

Palladium-Catalyzed Synthesis of Benzimidazoles and Quinazolinones from Common Precursors

Jessie E.R. Sadig, Radleigh Foster, Florian Wakenhut and Michael C. Willis*.

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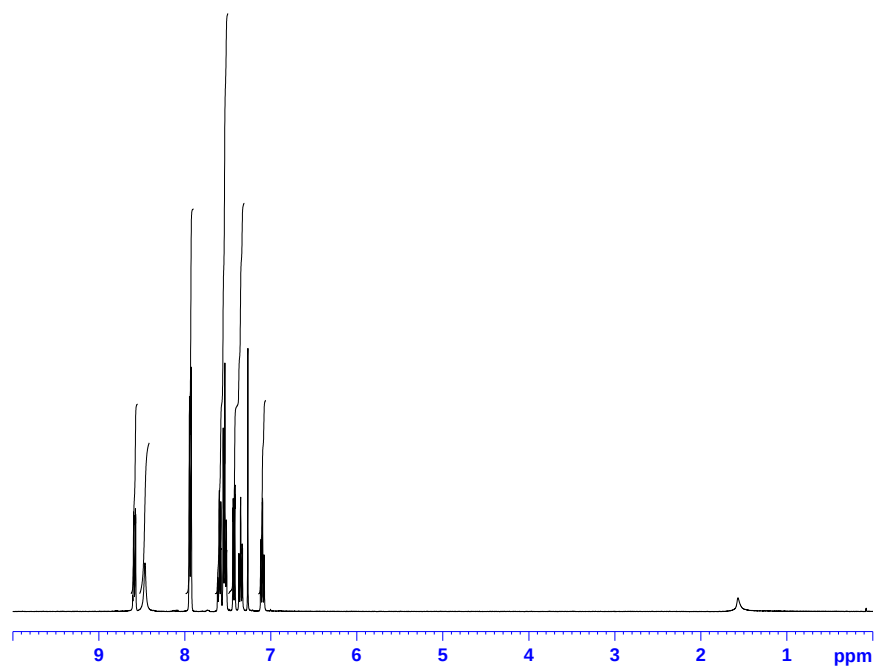
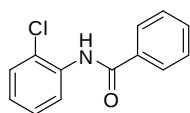
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Supporting Information

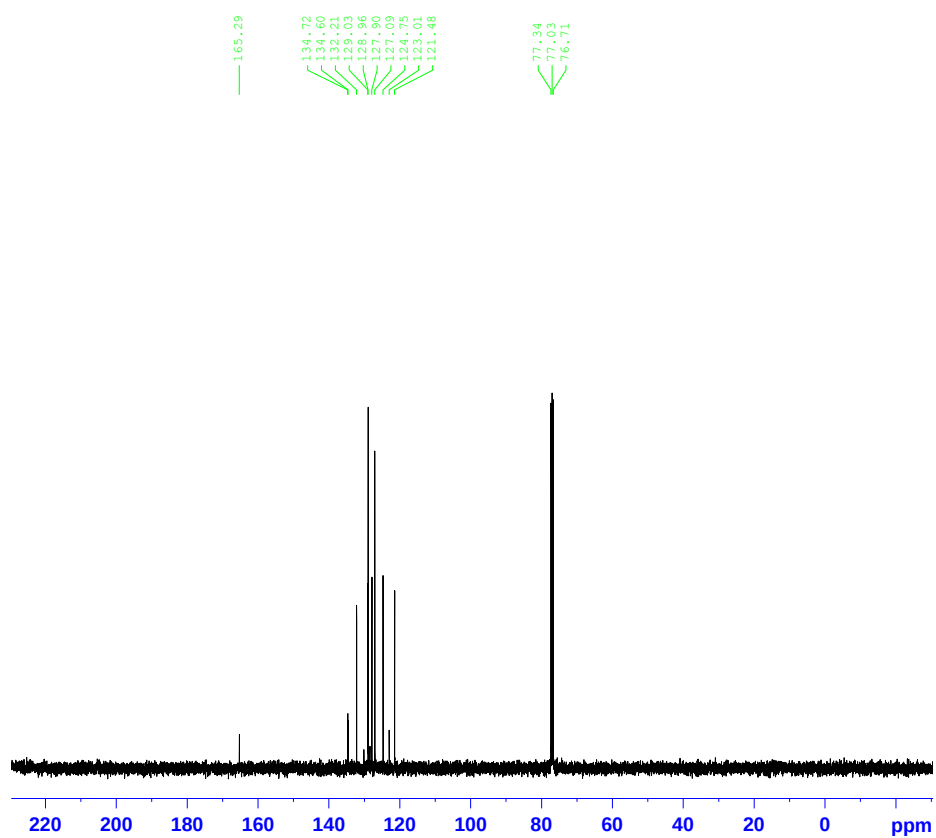
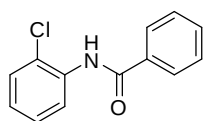
Contents

Amides 9a-9l NMR Spectra (^1H / ^{13}C)	2-13
Imidoyl chlorides 5a-5l NMR Spectra (^1H / ^{13}C)	14-25
Imidates 6a-6o NMR Spectra (^1H / ^{13}C)	26-40
Benzimidazoles 7a-7y NMR Spectra (^1H / ^{13}C)	41-65
Quinazolinones 8a-8r NMR Spectra (^1H / ^{13}C)	66-82
Amidine 11 NMR Spectra (^1H / ^{13}C)	83

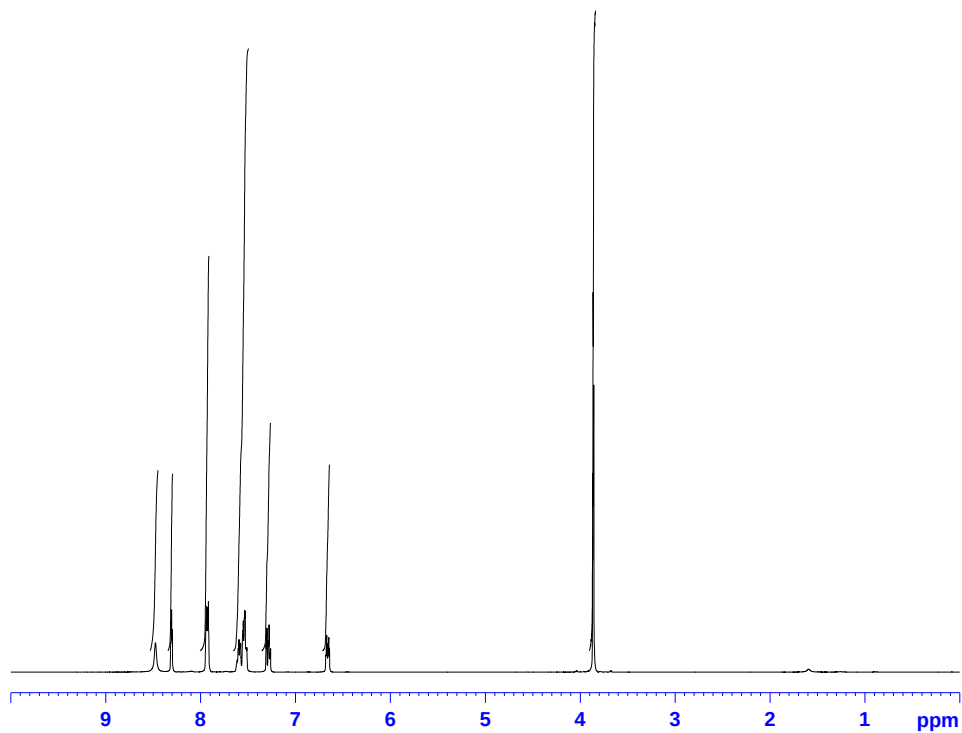
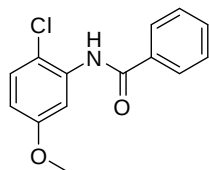
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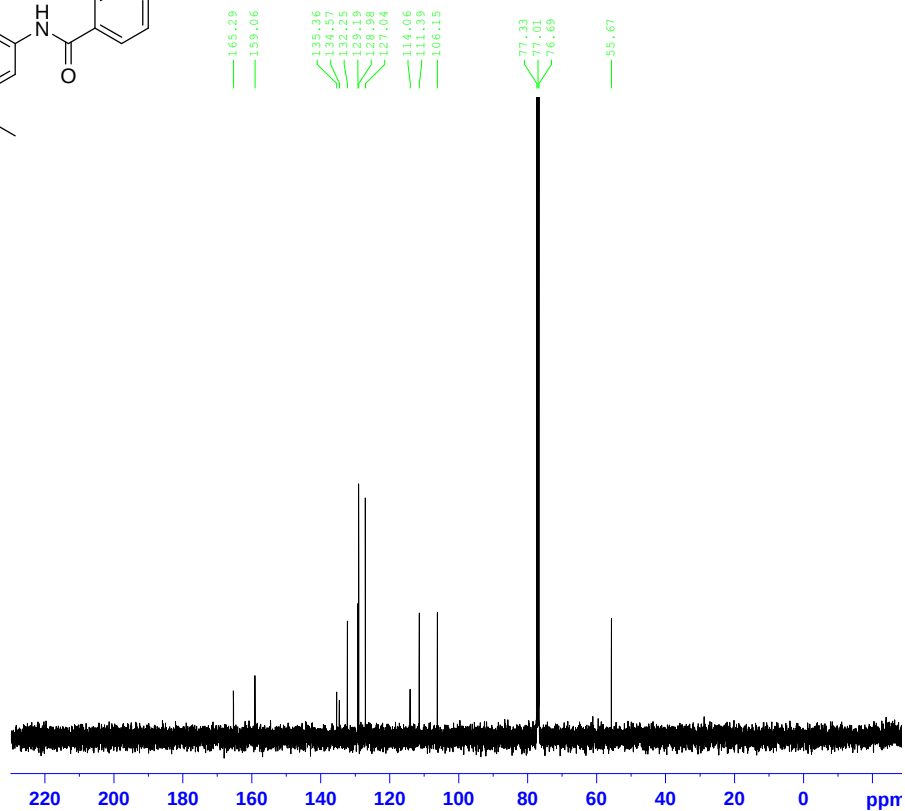
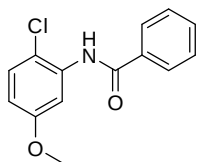
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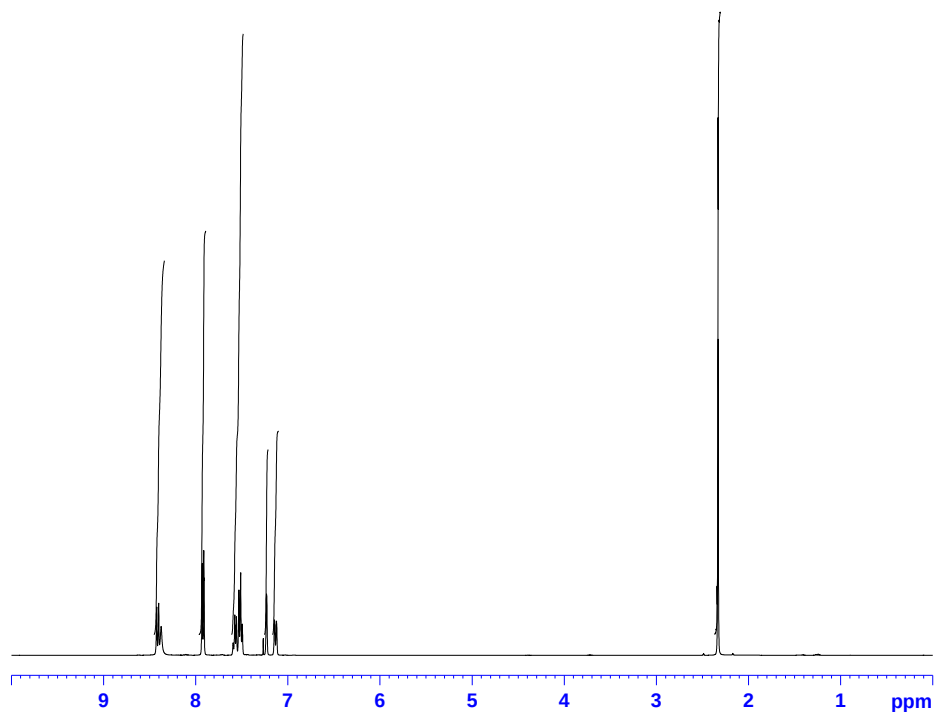
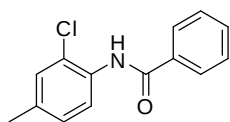
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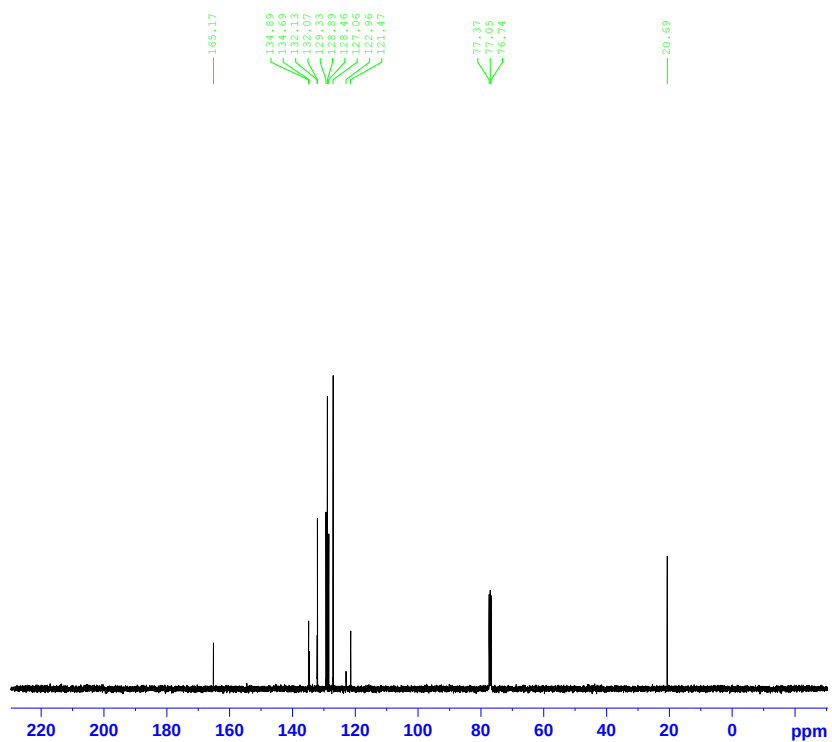
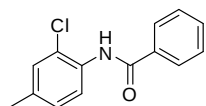
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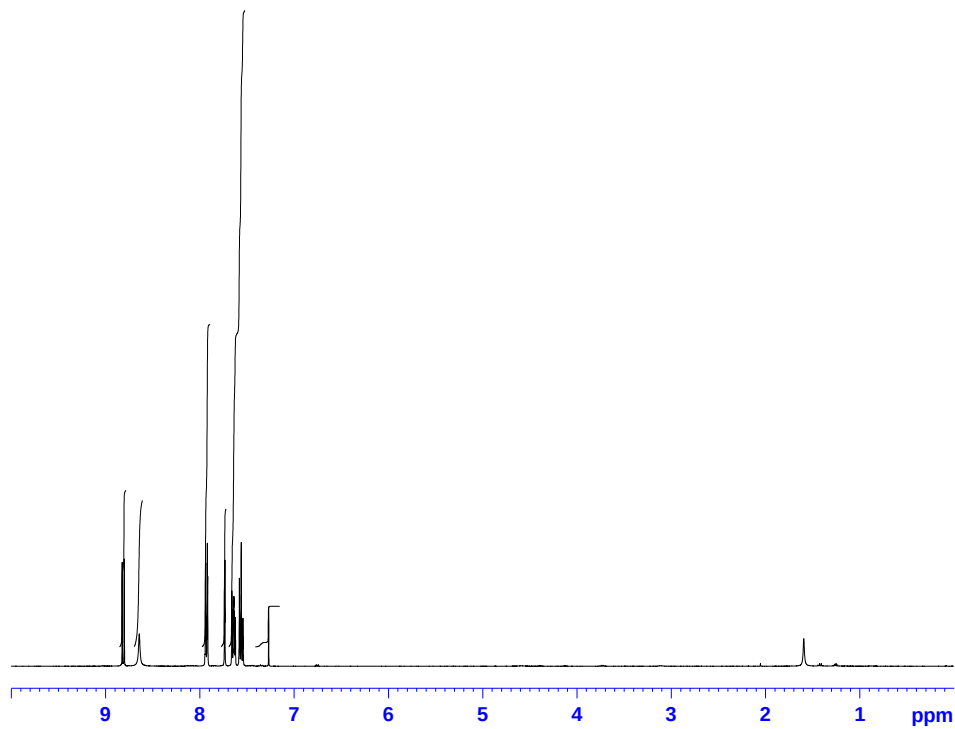
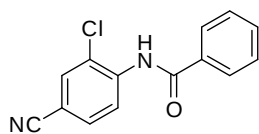
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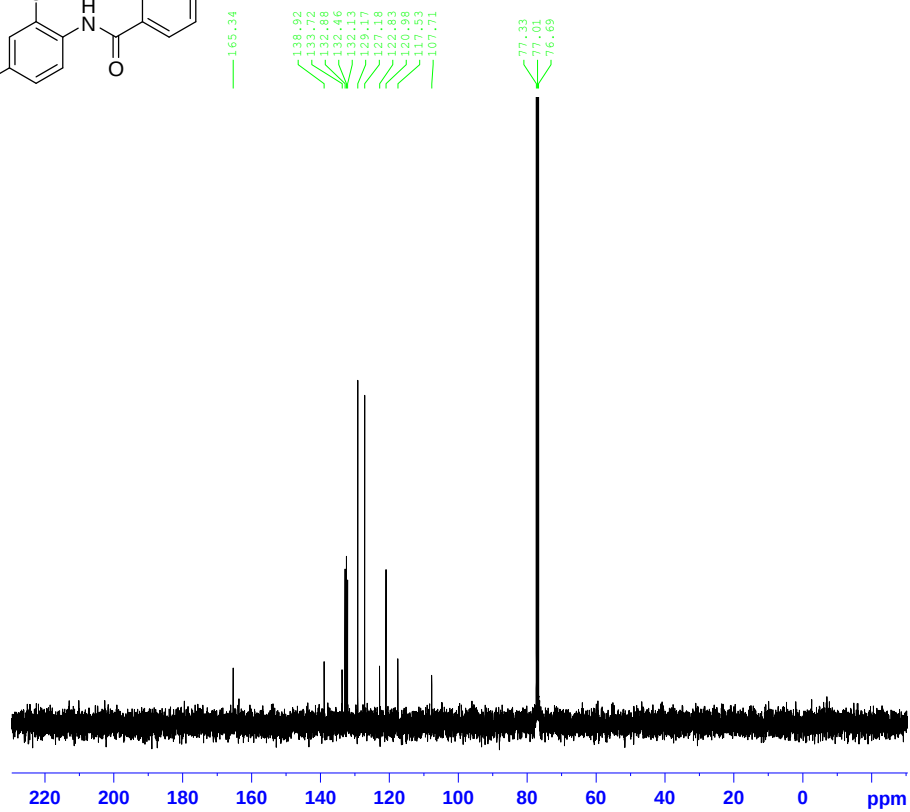
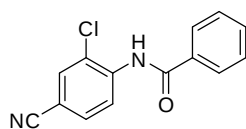
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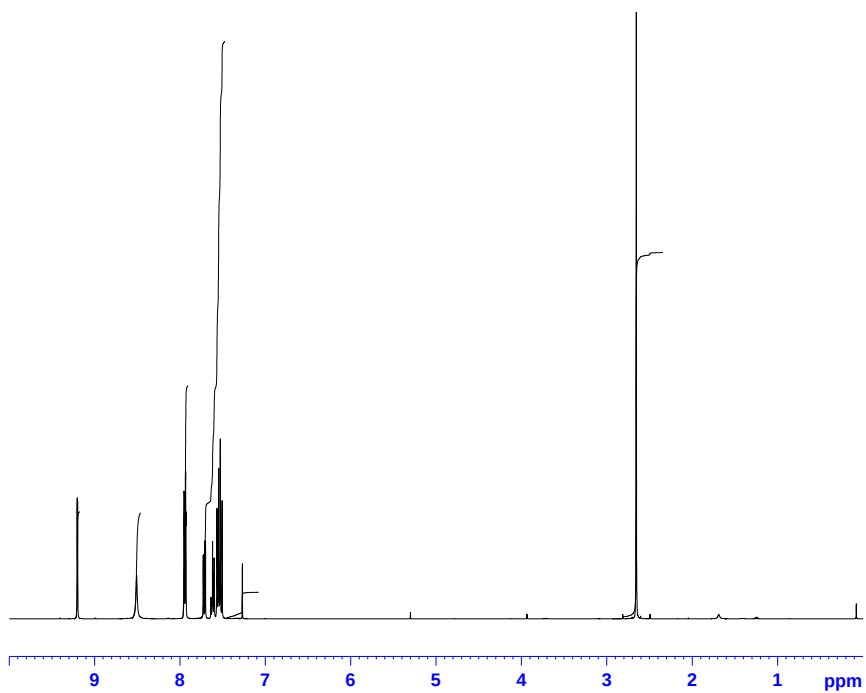
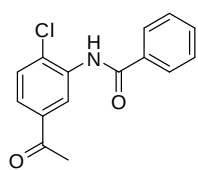
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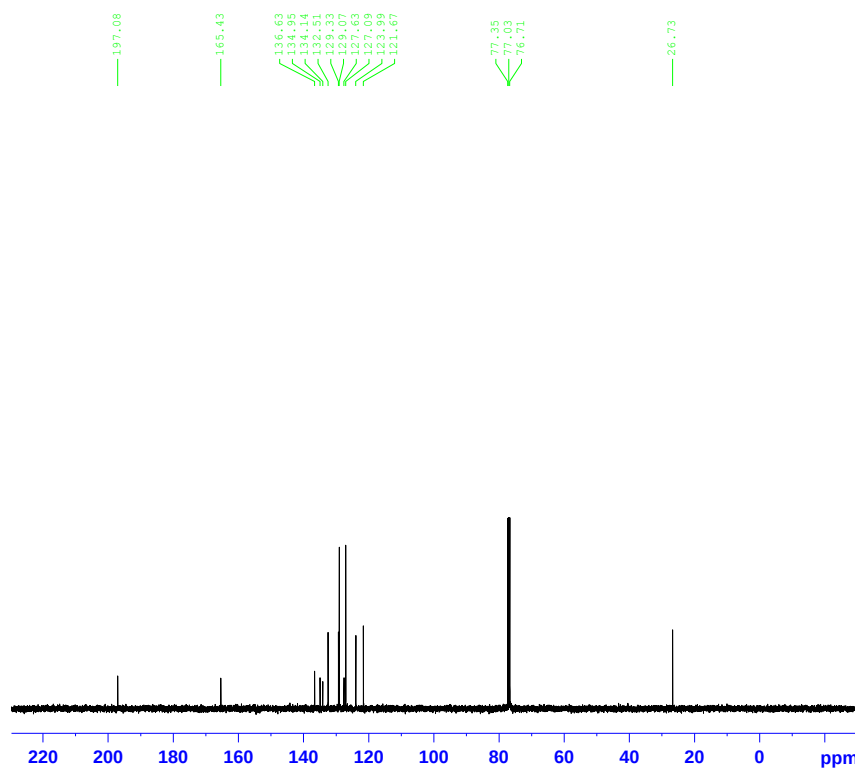
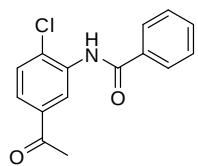
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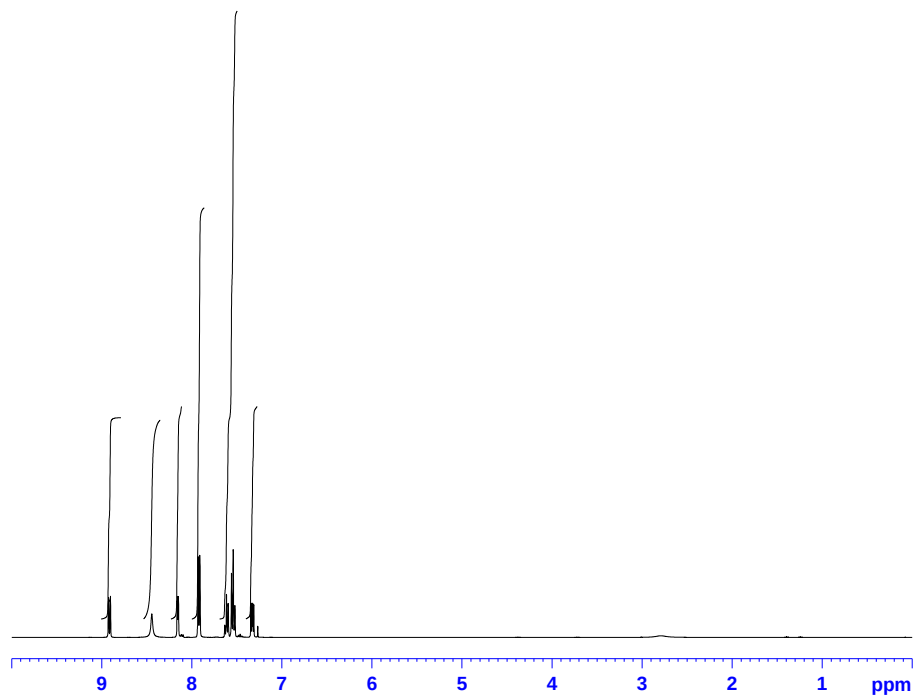
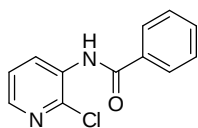
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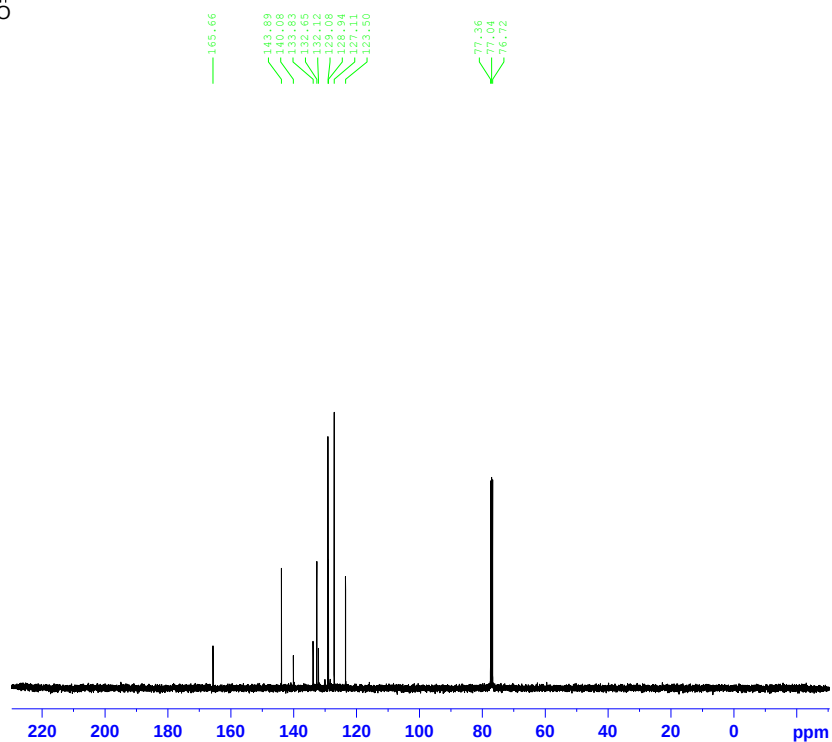
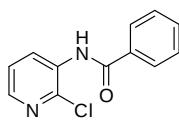
Amide 9f: ^{13}C -NMR (100 MHz, CDCl_3)



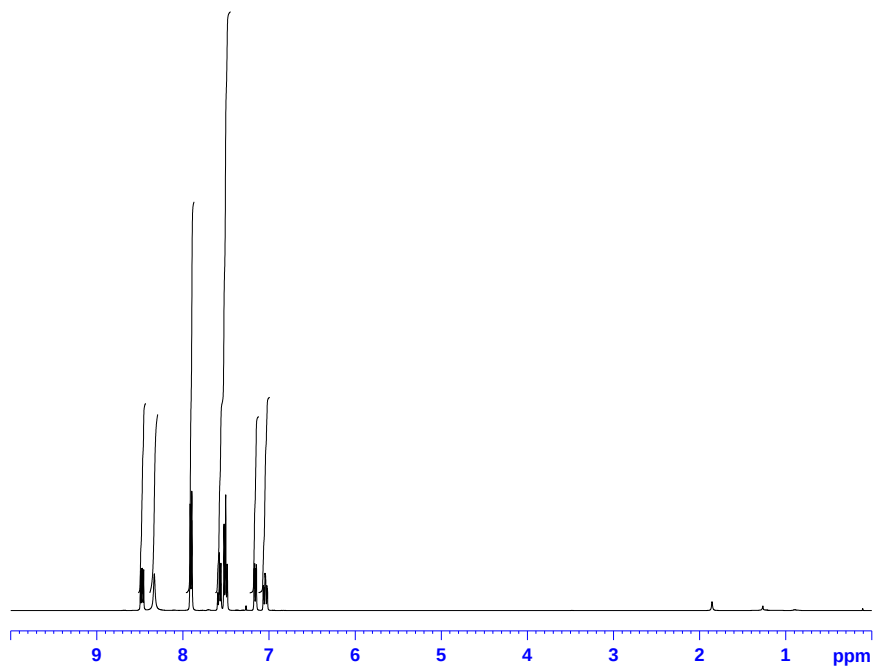
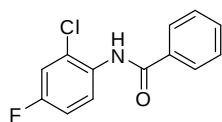
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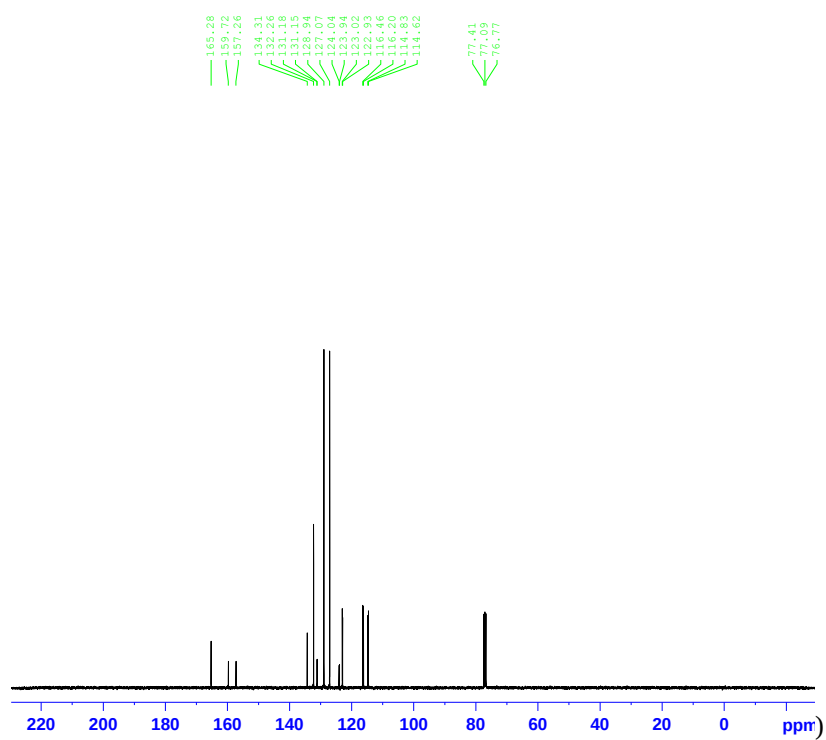
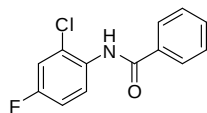
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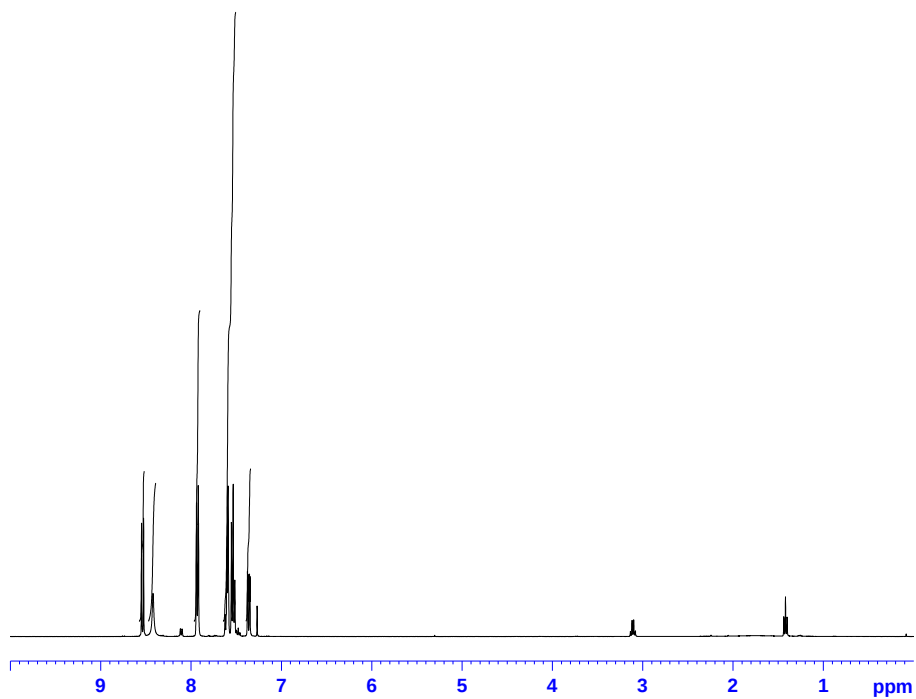
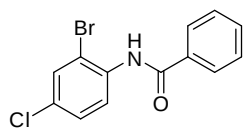
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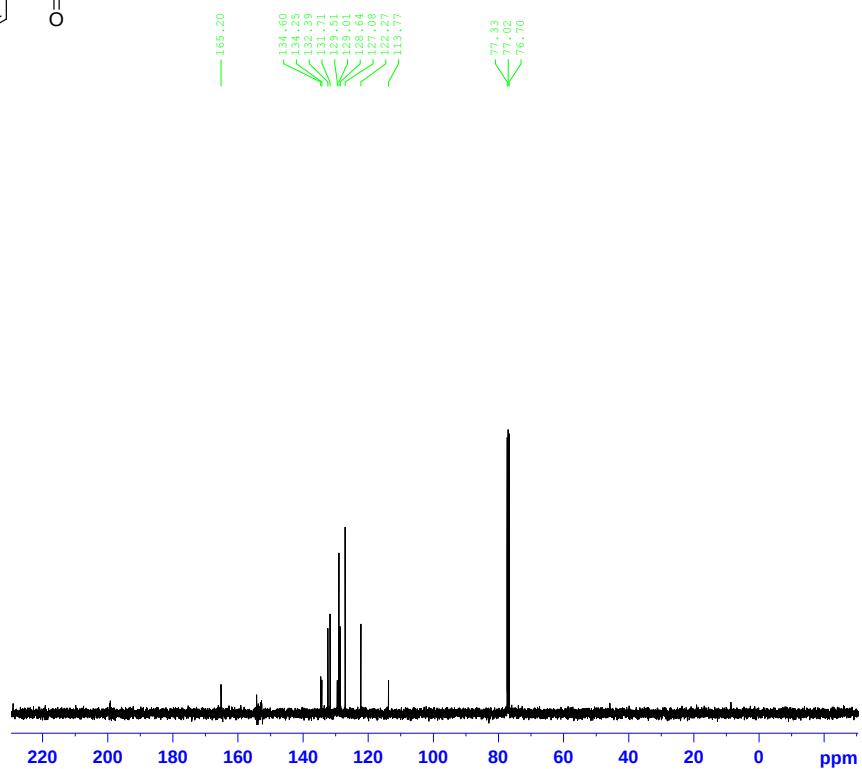
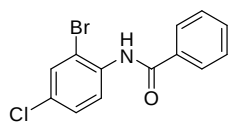
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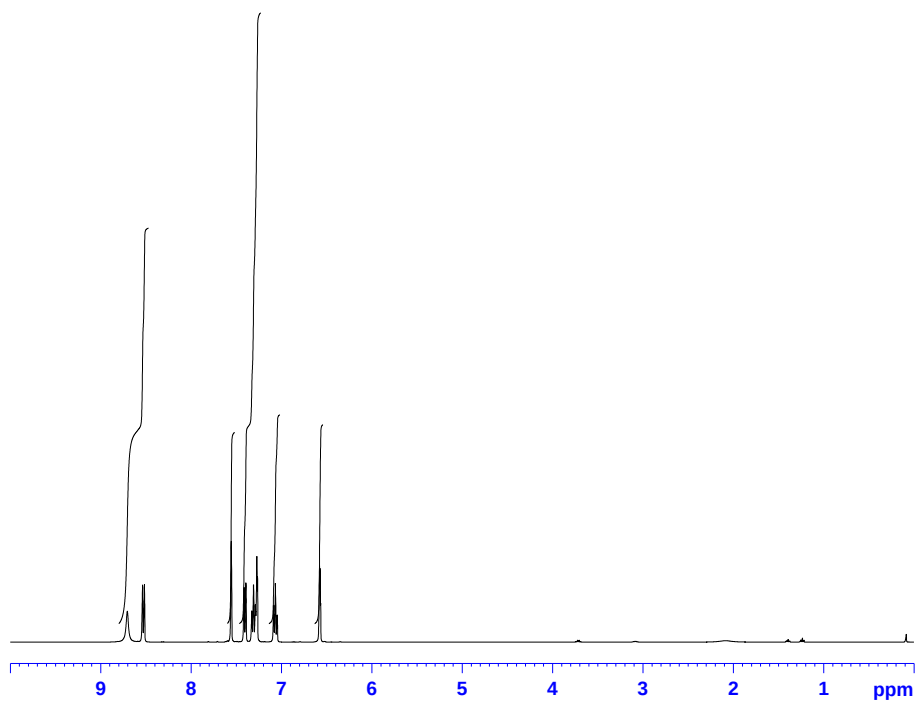
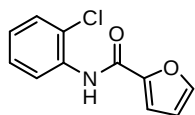
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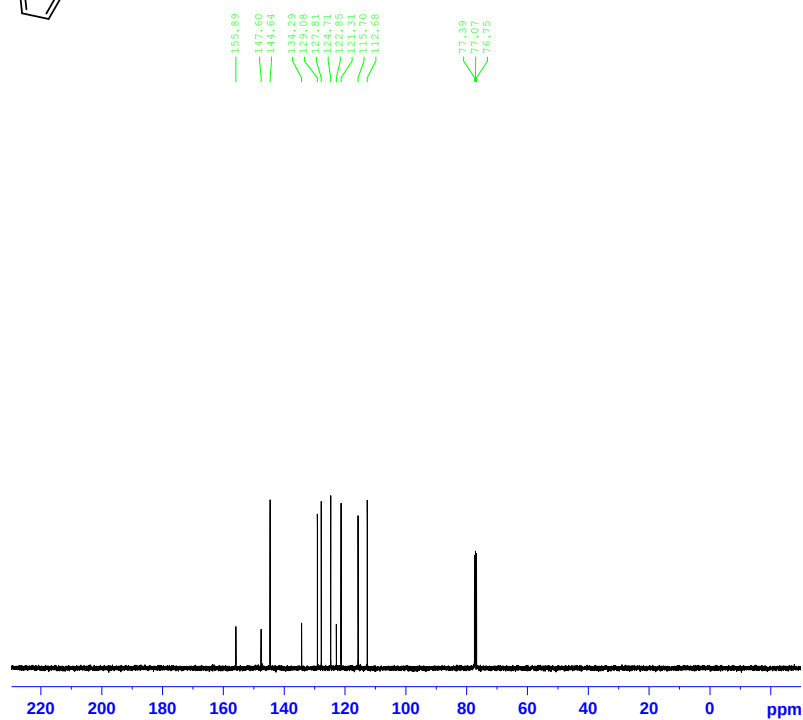
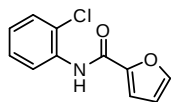
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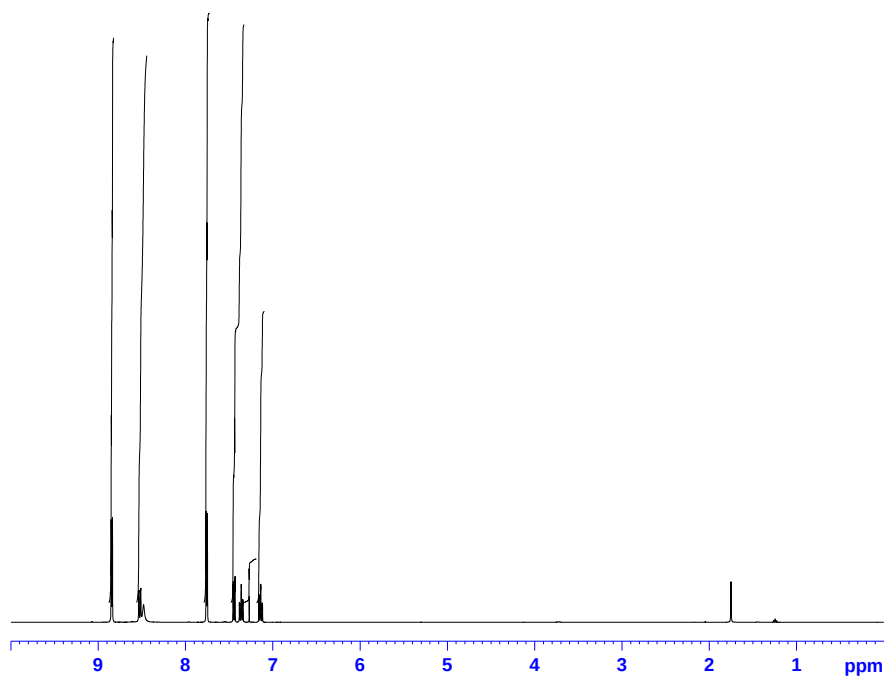
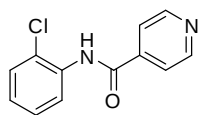
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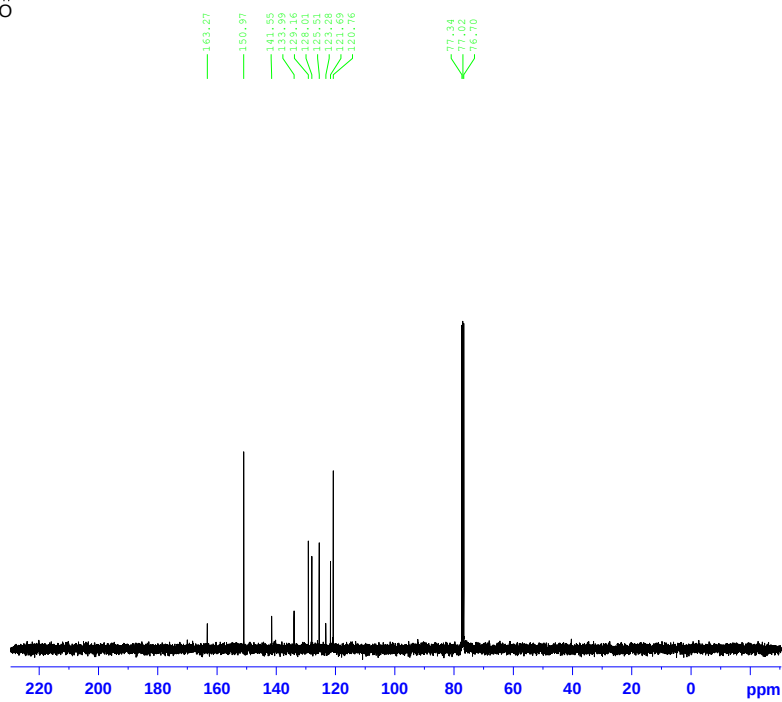
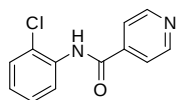
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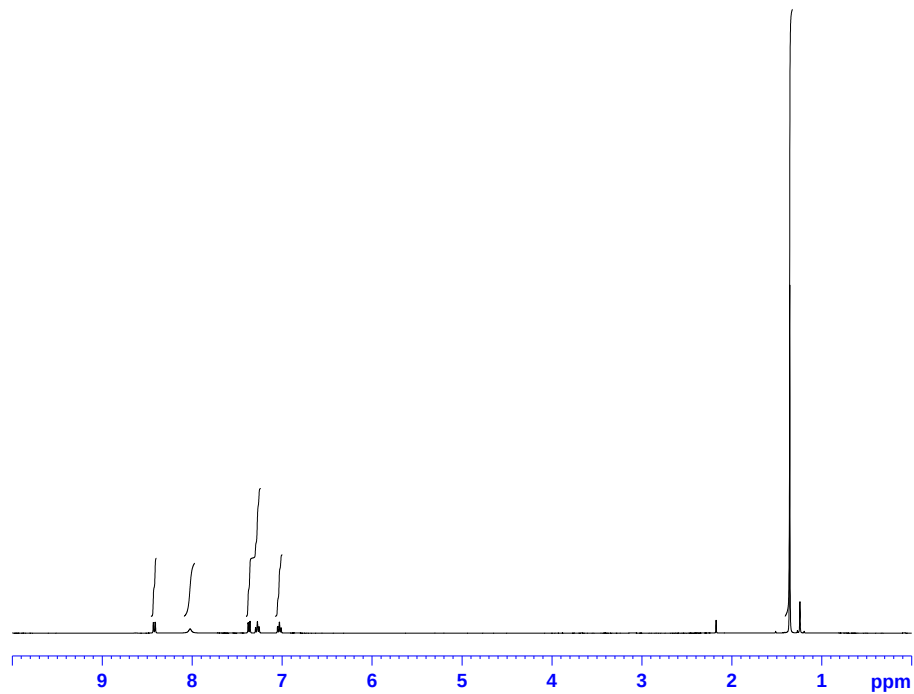
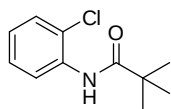
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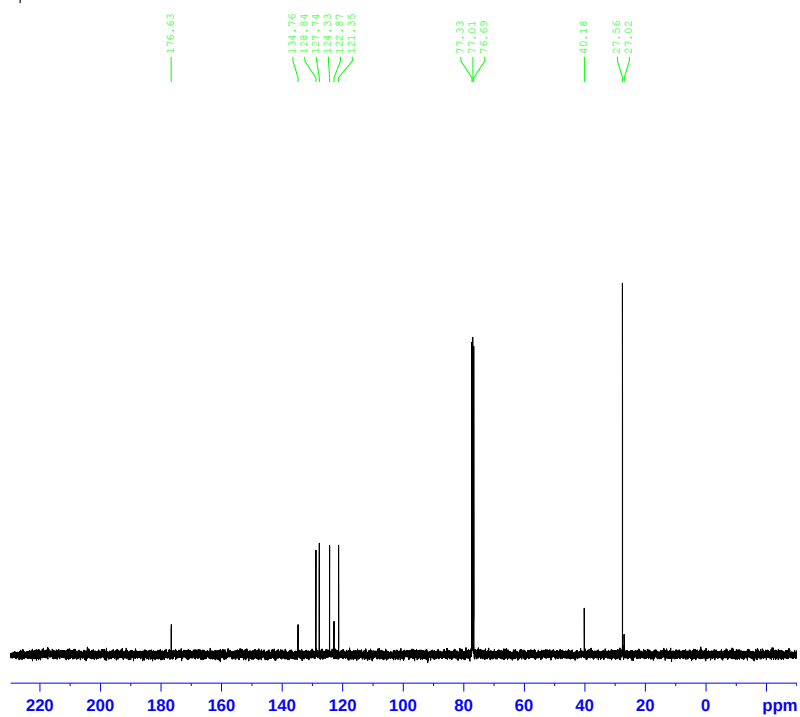
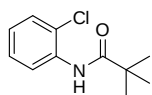
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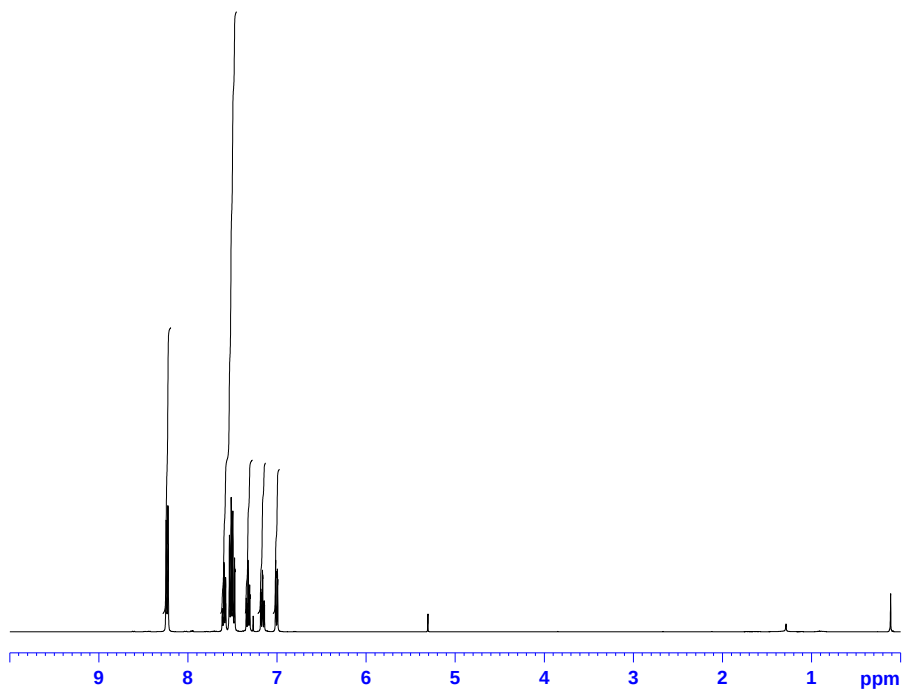
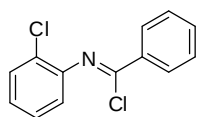
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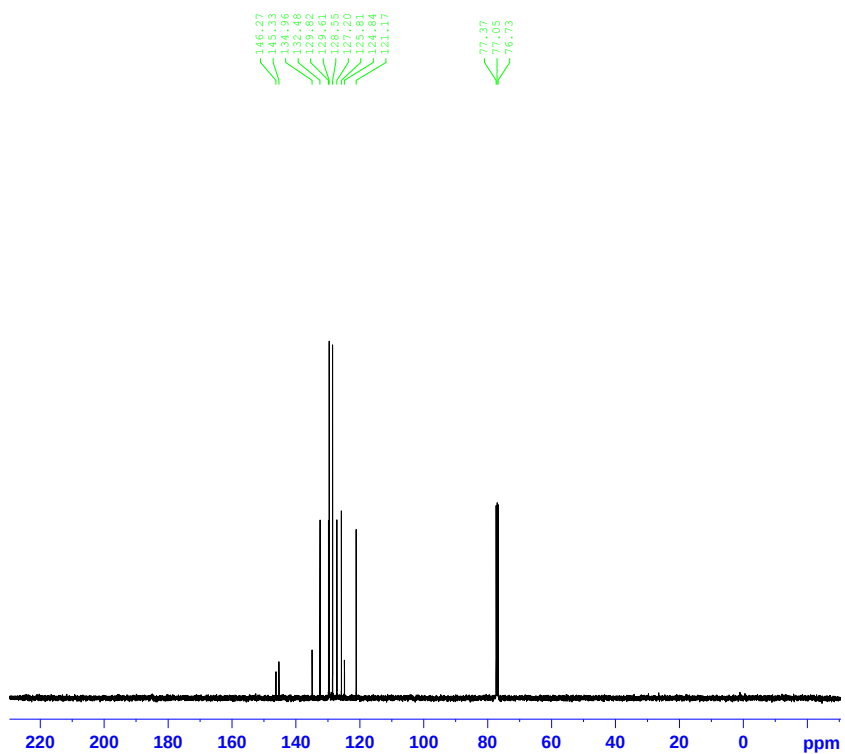
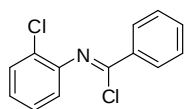
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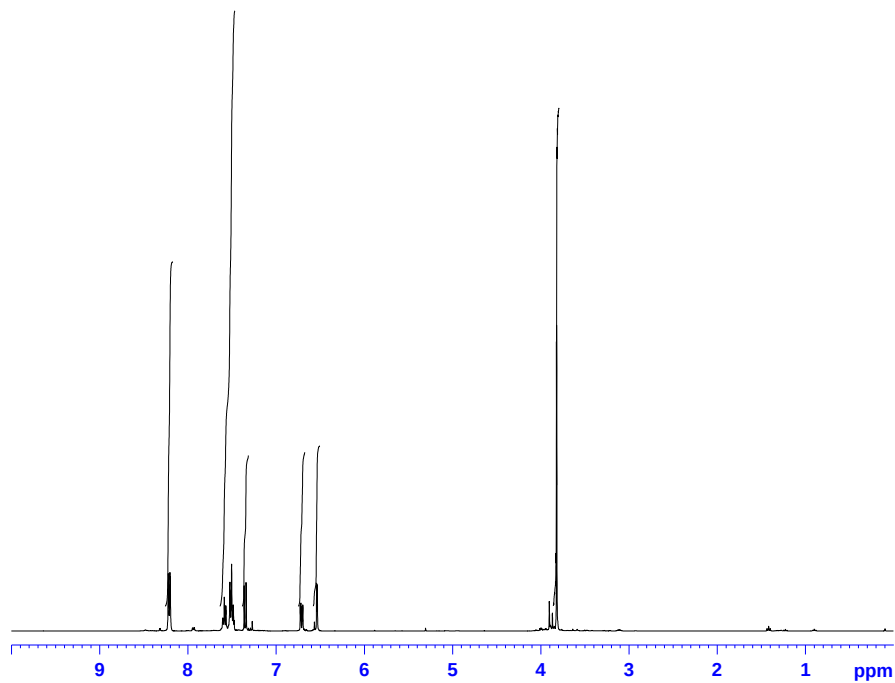
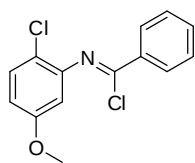
Imidoyl Chloride 5a: ^1H -NMR (400 MHz, CDCl_3)



