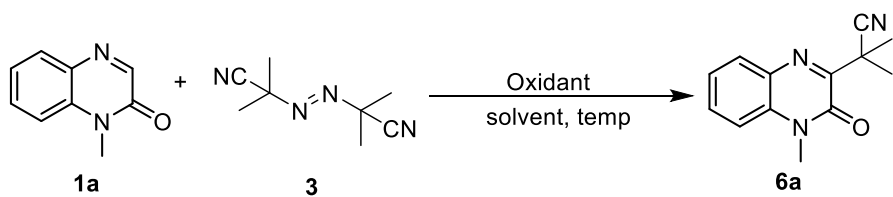


Supporting Information

CONTENTS:

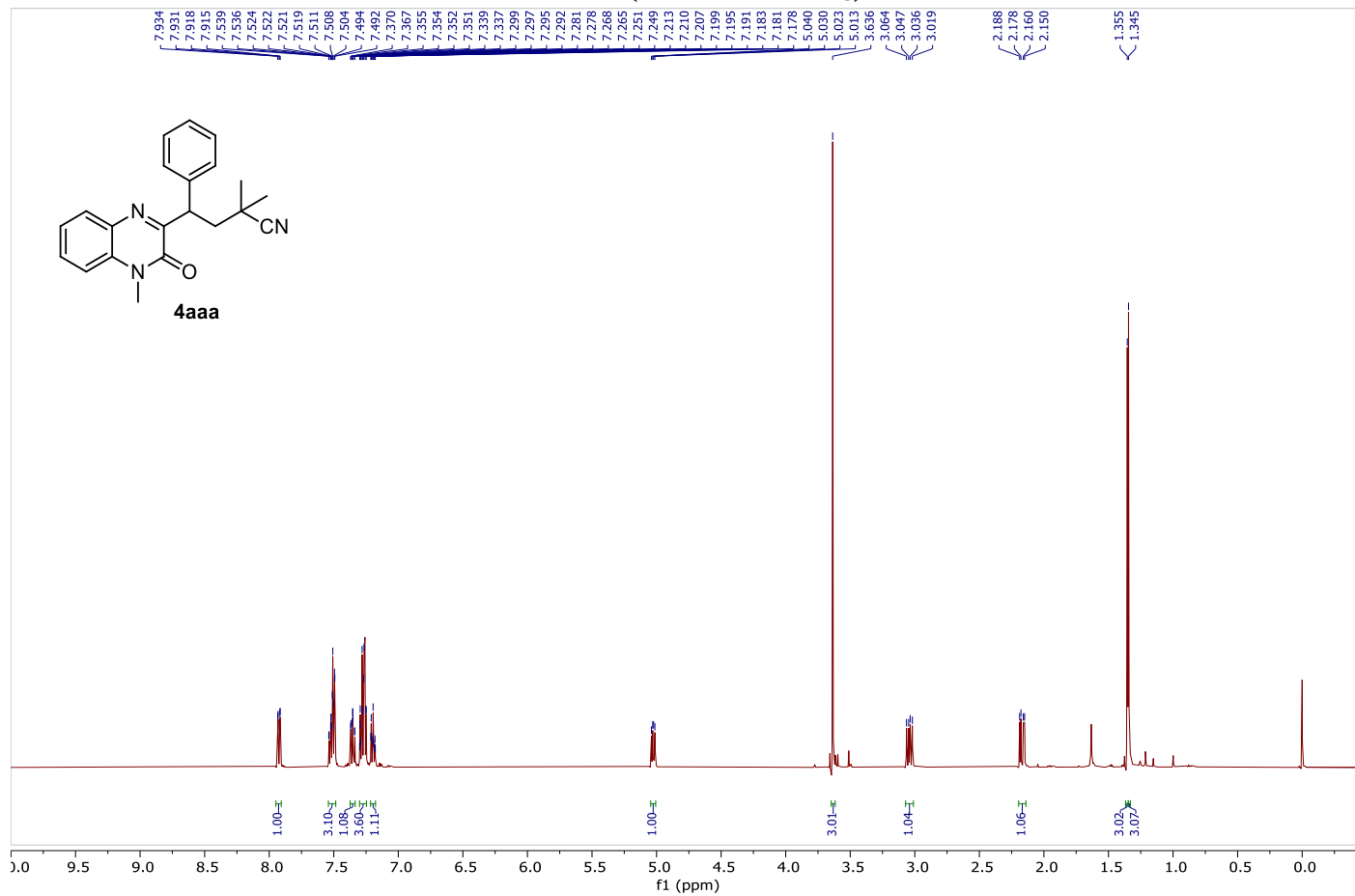
1. Optimization table for the synthesis of 6a	S2
2. ^1H NMR and ^{13}C NMR spectra of all synthesized compounds	S3-S40
3. NOESY – 4aka	S41

Table: Reaction optimization studies for the synthesis of **6a**^{a,b}

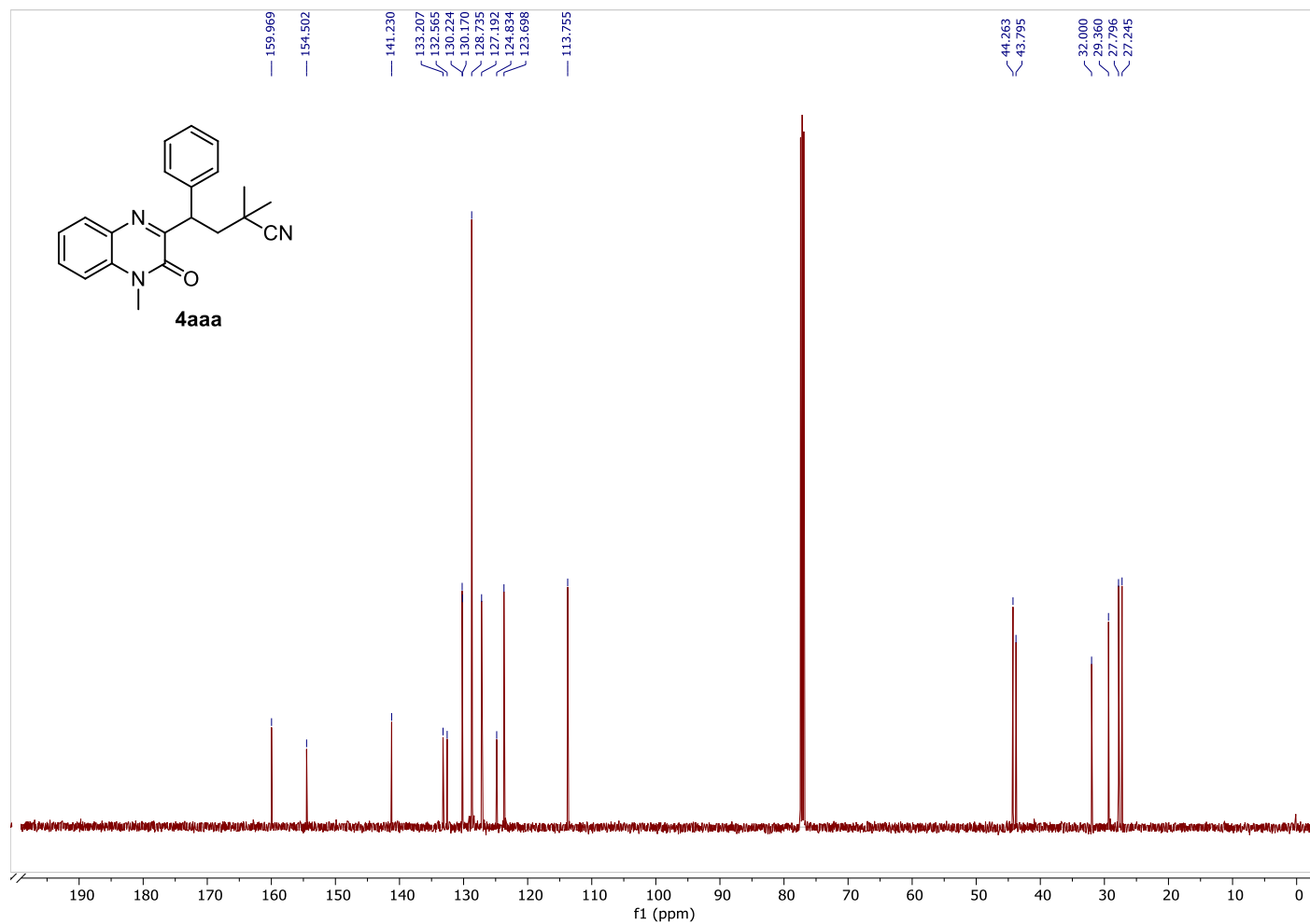
					
Entry	Oxidant (Equiv)	Additive	Solvent (2 mL)	Temp (°C)	Yield (%)
1	K ₂ S ₂ O ₈ (1.5)		EtOAc	80	20
2	K ₂ S ₂ O ₈ (1.5)		Cyclohexane	80	trace
3	K ₂ S ₂ O ₈ (1.5)		n-Hexane	60	n.r.
4	K₂S₂O₈ (1.5)		Cyclohexane	80	50
5	K ₂ S ₂ O ₈ (1.5)		DMF	80	trace
6	K ₂ S ₂ O ₈ (1.5)		CH ₃ CN: Cyclohexane (1:1)	80	25
7	K ₂ S ₂ O ₈ (1.5)		CH ₃ CN	80	35
8	K ₂ S ₂ O ₈ (1.5)	0.2 mL cyclohexene	CH ₃ CN	80	15

^aReaction conditions: A mixture of **1a** (0.2 mmol), **3** (0.3 mmol) in the presence of oxidant and solvent was stirred as mentioned above in the table. ^bisolated yields, n.r. = no reaction.

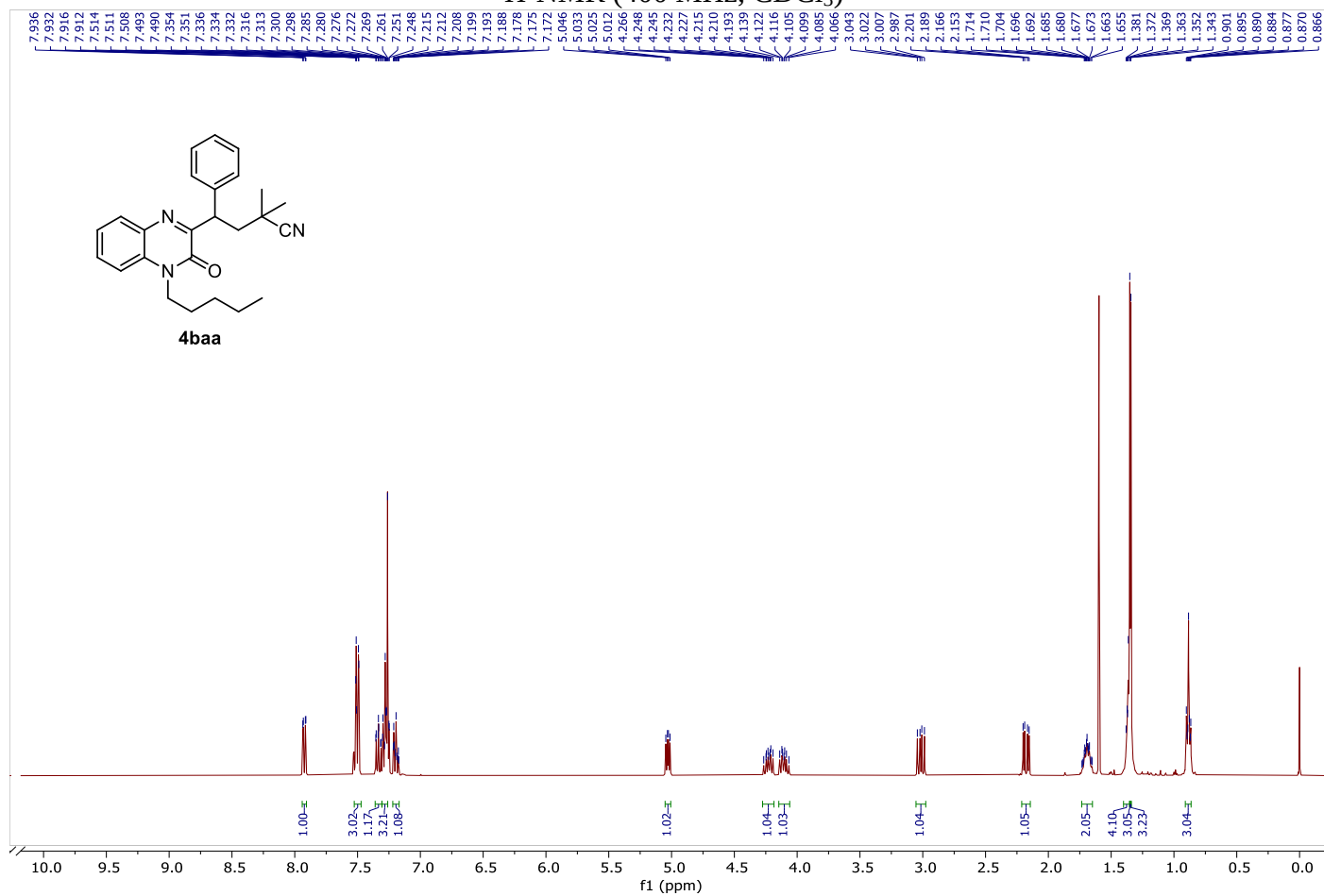
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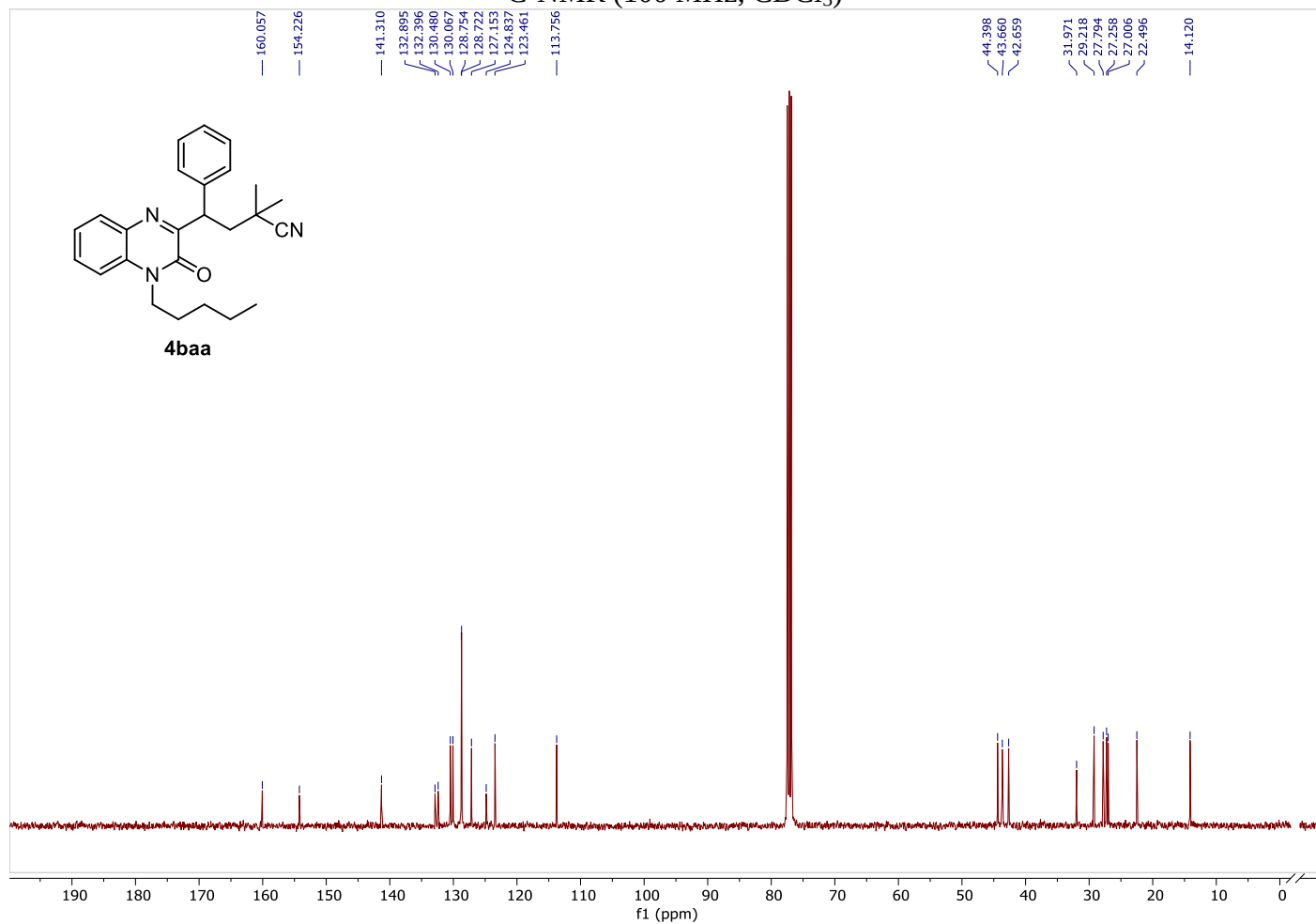
¹³C-NMR (125 MHz, CDCl₃)



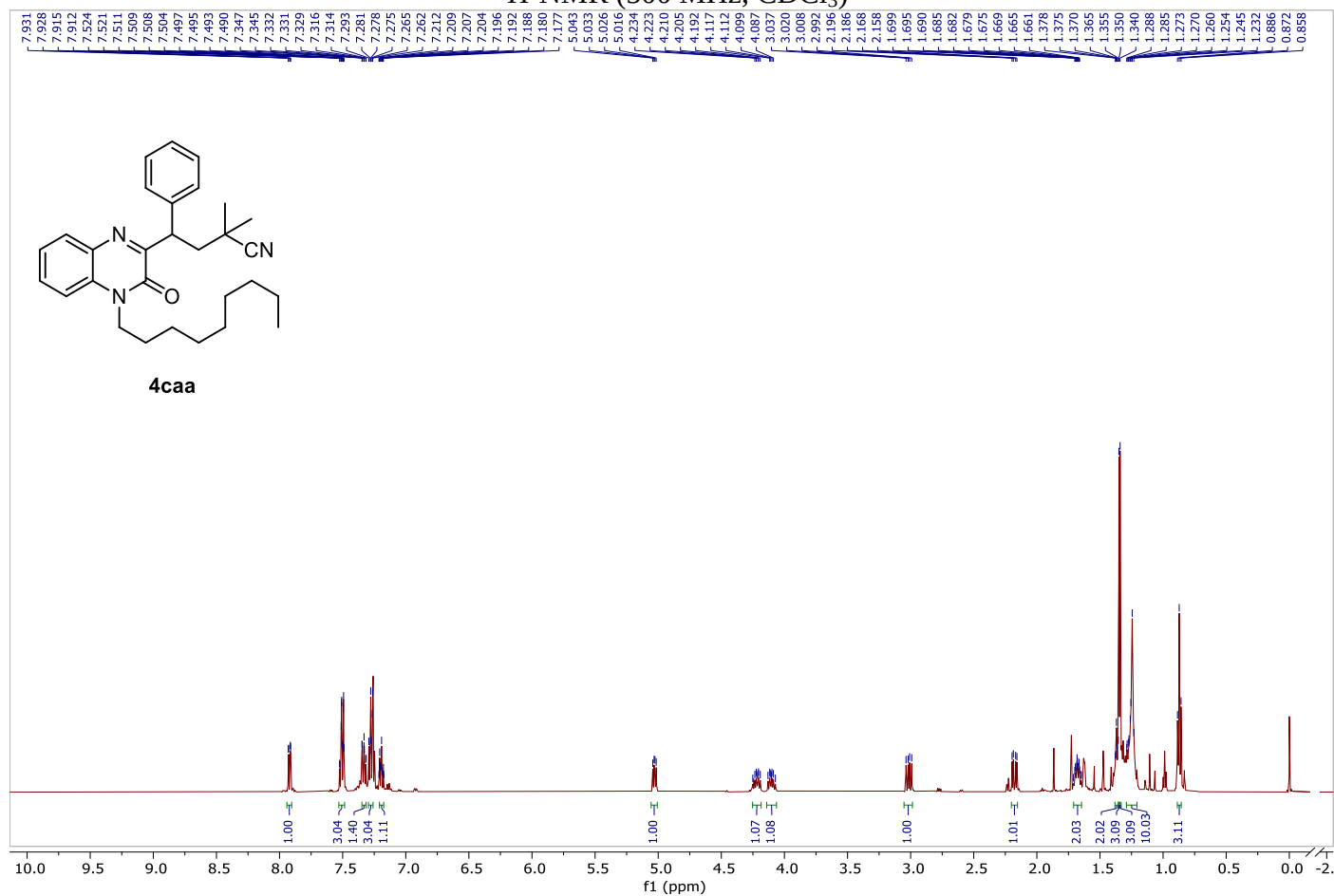
¹H-NMR (400 MHz, CDCl₃)



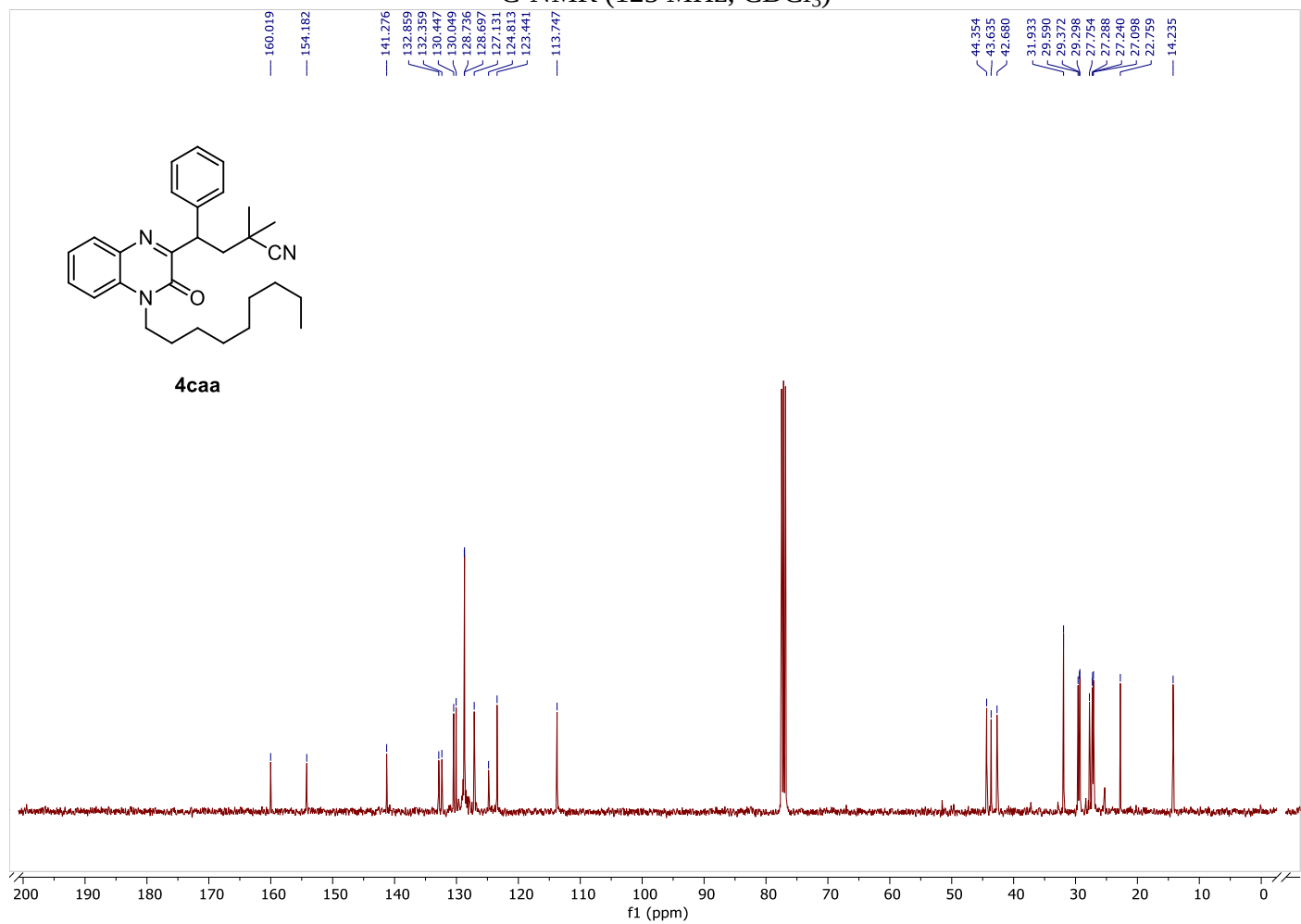
¹³C-NMR (100 MHz, CDCl₃)



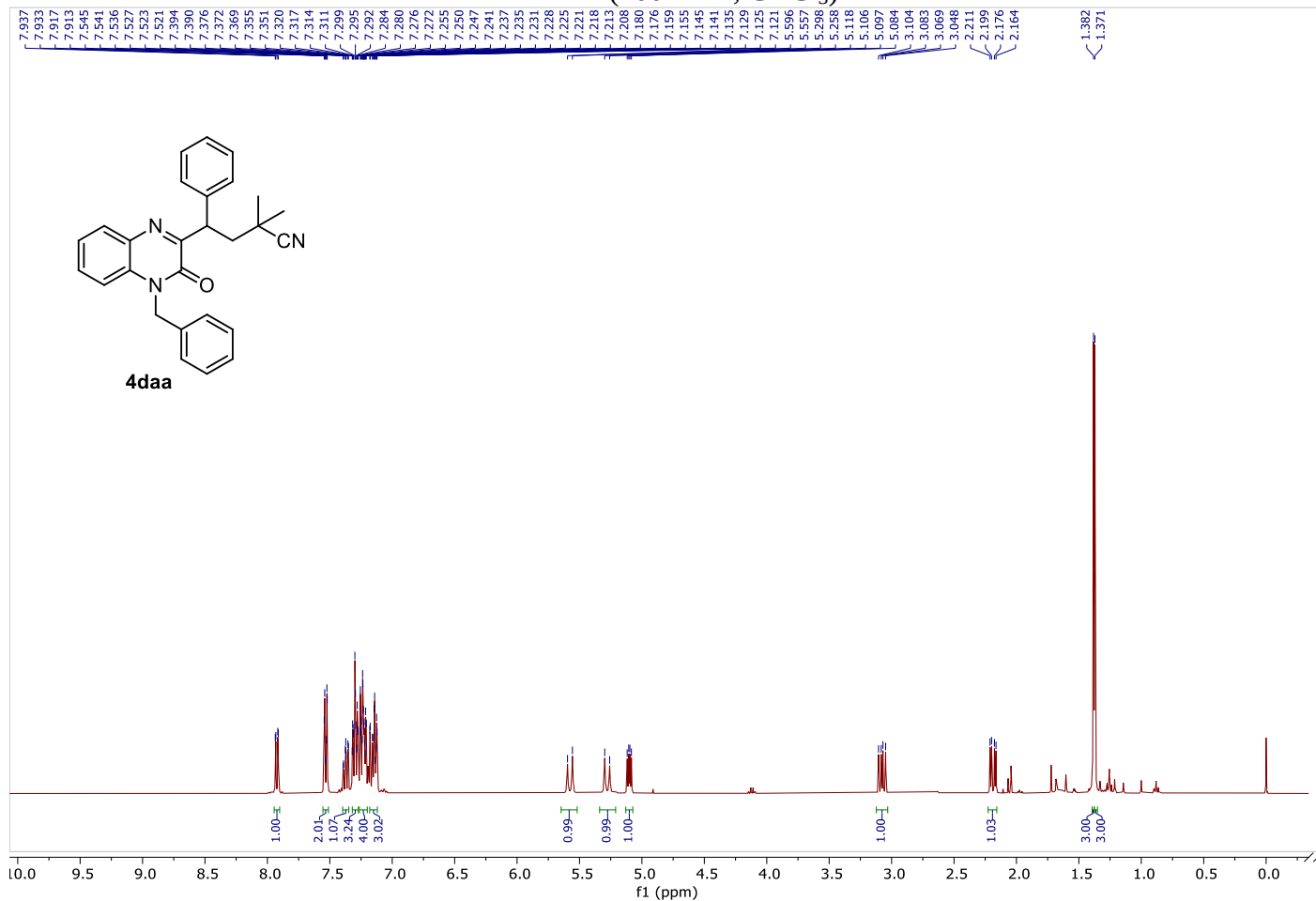
¹H-NMR (500 MHz, CDCl₃)



