

## Supplementary Materials

# Synthesis and structural confirmation of the thiazole alkaloids derived from *Peganum harmala* L.

Myeonghyeon Sim<sup>1</sup>, Sujin Lee<sup>2,\*</sup> and Young Taek Han<sup>1,\*</sup>

<sup>1</sup>College of Pharmacy, Dankook University, Cheonan 31116, Korea;

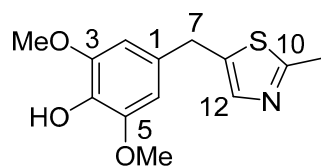
<sup>2</sup>College of Pharmacy, Daegu Catholic University, Gyungsan 38430, Korea;

\*Correspondence: hanyt@dankook.ac.kr (Y. T. Han); Tel.: +82-41-550-1431; sujinlee@cu.ac.kr (S. Lee)

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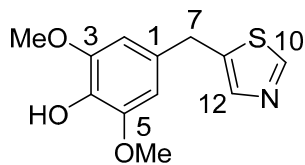
Table S1. <sup>1</sup>H- and <sup>13</sup>C-NMR assignment of Peganum B.



Position	Reported		Synthesized	
	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$
1		130.1		130.1
2	6.50(s)	105.8	6.51(s, 1H)	105.9
3		148.0		148.0
3-OCH <sub>3</sub>	3.71(s, 3H)	56.0	3.71(s, 3H)	56.0
4		134.1		134.2
4-OH	8.21(br s, 1H)		8.18(br s, 1H)	
5		148.0		148.0
5-OCH <sub>3</sub>	3.71(s, 3H)	56.0	3.71(s, 3H)	56.0
6	6.50(s, 1H)	105.8	6.51(s, 1H)	105.9
7	3.98(s, 2H)	32.3	3.98(s, 2H)	32.3
8		138.8		138.8
9				-
10		164.1		164.1
10-CH <sub>3</sub>	2.55(s, 3H)	18.8	2.55(s, 3H)	18.8
11				-
12	7.38 (s, 1H)	139.1	7.38 (s, 1H)	139.1

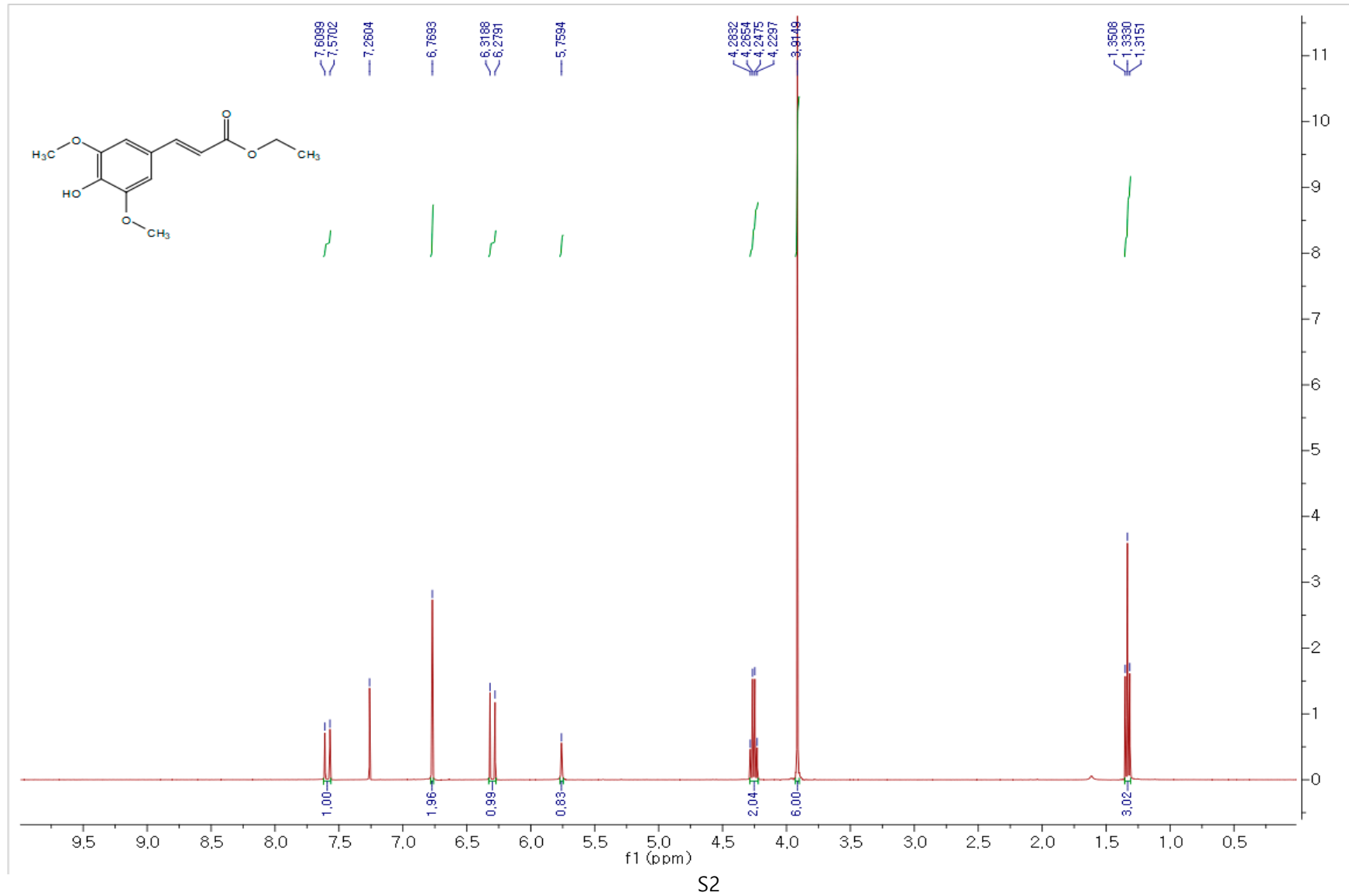
<sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded in DMSO at 500 MHz and 125 MHz, respectively.