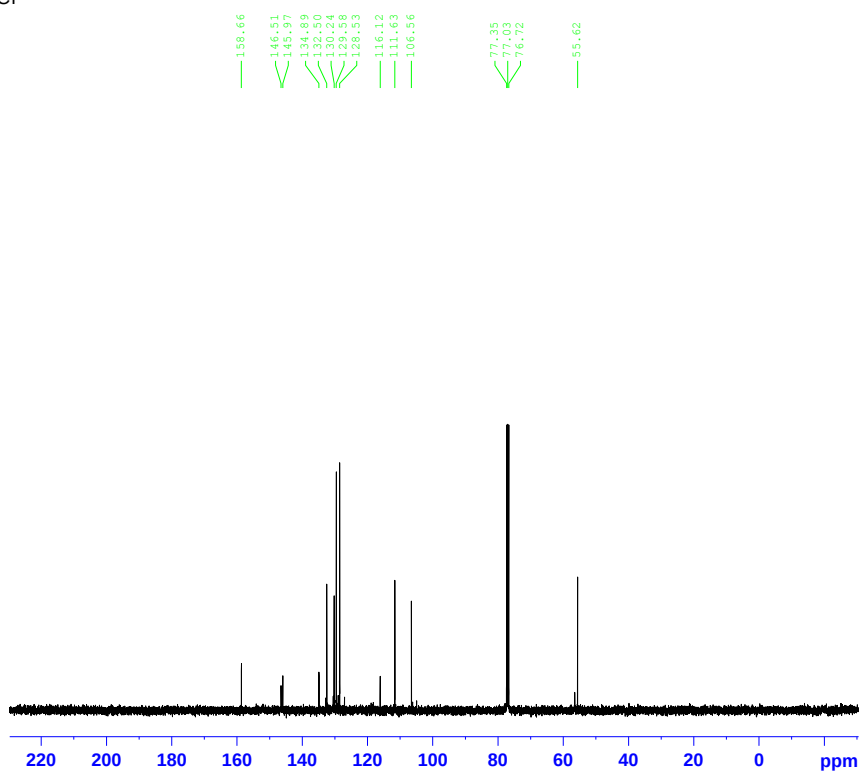
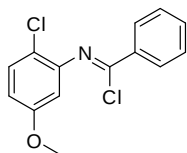
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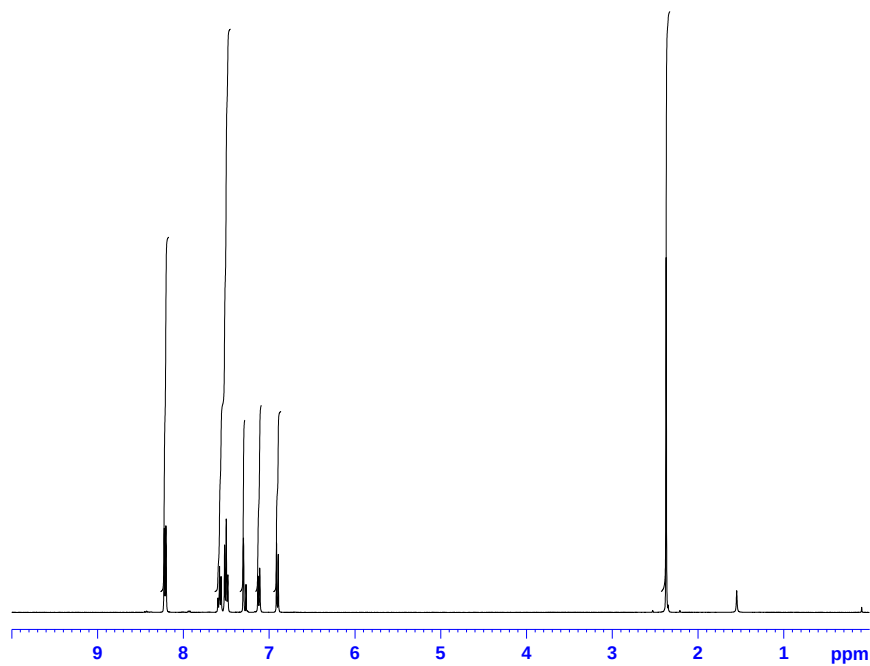
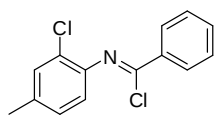
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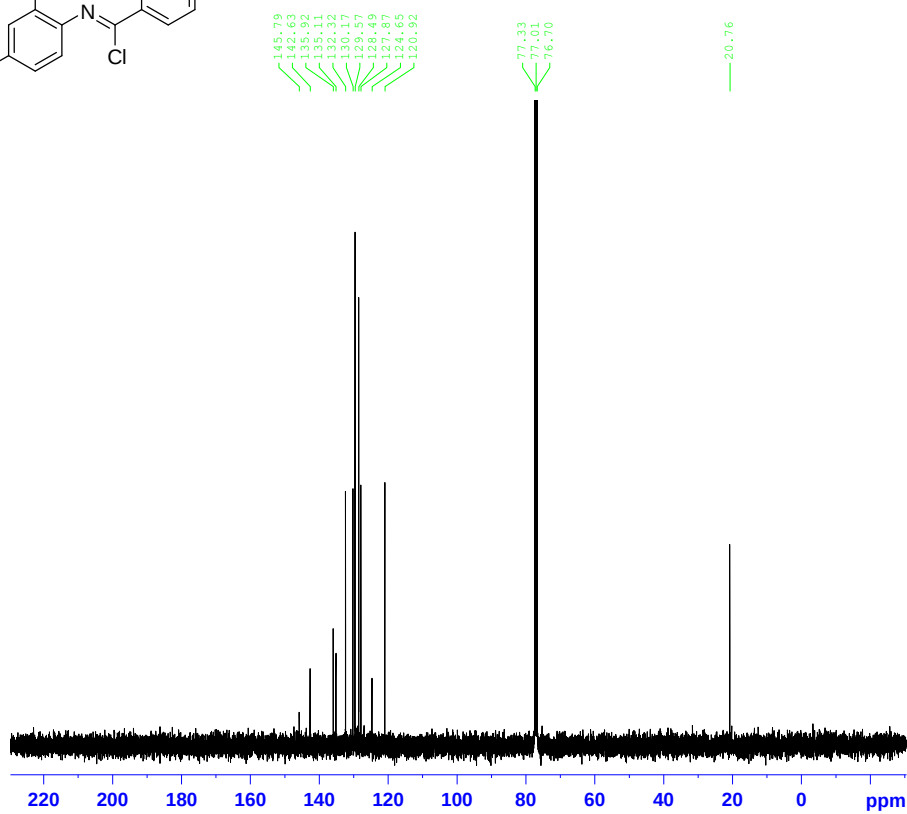
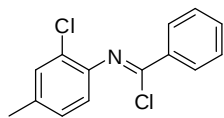
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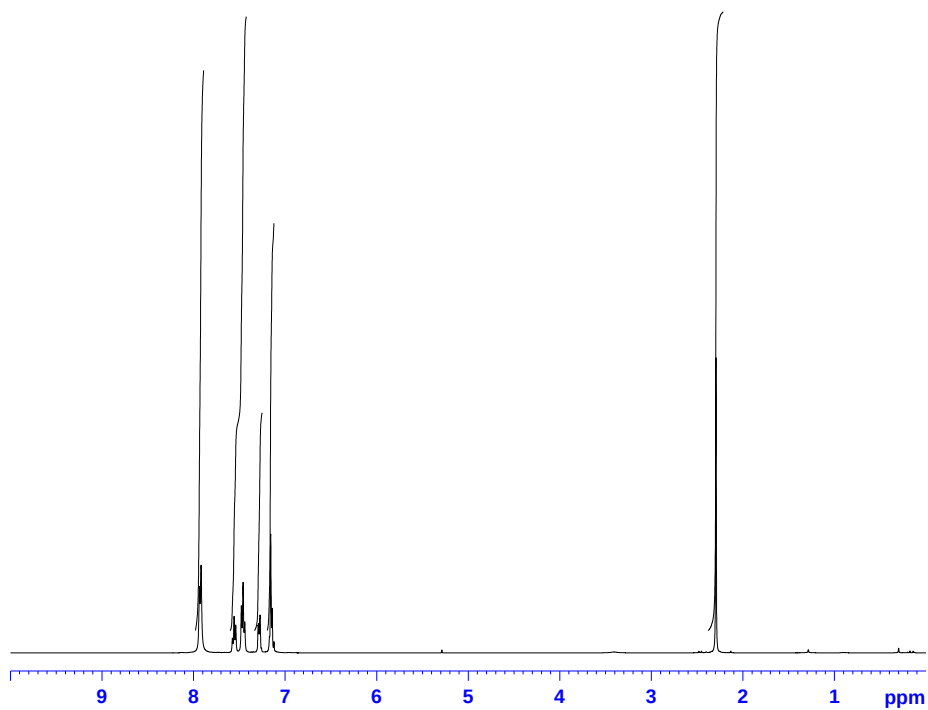
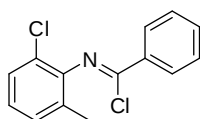
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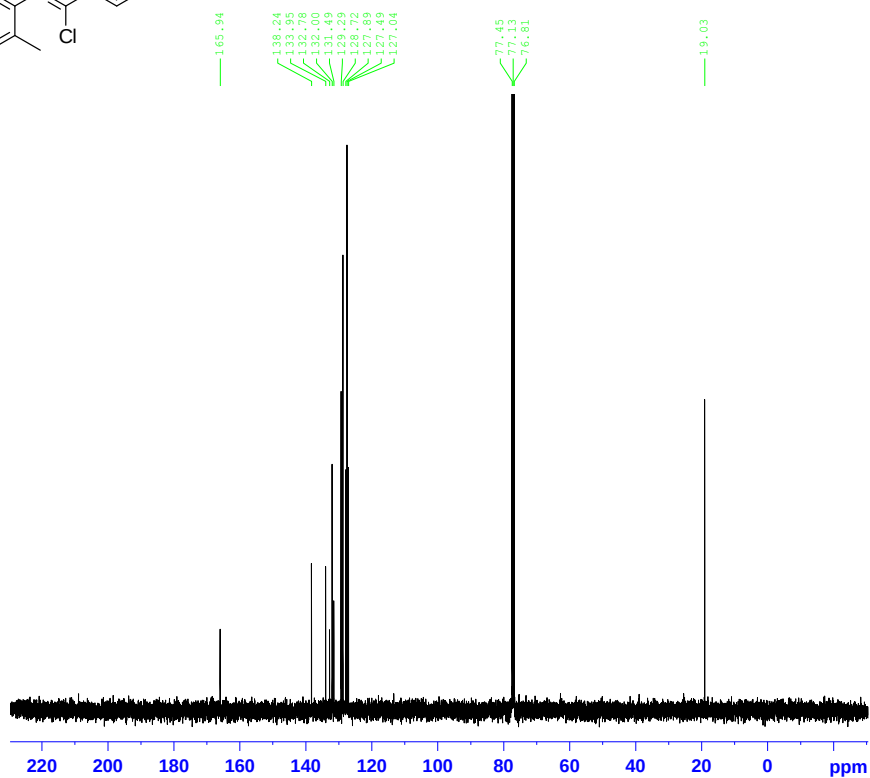
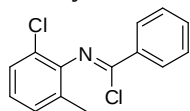
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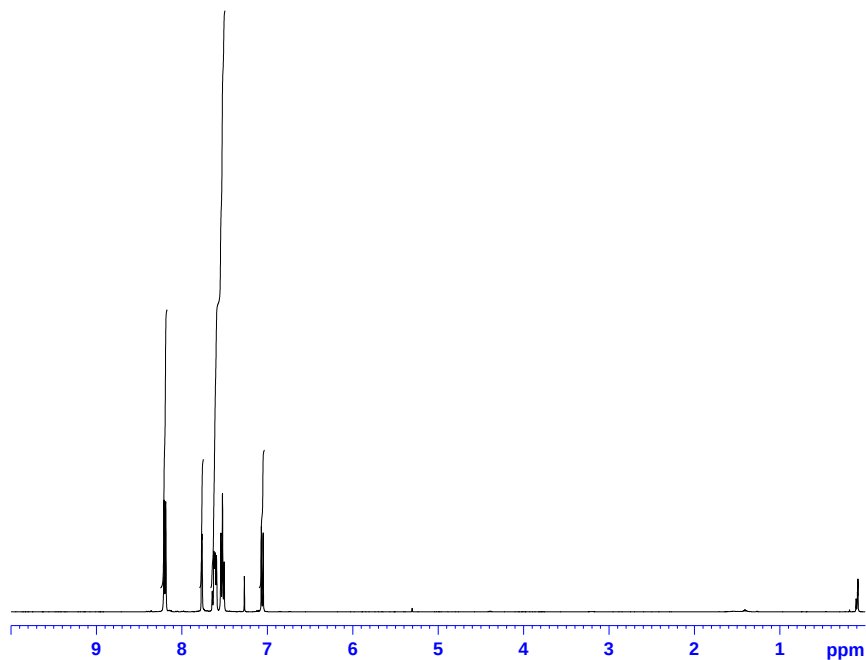
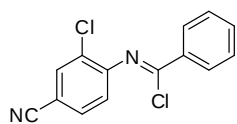
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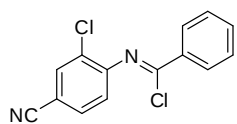
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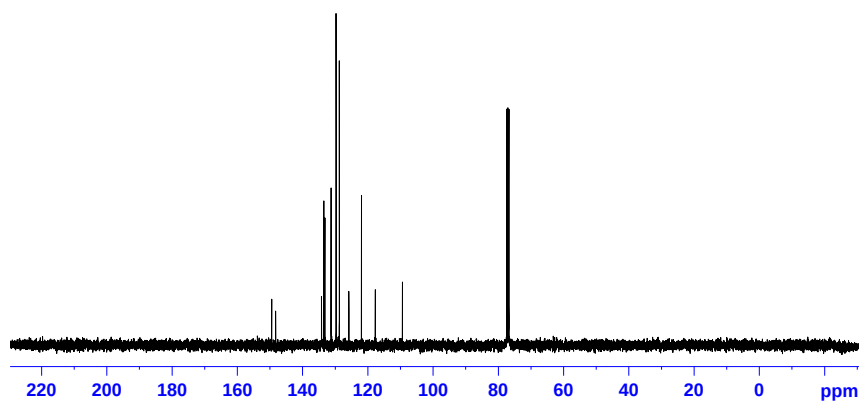
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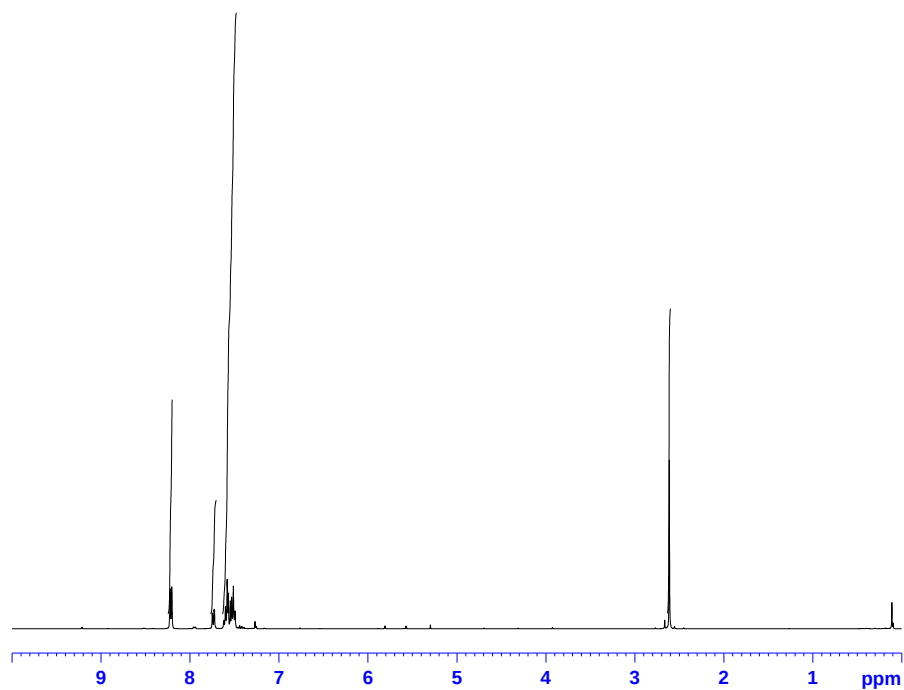
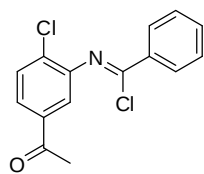
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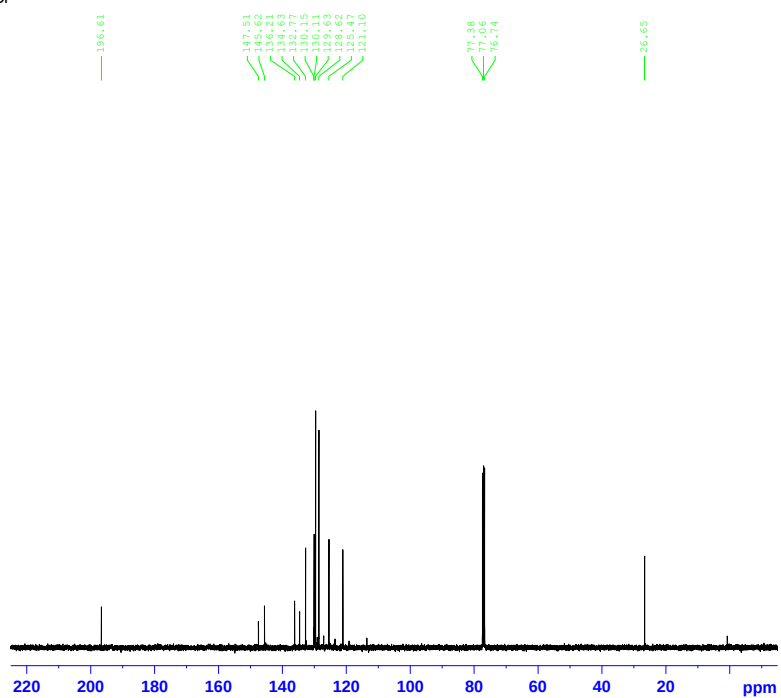
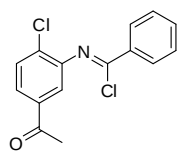
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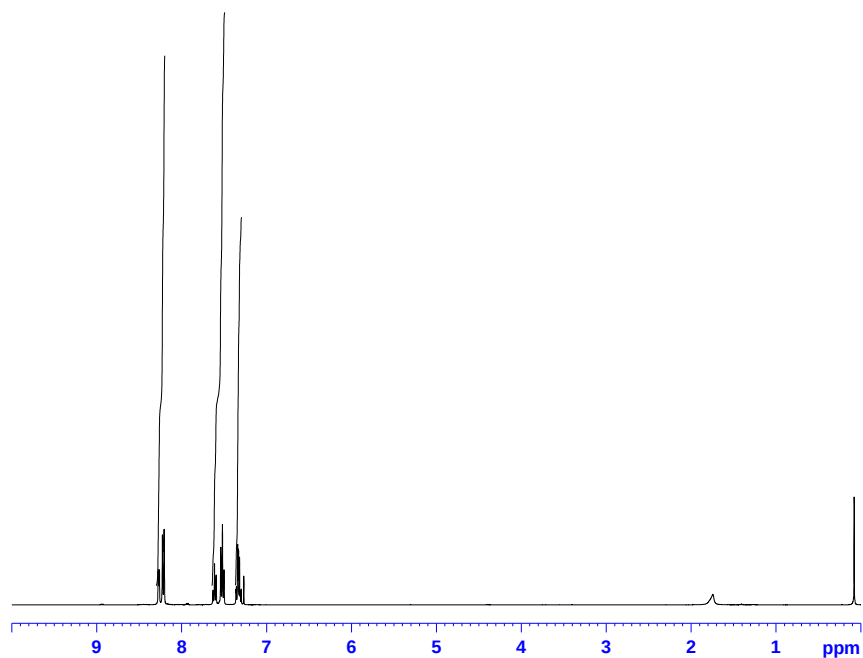
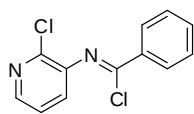
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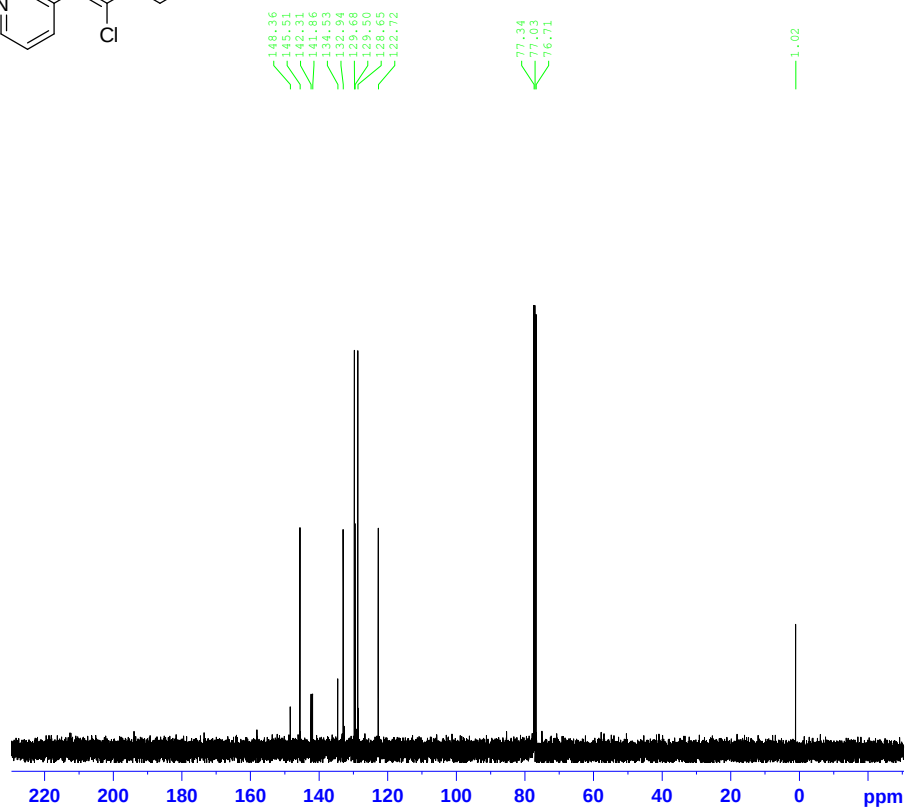
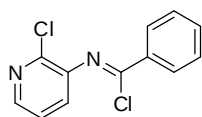
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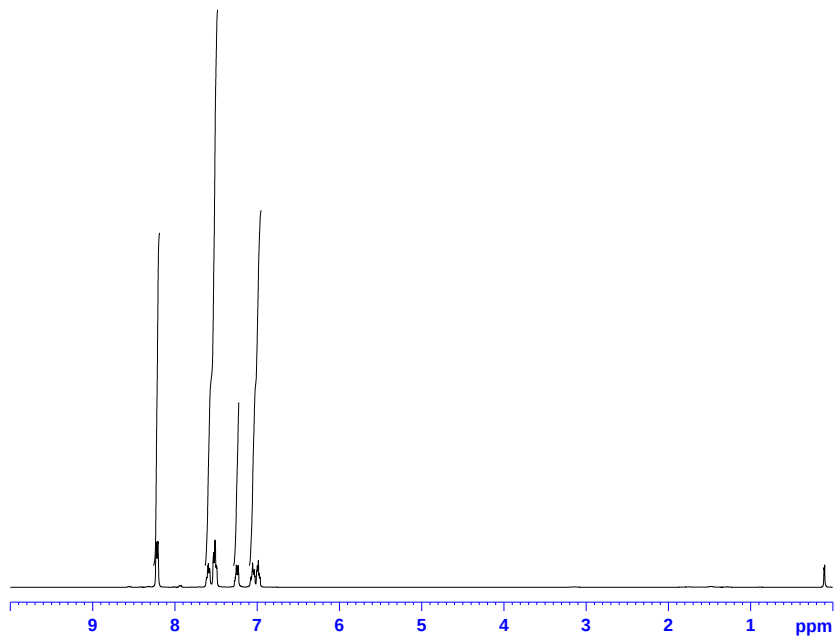
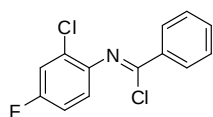
Imidoyl Chloride 5g: ^1H -NMR (400 MHz, CDCl_3)



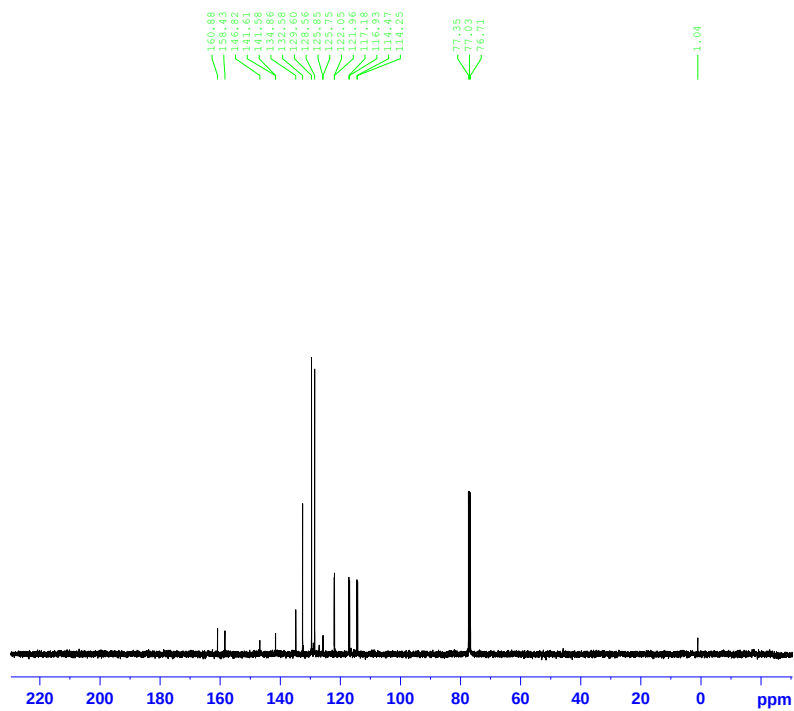
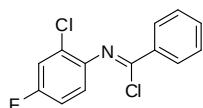
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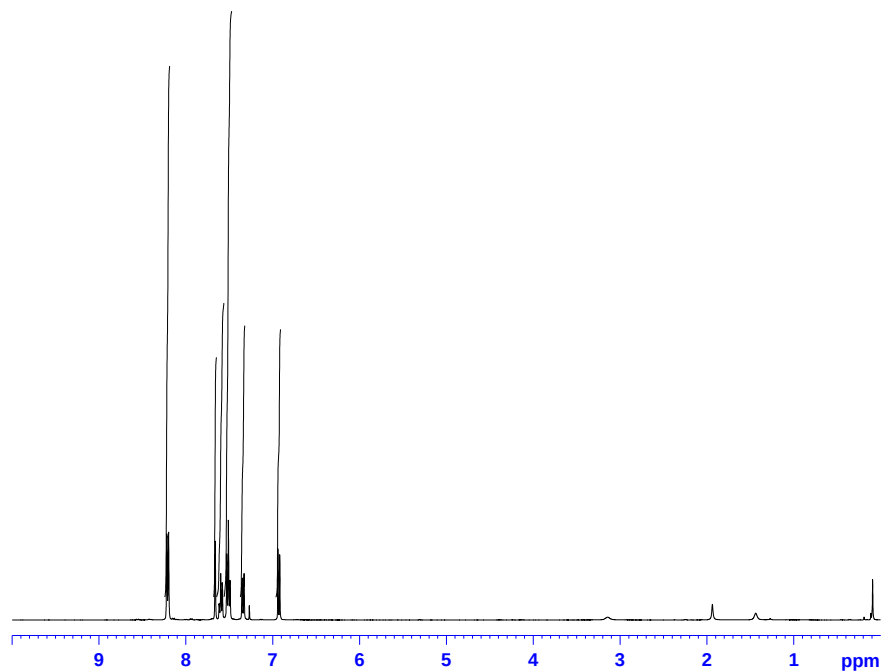
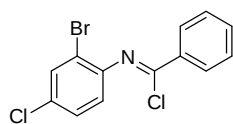
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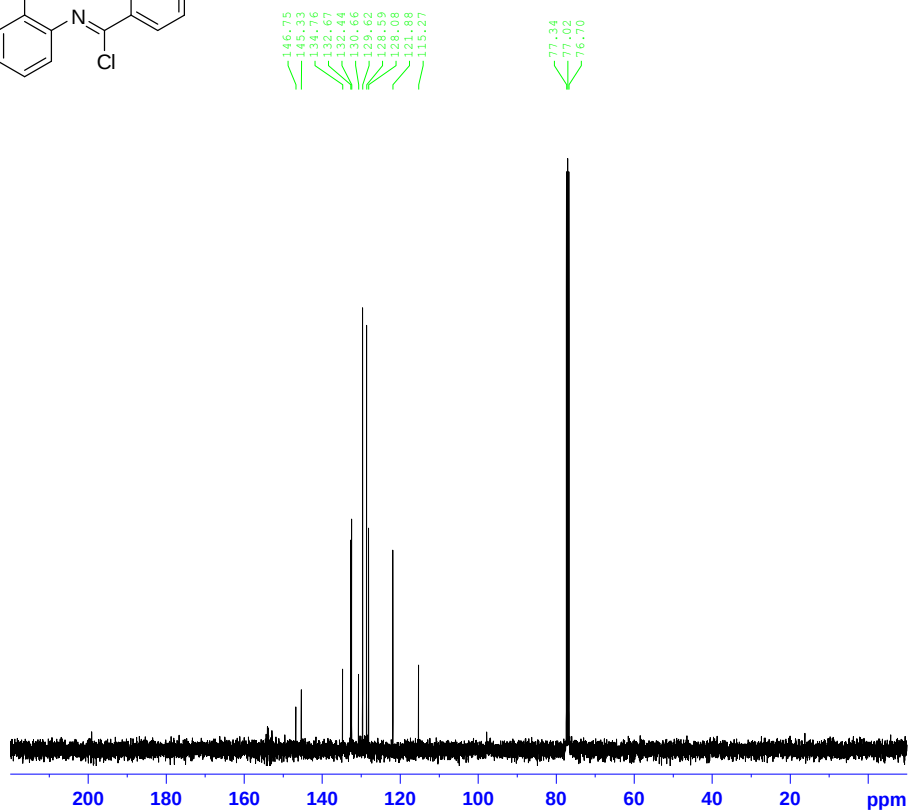
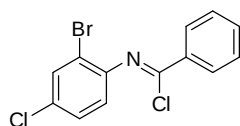
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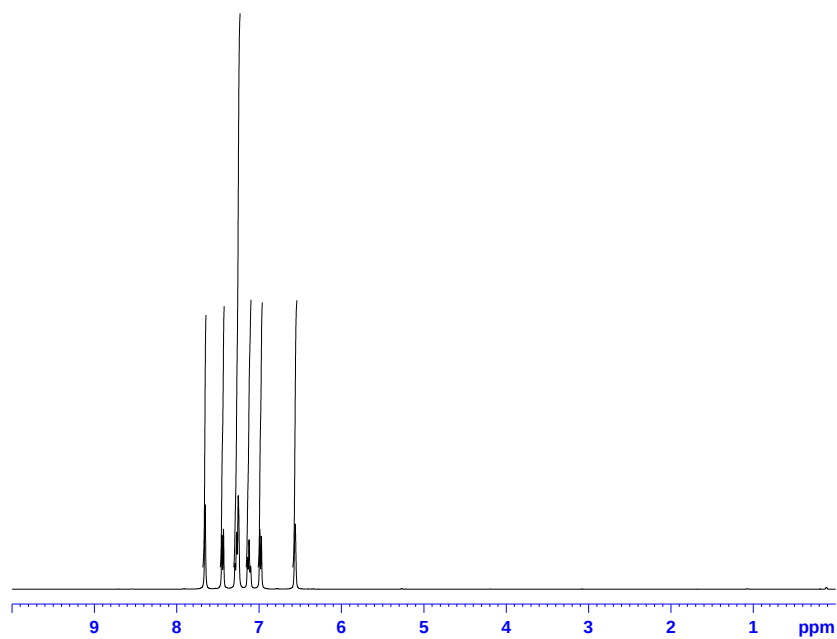
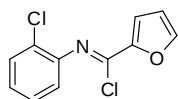
Imidoyl Chloride 5i: ^1H -NMR (400 MHz, CDCl_3)