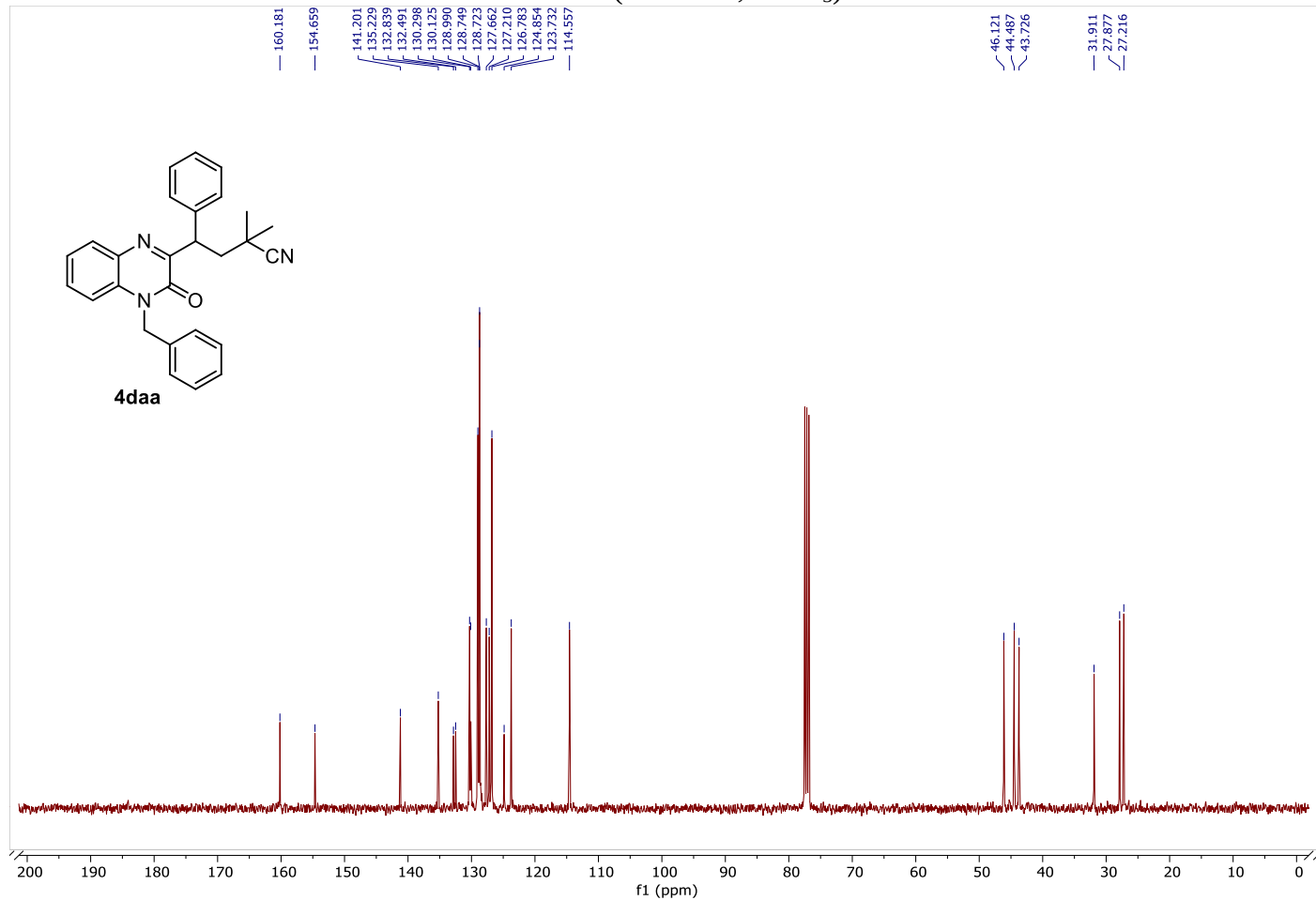
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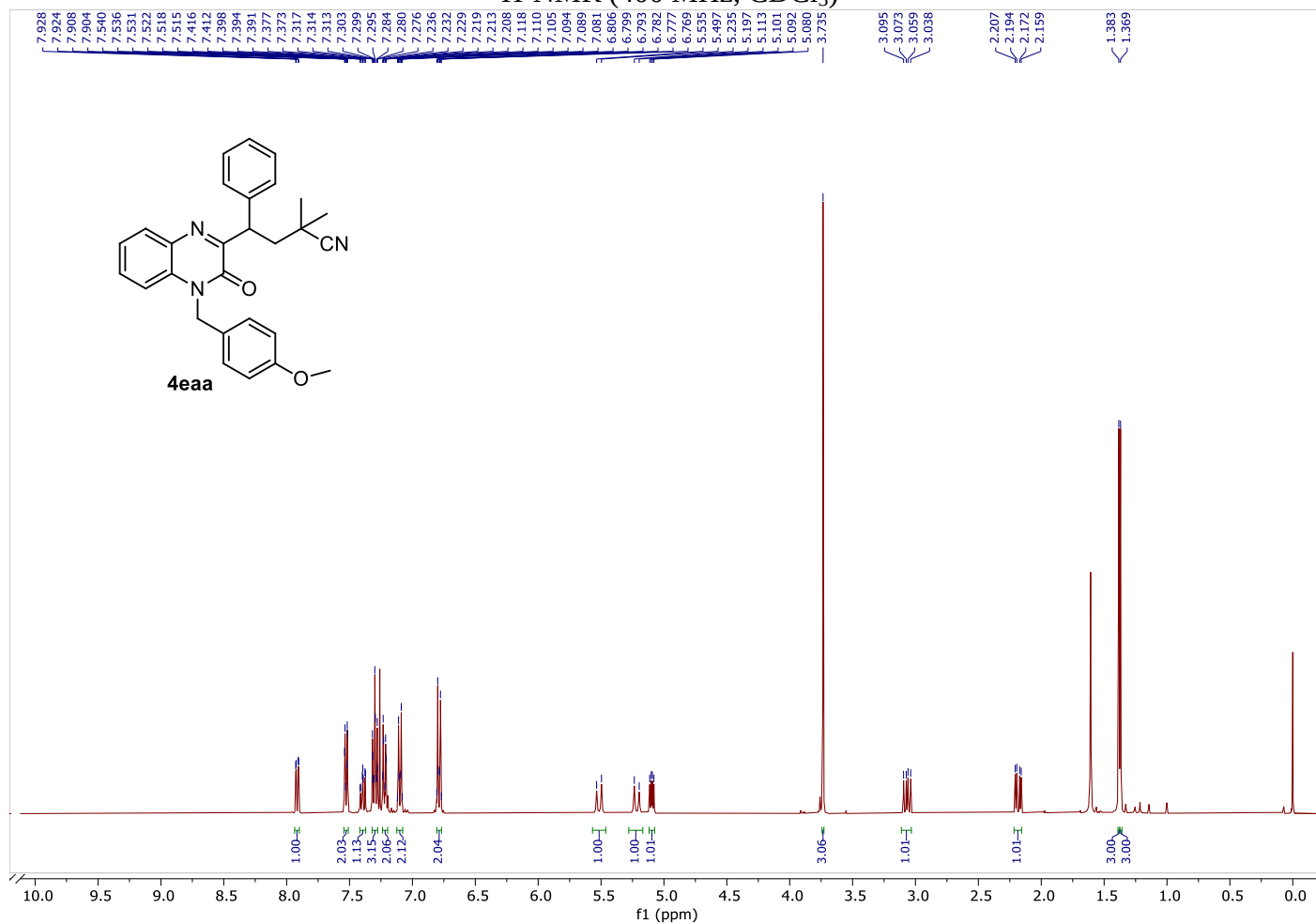
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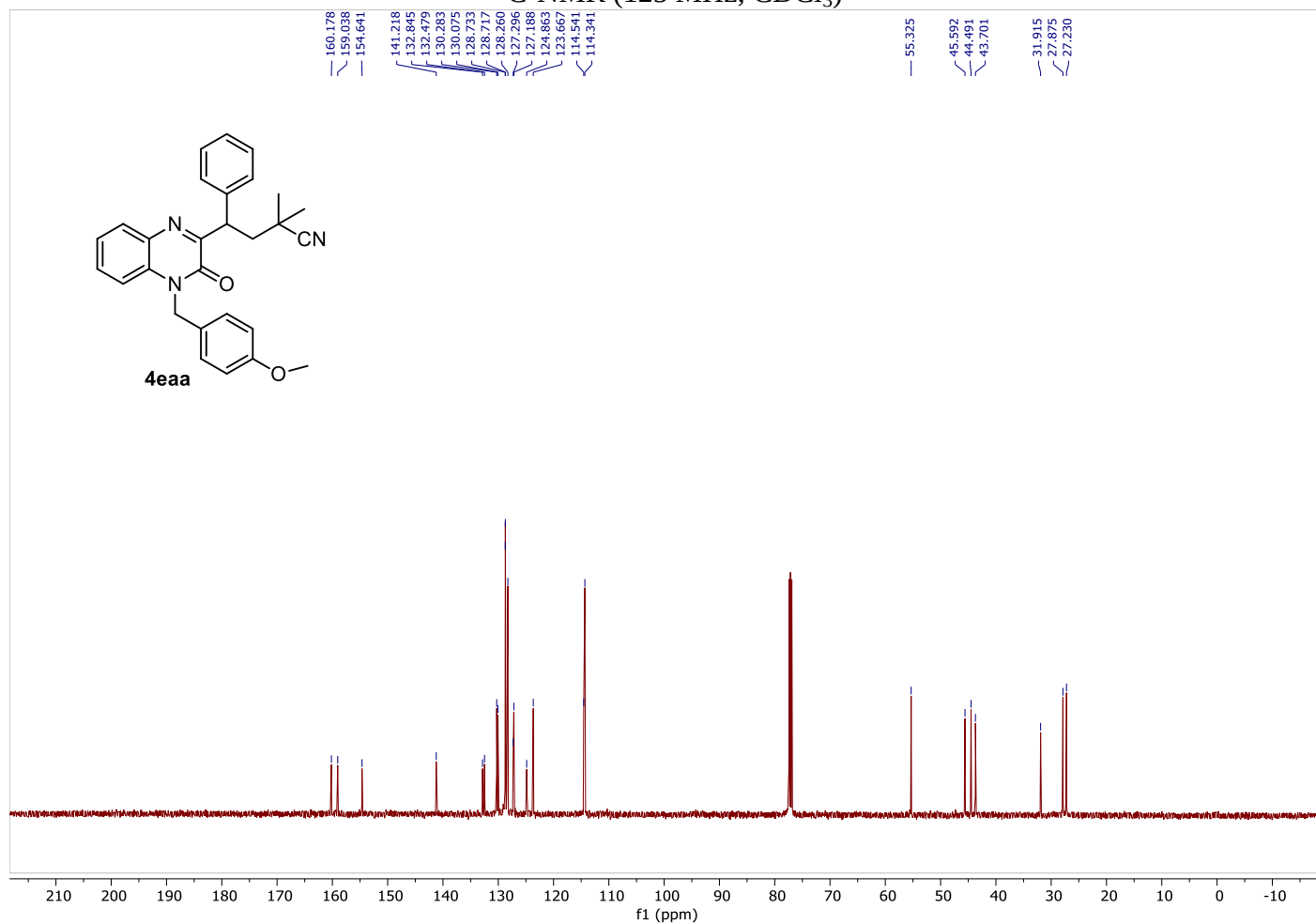
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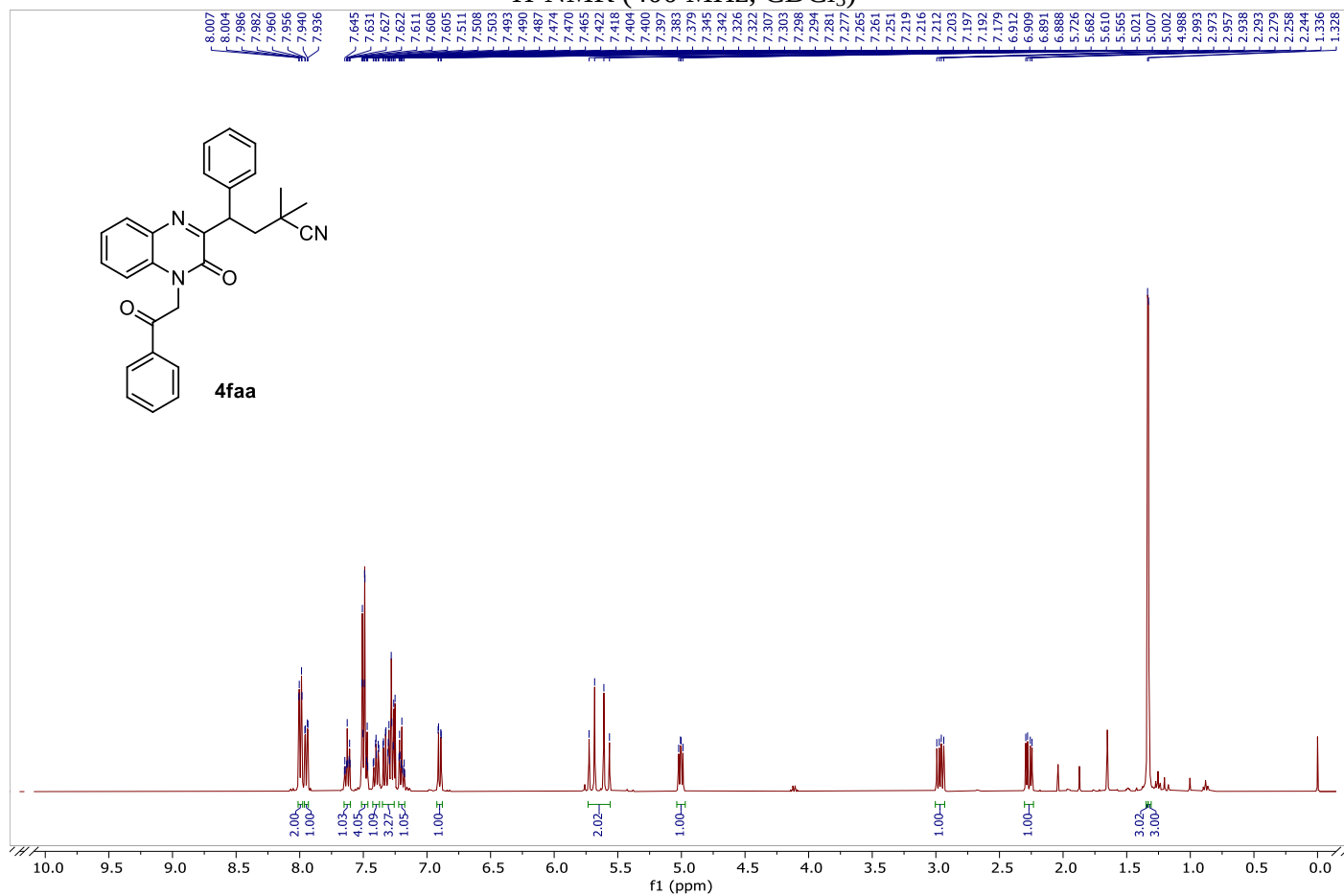
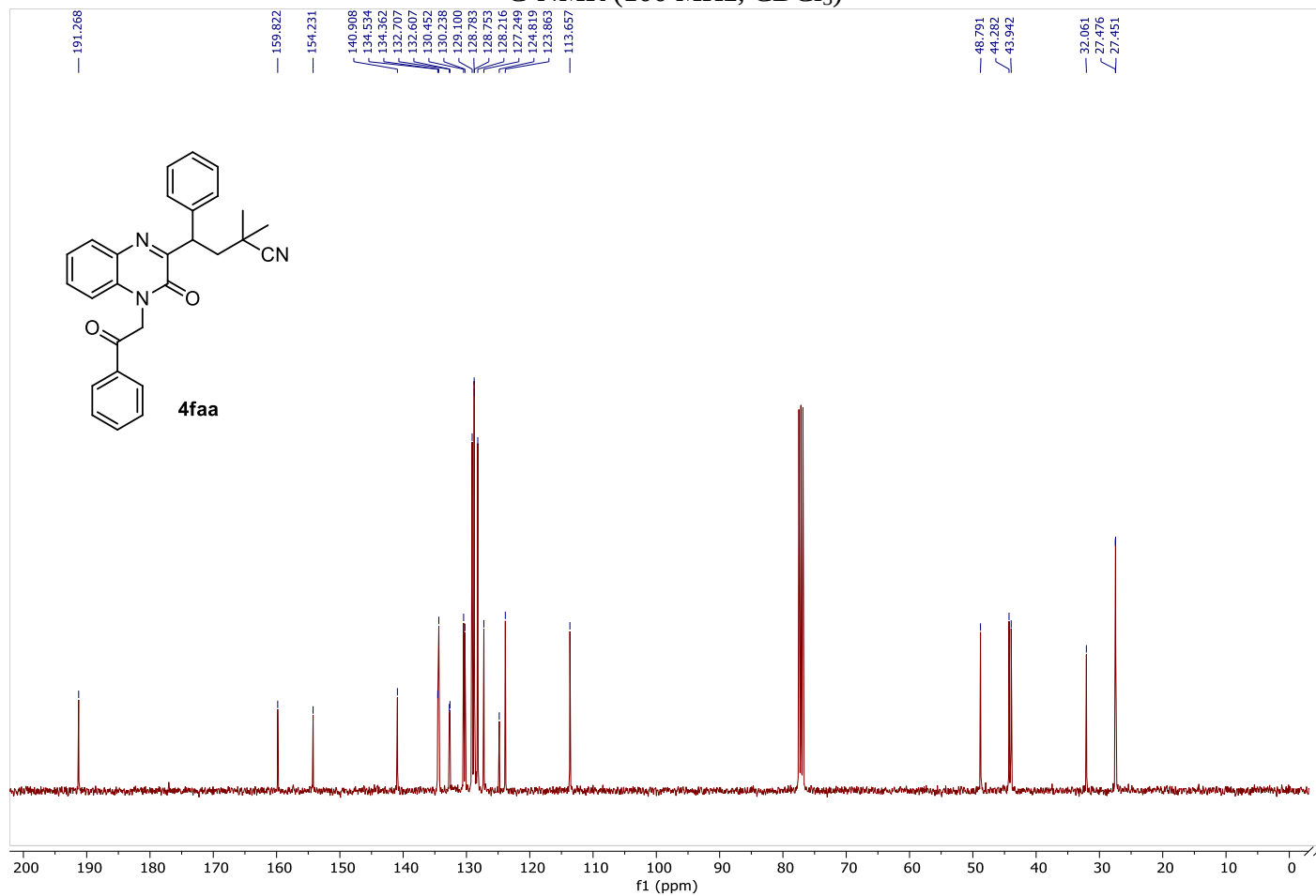


¹H-NMR (400 MHz, CDCl₃)

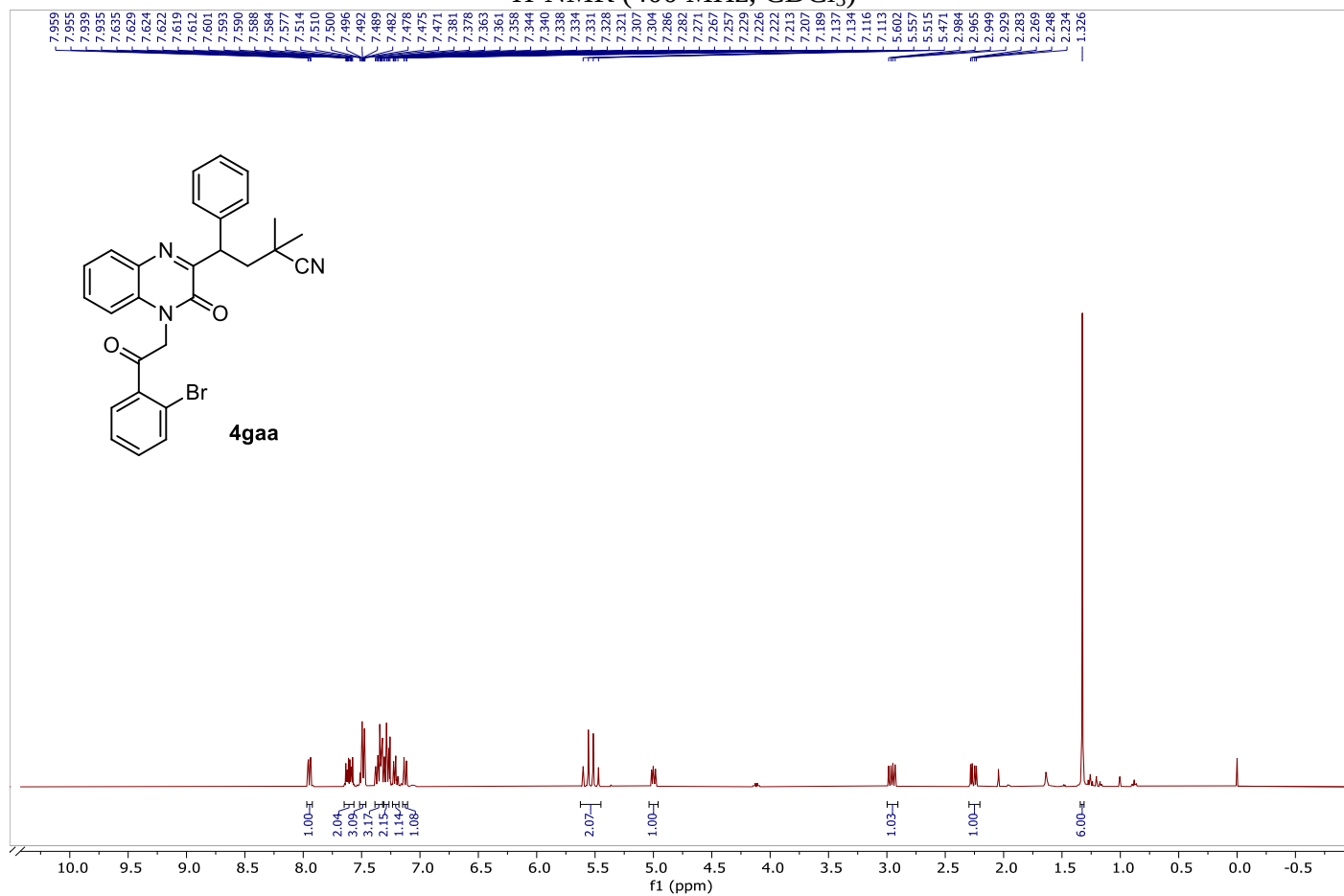


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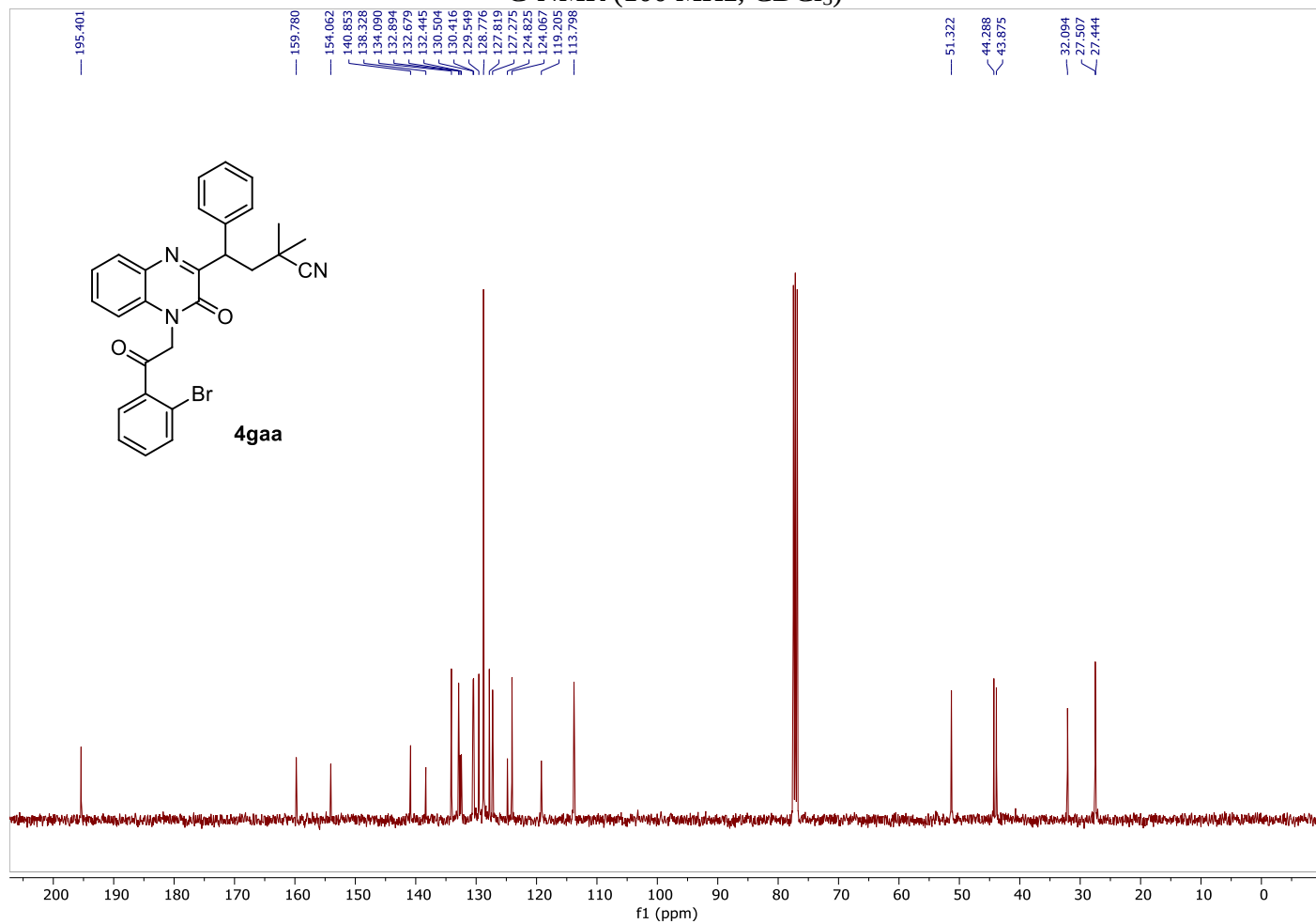


¹H-NMR (400 MHz, CDCl₃)¹³C-NMR (100 MHz, CDCl₃)