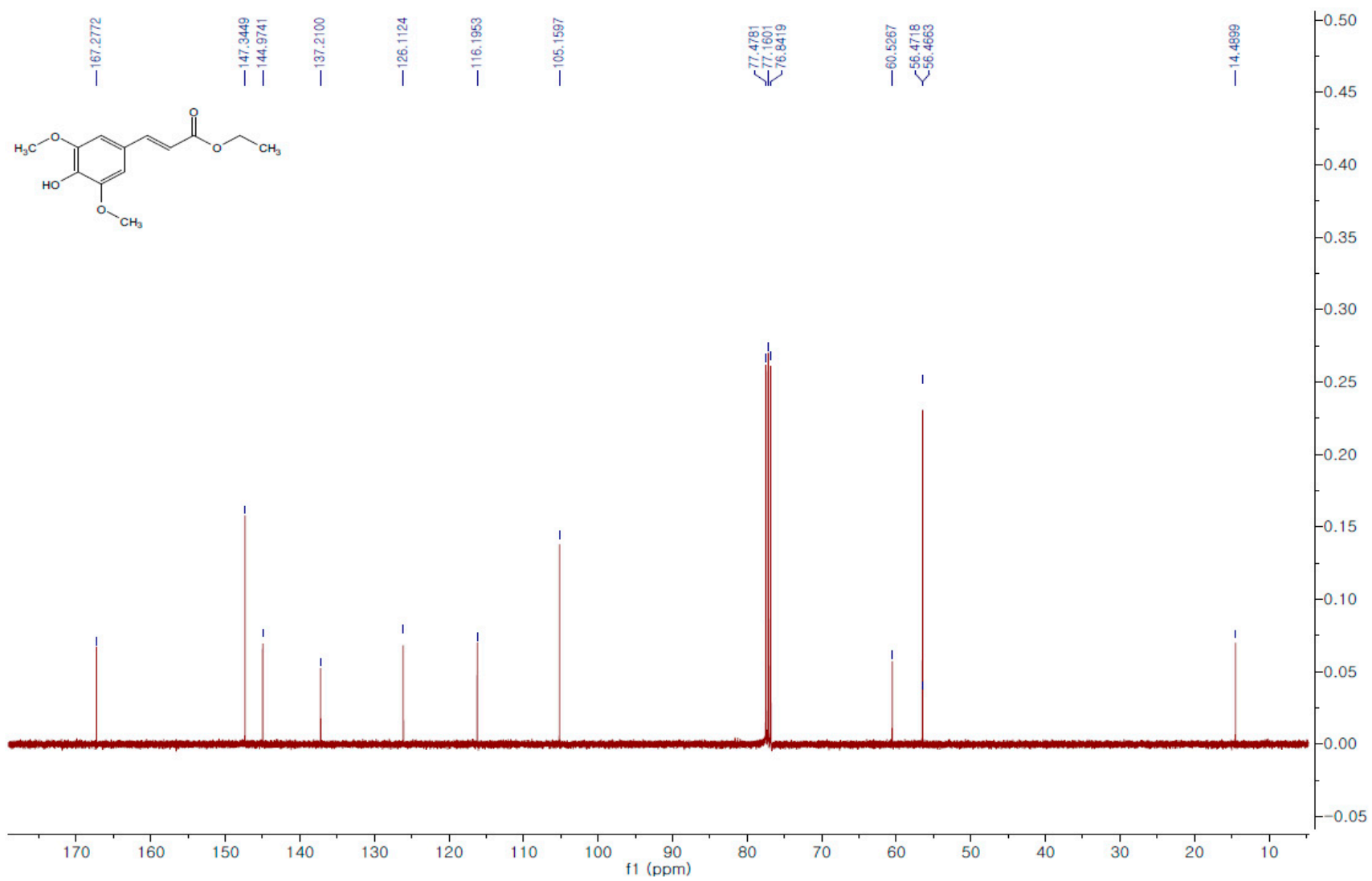
Table S2. <sup>1</sup>H- and <sup>13</sup>C-NMR assignment of Peganum A