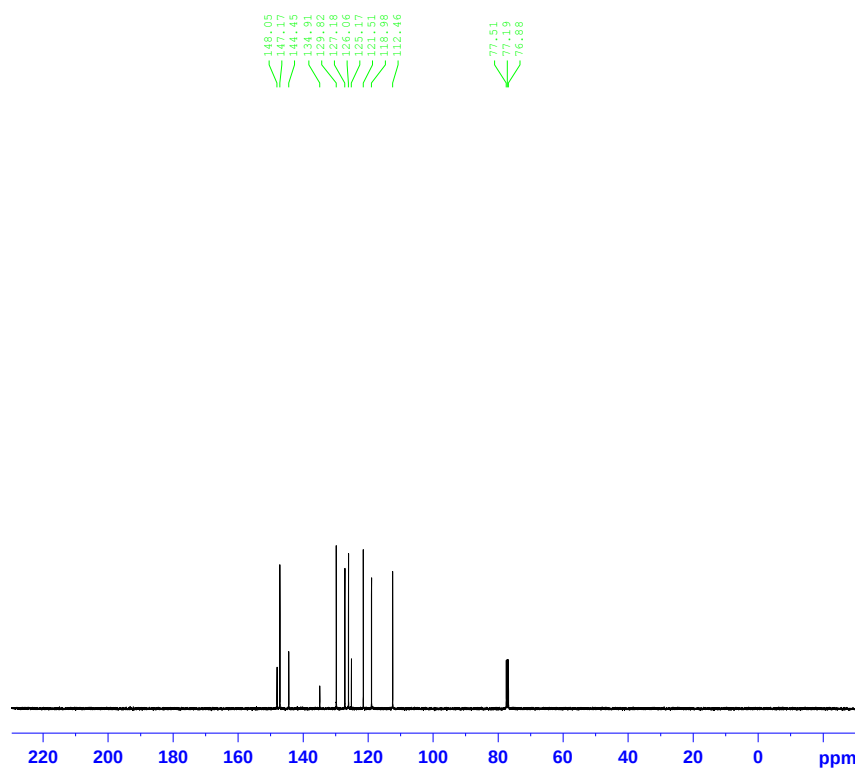
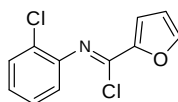
Imidoyl Chloride 5i: ^{13}C -NMR (100 MHz, CDCl_3)



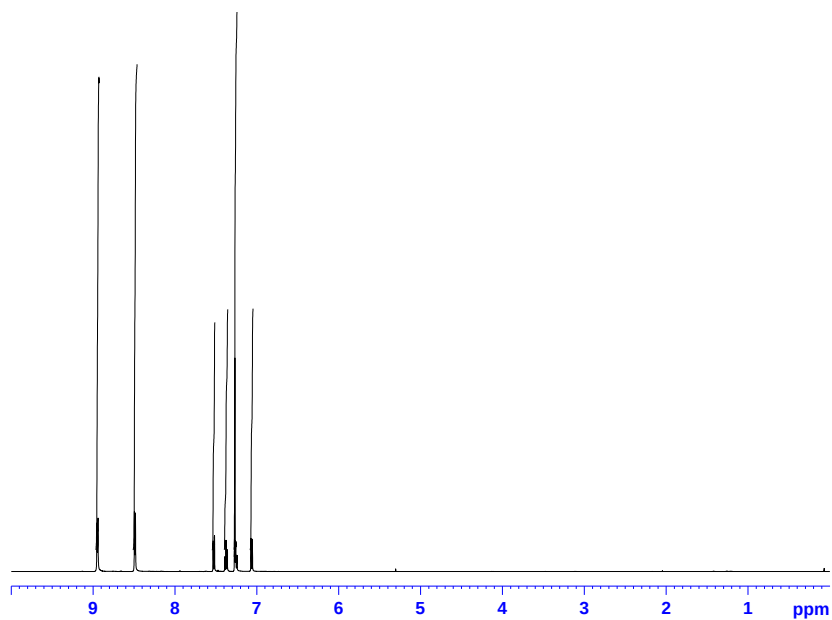
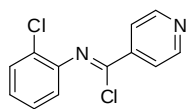
Imidoyl Chloride 5j: ^1H -NMR (400 MHz, CDCl_3)



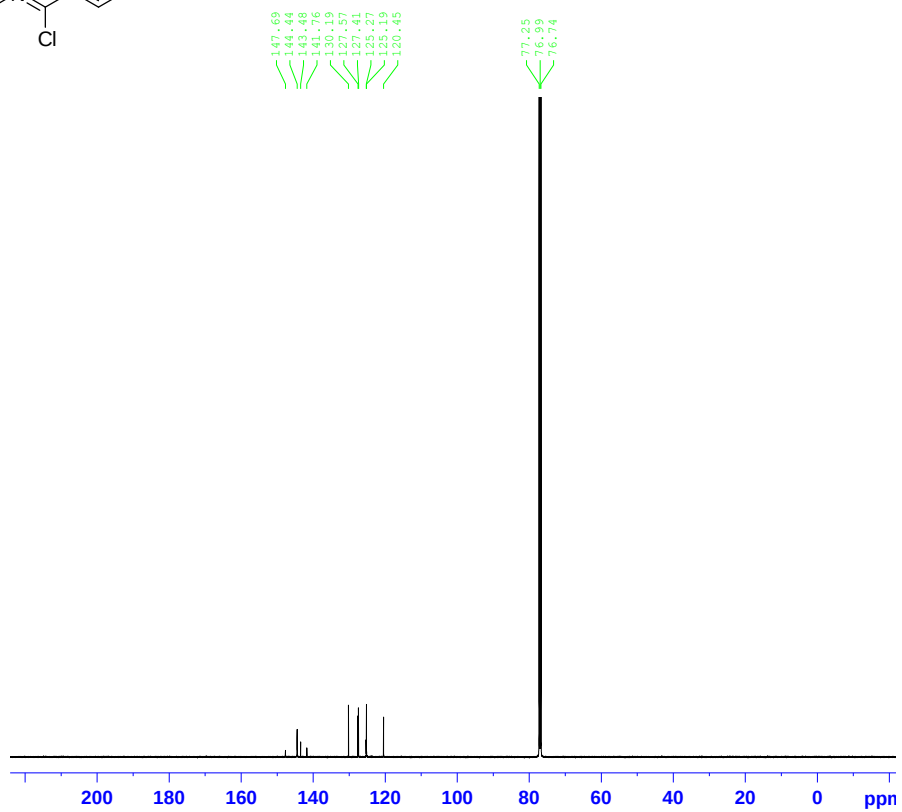
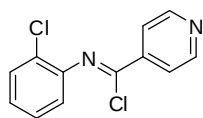
Imidoyl Chloride 5j: ^{13}C -NMR (100 MHz, CDCl_3)



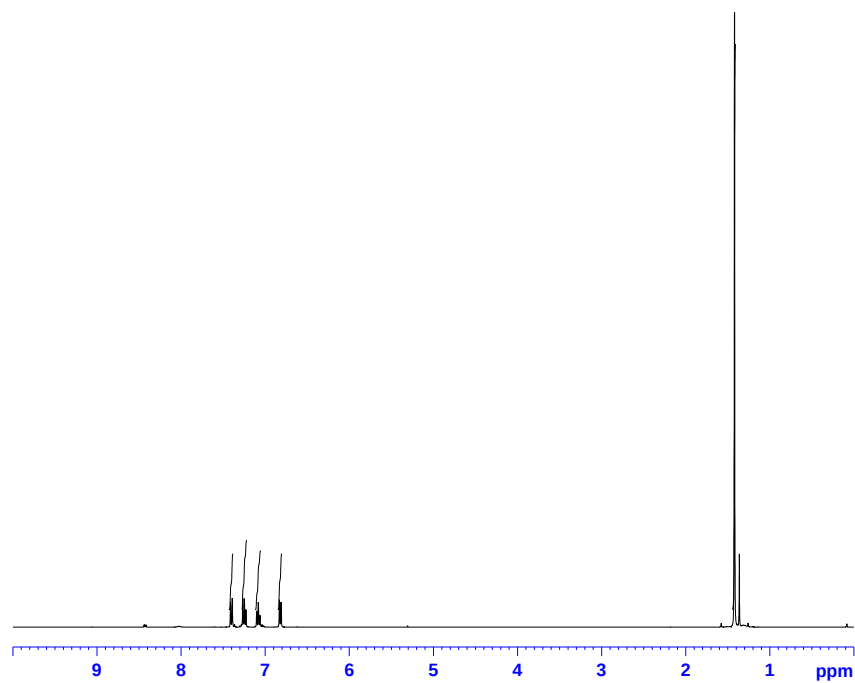
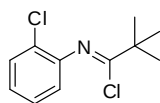
Imidoyl Chloride 5k: ^1H -NMR (500 MHz, CDCl_3)



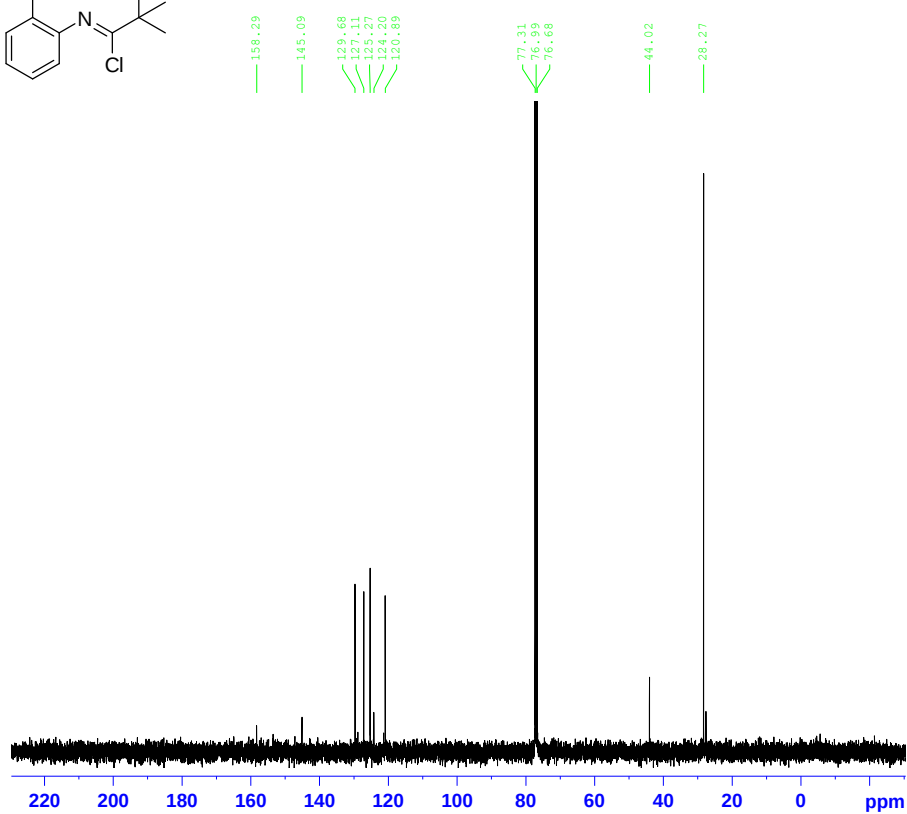
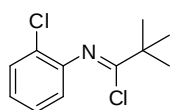
Imidoyl Chloride 5k: ^{13}C -NMR (125 MHz, CDCl_3)



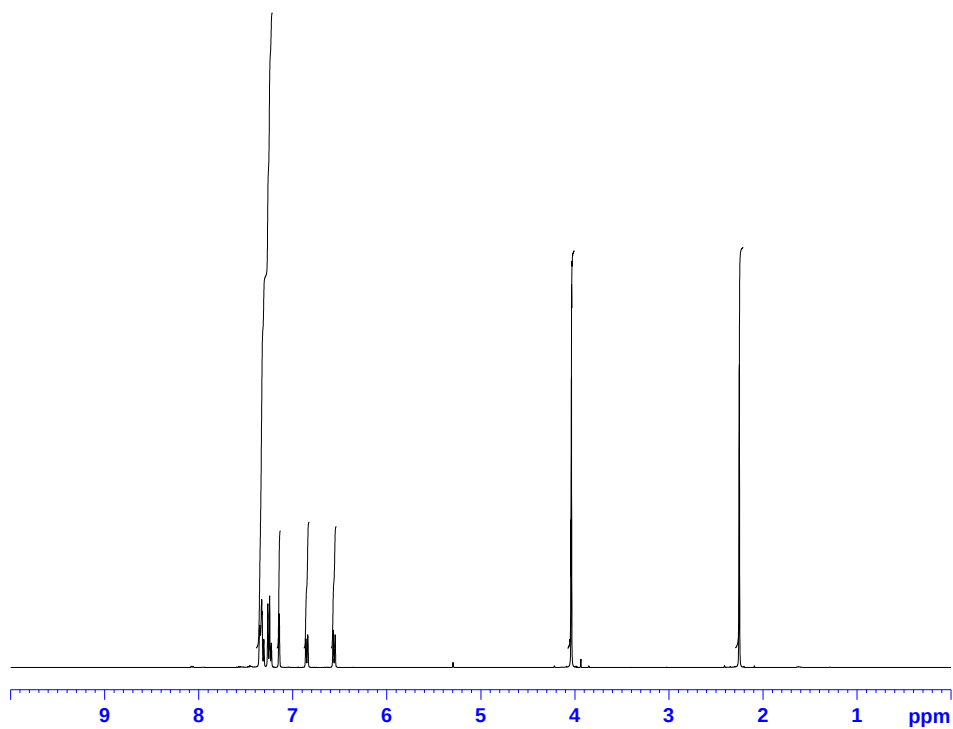
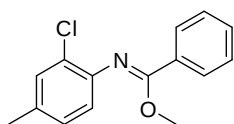
Imidoyl Chloride 5l: ^1H -NMR (400 MHz, CDCl_3)



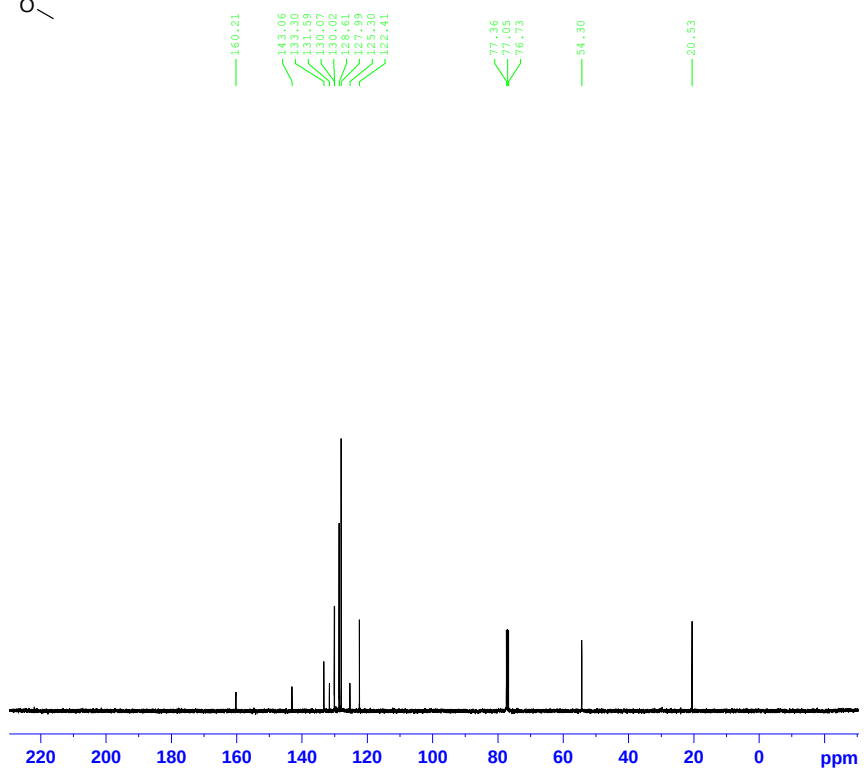
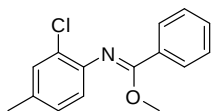
Imidoyl Chloride 5l: ^{13}C -NMR (100 MHz, CDCl_3)



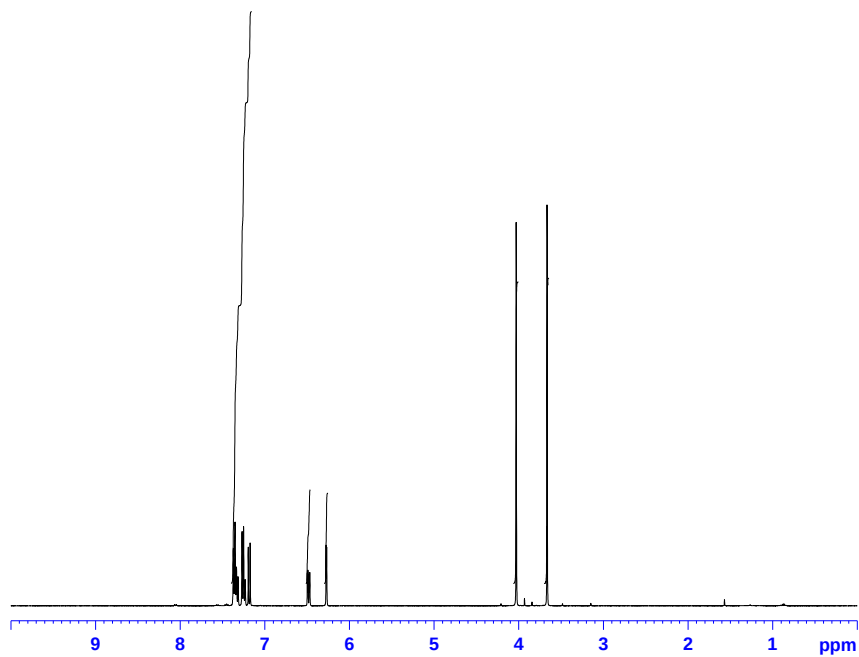
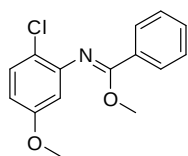
Imidate 6a: ^1H -NMR (400 MHz, CDCl_3)



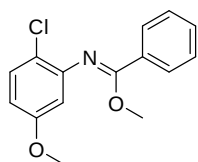
Imidate 6a: ^{13}C -NMR (100 MHz, CDCl_3)



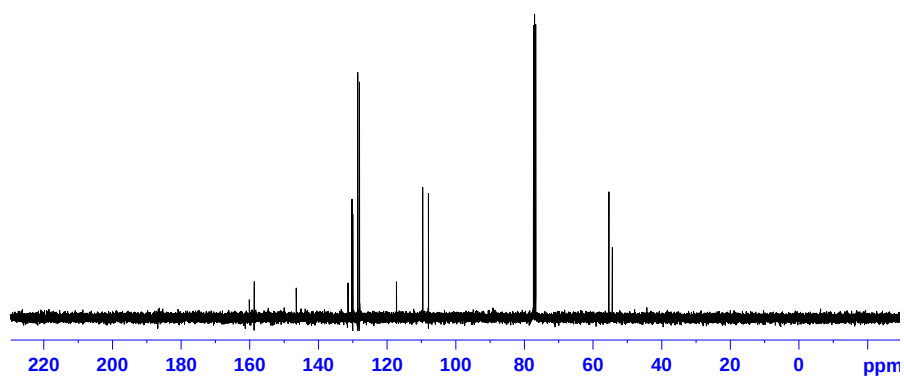
Imidate 6b: ^1H -NMR (400 MHz, CDCl_3)



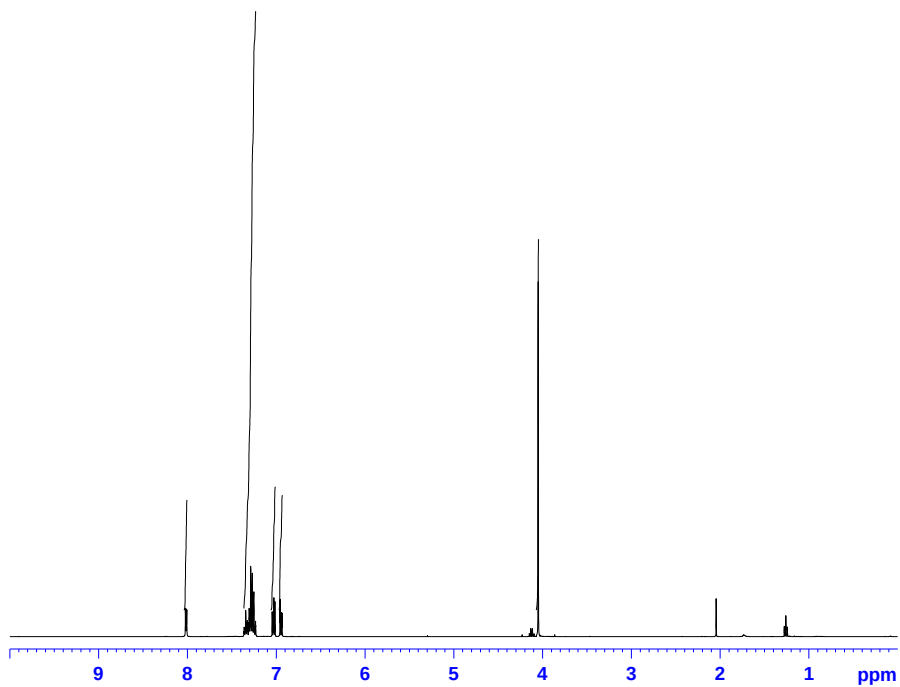
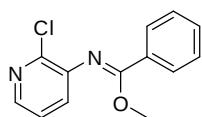
Imidate 6b: ^{13}C -NMR (100 MHz, CDCl_3)



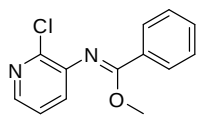
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77.01
76.70
55.41
54.38



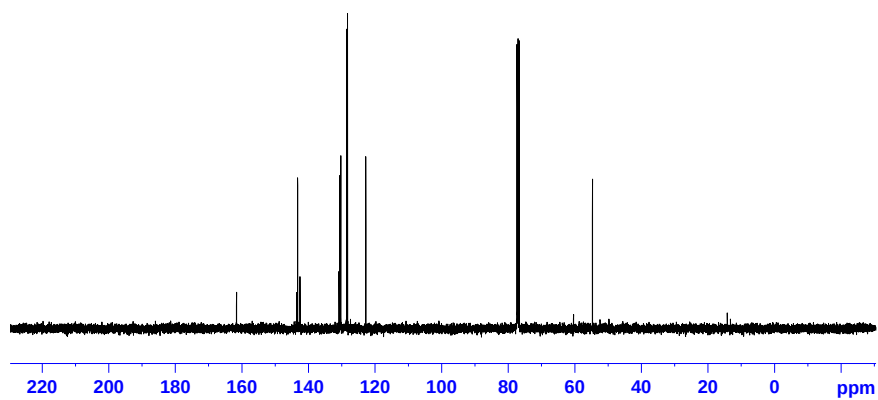
Imidate 6c: ^1H -NMR (400 MHz, CDCl_3)



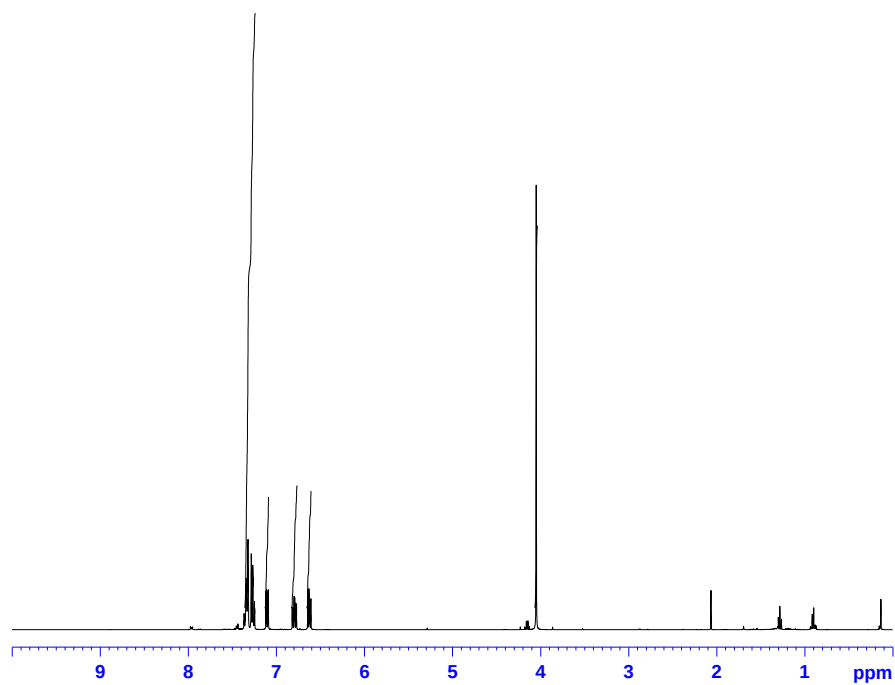
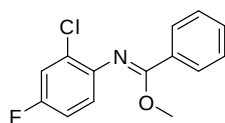
Imidate 6c: ^{13}C -NMR (100 MHz, CDCl_3)



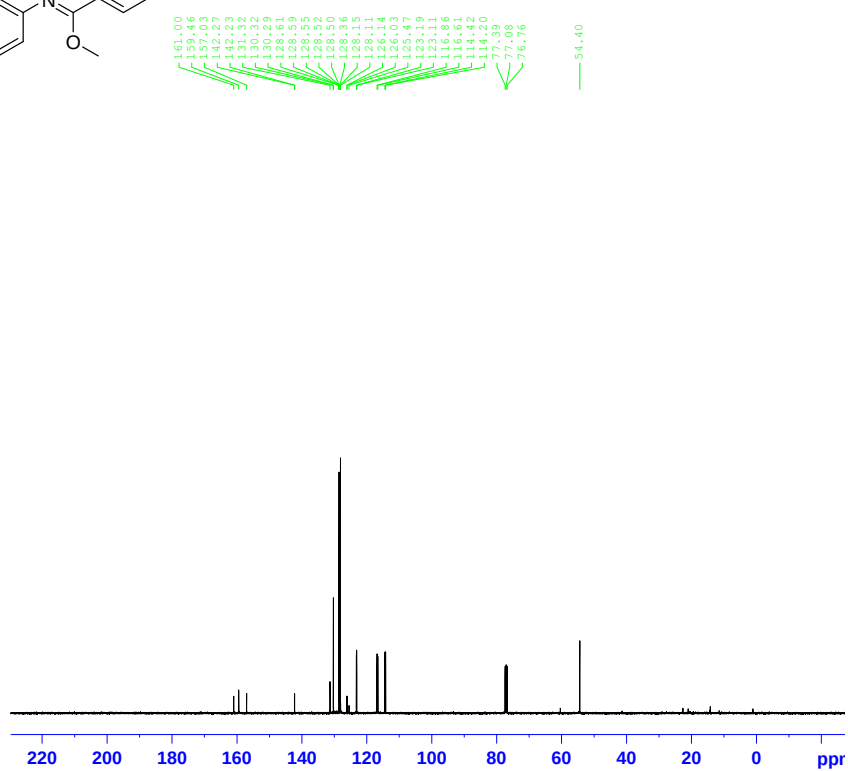
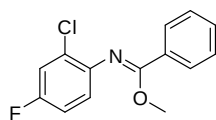
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128.53
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122.78
77.34
77.03
76.71
54.68



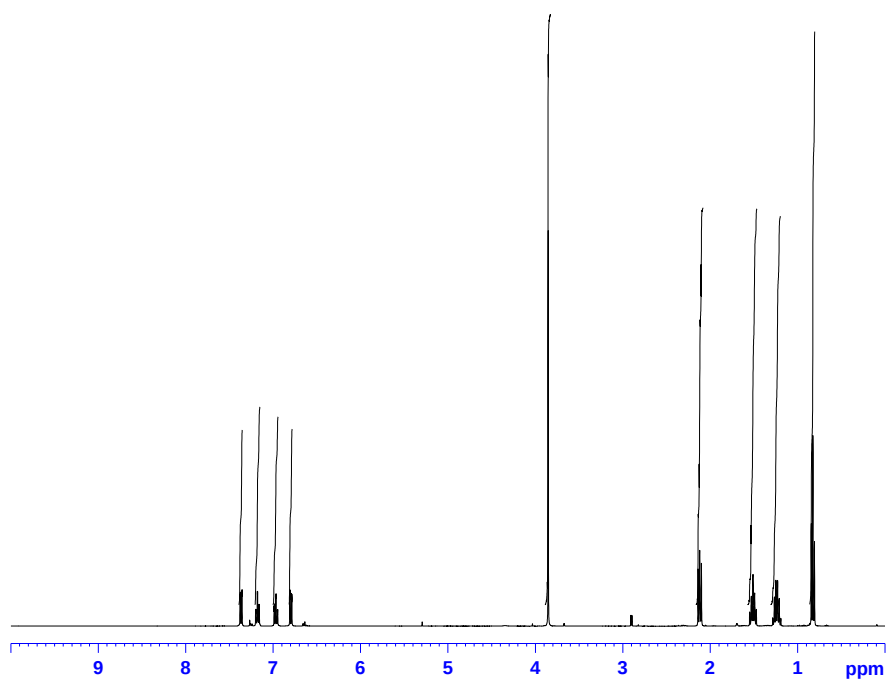
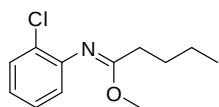
Imidate 6d: ^1H -NMR (400 MHz, CDCl_3)



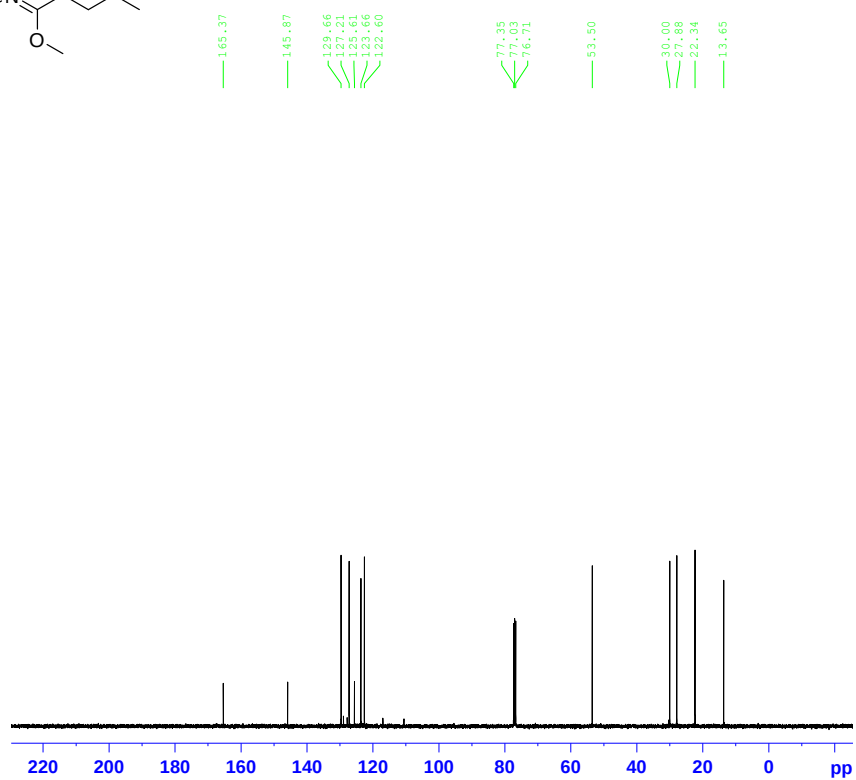
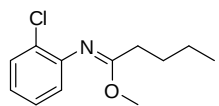
Imidate 6d: ^{13}C -NMR (100 MHz, CDCl_3)



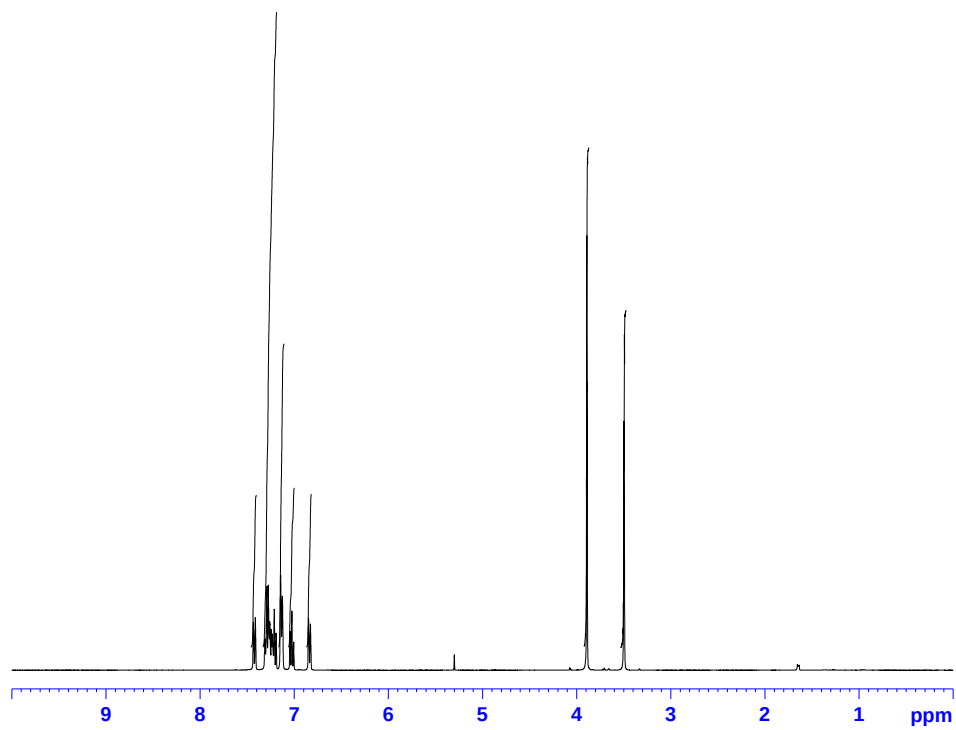
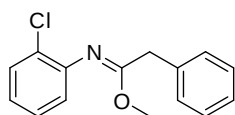
Imidate 6e: ^1H -NMR (400 MHz, CDCl_3)



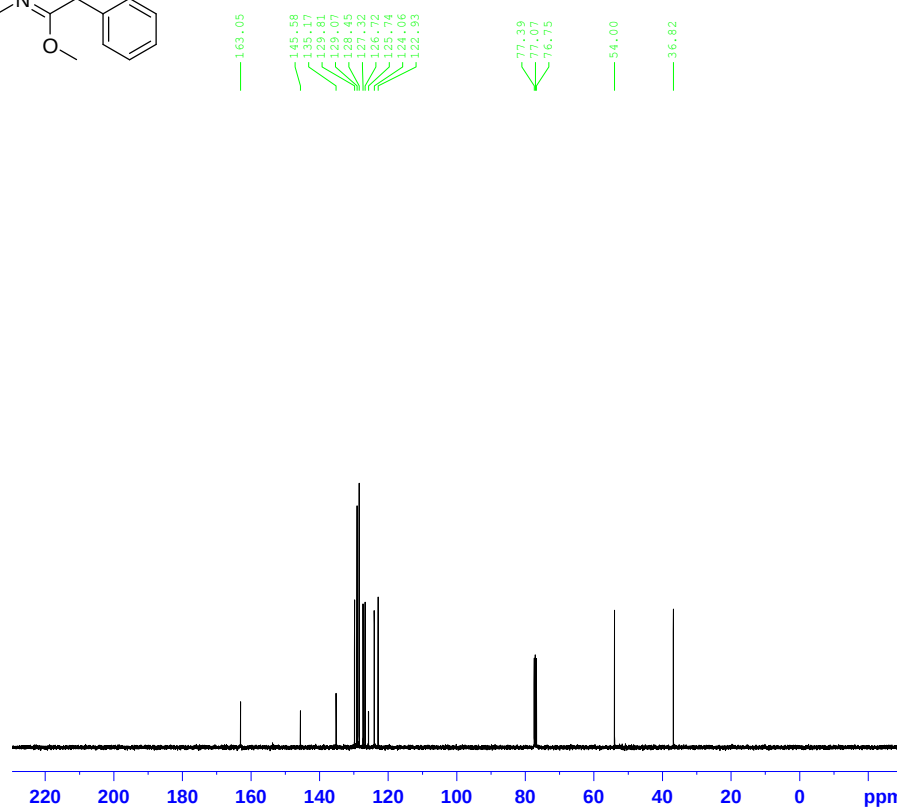
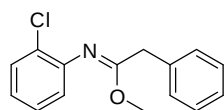
Imidate 6e: ^{13}C -NMR (100 MHz, CDCl_3)



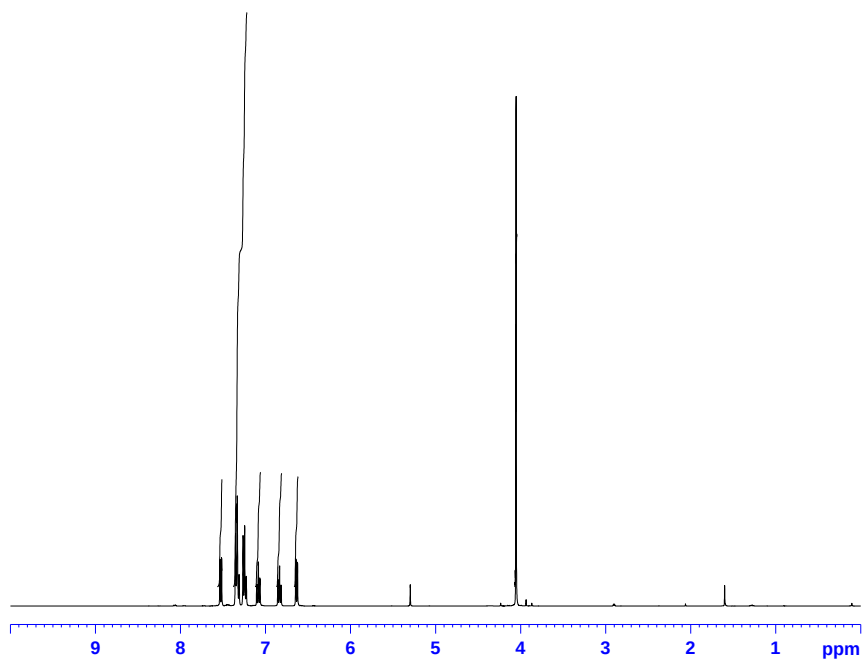
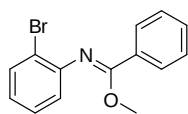
Imidate 6f: ^1H -NMR (400 MHz, CDCl_3)



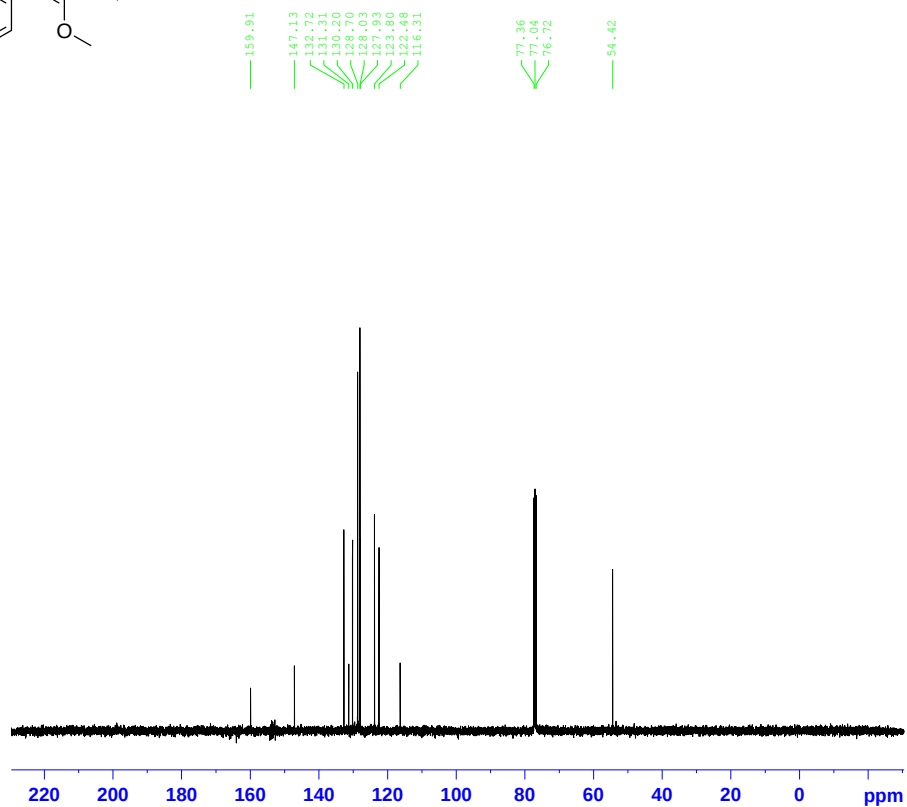
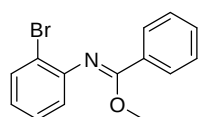
Imidate 6f: ^{13}C -NMR (100 MHz, CDCl_3)



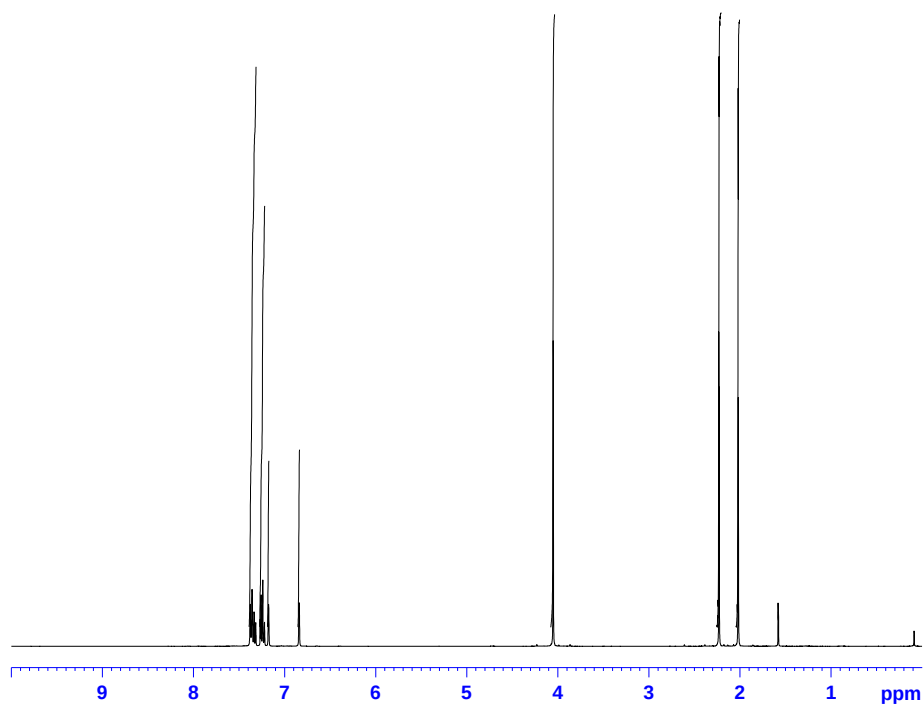
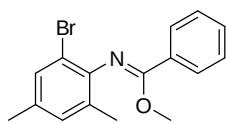
Imidate 6g: ^1H -NMR (400 MHz, CDCl_3)



