

*Supporting Information*

**Dual antitubercular and anti-leishmanial profiles of quinoxaline di-N-oxides containing an amino acidic side chain**

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## 1. Numerical biological data

**Table S1.** Antibacterial activity against Mtb H37Rv \*

Entry	Compound	IC <sub>50</sub> (μM)	IC <sub>90</sub> (μM)	MIC (μM)
1	<b>4a</b>	26.30	55.50	100
2	<b>4b</b>	40.64	69.83	100
3	<b>4c</b>	13.19	25.90	50
4	<b>4d</b>	28.57	47.72	50
5	<b>4e</b>	25.17	47.86	100
6	<b>4f</b>	21.91	47.93	50
7	<b>4g</b>	49.95	71.87	100
8	<b>4h</b>	8.46	12.42	50
9	<b>4i</b>	47.2	66.5	100
10	<b>4j</b>	12.87	24.60	50
11	<b>4k</b>	25.87	44.60	100
12	<b>4l</b>	7.20	15.5	50
13	<b>4m</b>	18.28	36.50	50
14	<b>4n</b>	11.91	27.93	50
15	<b>5f</b>	4.28	9.86	25
16	<b>5h</b>	16.38	21.97	50
17	<b>5m</b>	17.20	3505	50
18	<b>6</b>	44.95	76.38	100
19	7	28.28	66.50	100
20	Amikacin	0.07	0.08	0.16
21	Cycloserine	12.47	13.49	25
22	Ethambutol	1.56	32.79	12.5
23	Isoniazid	0.18	0.29	0.31
24	Pyrimethamine	37.35	74.96	100

\* None of the compounds showed cytotoxicity in Vero cells at concentrations up to 6.25 μg/mL.

**Table S2.** Antileishmanial promastigote activity, cytotoxicity and selectivity indexes\*

Entry	Compound	<i>L. amazonensis</i> IC <sub>50</sub> , μM (SI)	<i>L. donovani</i> IC <sub>50</sub> , μM (SI)	Toxicity against J774 macrophages CC <sub>50</sub> , μM
1	<b>4a</b>	171.0 ± 8.5 (5.0)	103.4 ± 9.8 (8.2)	849.8
2	<b>4b</b>	157.4 ± 7.8 (9.9)	261.1 ± 7.8 (6.0)	1566.6
3	<b>4c</b>	> 237.5 (> 30)	> 237.5 (> 30)	6960.1
4	<b>4d</b>	124.9 ± 1.43 (4.3)	164.9 ± 10.24 (3.3)	539.1
5	<b>4e</b>	25.1 ± 0.56 (0.7)	34.0 ± 5.2 (0.5)	18.5 ± 3.4
6	<b>4f</b>	> 261.1 (> 30.0)	> 261.1 (30.0)	7832.9
7	<b>4g</b>	111.8 ± 13.7 (64.3)	40.0 ± 6.7 (179.9)	7194.2
8	<b>4h</b>	122.0 ± 9.9 (4.5)	25.3 ± 1.55 (21.9)	554.3
9	<b>4i</b>	116.9 ± 8.0 (3.2)	46.9 ± 14.2 (12.2)	379.0 ± 49.9
10	<b>4j</b>	110.8 ± 4.0 (2.9)	13.8 ± 9.5 (23.2)	318.6 ± 0.84
11	<b>4k</b>	117.4 ± 14.3 (2.8)	23.9 ± 2.2 (13.8)	330.0 ± 75.5
12	<b>4l</b>	> 229.9 (> 6.0)	229.9 (> 6.0)	1380
13	<b>4m</b>	62.8 ± 1.6 (7.2)	84.8 ± 8.9 (5.4)	454.5
14	<b>4n</b>	97.3 ± 4.3 (2.0)	43.5 ± 1.1 (4.4)	191.3 ± 29.3
15	<b>5d</b>	> 280.1 (> 3.0)	> 280.1 (> 3.0)	840
16	<b>5f</b>	> 271.0 (> 30)	> 271.0 (> 30)	8130
17	<b>5h</b>	> 228.8 (> 8)	> 228.8 (> 8)	1831
18	<b>5m</b>	> 269.5 (> 30)	> 269.5 (> 30)	8086
19	<b>6</b>	20.5 ± 2.5 (20.7)	6.2 ± 0.2 (68.4)	424.0
20	Miltefosine	47.9 ± 4.9 (2.8)	0.2 ± 0.02 (680.5)	136.1 ± 10.3

\* SI, selectivity index.

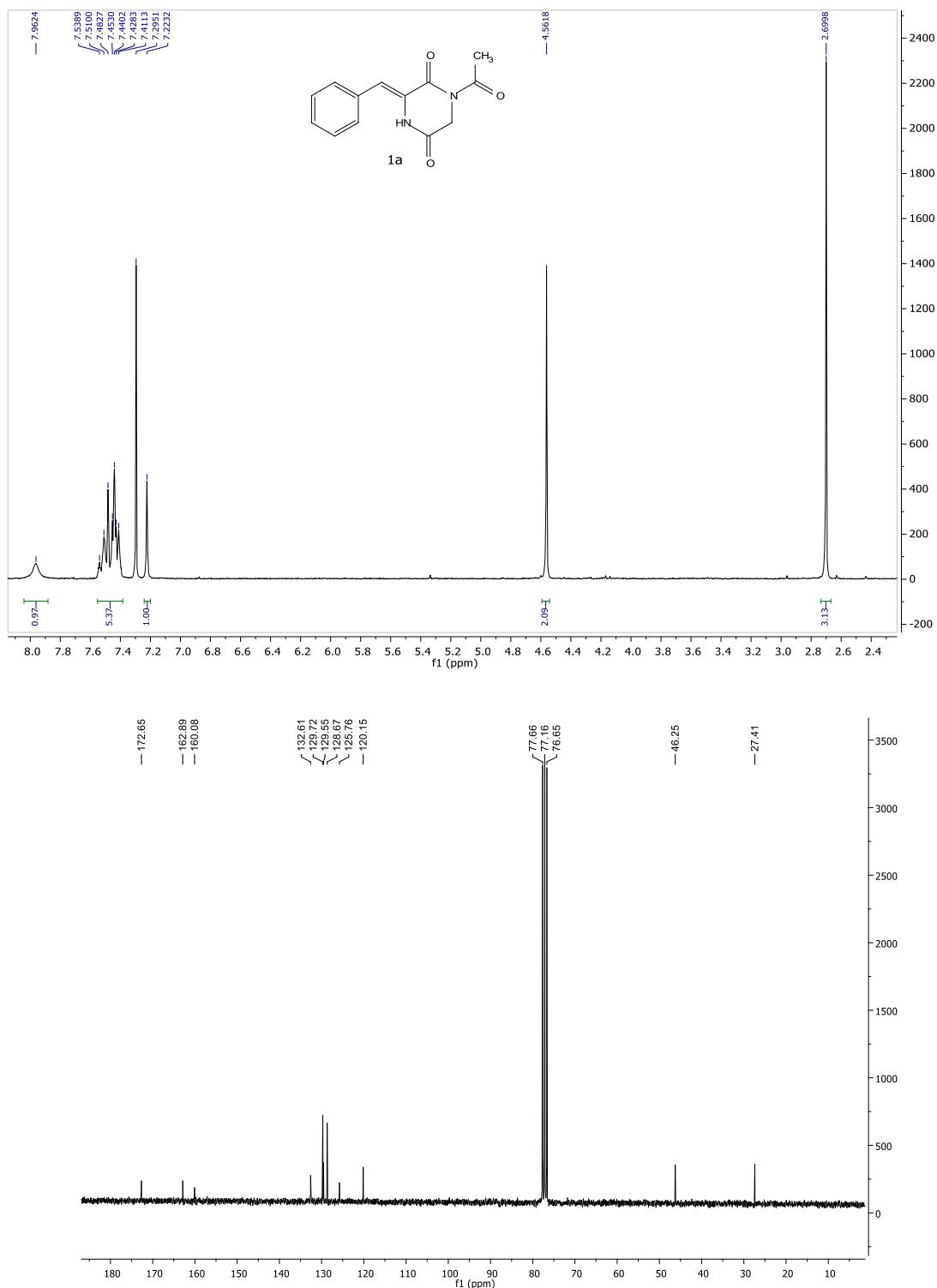
**Table S3.** Anti-amastigote activity, cytotoxicity and selectivity of selected compounds\*

Entry	Compound	<i>L. amazonensis</i> IC <sub>50</sub> , μM (SI)	<i>L. donovani</i> IC <sub>50</sub> , μM (SI)	Toxicity against J774 macrophages CC <sub>50</sub> , μM
1	<b>4a</b>	12.6 ± 0.3 (67.3)	ND	850
2	<b>4d</b>	9.8 ± 1.0 (54.9)	234.2 ± 5.9 (2.3)	539
3	<b>4g</b>	23.2 ± 4.1 (310.6)	77.5 ± 6.2 (92.8)	7194
4	<b>4h</b>	20.9 ± 4.0 (26.5)	39.5 ± 7.5 (14.0)	554
5	<b>4i</b>	12.9 ± 1.7 (29.9)	71.0 ± 11.0 (5.3)	379
6	<b>4k</b>	7.2 ± 0.5 (45.6)	72.2 ± 18.6 (4.6)	330
7	<b>4m</b>	74.4 ± 19.3 (6.11)	284.9 ± 114.8 (1.6)	454
8	<b>6</b>	31.9 ± 13.2 (13.3)	ND	424
9	Miltefosine	47.6 ± 7.4 (2.9)	7.1 (19.1)	136

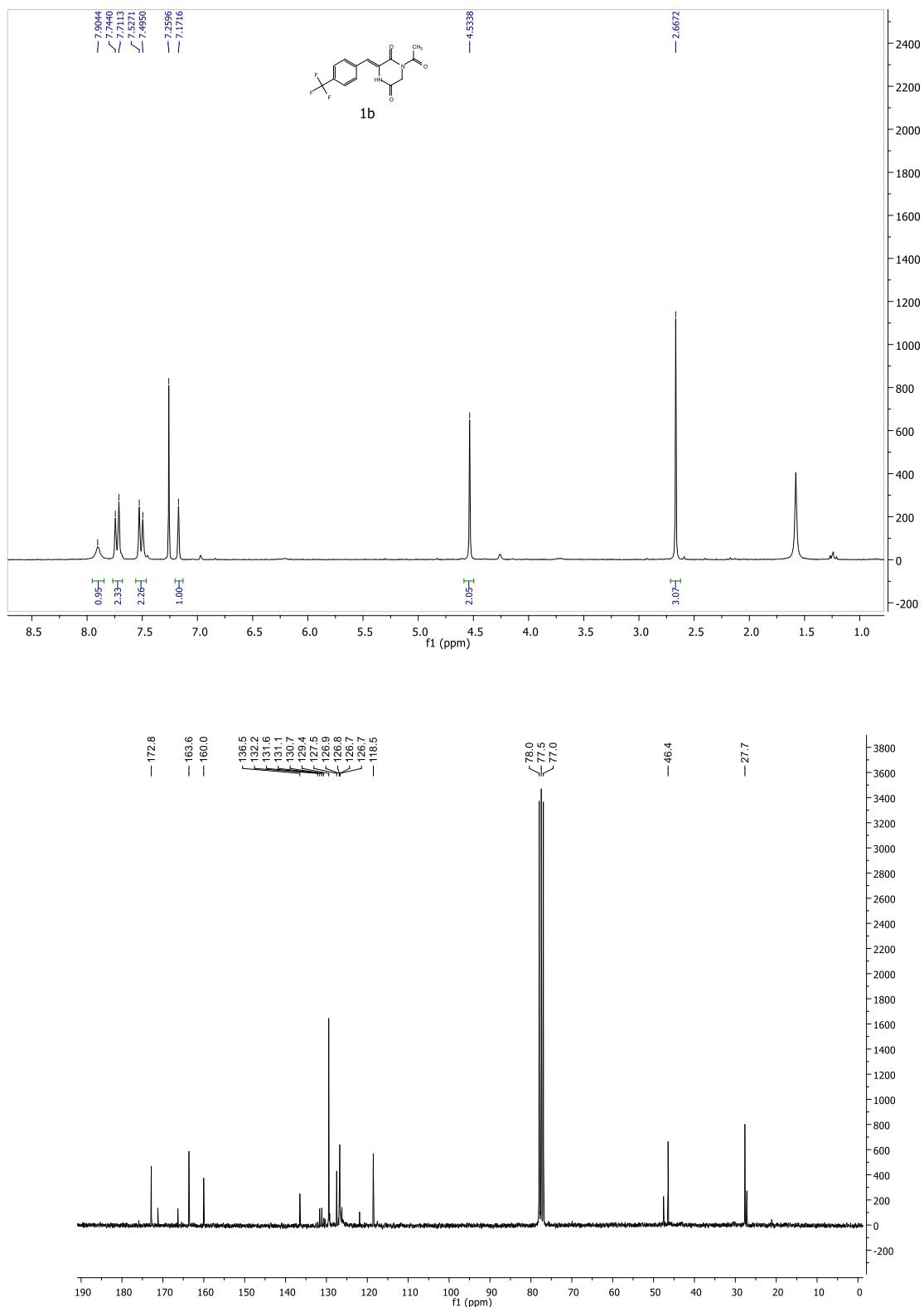
\* SI, selectivity index.