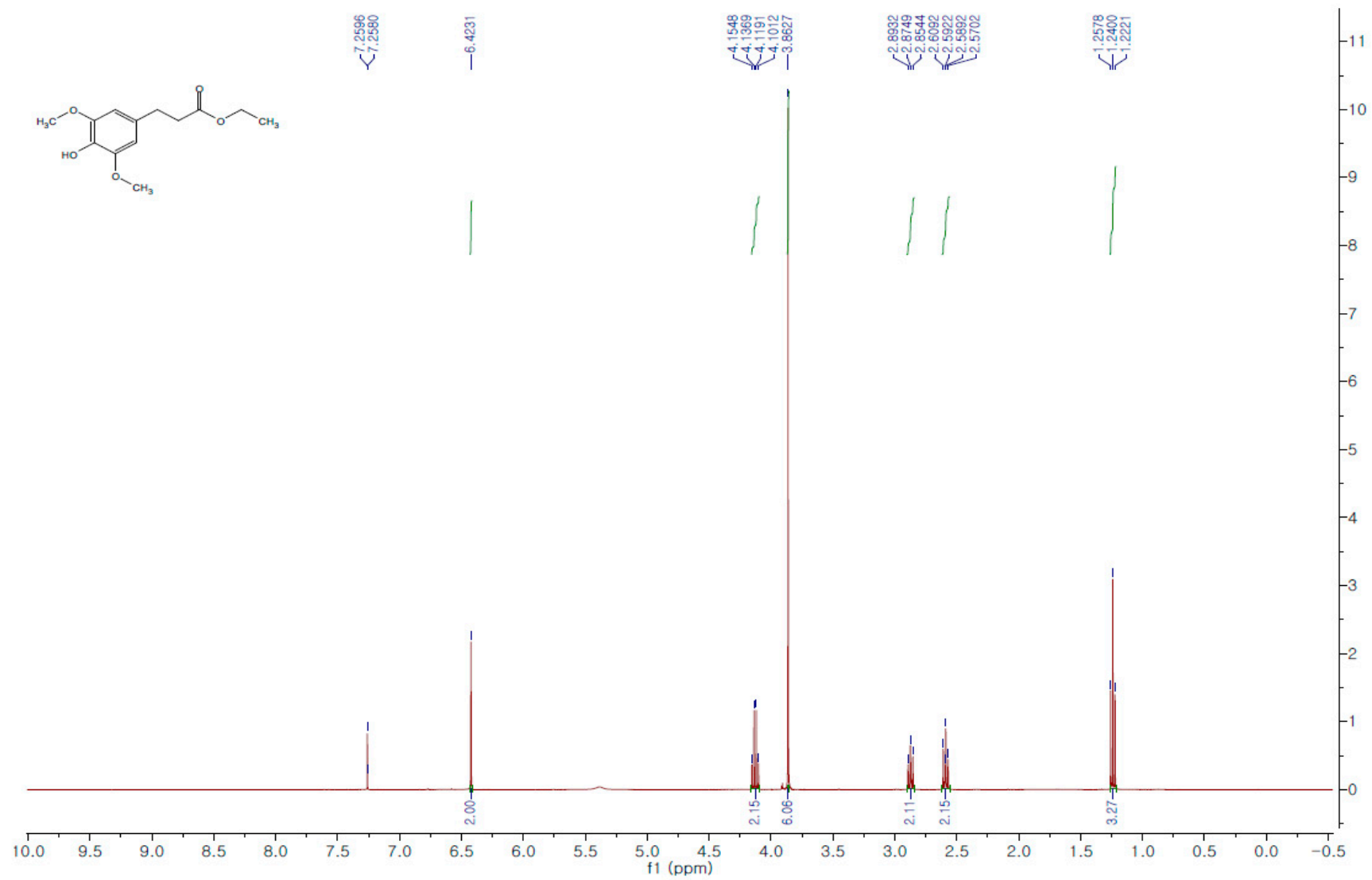
Position	Reported		Synthesized	
	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$
1		130.0		130.0
2	6.52 (s, 1H)	105.9	6.52 (s, 1H)	105.9
3		148.0		148.0
3-OCH <sub>3</sub>	3.71 (s, 3H)	56.0	3.71 (s, 3H)	56.0
4		134.2		134.2
4-OH	8.22 (brs, 1H)		8.21 (s, 1H)	
5		148.0		148.0
5-OCH <sub>3</sub>	3.71 (s, 3H)	56.0	3.71 (s, 3H)	56.0
6	6.52 (s, 1H)	105.9	6.52 (s, 1H)	105.9
7	4.08 (s, 2H)	31.9	4.08 (s, 2H)	31.9
8		139.4		139.4
9				
10	8.91 (d, 0.5Hz, 1H)	153.1	8.91 (d, 0.6Hz, 1H)	153.1
11				
12	7.70 (d, 0.5Hz, 1H)	140.5	7.70 (d, 0.6Hz, 1H)	140.5

<sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded in DMSO at 500 MHz and 125 MHz, respectively.