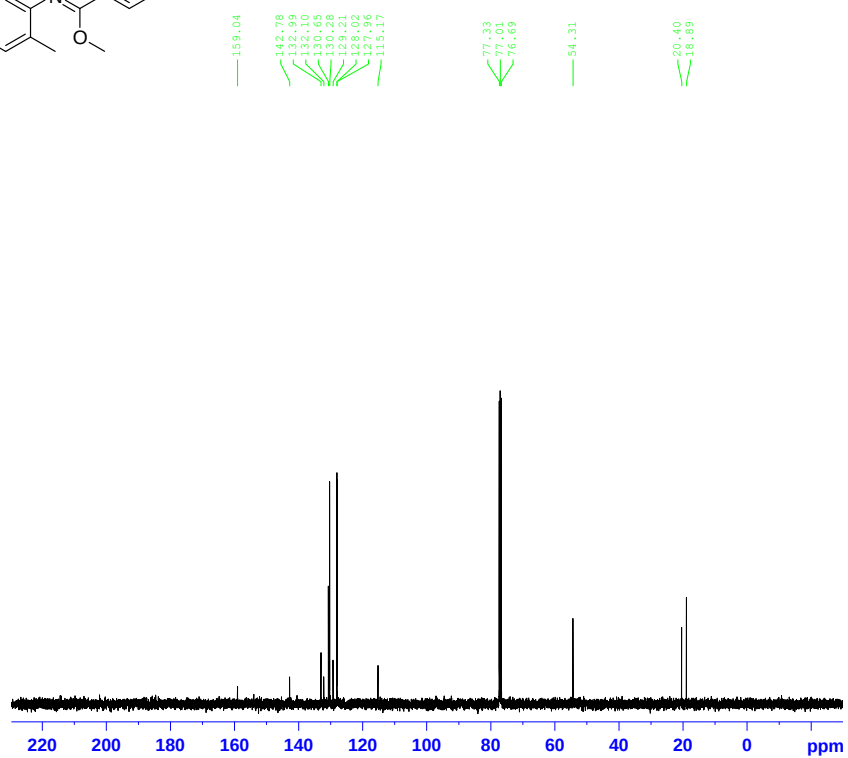
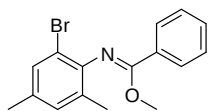
Imidate 6g: ^{13}C -NMR (100 MHz, CDCl_3)



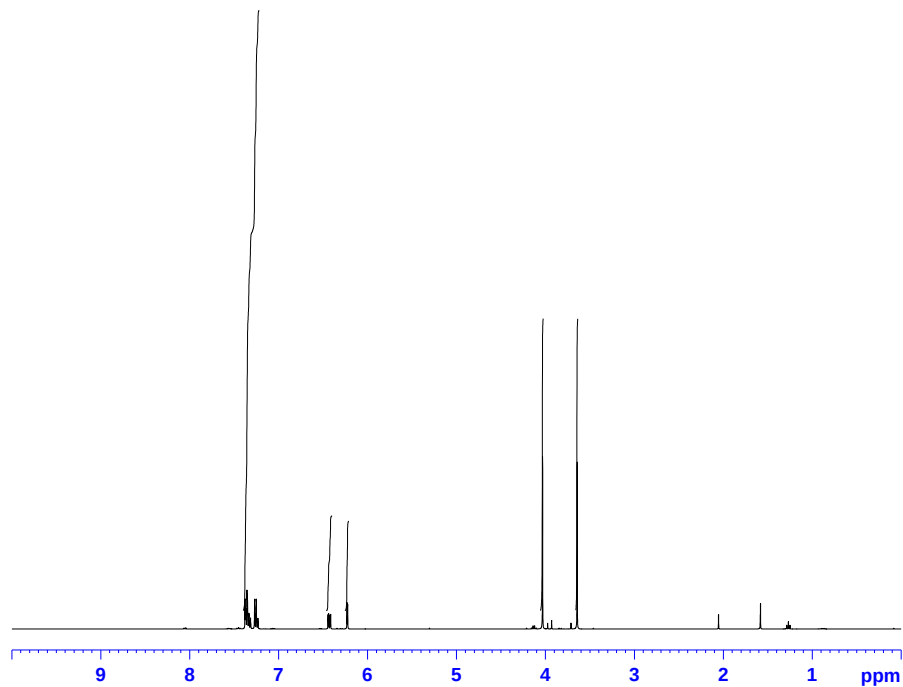
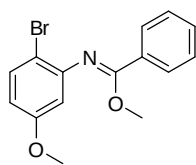
Imidate 6h: ^1H -NMR (400 MHz, CDCl_3)



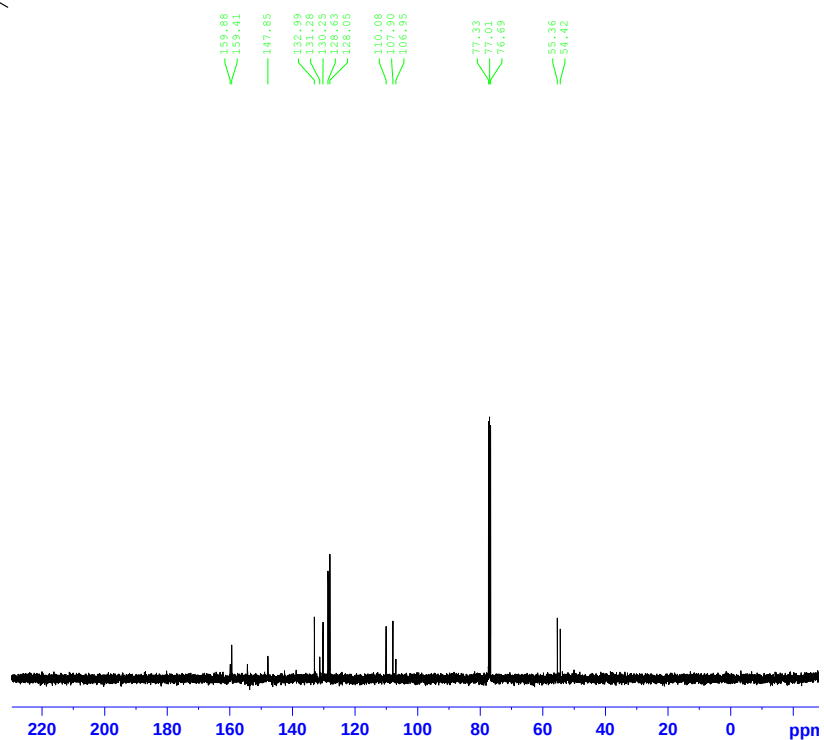
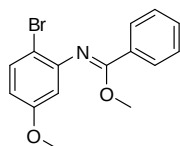
Imidate 6h: ^{13}C -NMR (100 MHz, CDCl_3)



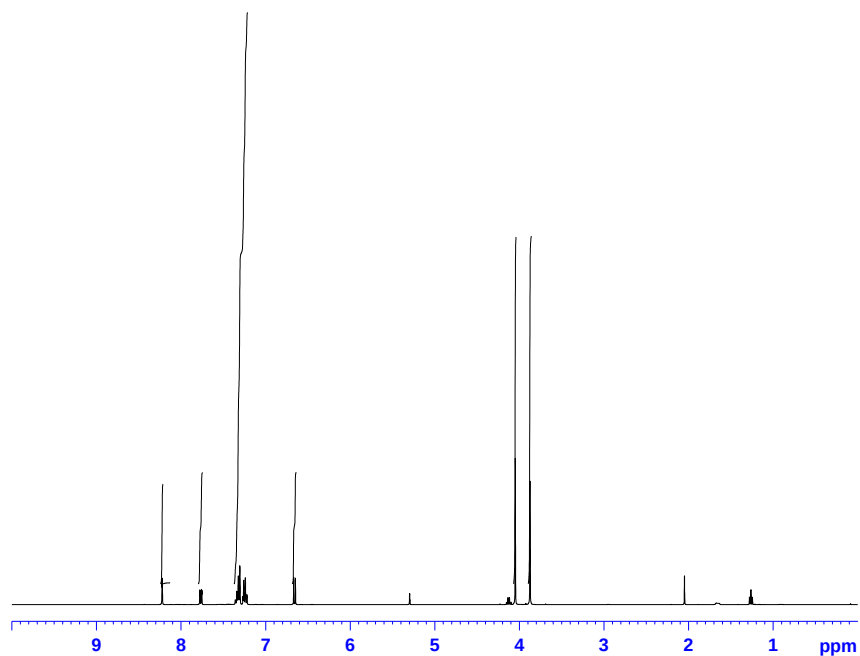
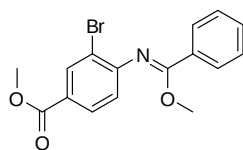
Imidate 6i: ^1H -NMR (400 MHz, CDCl_3)



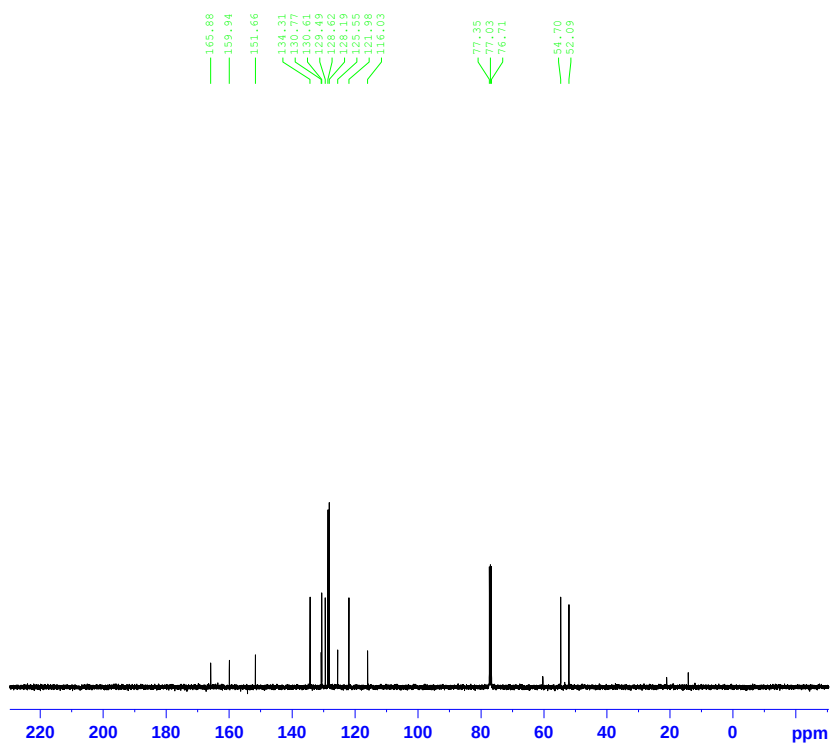
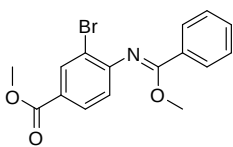
Imidate 6i: ^{13}C -NMR (100 MHz, CDCl_3)



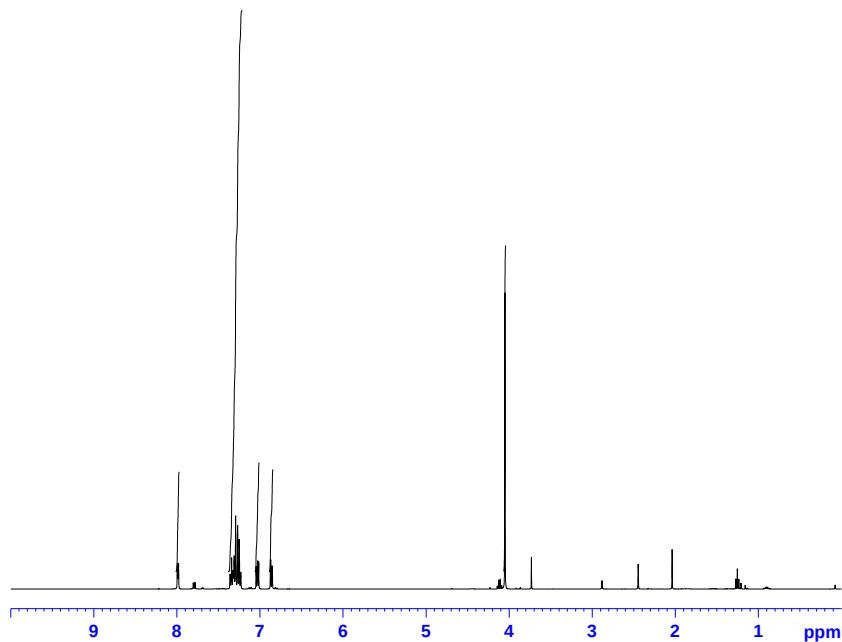
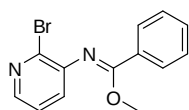
Imidate 6j: ^1H -NMR (400 MHz, CDCl_3)



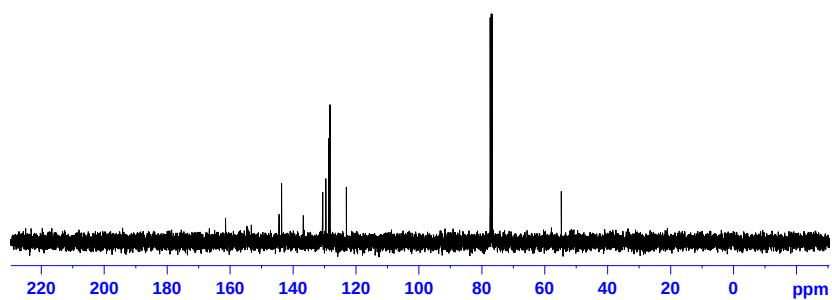
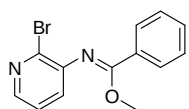
Imidate 6j: ^{13}C -NMR (100 MHz, CDCl_3)



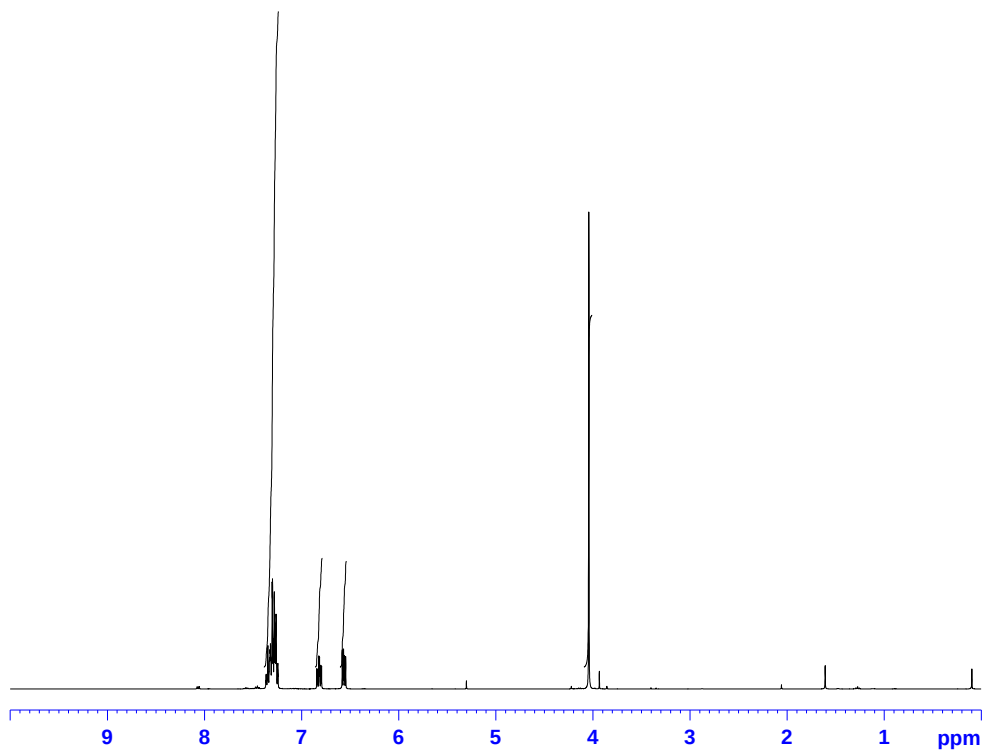
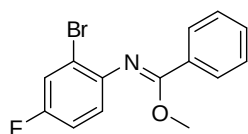
Imidate 6k: ^1H -NMR (400 MHz, CDCl_3)



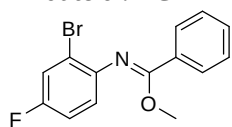
Imidate 6k: ^{13}C -NMR (100 MHz, CDCl_3)



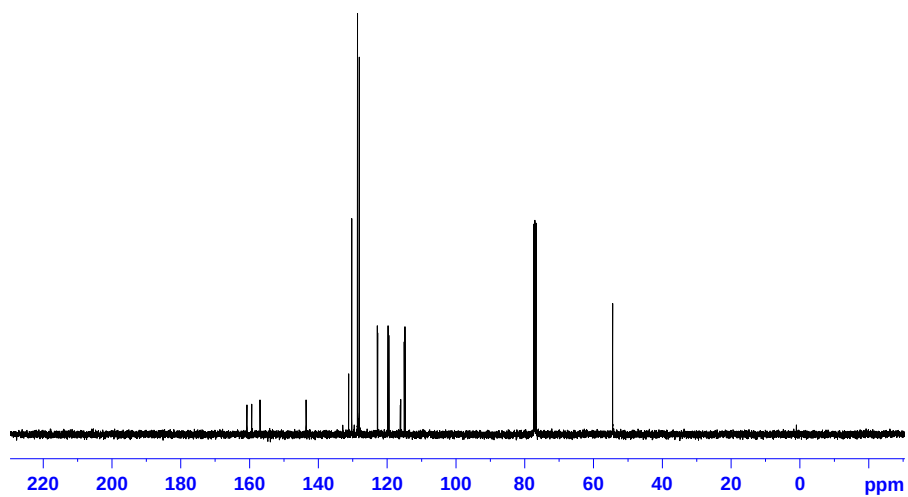
Imidate 6l: ^1H -NMR (400 MHz, CDCl_3)



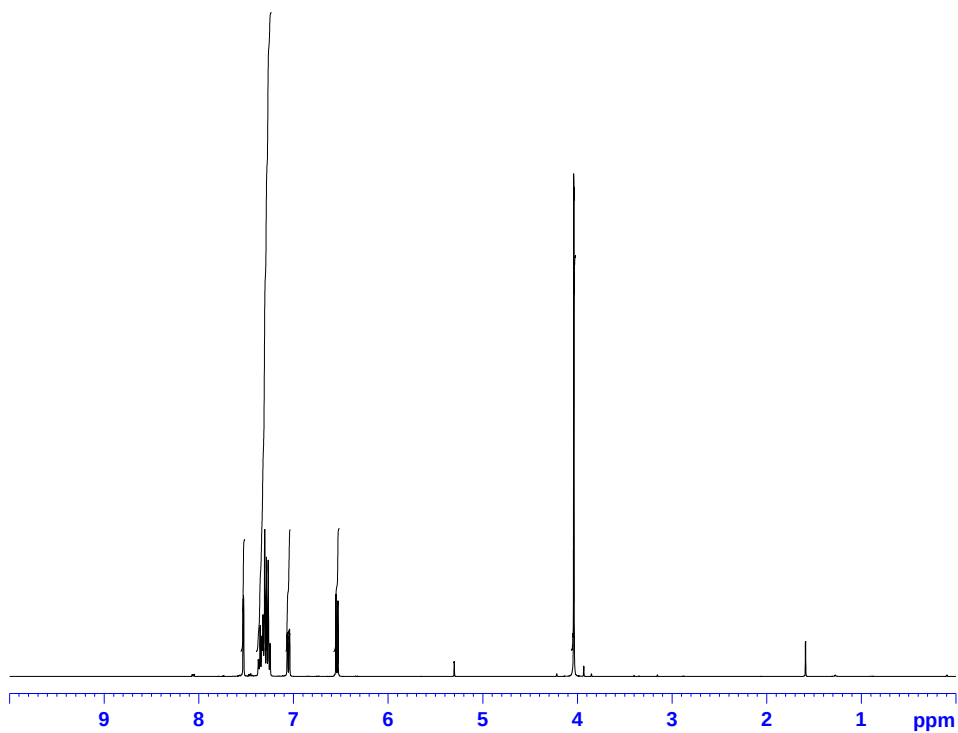
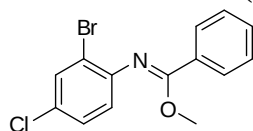
Imidate 6l: ^{13}C -NMR (100 MHz, CDCl_3)



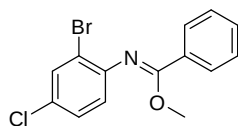
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115.03
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77.23
77.03
76.71
54.46



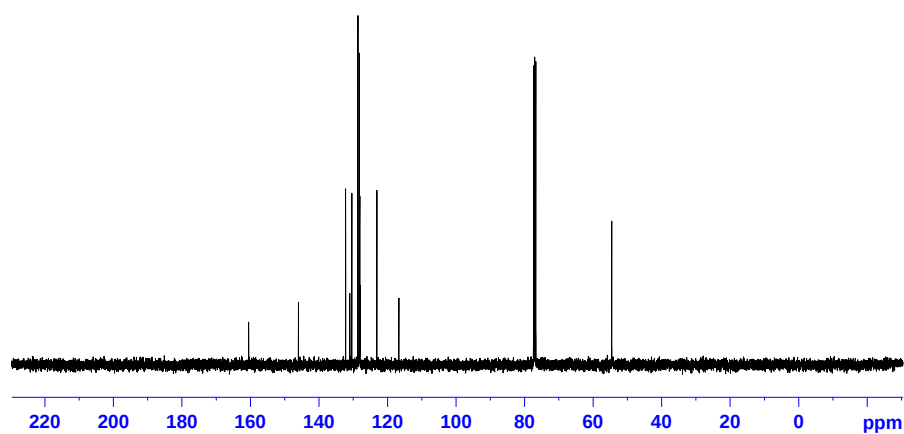
Imidat 6m: ^1H -NMR (400 MHz, CDCl_3)



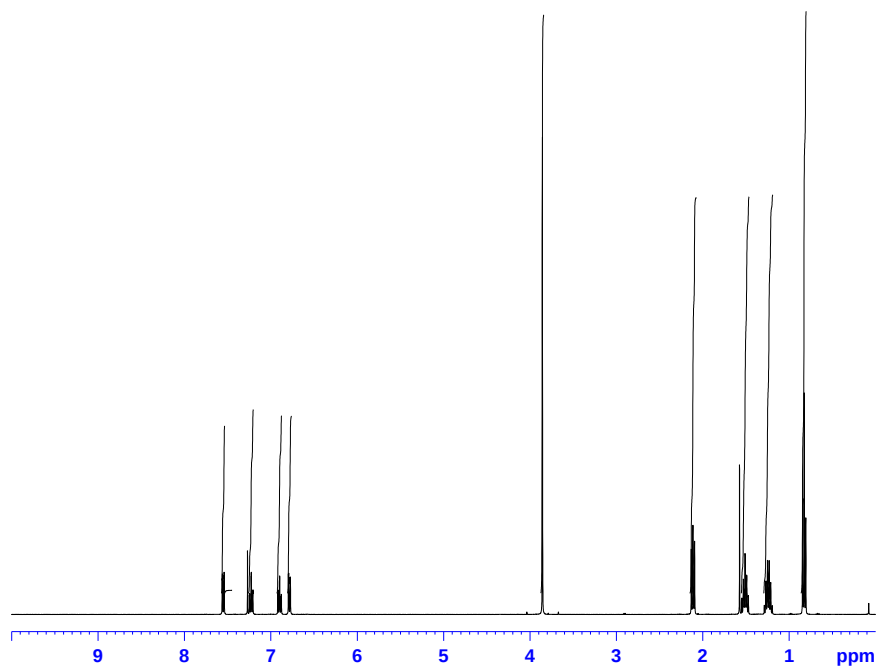
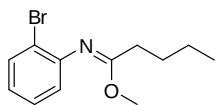
Imidate 6m: ^{13}C -NMR (100 MHz, CDCl_3)



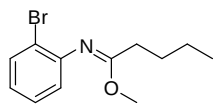
^{13}C -NMR chemical shifts (ppm):
 160.53, 145.99, 132.21, 131.00, 130.41, 128.63, 128.17, 128.08, 123.09, 123.09, 116.68, 77.55, 77.03, 76.71, 54.55



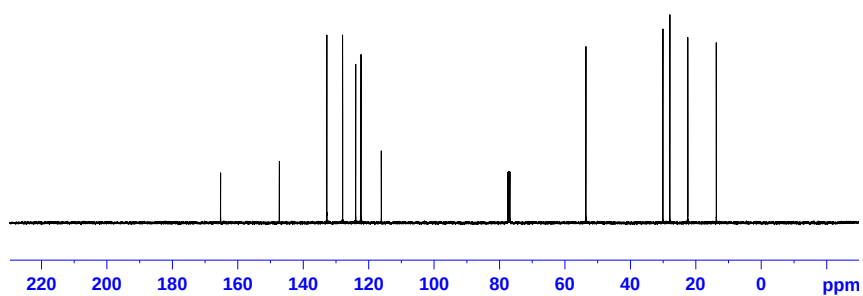
Imide 6n: ^1H -NMR (400 MHz, CDCl_3)



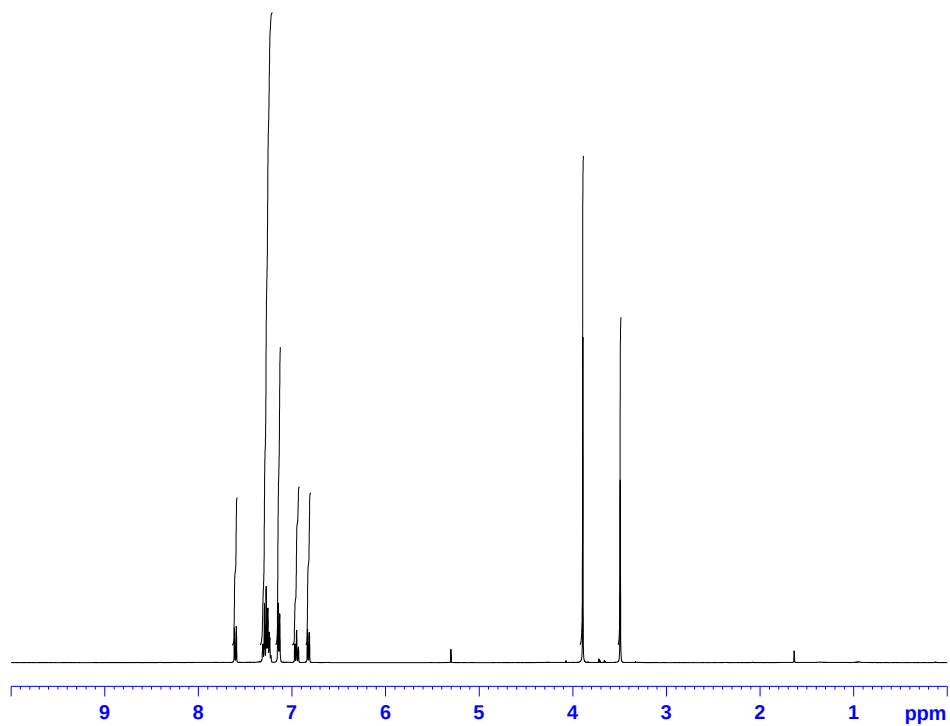
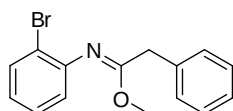
Imide 6n: ^{13}C -NMR (100 MHz, CDCl_3)



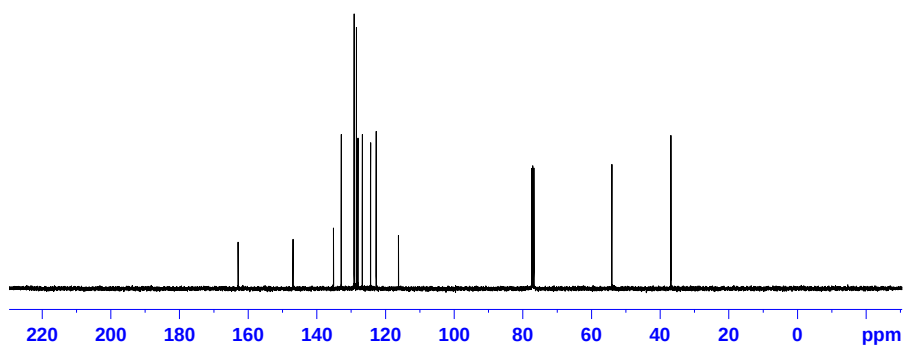
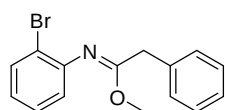
^{13}C -NMR chemical shifts (ppm): 165.22, 147.25, 132.74, 132.61, 129.91, 129.32, 122.32, 116.10, 77.41, 77.09, 76.77, 53.55, 30.01, 27.89, 22.59, 13.68.



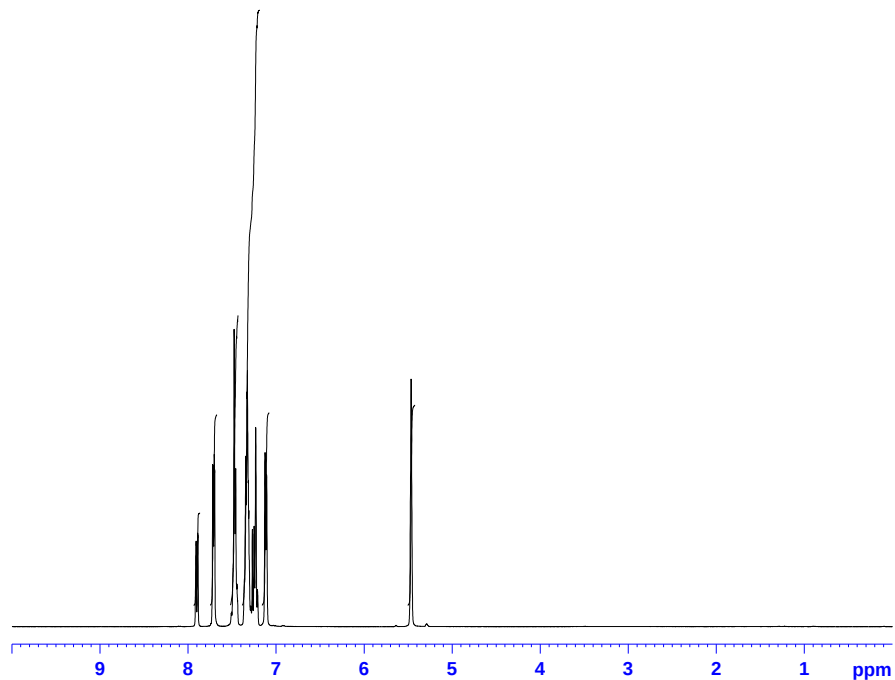
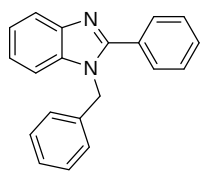
Imidate 6o: ^1H -NMR (400 MHz, CDCl_3)



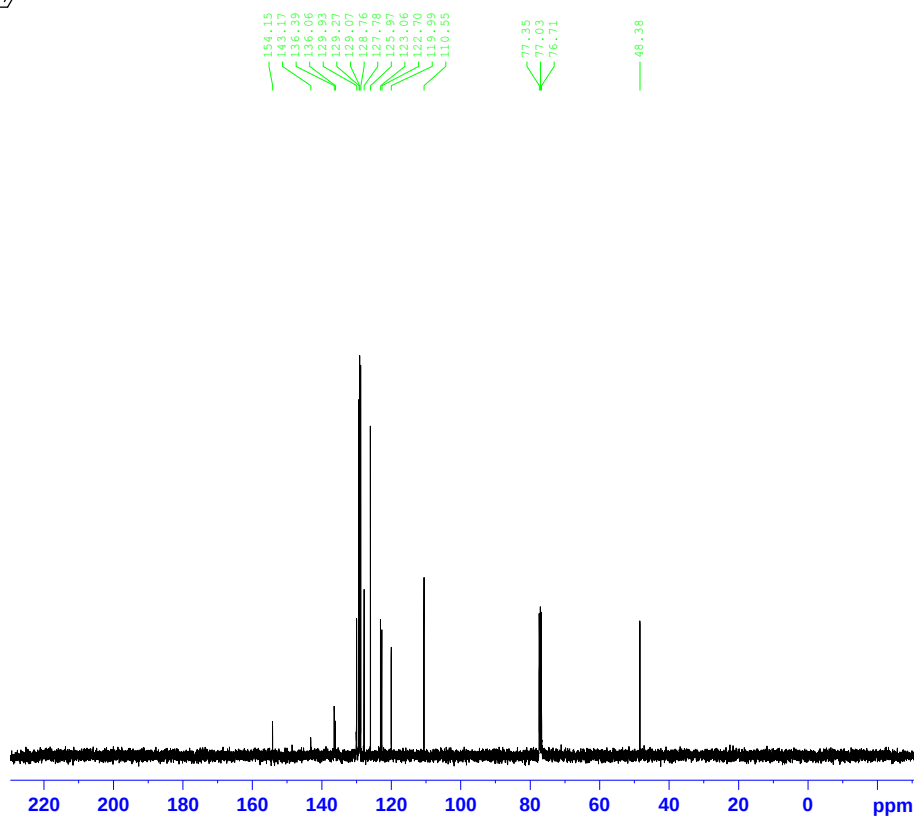
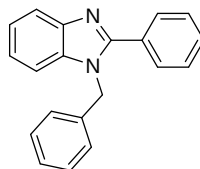
Imidate 6o: ^{13}C -NMR (100 MHz, CDCl_3)



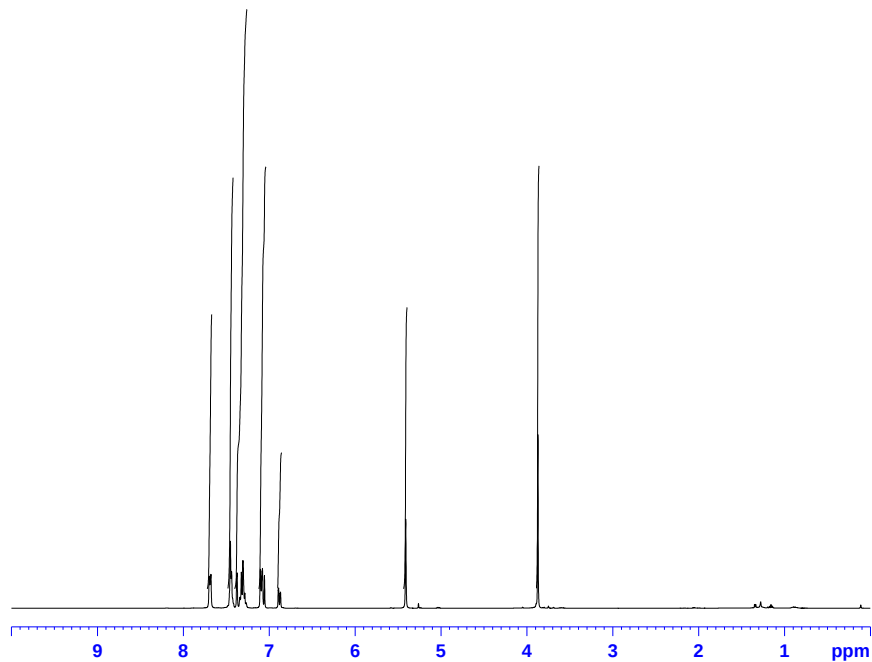
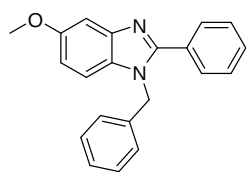
Benzimidazole 7a: ^1H -NMR (400 MHz, CDCl_3)



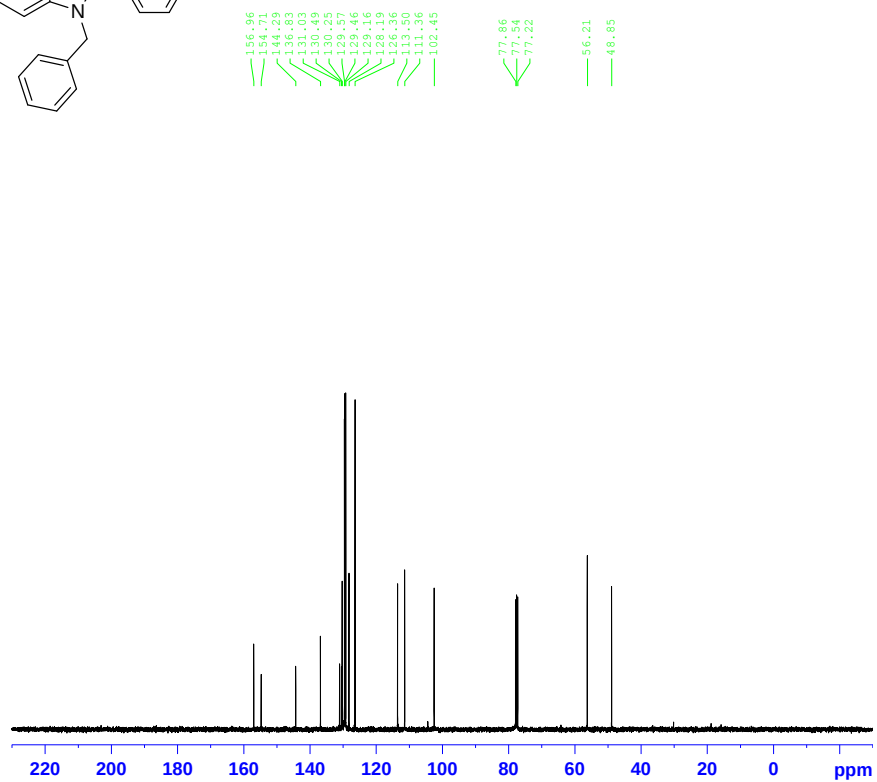
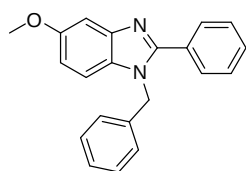
Benzimidazole 7a: ^{13}C -NMR (400 MHz, CDCl_3)



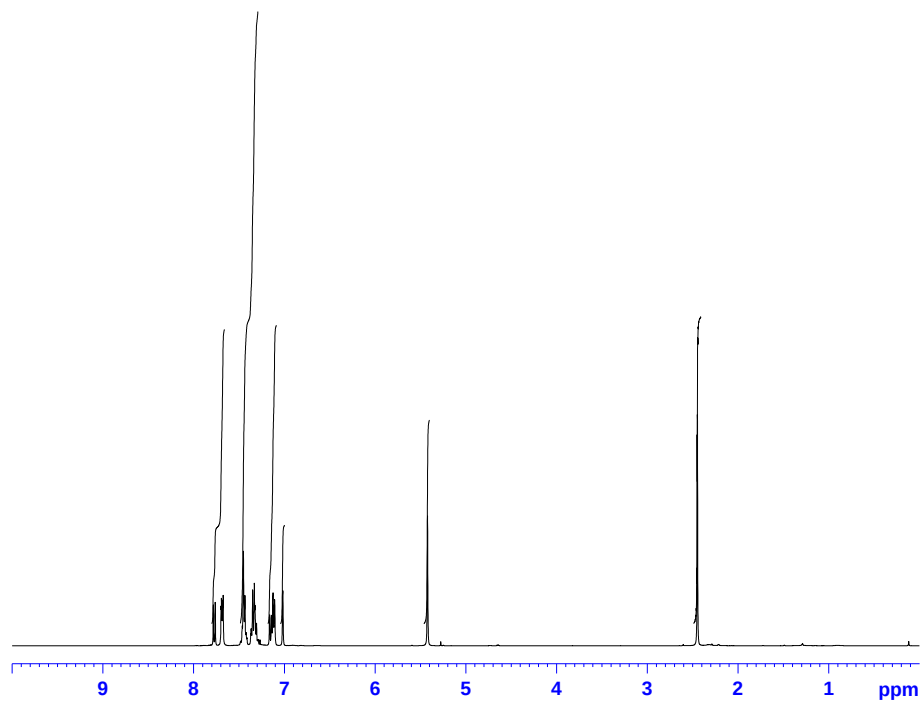
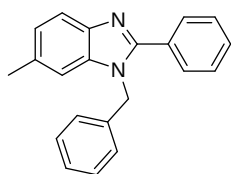
Benzimidazole 7b: ^1H -NMR (400 MHz, CDCl_3)



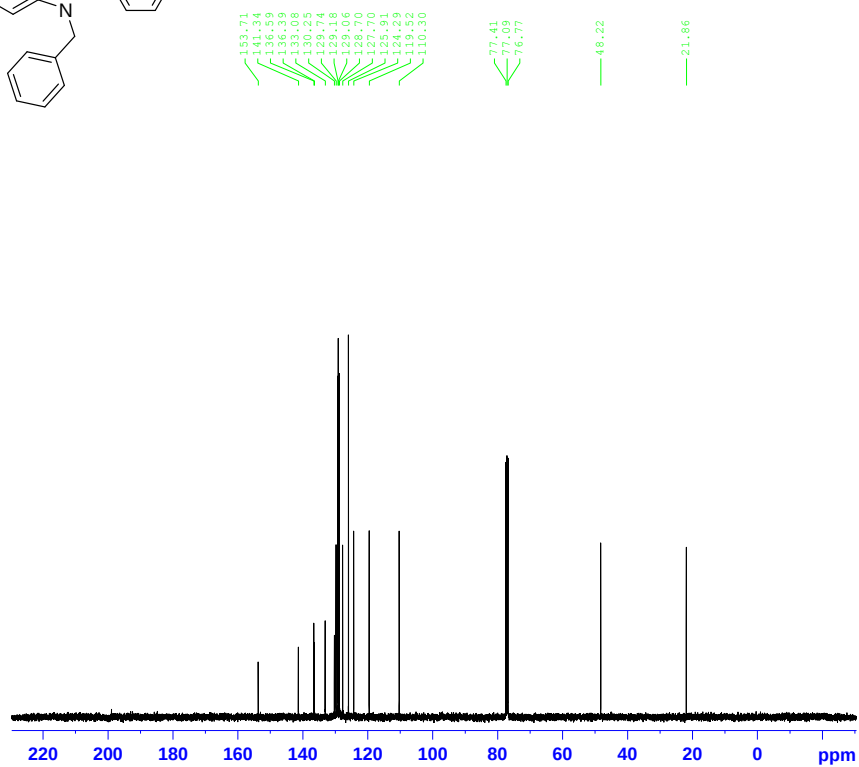
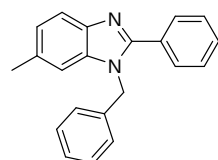
Benzimidazole 7b: ^{13}C -NMR (100 MHz, CDCl_3)



