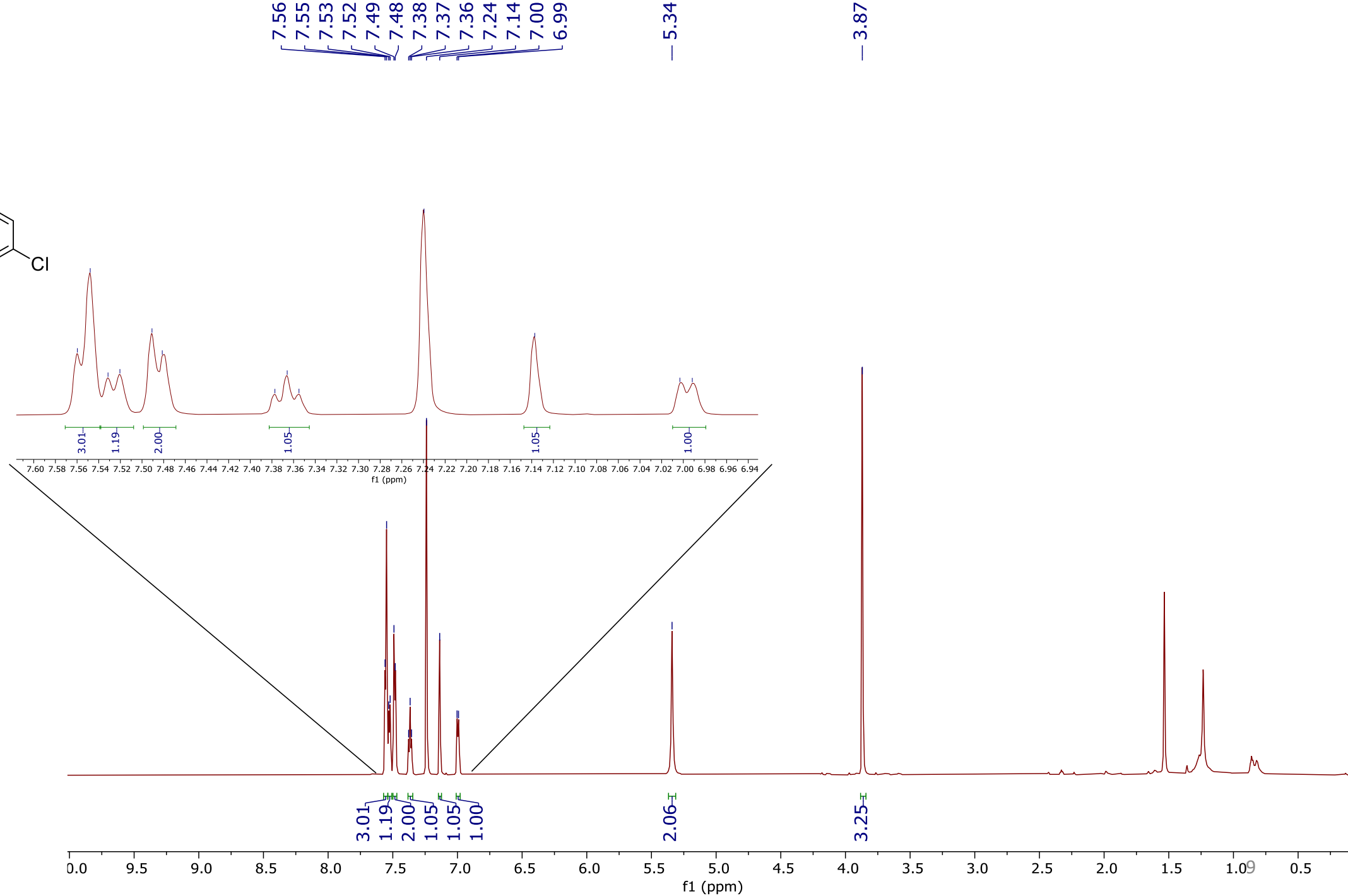
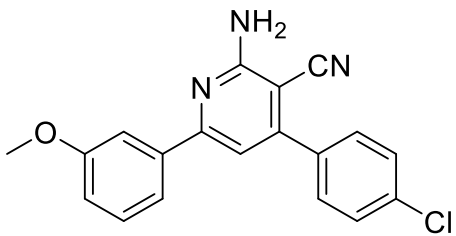