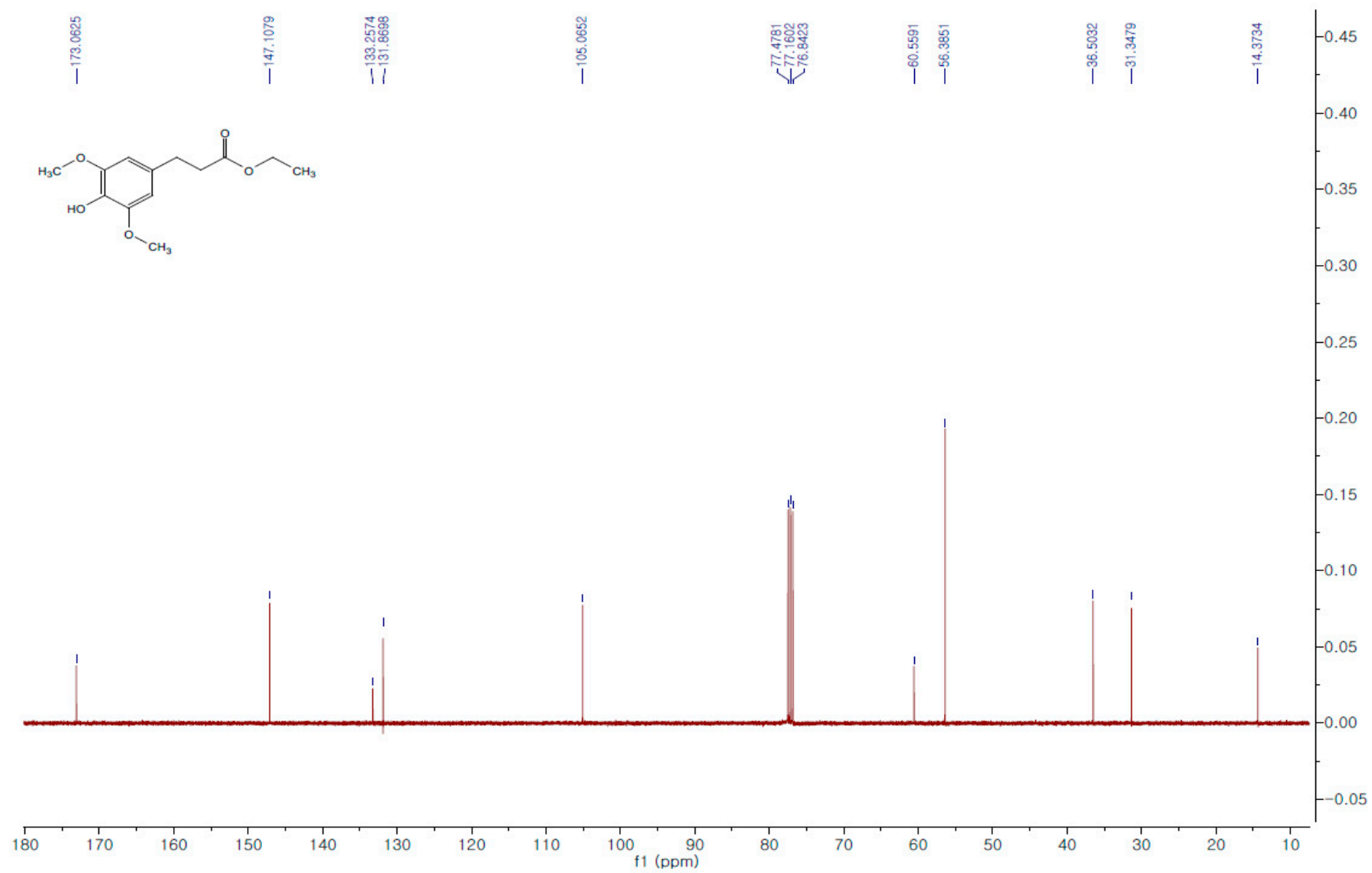




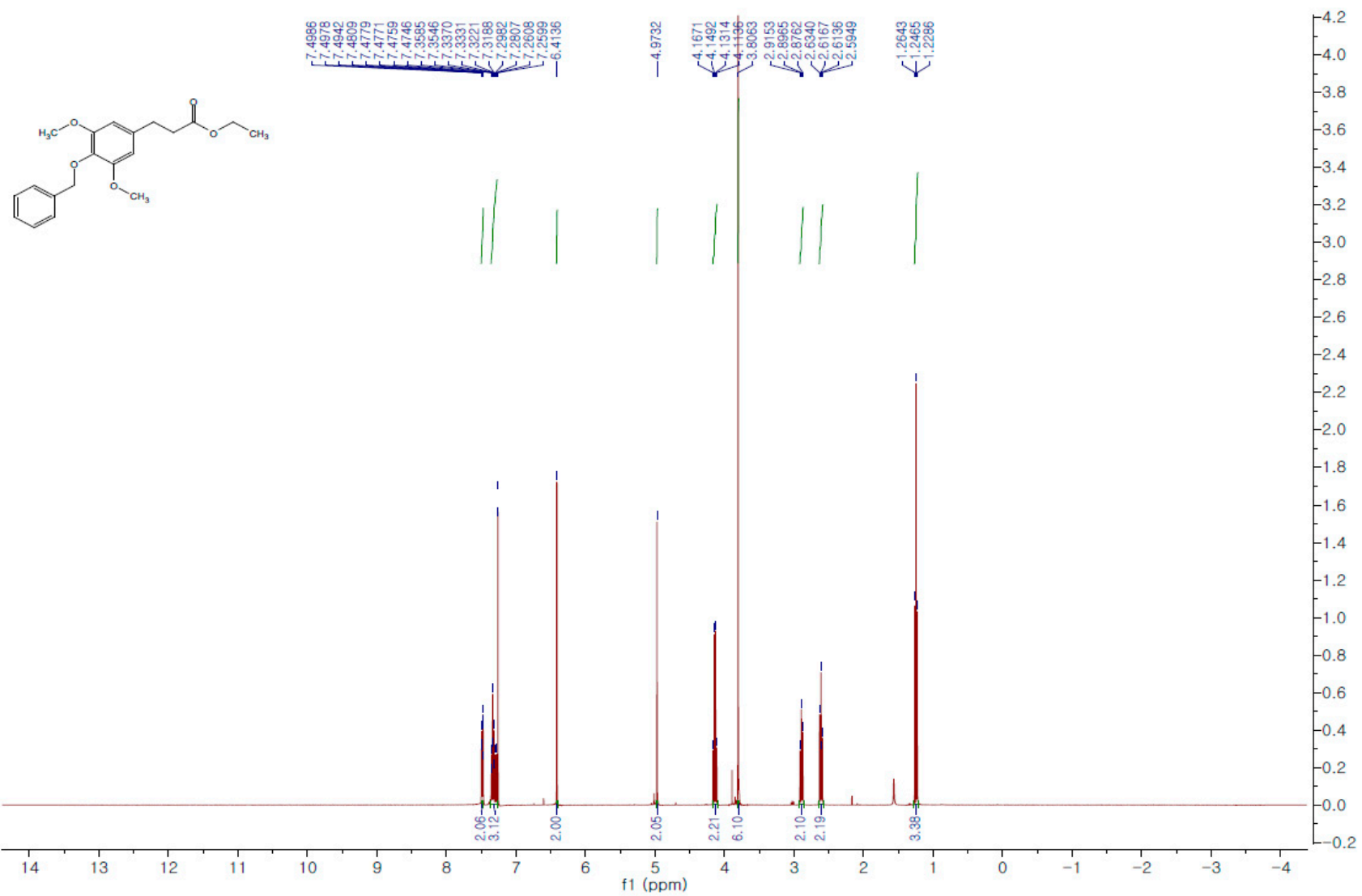