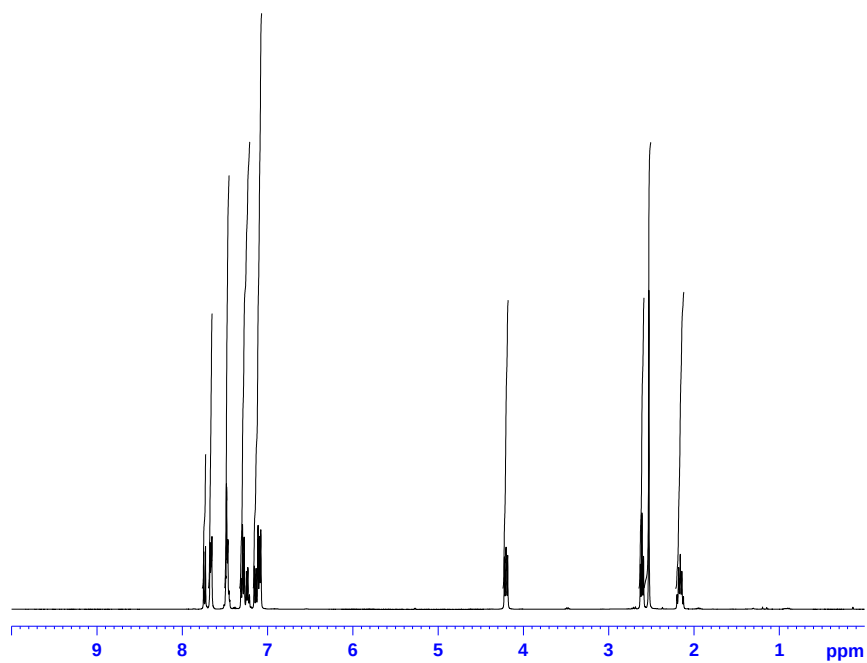
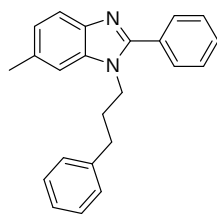
Benzimidazole 7c: ^1H -NMR (400 MHz, CDCl_3)



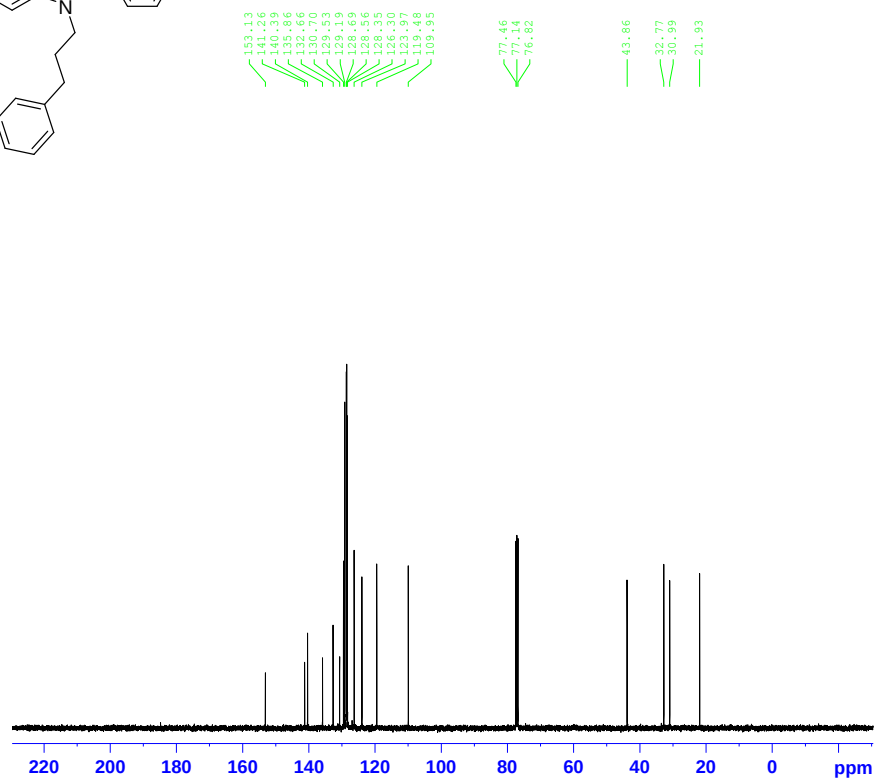
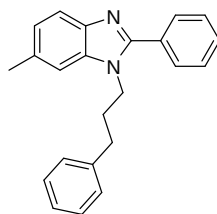
Benzimidazole 7c: ^{13}C -NMR (100 MHz, CDCl_3)



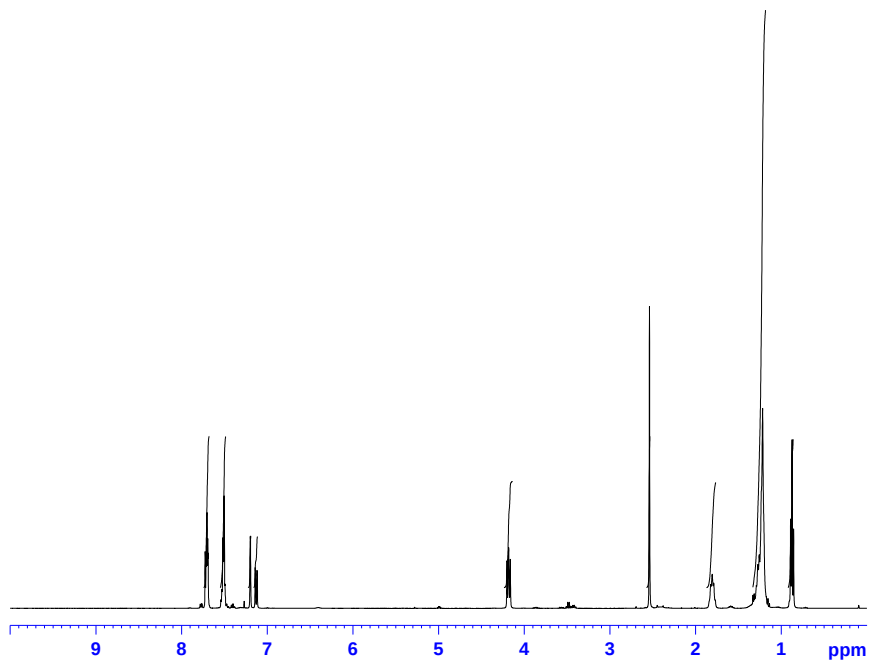
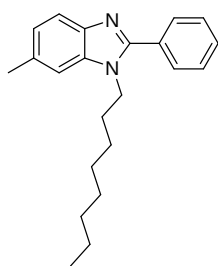
Benzimidazole 7d: ^1H -NMR (400 MHz, CDCl_3)



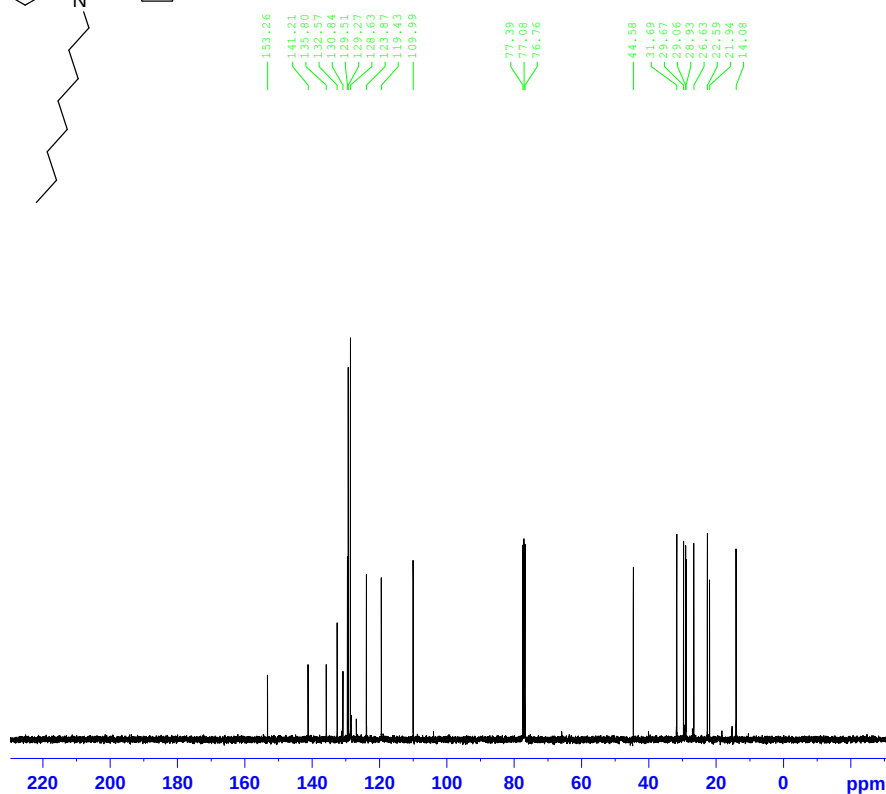
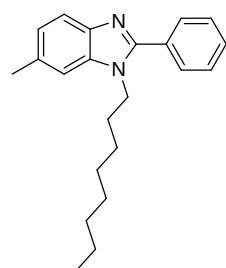
Benzimidazole 7d: ^{13}C -NMR (100 MHz, CDCl_3)



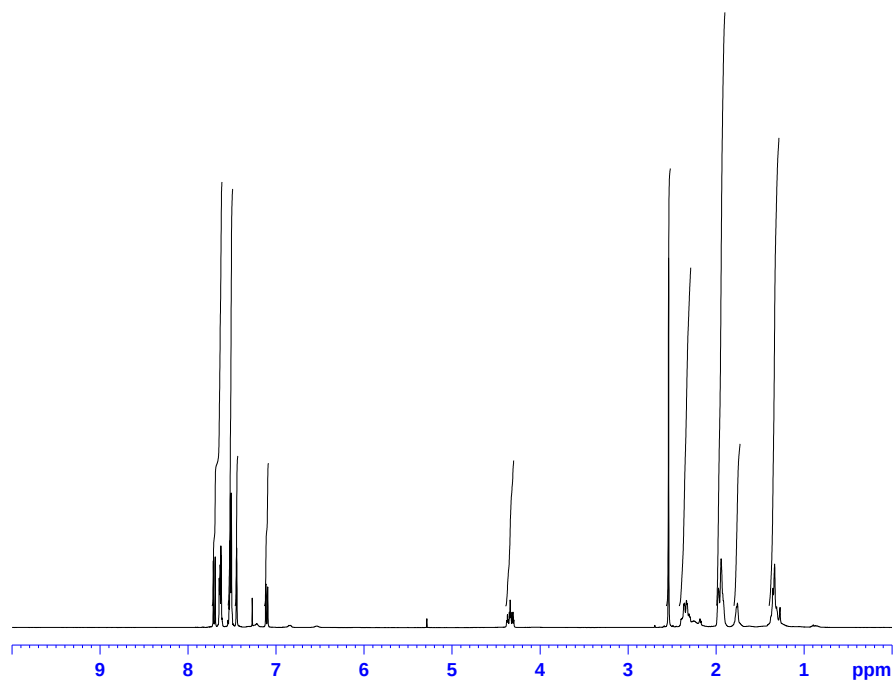
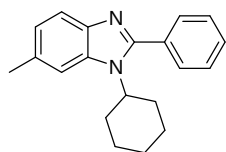
Benzimidazole 7e: ^1H -NMR (400 MHz, CDCl_3)



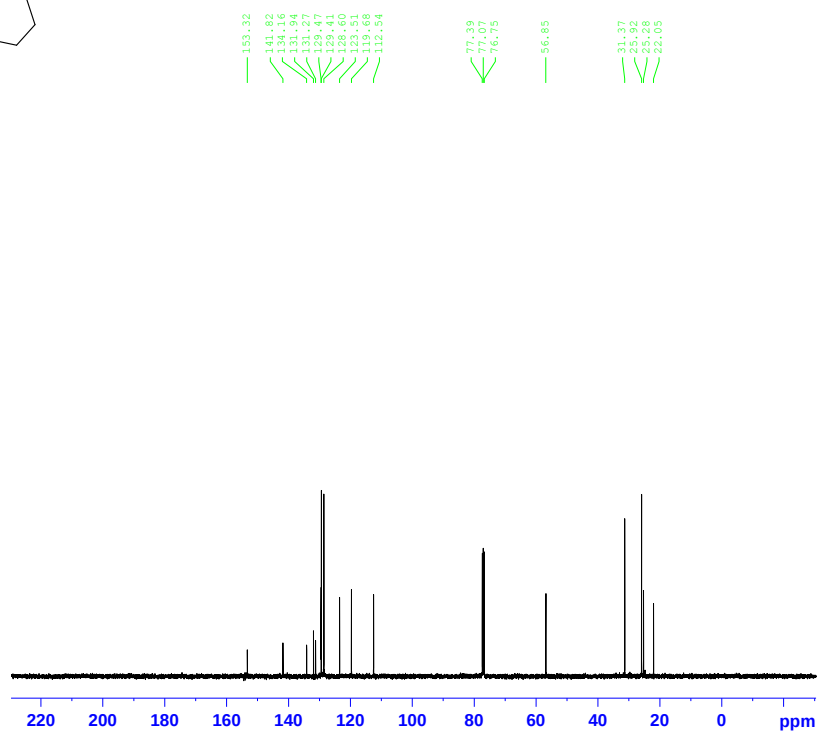
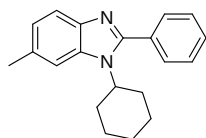
Benzimidazole 7e: ^{13}C -NMR (100 MHz, CDCl_3)



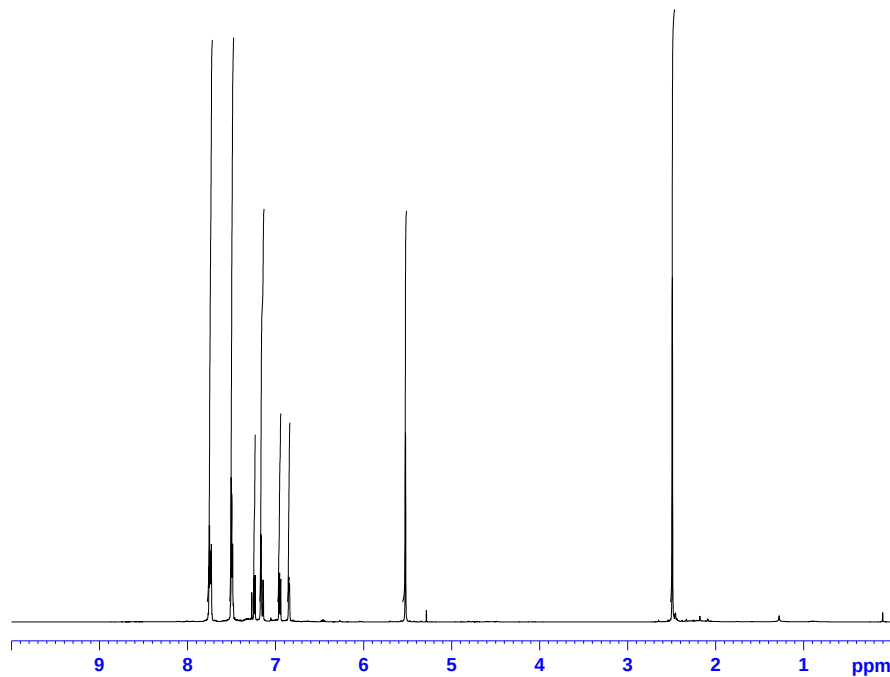
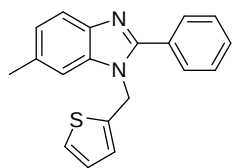
Benzimidazole 7f: ^1H -NMR (400 MHz, CDCl_3)



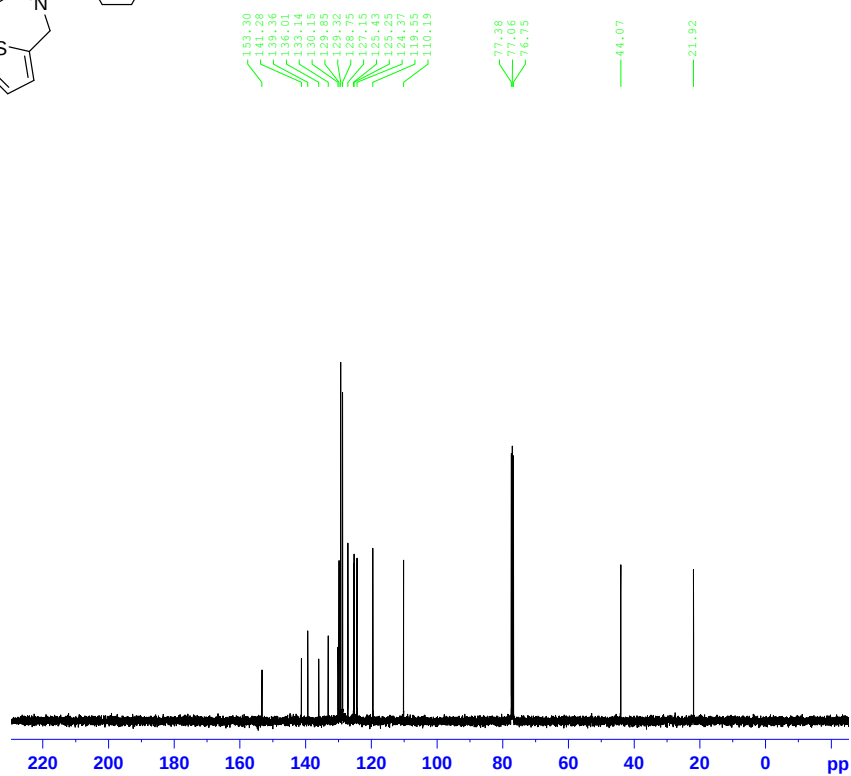
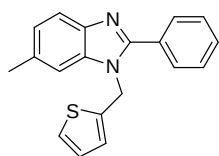
Benzimidazole 7f: ^{13}C -NMR (100 MHz, CDCl_3)



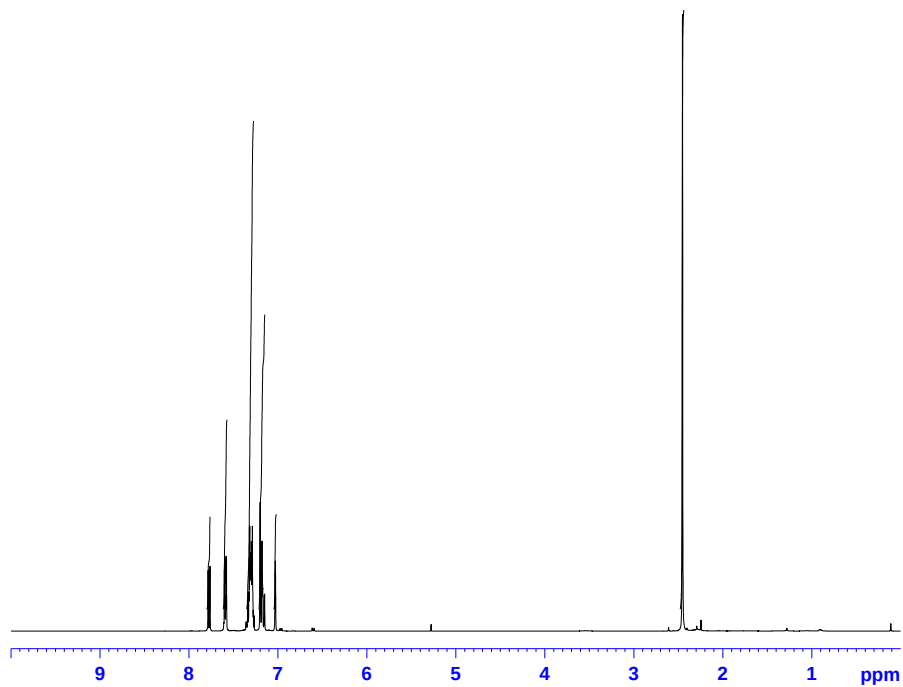
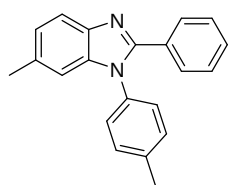
Benzimidazole 7g: ^1H -NMR (400 MHz, CDCl_3)



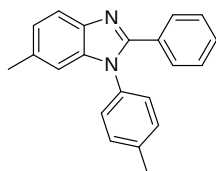
Benzimidazole 7g: ^{13}C -NMR (100 MHz, CDCl_3)



Benzimidazole 7h: ^1H -NMR (400 MHz, CDCl_3)



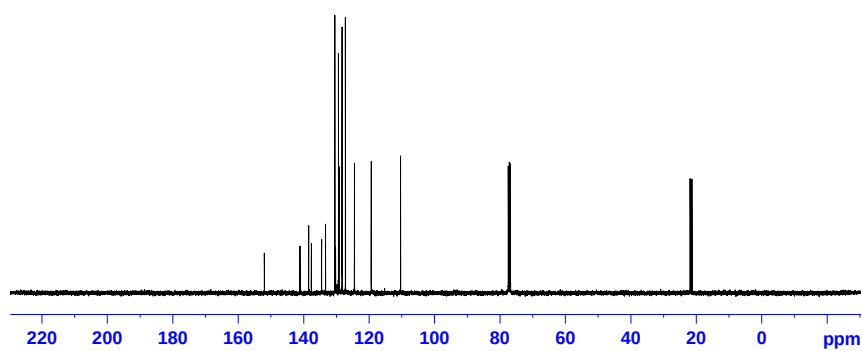
Benzimidazole 7h: ^{13}C -NMR (100 MHz, CDCl_3)



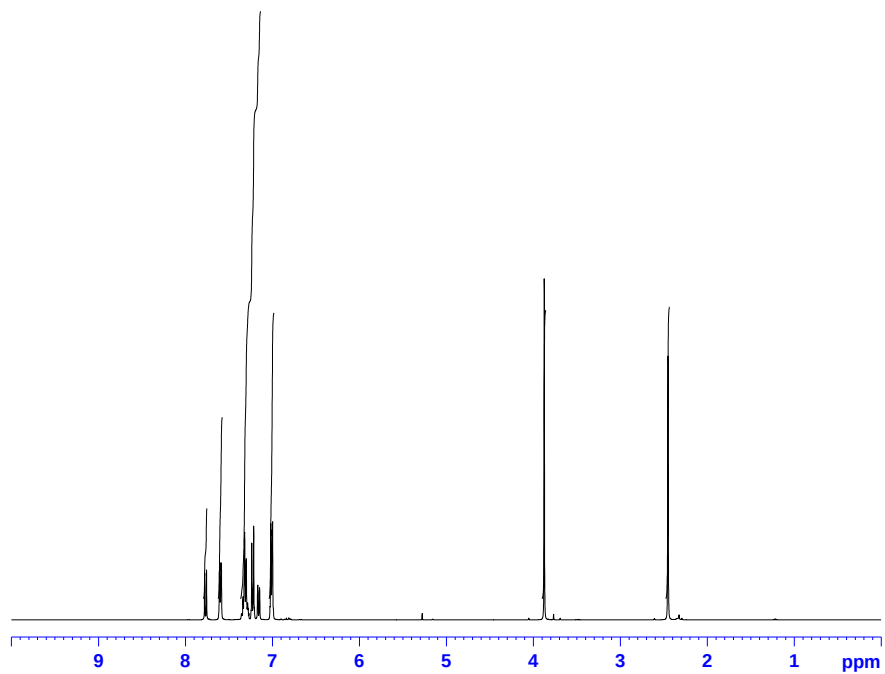
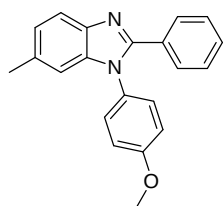
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141.09
138.46
137.61
134.59
131.59
130.44
130.21
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128.12
127.19
124.44
119.30
110.35

77.40
77.09
76.77

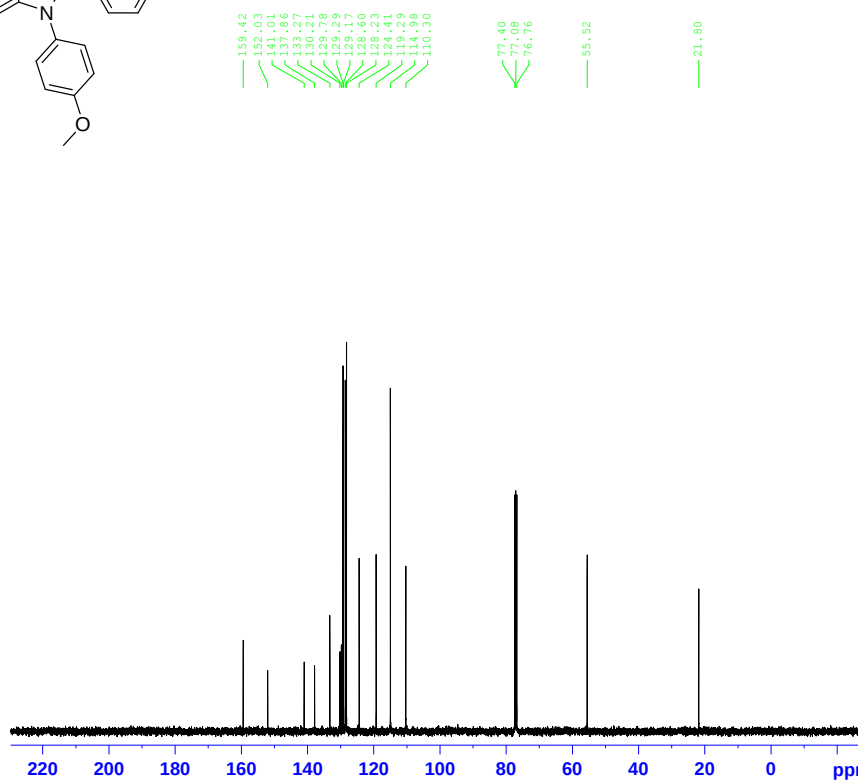
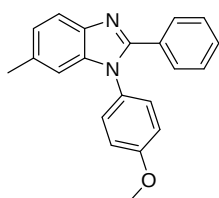
21.81
21.26



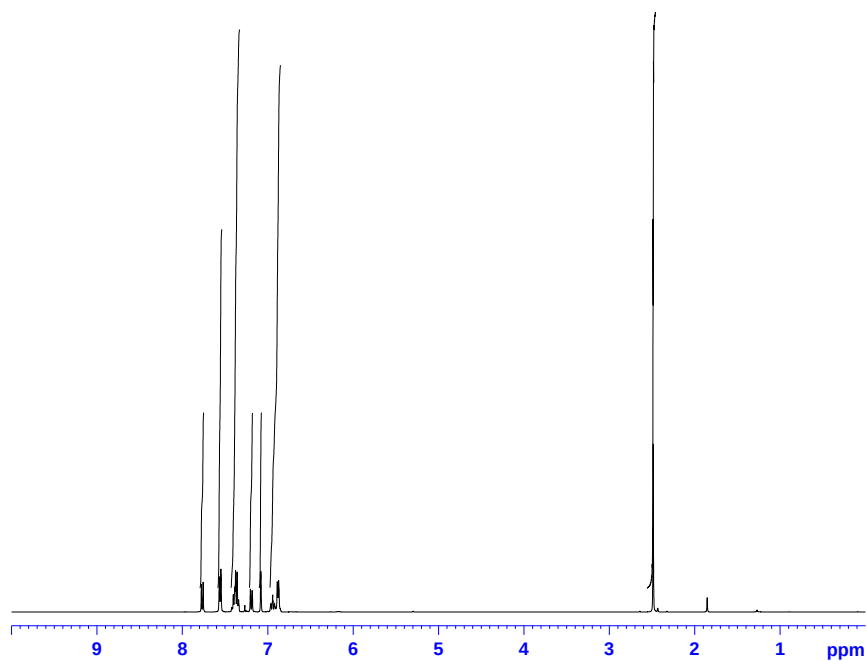
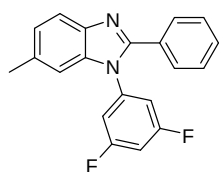
Benzimidazole 7i: ^1H -NMR (400 MHz, CDCl_3)



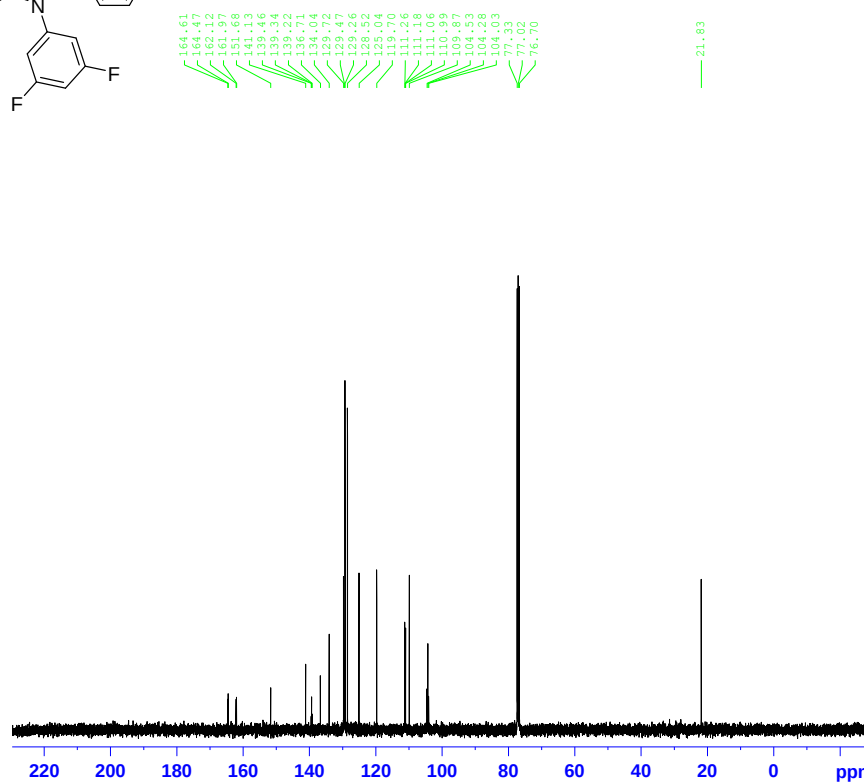
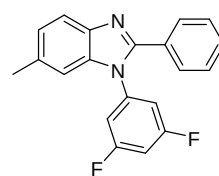
Benzimidazole 7i: ^{13}C -NMR (100 MHz, CDCl_3)



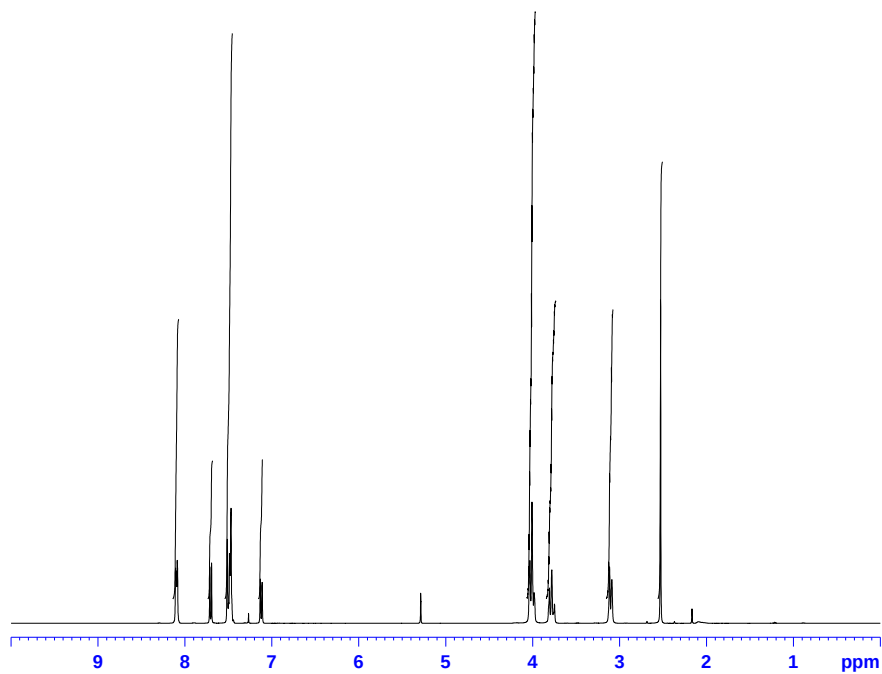
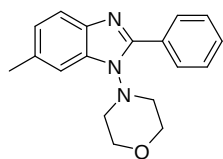
Benzimidazole 7j: ^1H -NMR (400 MHz, CDCl_3)



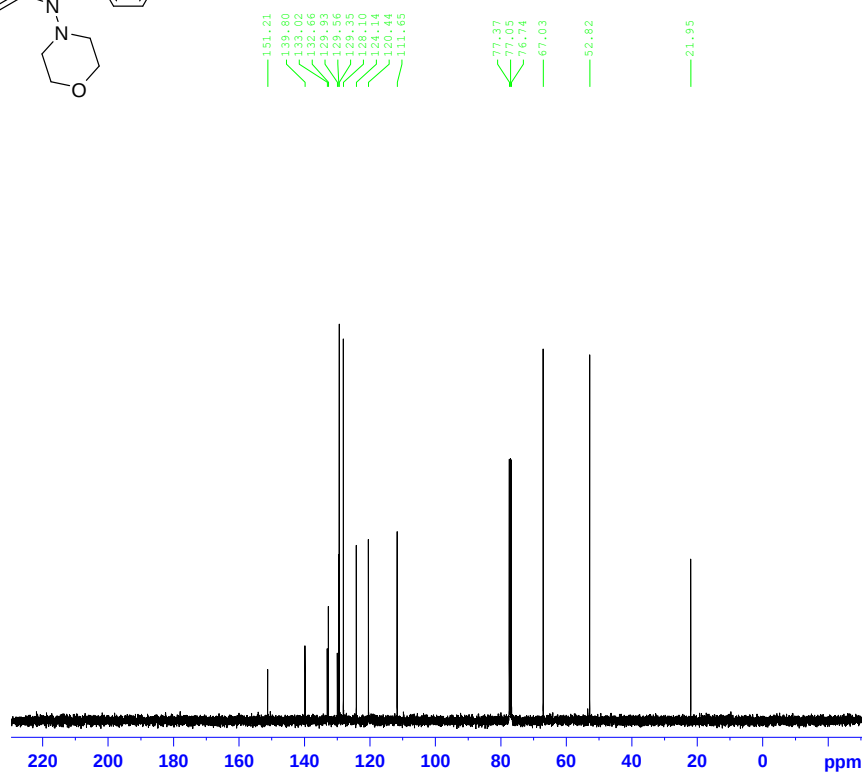
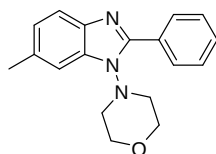
Benzimidazole 7j: ^{13}C -NMR (100 MHz, CDCl_3)



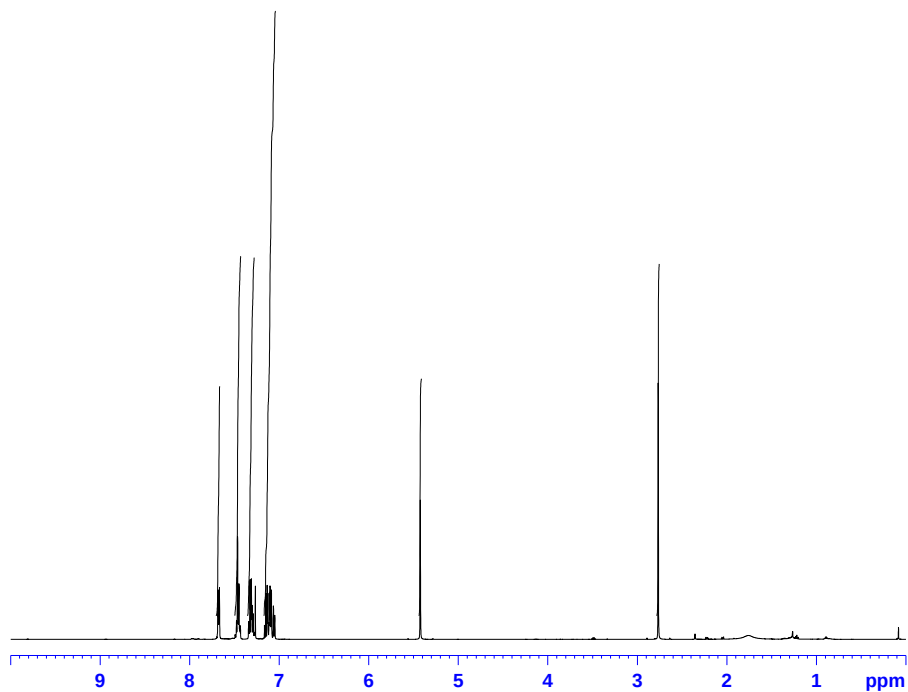
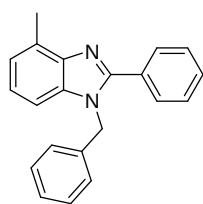
Benzimidazole 7k: ^1H -NMR (400 MHz, CDCl_3)



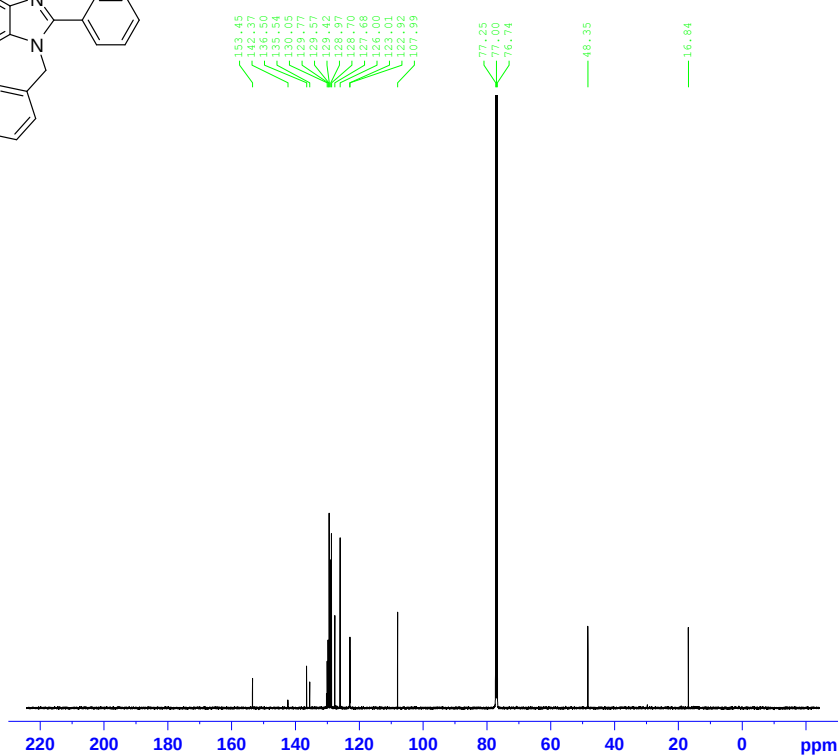
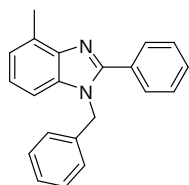
Benzimidazole 7k: ^{13}C -NMR (100 MHz, CDCl_3)



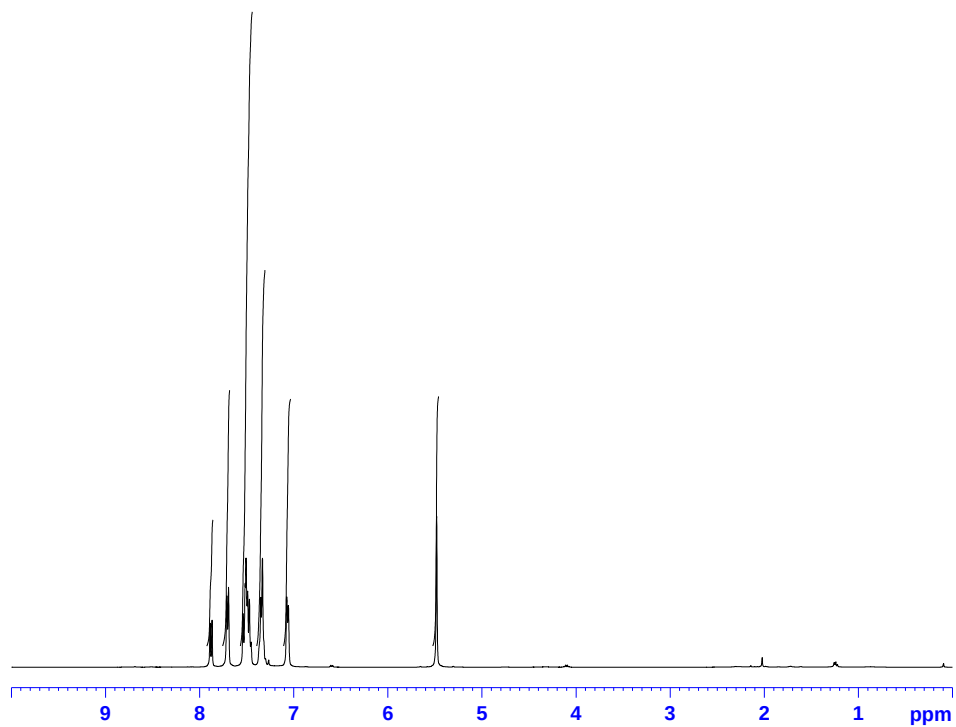
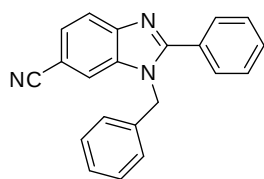
Benzimidazole 7l: ^1H -NMR (500 MHz, CDCl_3)



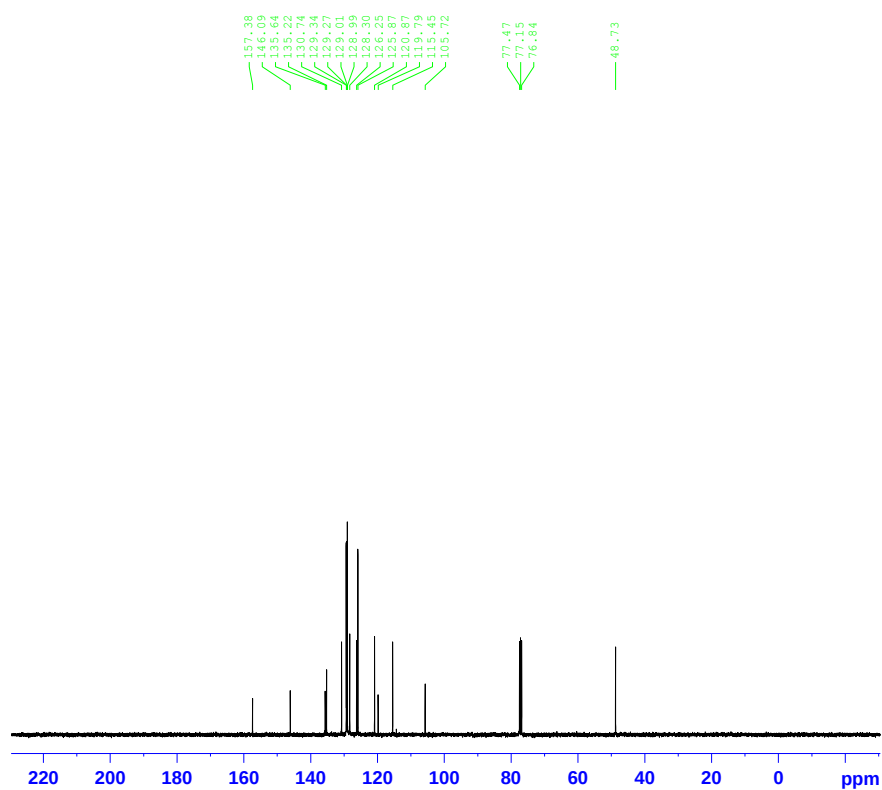
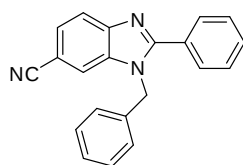
Benzimidazole 7l: ^{13}C -NMR (125 MHz, CDCl_3)