Exact Mass = 301.1215

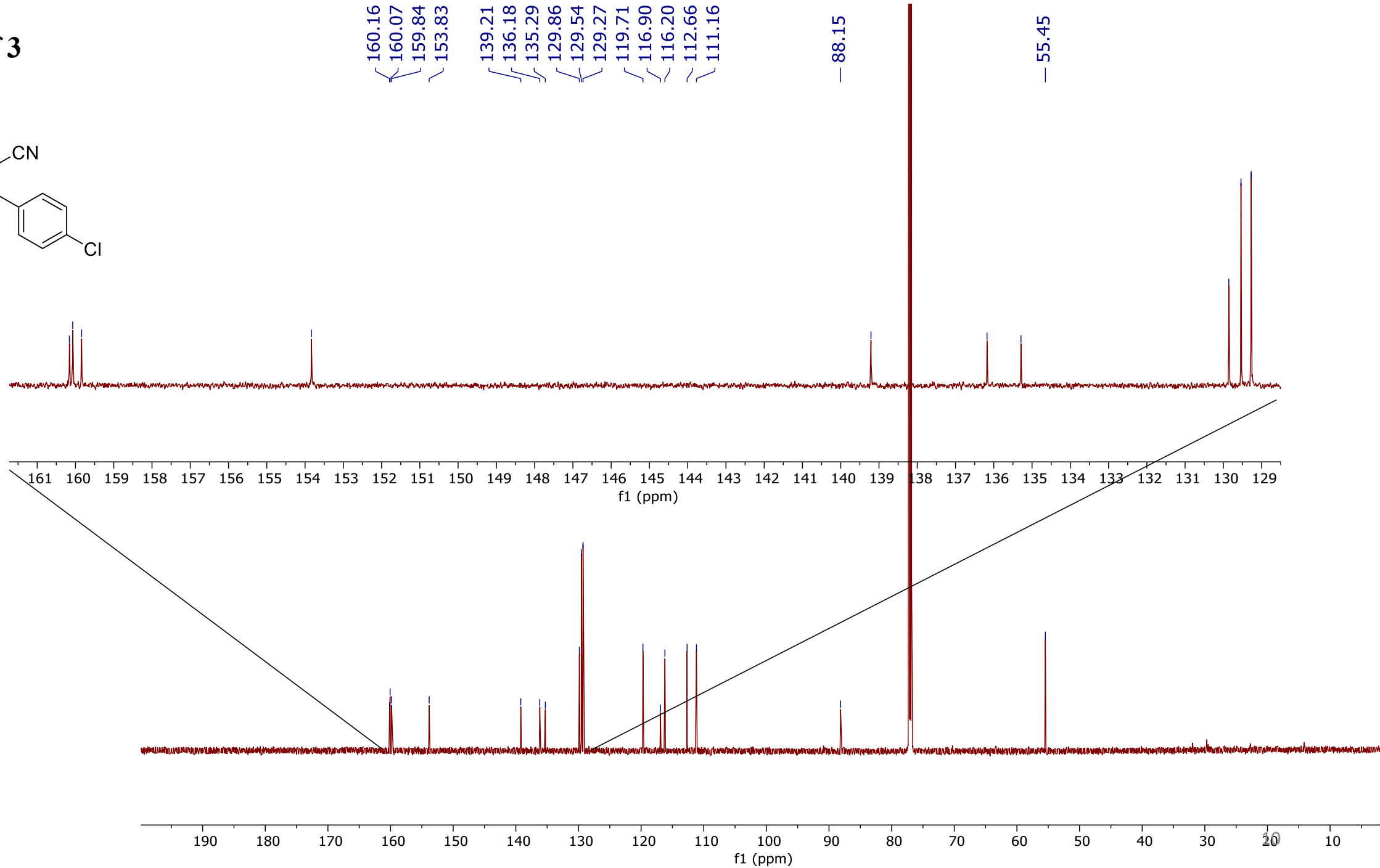
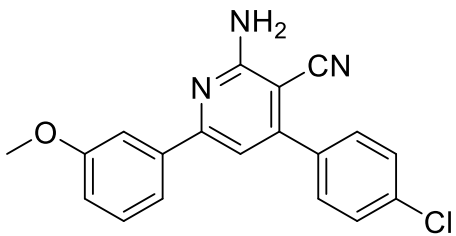
$m/z = 302.0671$ $[M+H]^+$; 324.0705 $[M+Na]^+$



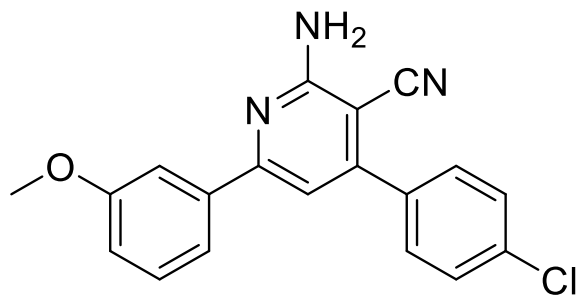
¹H-NMR of 3



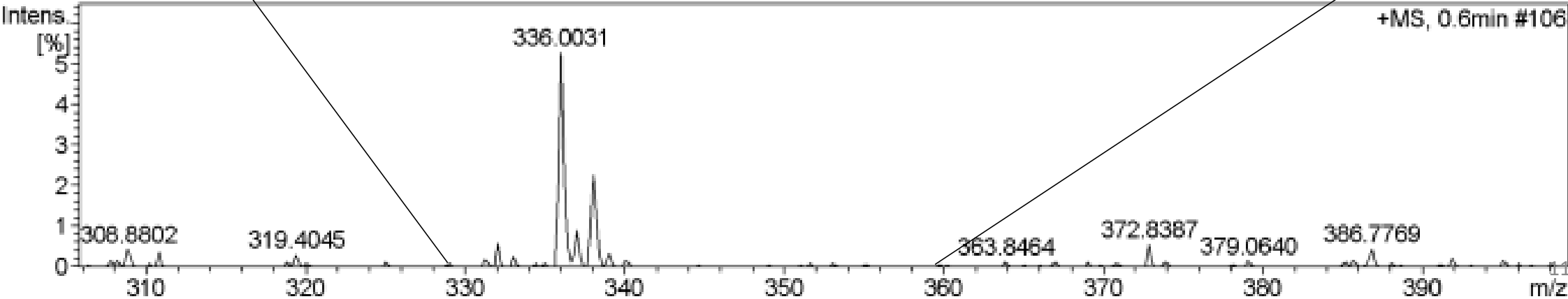
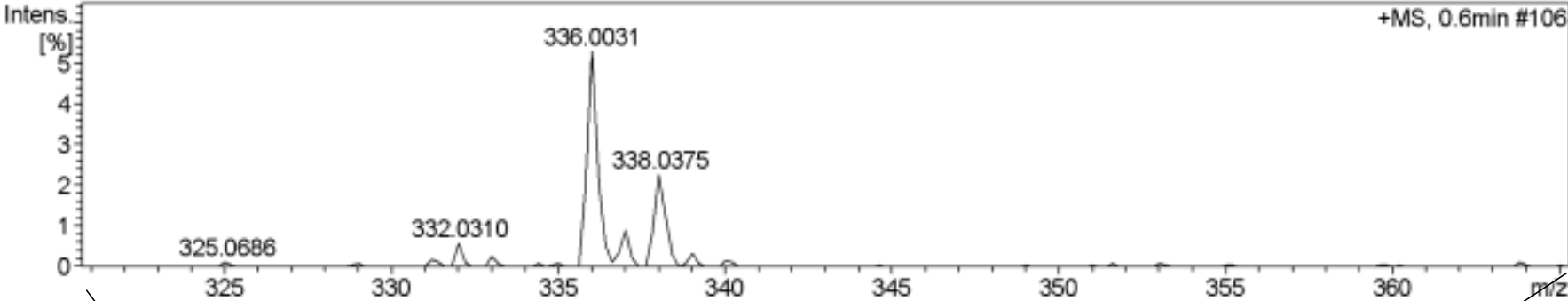
¹³C-NMR of **3**