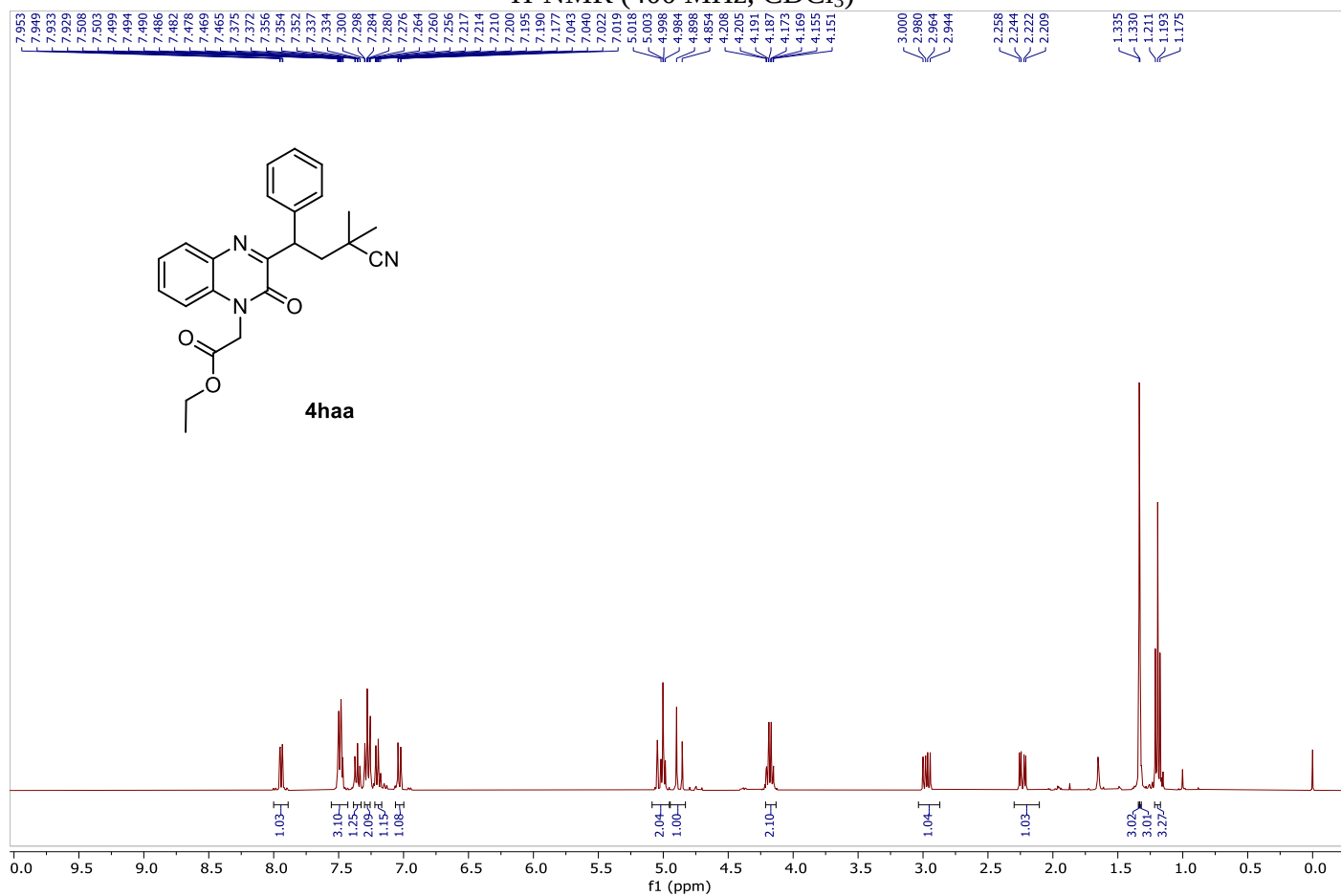
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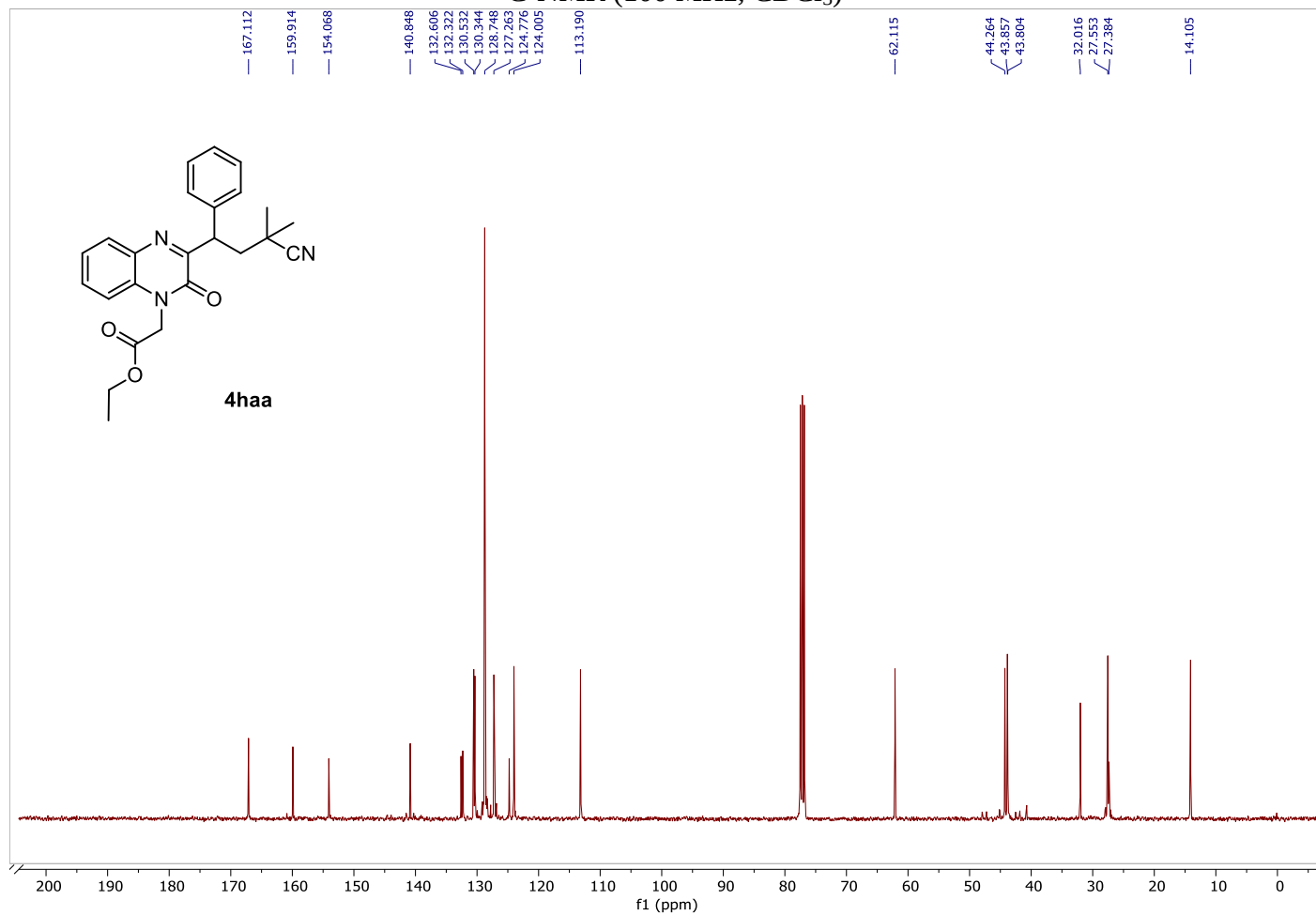
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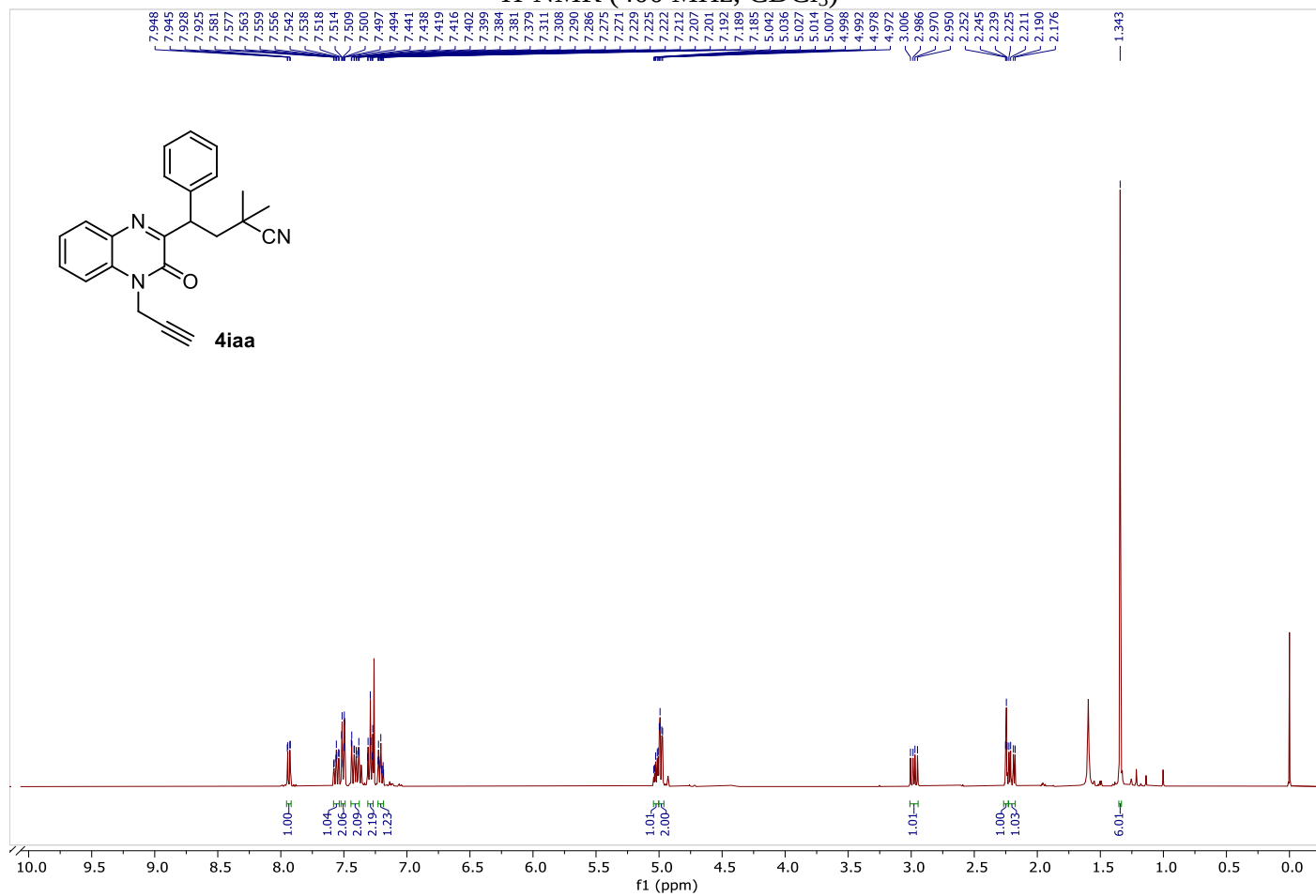
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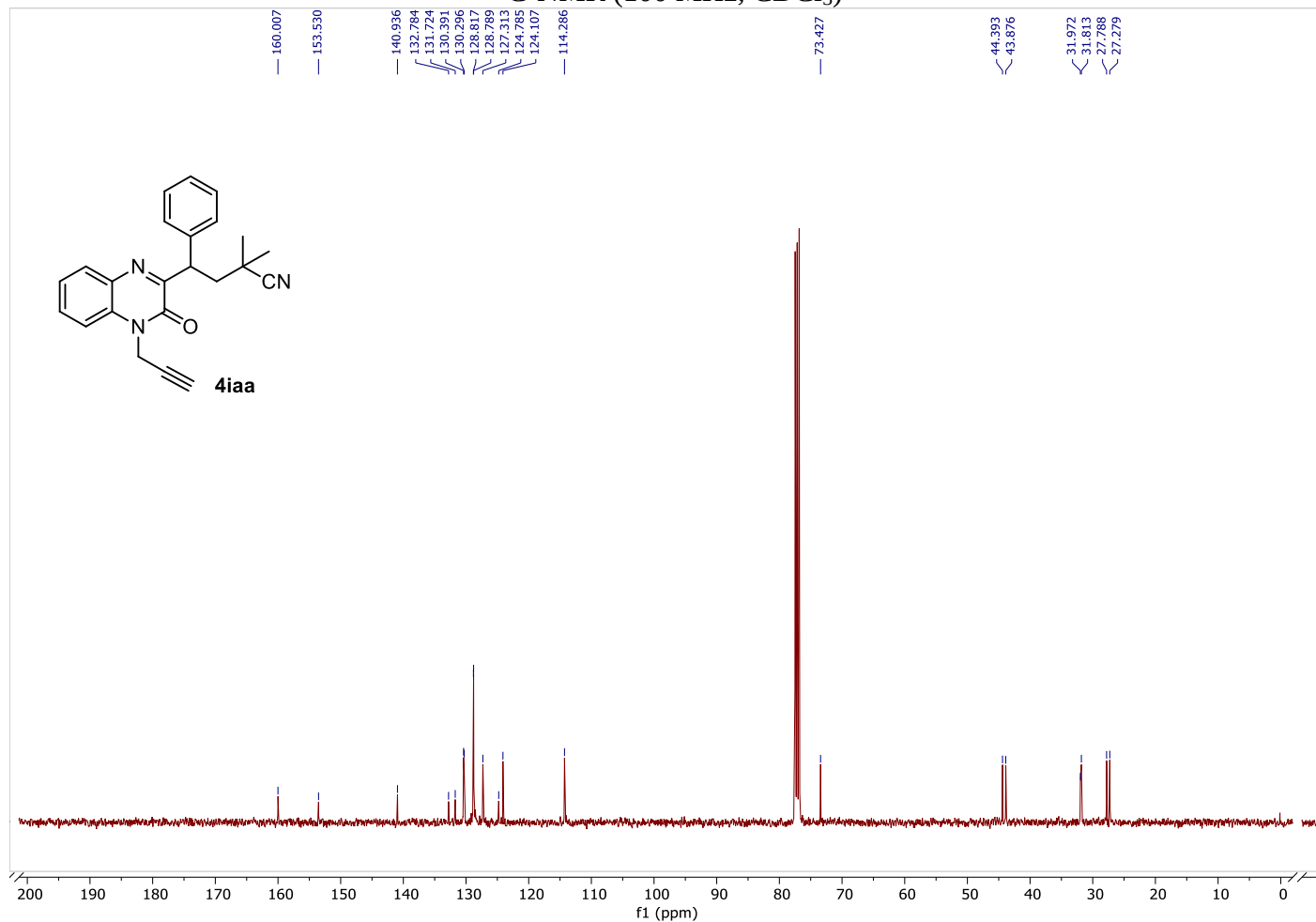
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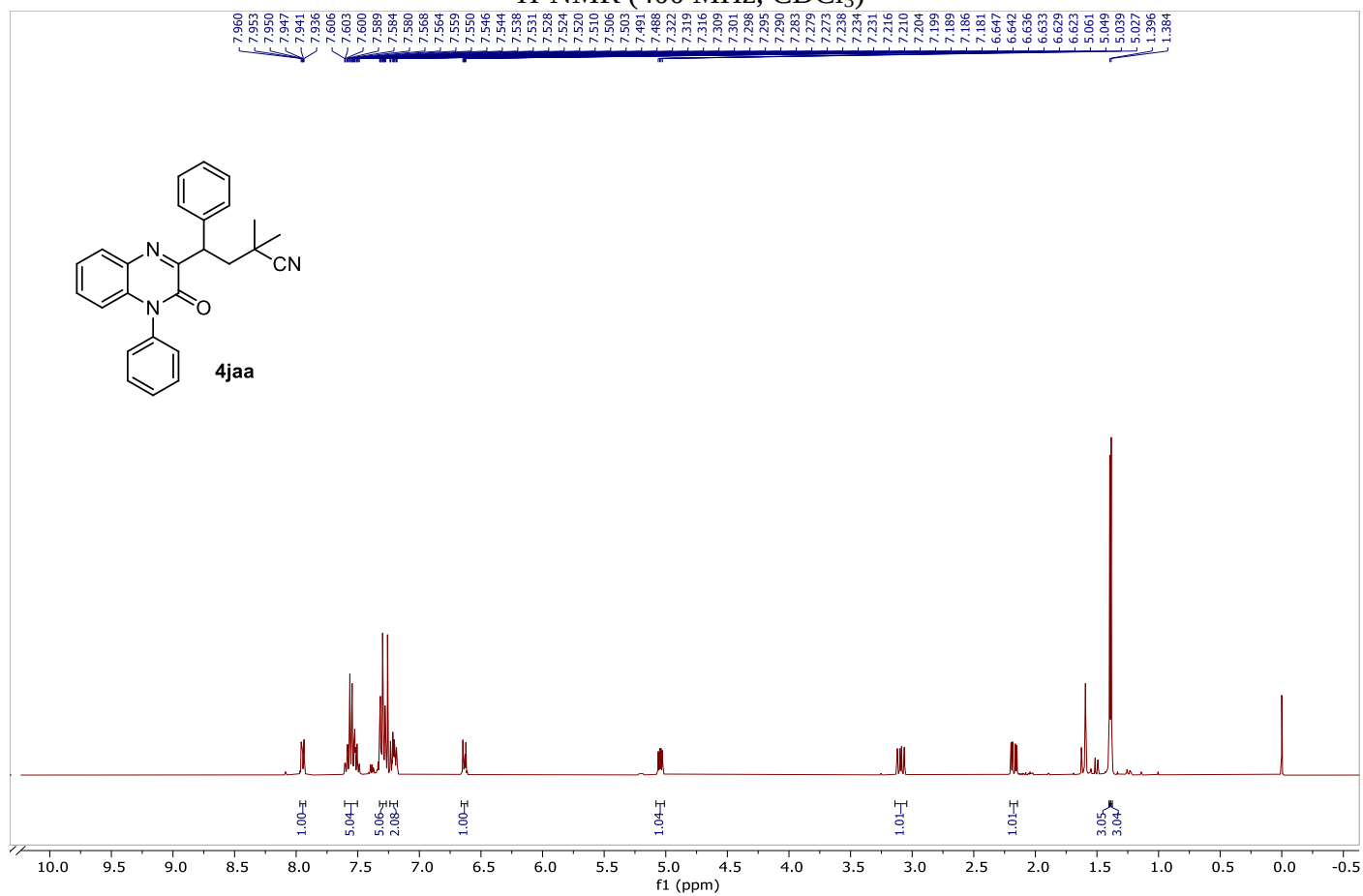
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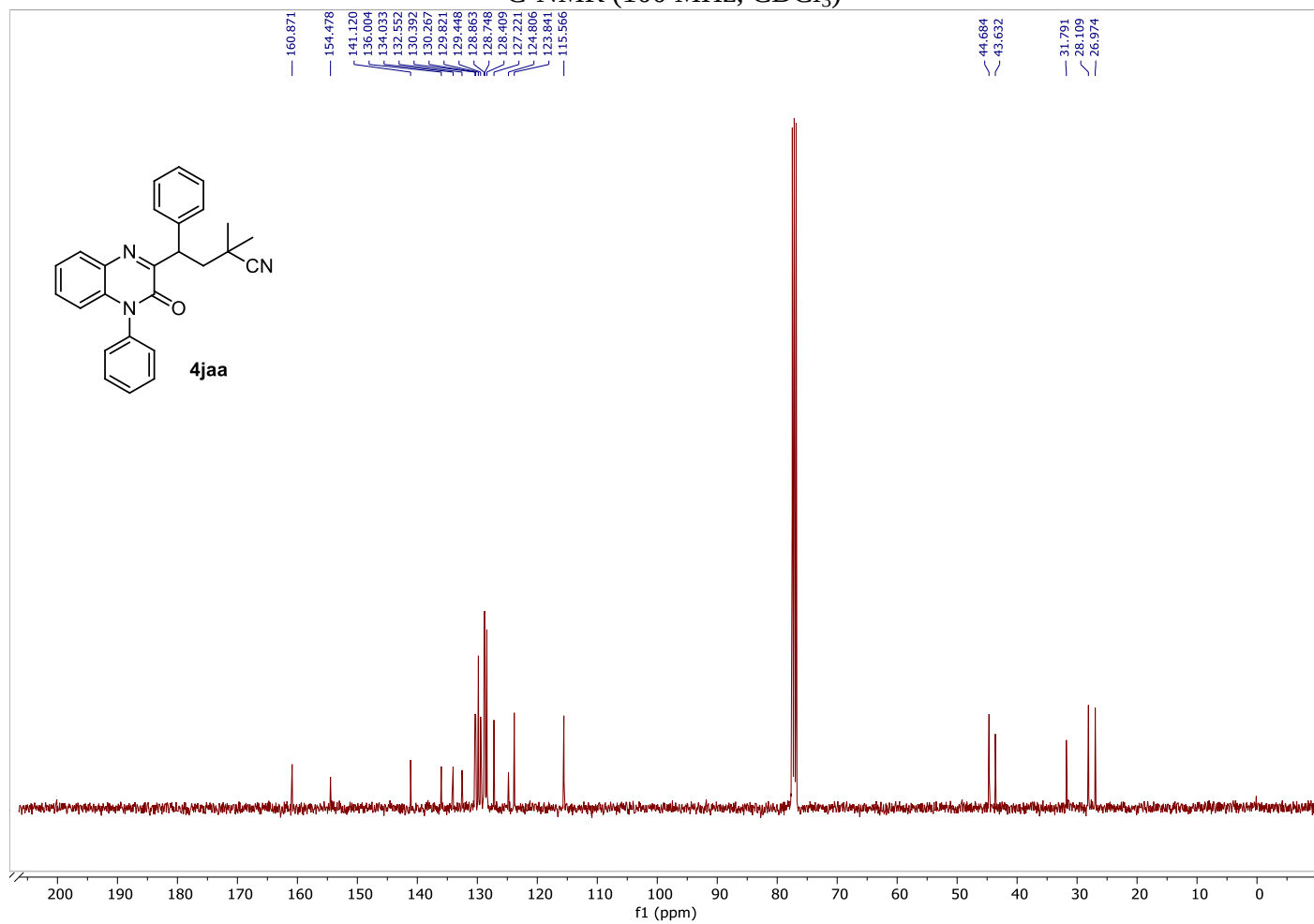
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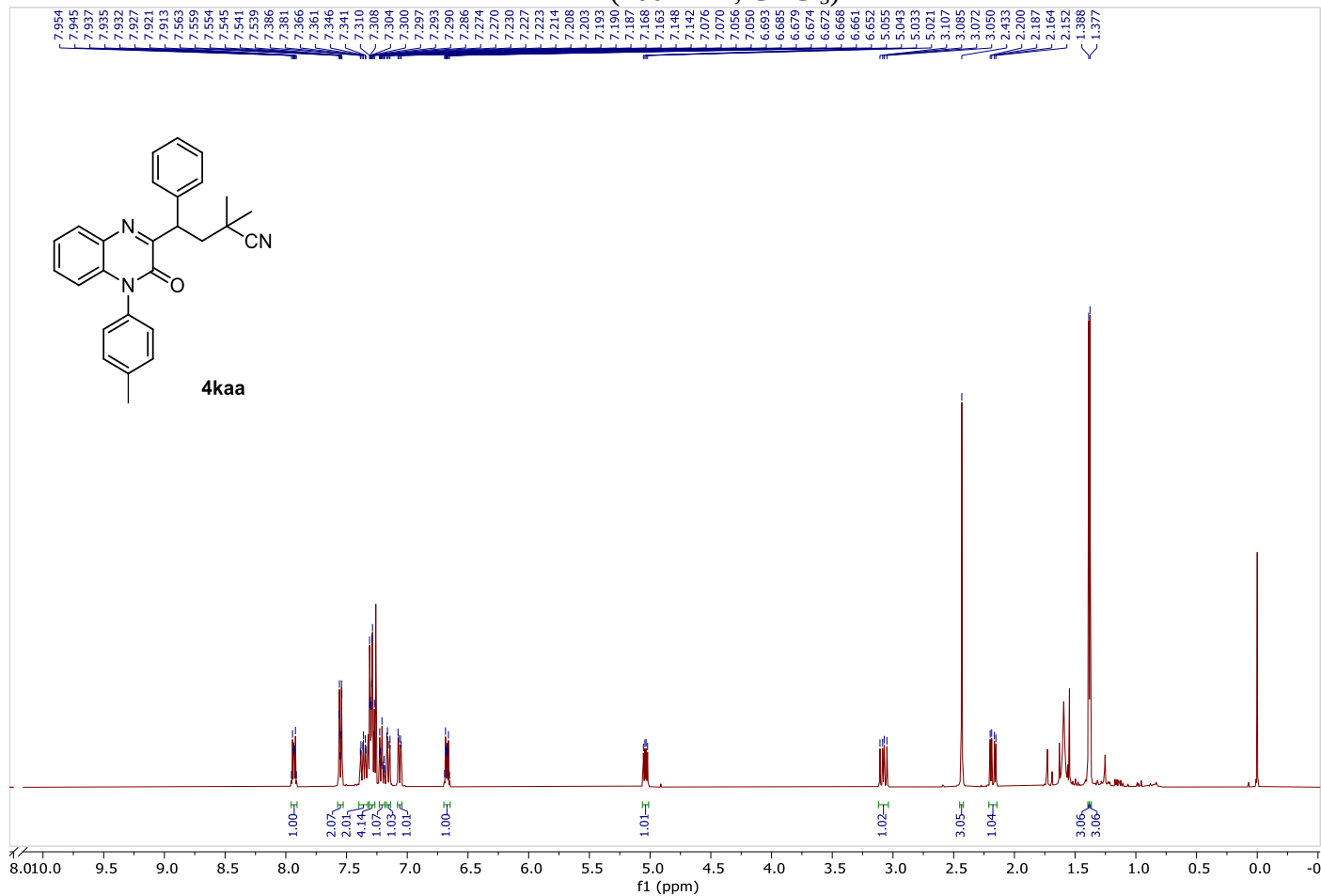
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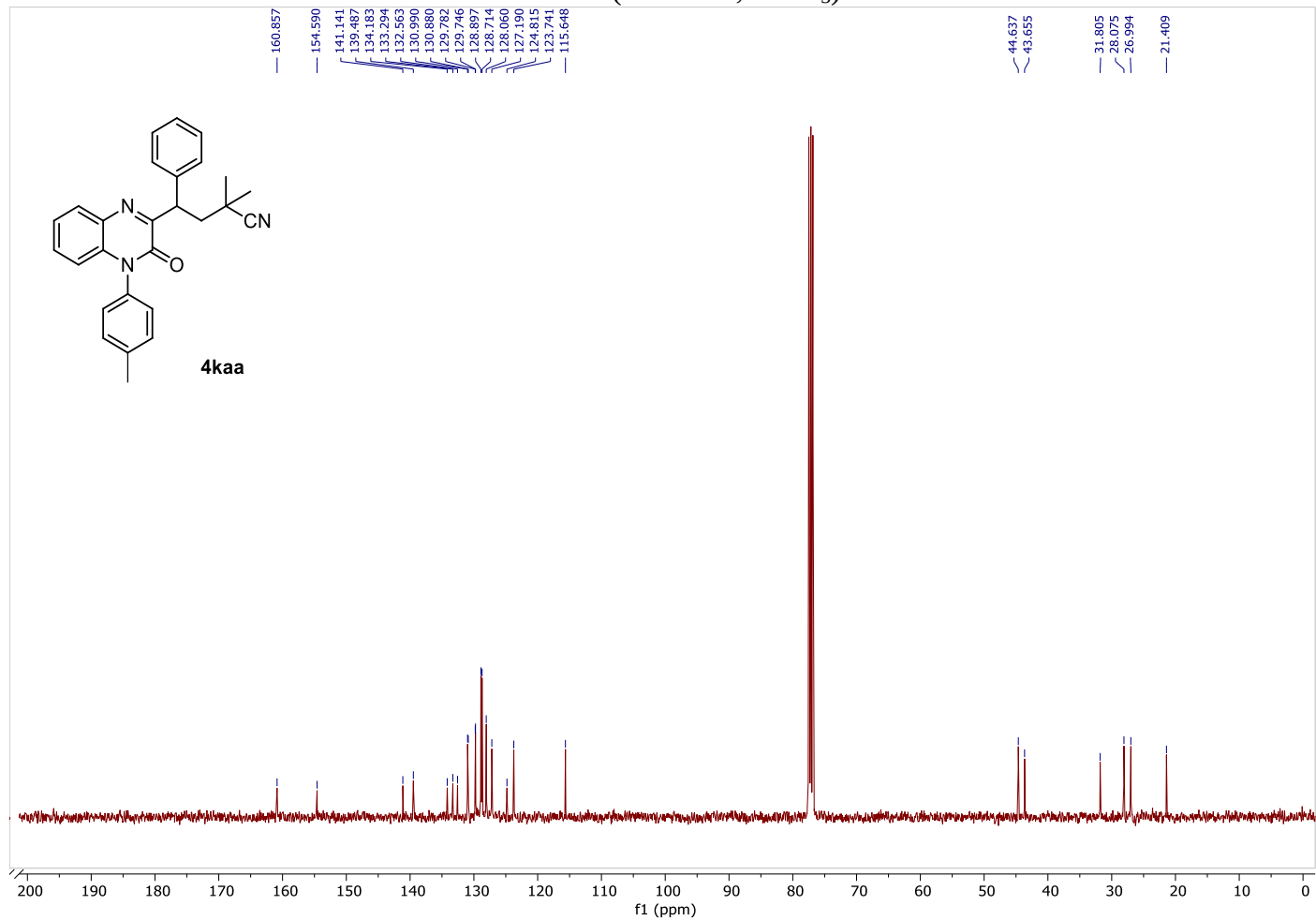
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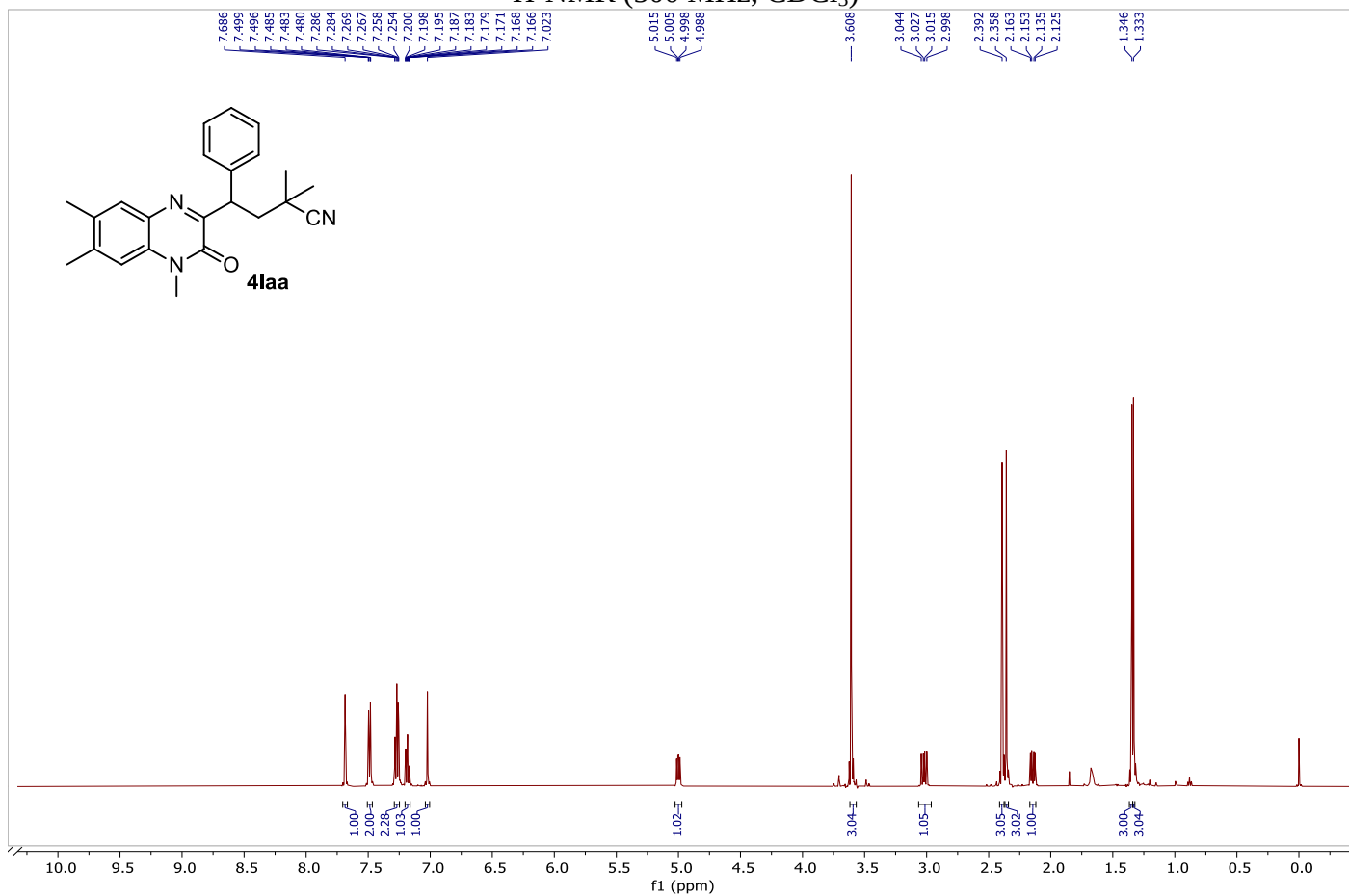
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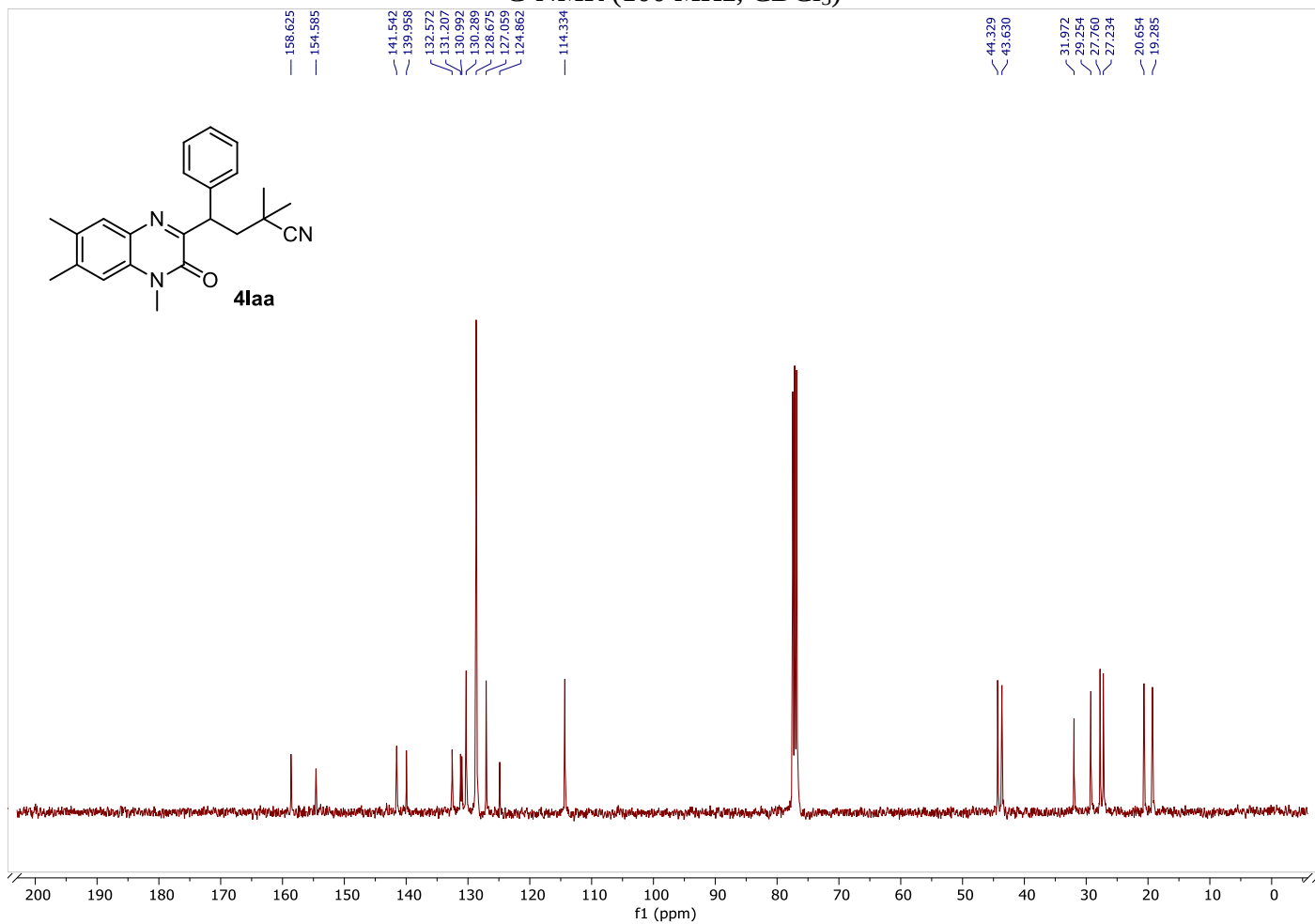