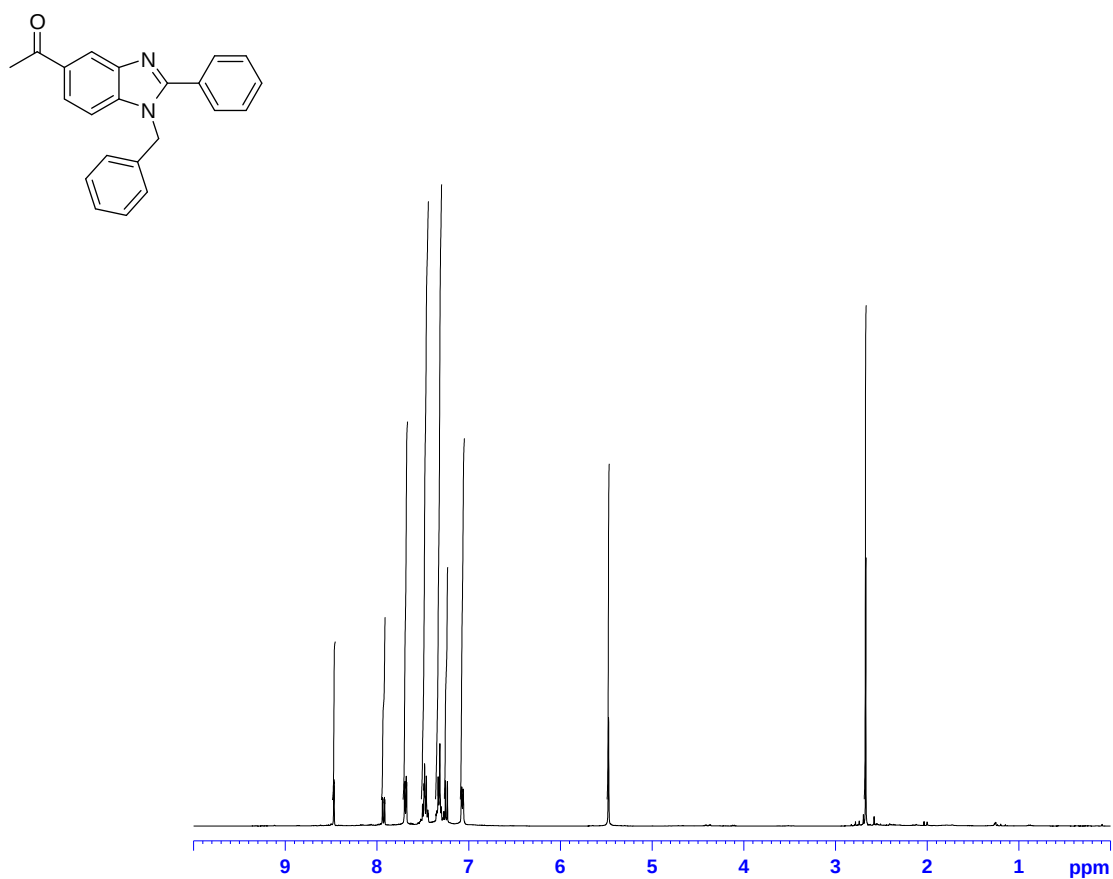
Benzimidazole 7m: ^1H -NMR (400 MHz, CDCl_3)



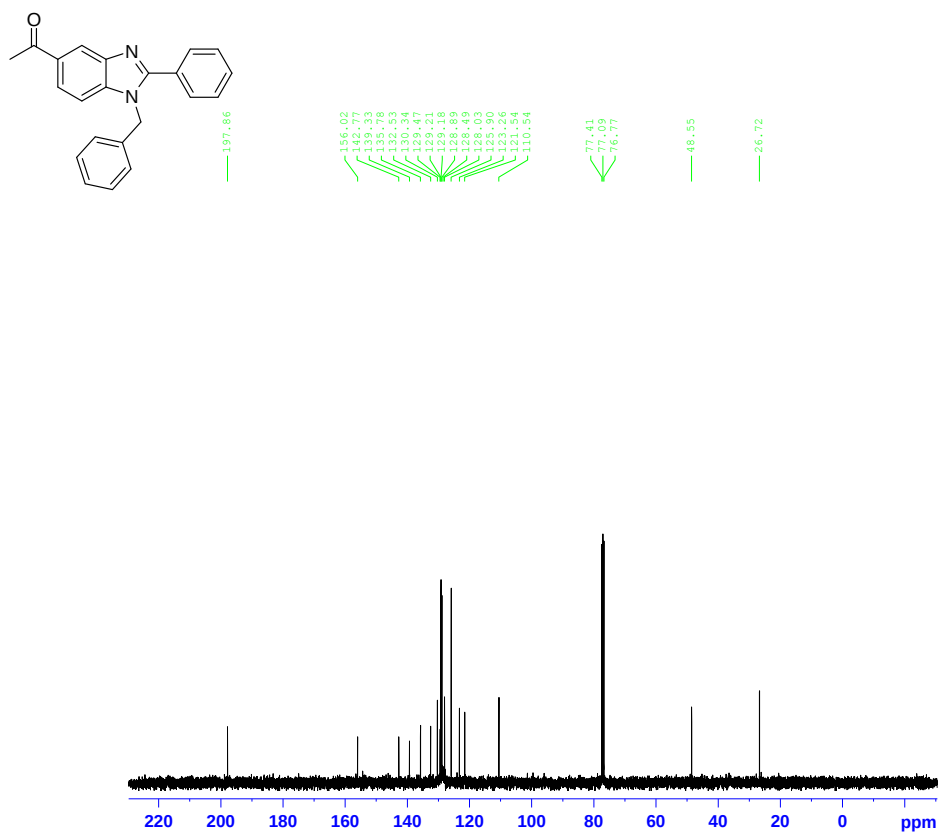
Benzimidazole 7m: ^{13}C -NMR (100 MHz, CDCl_3)



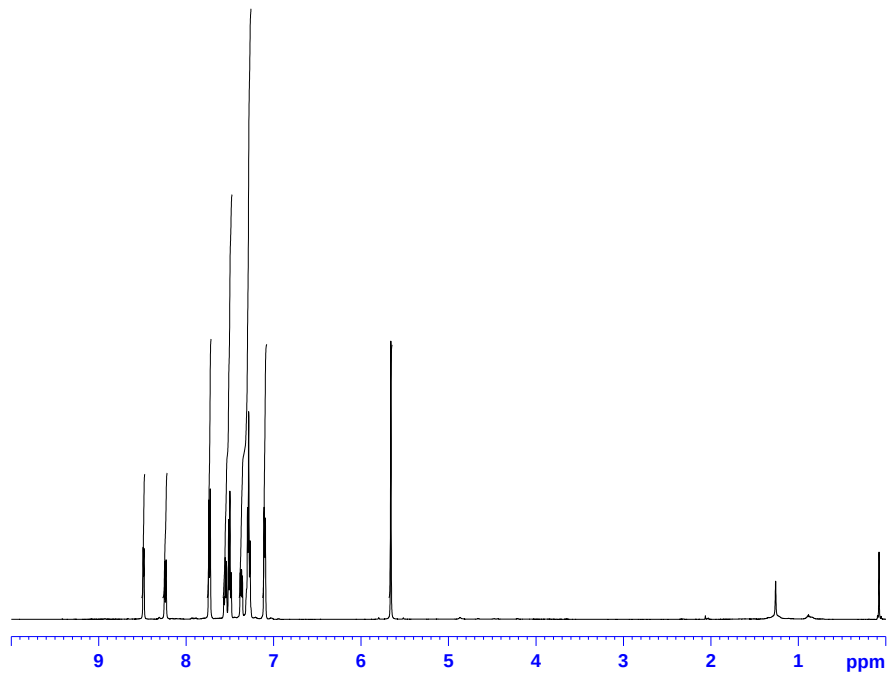
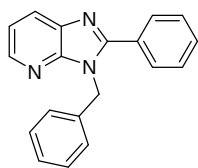
Benzimidazole 7n: ^1H -NMR (400 MHz, CDCl_3)



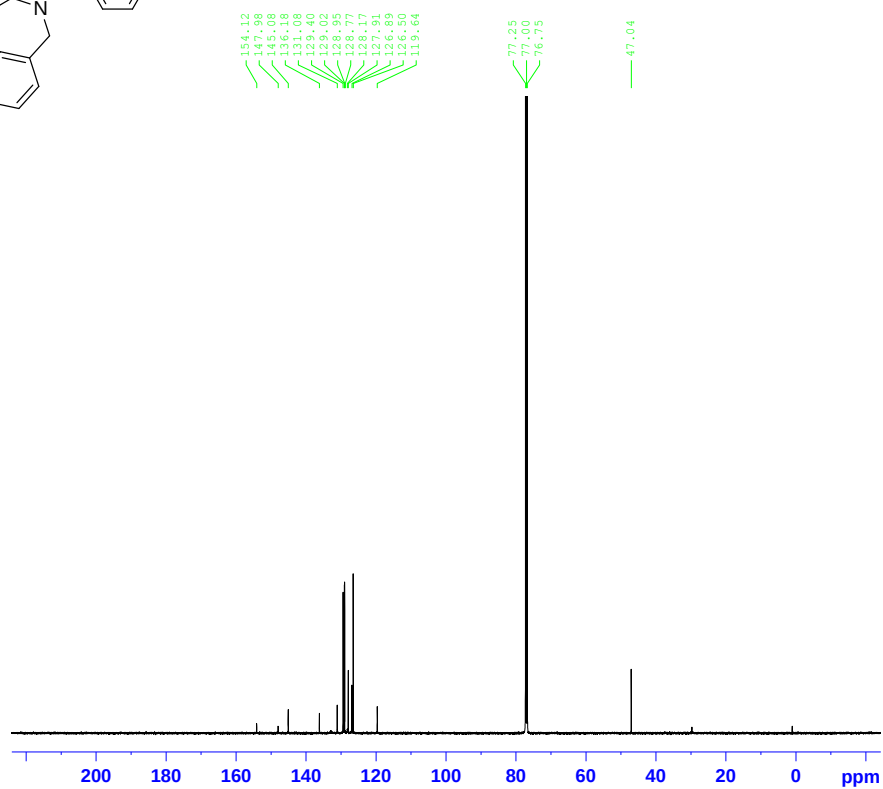
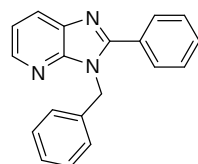
Benzimidazole 7n: ^{13}C -NMR (100 MHz, CDCl_3)



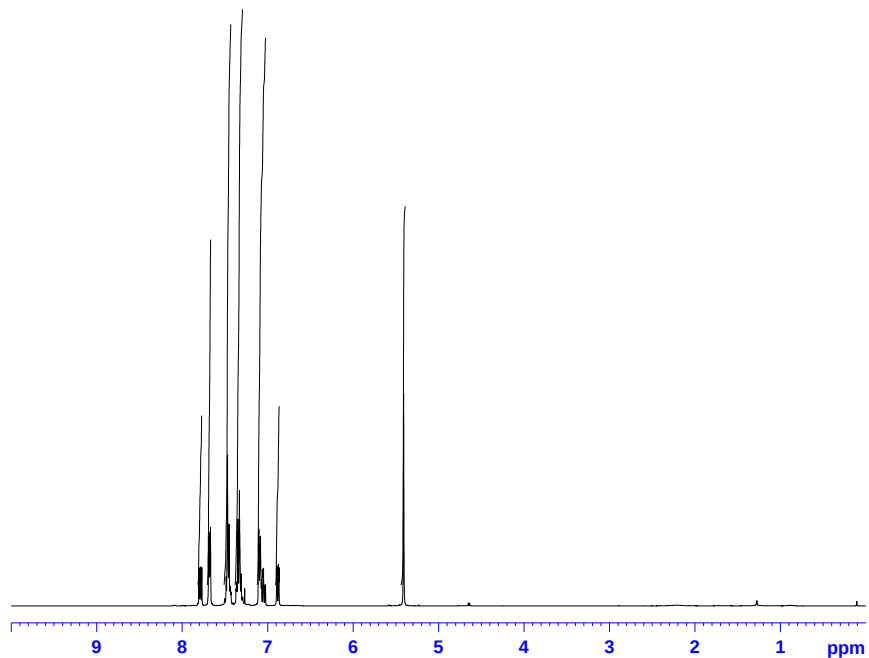
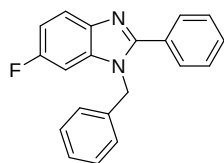
Benzimidazole 7o: ^1H -NMR (500 MHz, CDCl_3)



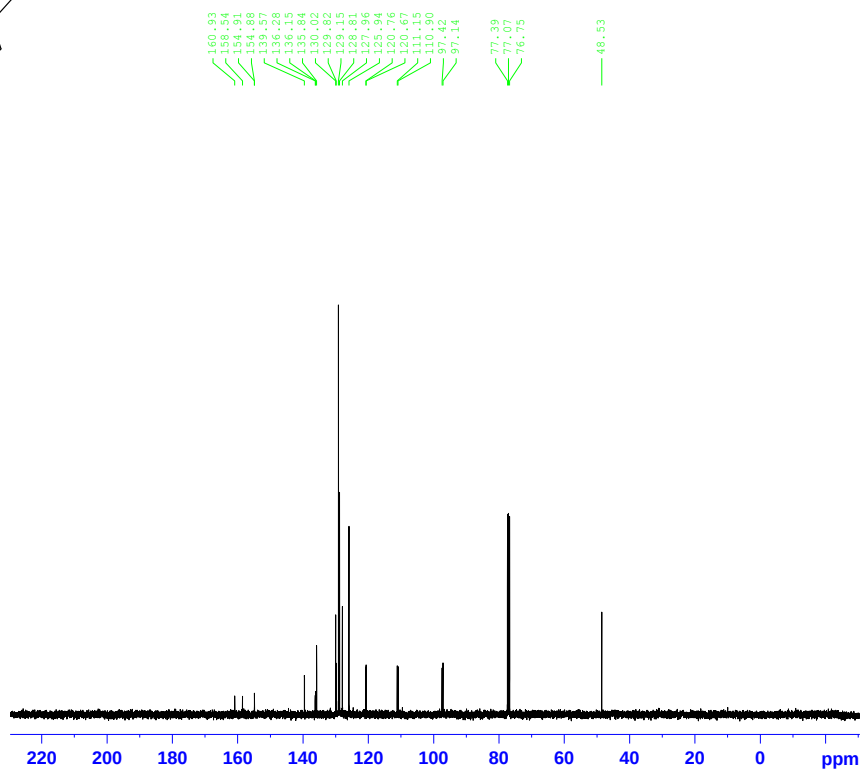
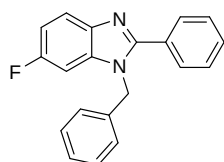
Benzimidazole 7o: ^{13}C -NMR (125 MHz, CDCl_3)



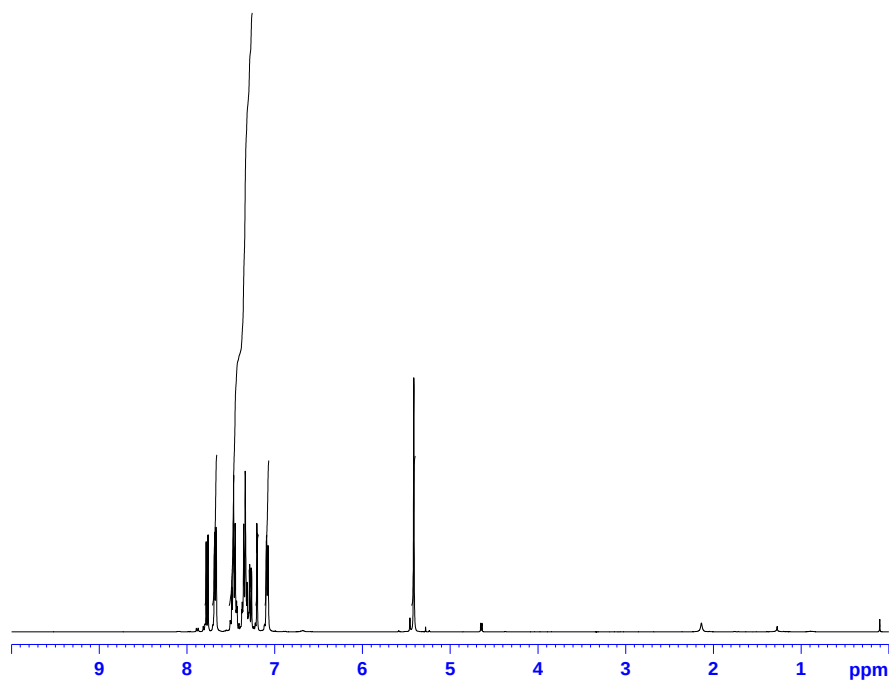
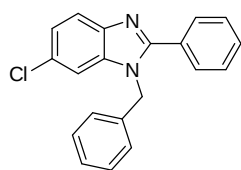
Benzimidazole 7p: ^1H -NMR (400 MHz, CDCl_3)



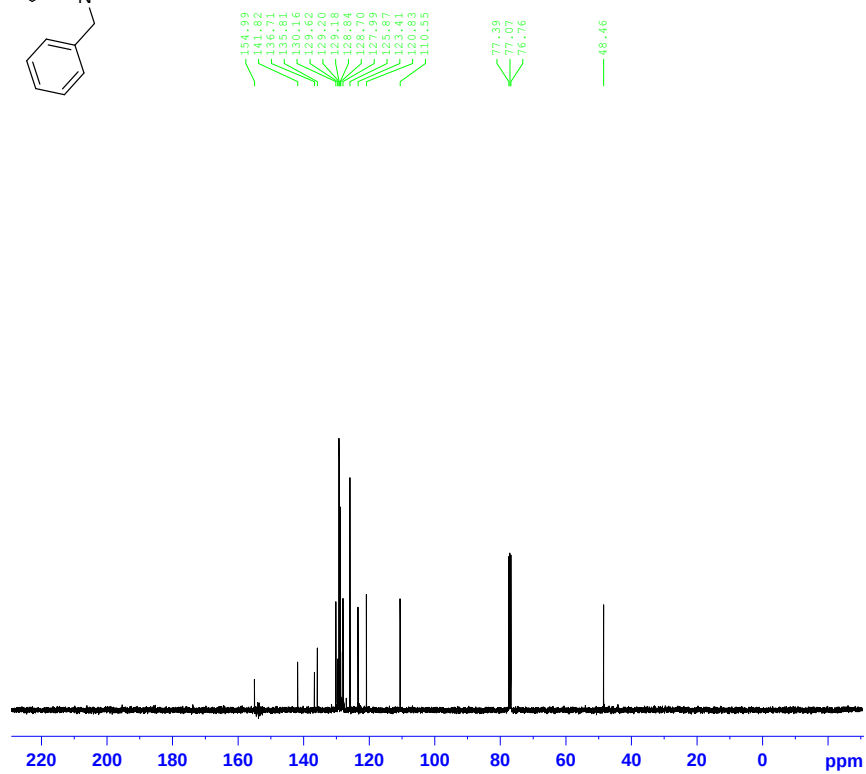
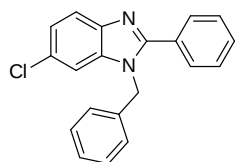
Benzimidazole 7p: ^{13}C -NMR (100 MHz, CDCl_3)



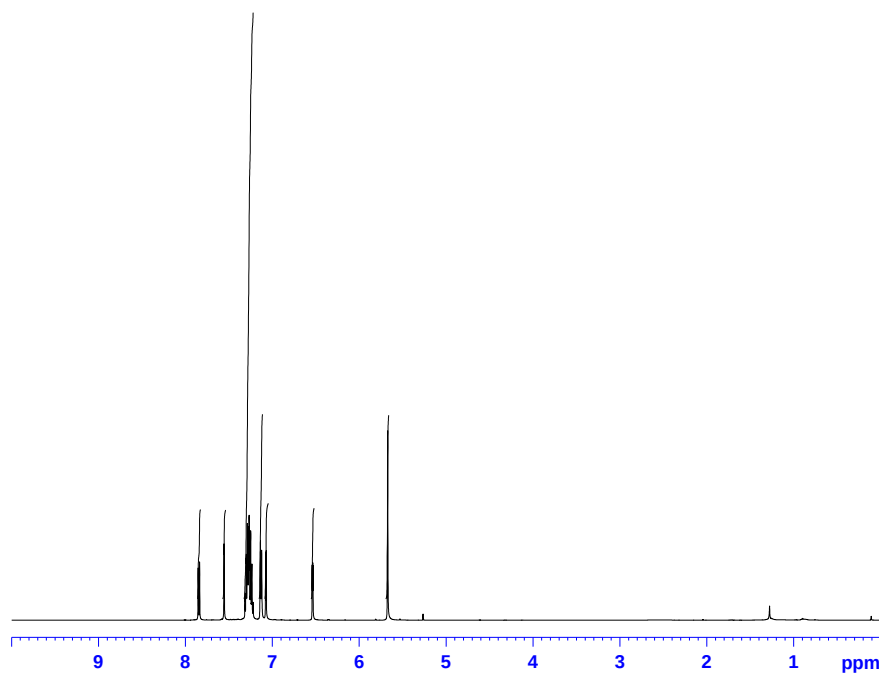
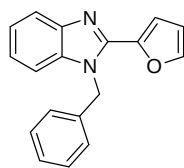
Benzimidazole 7q: ^1H -NMR (400 MHz, CDCl_3)



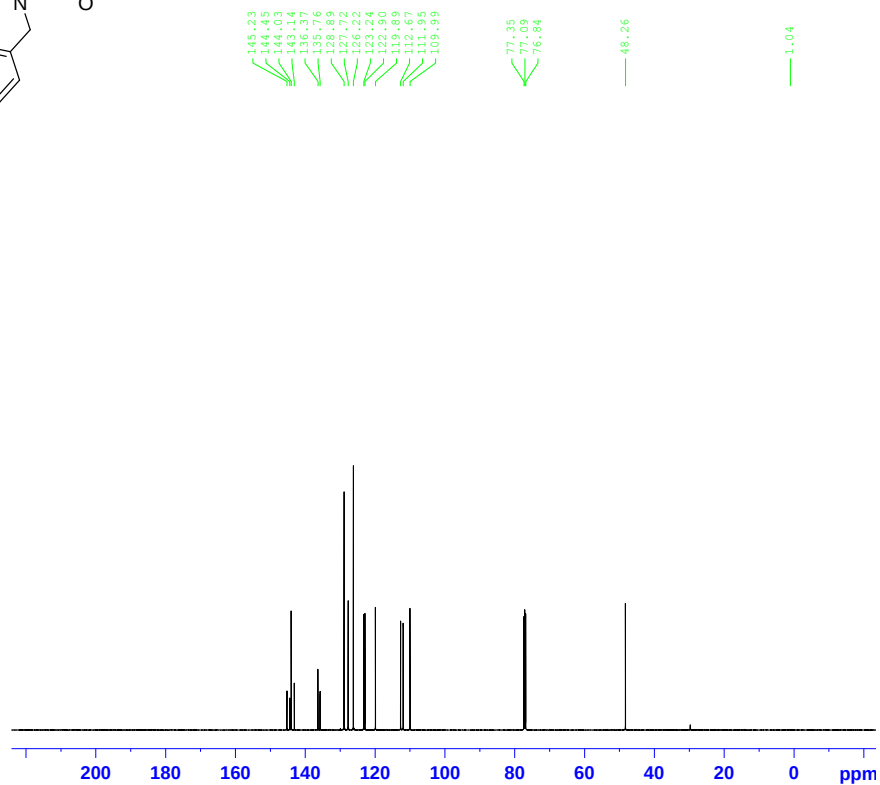
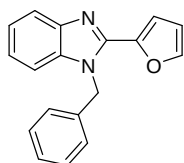
Benzimidazole 7q: ^{13}C -NMR (100 MHz, CDCl_3)



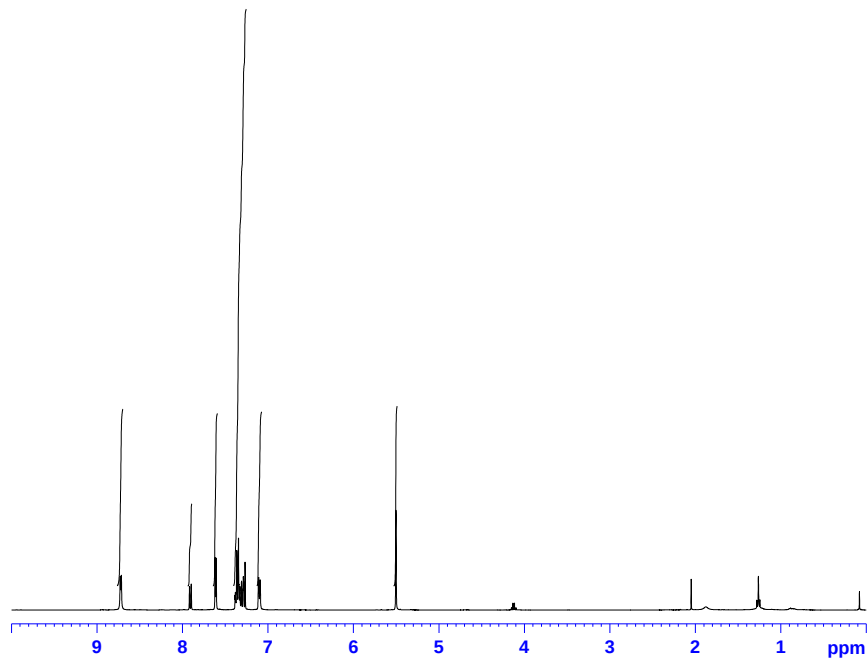
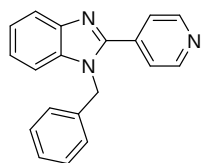
Benzimidazole 7r: ^1H -NMR (500 MHz, CDCl_3)



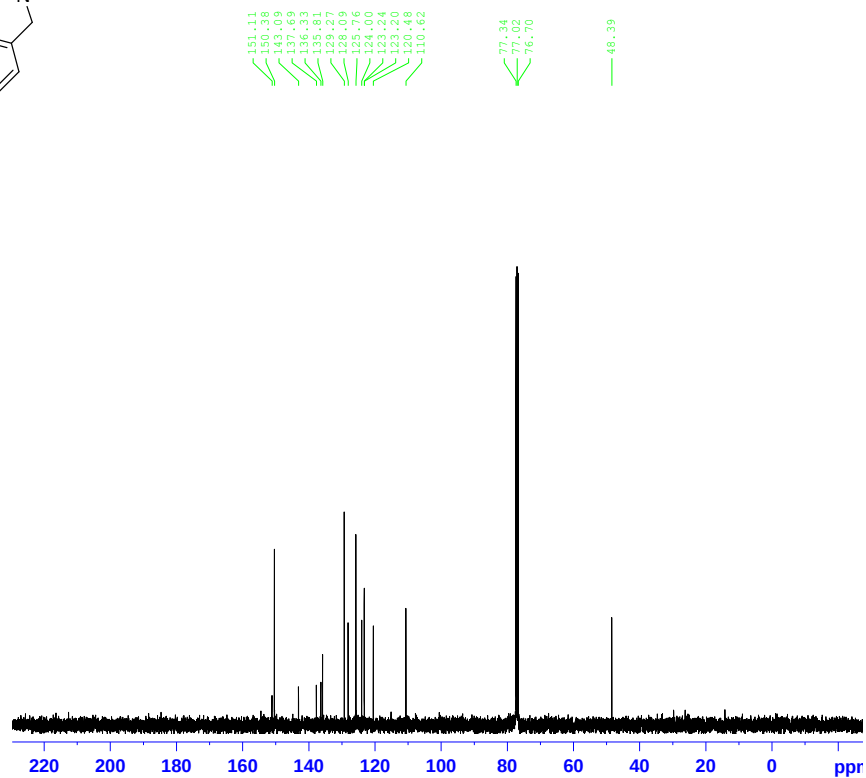
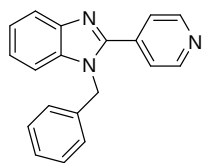
Benzimidazole 7r: ^{13}C -NMR (125 MHz, CDCl_3)



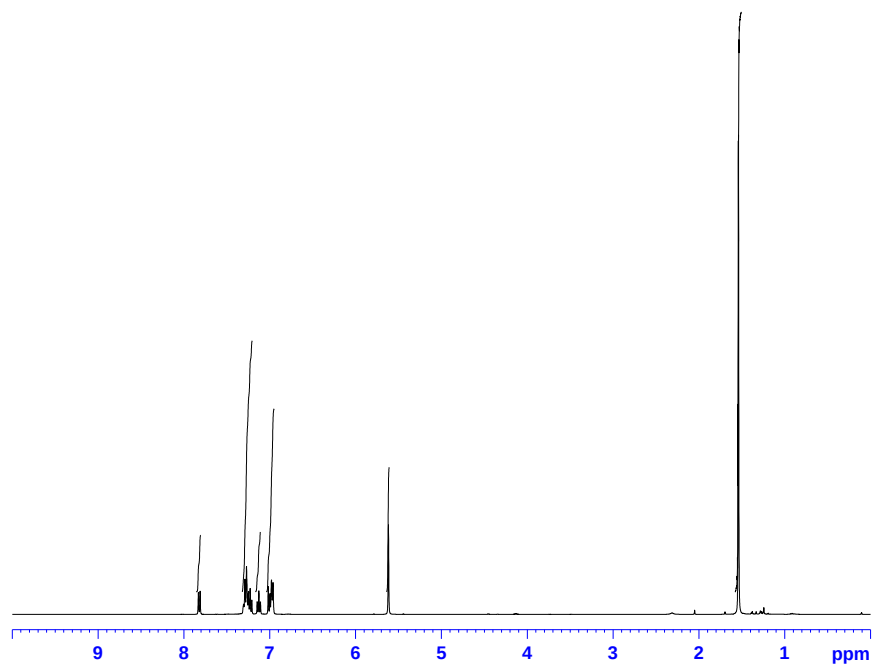
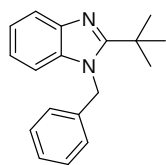
Benzimidazole 7s: ^1H -NMR (400 MHz, CDCl_3)



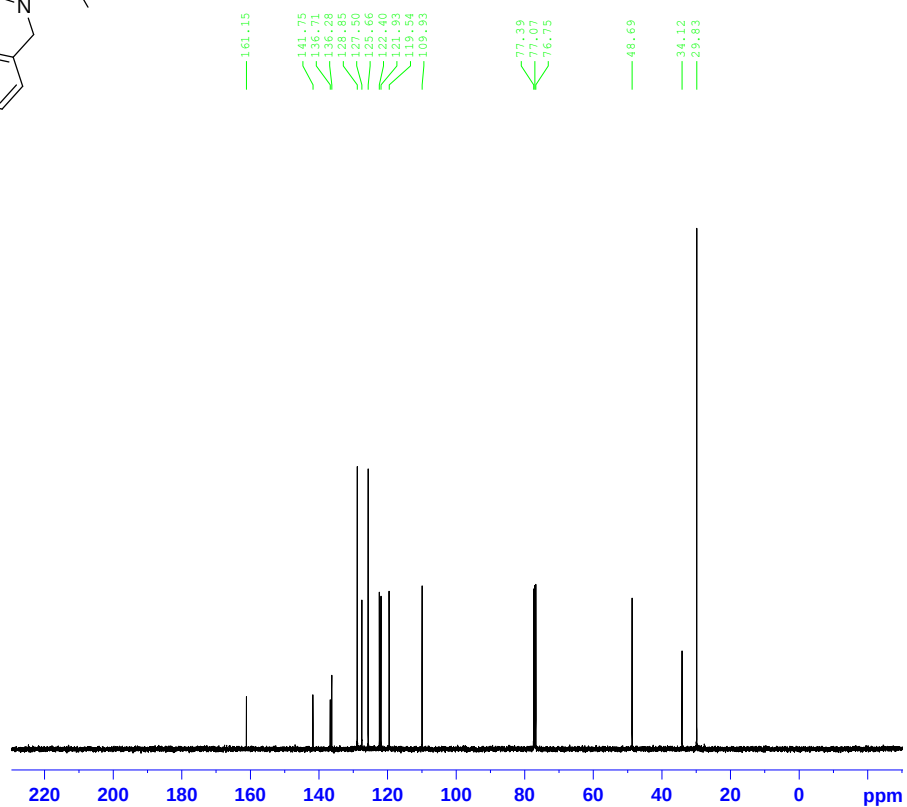
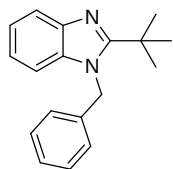
Benzimidazole 7s: ^{13}C -NMR (100 MHz, CDCl_3)



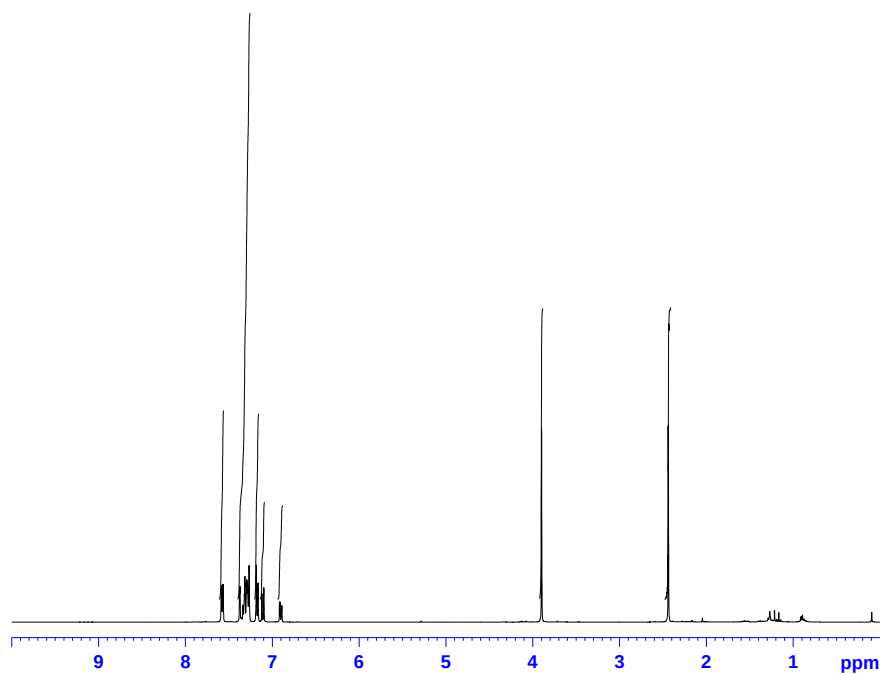
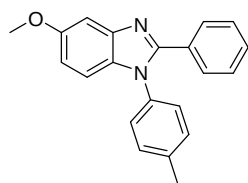
Benzimidazole 7t: ^1H -NMR (400 MHz, CDCl_3)



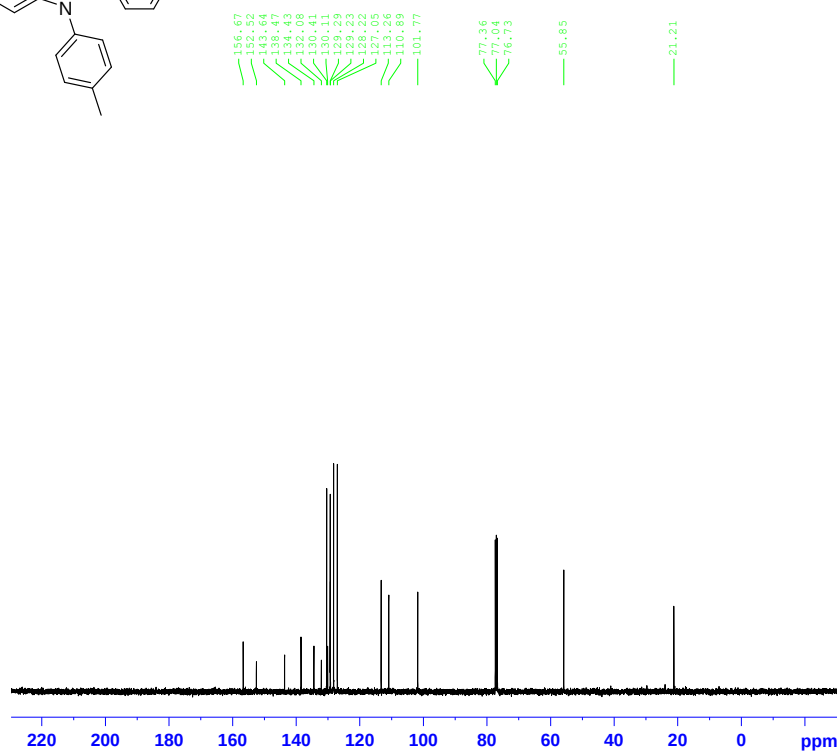
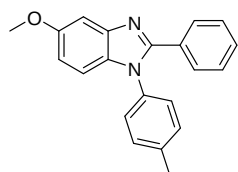
Benzimidazole 7t: ^{13}C -NMR (100 MHz, CDCl_3)



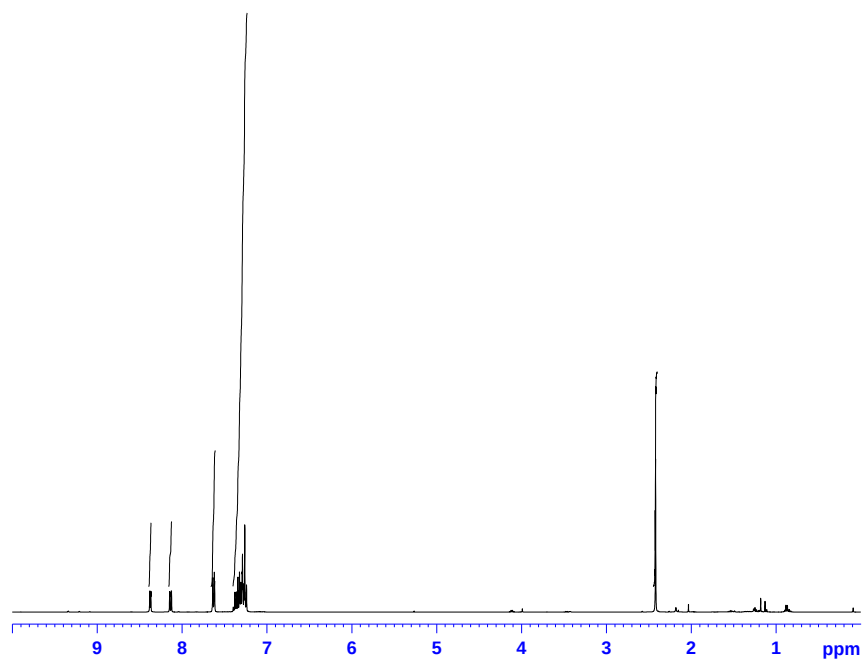
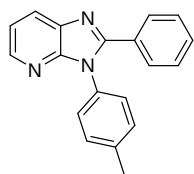
Benzimidazole 7u: ^1H -NMR (400 MHz, CDCl_3)



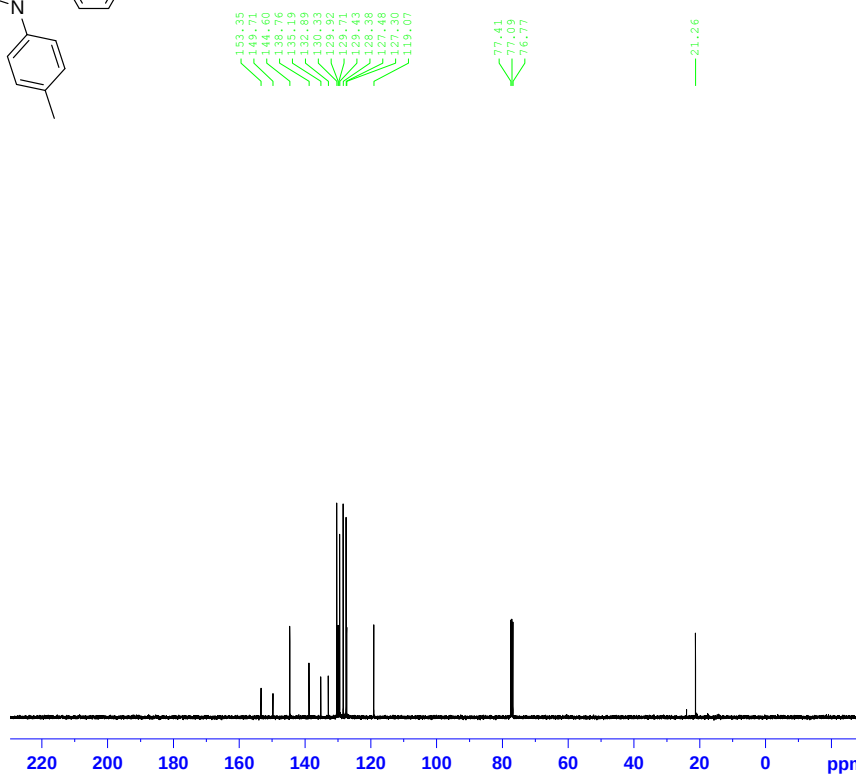
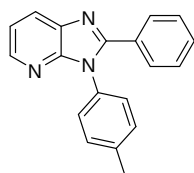
Benzimidazole 7u: ^{13}C -NMR (100 MHz, CDCl_3)