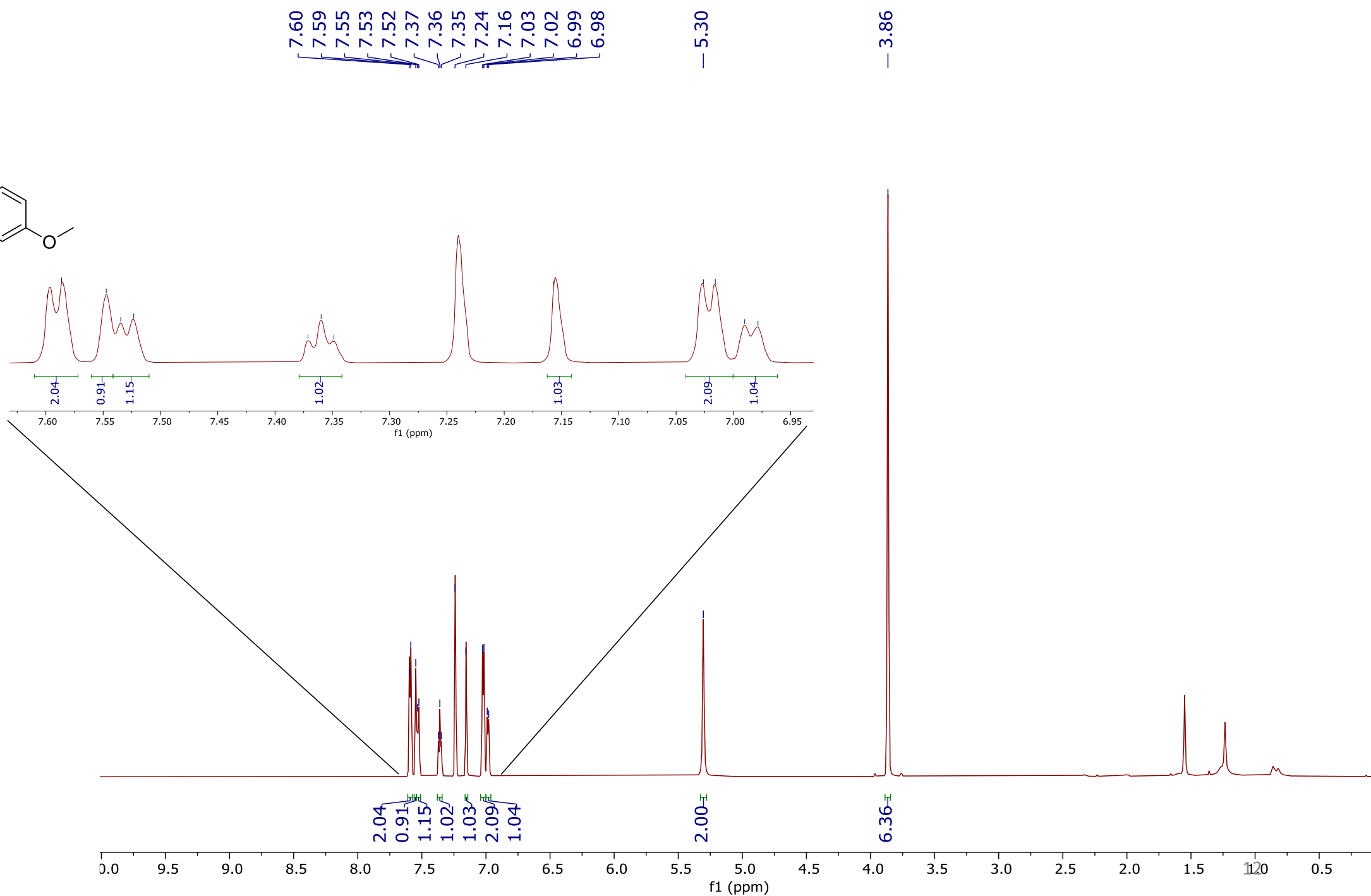
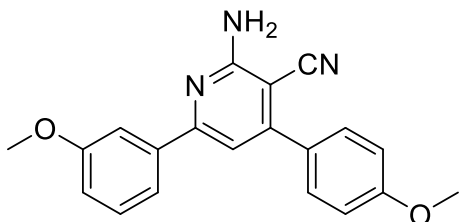
Mass Spectra of 3



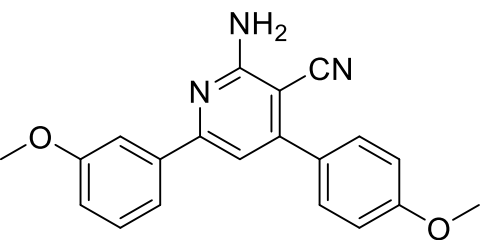
Exact Mass = 335.0825
 m/z 336.0031 $[M(^{35}\text{Cl})+H]^+$; 338.0375 $[M(^{37}\text{Cl})+H]^+$.