## 2. Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra

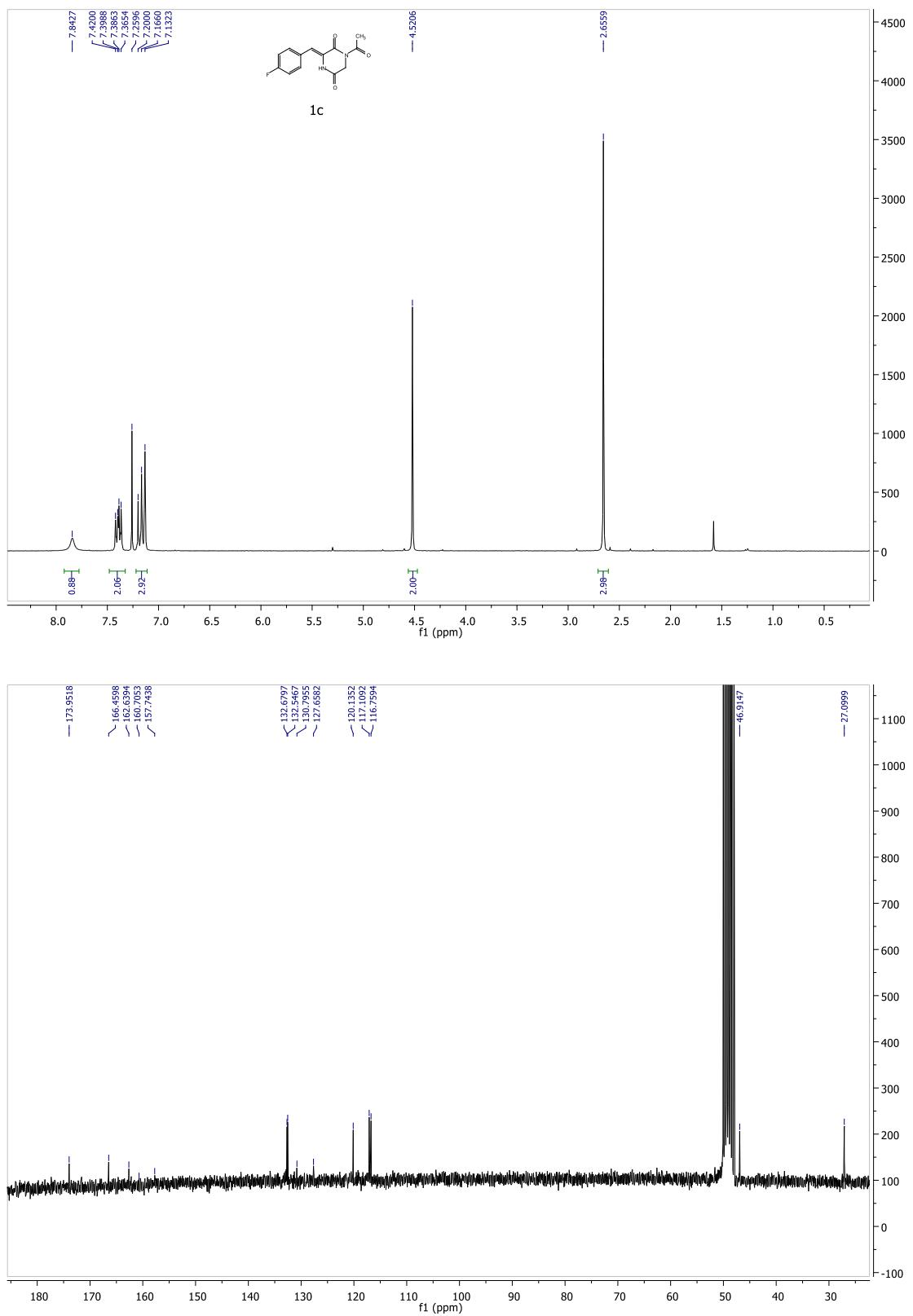
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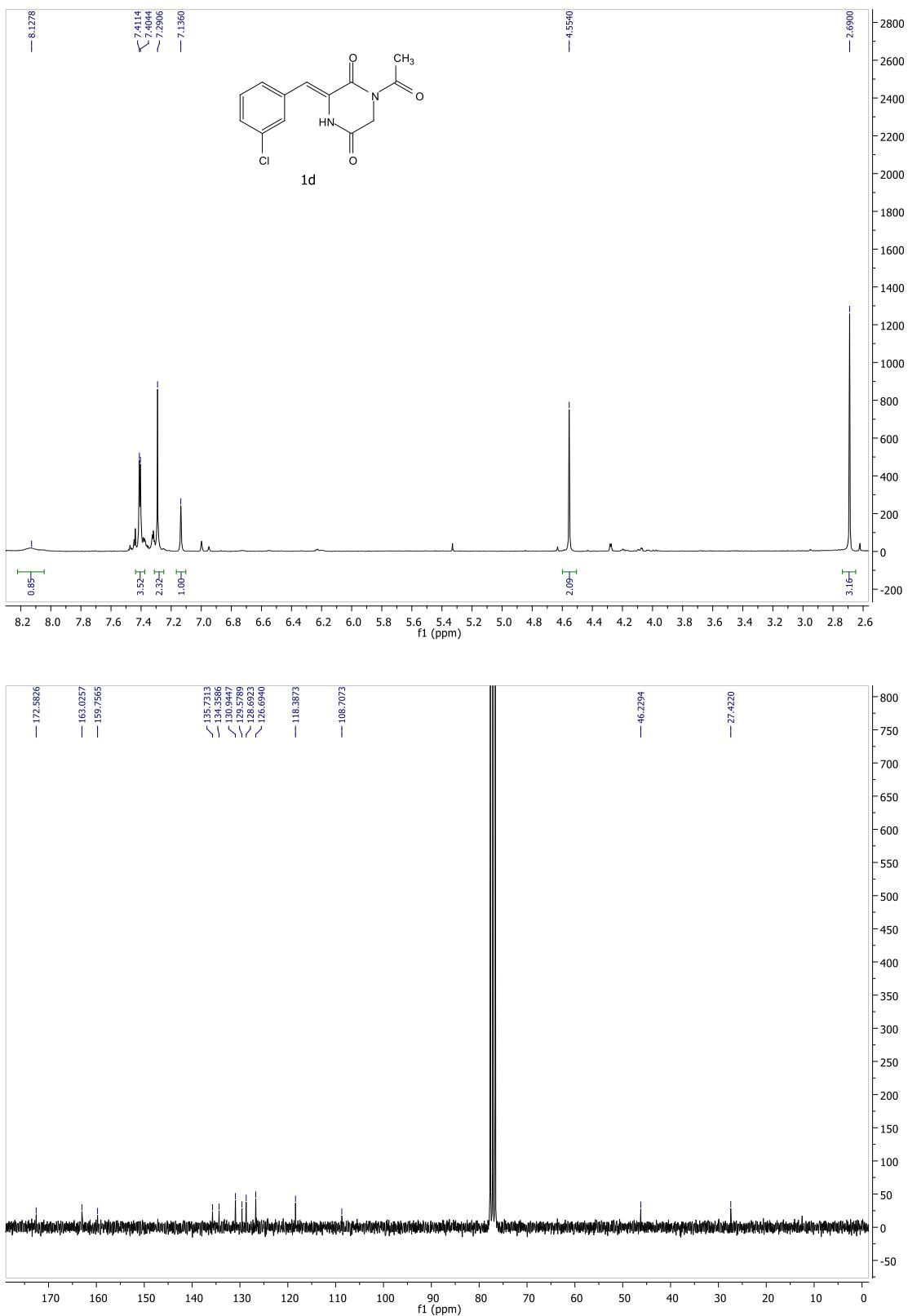
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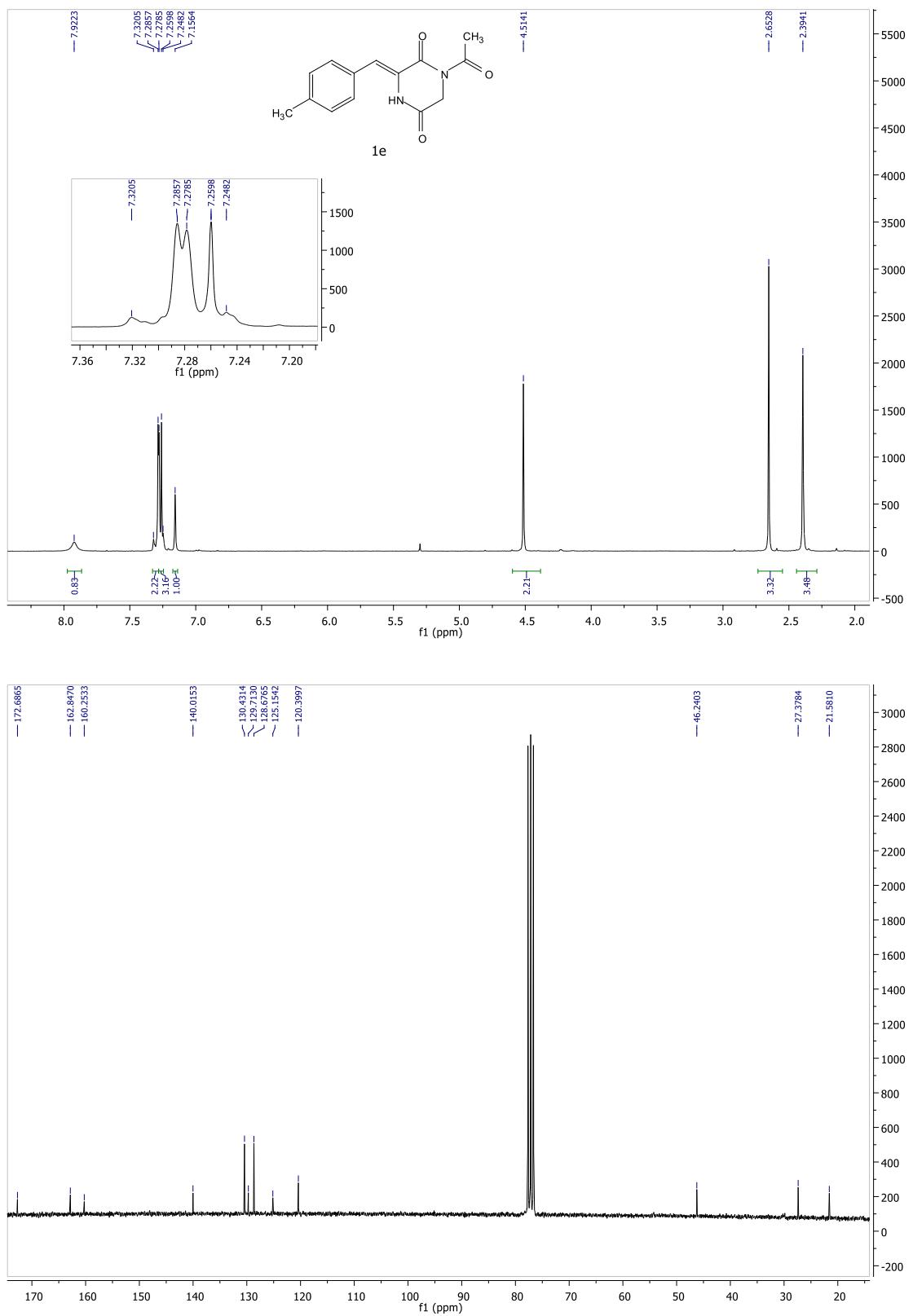
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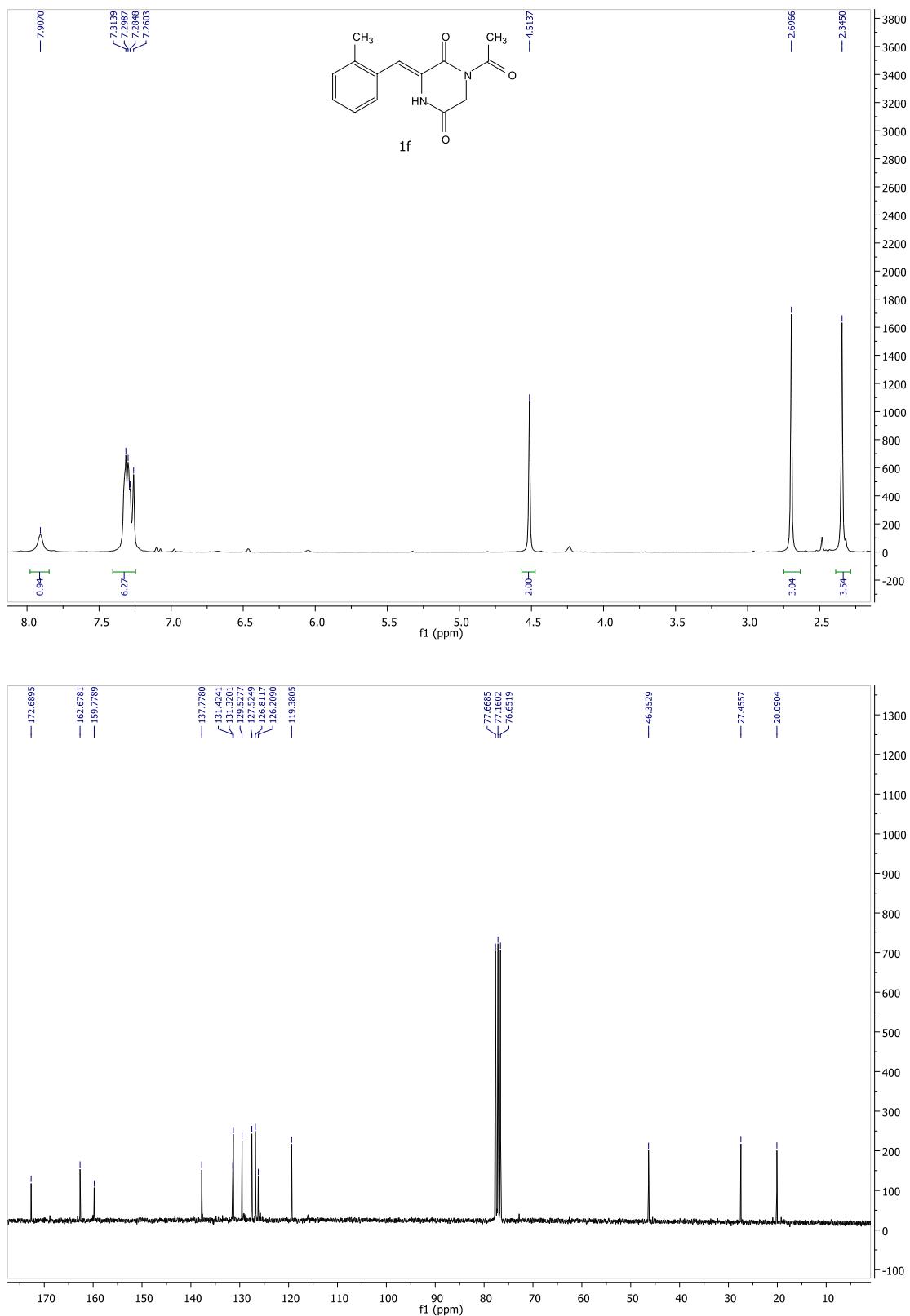
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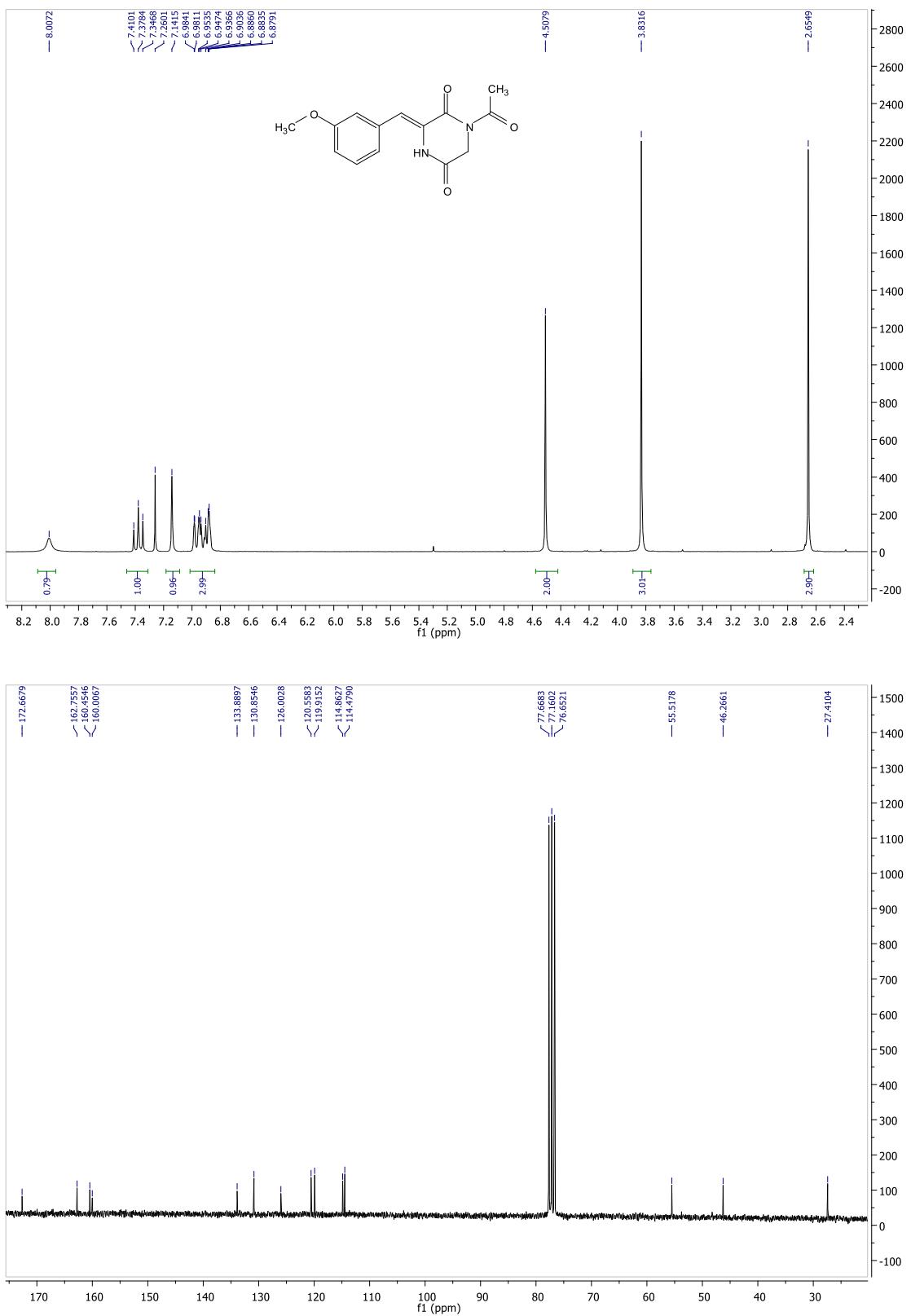
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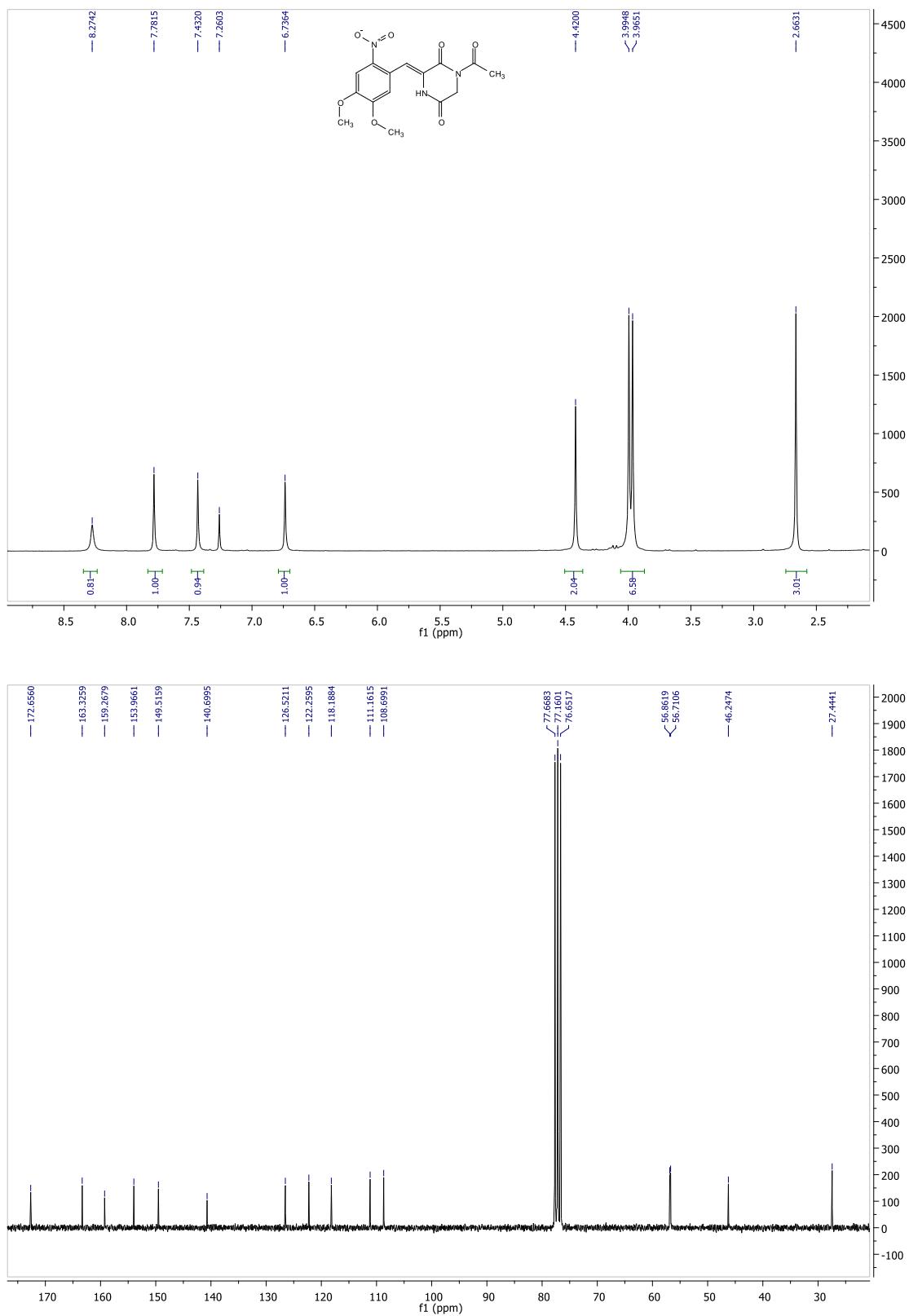