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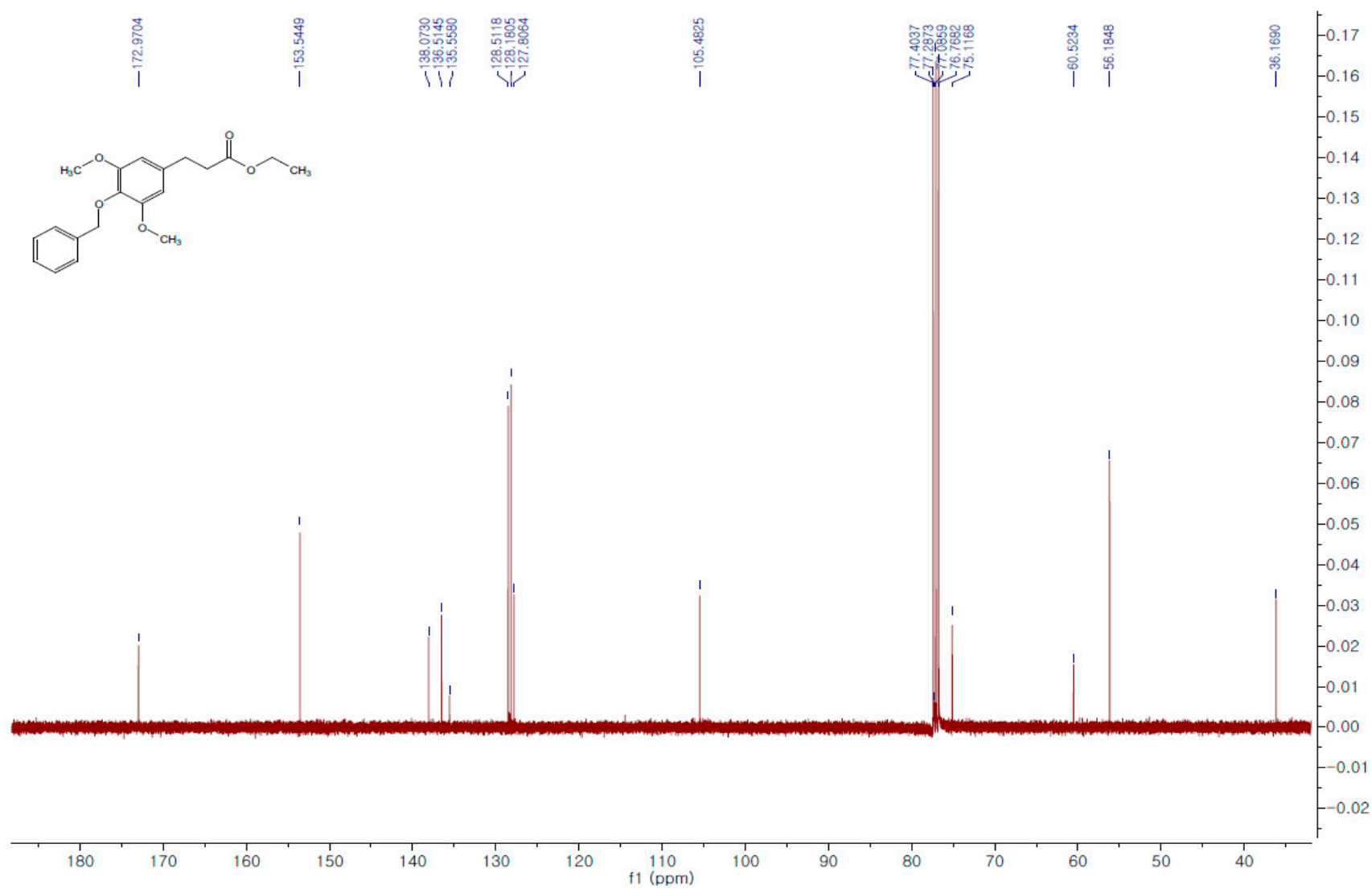