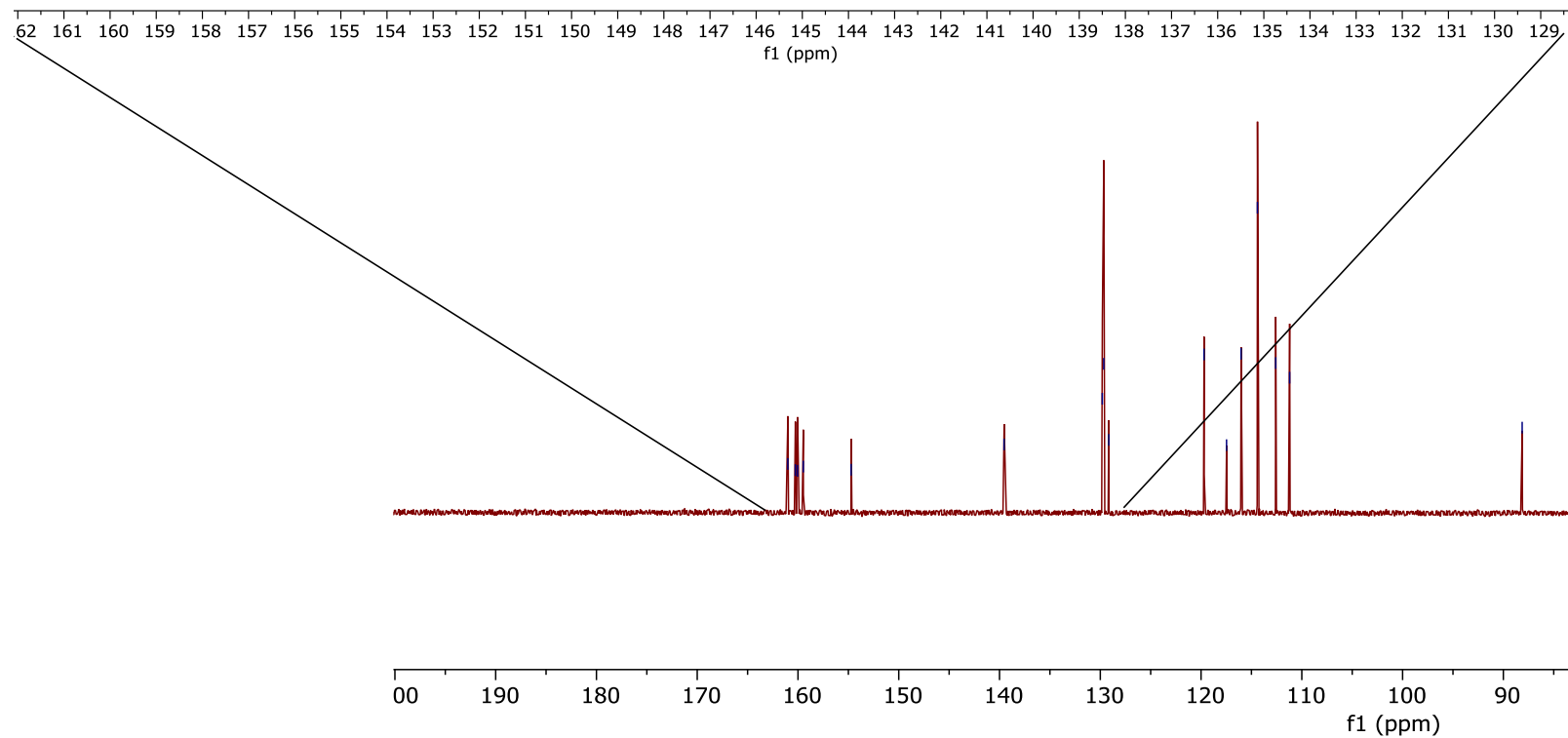
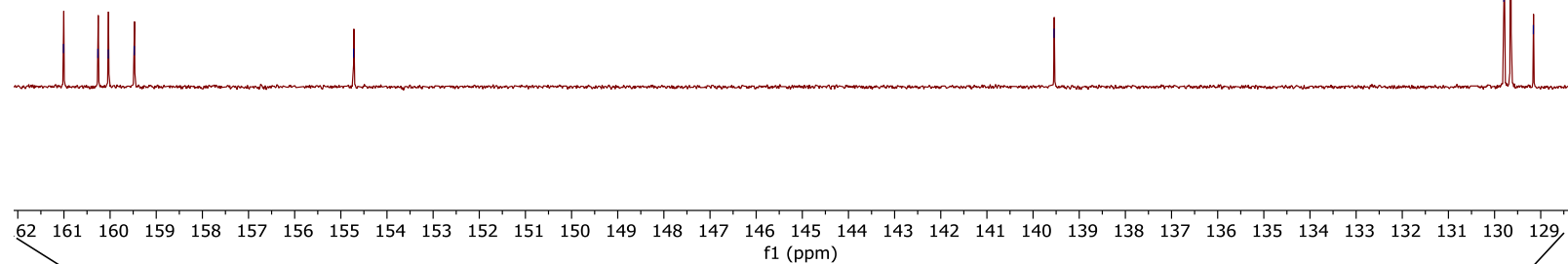
¹H-NMR of 4