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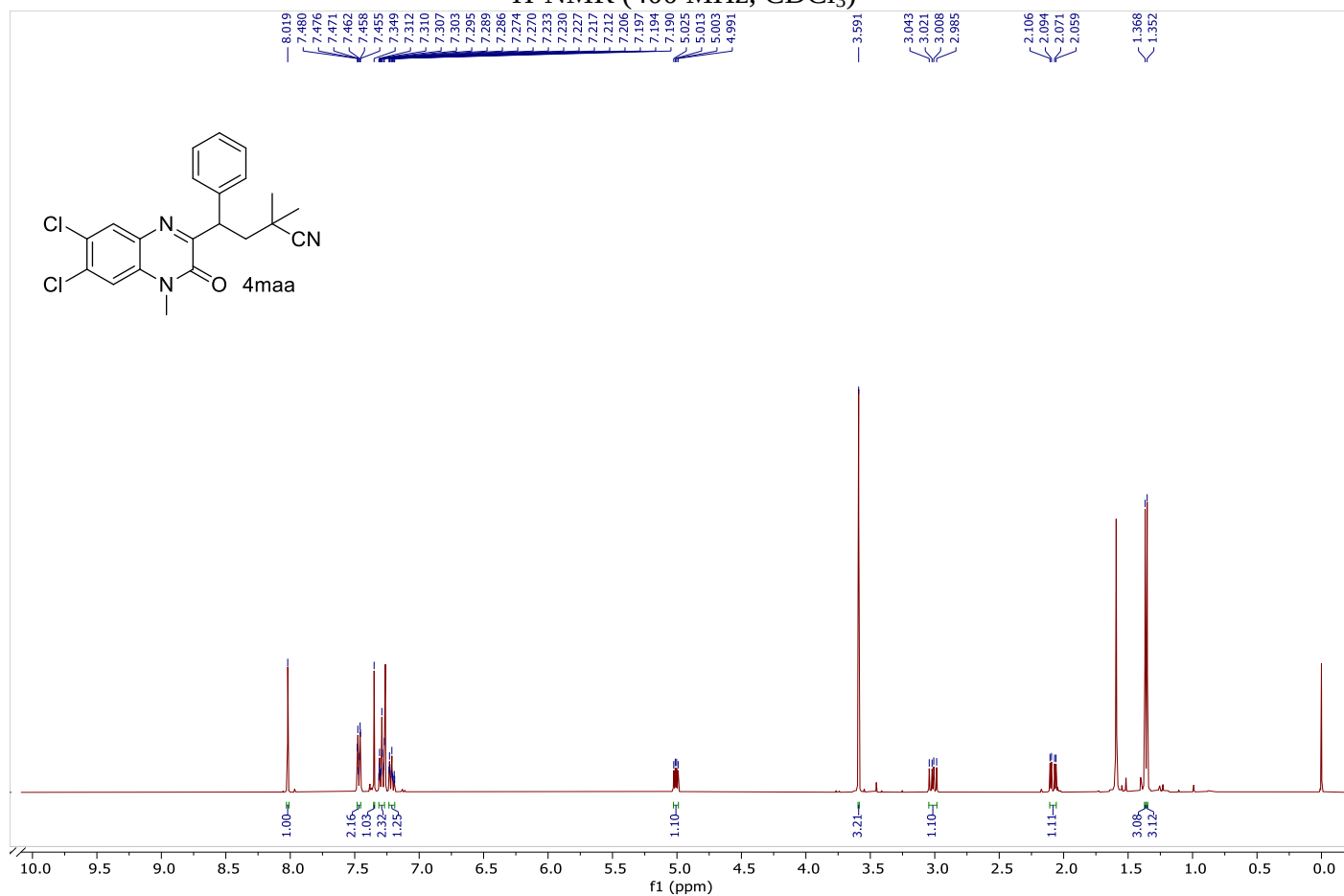
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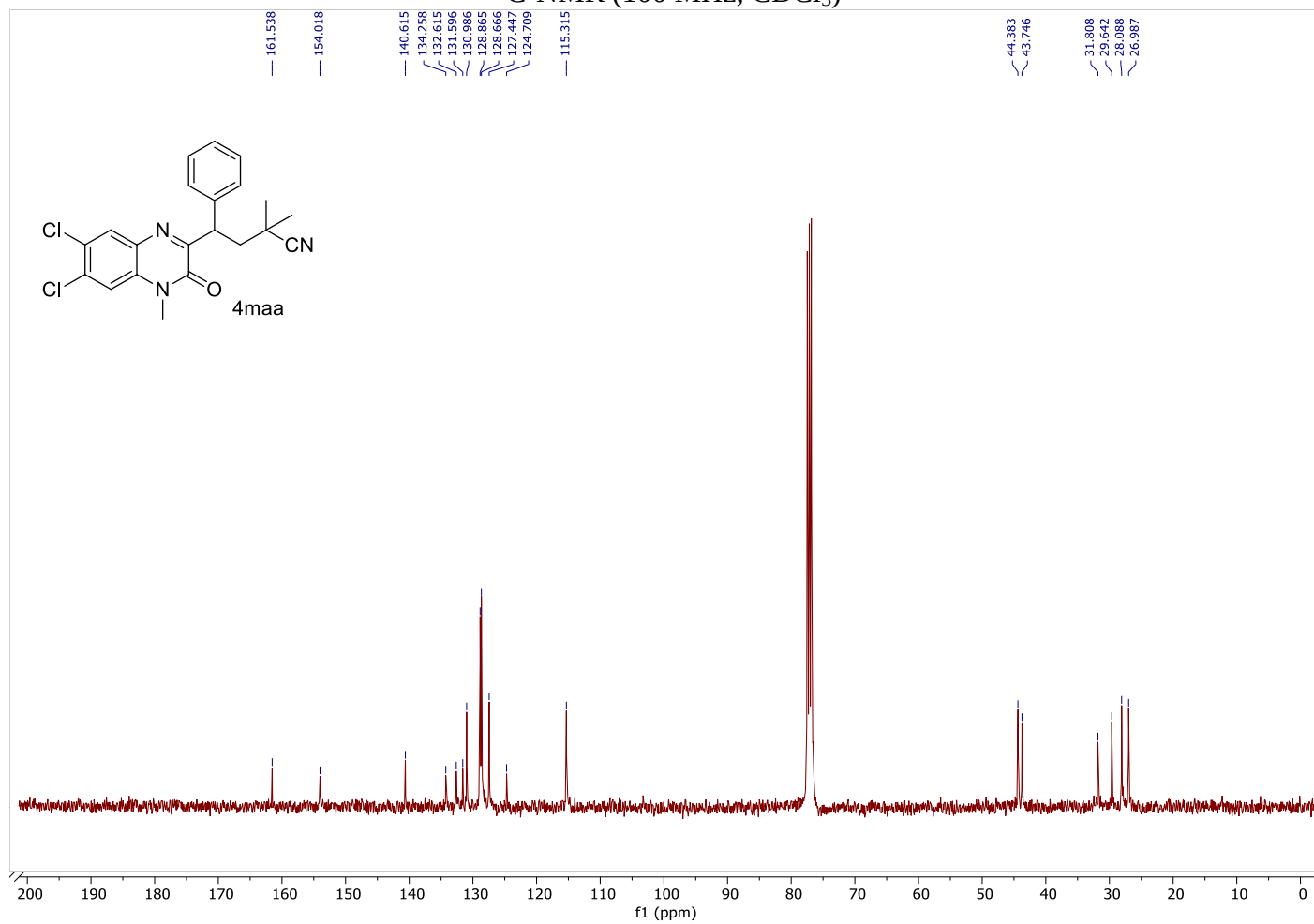
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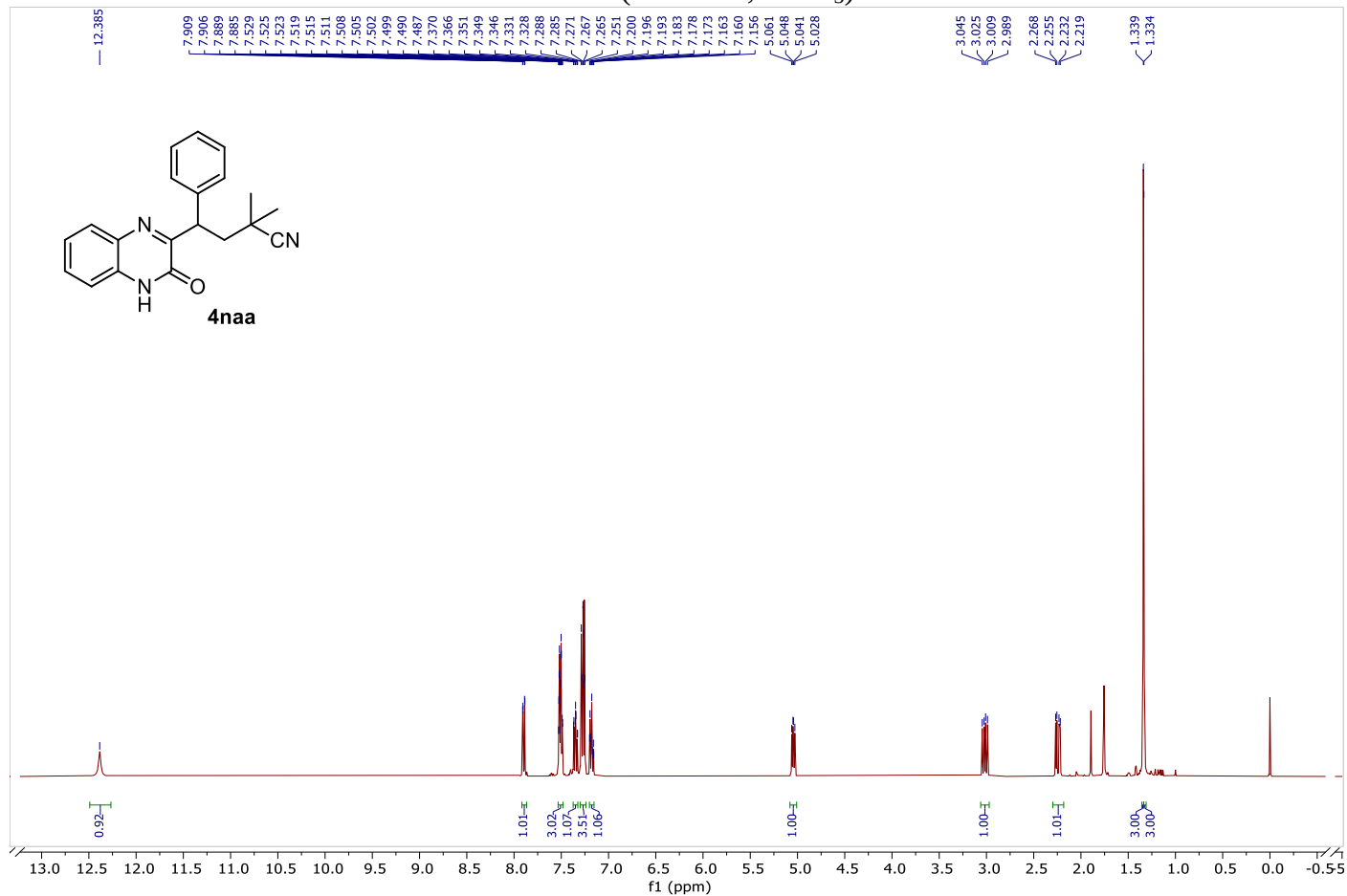
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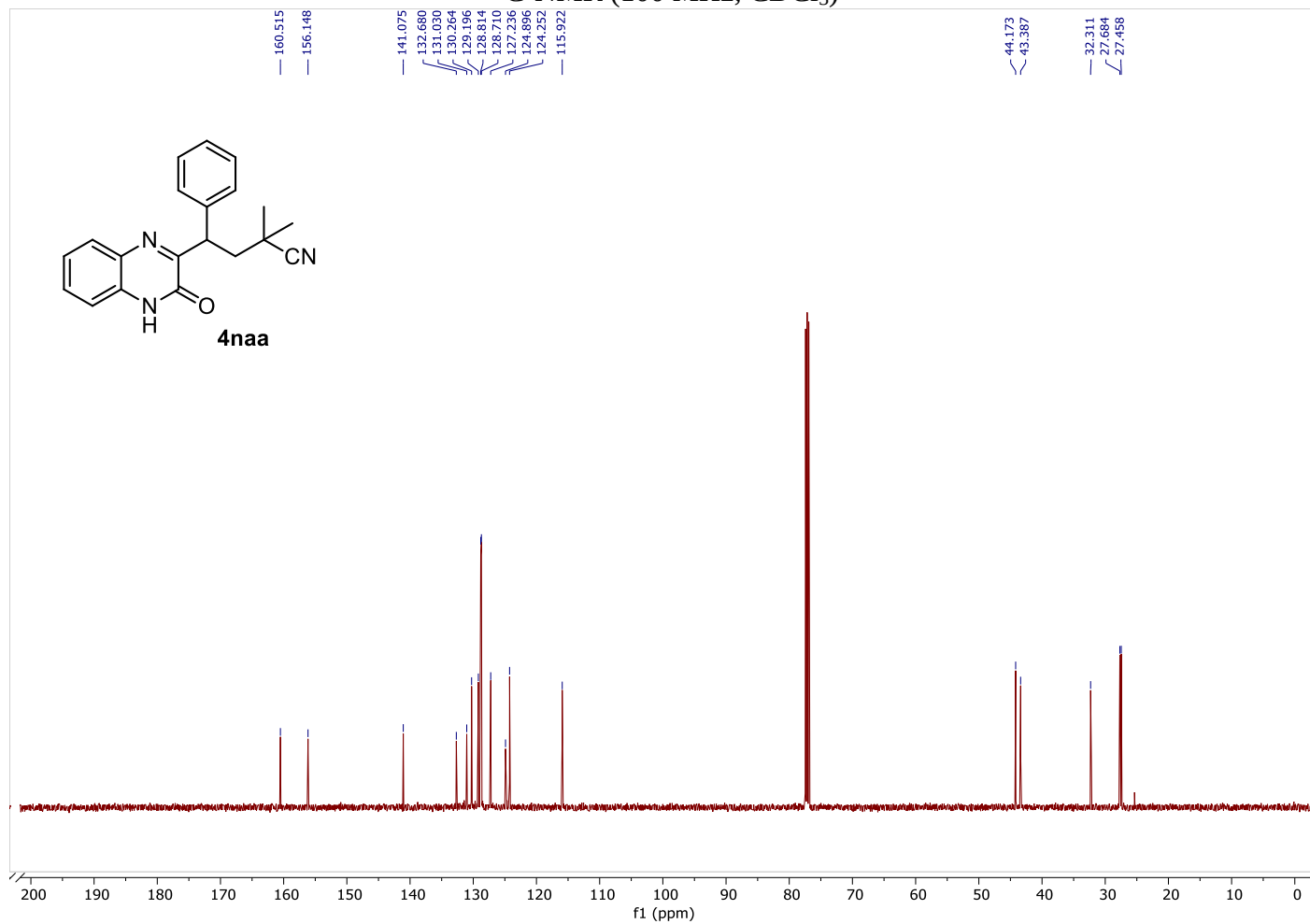
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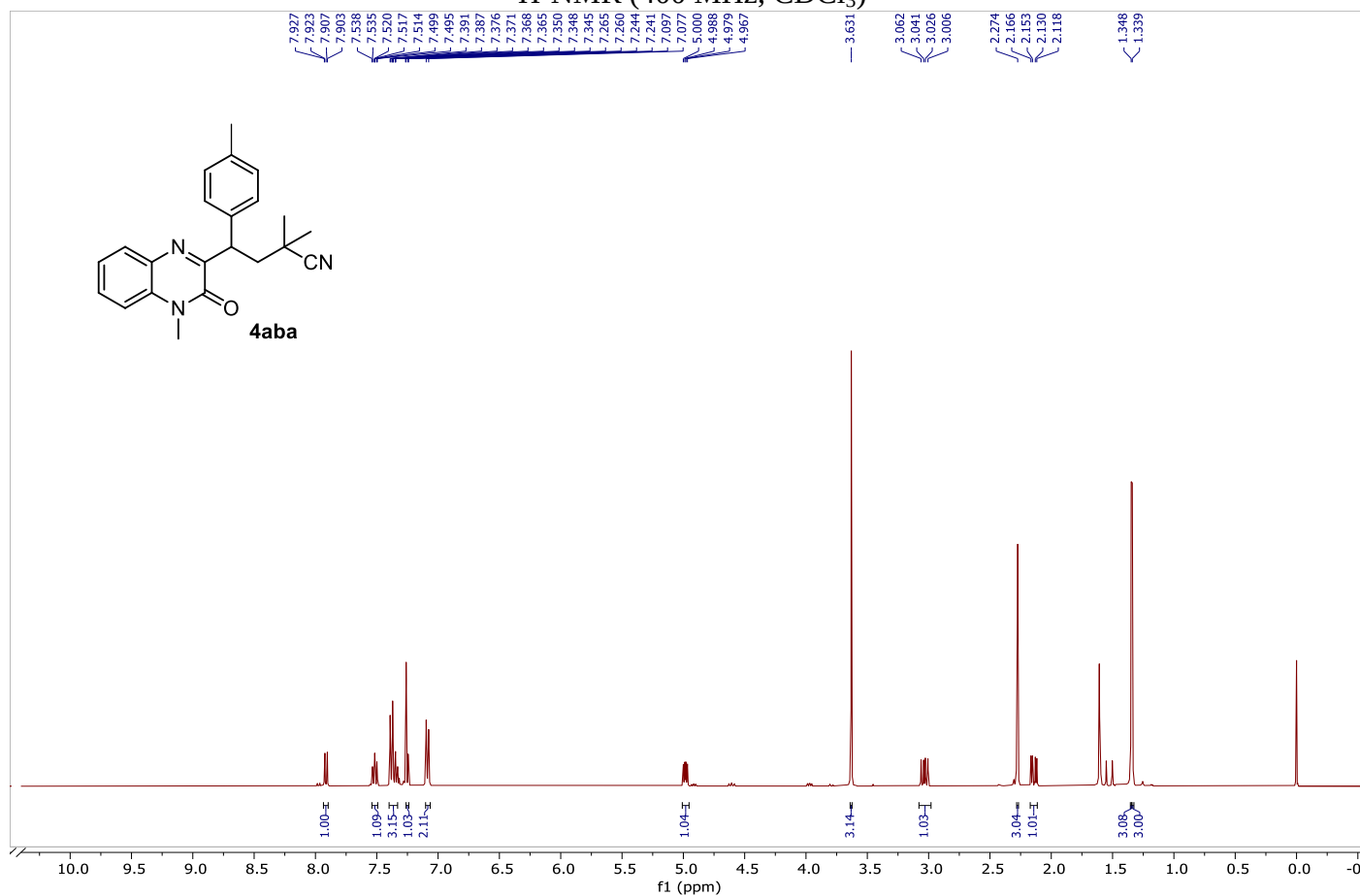
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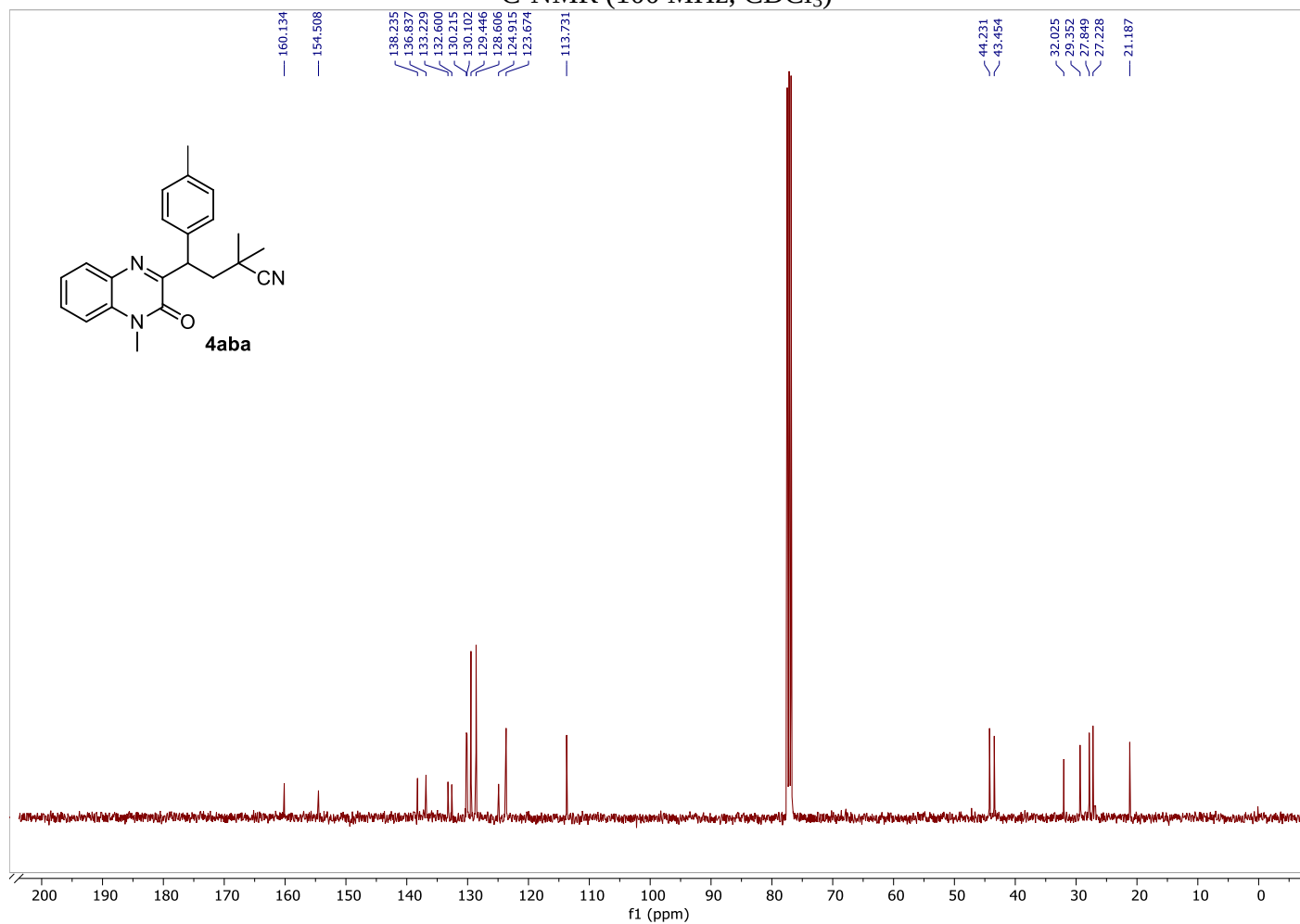
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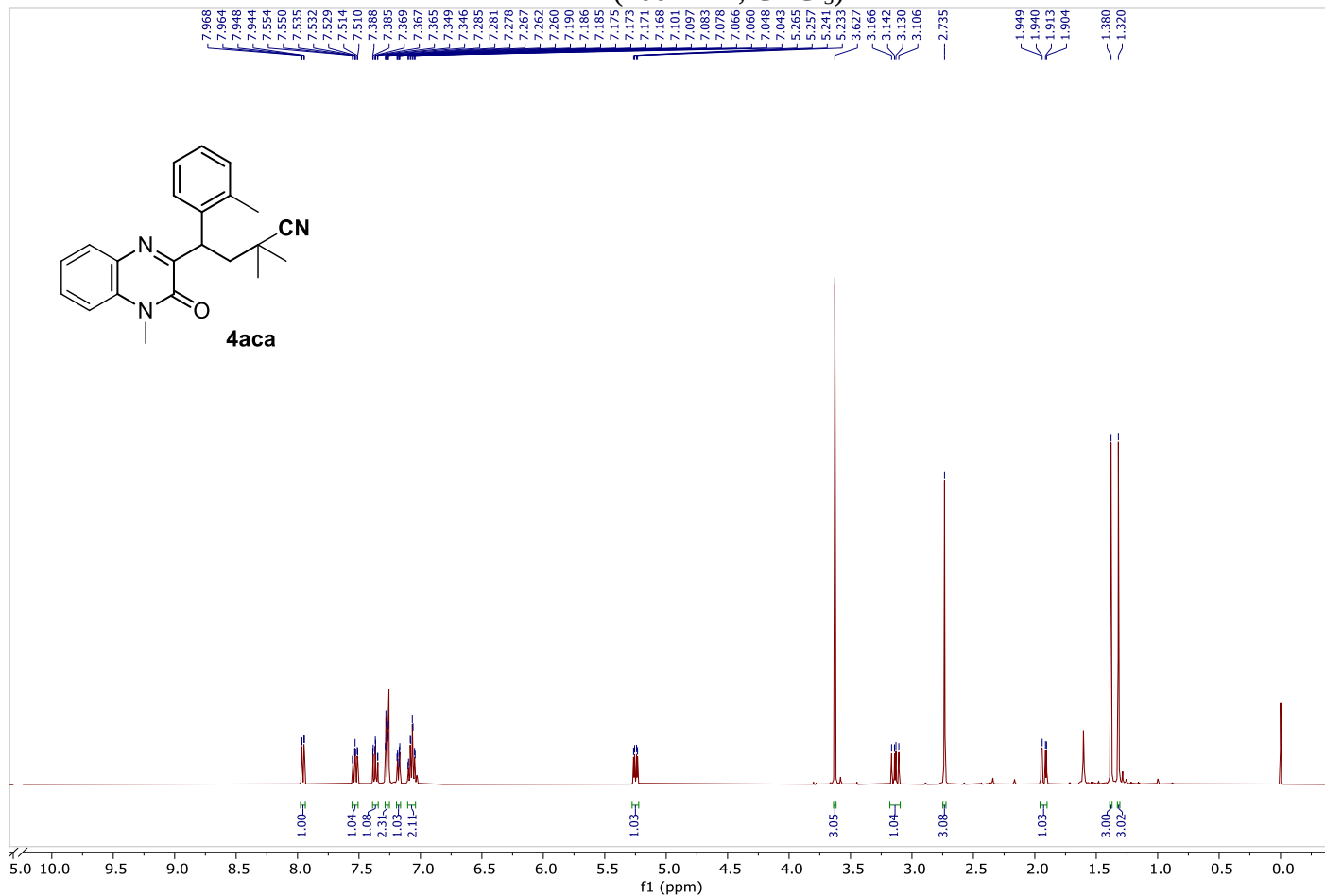
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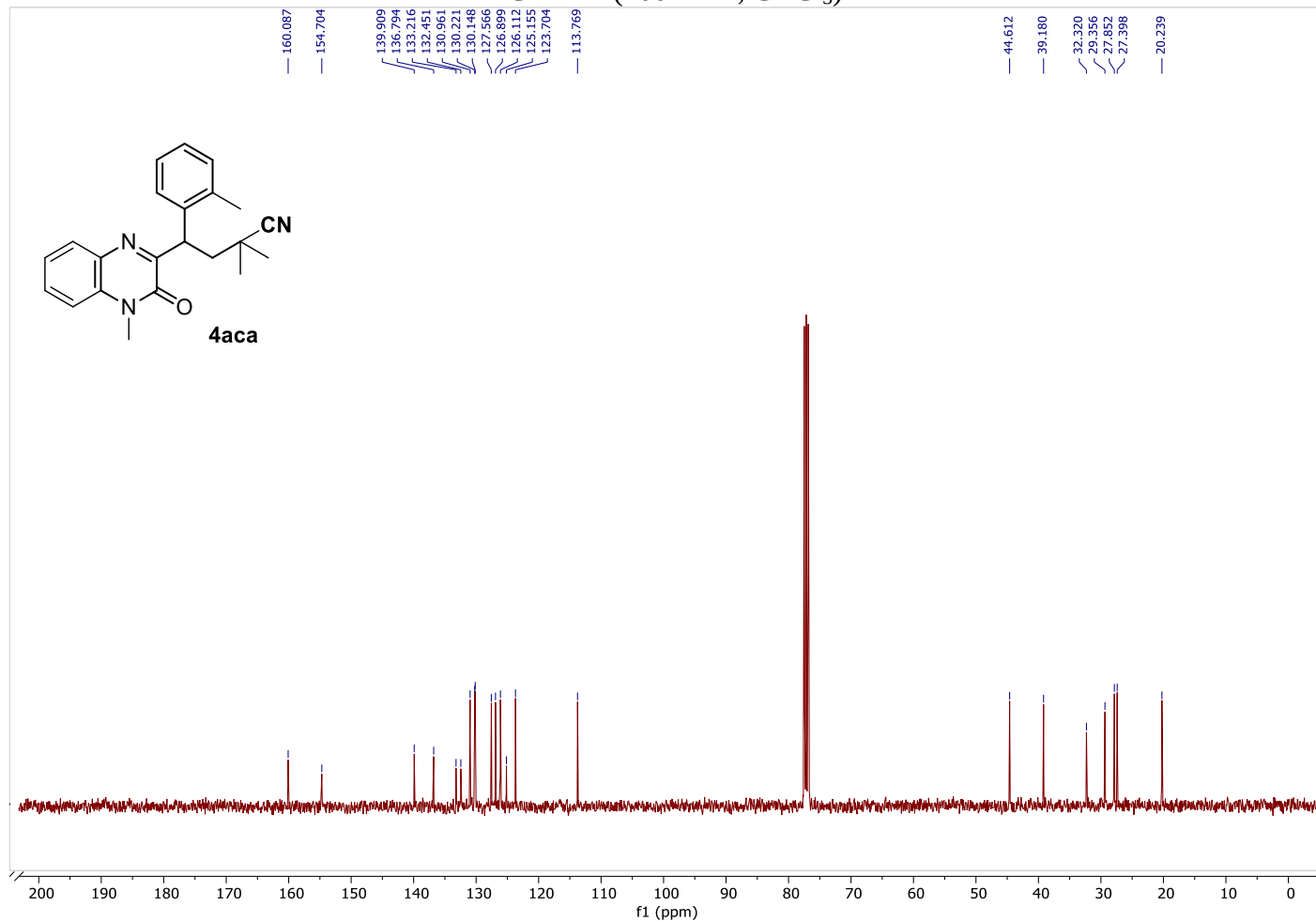
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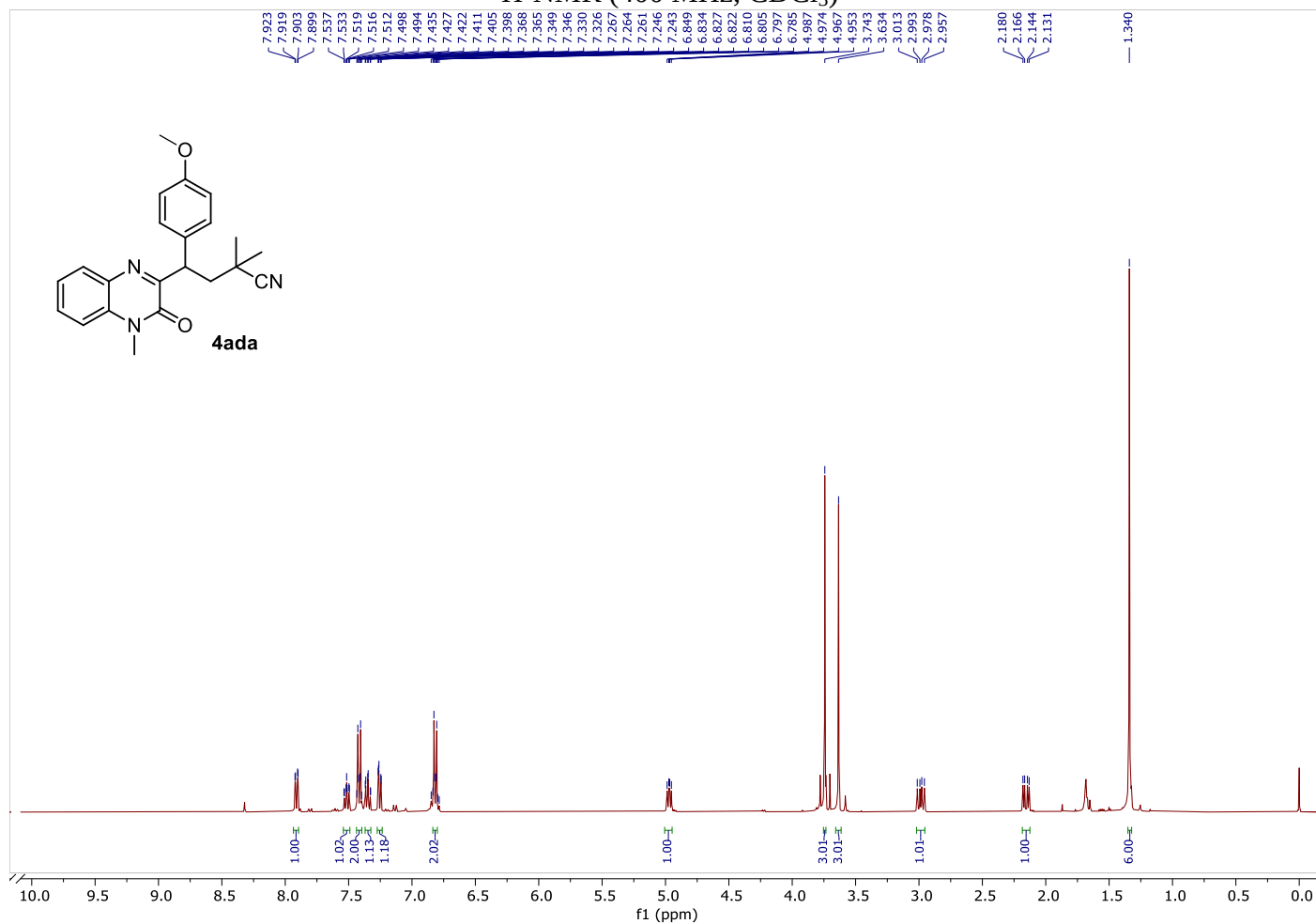
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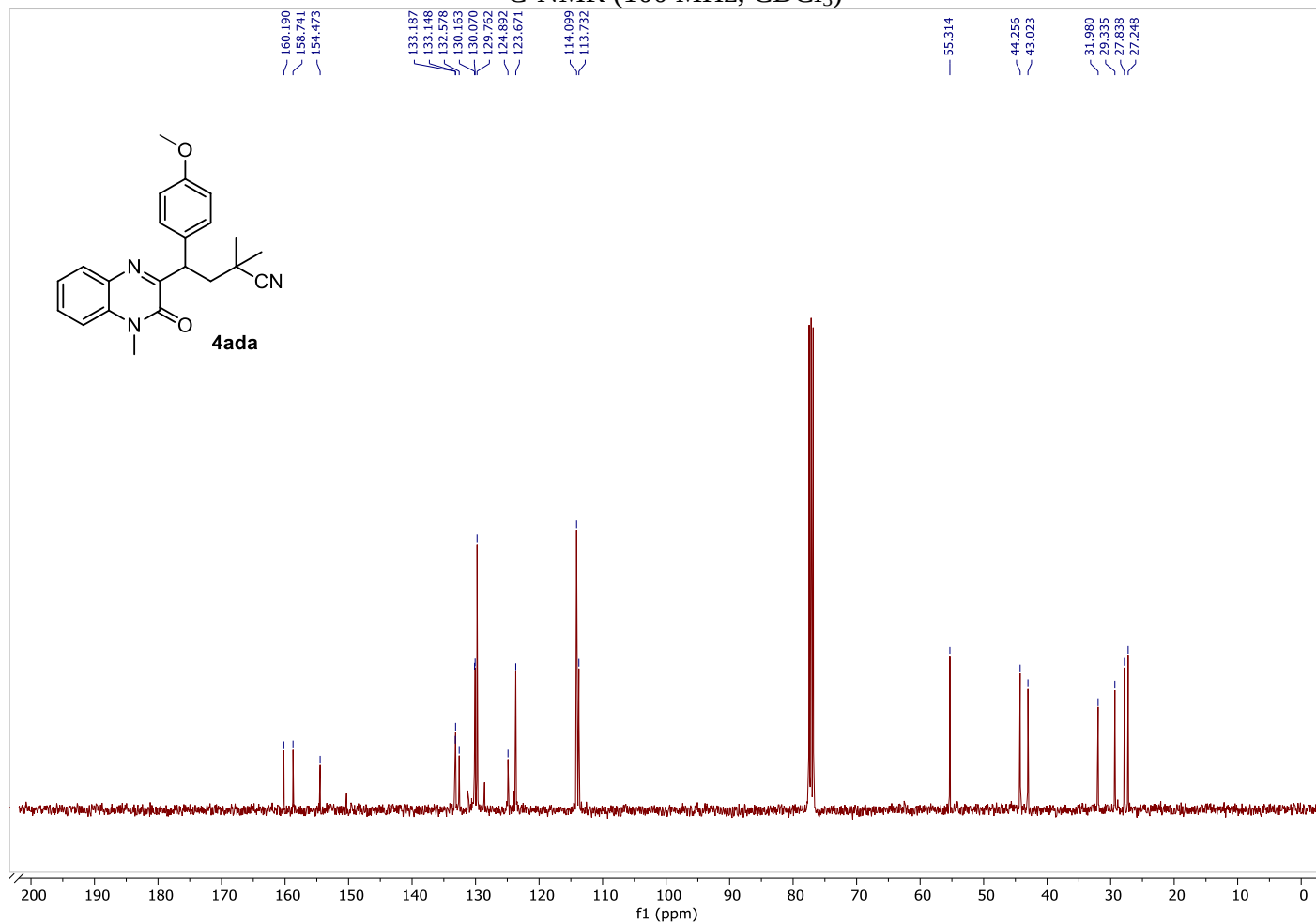