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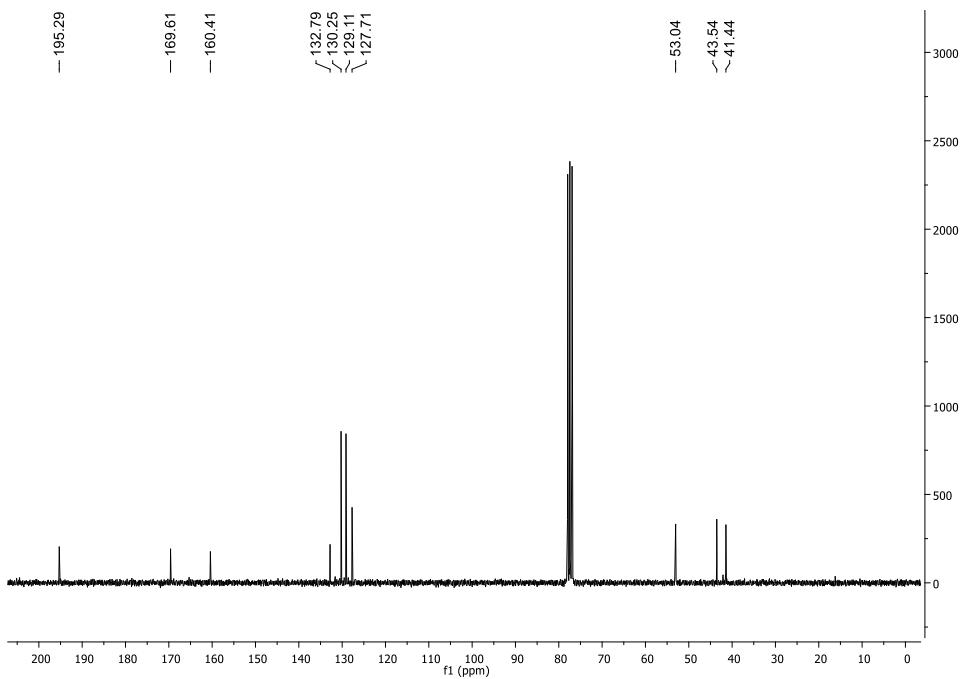
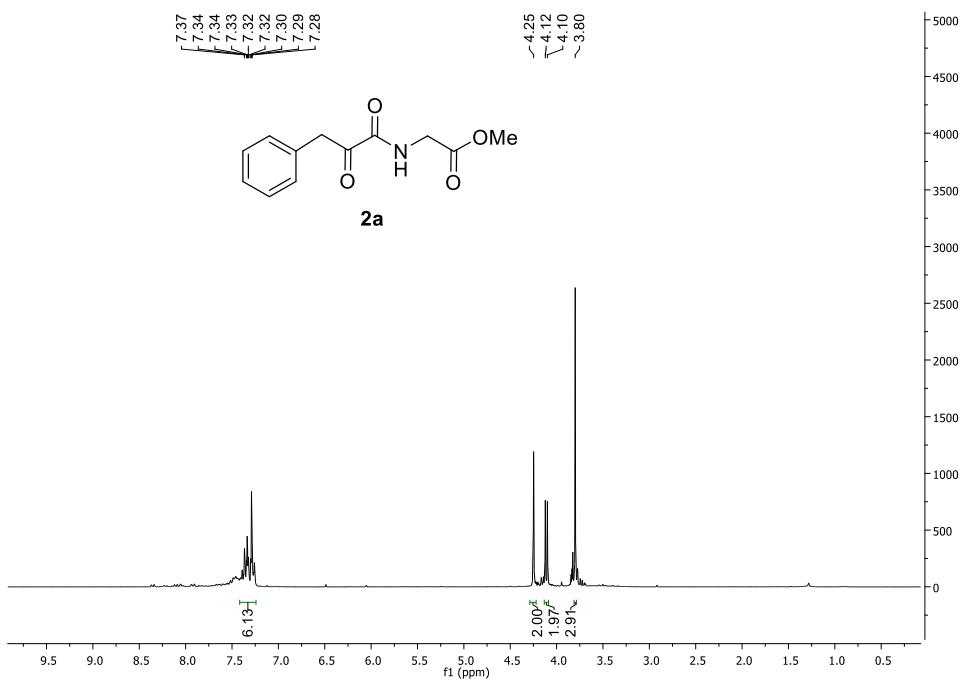
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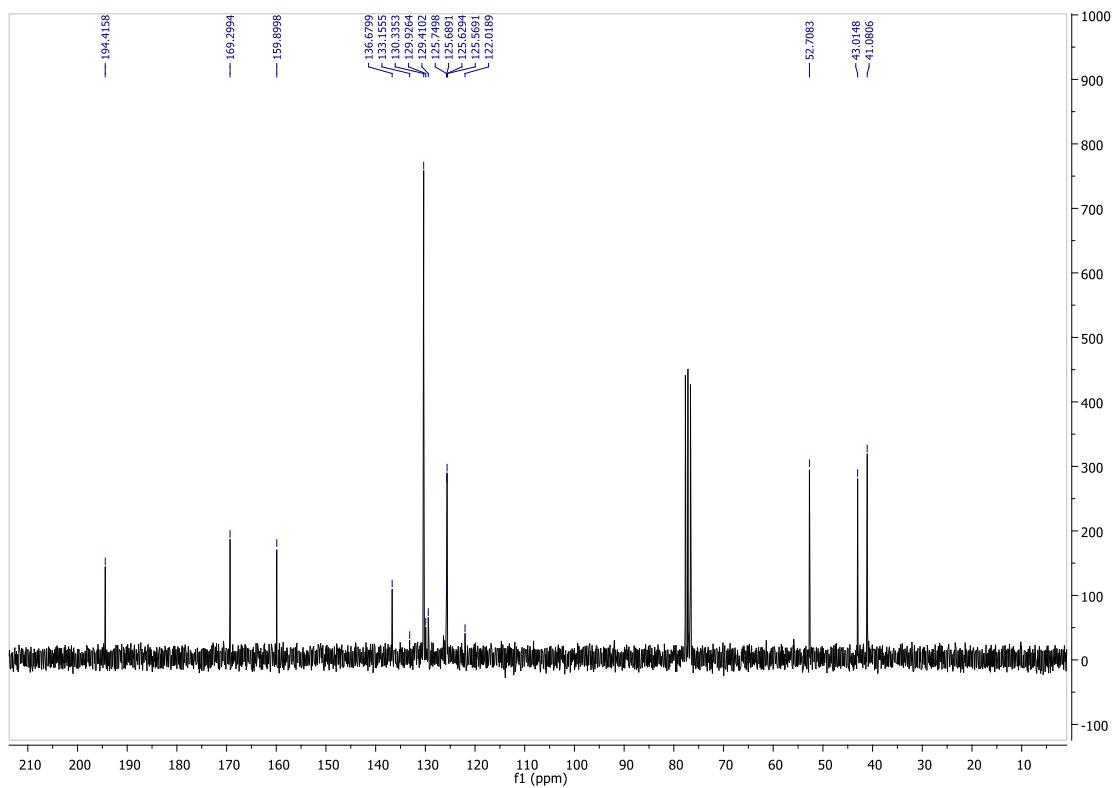
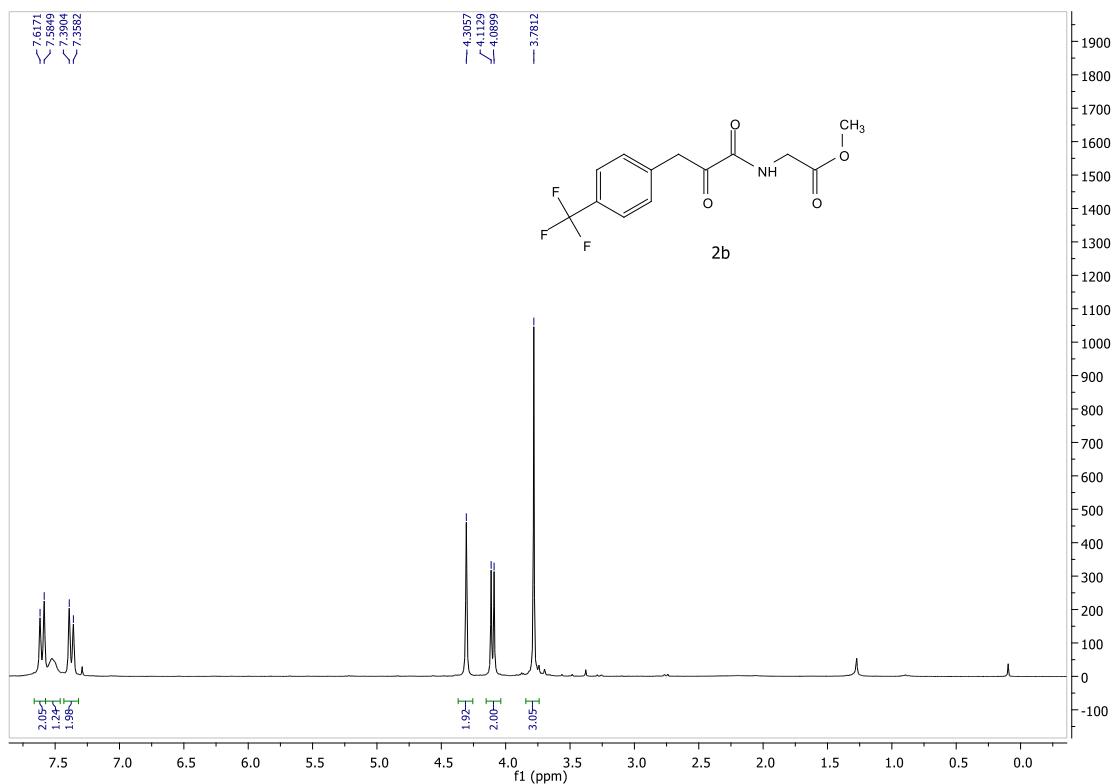
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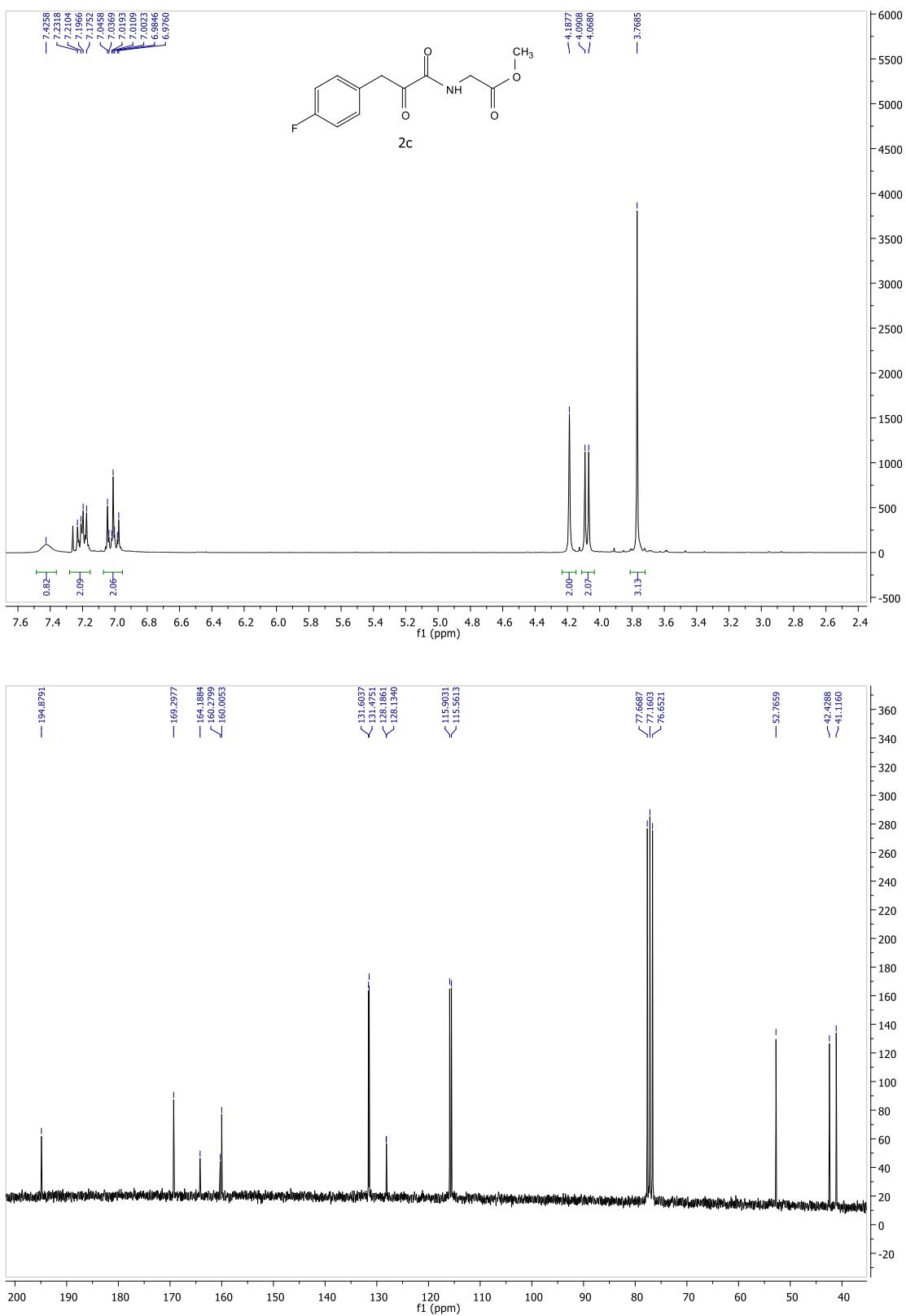
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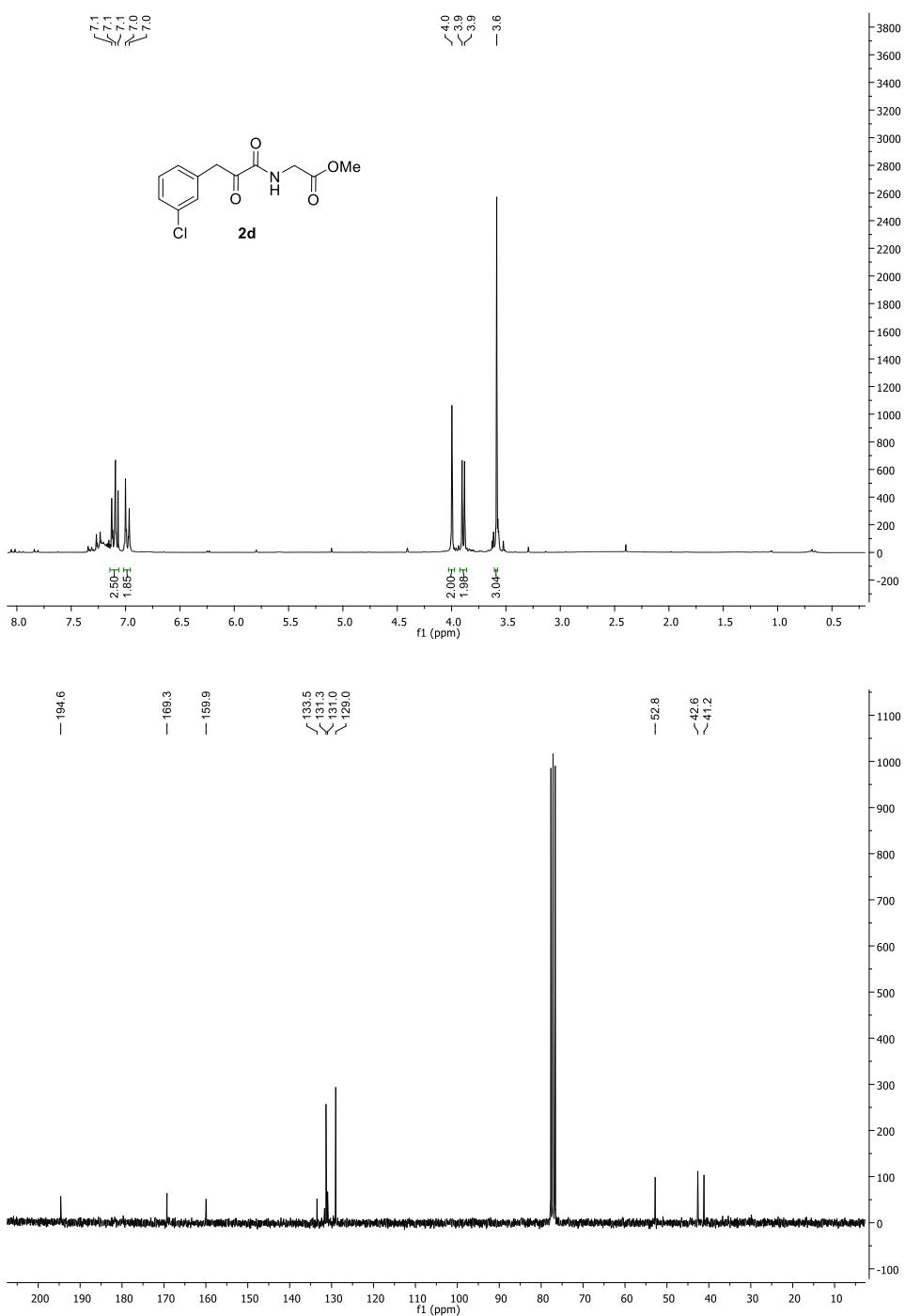
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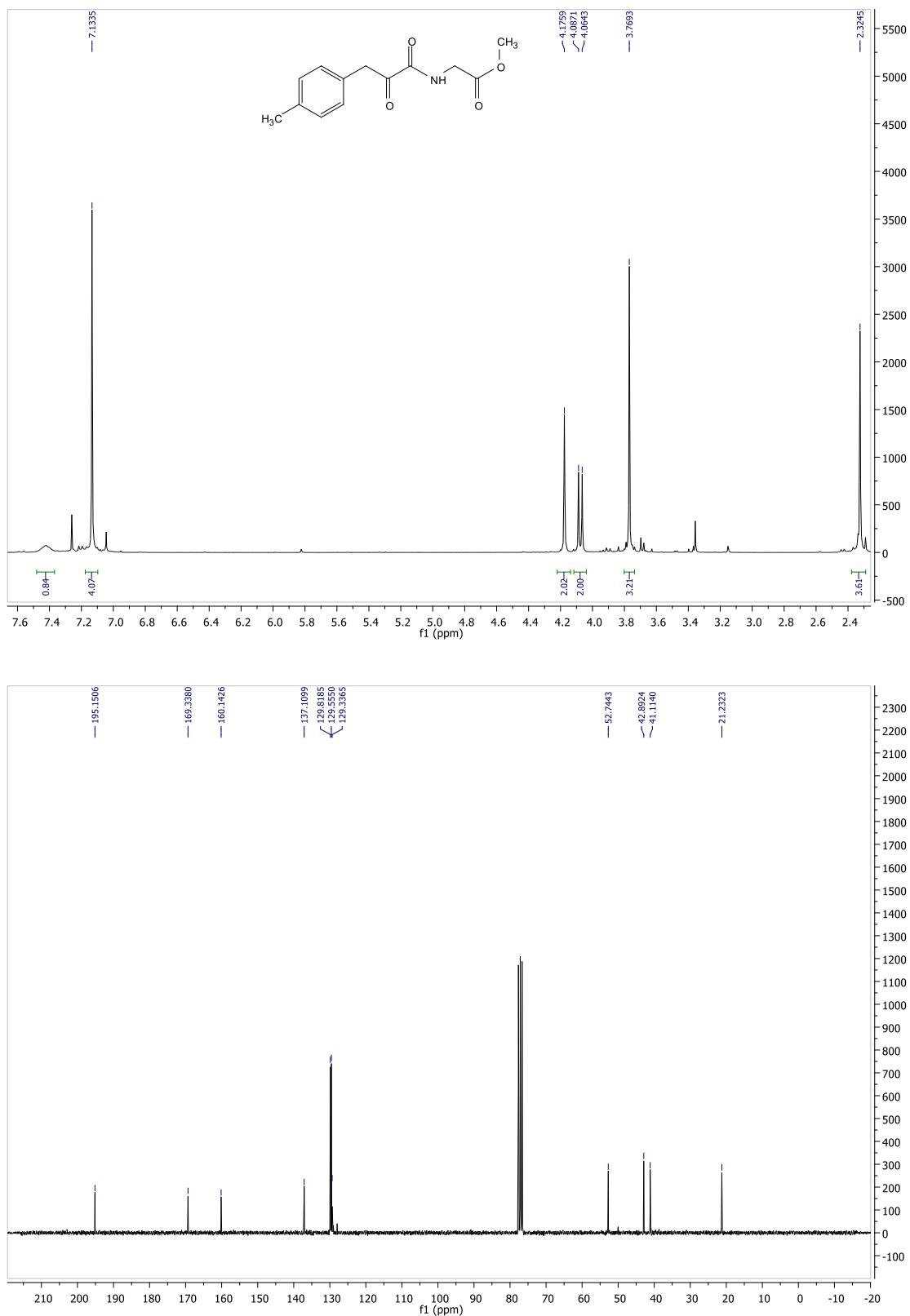