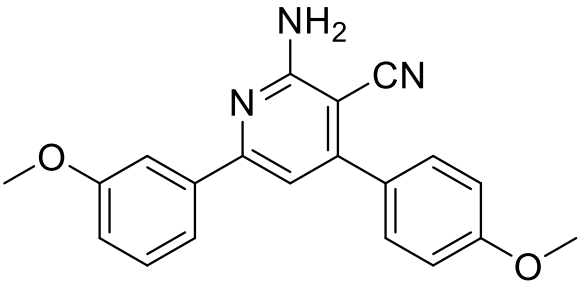
¹³C-NMR of **4**



161.01
160.26
160.04
159.48
154.72
— 139.55
129.80
129.65
129.16
119.71
117.47
116.03
114.40
112.59
111.21
— 88.14
55.45
55.44

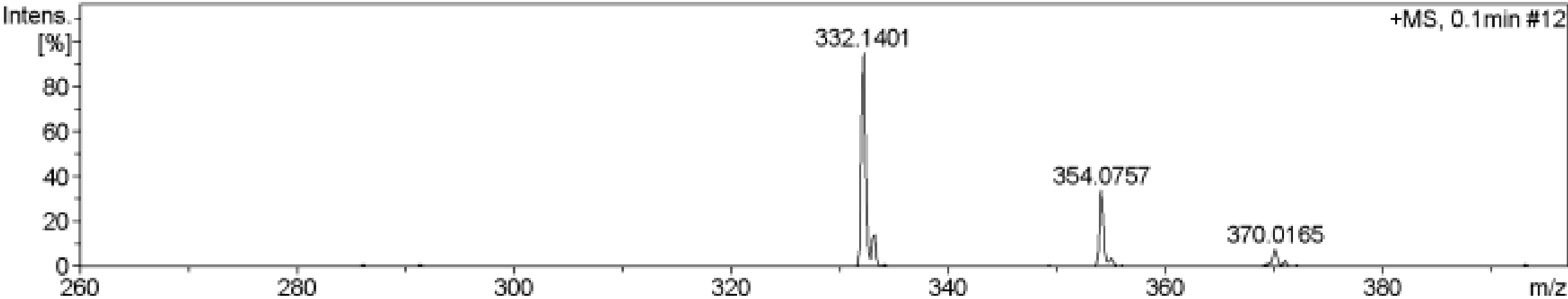


Mass Spectra of 4

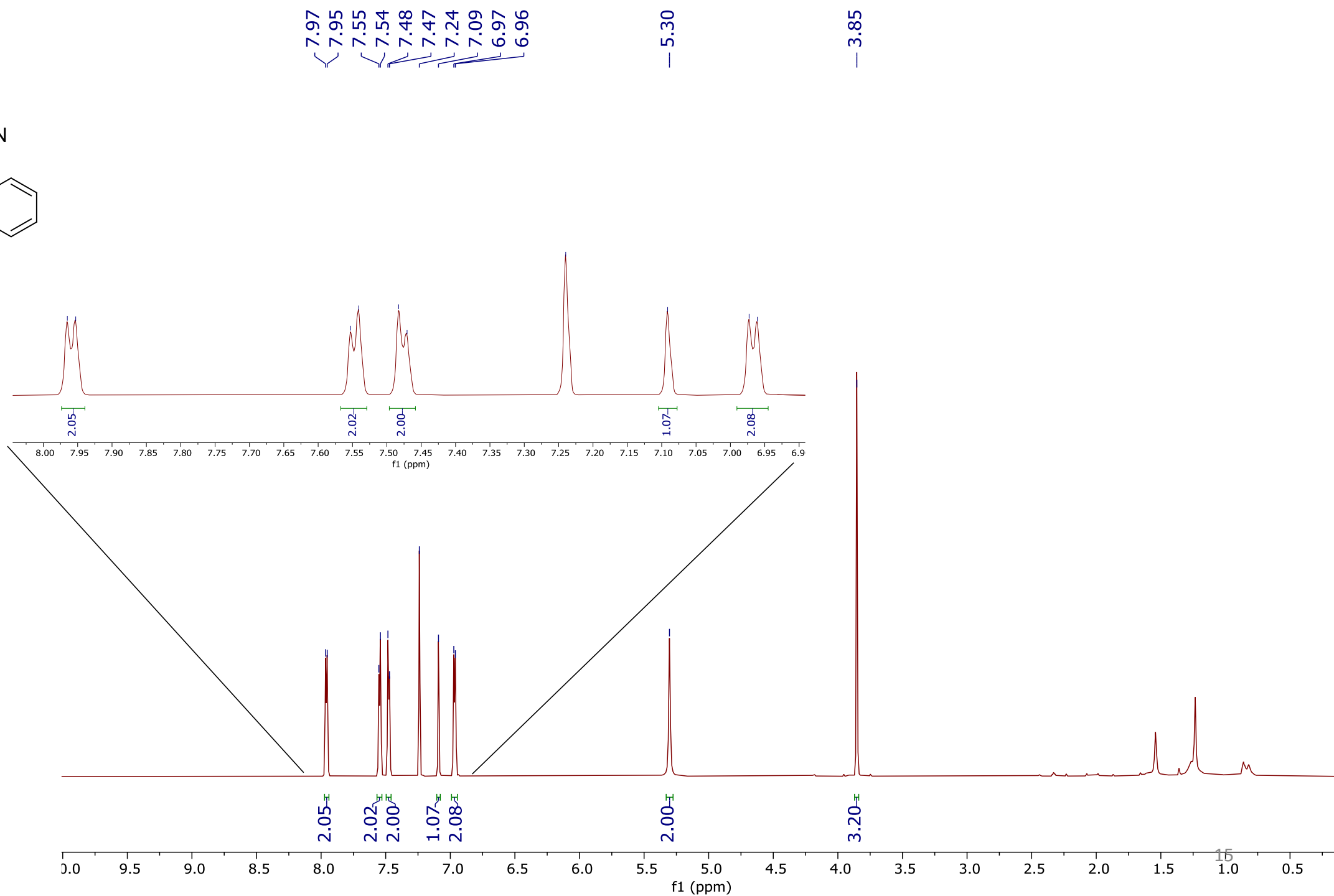
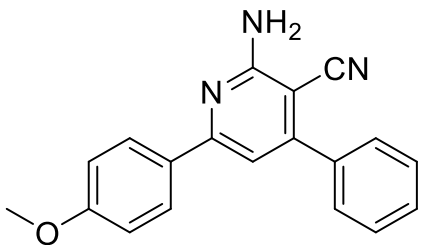