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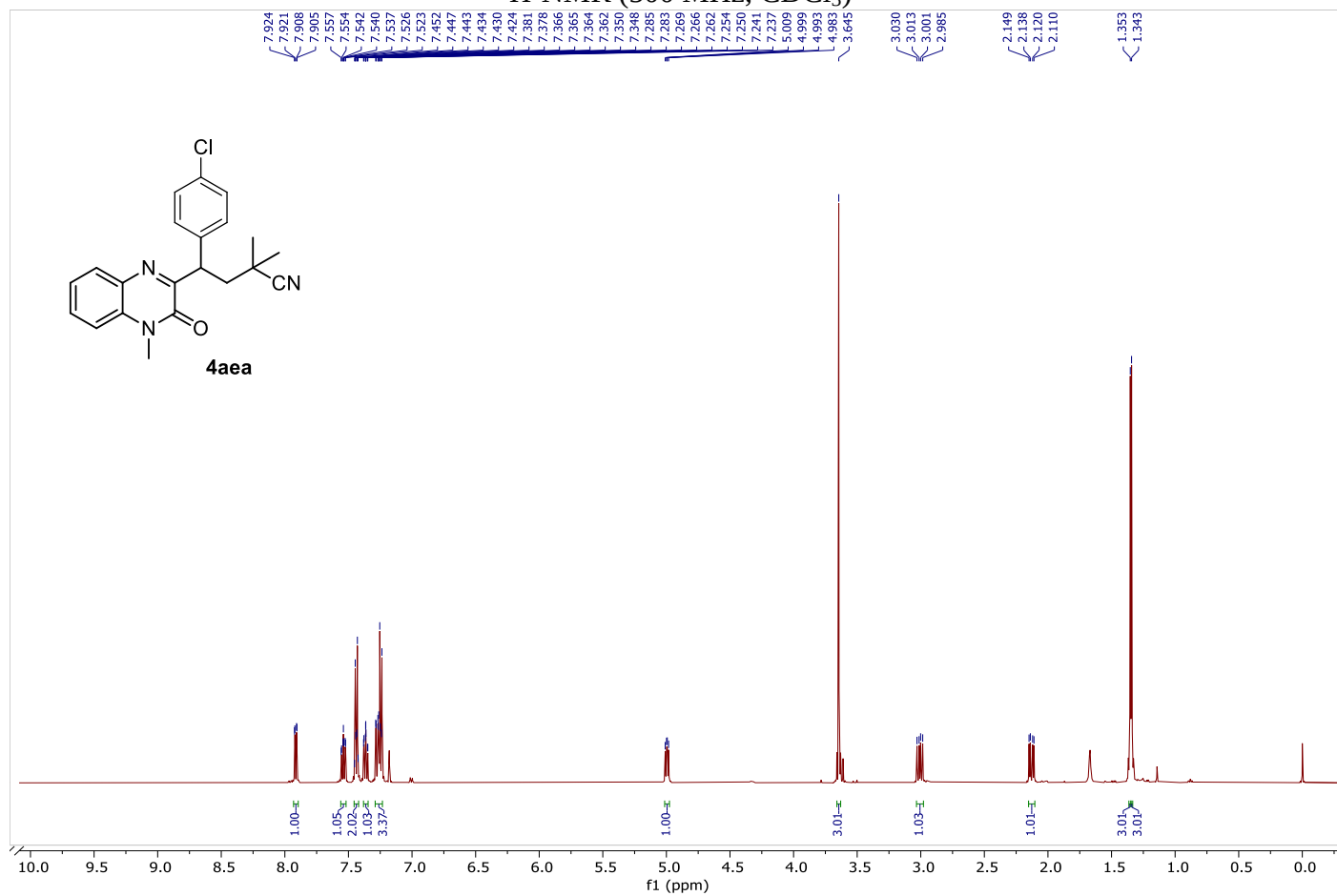
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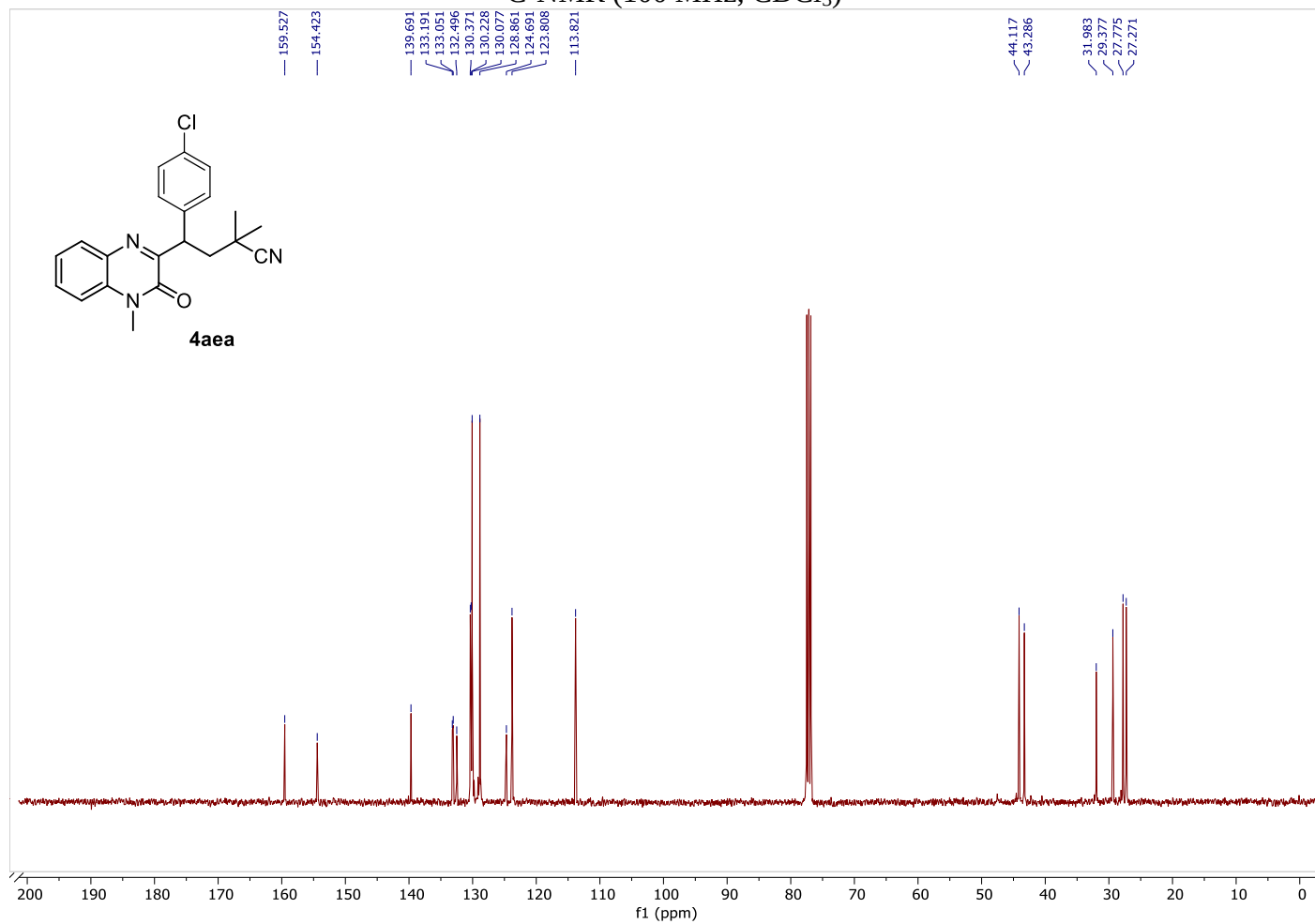
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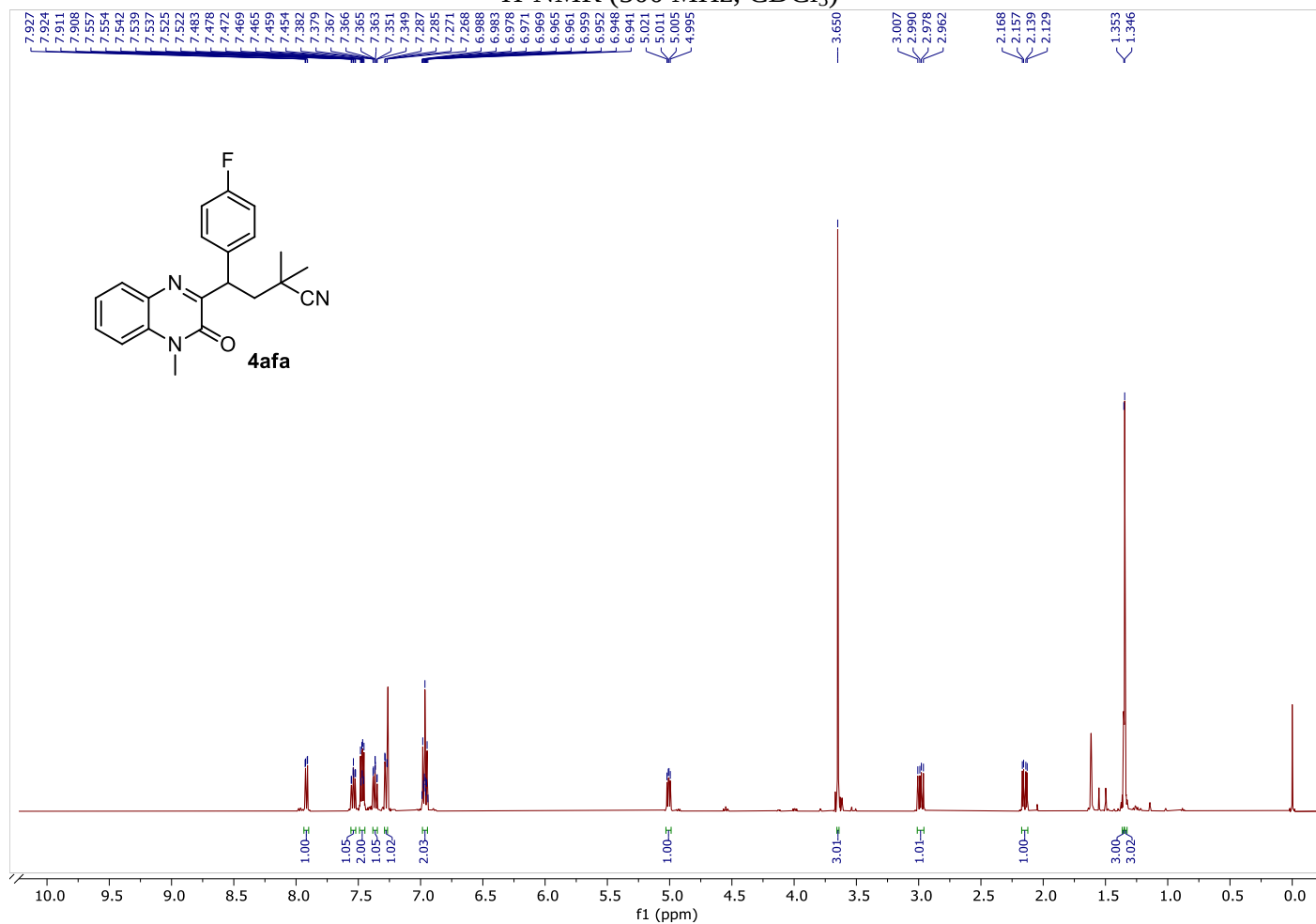
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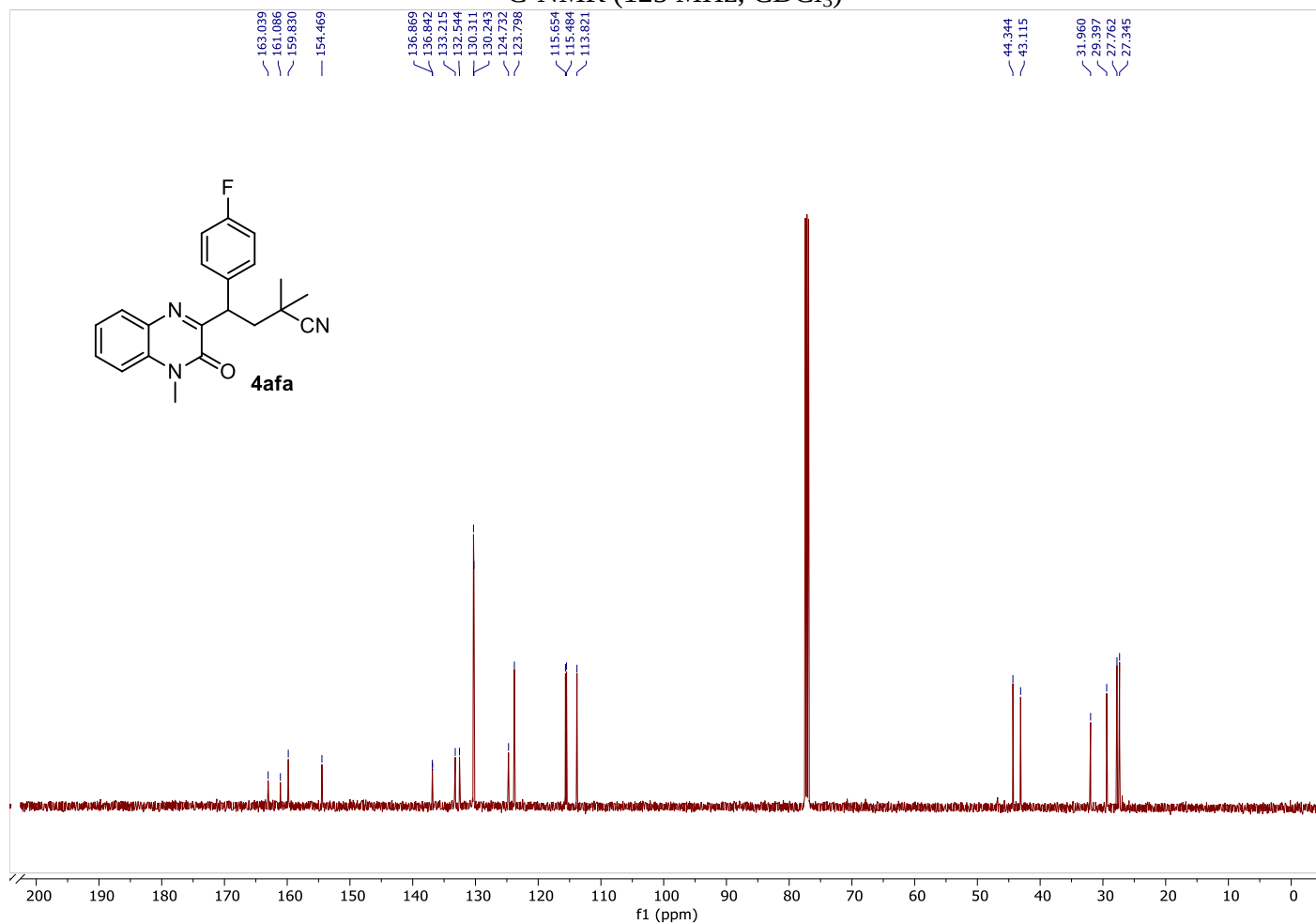
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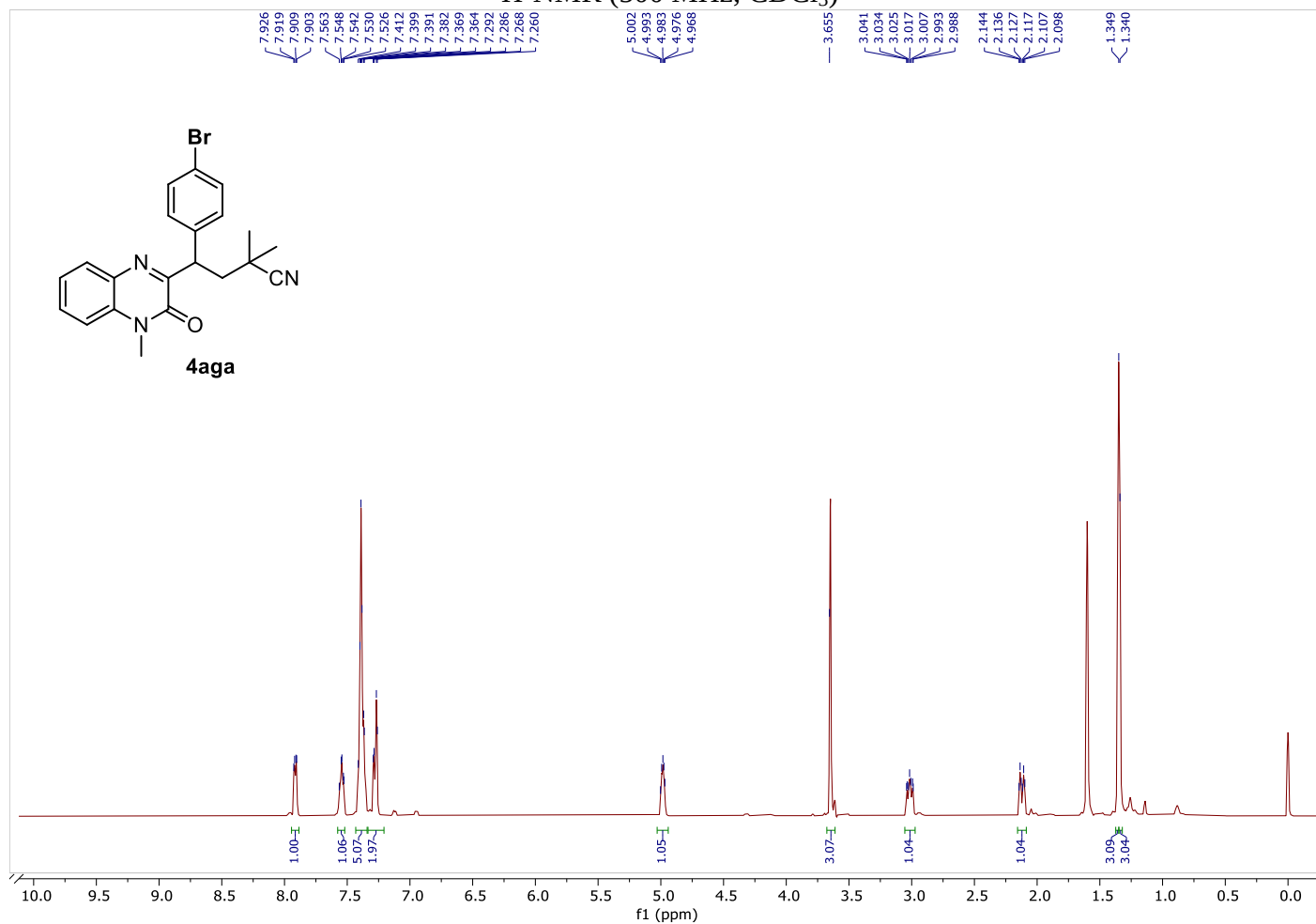
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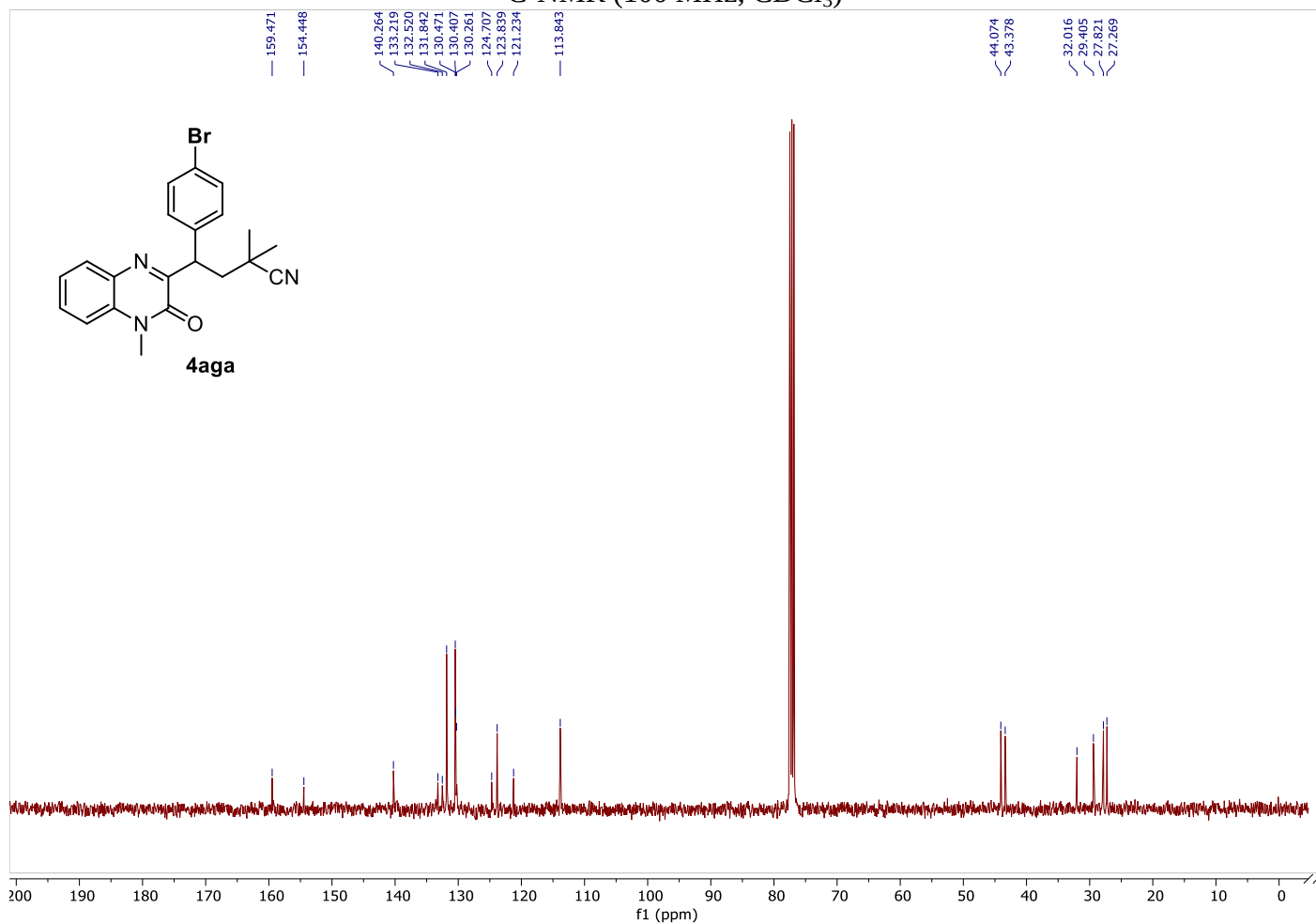
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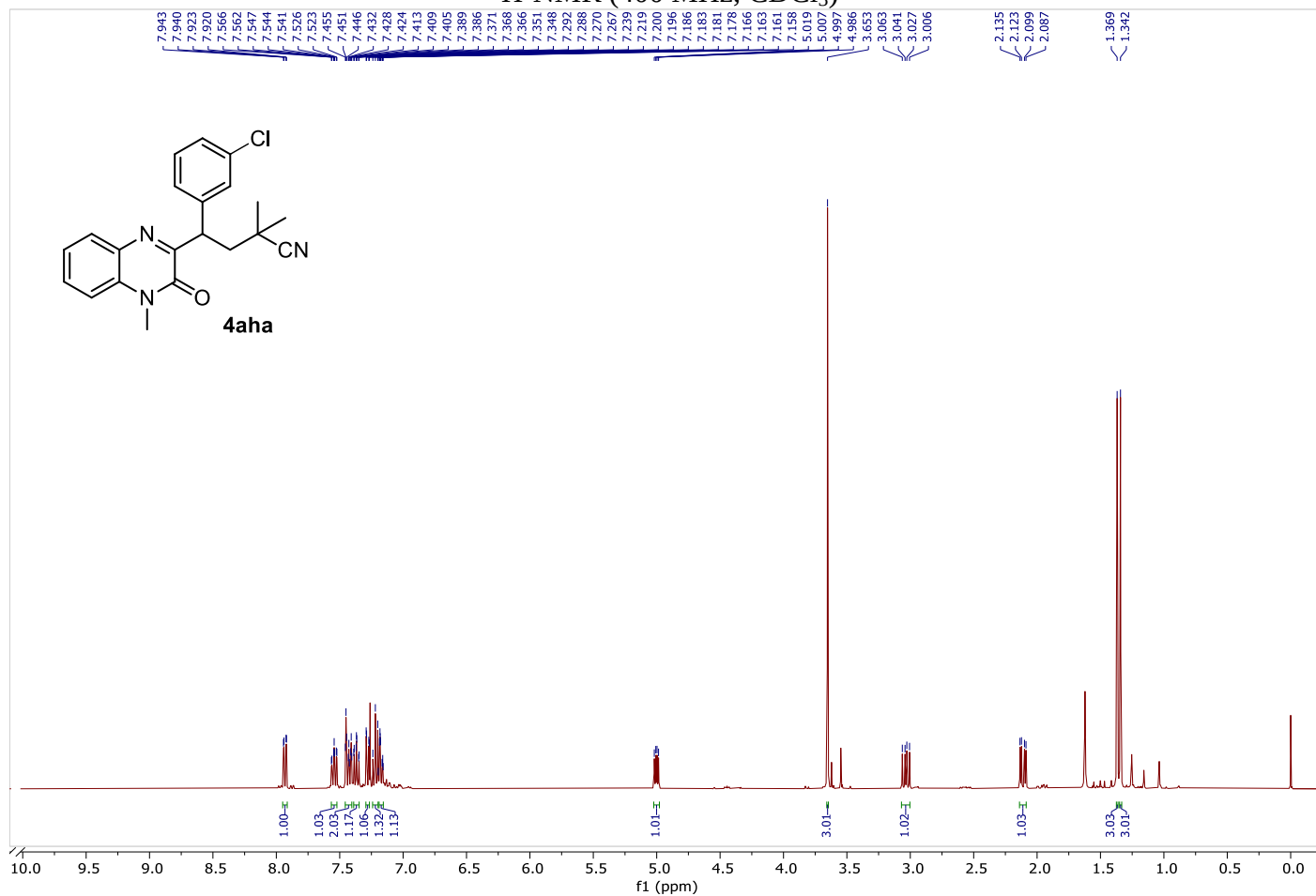
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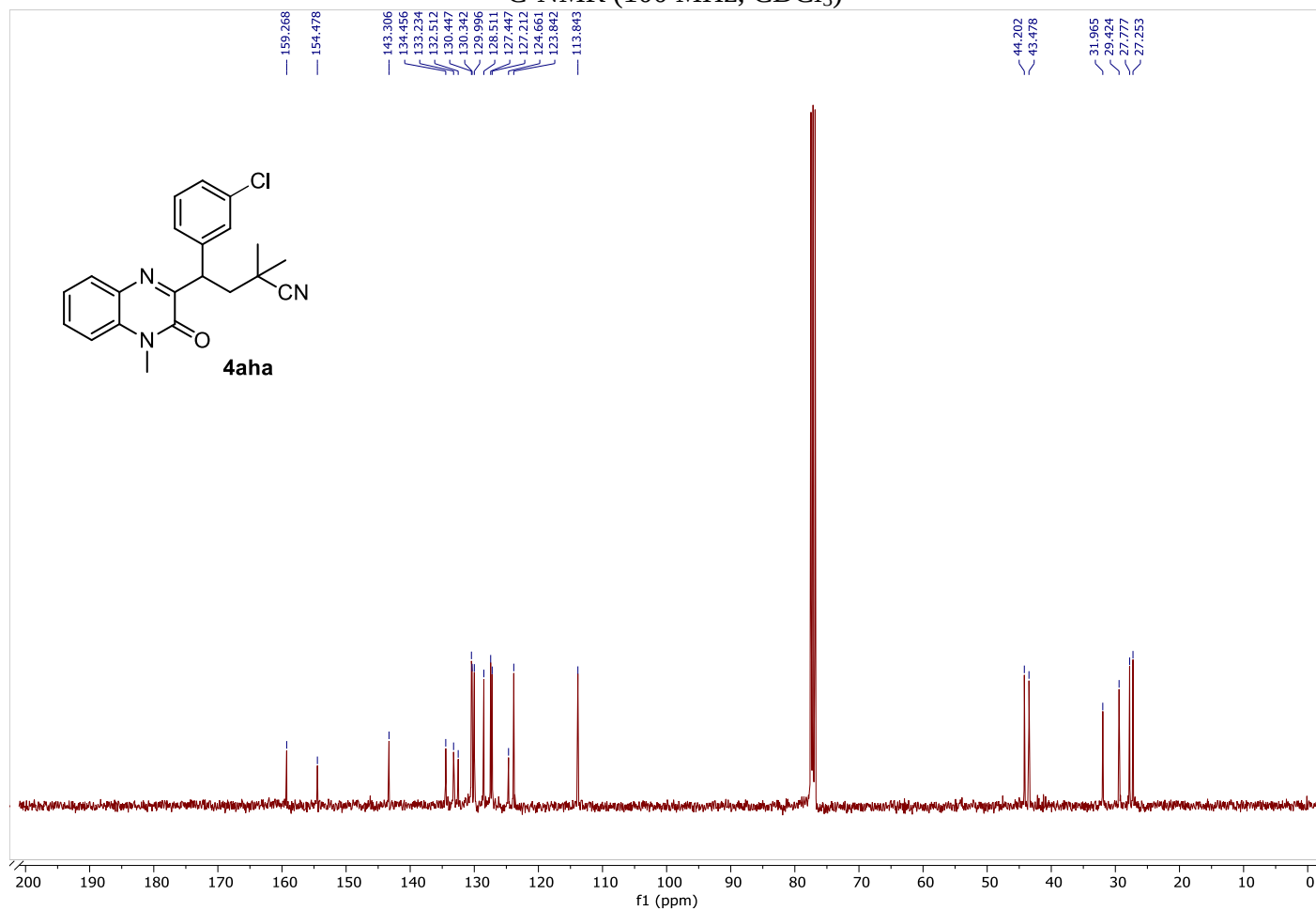
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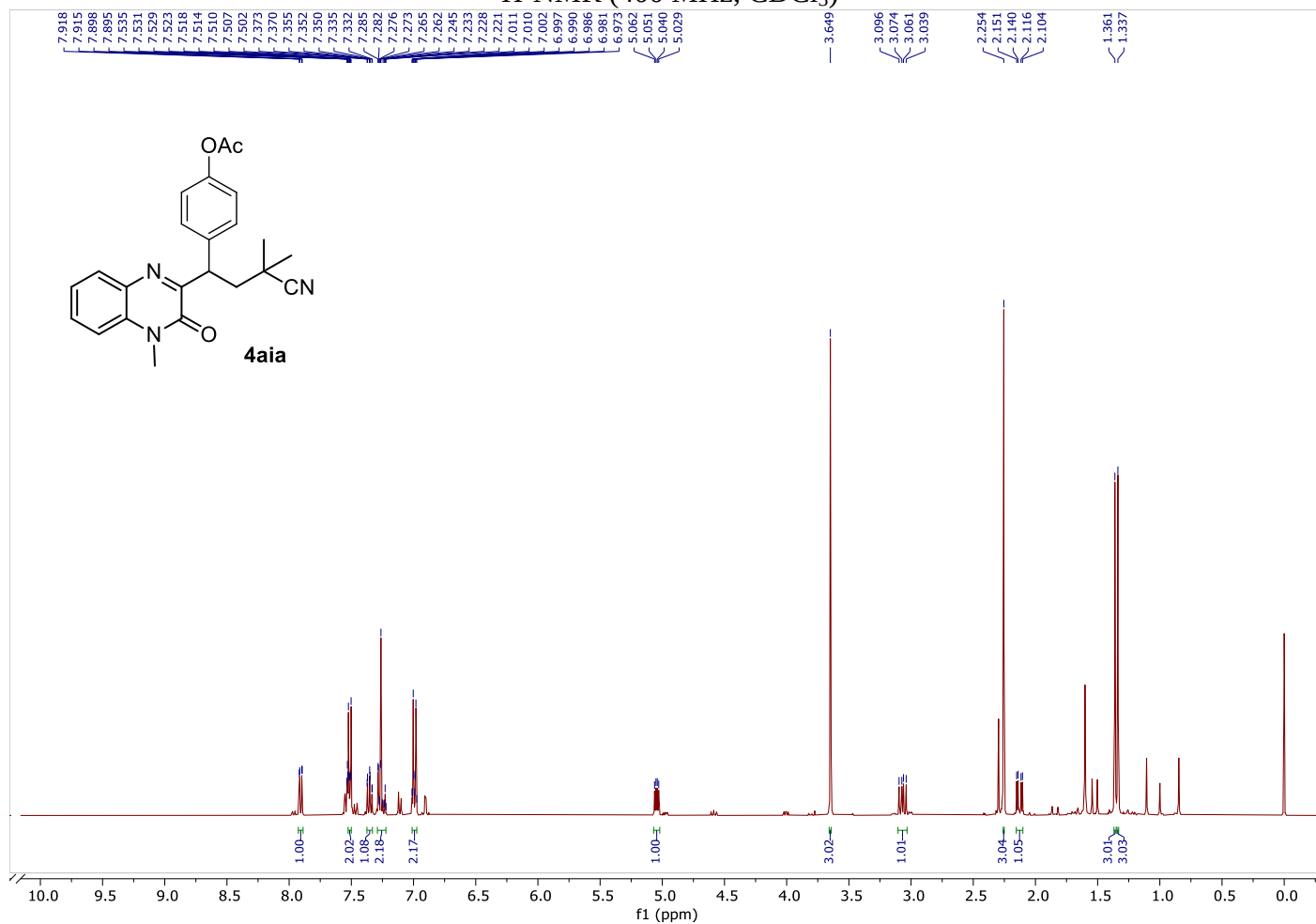