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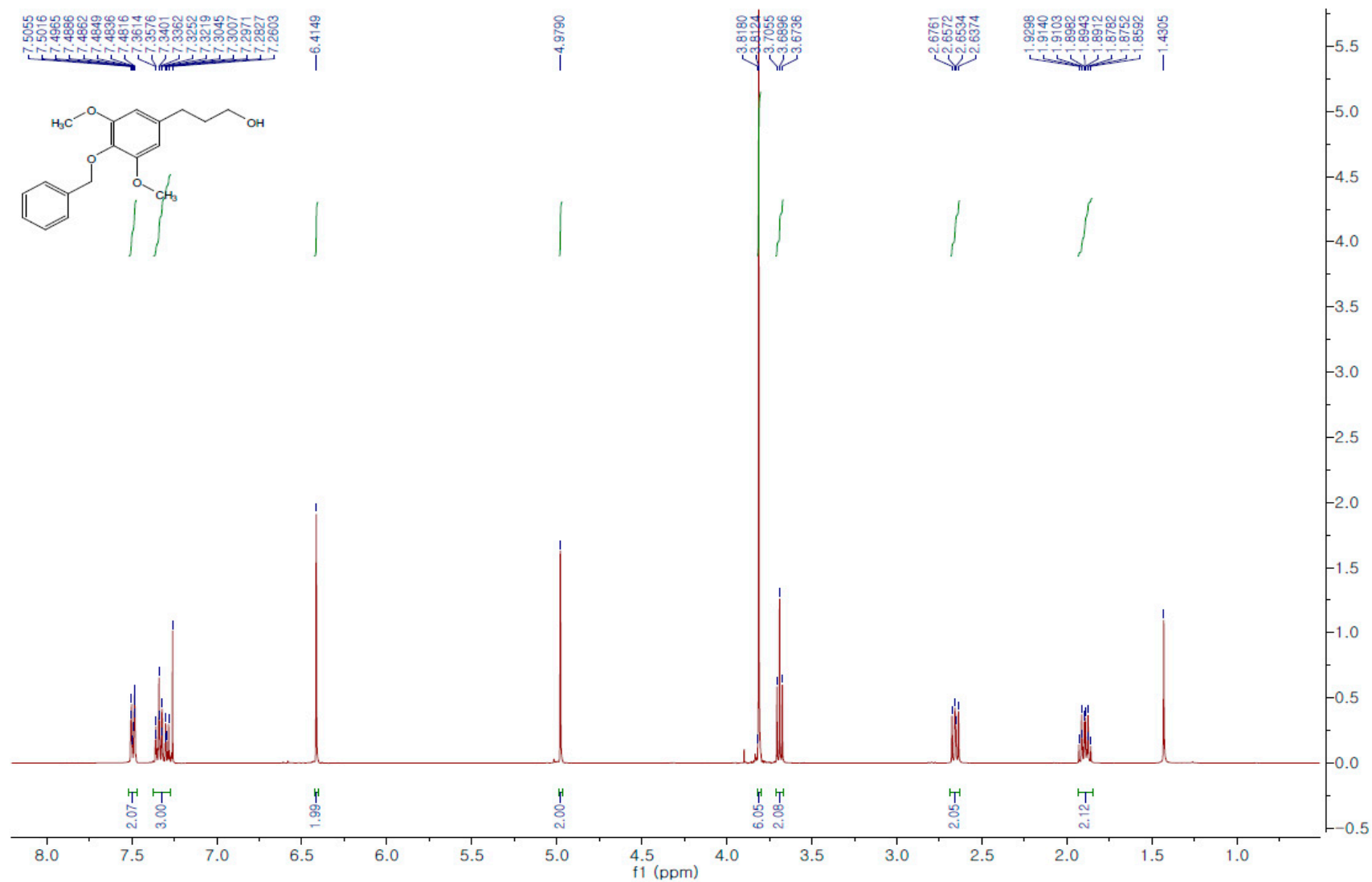