Exact Mass = 331.1321

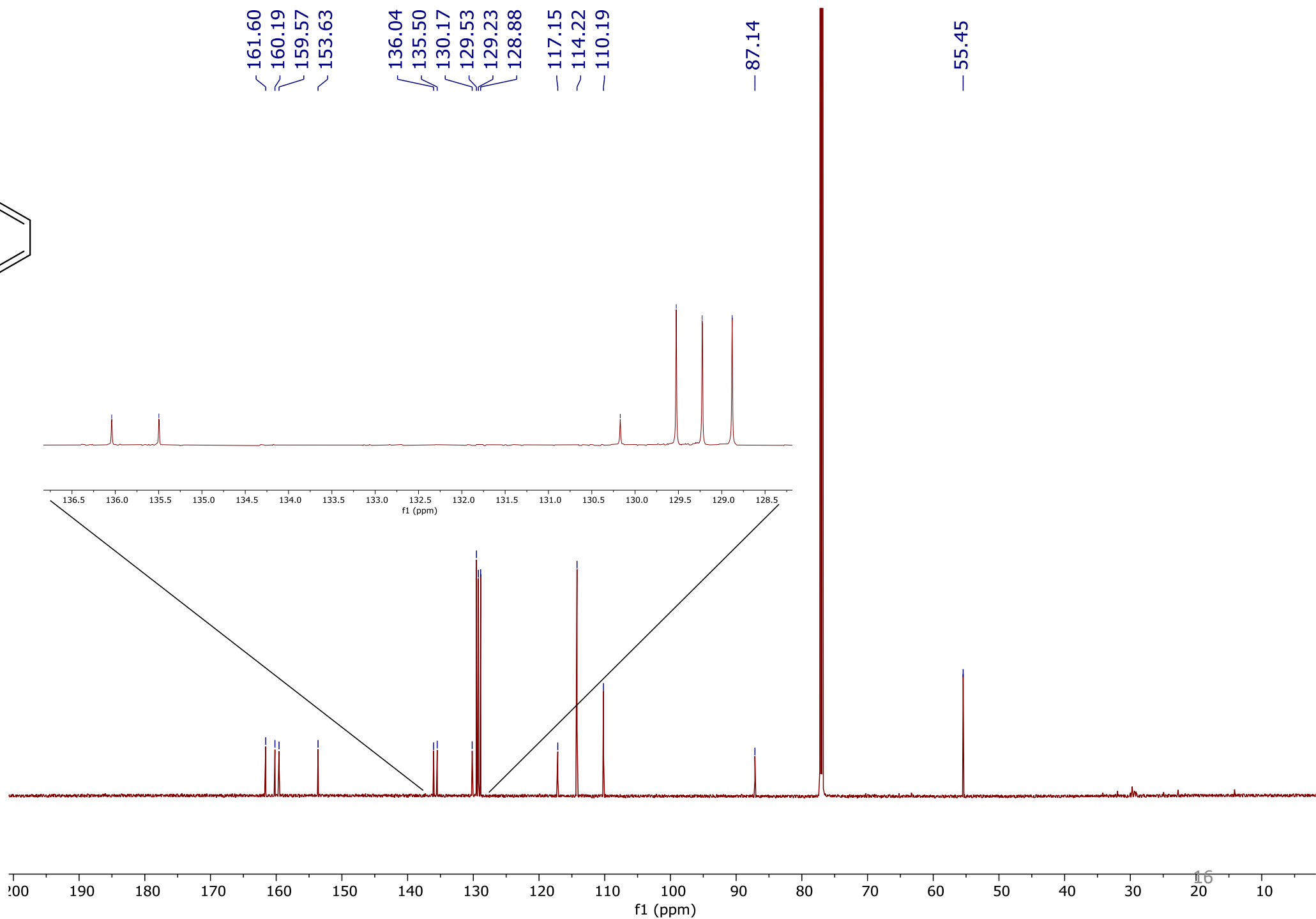
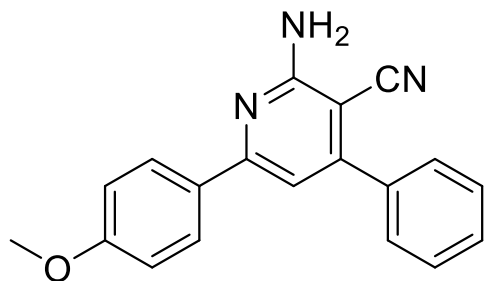
$m/z = 332.1401$ [M+H]⁺; 354.0757 [M+Na]⁺; 370.0165 [M+K]⁺;