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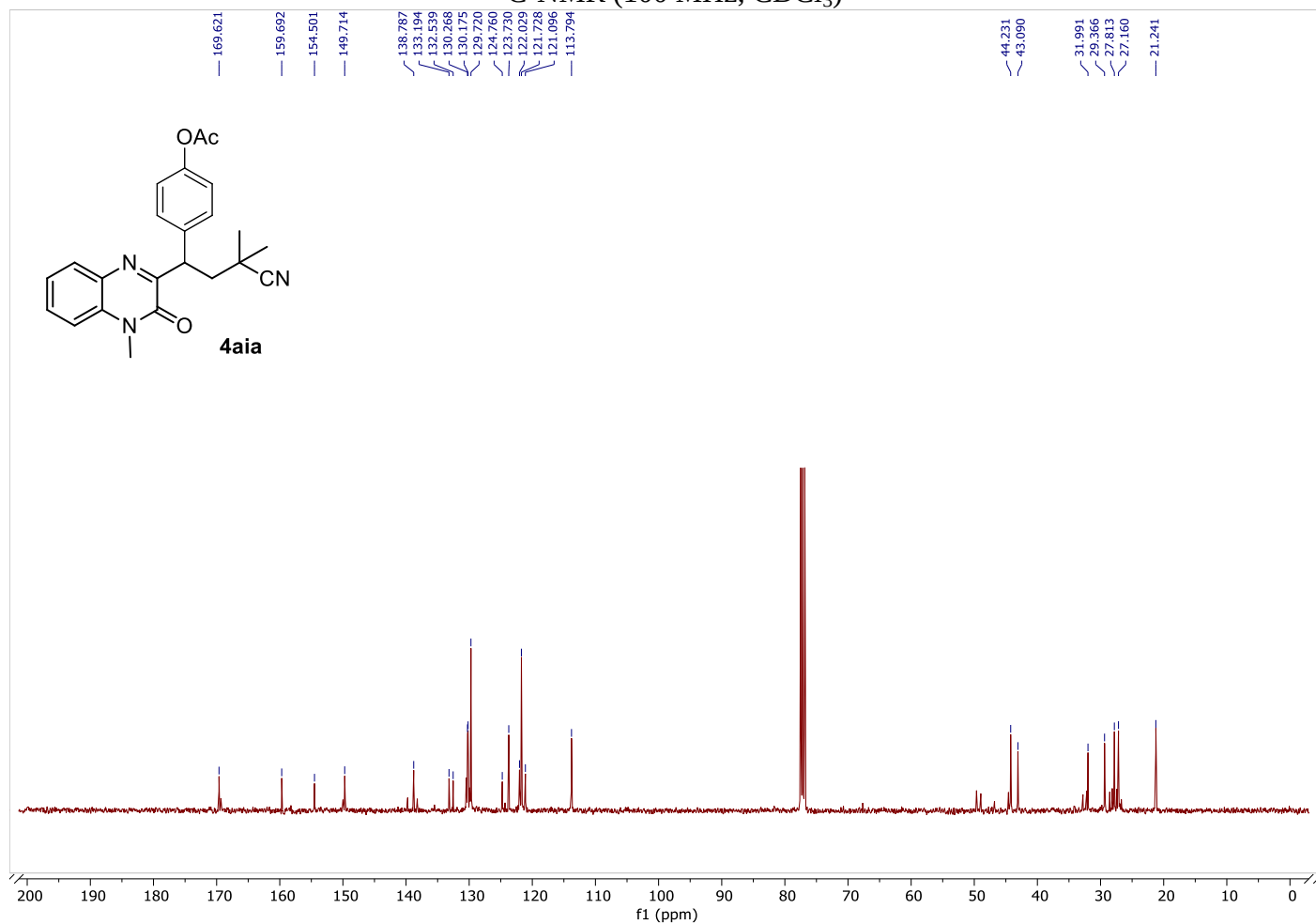
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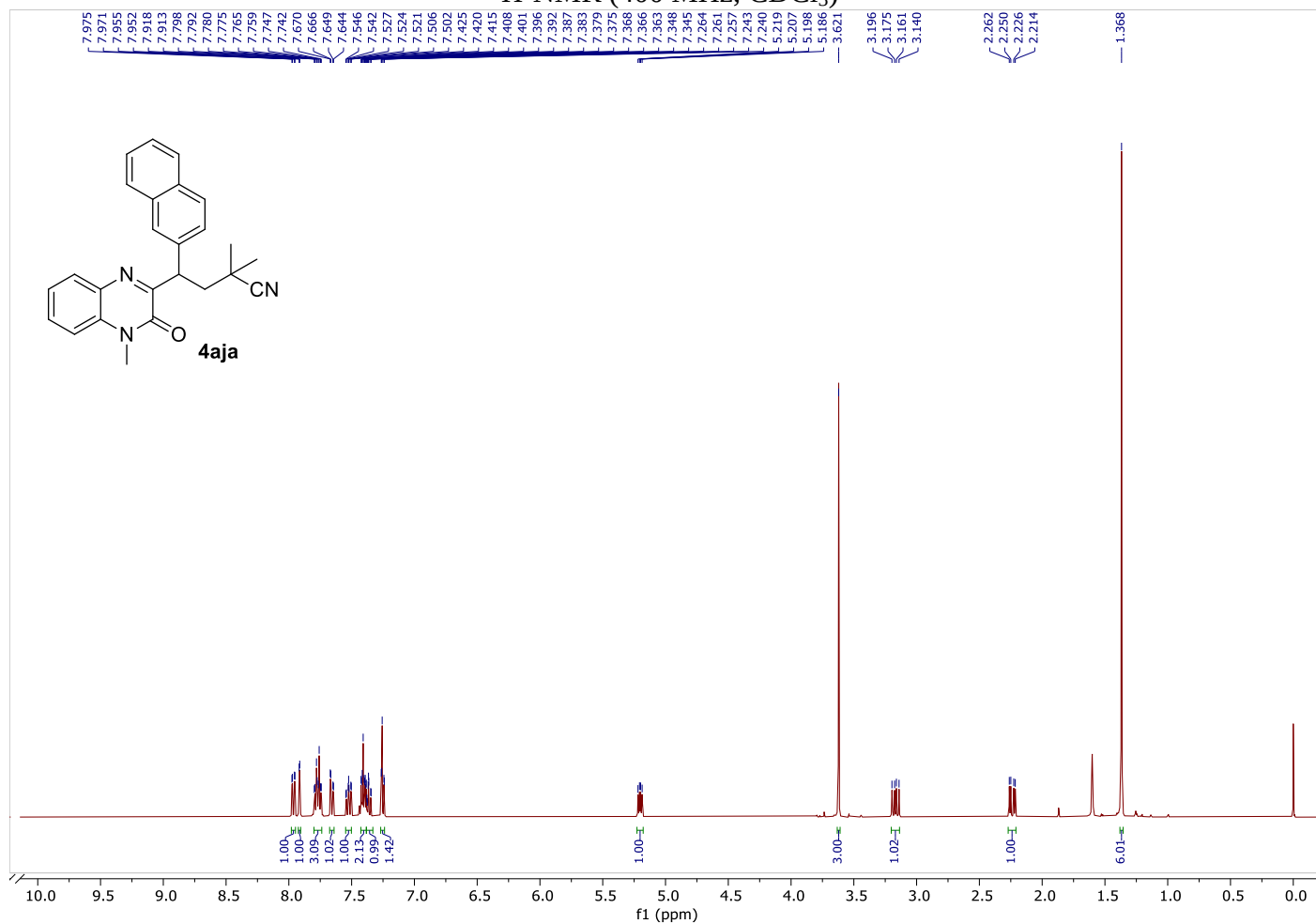
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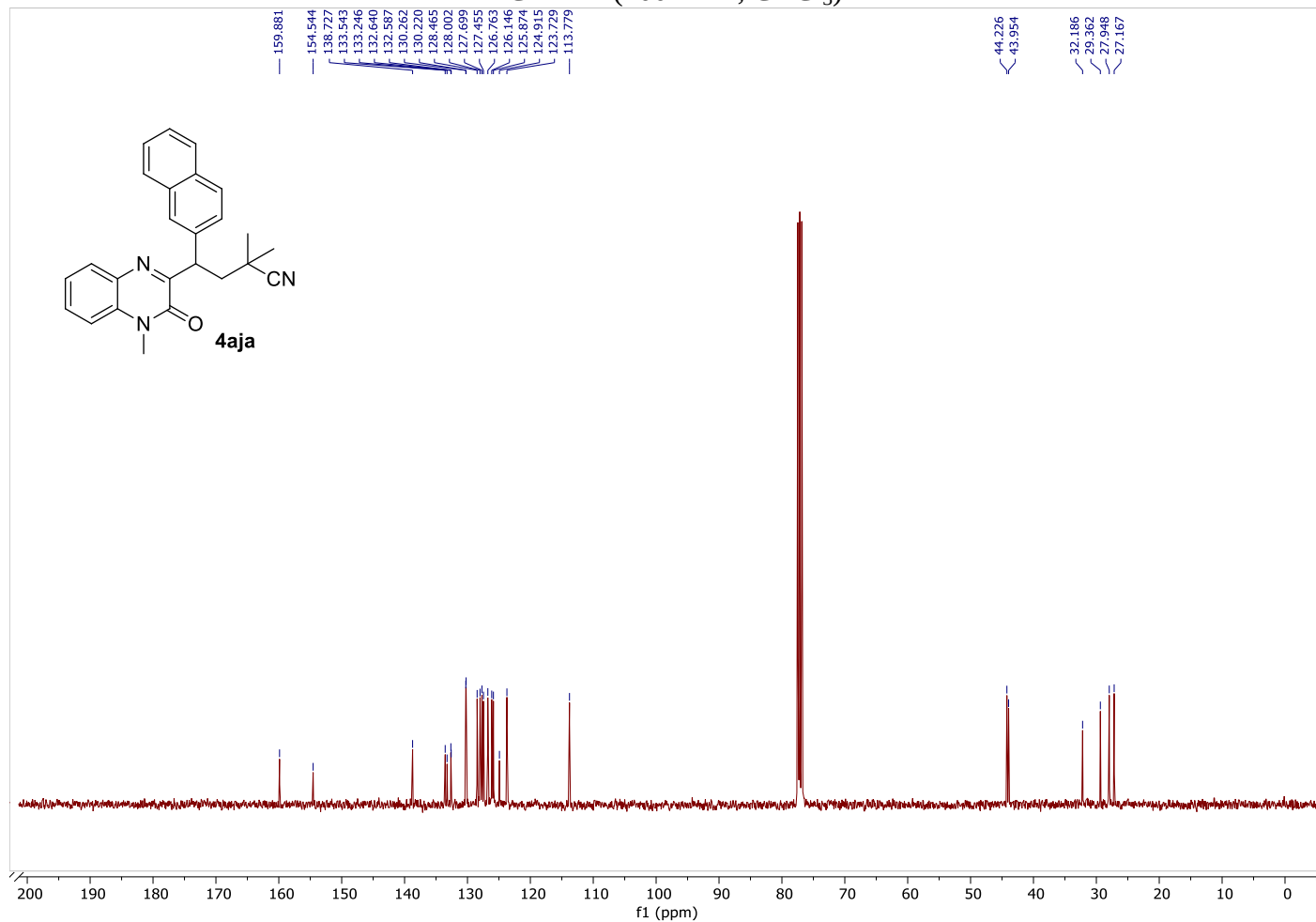
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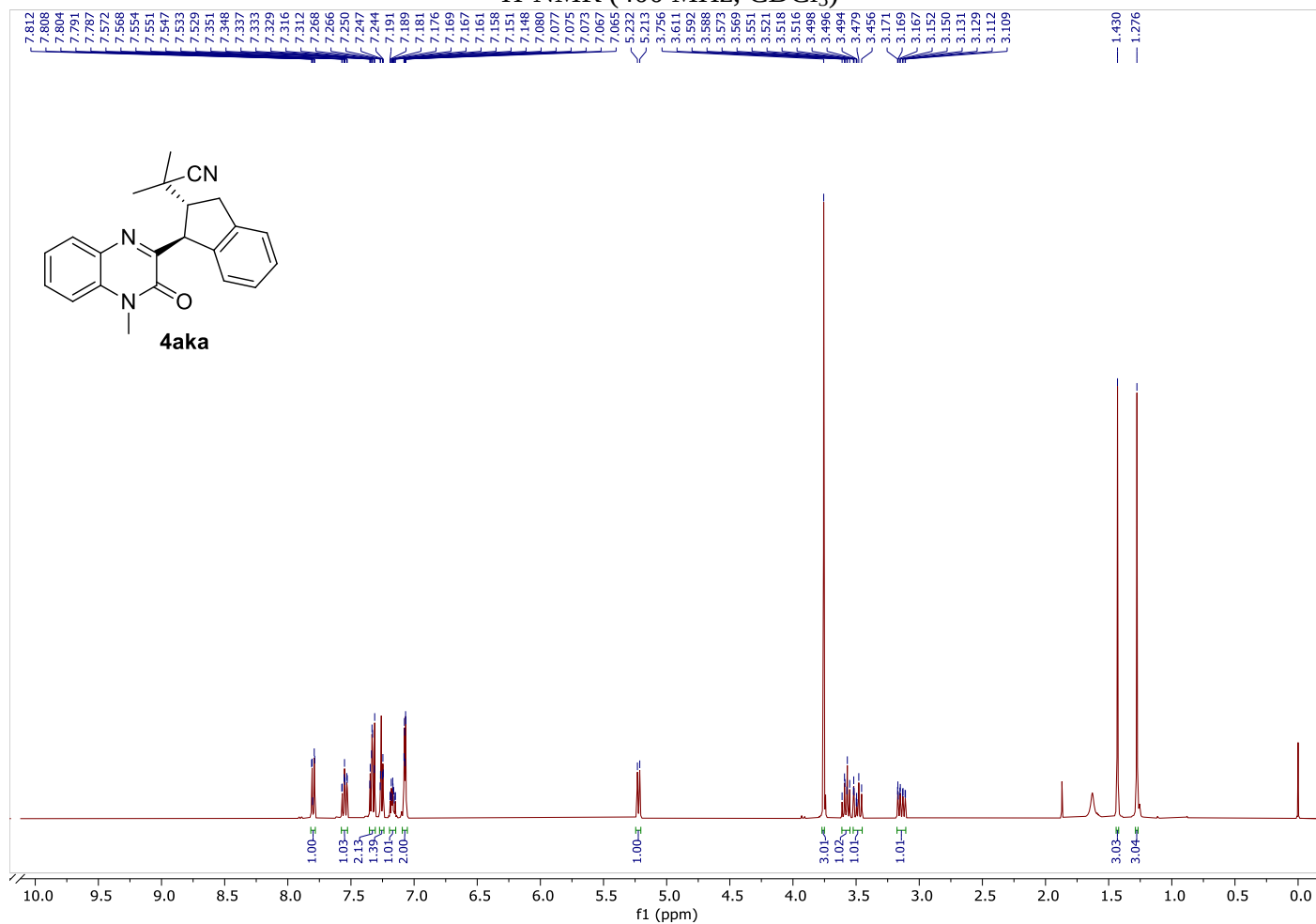
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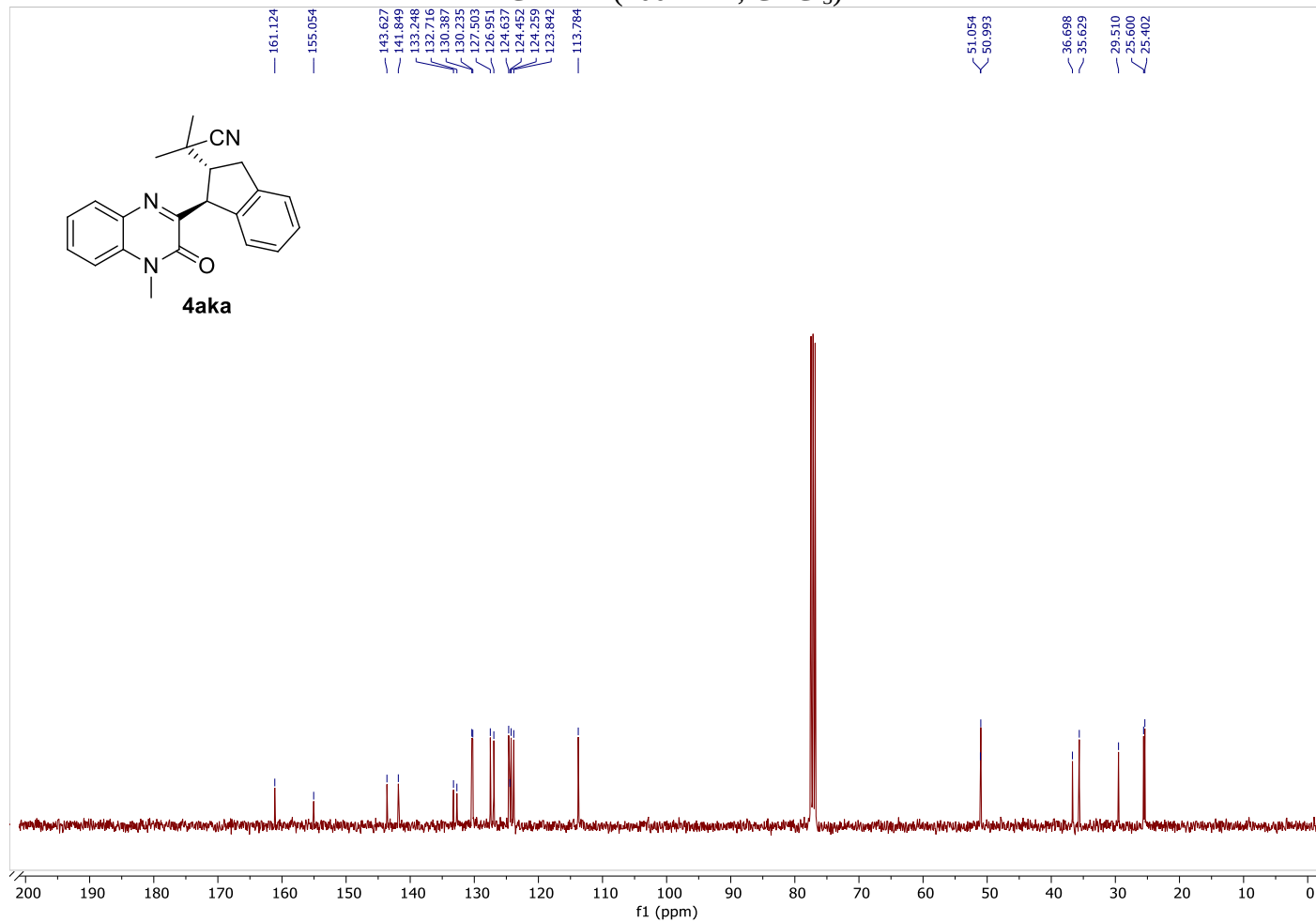
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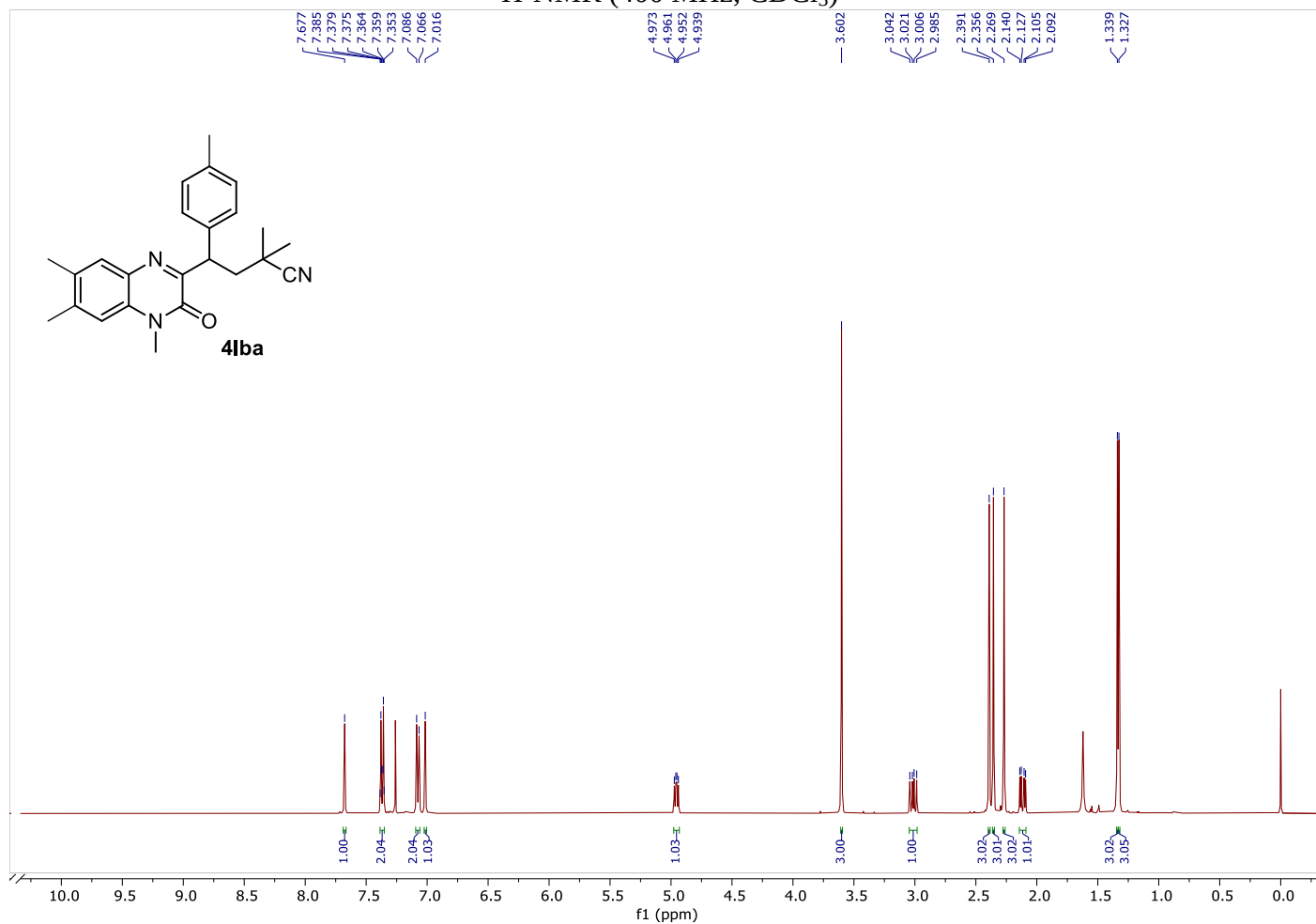
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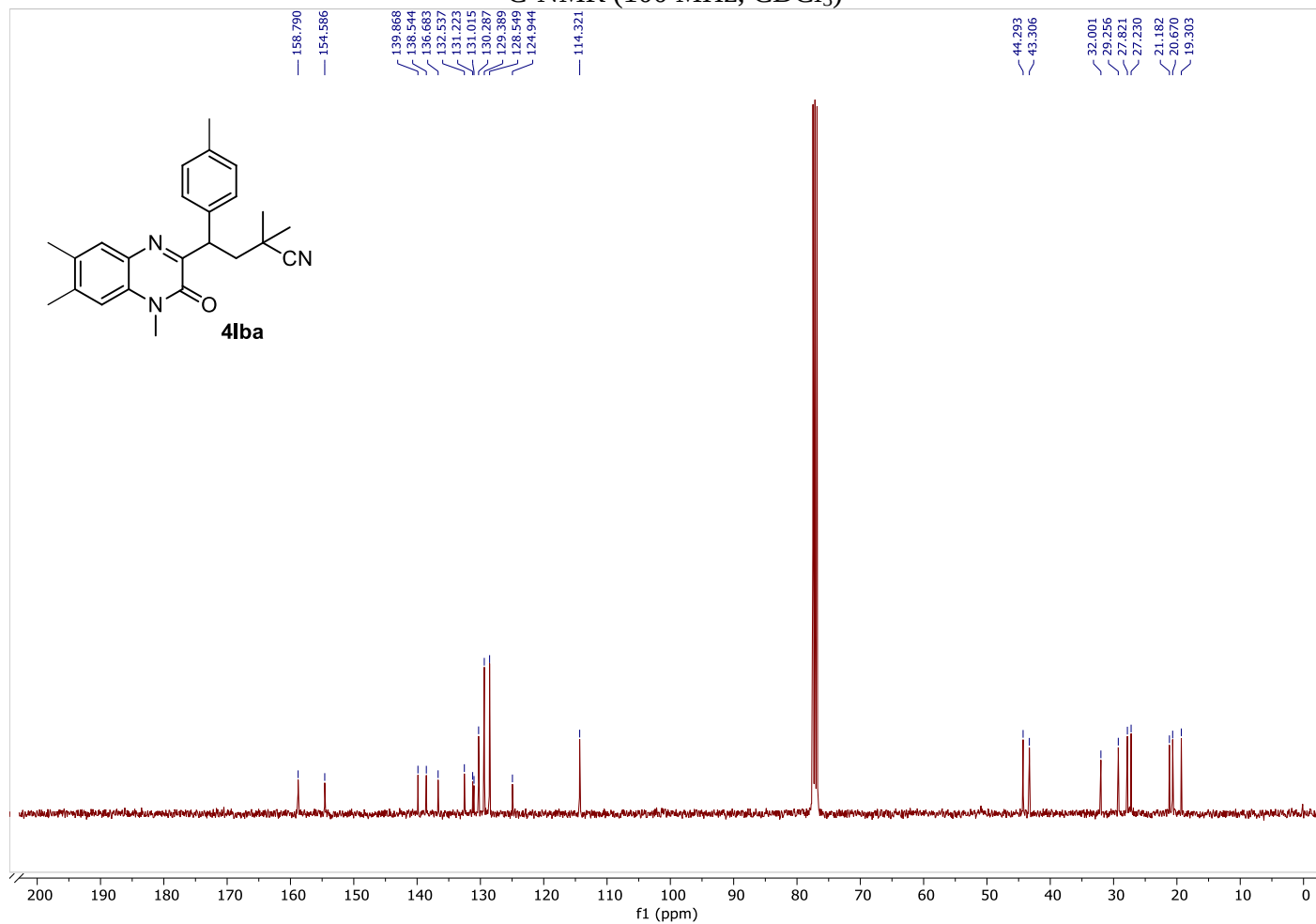
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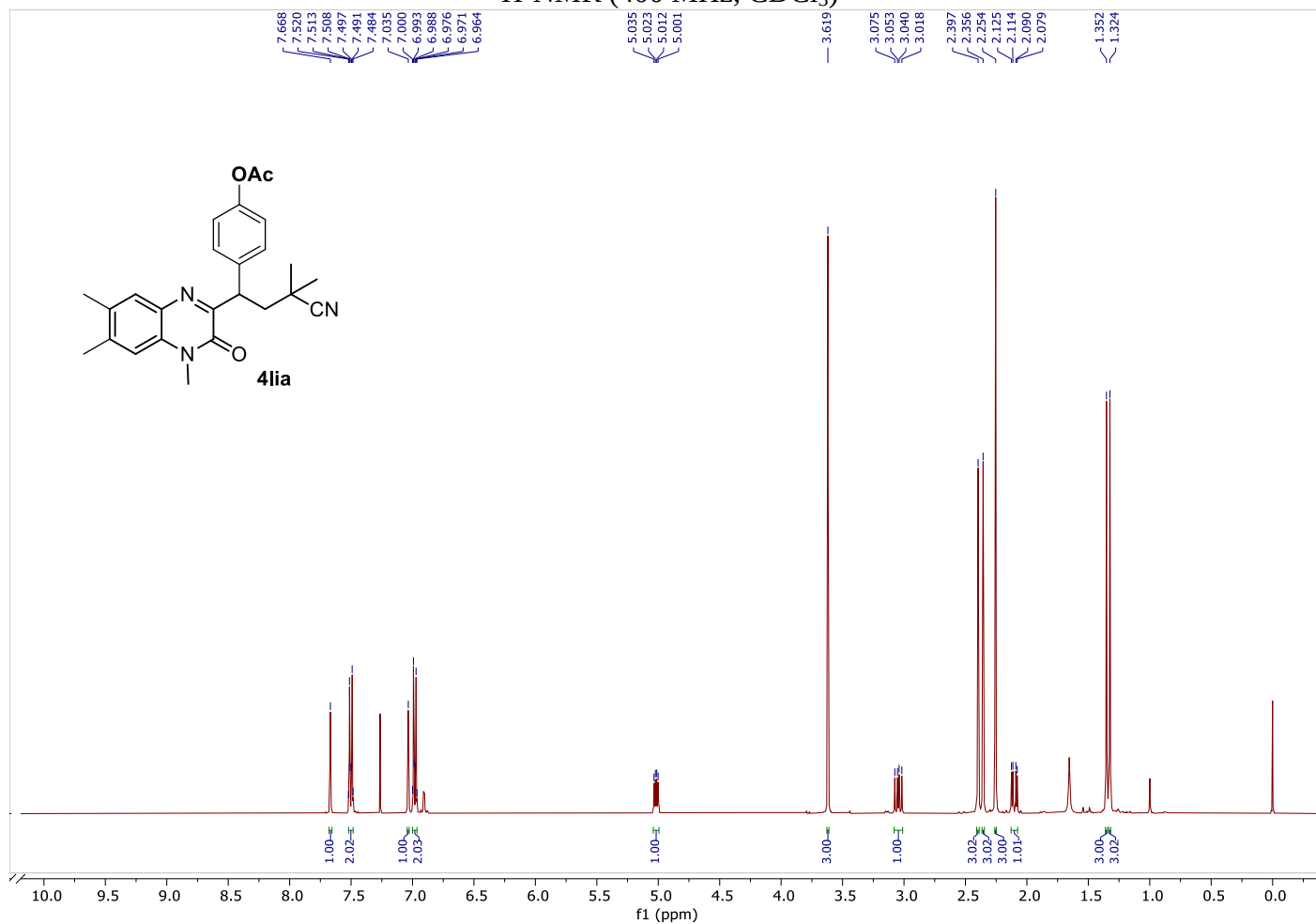
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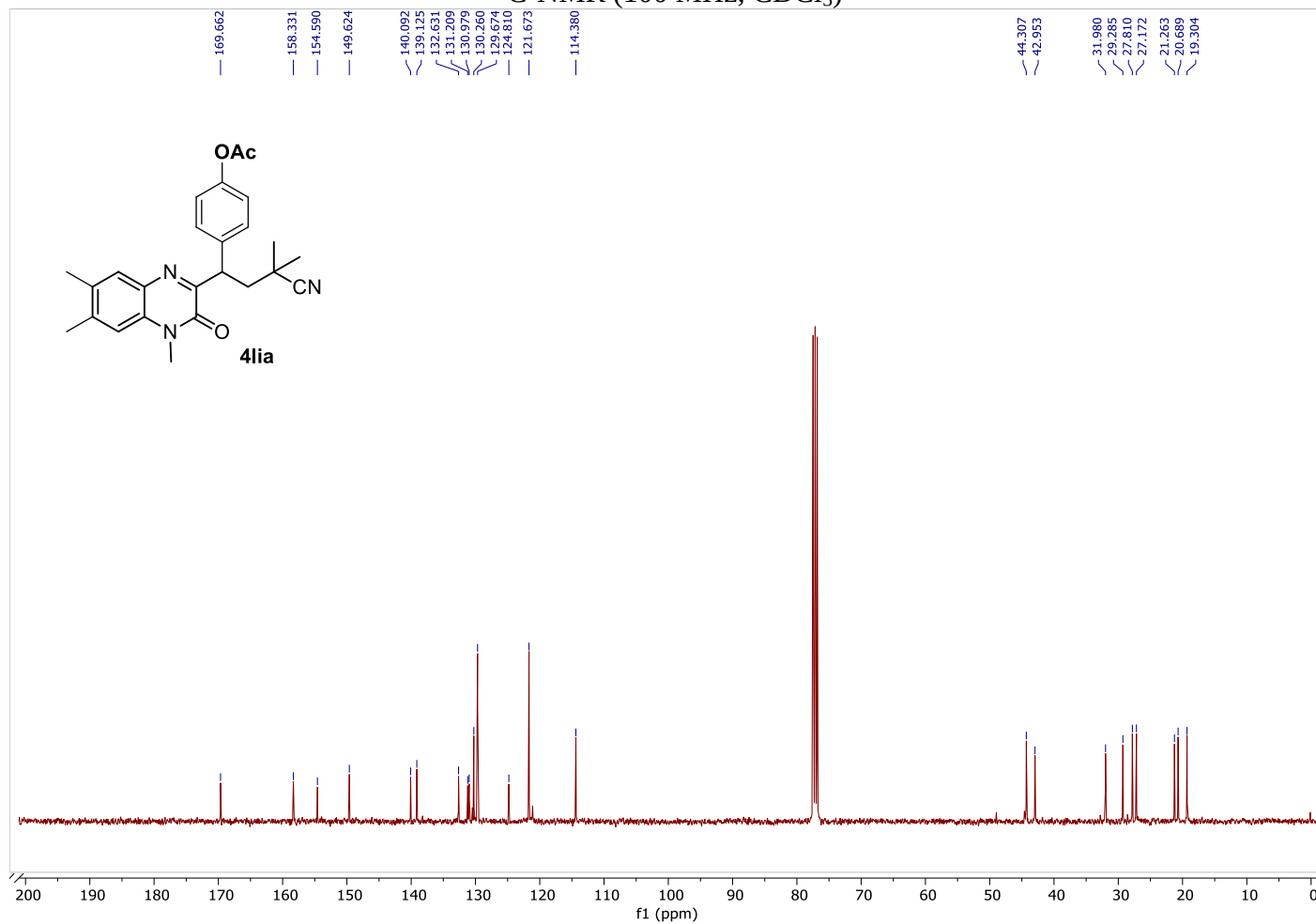
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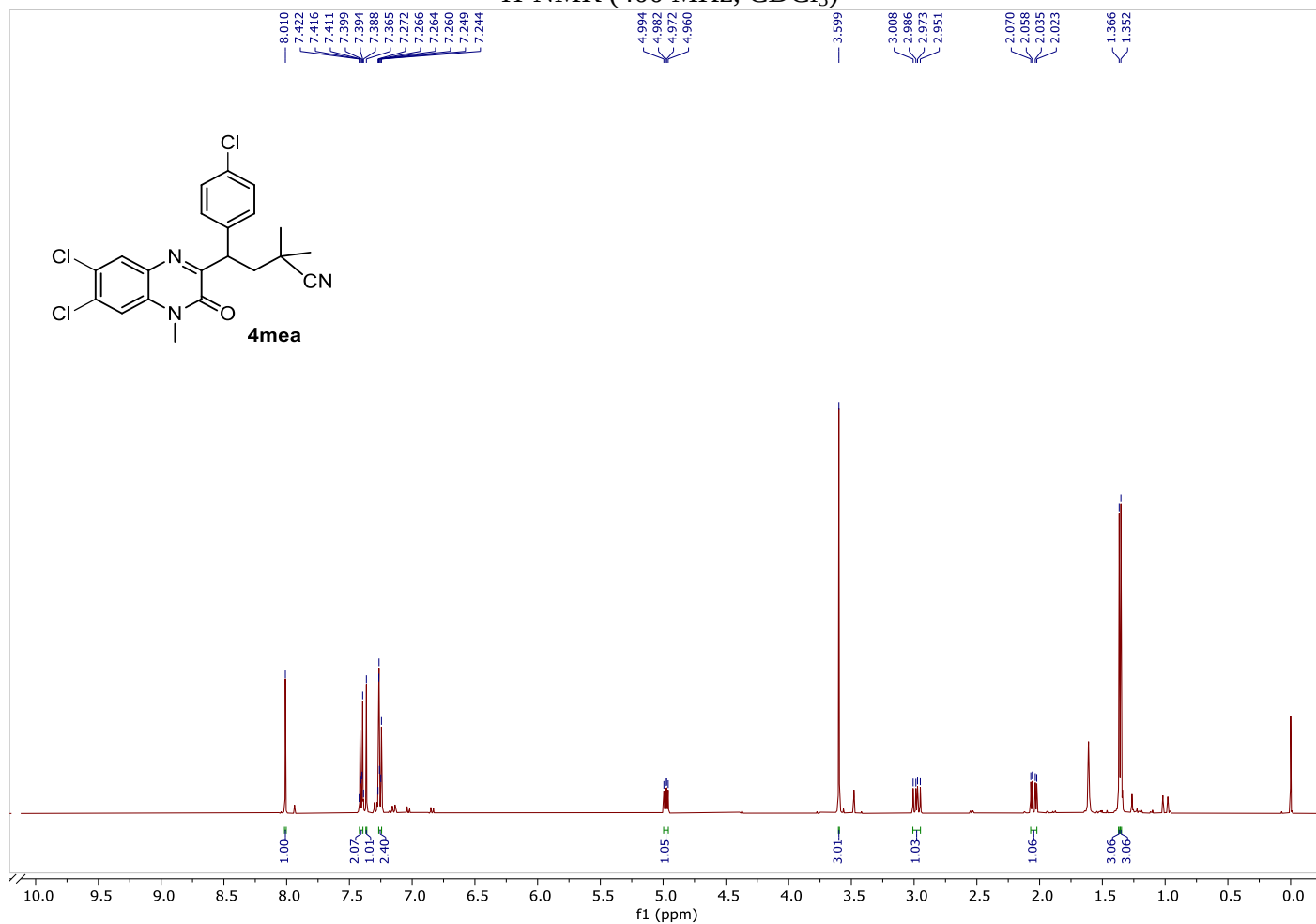