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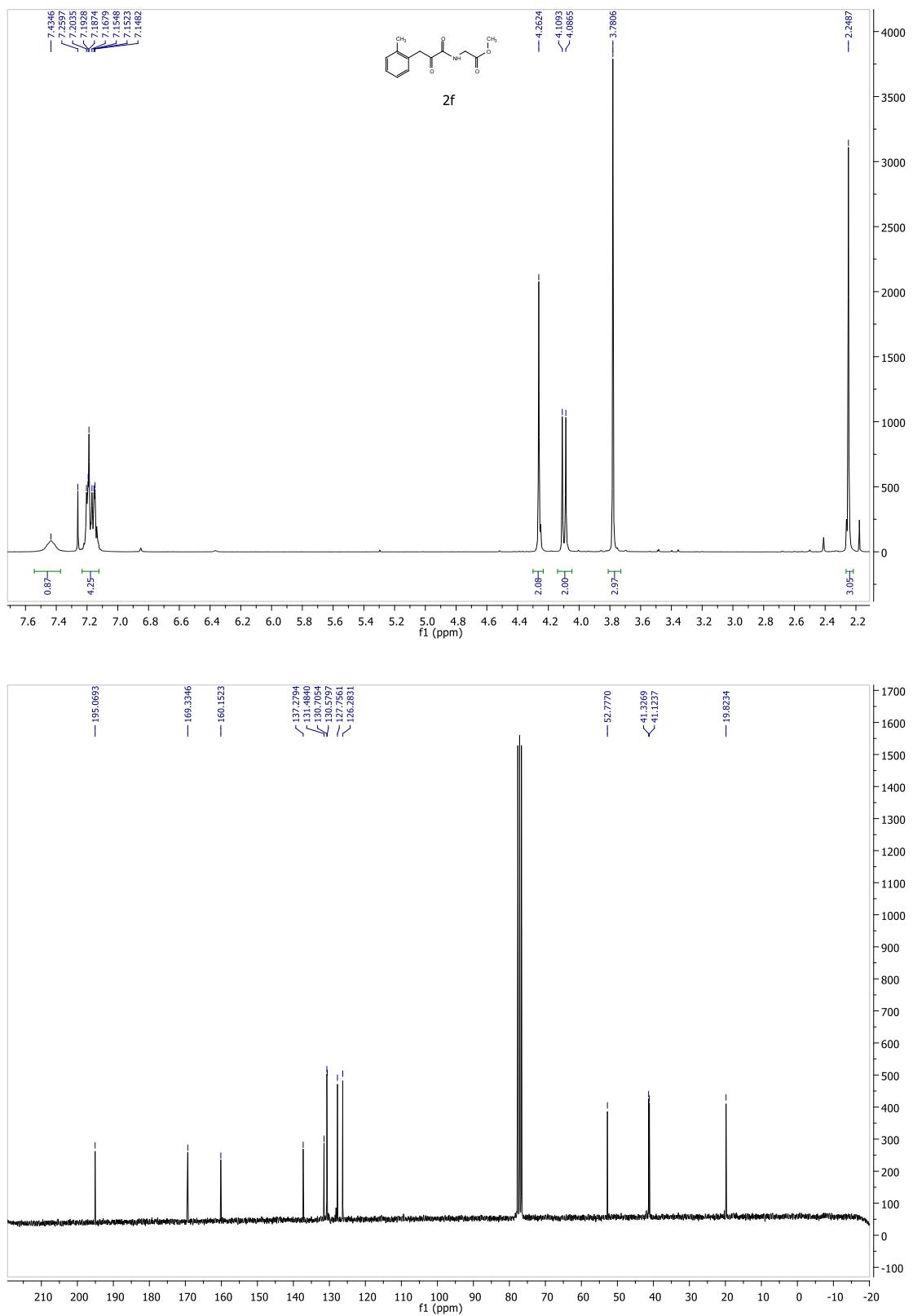
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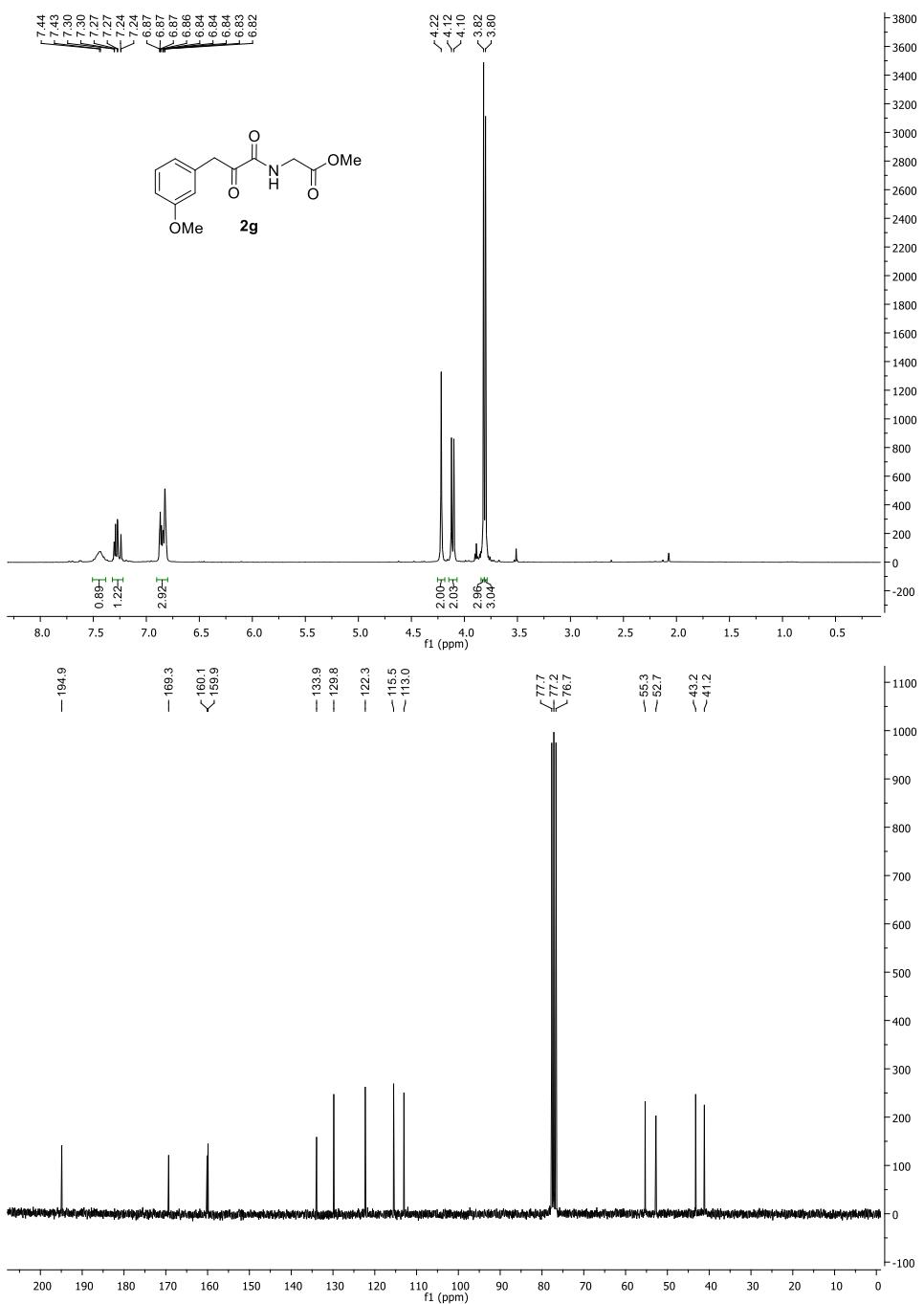
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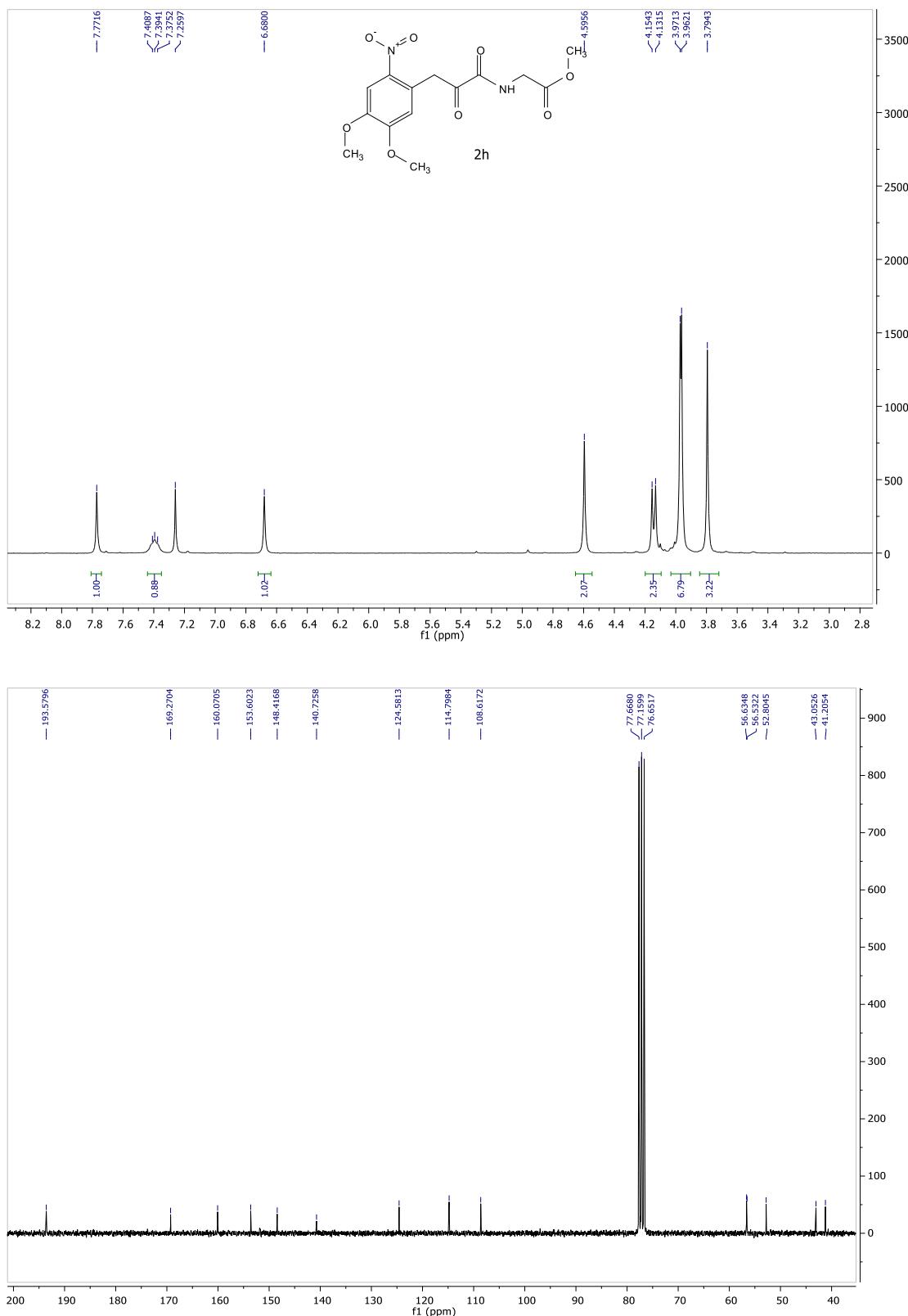
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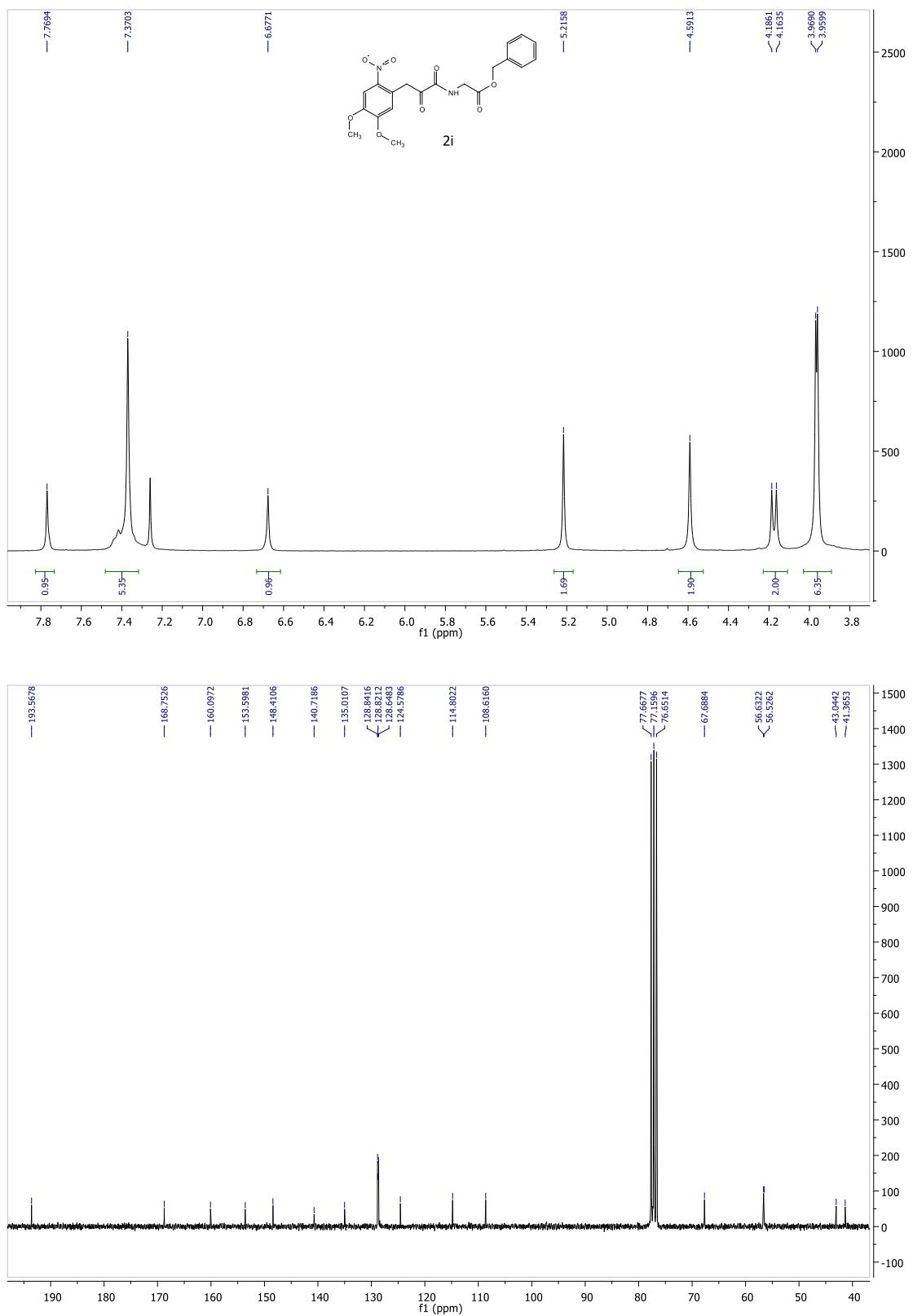
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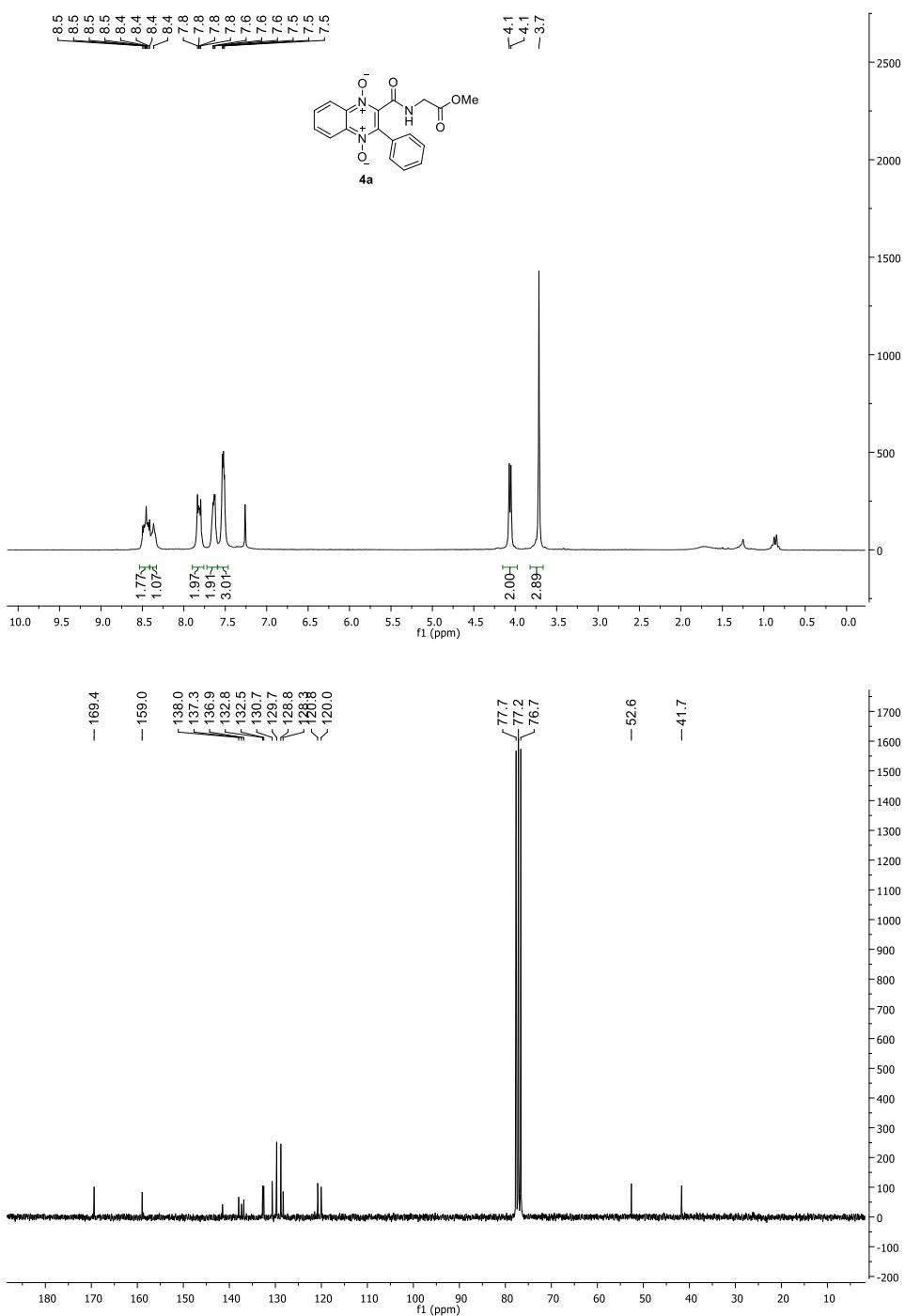
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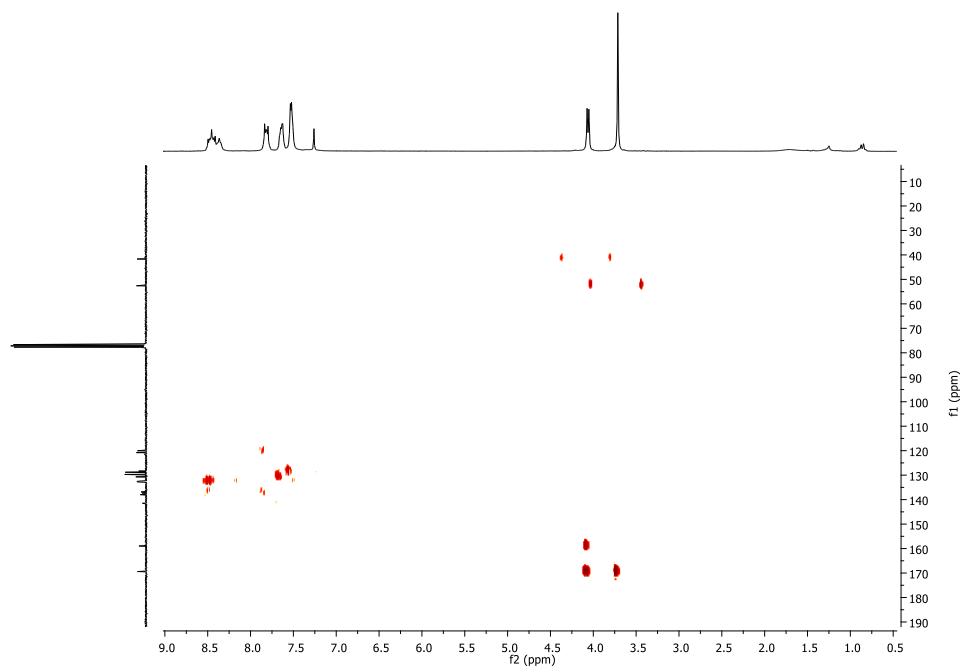
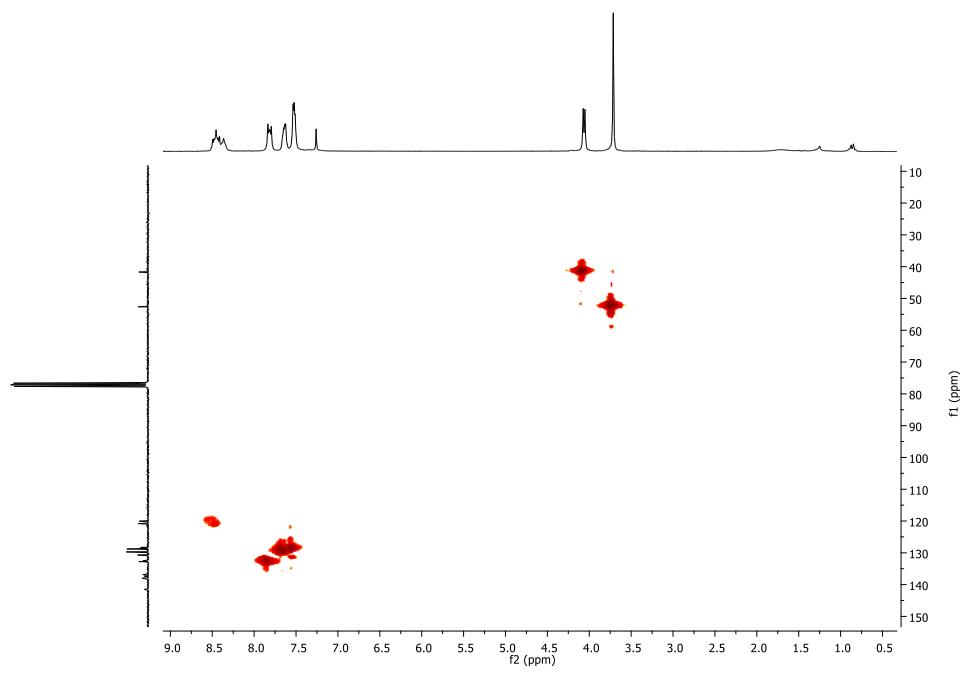