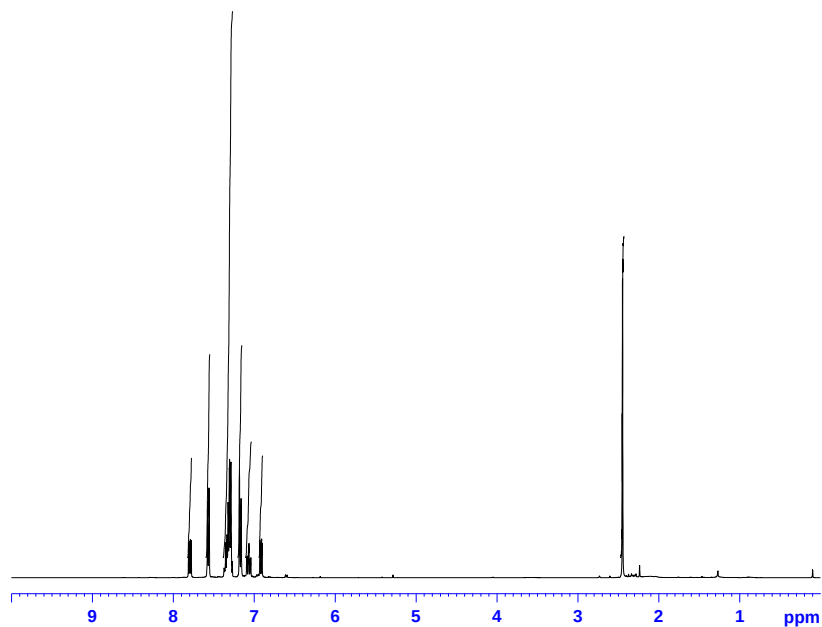
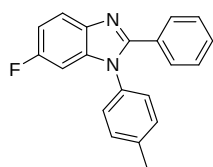
Benzimidazole 7v: ^1H -NMR (400 MHz, CDCl_3)



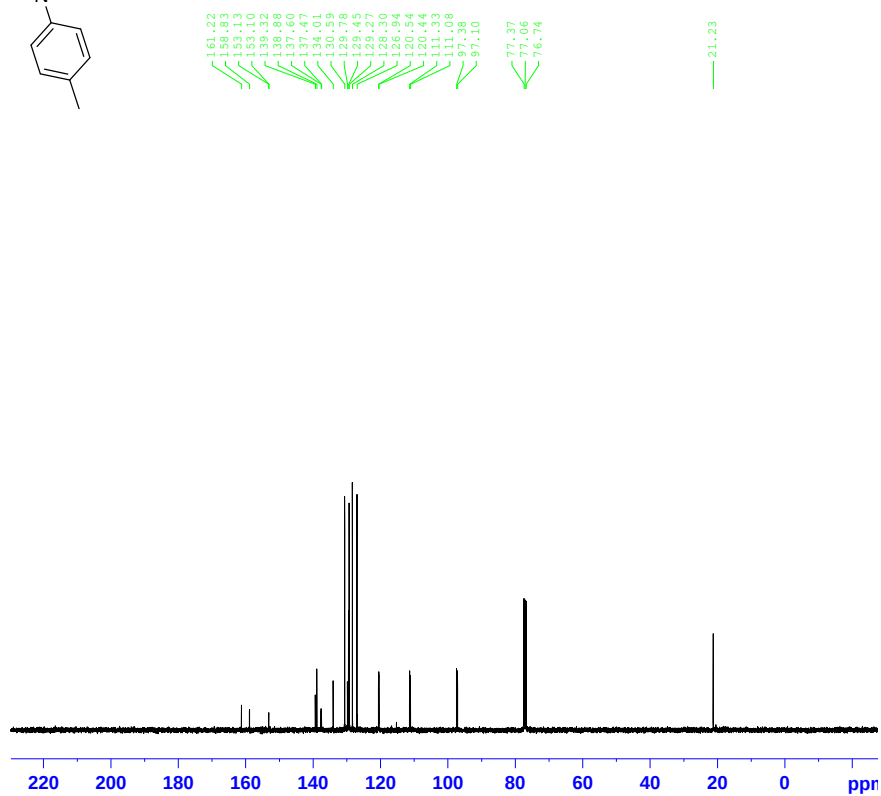
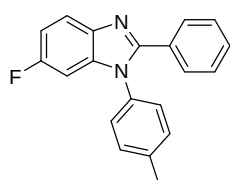
Benzimidazole 7v: ^{13}C -NMR (100 MHz, CDCl_3)



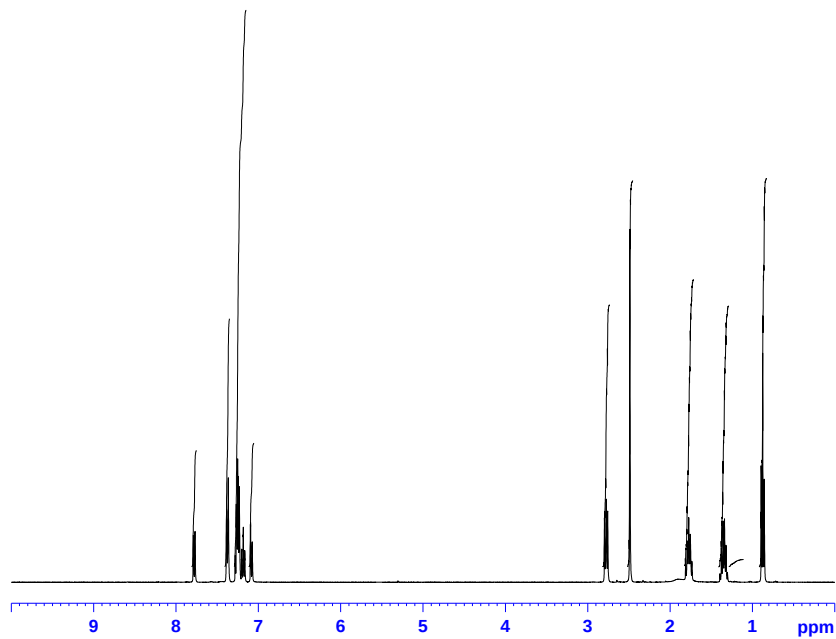
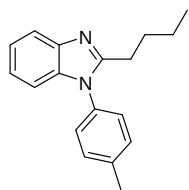
Benzimidazole 7w: ^1H -NMR (400 MHz, CDCl_3)



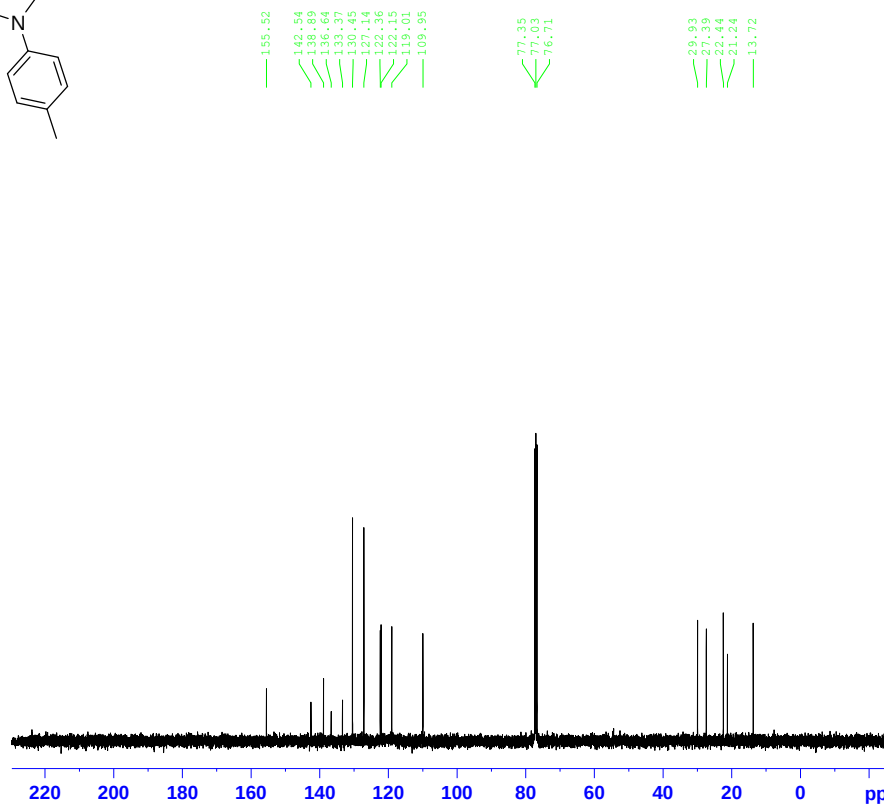
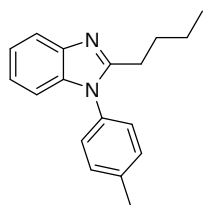
Benzimidazole 7w: ^{13}C -NMR (100 MHz, CDCl_3)



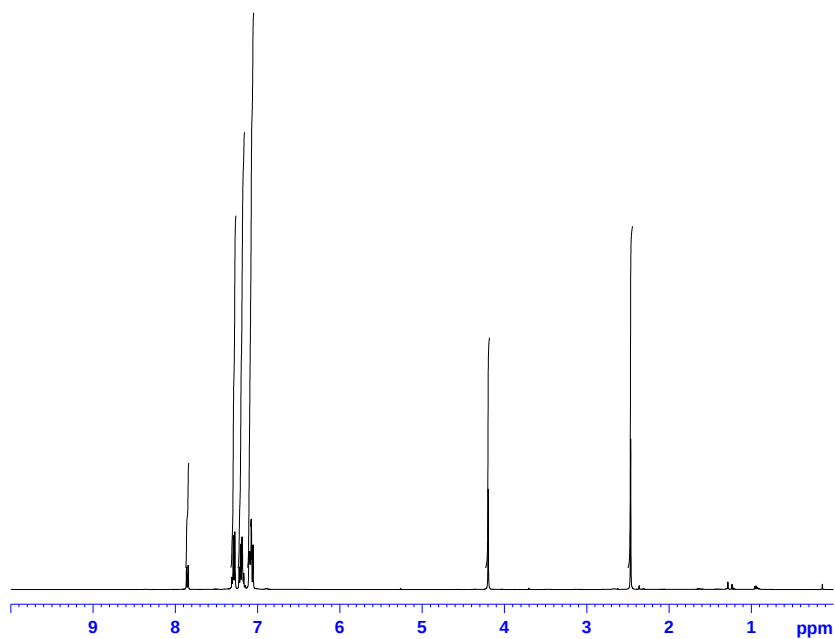
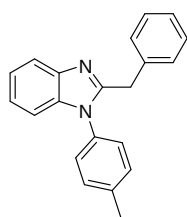
Benzimidazole 7x: ^1H -NMR (400 MHz, CDCl_3)



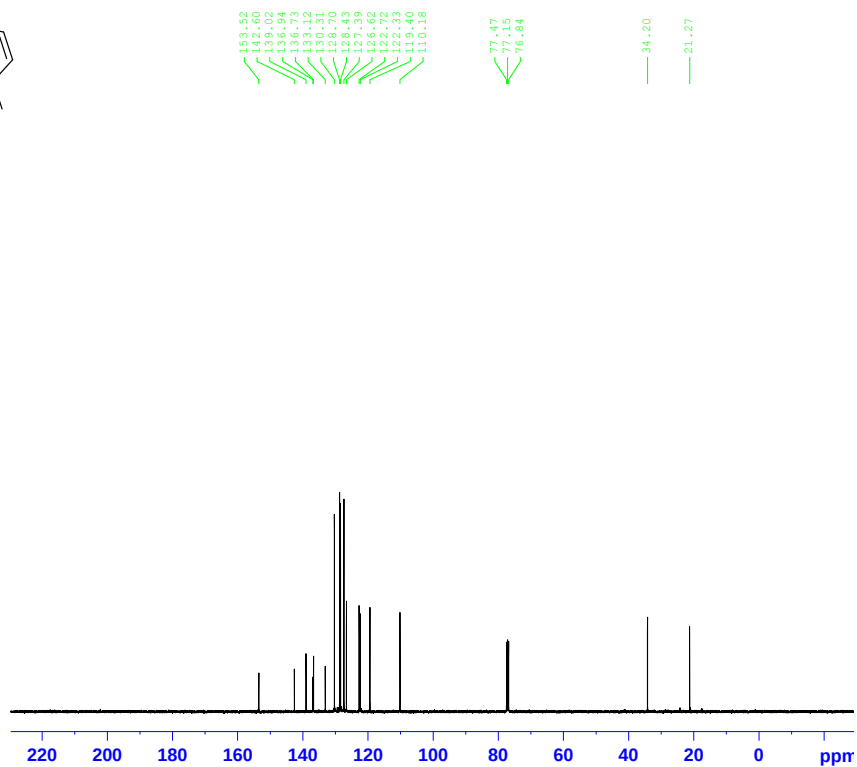
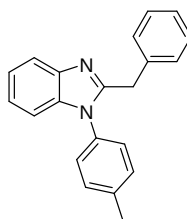
Benzimidazole 7x: ^{13}C -NMR (100 MHz, CDCl_3)



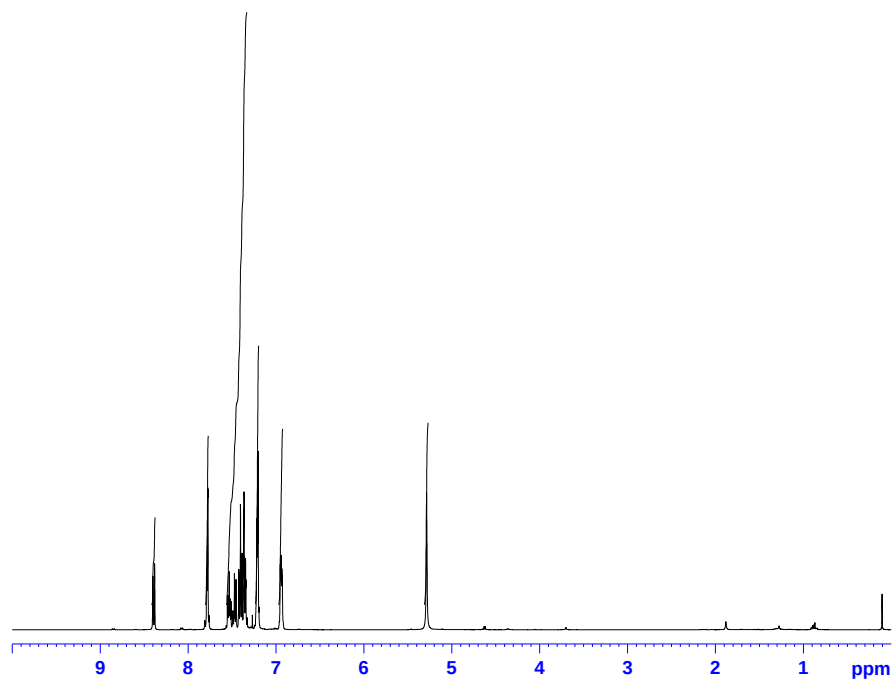
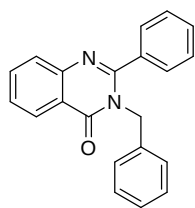
Benzimidazole 7y: ^1H -NMR (400 MHz, CDCl_3)



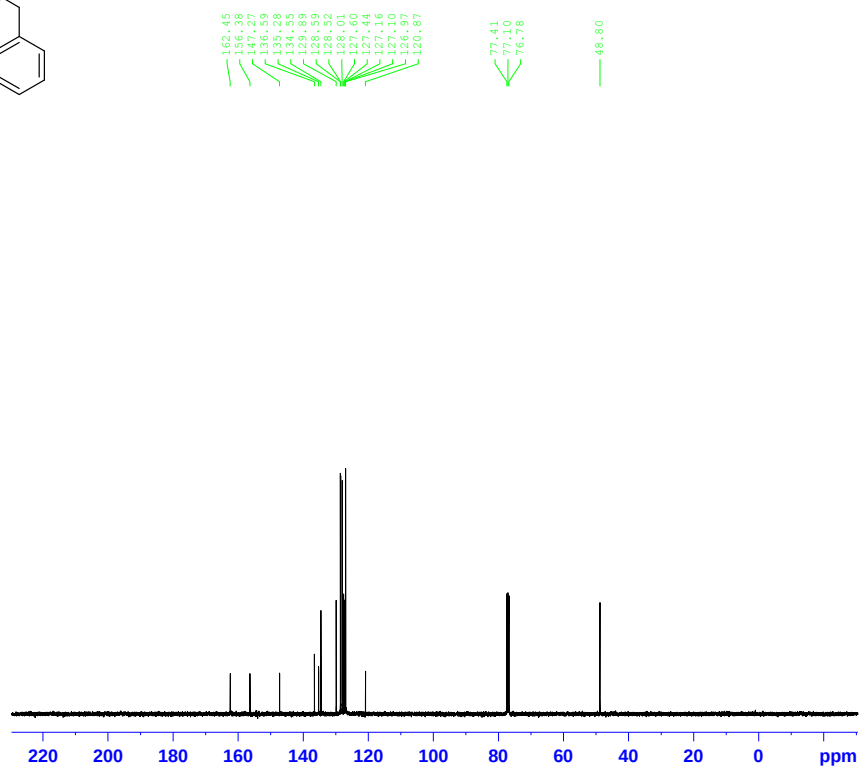
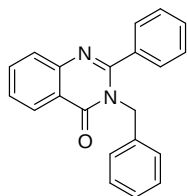
Benzimidazole 7y: ^{13}C -NMR (100 MHz, CDCl_3)



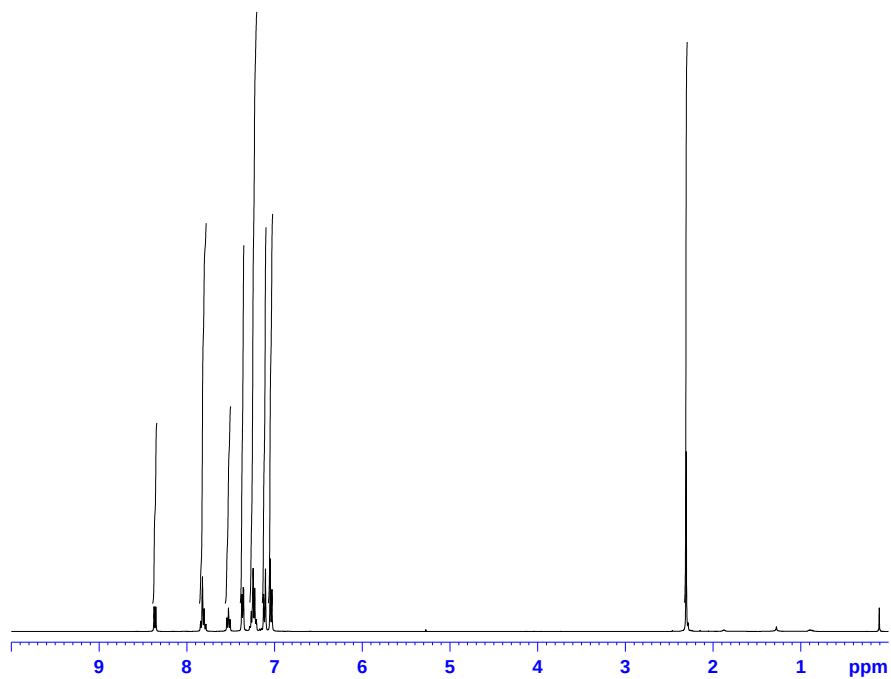
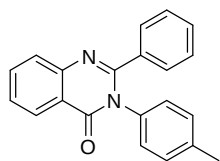
Quinazolinone 8a: ^1H -NMR (400 MHz, CDCl_3)



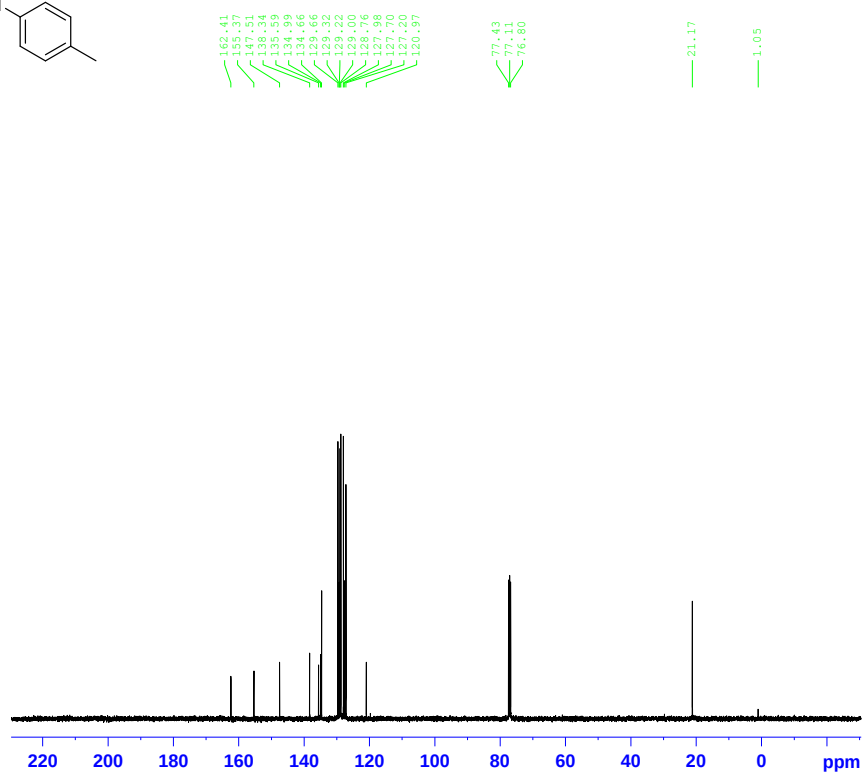
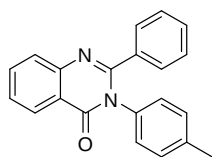
Quinazolinone 8a: ^{13}C -NMR (100 MHz, CDCl_3)



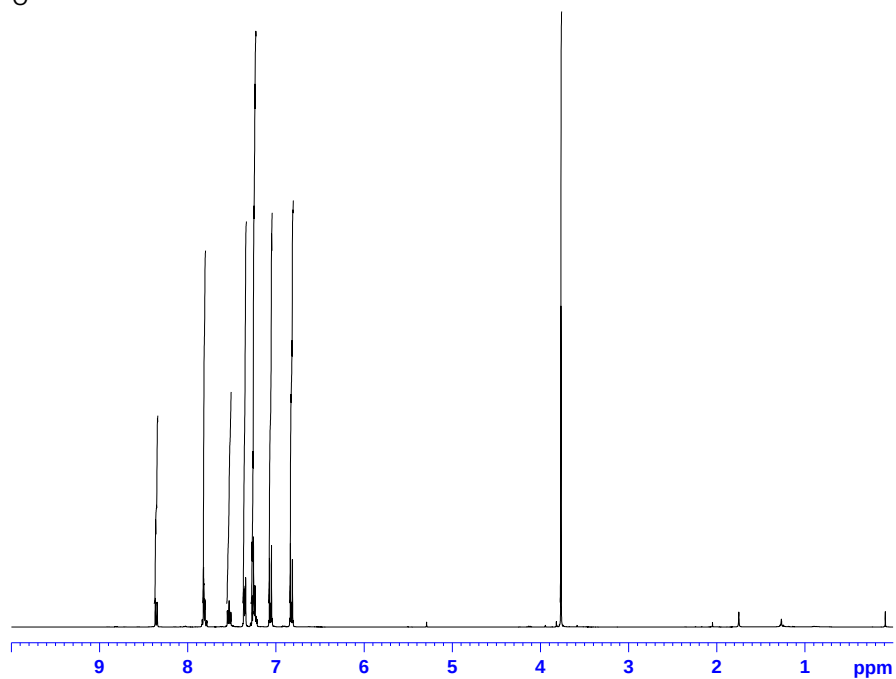
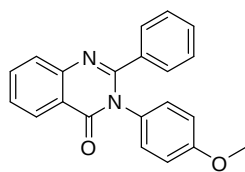
Quinazolinone 8b: ^1H -NMR (400 MHz, CDCl_3)



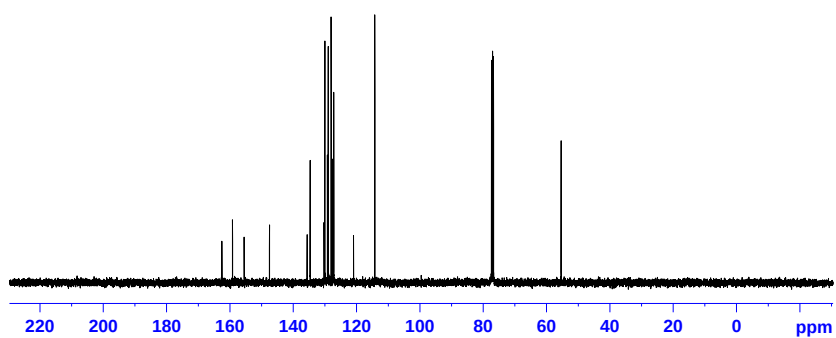
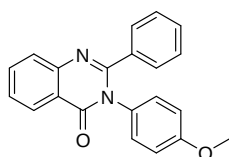
Quinazolinone 8b: ^{13}C -NMR (100 MHz, CDCl_3)



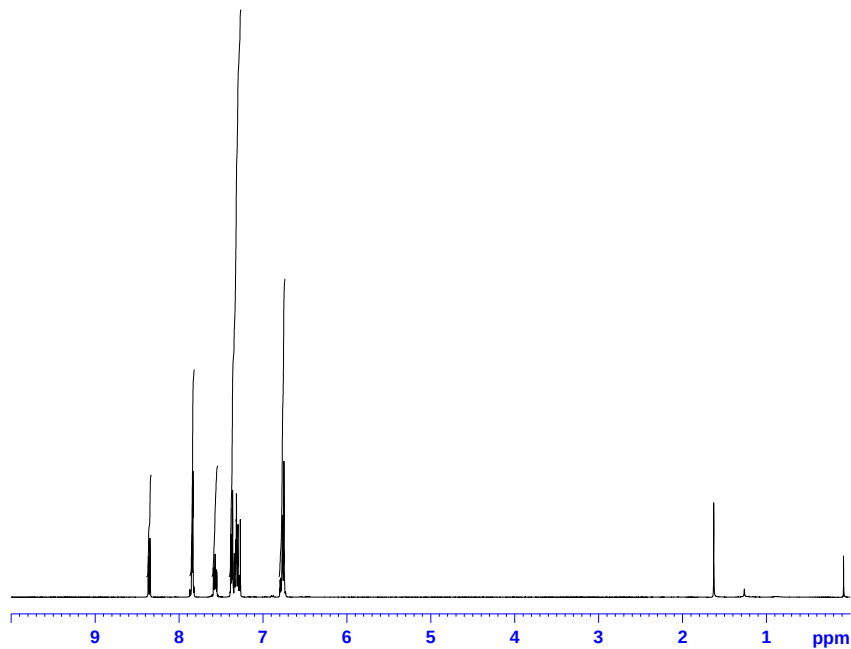
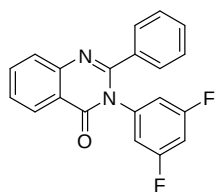
Quinazolinone 8c: ^1H -NMR (400 MHz, CDCl_3)



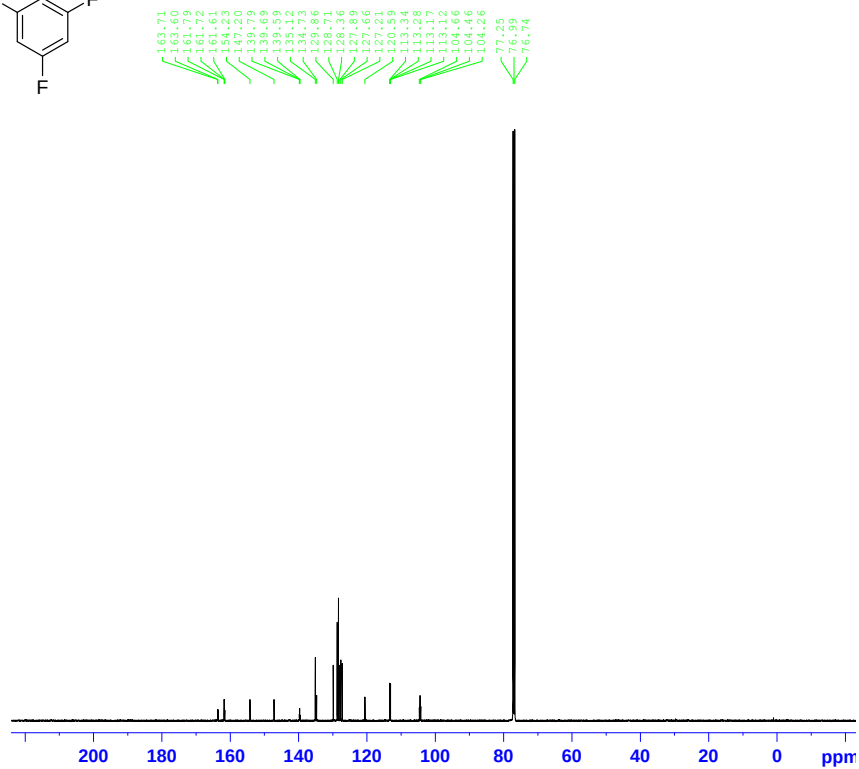
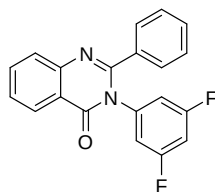
Quinazolinone 8c: ^{13}C -NMR (100 MHz, CDCl_3)



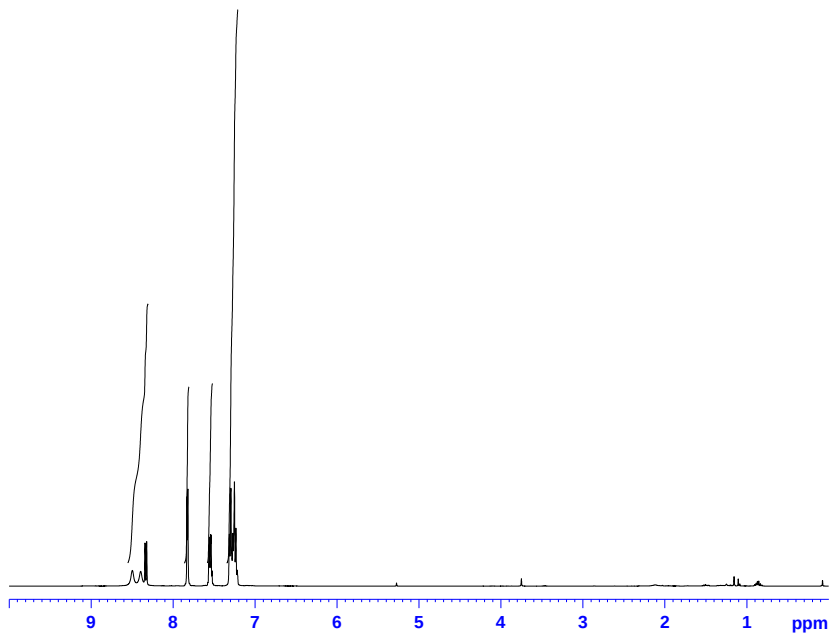
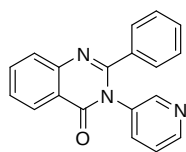
Quinazolinone 8d: ^1H -NMR (400 MHz, CDCl_3)



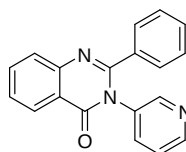
Quinazolinone 8d: ^{13}C -NMR (125 MHz, CDCl_3)



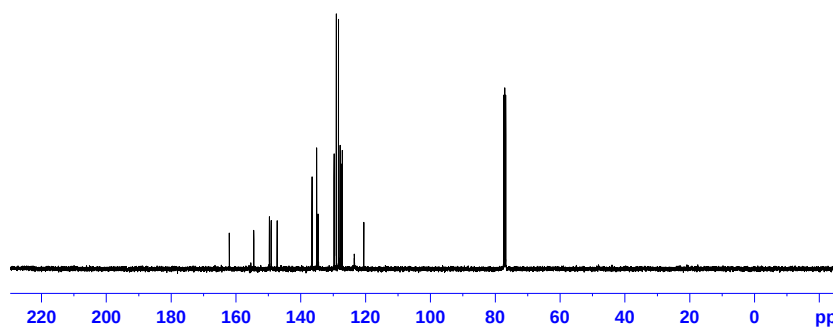
Quinazolinone 8e: ^1H -NMR (400 MHz, CDCl_3)



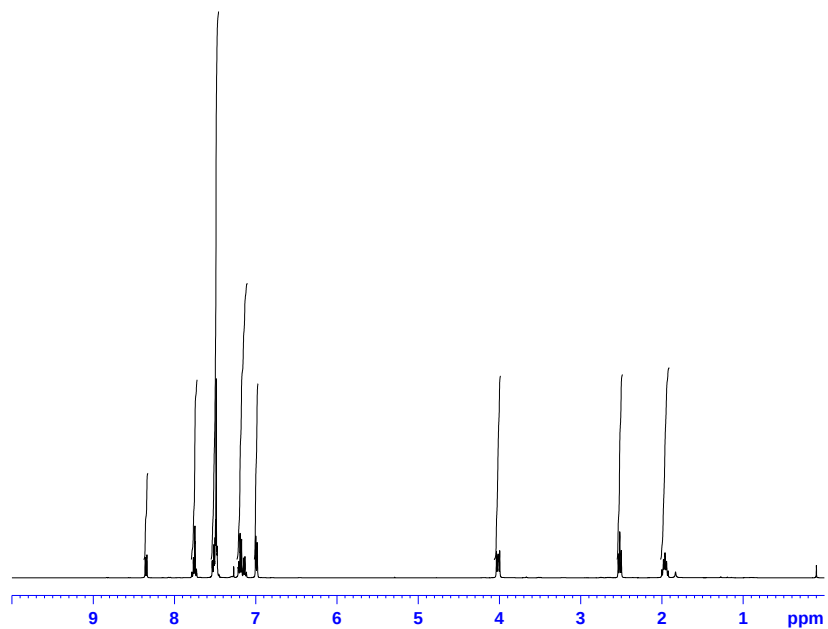
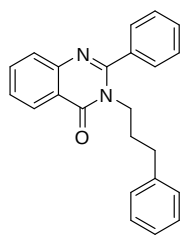
Quinazolinone 8e: ^{13}C -NMR (100 MHz, CDCl_3)



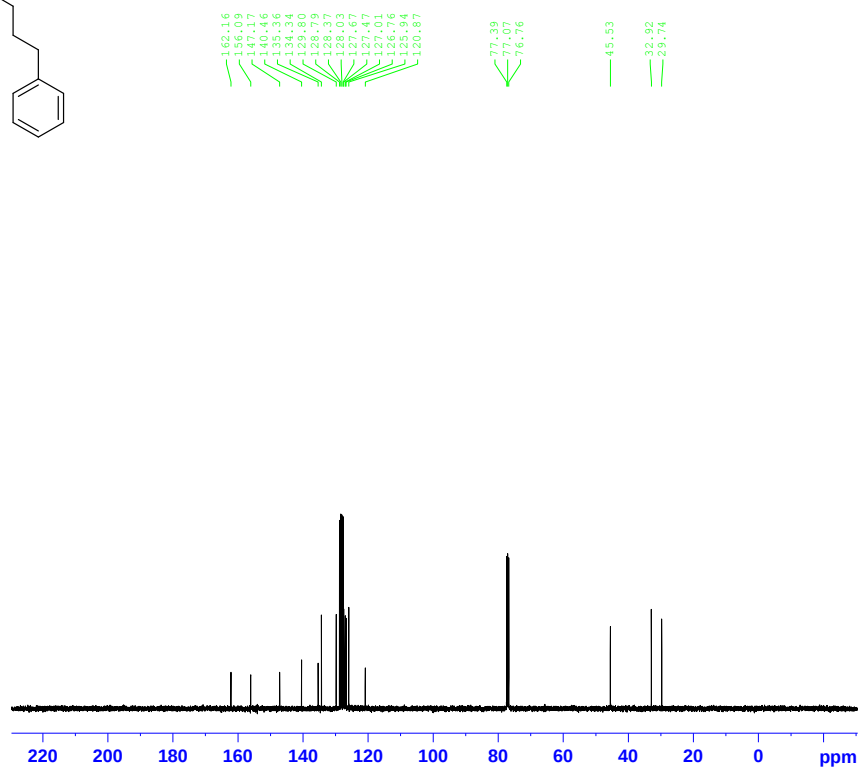
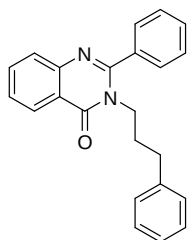
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147.32
136.56
135.13
134.71
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129.06
128.40
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127.64
127.19
123.51
120.58
77.42
77.11
76.79



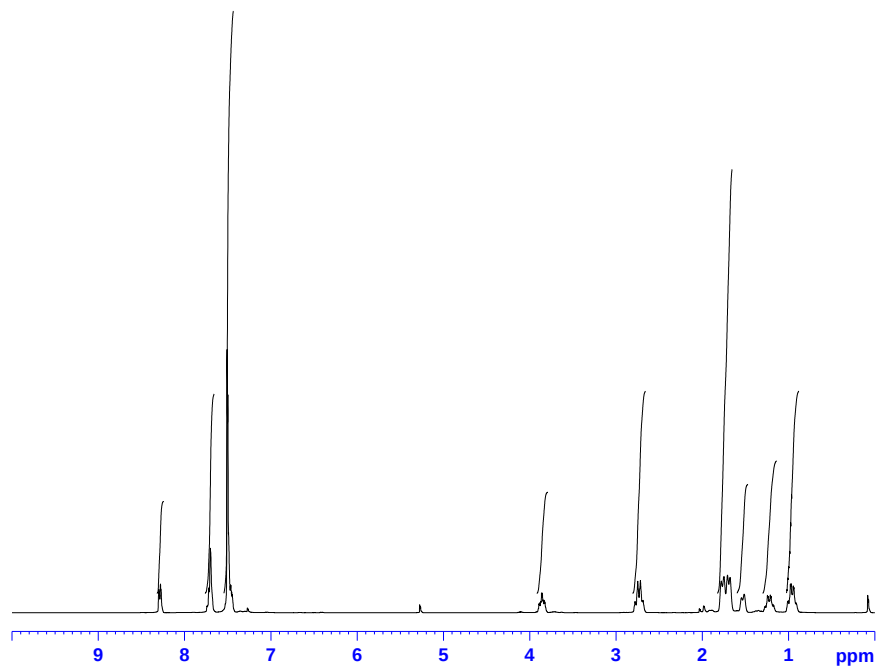
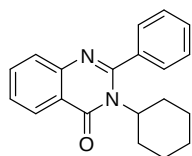
Quinazolinone 8f: ^1H -NMR (400 MHz, CDCl_3)



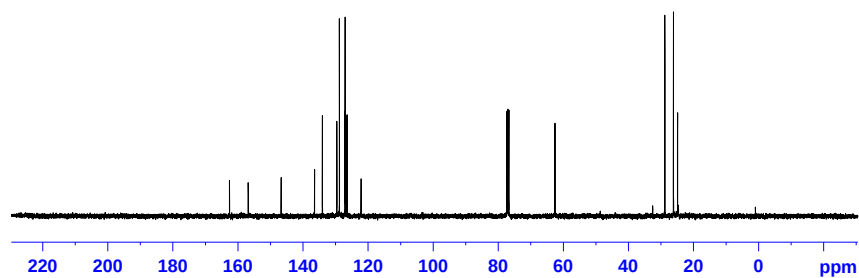
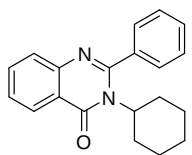
Quinazolinone 8f: ^{13}C -NMR (100 MHz, CDCl_3)



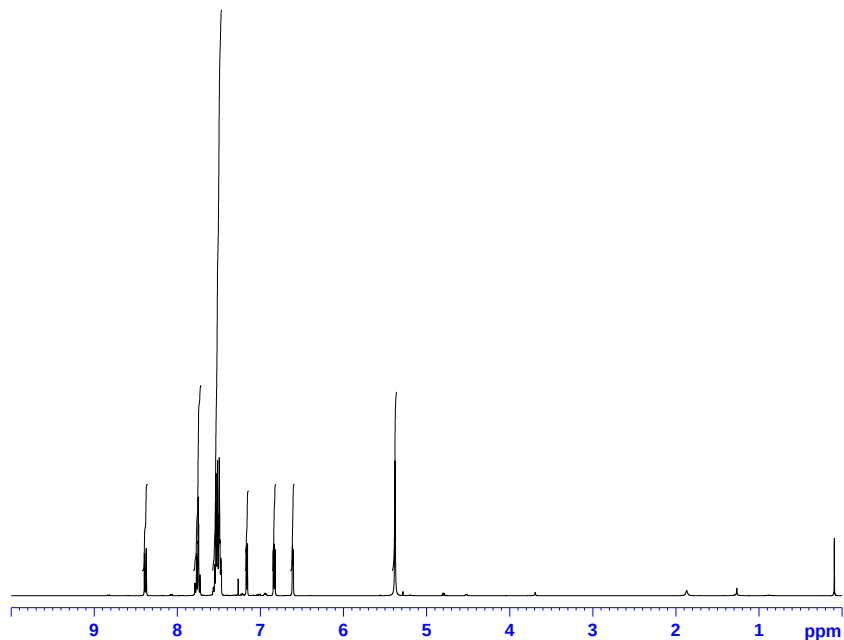
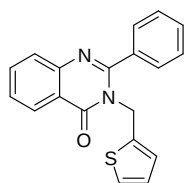
Quinazolinone 8g: ^1H -NMR (400 MHz, CDCl_3)



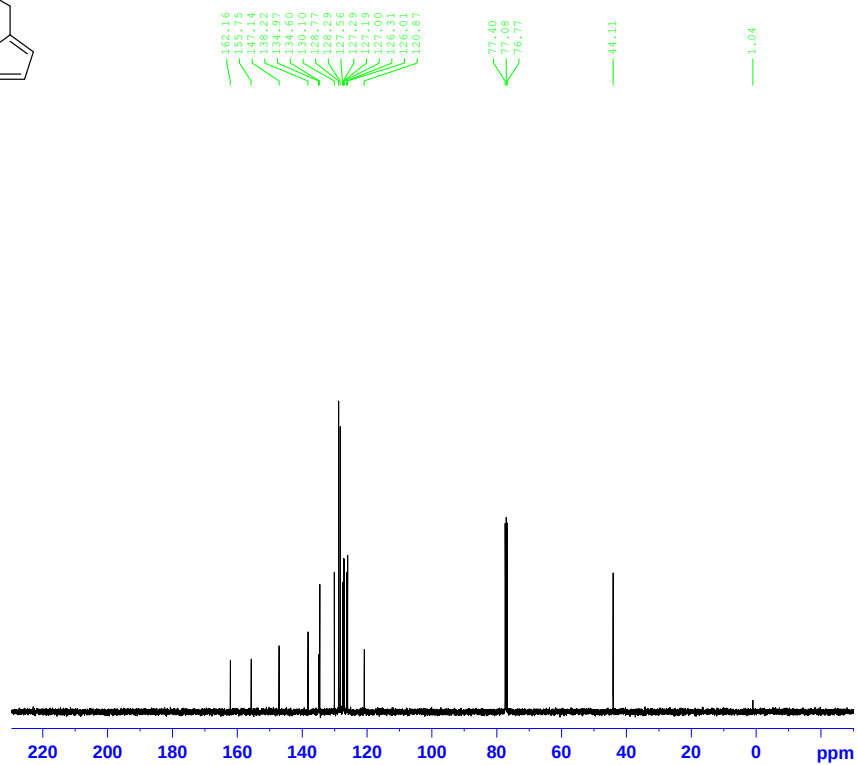
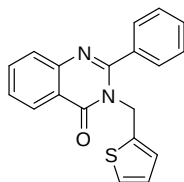
Quinazolinone 8g: ^{13}C -NMR (100 MHz, CDCl_3)