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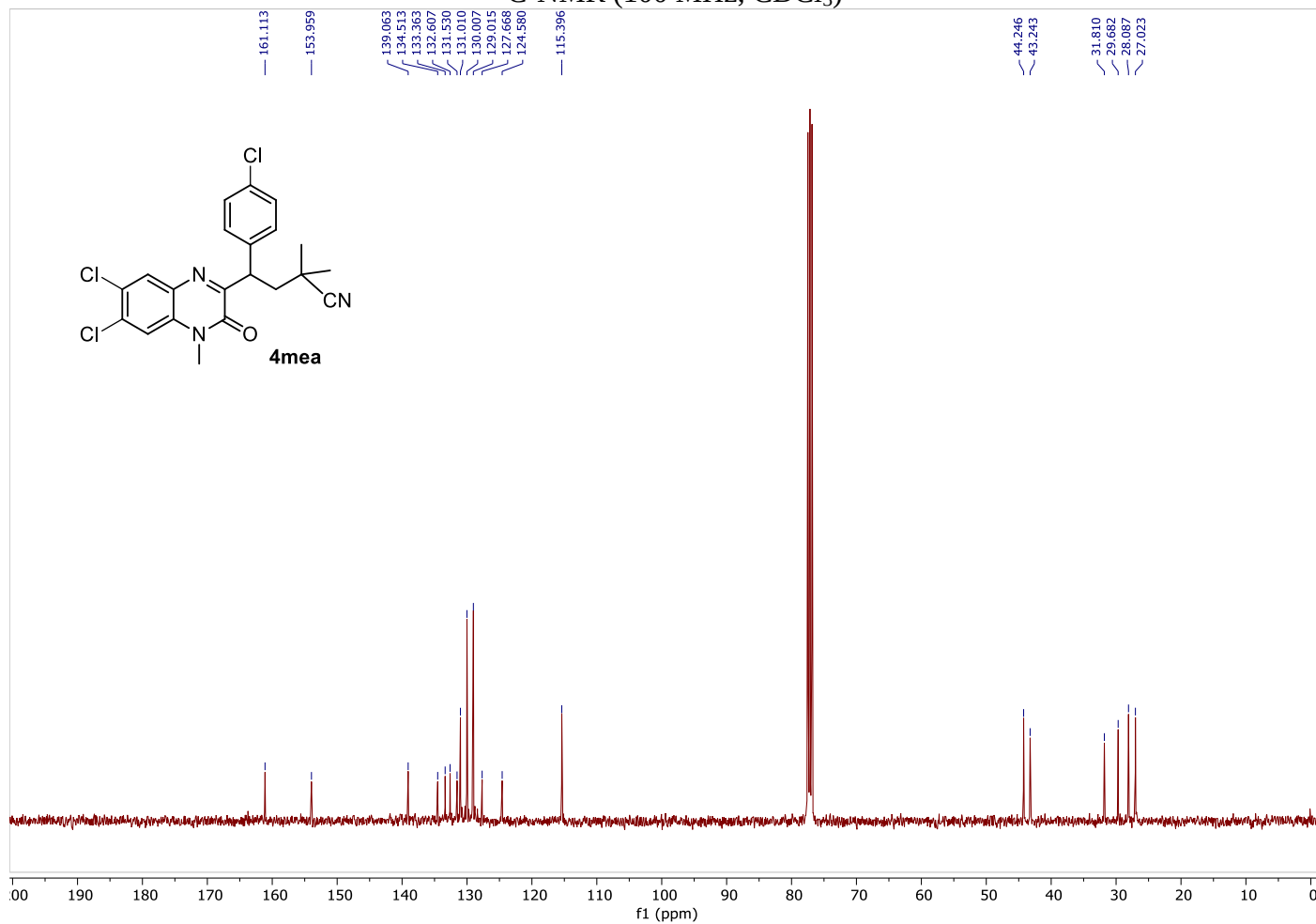
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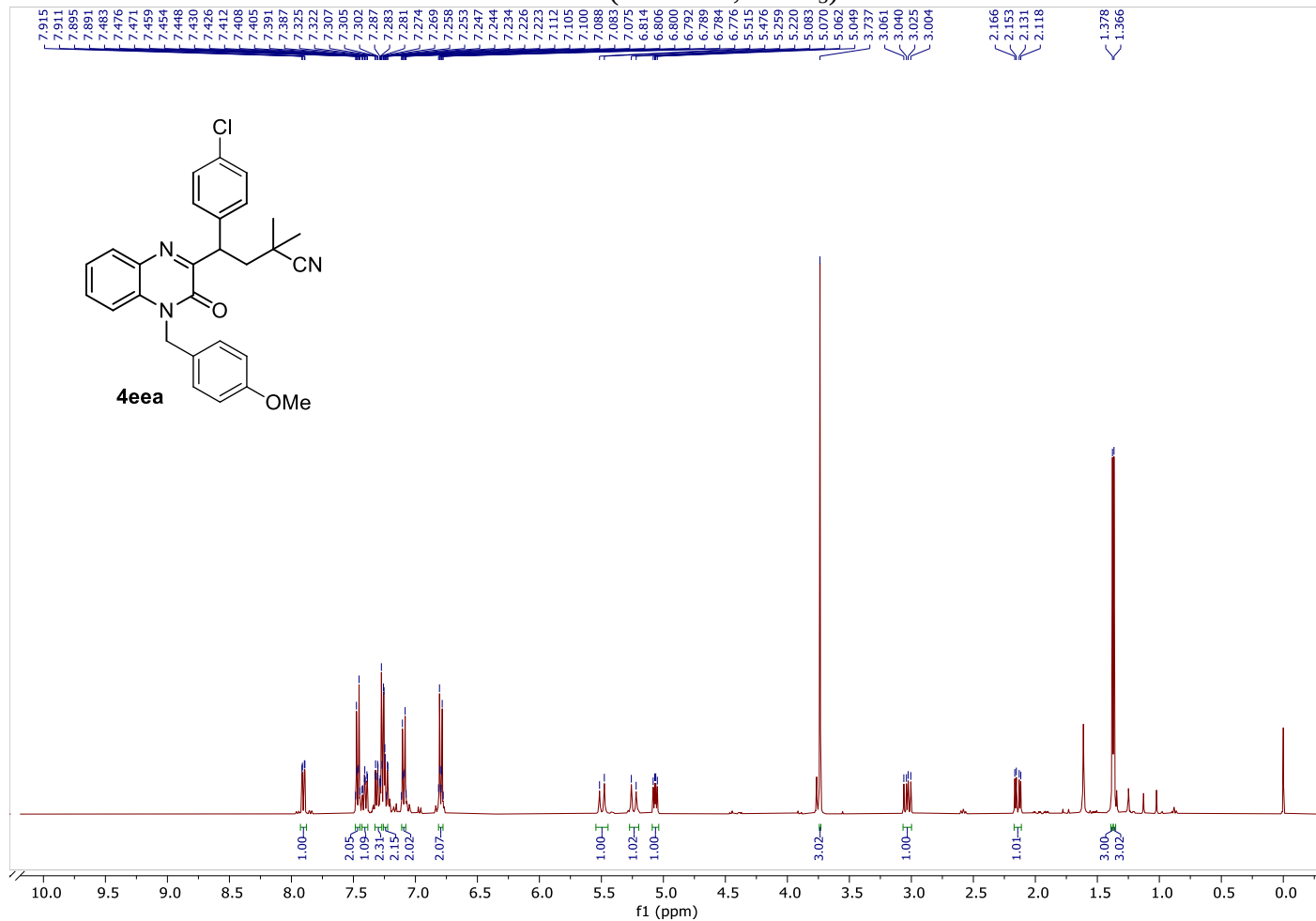
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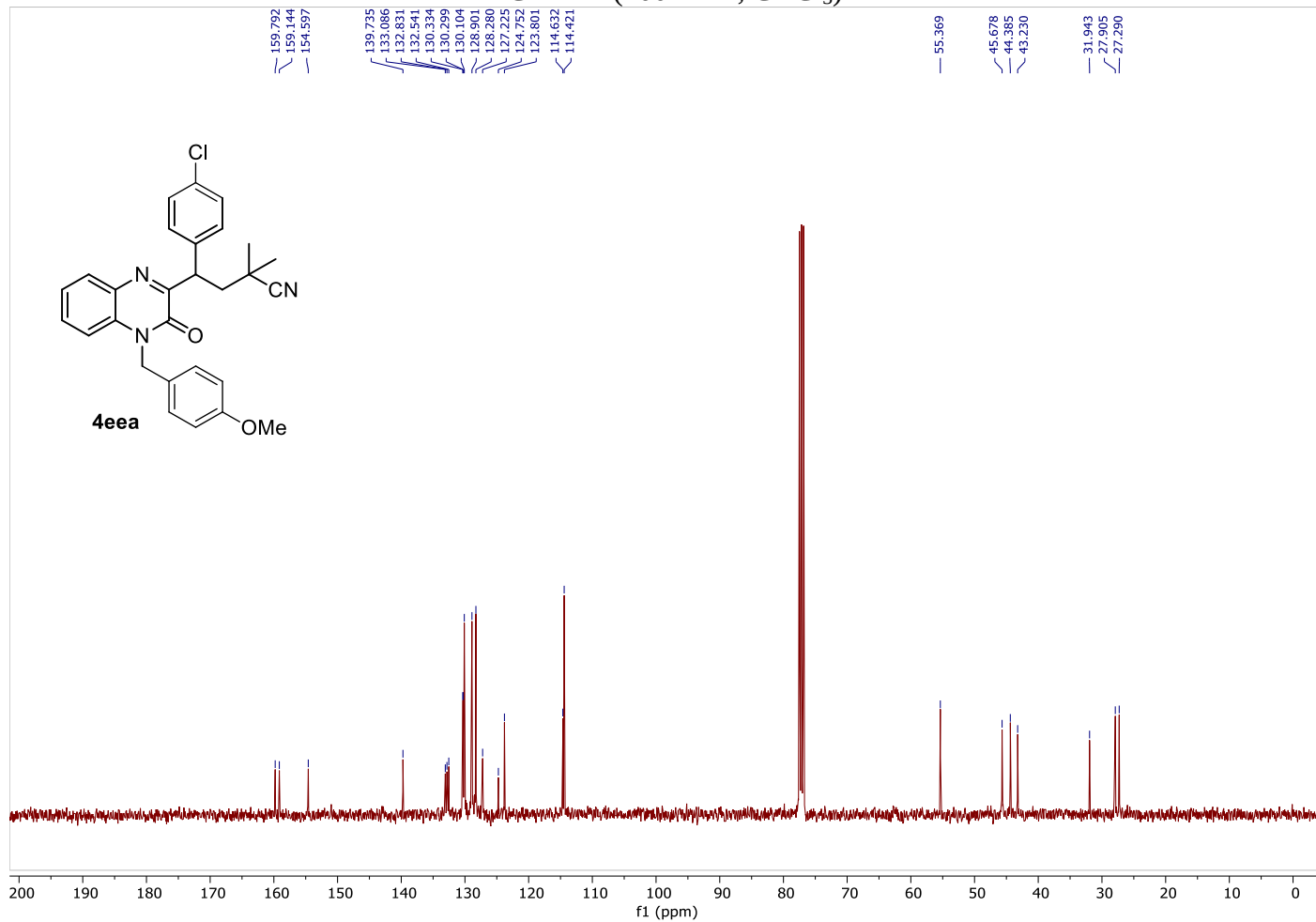
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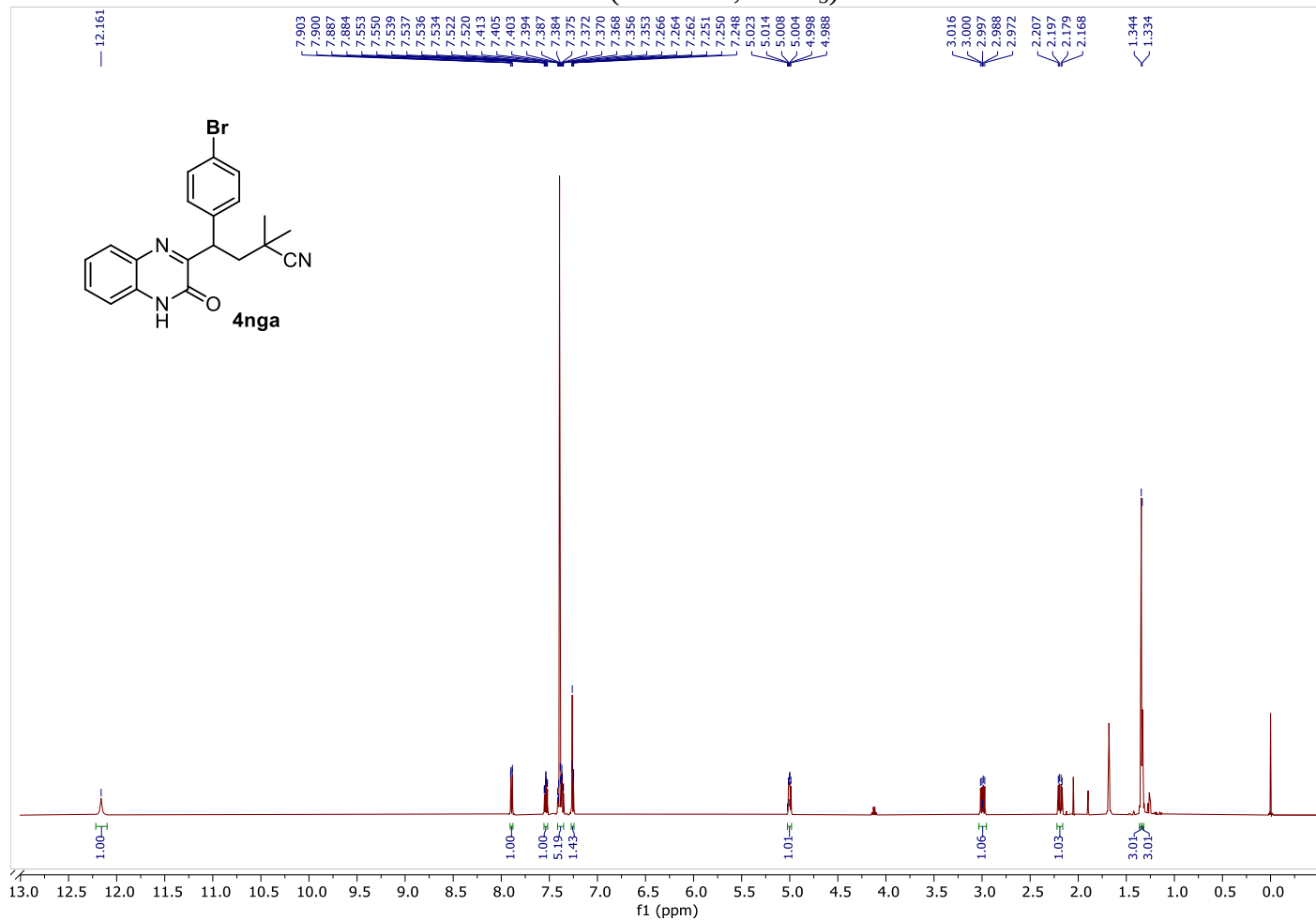
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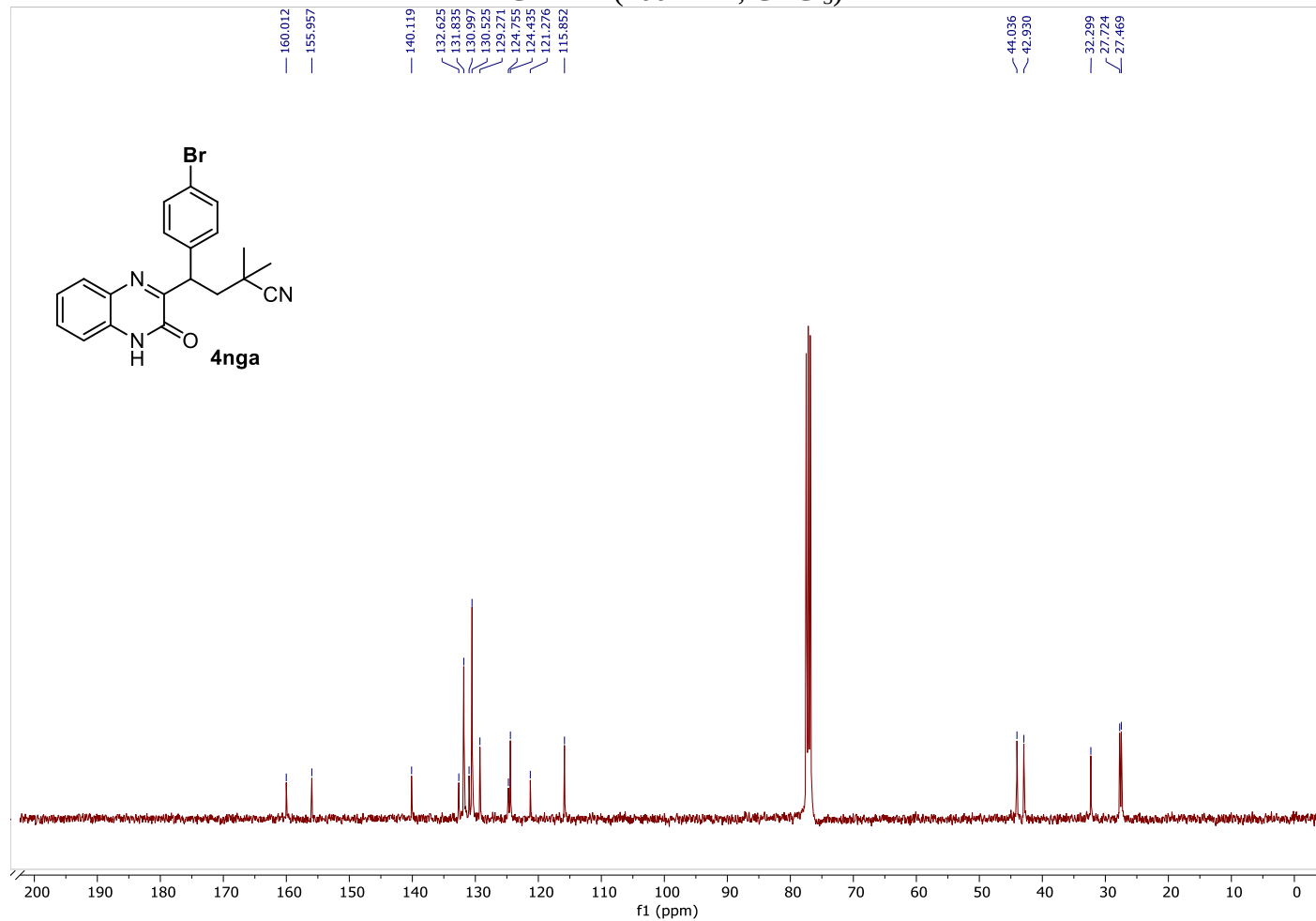
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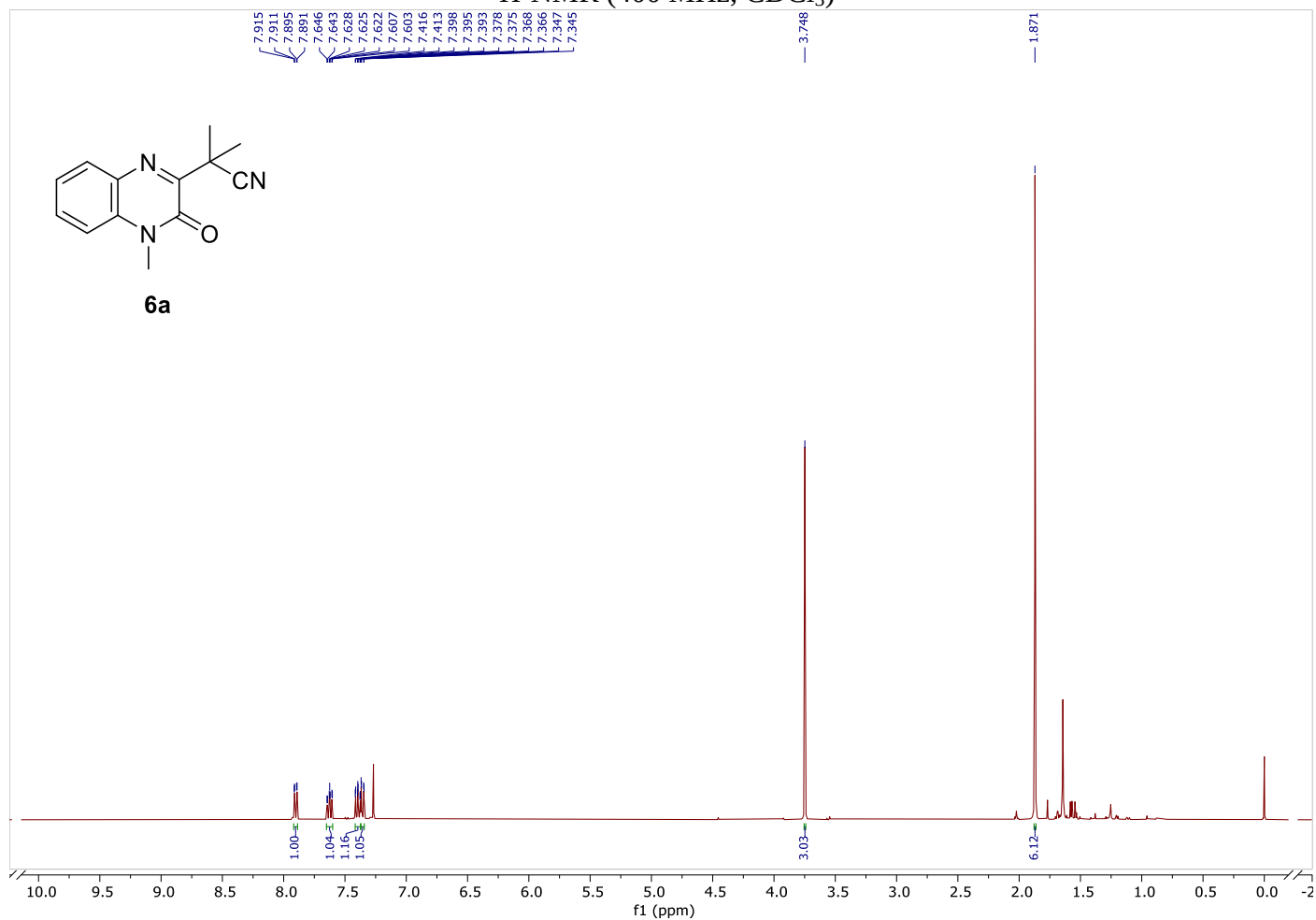
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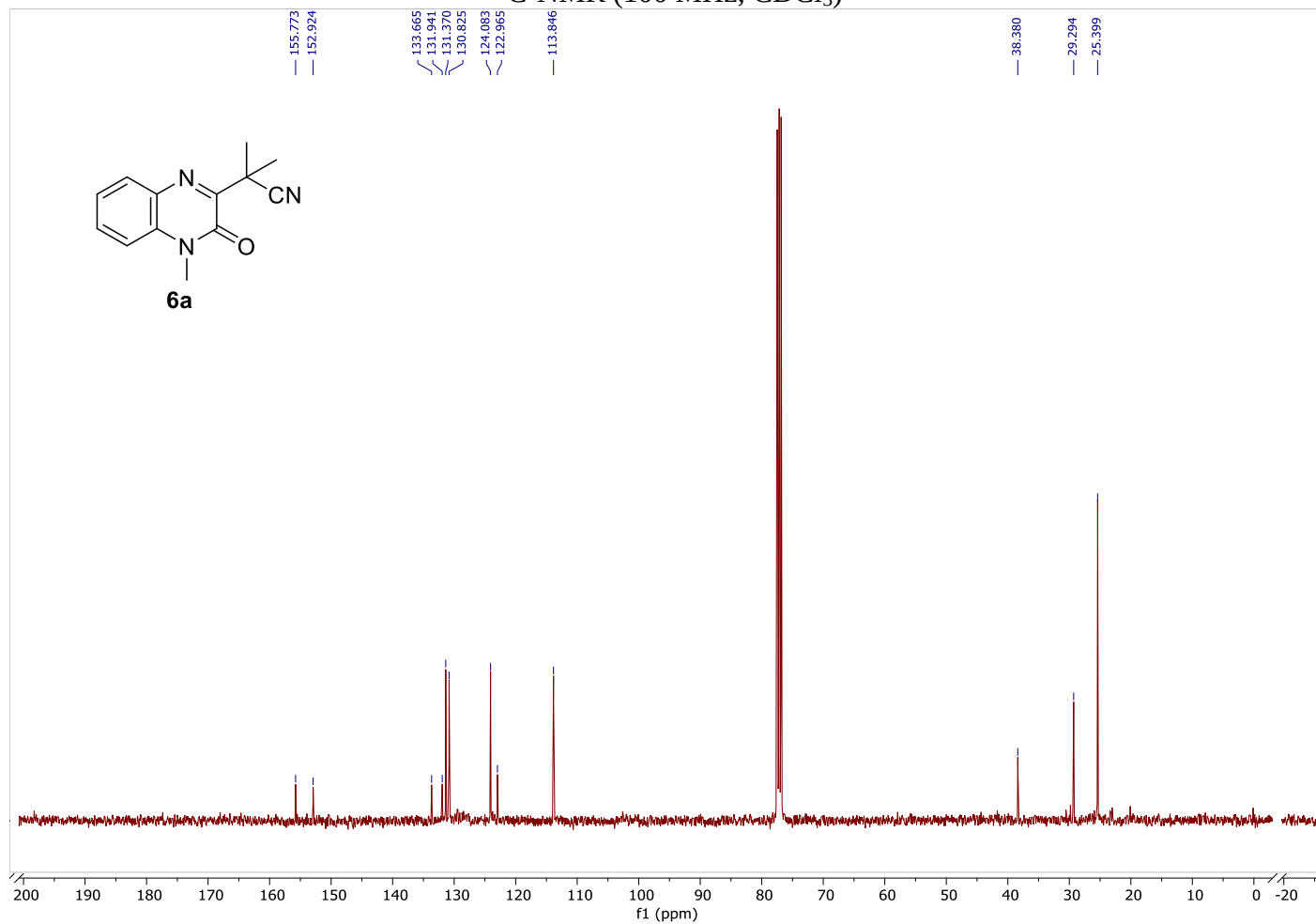
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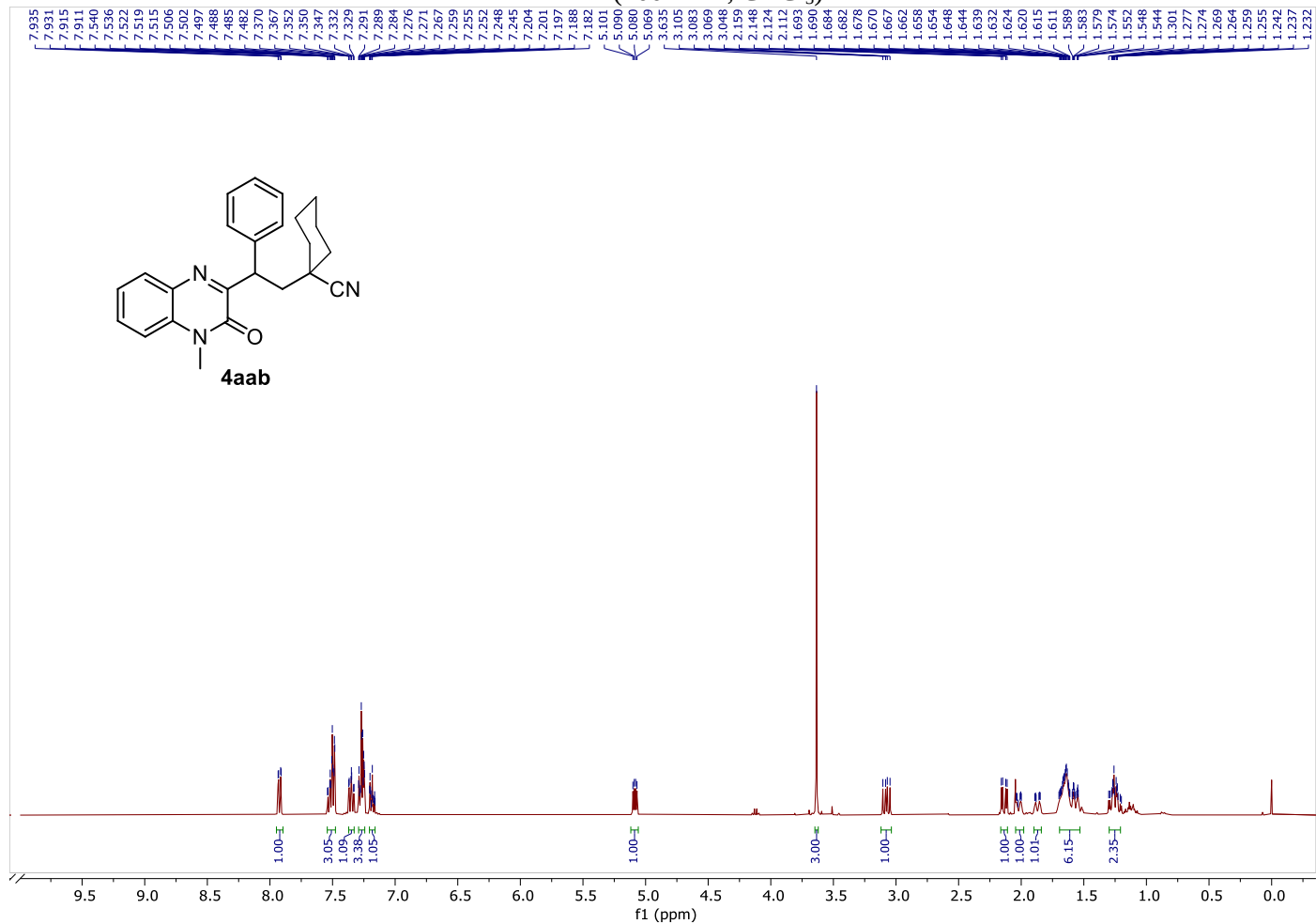
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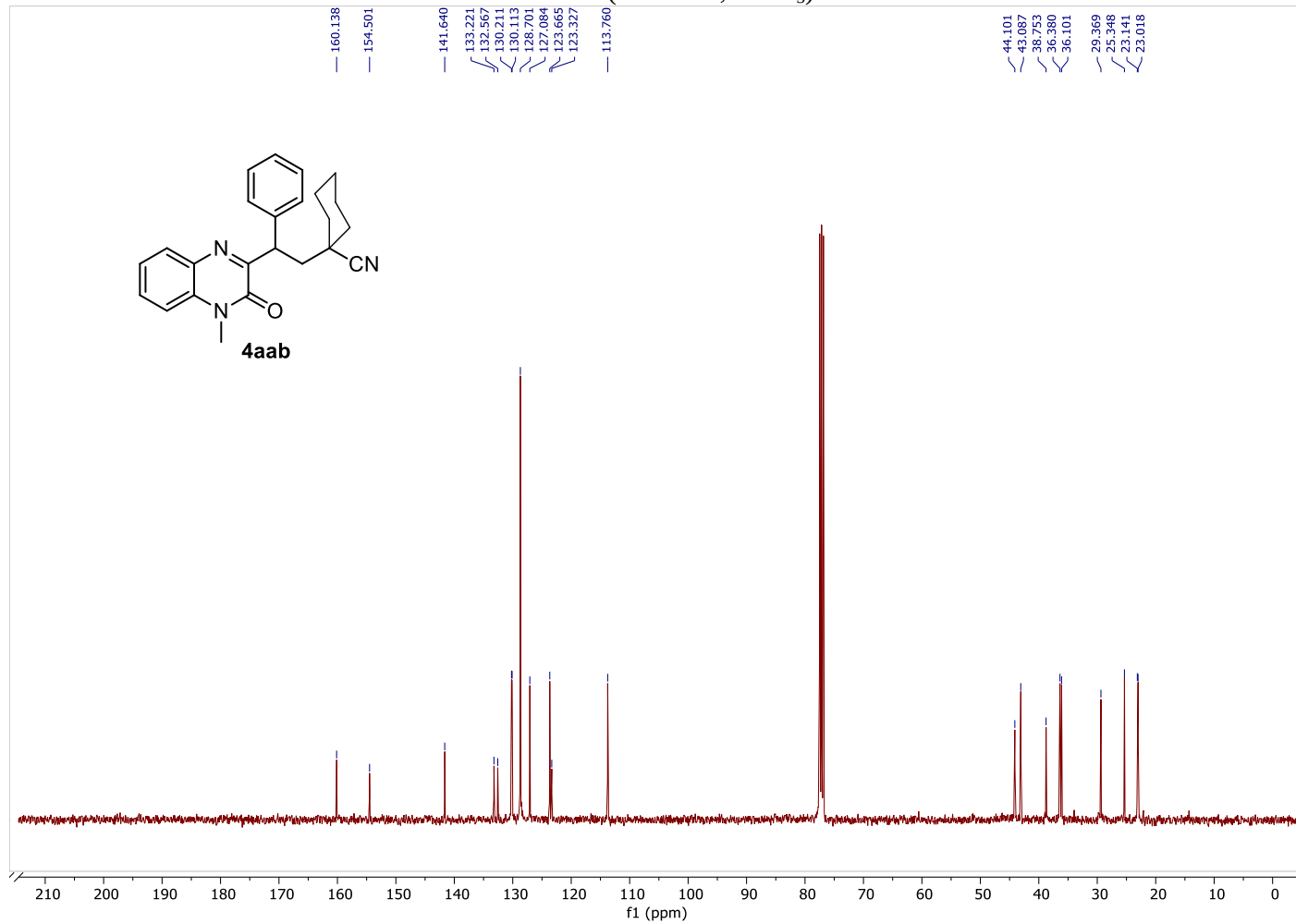
¹³C-NMR (100 MHz, CDCl₃)