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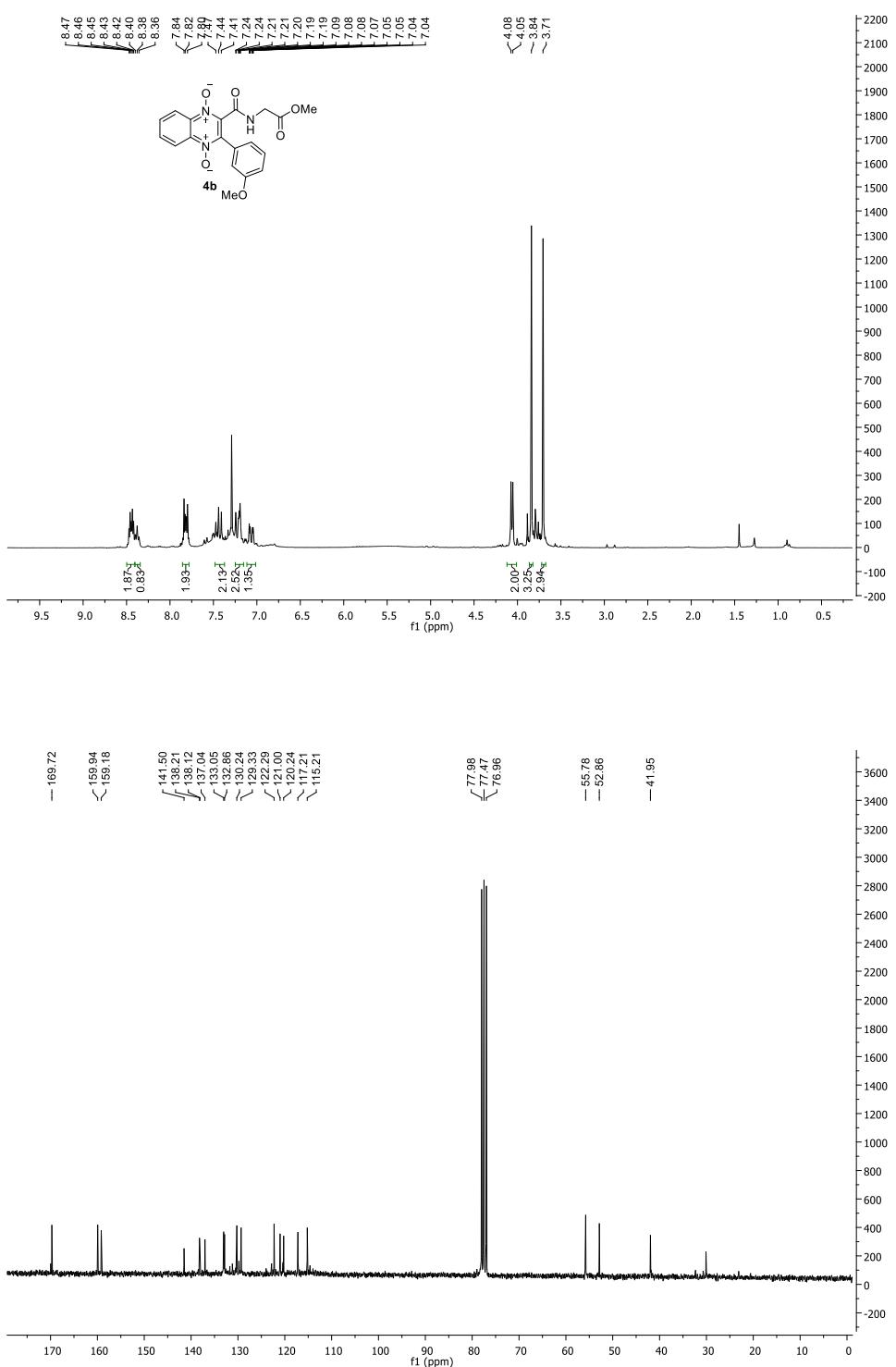