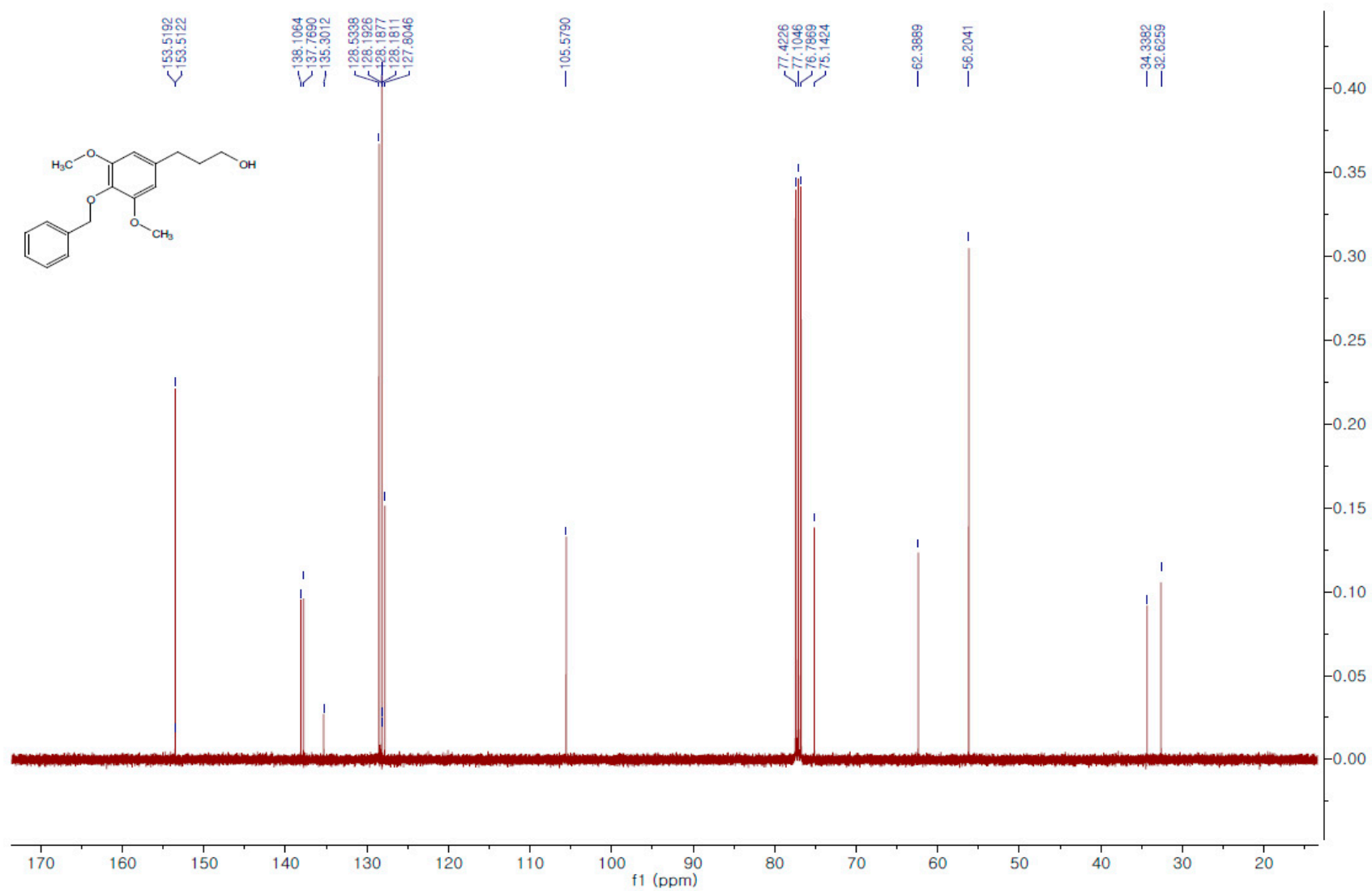
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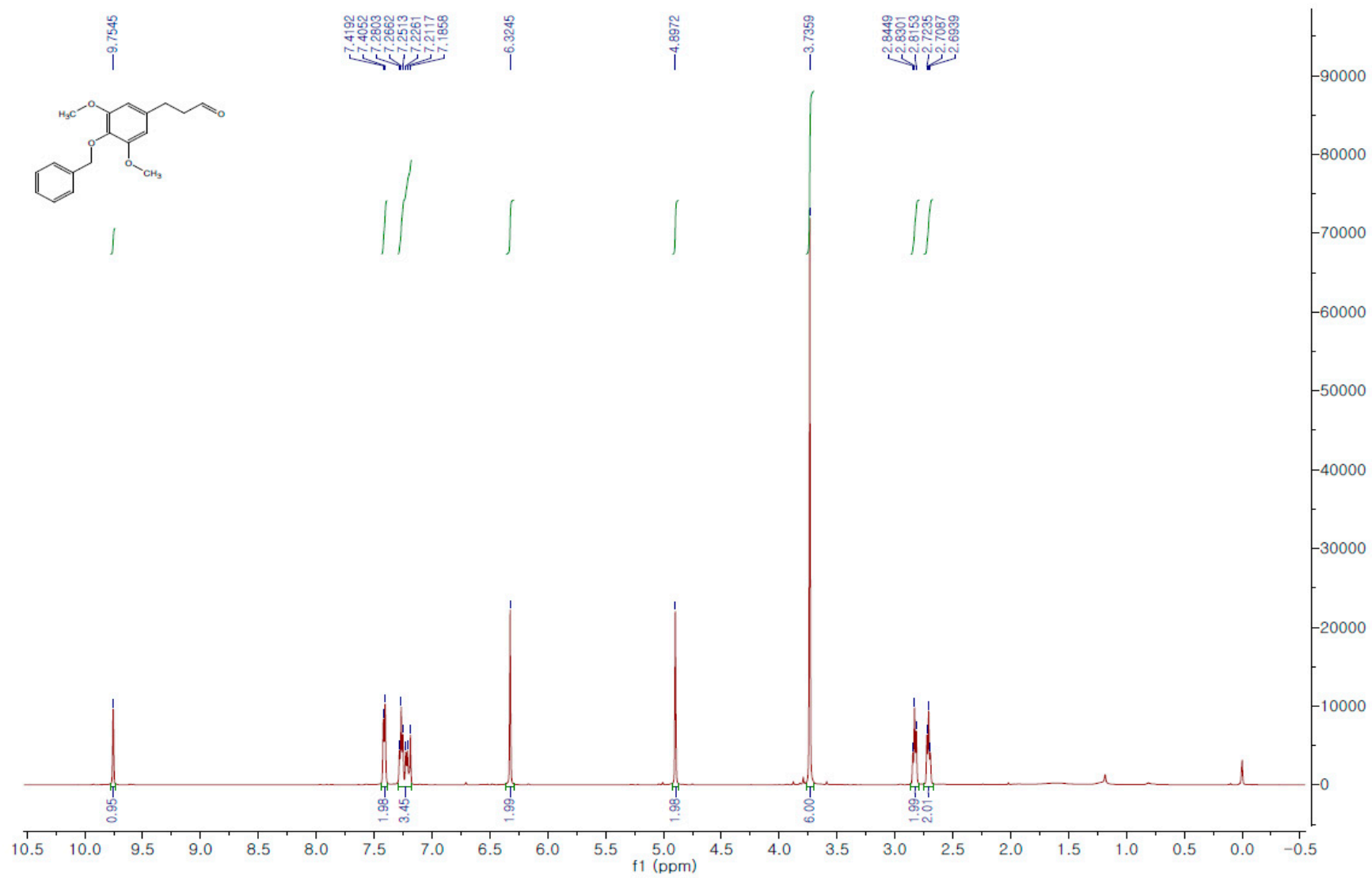