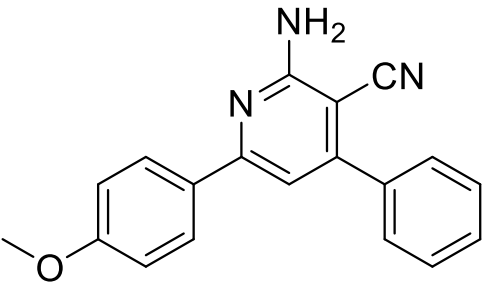
^1H -NMR of **5**



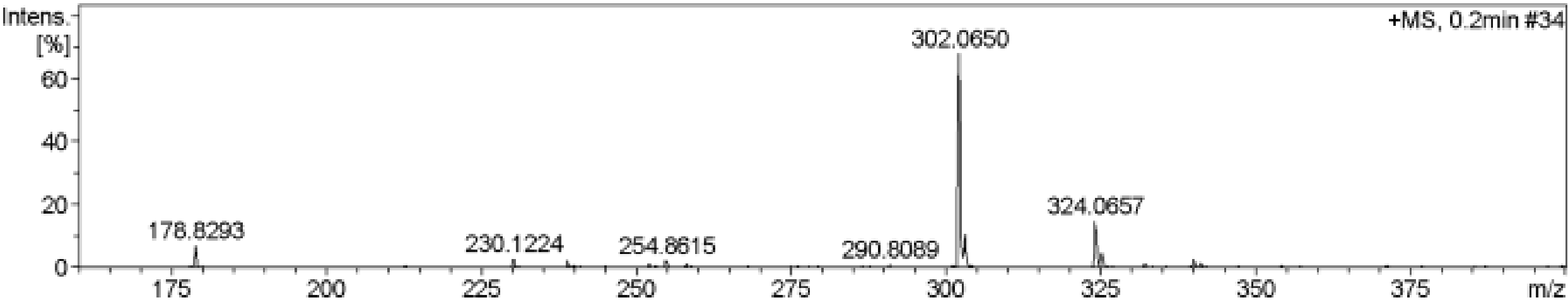
¹³C-NMR of **5**



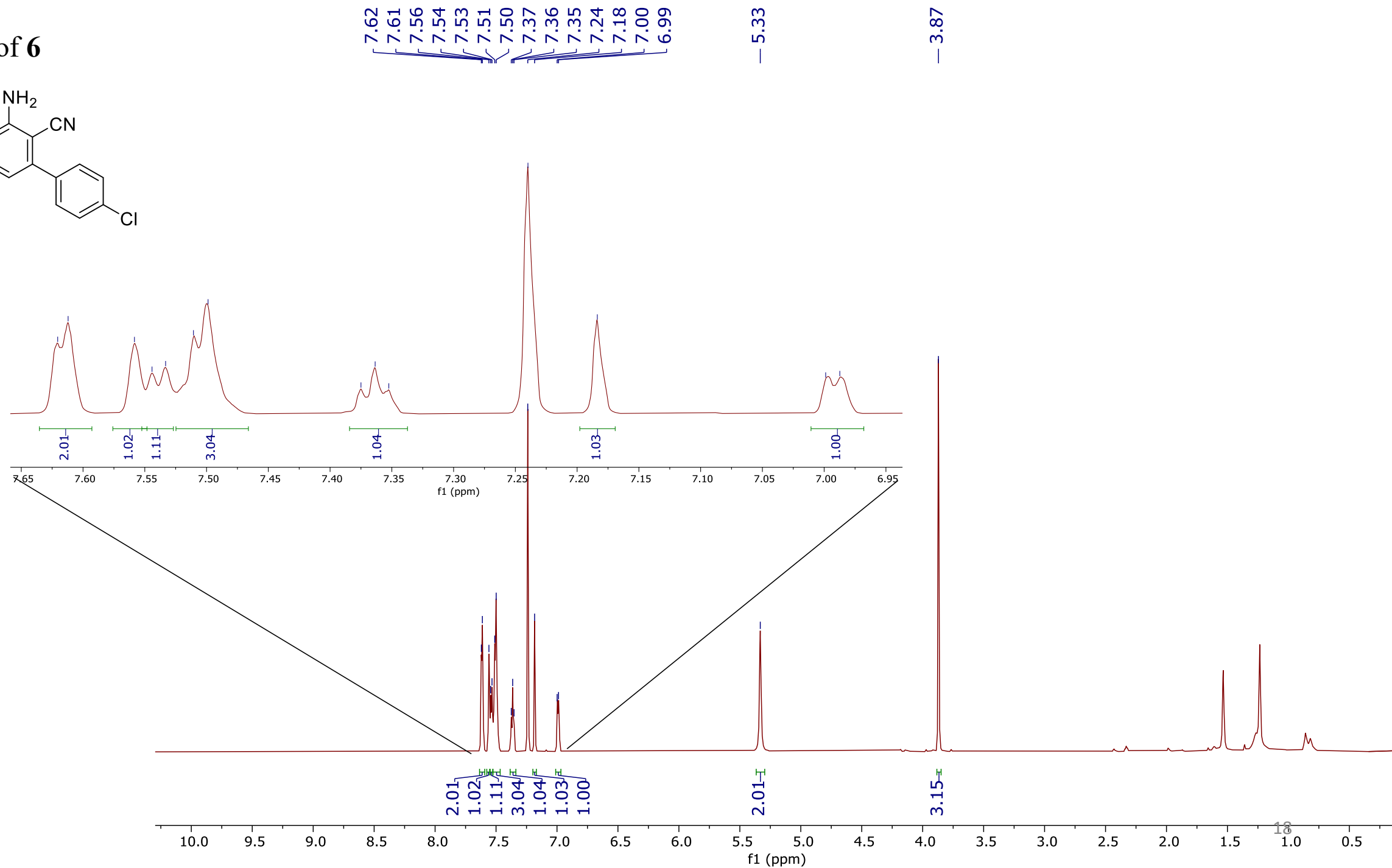
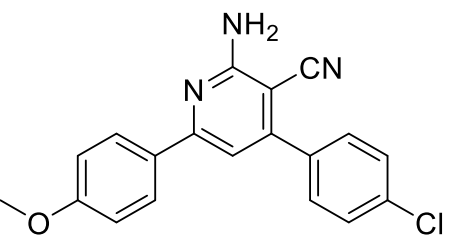
Mass Spectra of 5