¹H-NMR (400 MHz, CDCl₃)



¹³C-NMR (100 MHz, CDCl₃)



4aeb

CN1C(=O)N=C2C(=C1)C=CC=C2C(=C3C(=CC=C(C=C3)Cl)C4CC5C(C4)CC(C5)C#N)C

1H NMR spectrum (CDCl₃) of compound **4aeb**. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 10.0. The spectrum shows several peaks, with integration values indicated below the baseline. The peaks are labeled with their corresponding chemical shifts and integration values.

Chemical Shift (ppm)	Integration
~7.2	1.00
~7.4	1.03
~7.5	2.00
~7.6	1.06
~7.7	3.49
~7.8	1.00
~7.9	3.00
~8.0	1.00
~8.1	1.00
~8.2	1.09
~8.3	1.04
~8.4	6.30
~8.5	2.49

4aeb

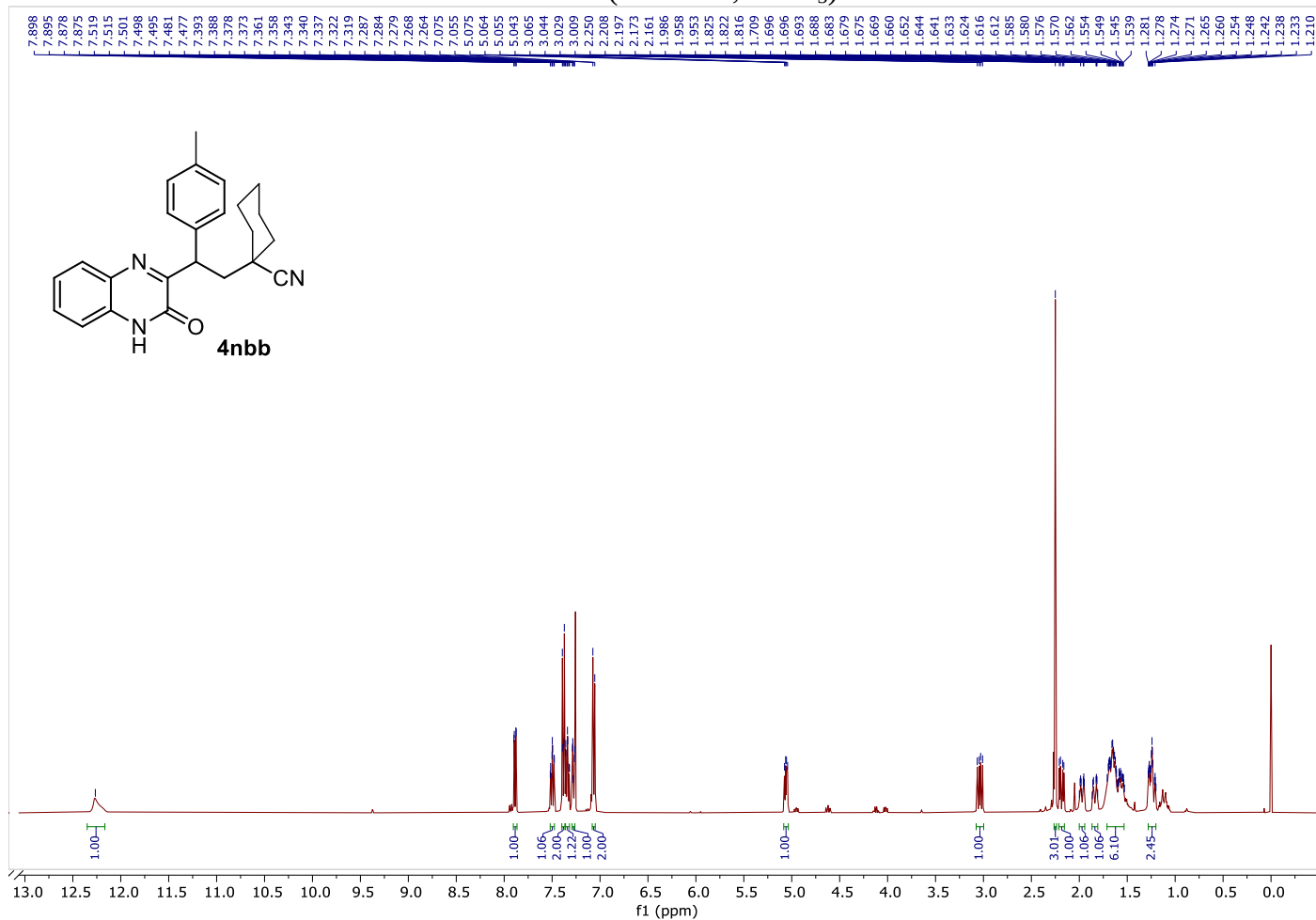
CN1C(=O)C(=Nc2ccccc2N1C)C(C#N)C3CC4C(C1)CC5C(C4)CC(C3)C5

Chemical structure of compound **4aeb** is shown. The structure features a 1-methyl-2-(4-chlorophenyl)-1H-benzotriazin-4(1H)-one core, substituted with a 1-cyano-2-phenyl-2-phenylpropan-1-yl group.

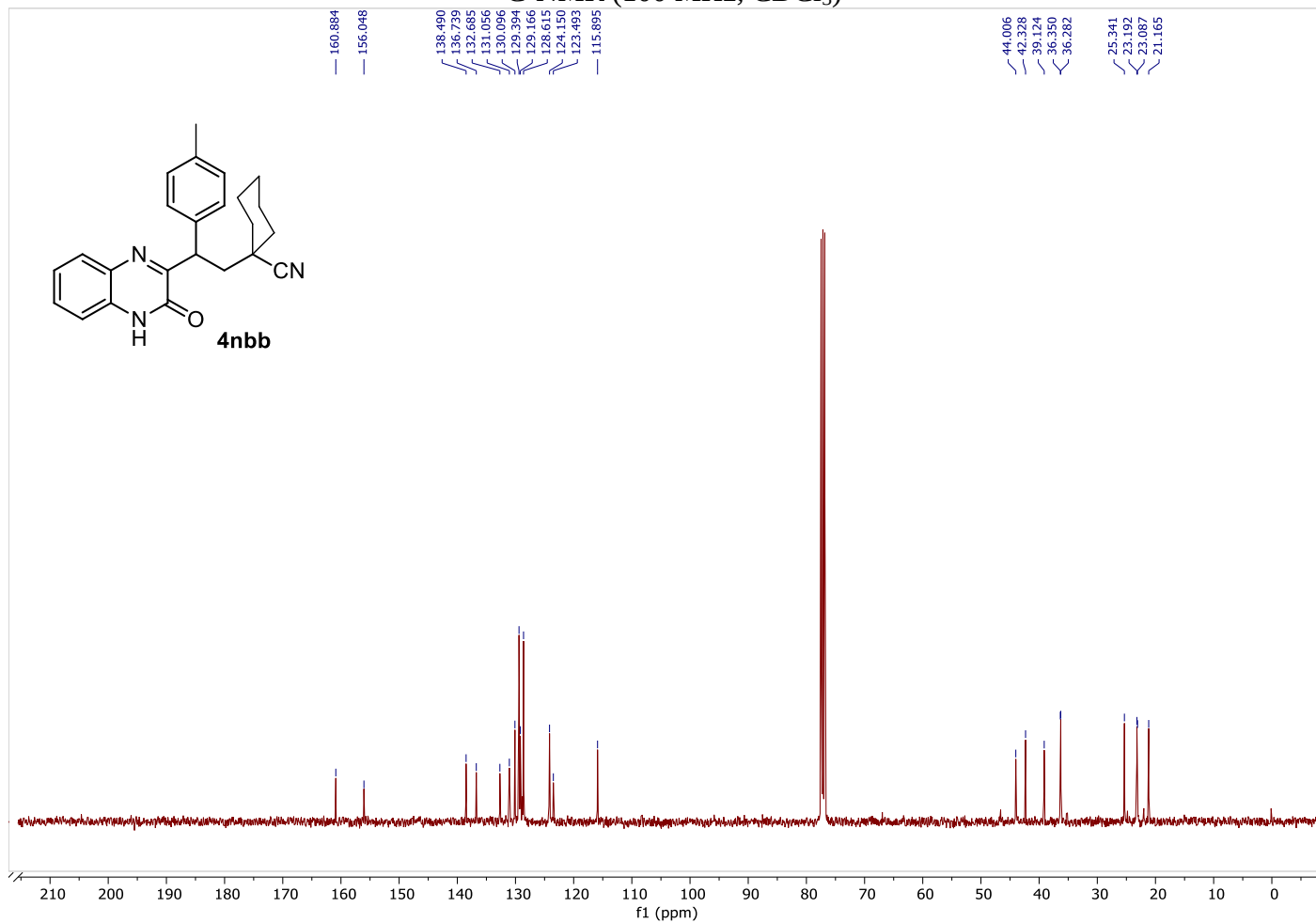
¹³C NMR spectrum (CDCl₃) of compound **4aeb** is displayed. The spectrum shows peaks corresponding to the structure, with the following chemical shifts (ppm) labeled:

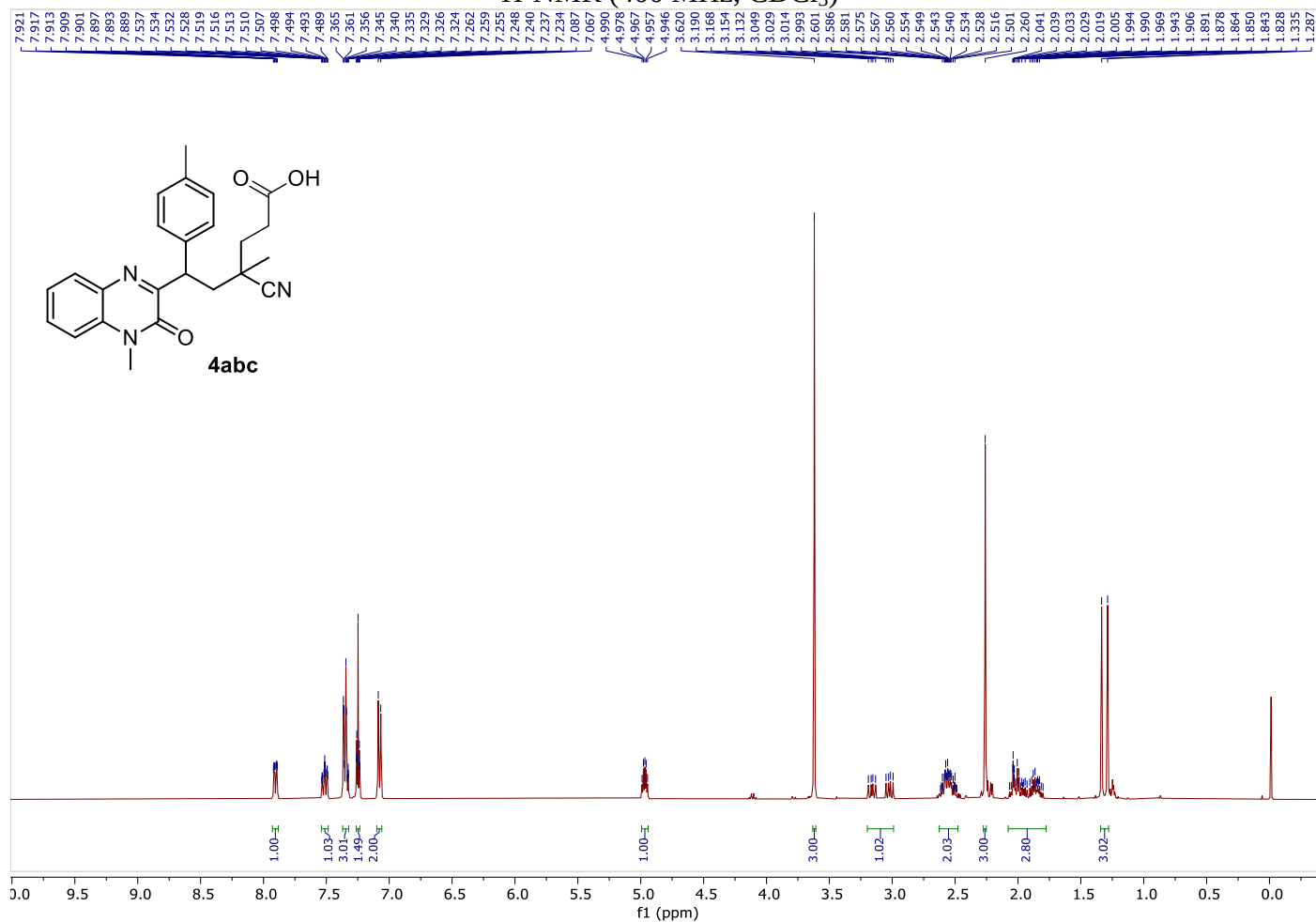
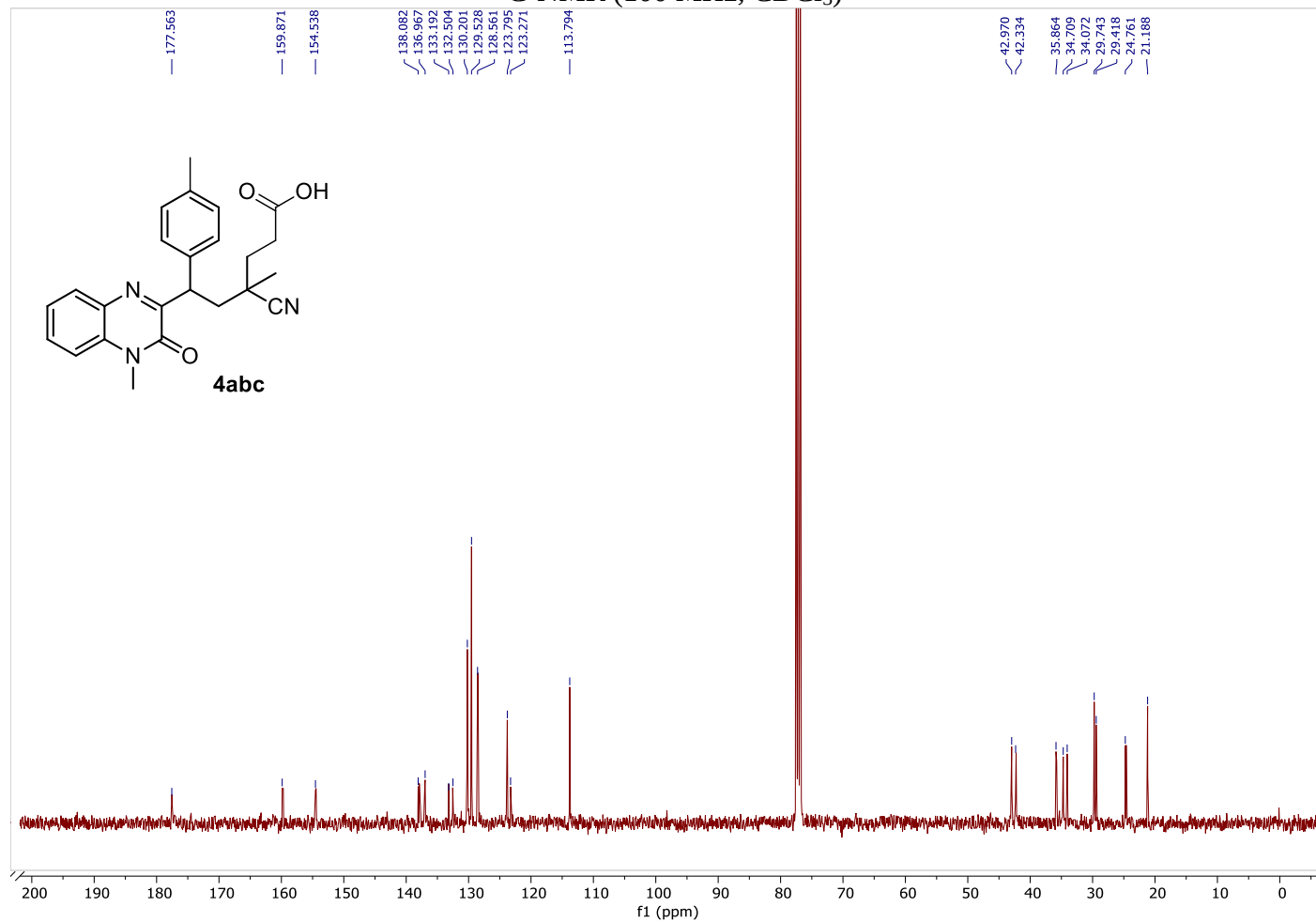
Chemical Shift (ppm)
159.733
154.424
140.092
133.227
132.951
132.516
130.316
130.235
130.056
128.845
123.778
123.216
113.825
43.963
42.603
38.750
36.391
36.182
29.397
25.321
23.129
23.007

¹H-NMR (400 MHz, CDCl₃)

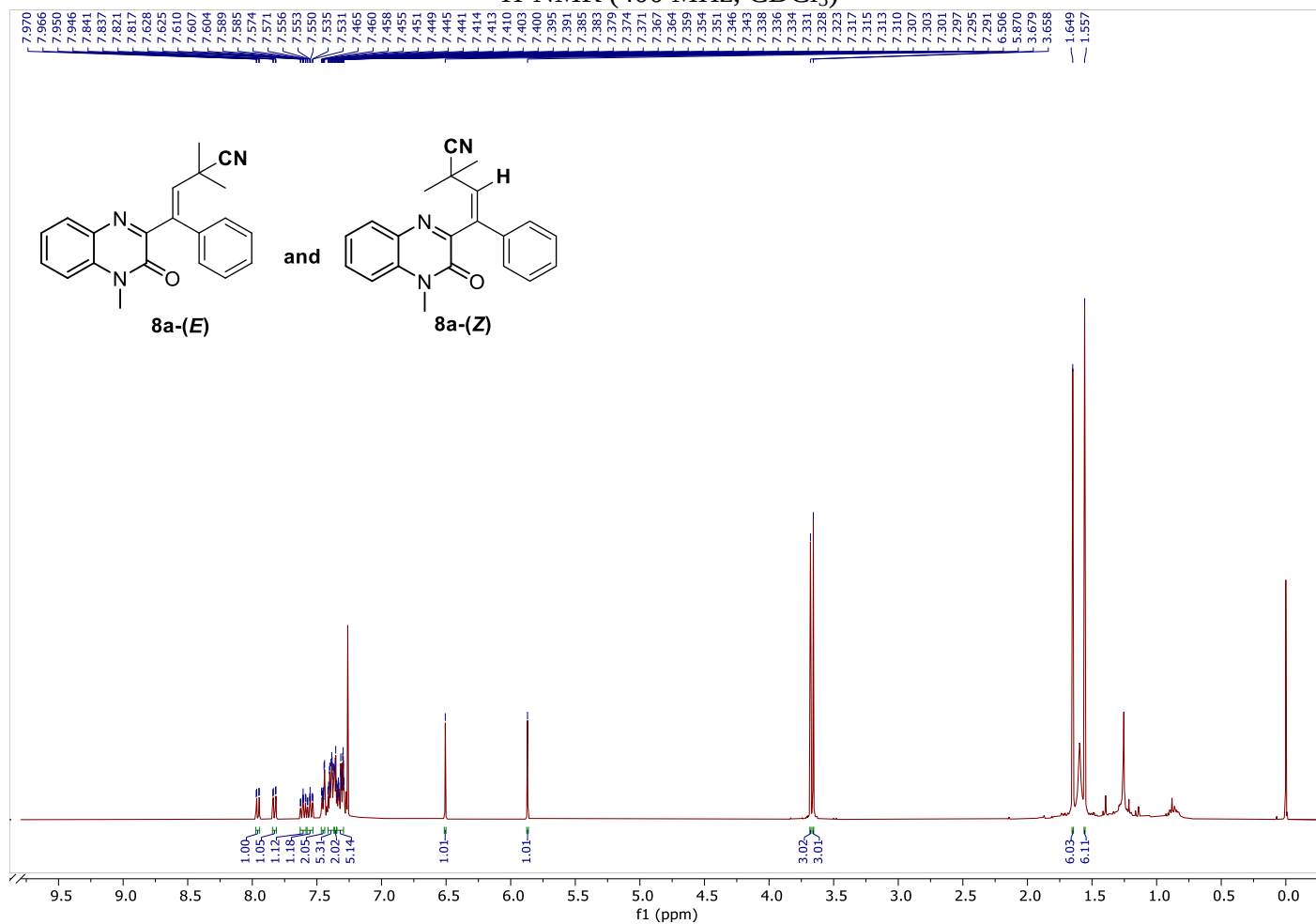


¹³C-NMR (100 MHz, CDCl₃)

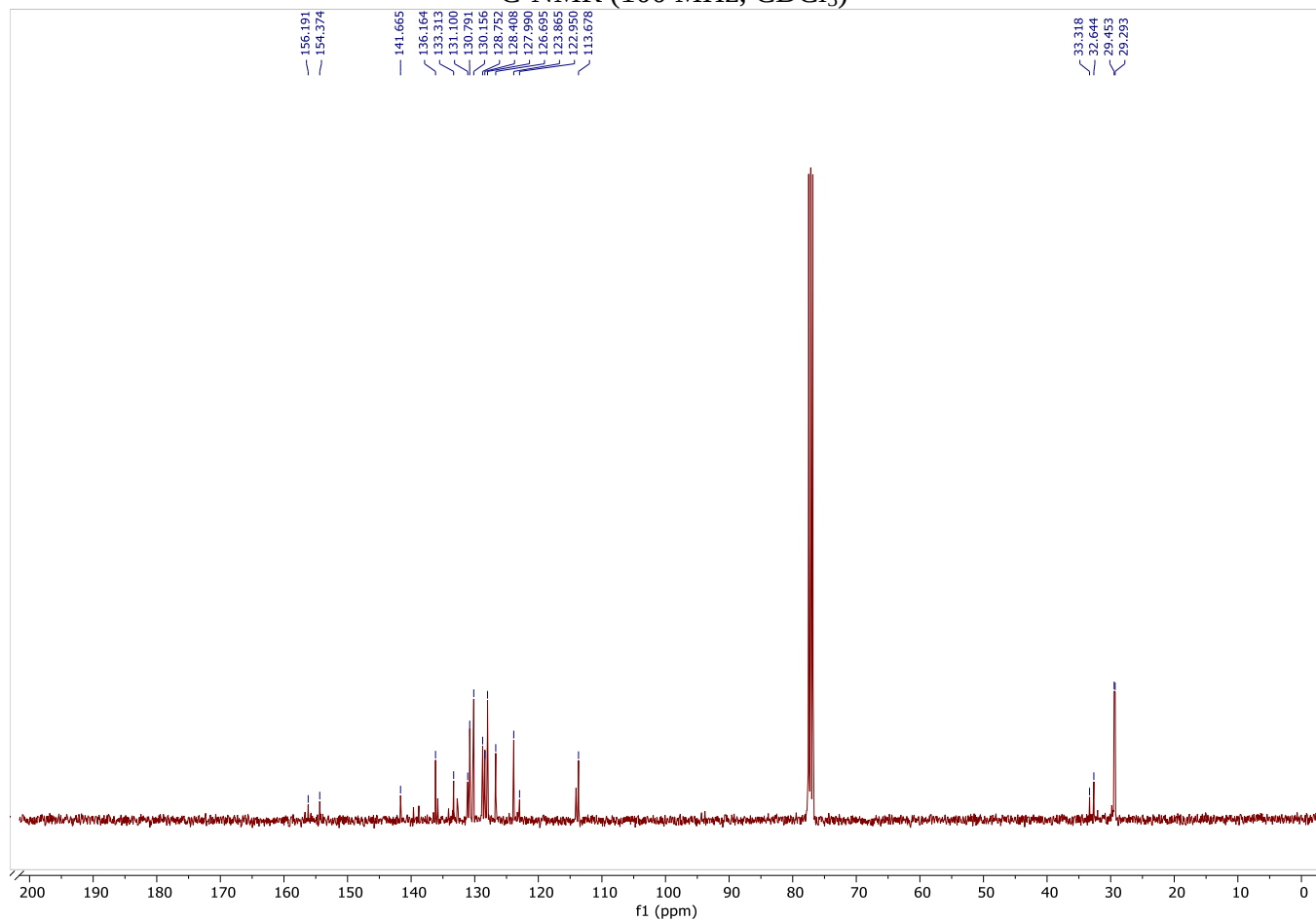


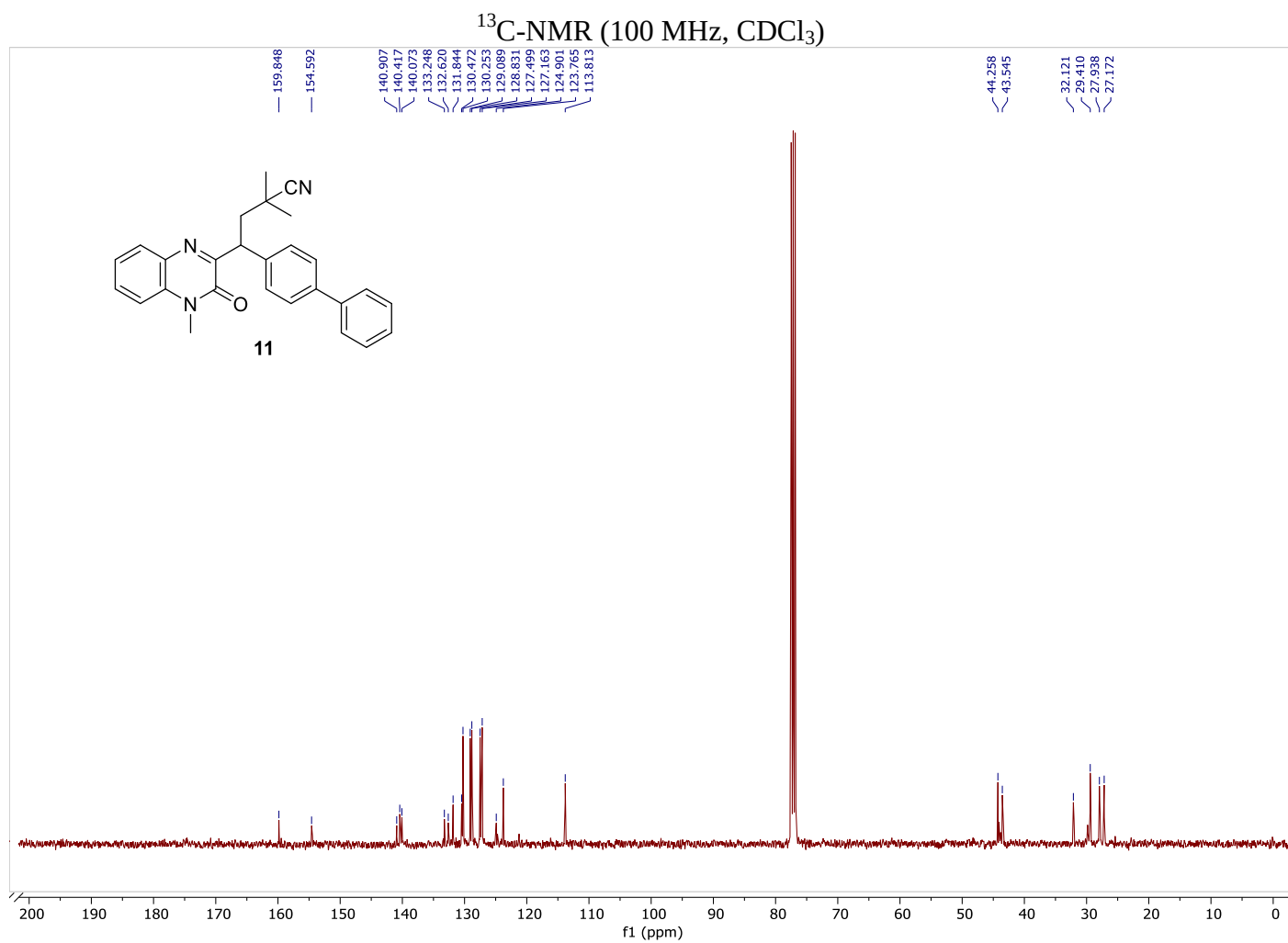
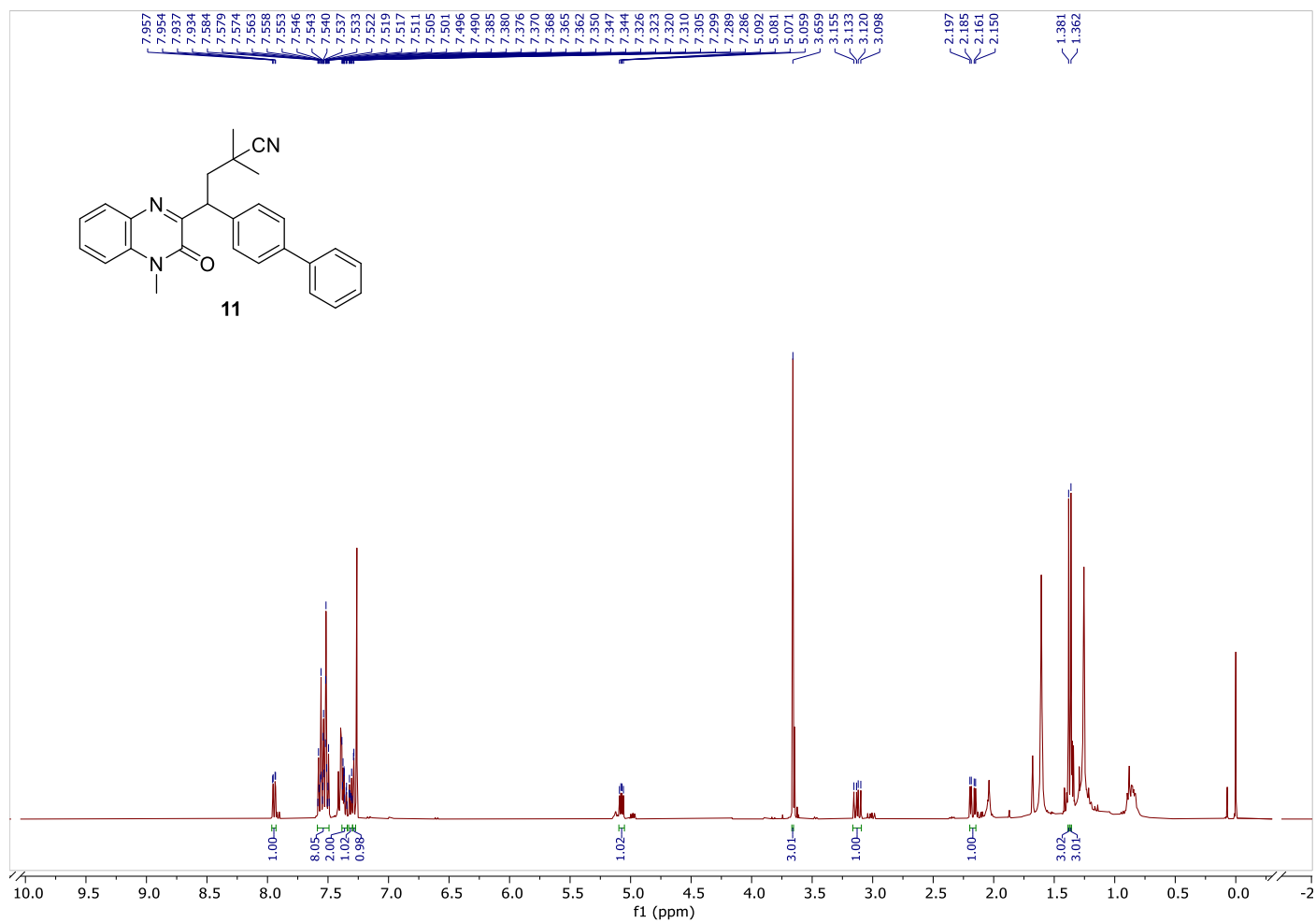
¹H-NMR (400 MHz, CDCl₃)¹³C-NMR (100 MHz, CDCl₃)

¹H-NMR (400 MHz, CDCl₃)



¹³C-NMR (100 MHz, CDCl₃)





➤ NOESY- **4aka**: No NOE observed between H_a and H_b.