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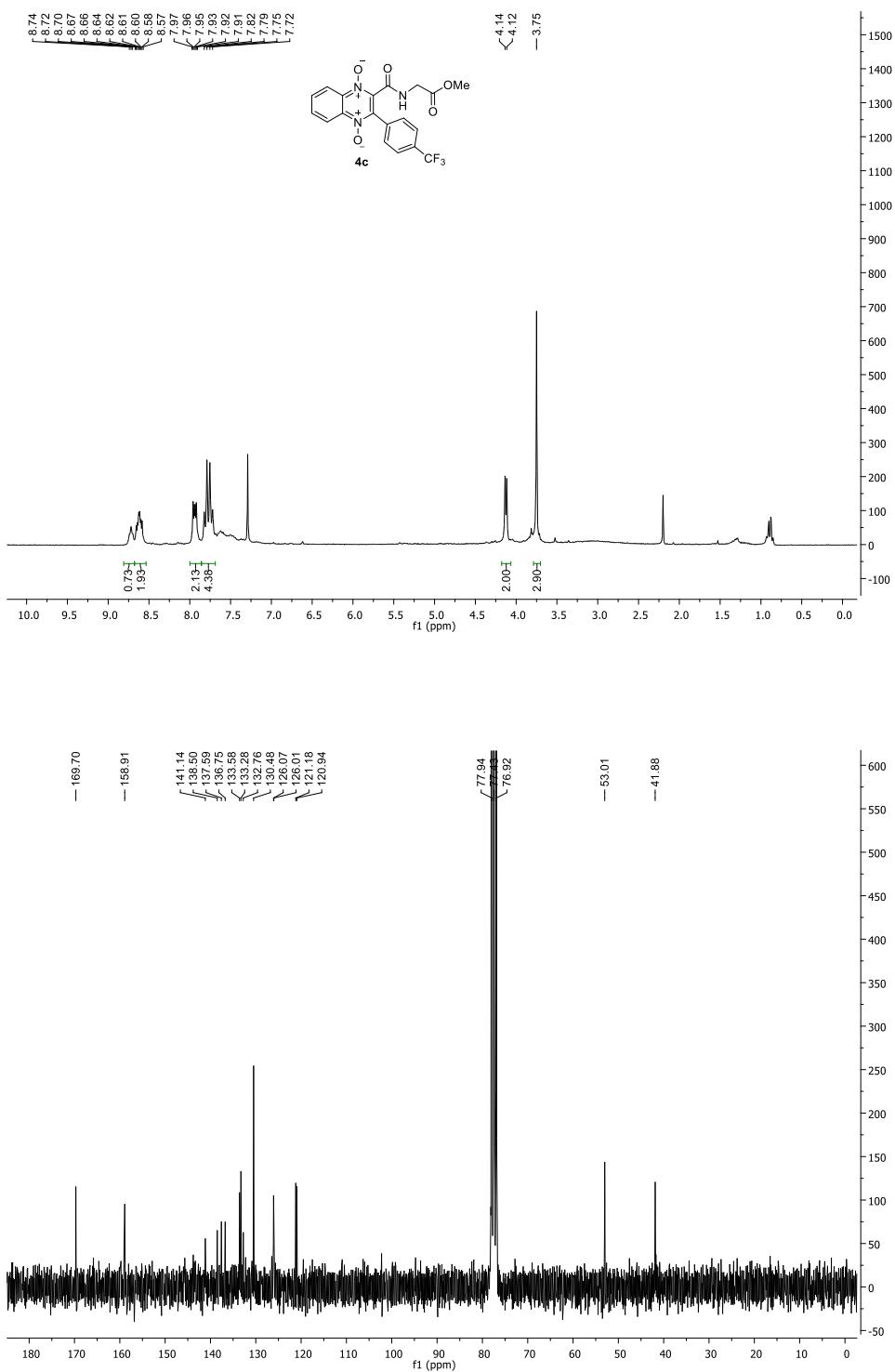