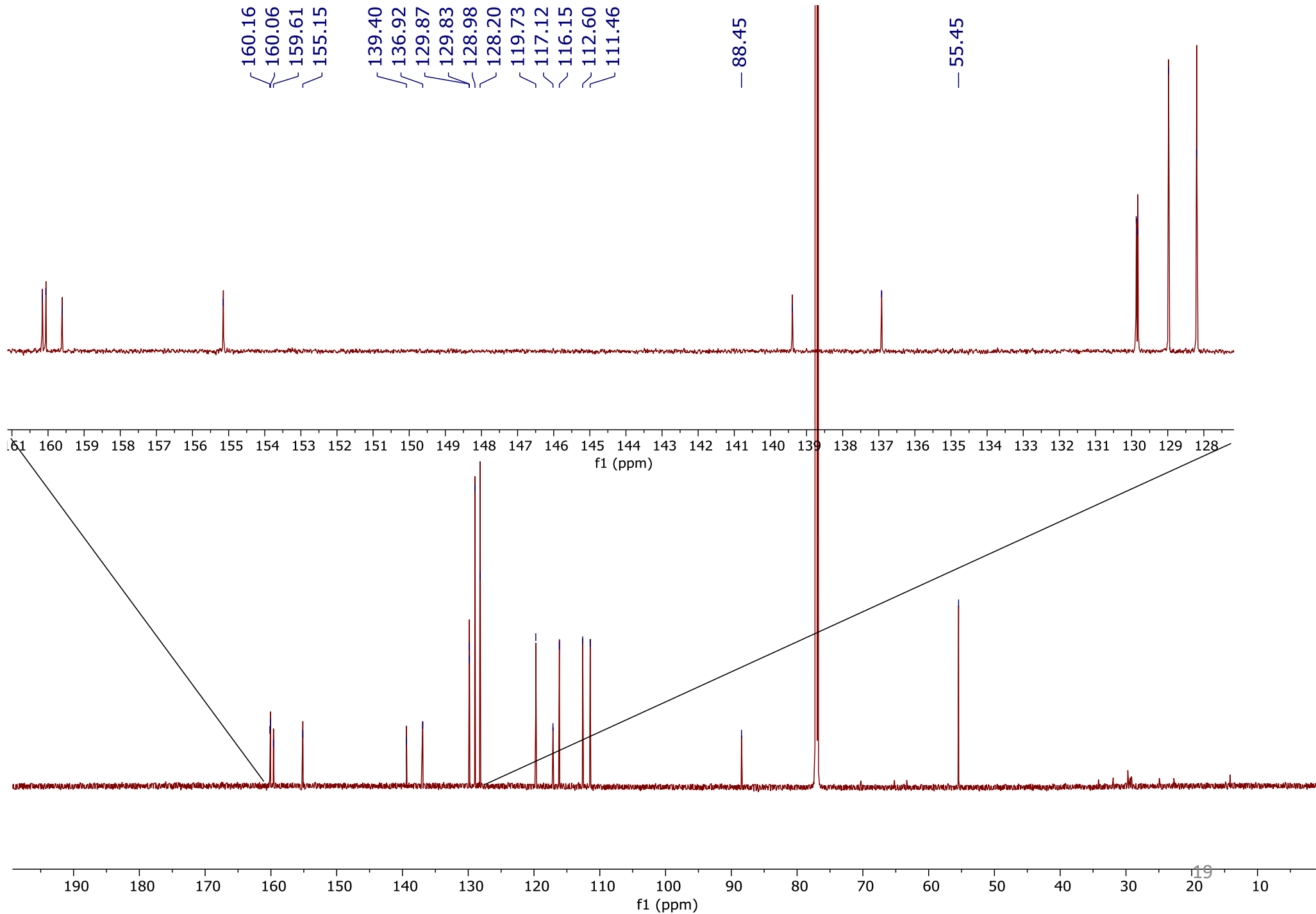
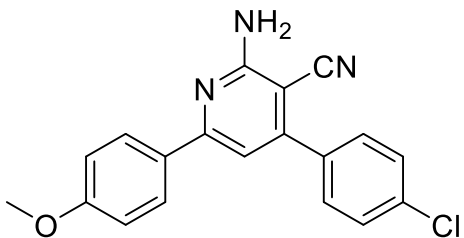
Exact Mass = 301.1215
 $m/z = 302.0650$ [M+H]⁺; 324.0657 [M+Na]⁺



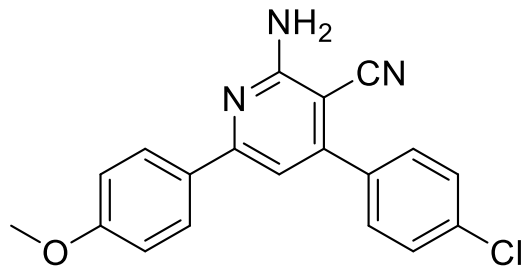
¹H-NMR of 6



¹³C-NMR of **6**



Mass Spectra of **6**



Exact Mass = 335.0825

m/z 336.116 $[M(^{35}\text{Cl})+H]^+$; 338.0885 $[M(^{37}\text{Cl})+H]^+$; 358.0559 $[M(^{35}\text{Cl})+Na]^+$; 359.9924 $[M(^{37}\text{Cl})+Na]^+$.