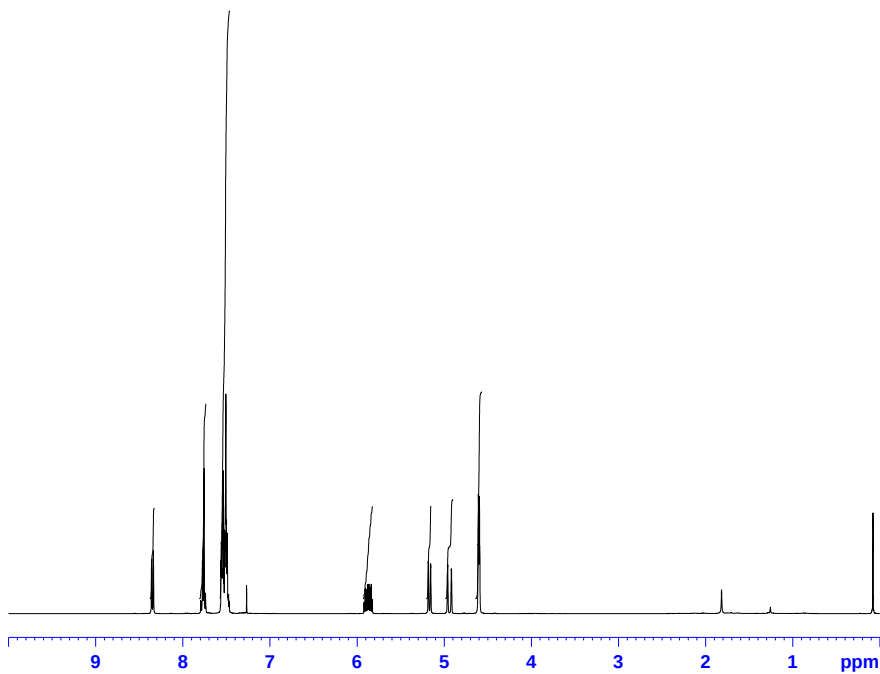
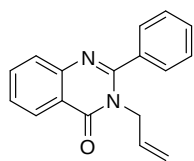
Quinazolinone 8h: ^1H -NMR (400 MHz, CDCl_3)



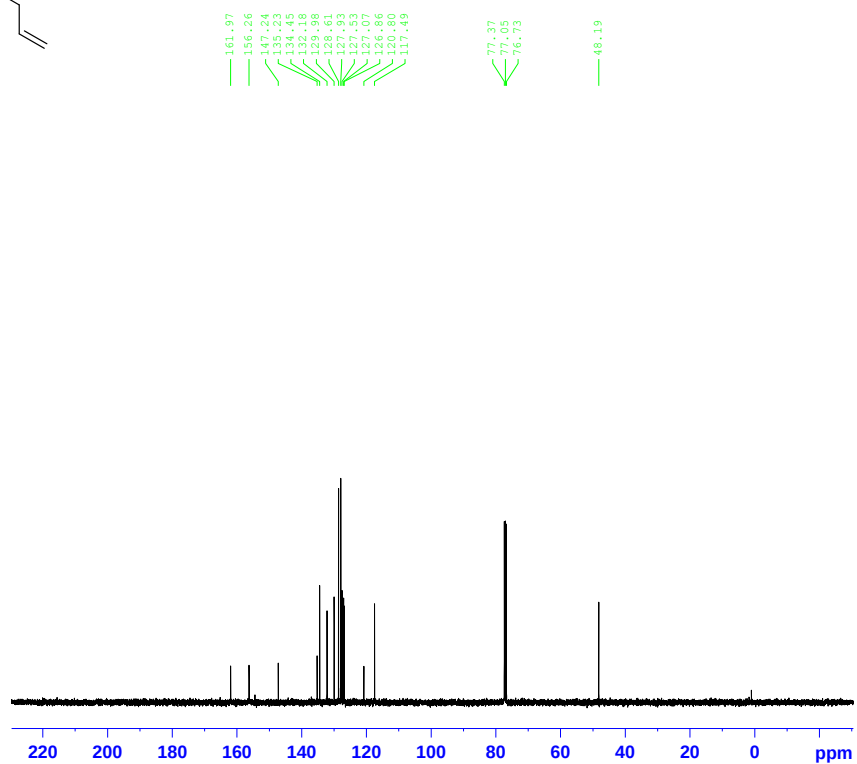
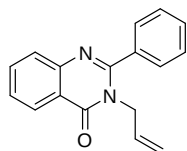
Quinazolinone 8h: ^{13}C -NMR (100 MHz, CDCl_3)



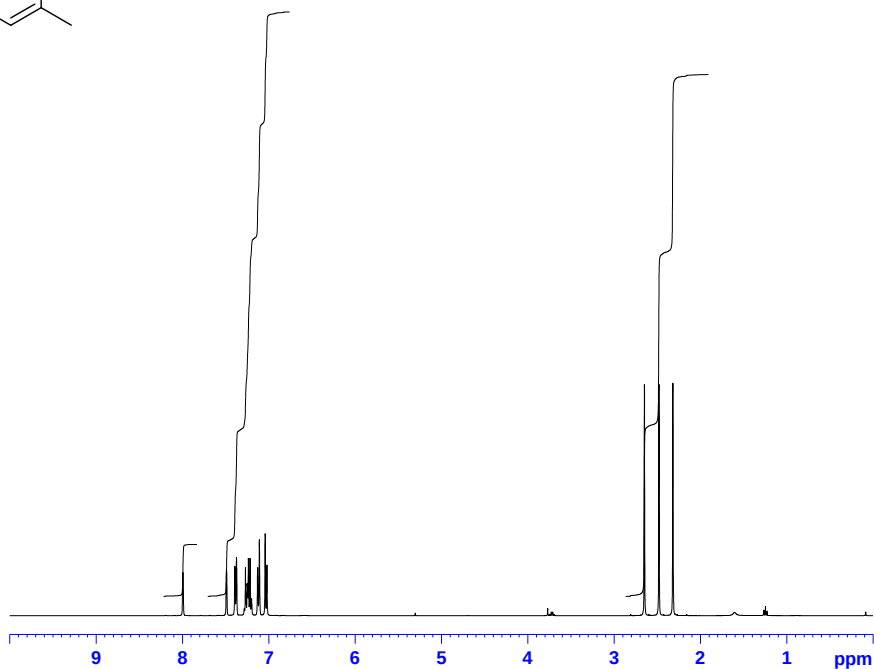
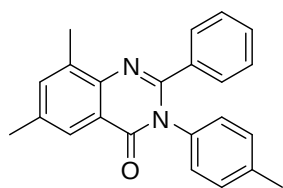
Quinazolinone 8i: ^1H -NMR (400 MHz, CDCl_3)



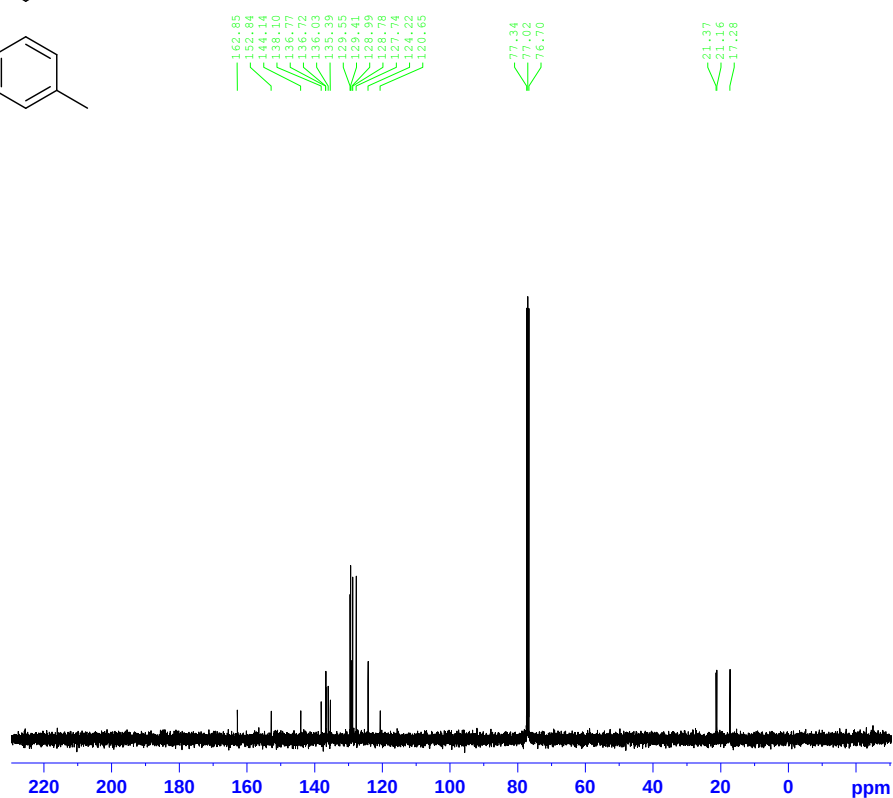
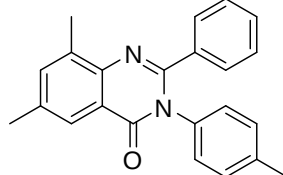
Quinazolinone 8i: ^{13}C -NMR (100 MHz, CDCl_3)



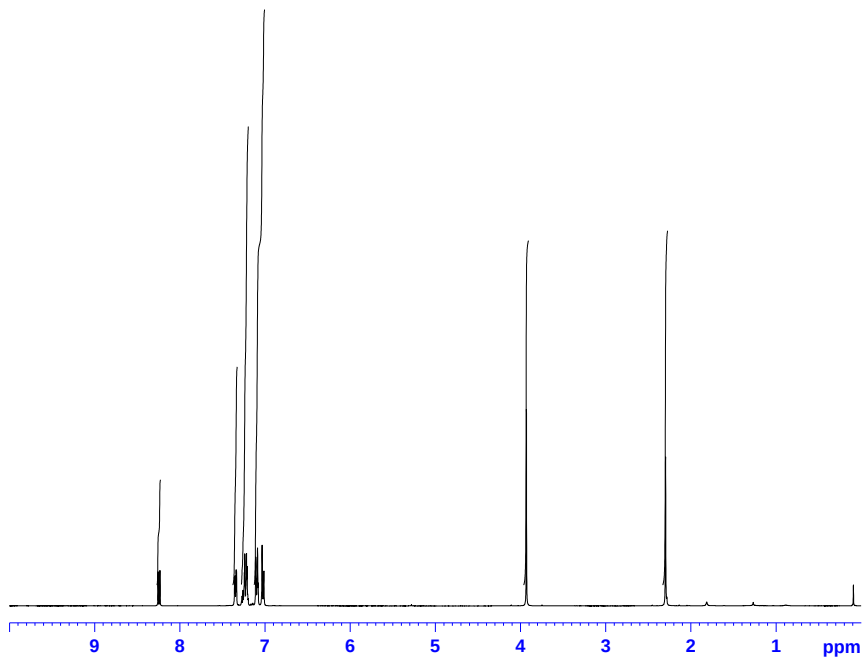
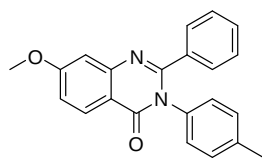
Quinazolinone 8j: ^1H -NMR (400 MHz, CDCl_3)



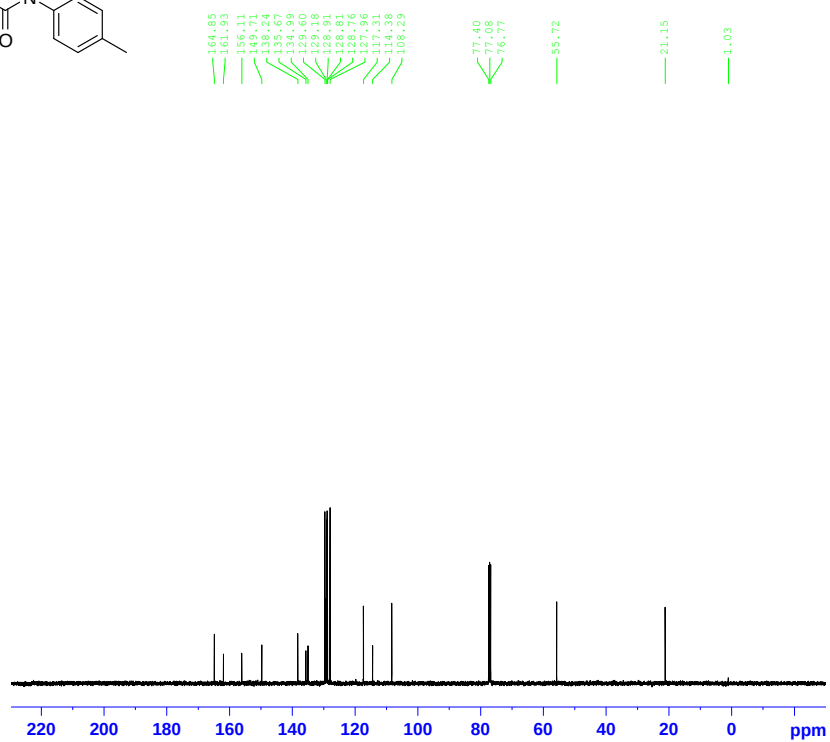
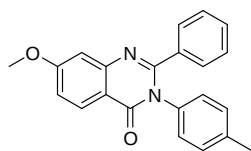
Quinazolinone 8j: ^{13}C -NMR (100 MHz, CDCl_3)



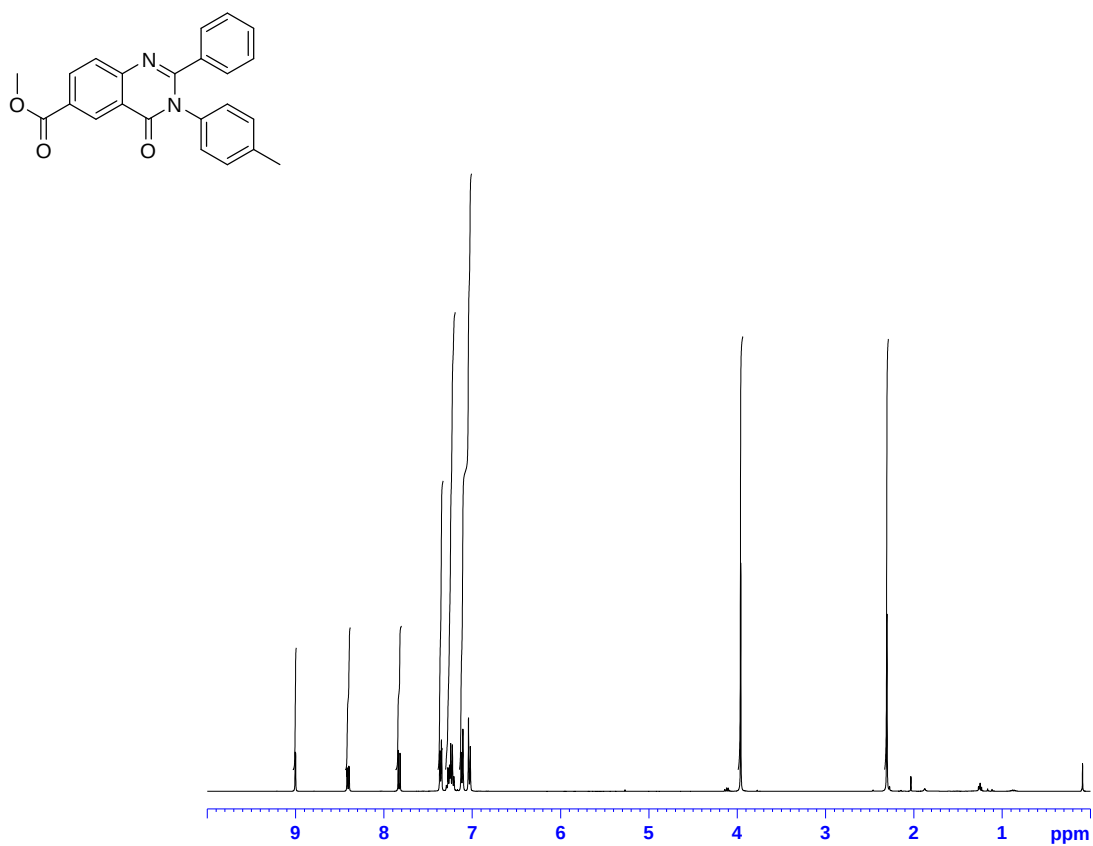
Quinazolinone 8k: $^1\text{H-NMR}$ (400 MHz, CDCl_3)



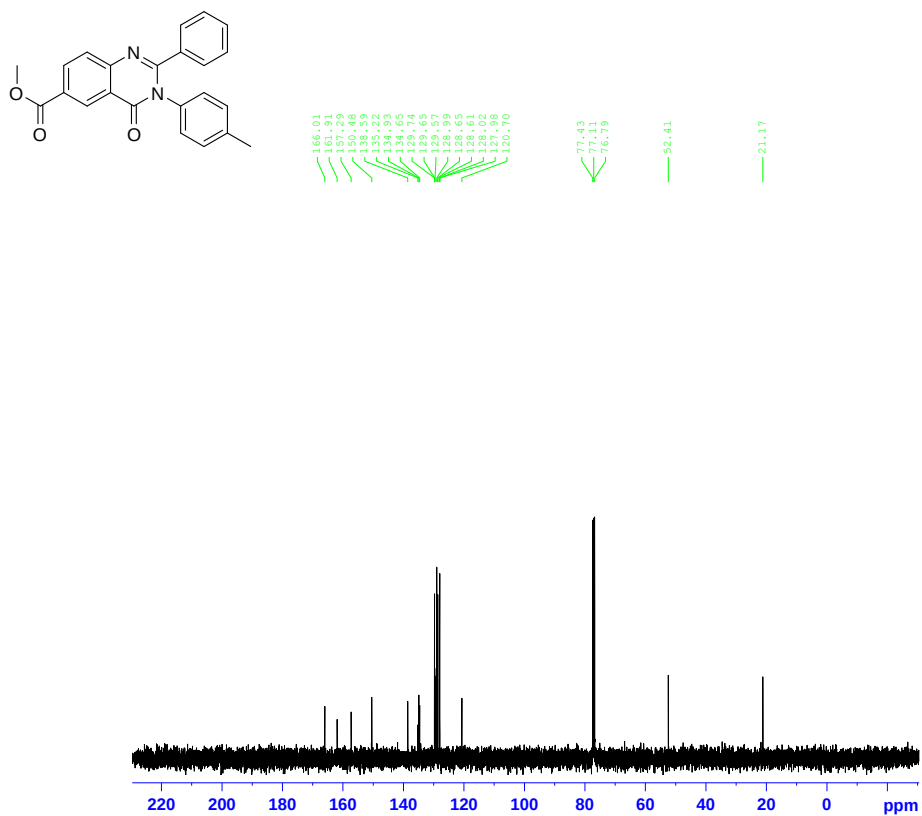
Quinazolinone 8k: $^{13}\text{C-NMR}$ (100 MHz, CDCl_3)



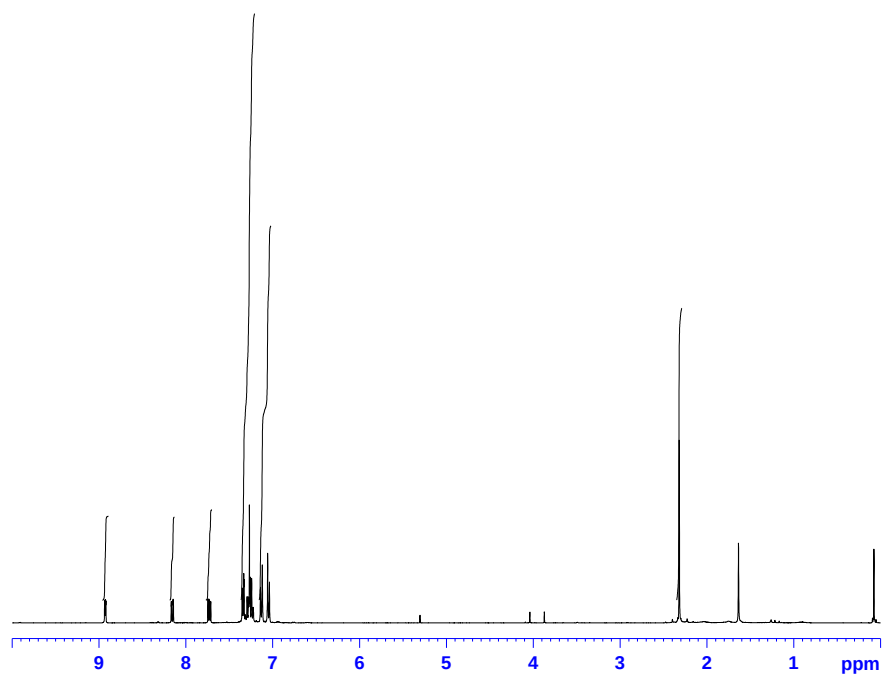
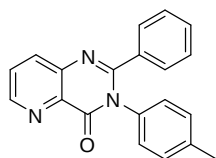
Quinazolinone 8l: ^1H -NMR (400 MHz, CDCl_3)



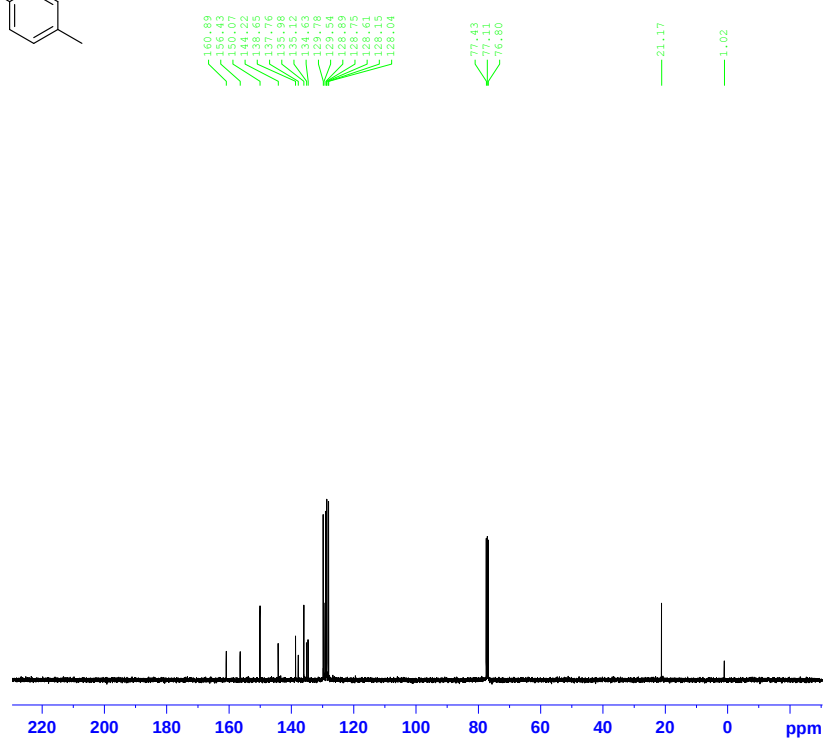
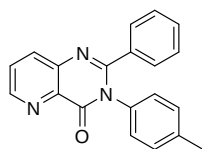
Quinazolinone 8l: ^{13}C -NMR (100 MHz, CDCl_3)



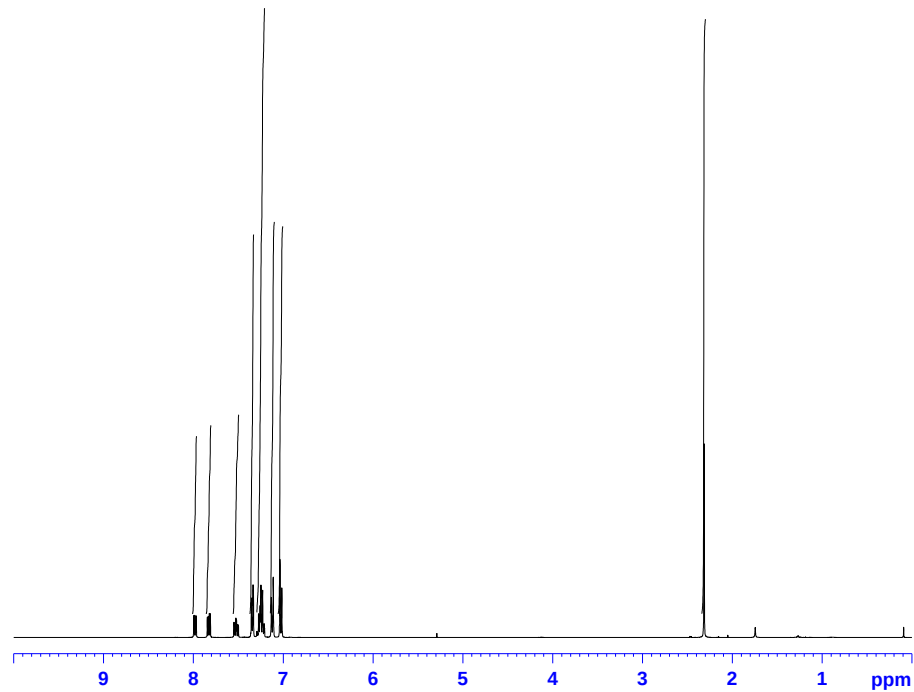
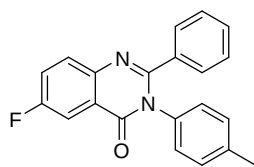
Quinazolinone 8m: ^1H -NMR (400 MHz, CDCl_3)



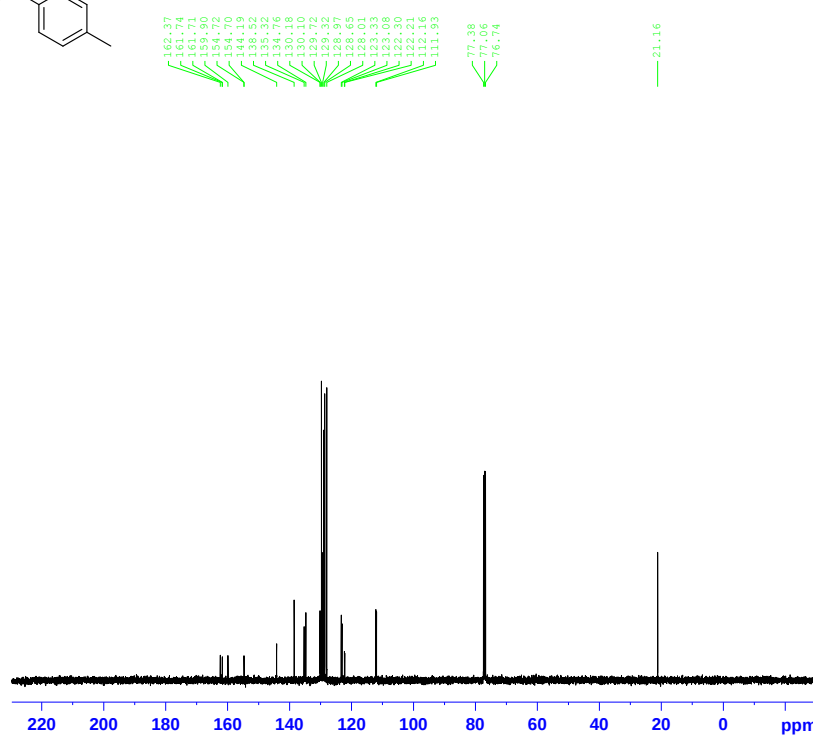
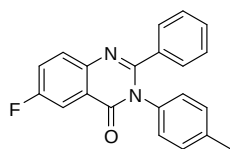
Quinazolinone 8m: ^{13}C -NMR (100 MHz, CDCl_3)



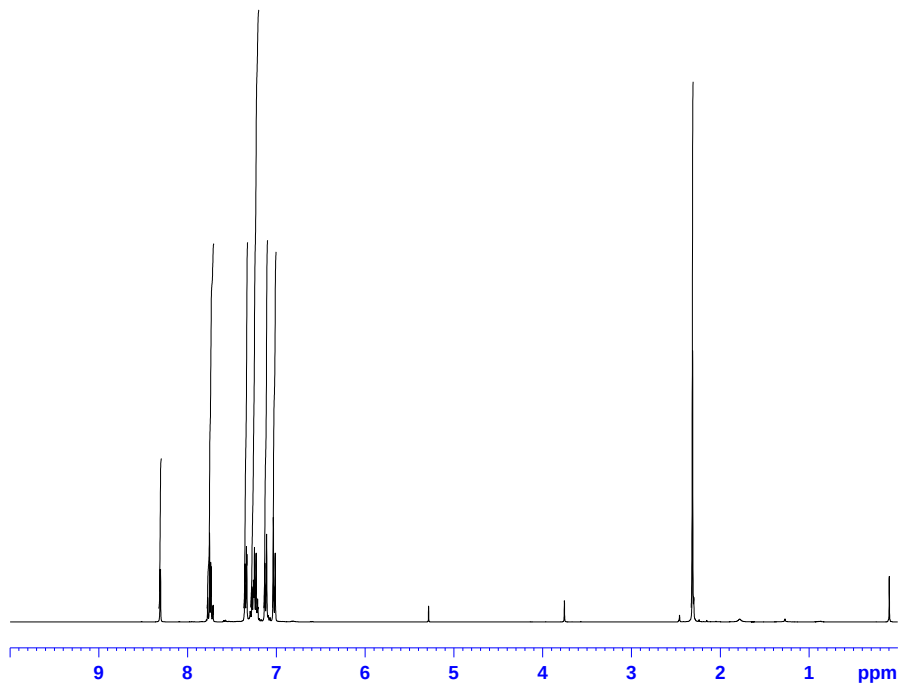
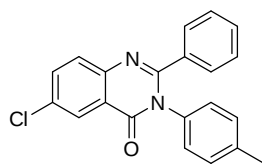
Quinazolinone 8n: ^1H -NMR (400 MHz, CDCl_3)



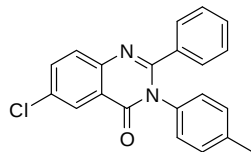
Quinazolinone 8n: ^{13}C -NMR (100 MHz, CDCl_3)



Quinazolinone 8o: ^1H -N MR (400 MHz, CDCl_3)



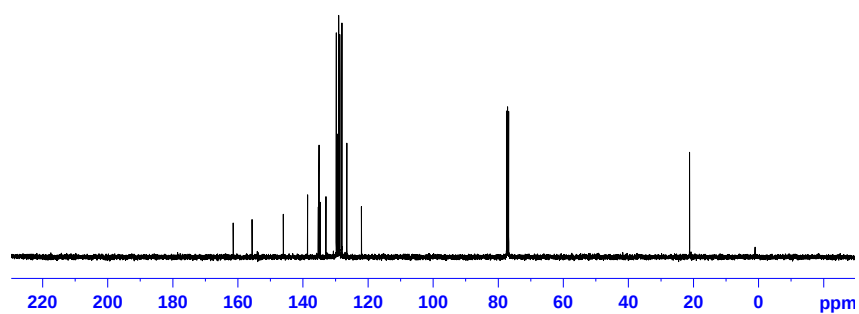
Quinazolinone 8o: ^{13}C -NMR (100 MHz, CDCl_3)



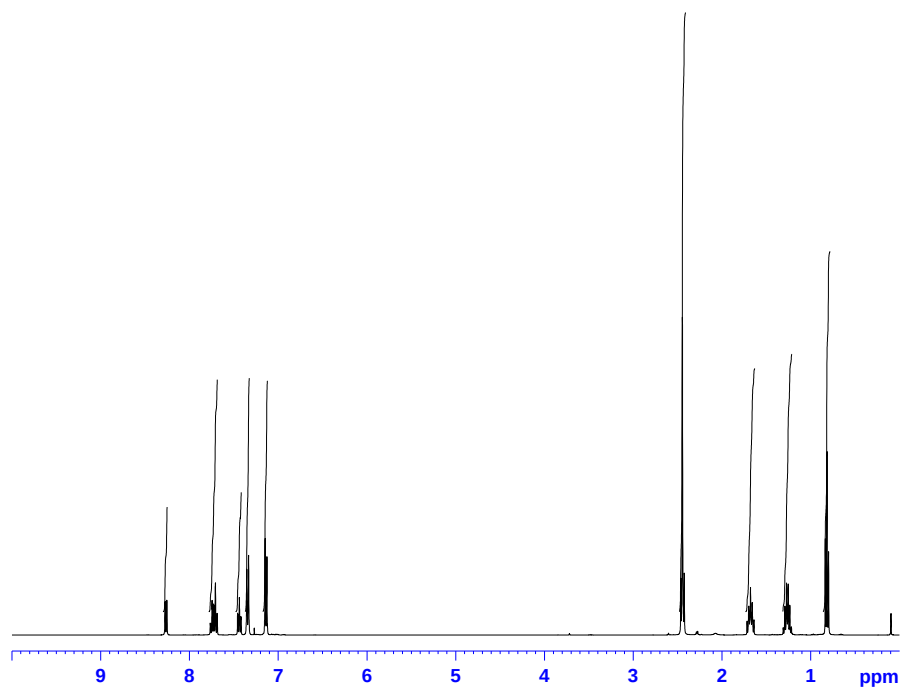
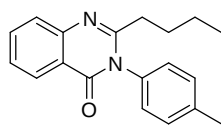
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126.49
122.02

77.40
77.08
76.76

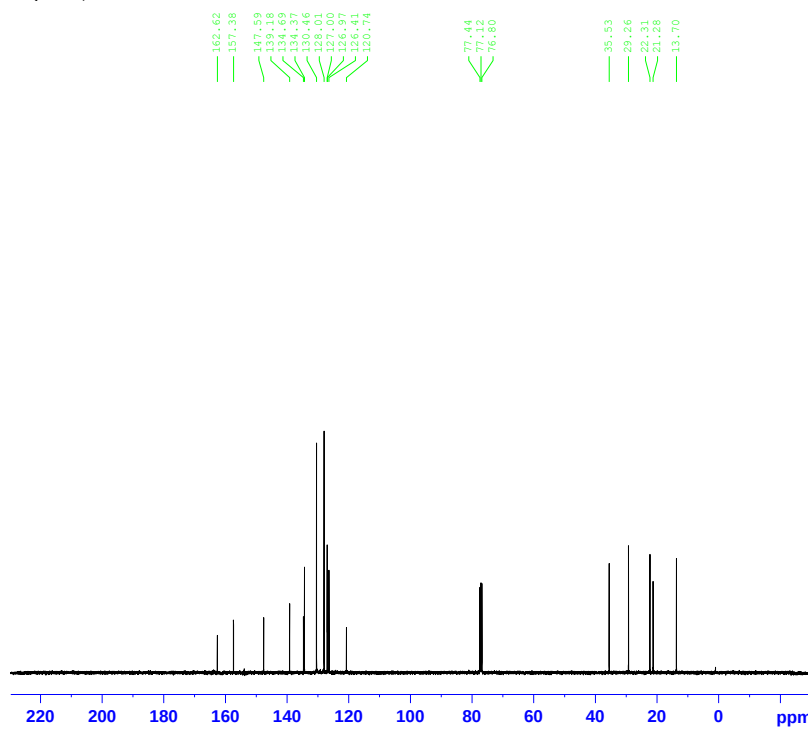
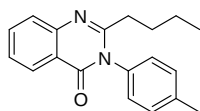
21.17



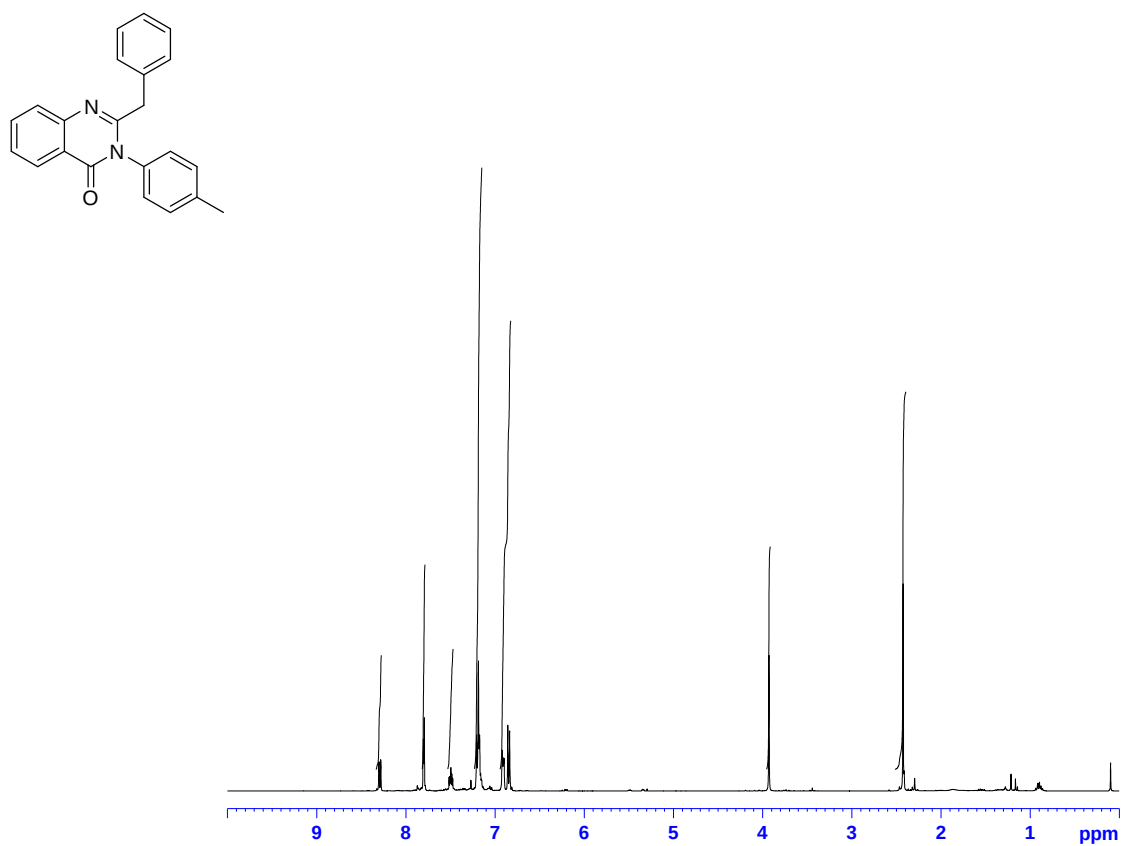
Quinazolinone 8p: ^1H -NMR (400 MHz, CDCl_3)



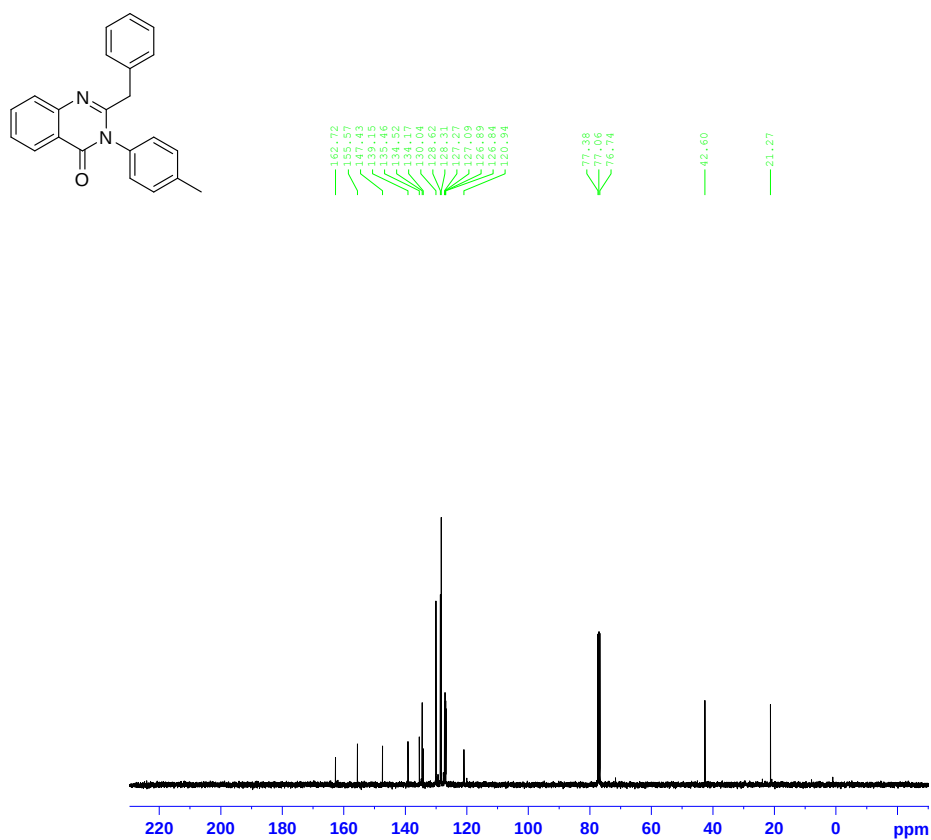
Quinazolinone 8p: ^{13}C -NMR (100 MHz, CDCl_3)



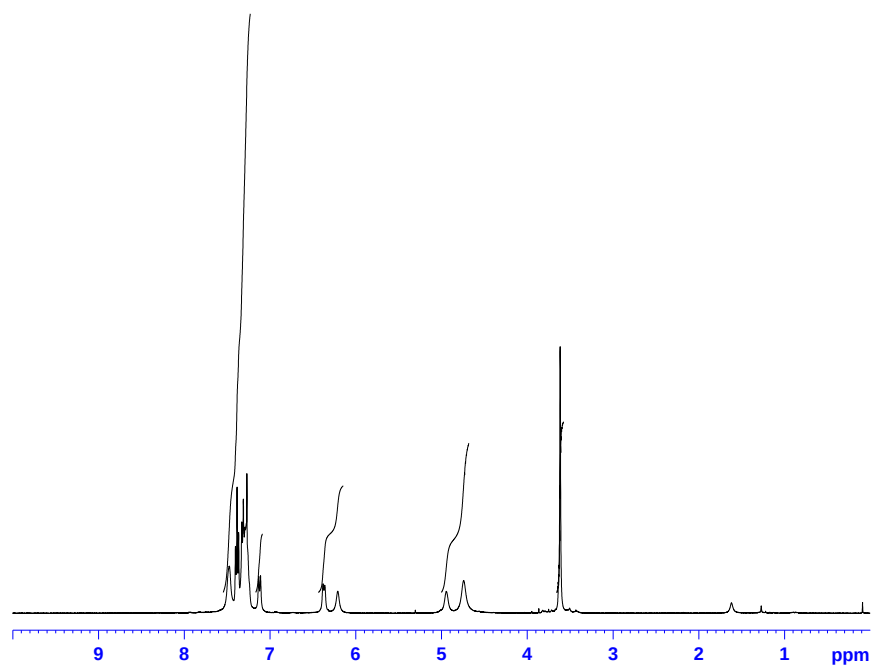
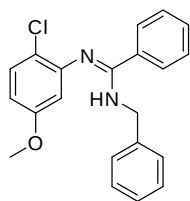
Quinazolinone 8q: ^1H -NMR (400 MHz, CDCl_3)



Quinazolinone 8q: ^{13}C -NMR (100 MHz, CDCl_3)



Amidine 11: ^1H -NMR (400 MHz, CDCl_3)



Amidine 11: ^{13}C -NMR (100 MHz, CDCl_3)