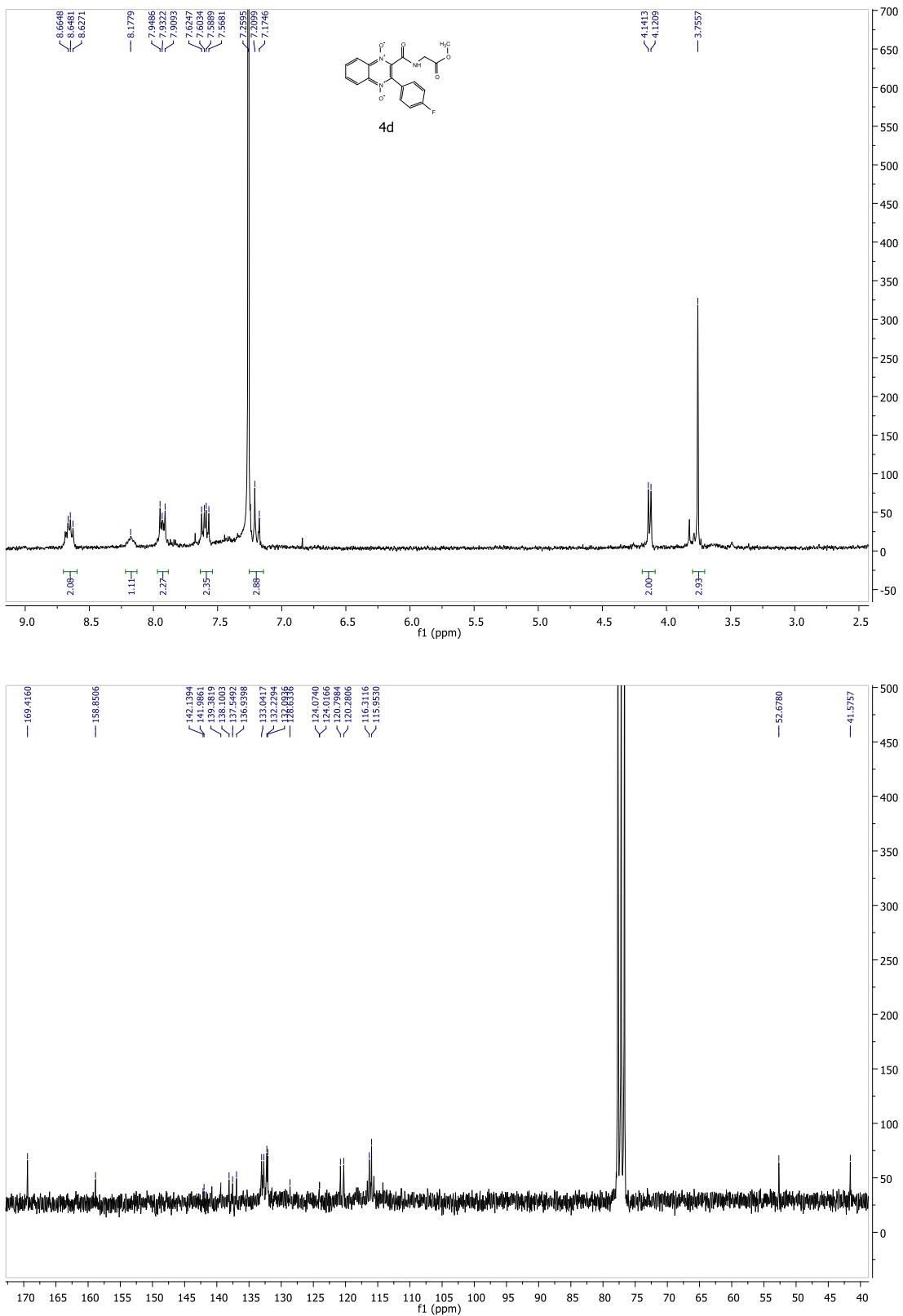
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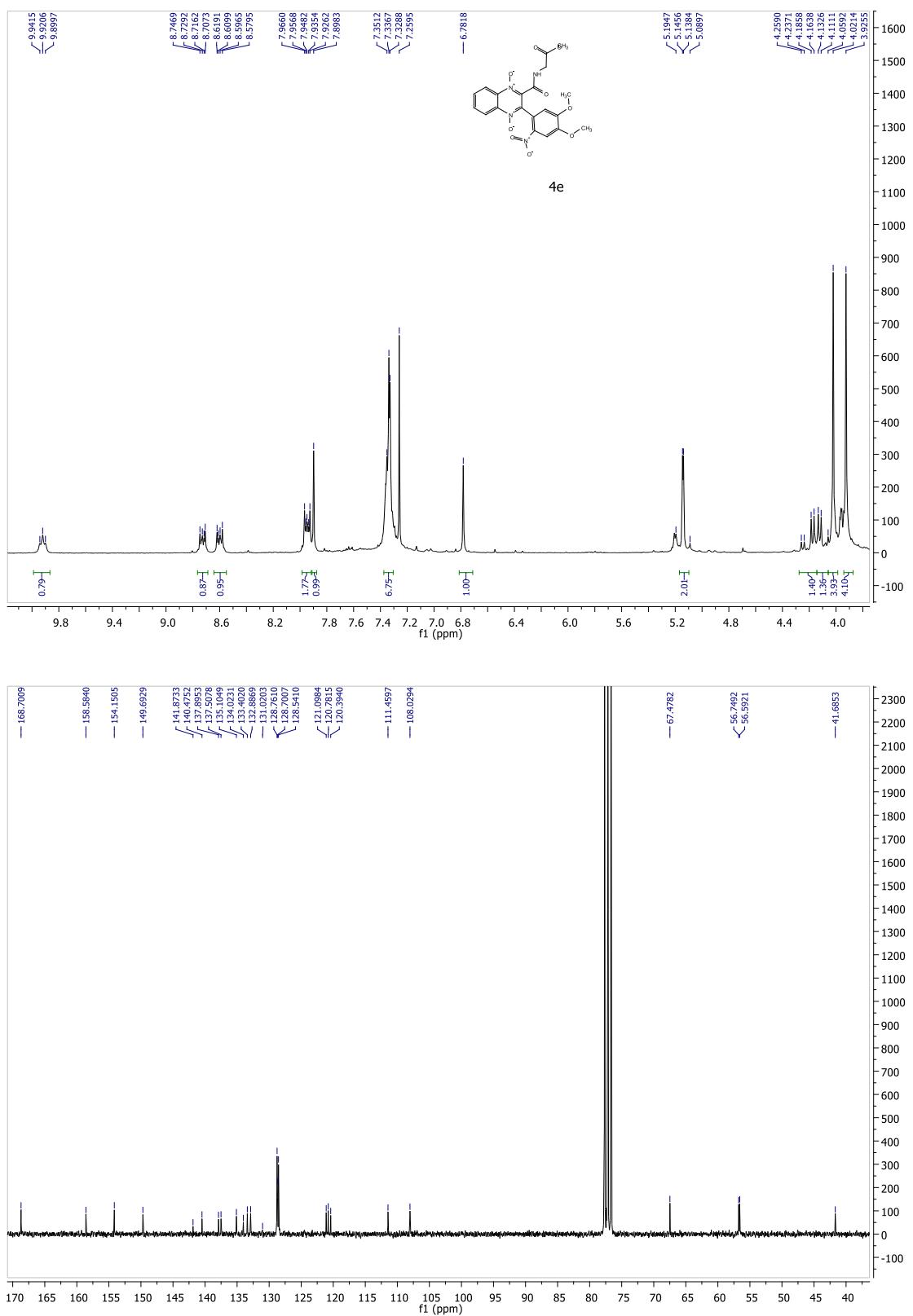
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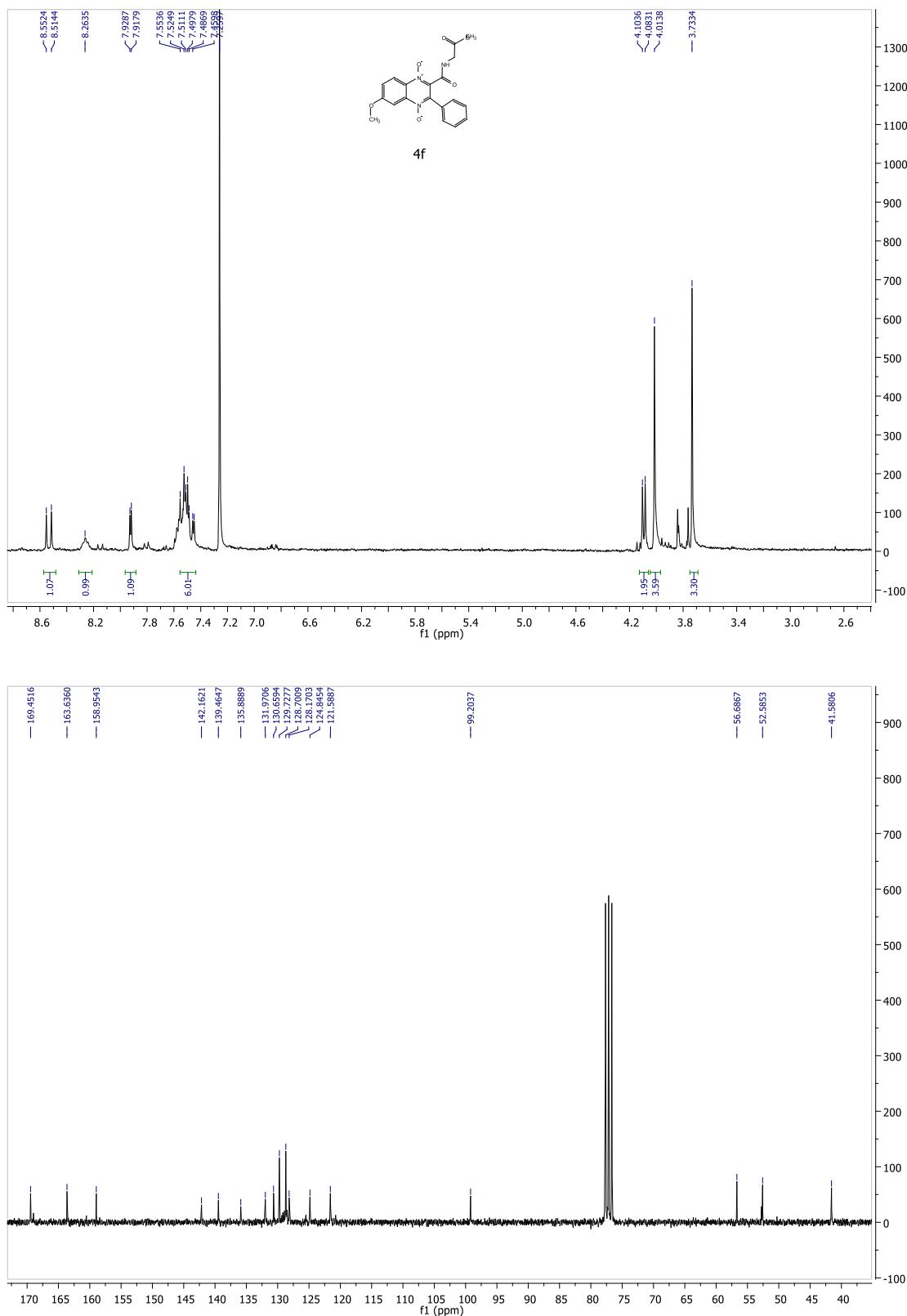
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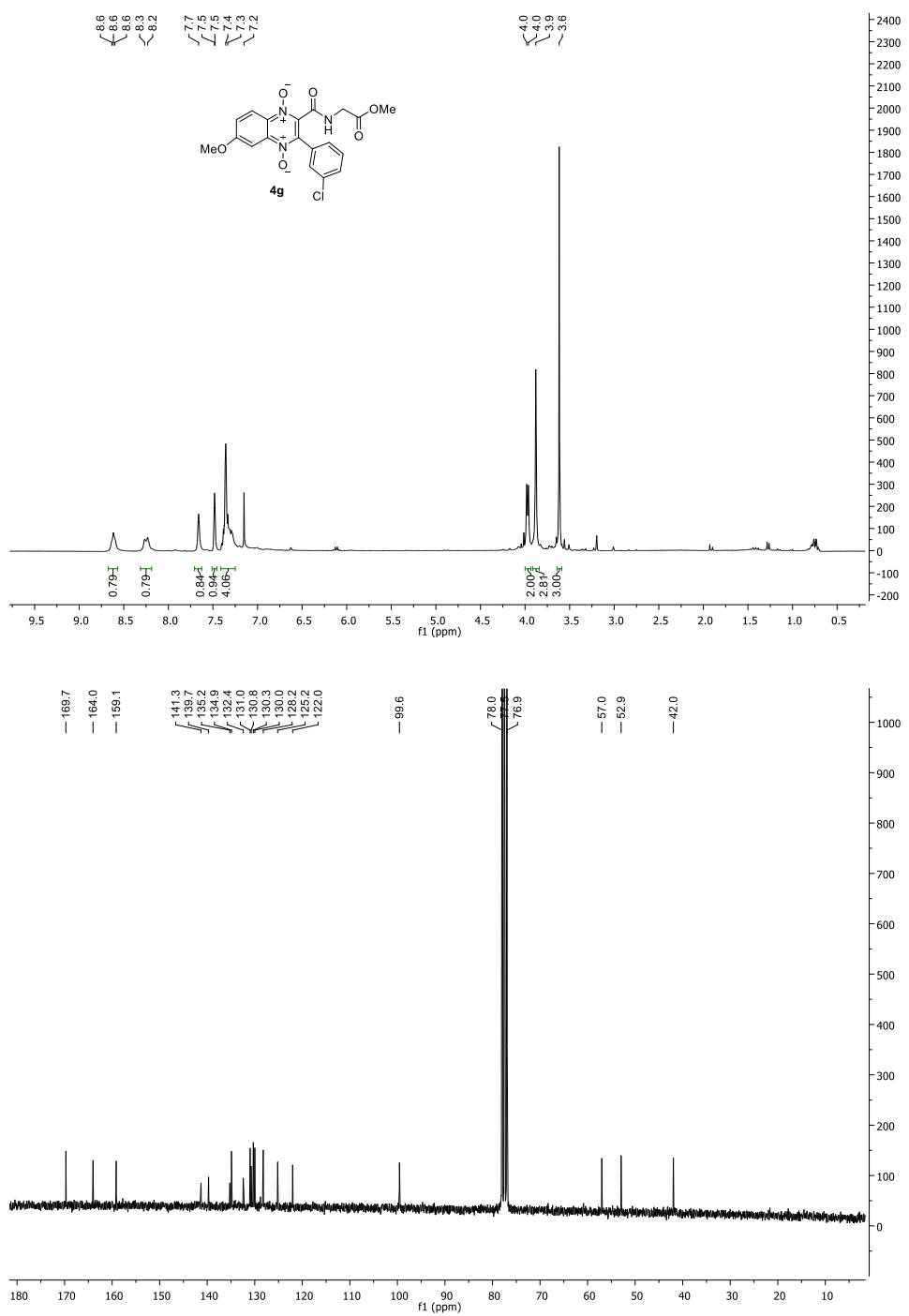
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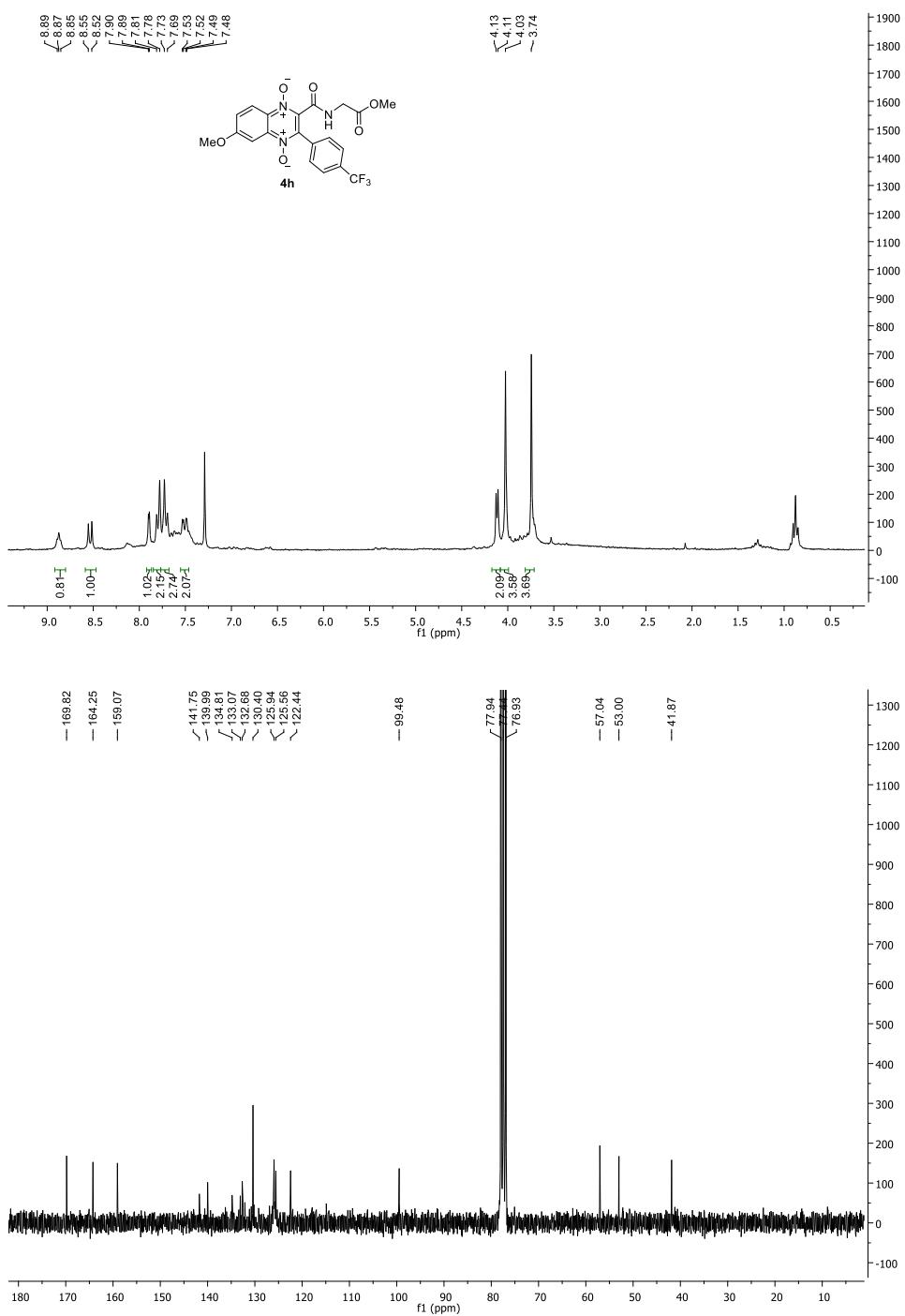
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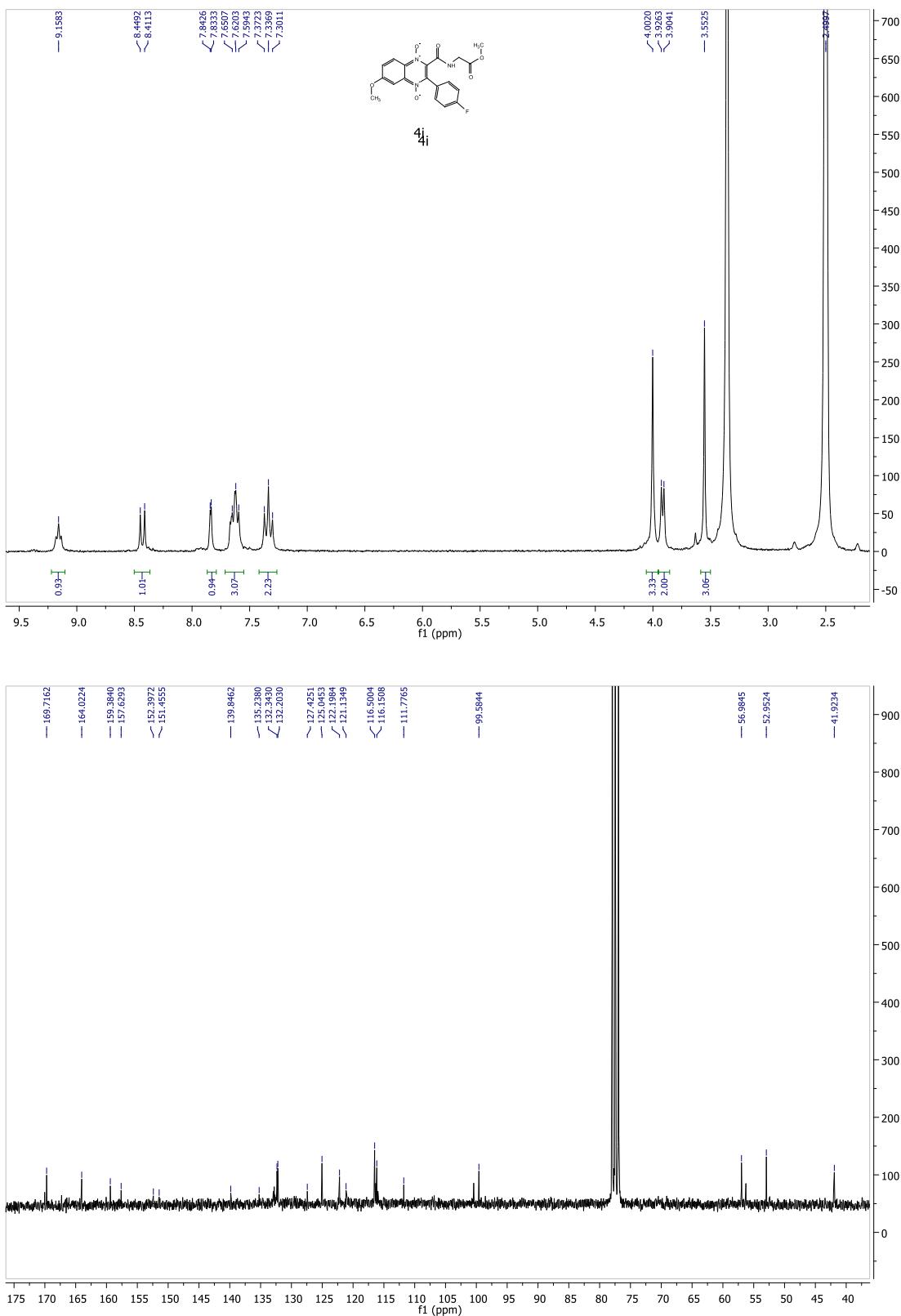
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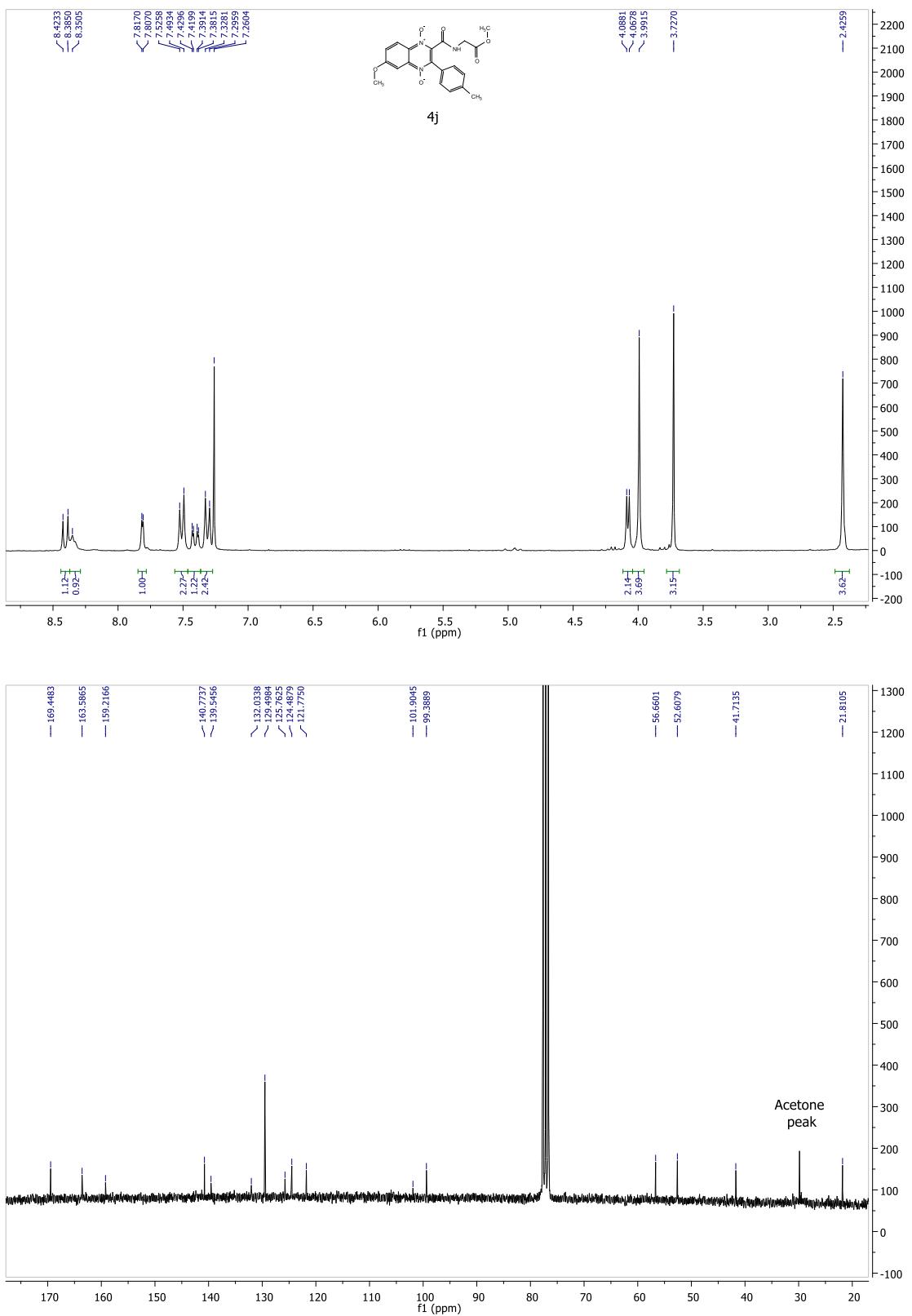
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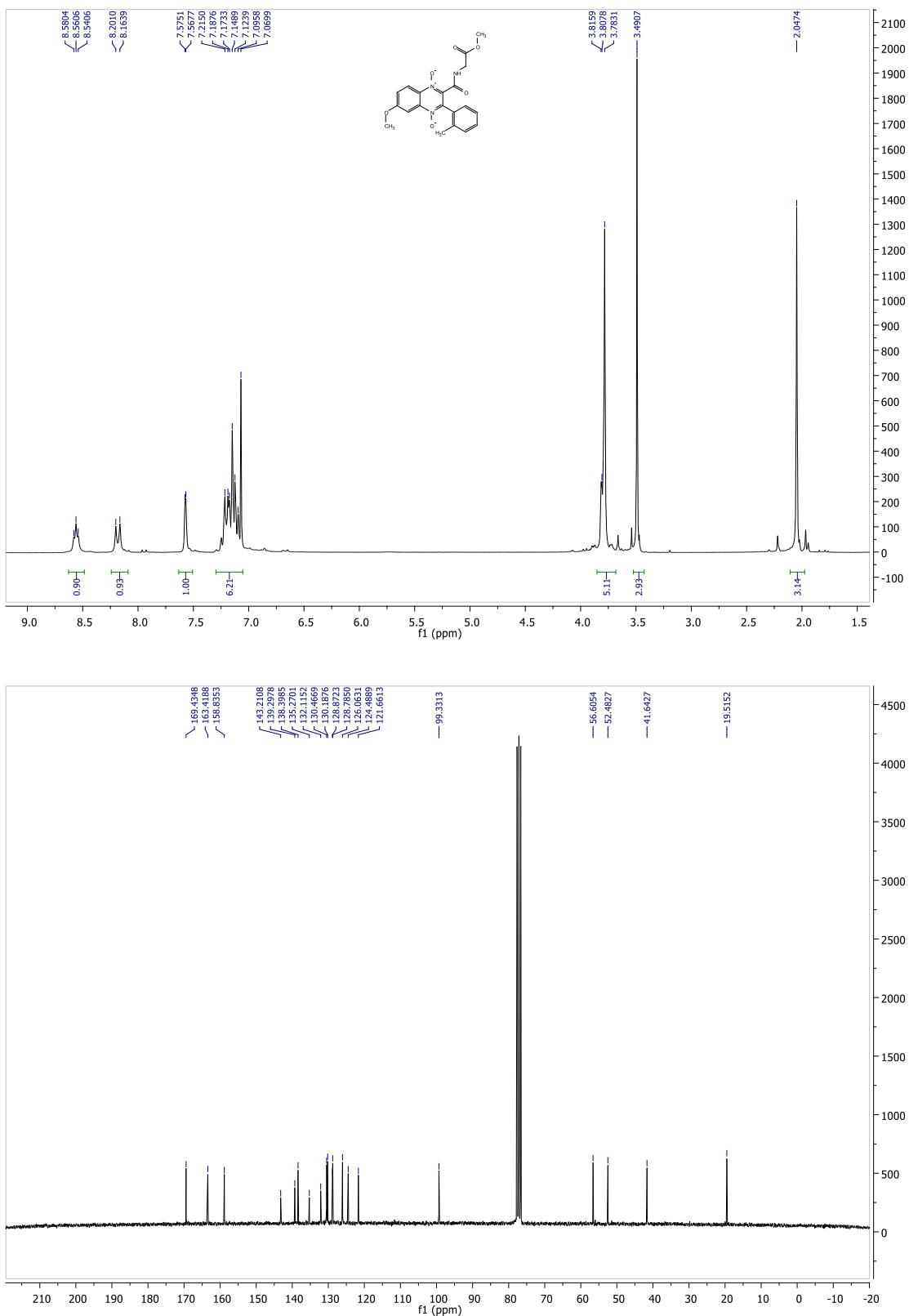
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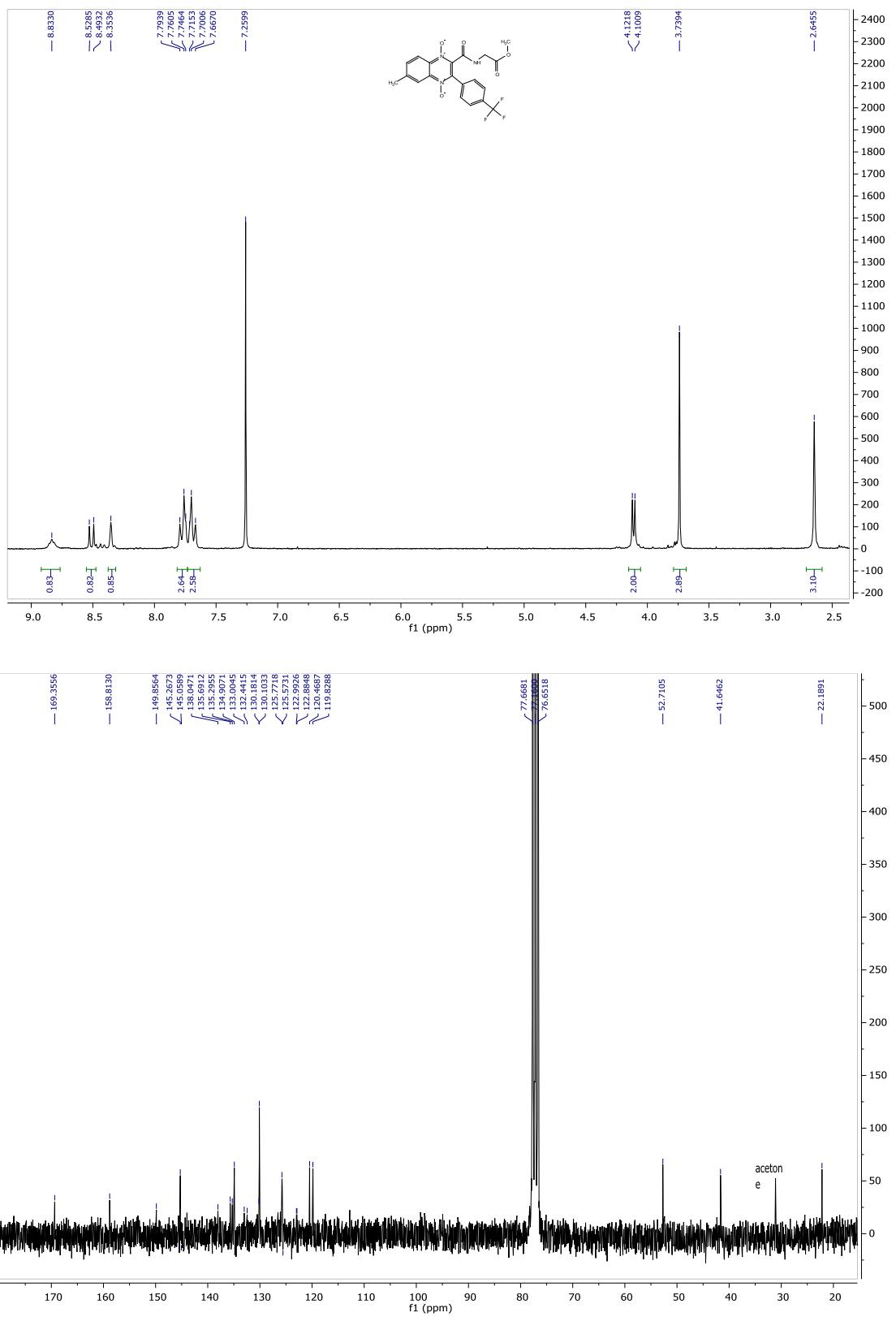
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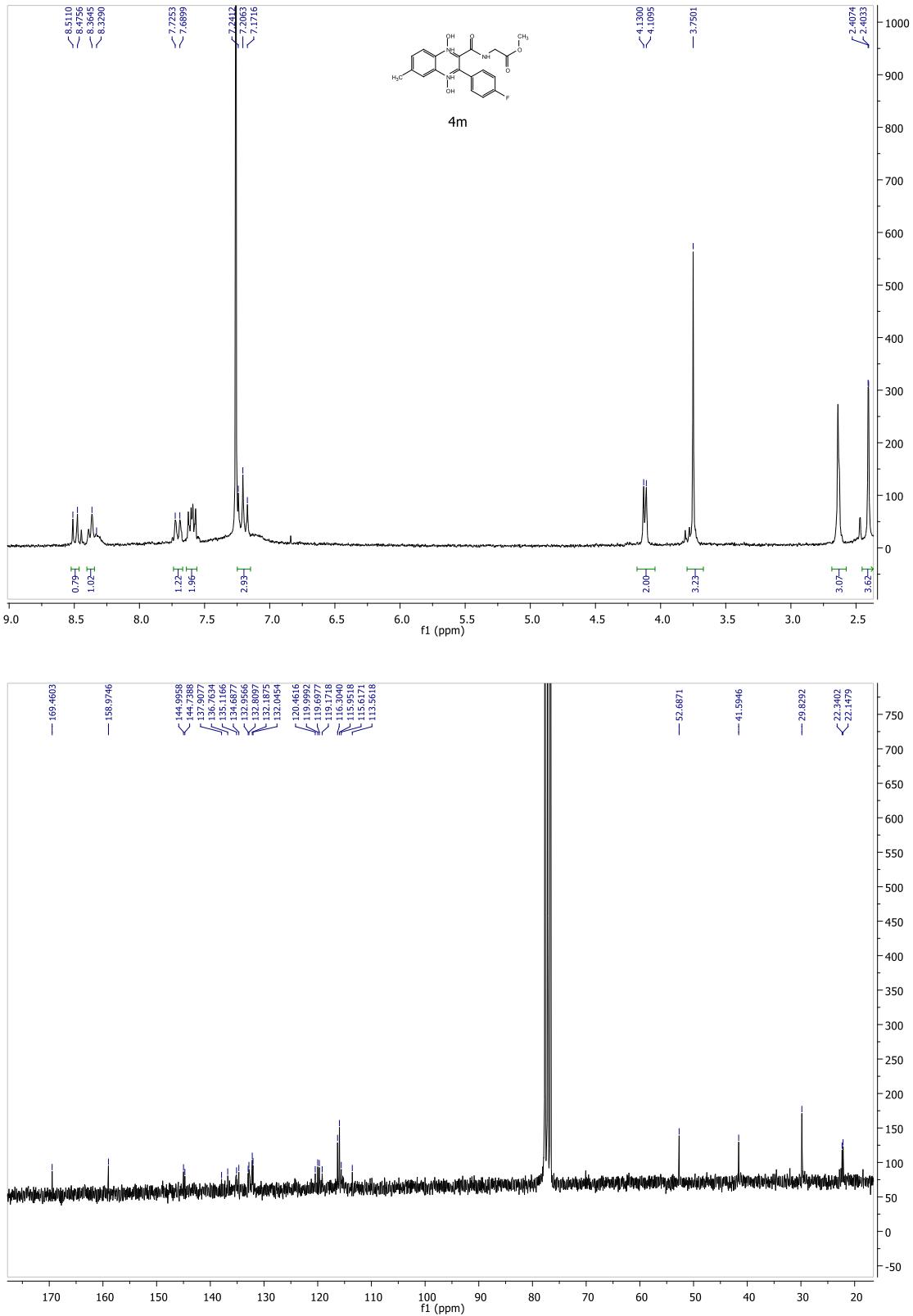
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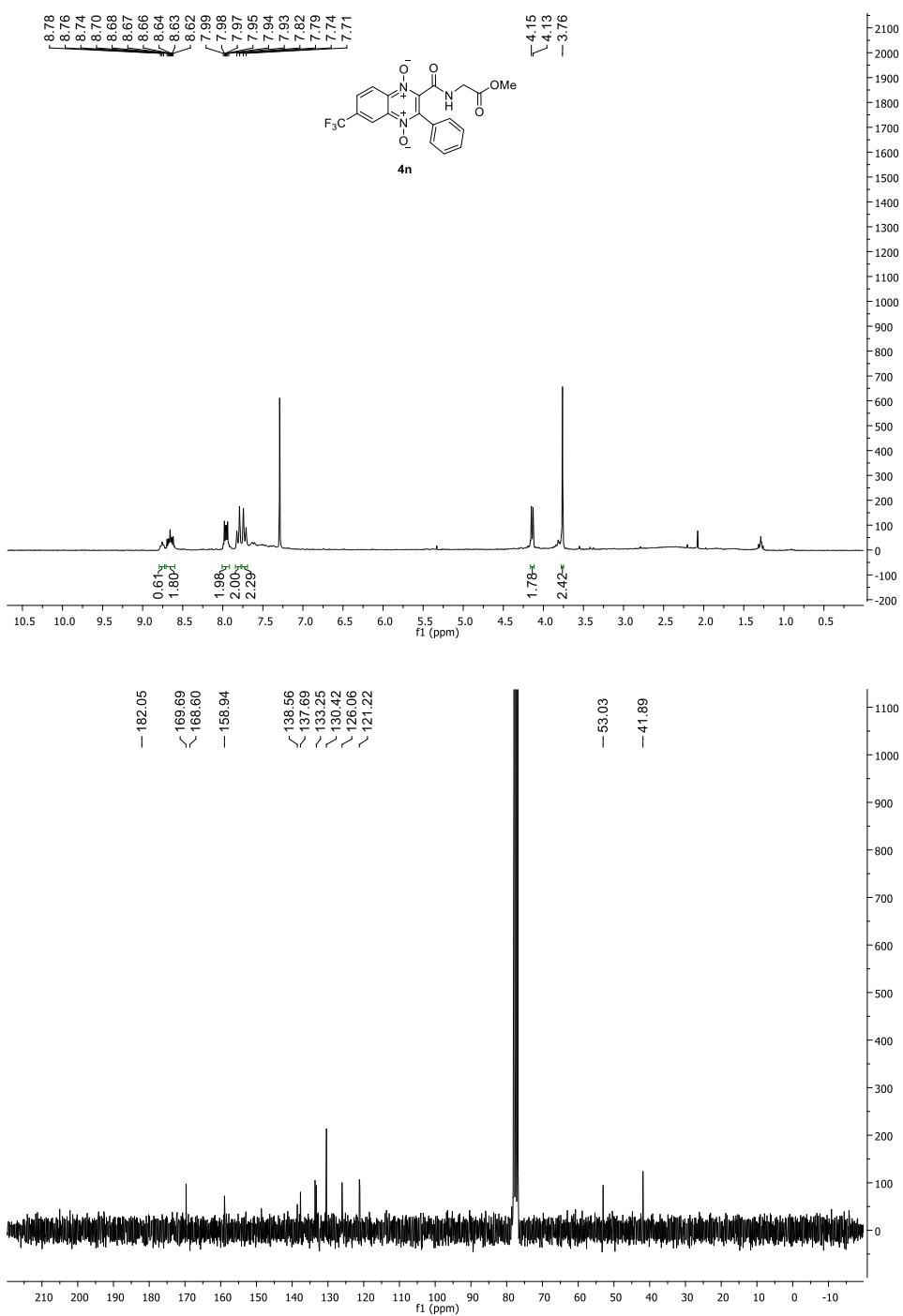
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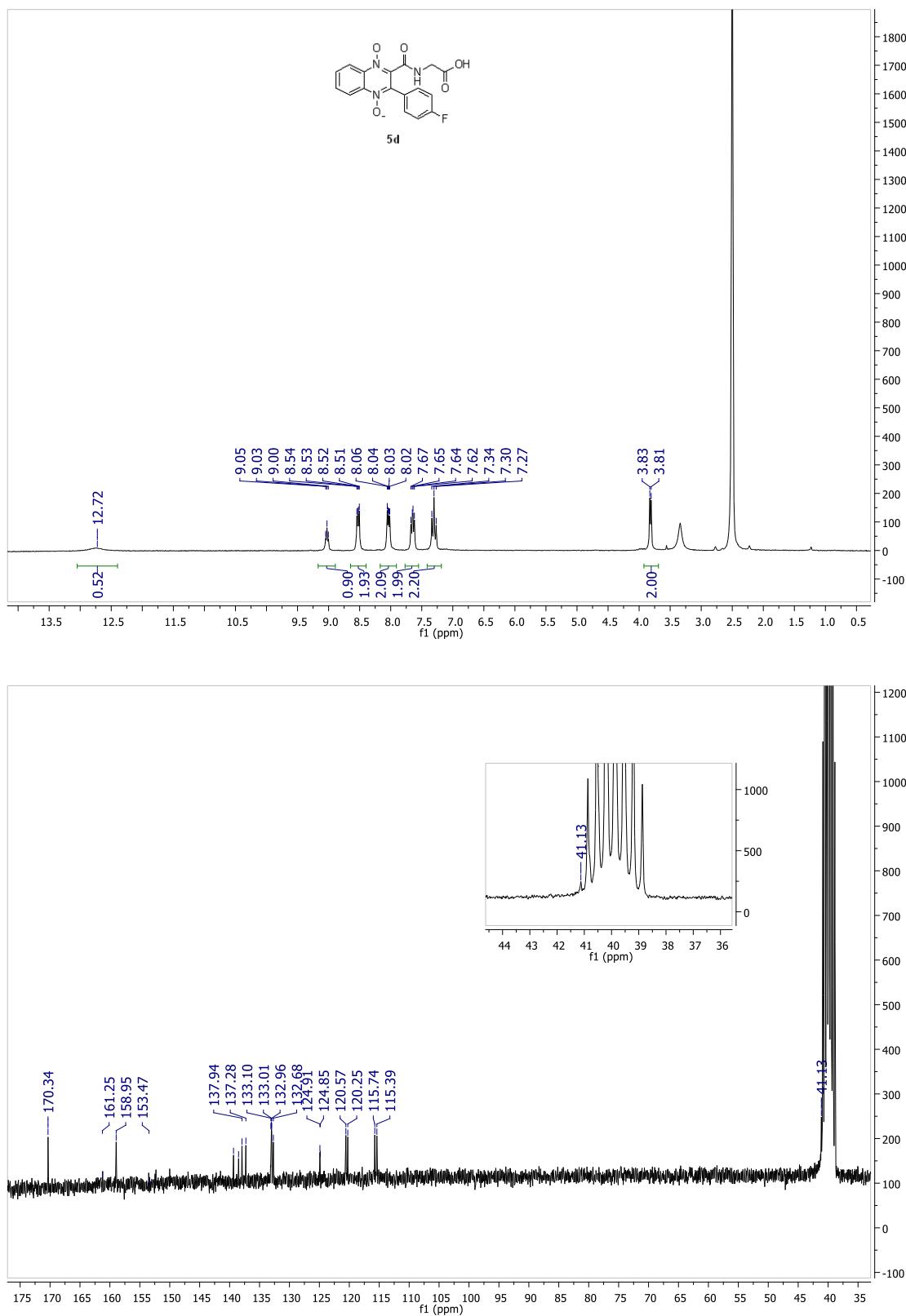
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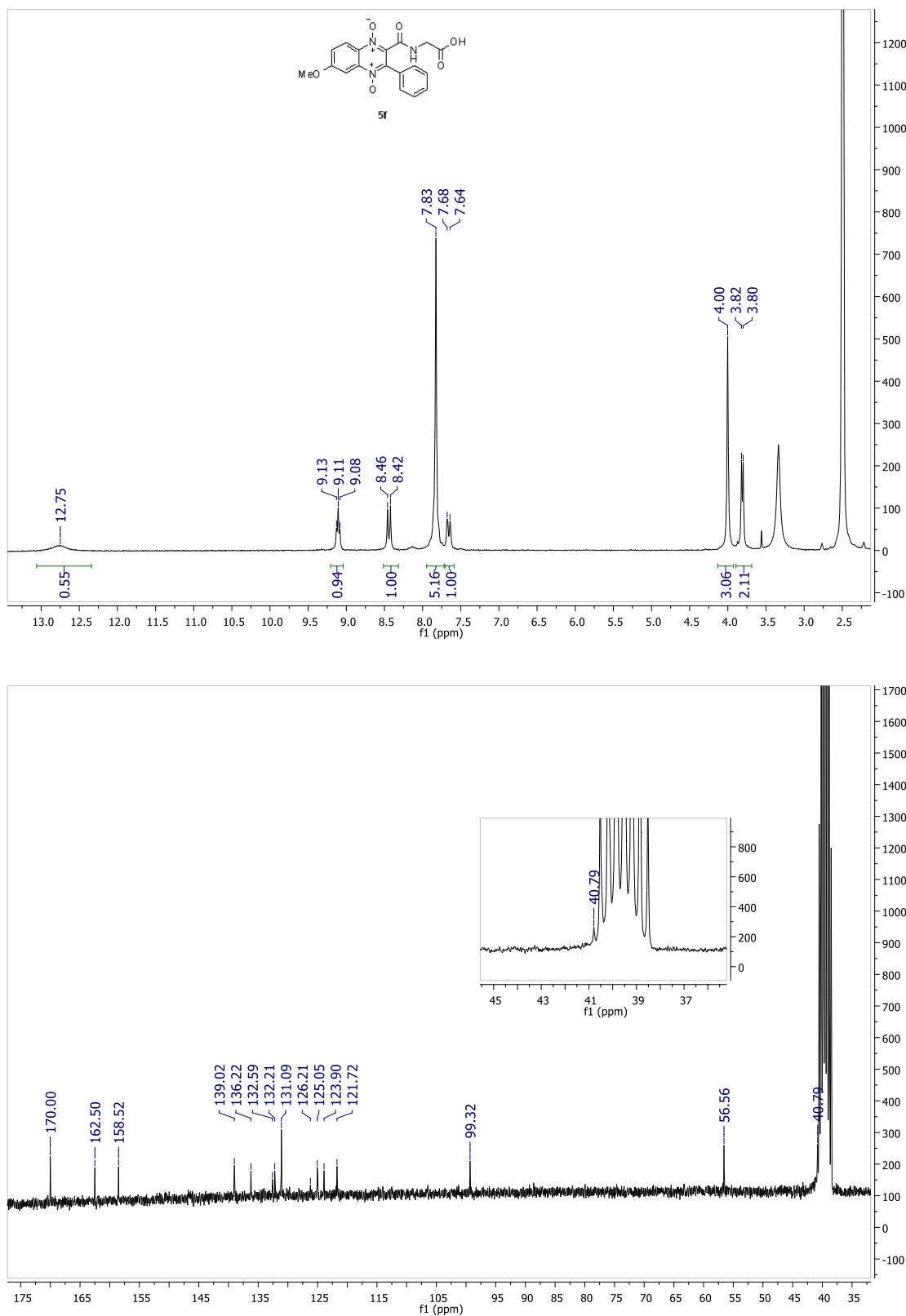
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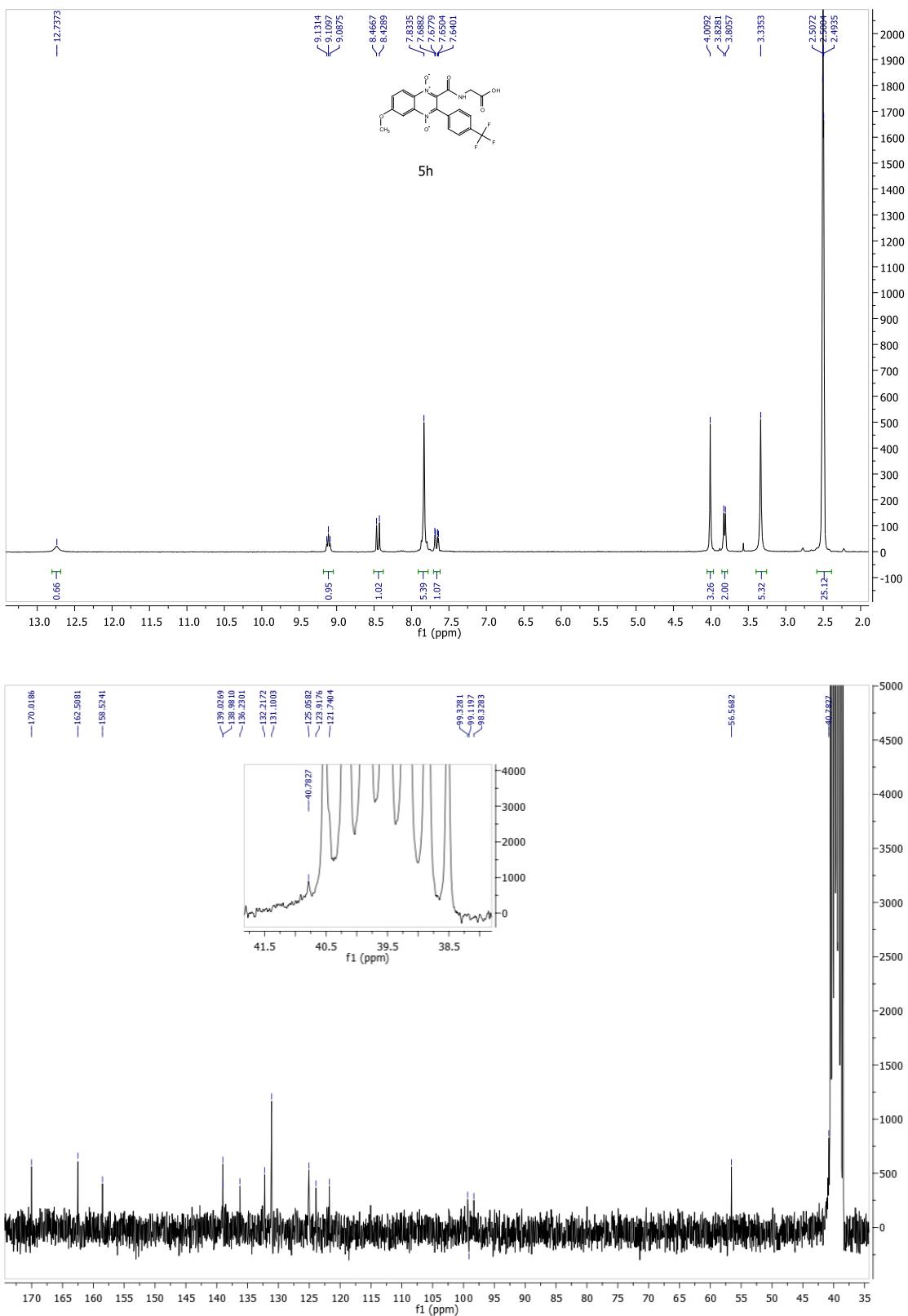
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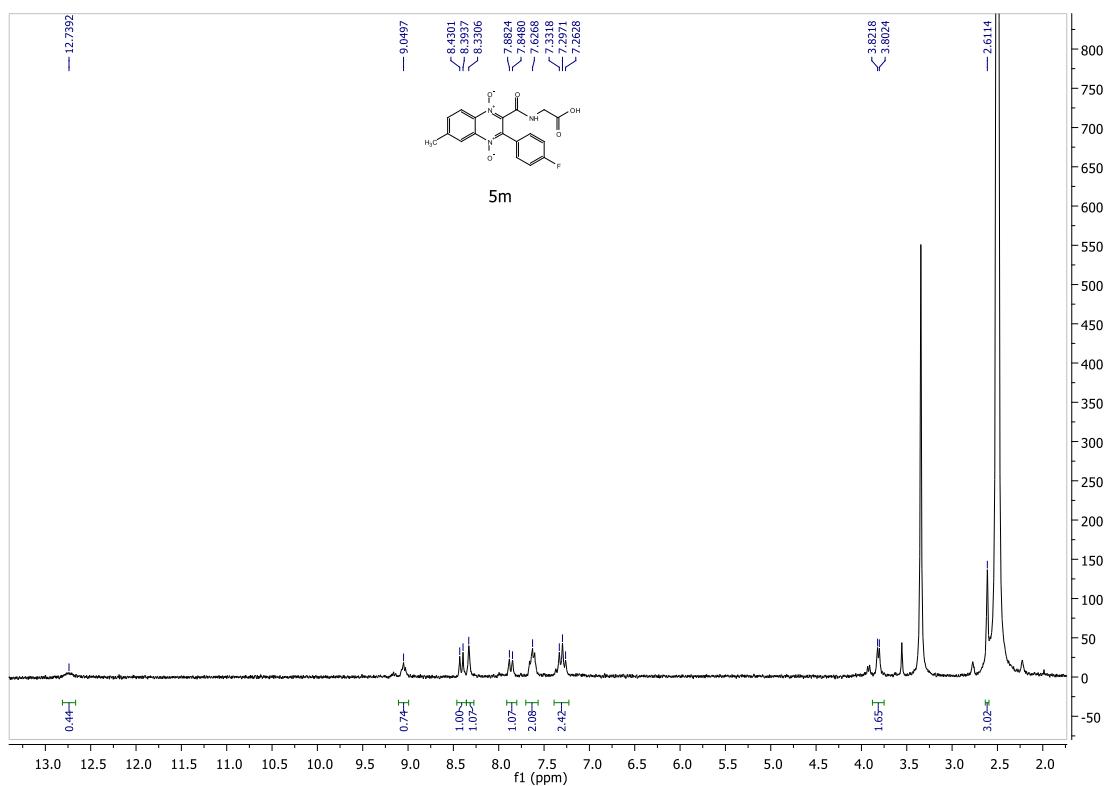
### Compound 5f



## Compound 5h



## Compound 5m



## Compound 6