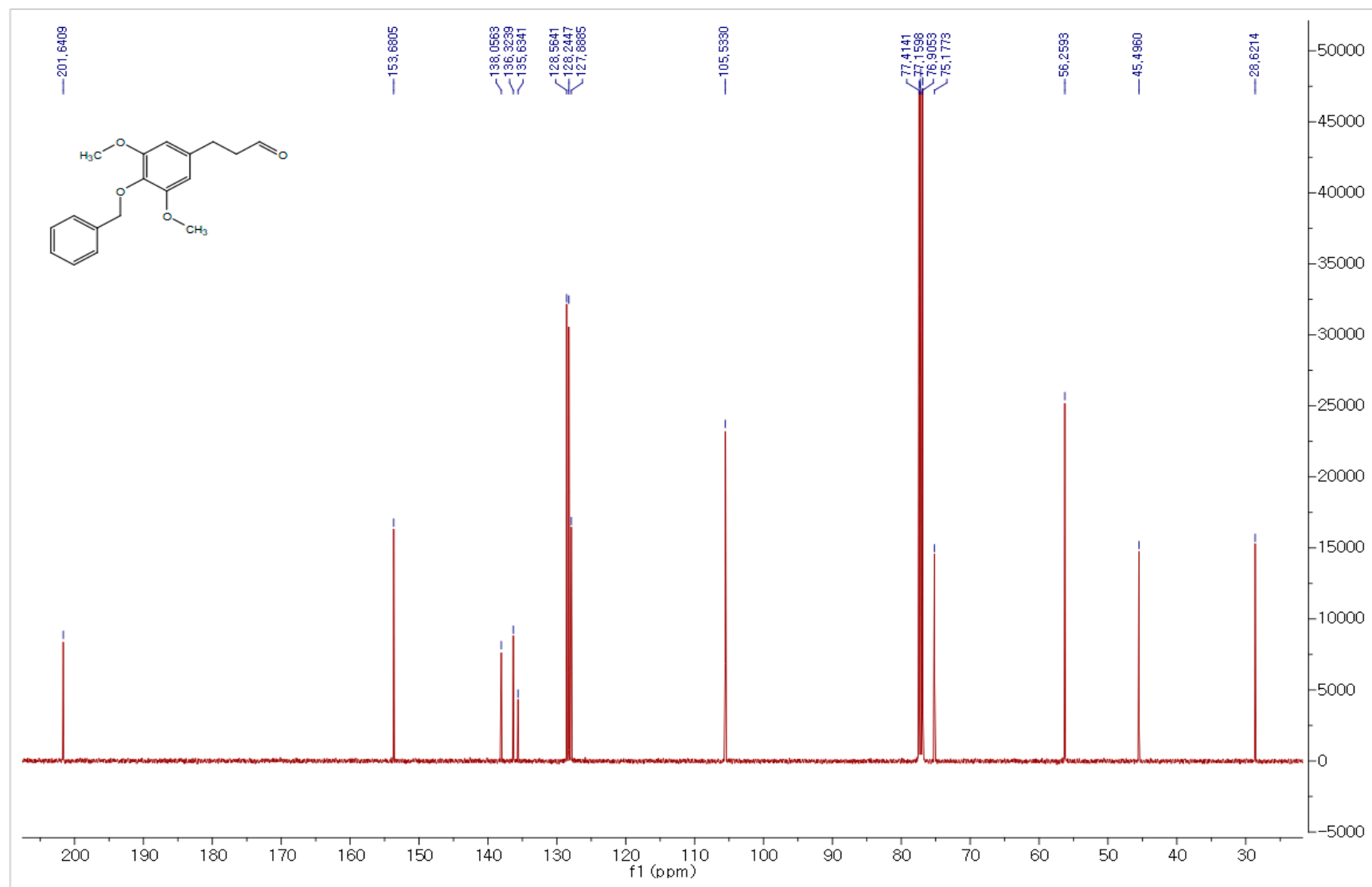




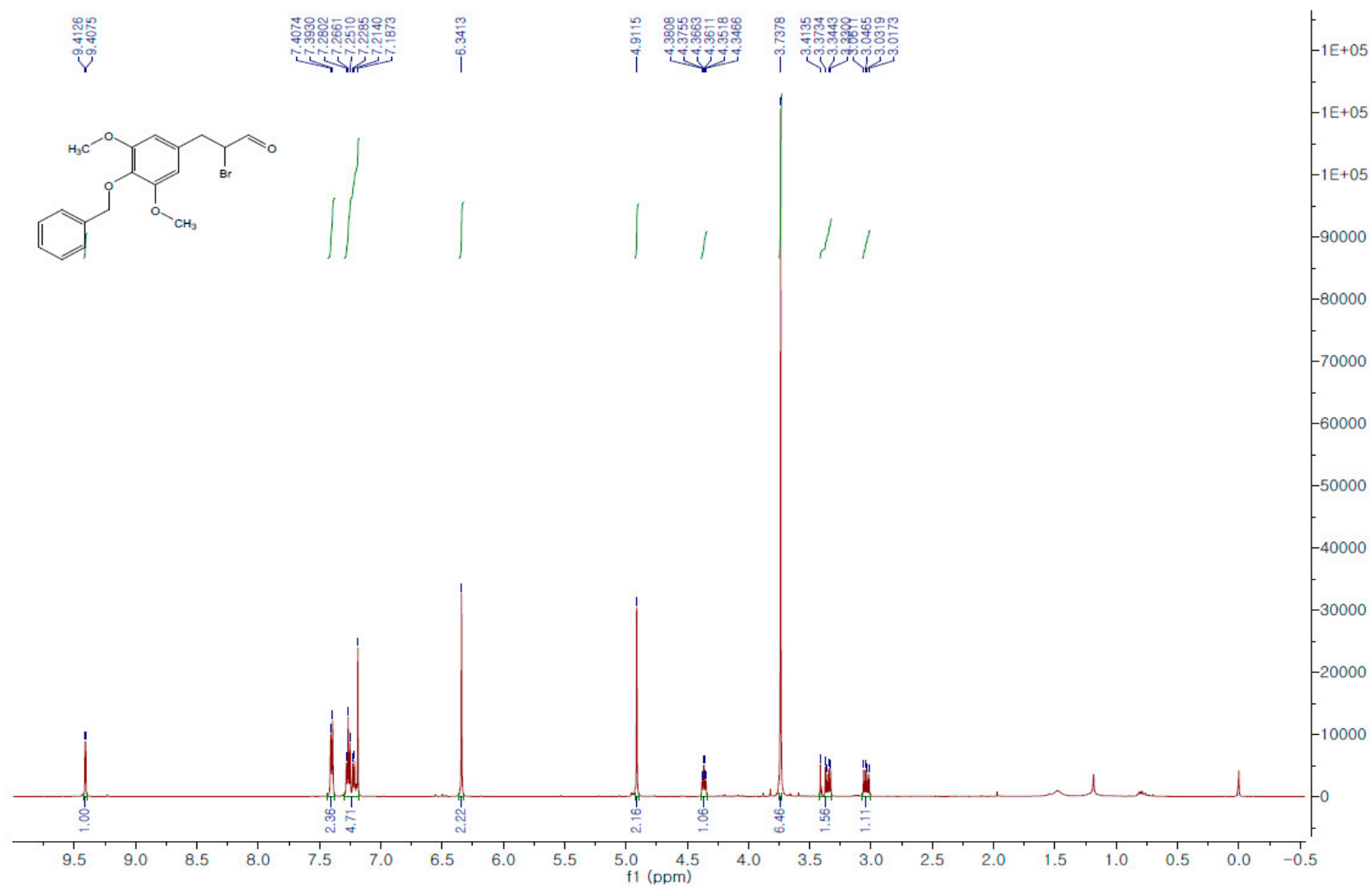




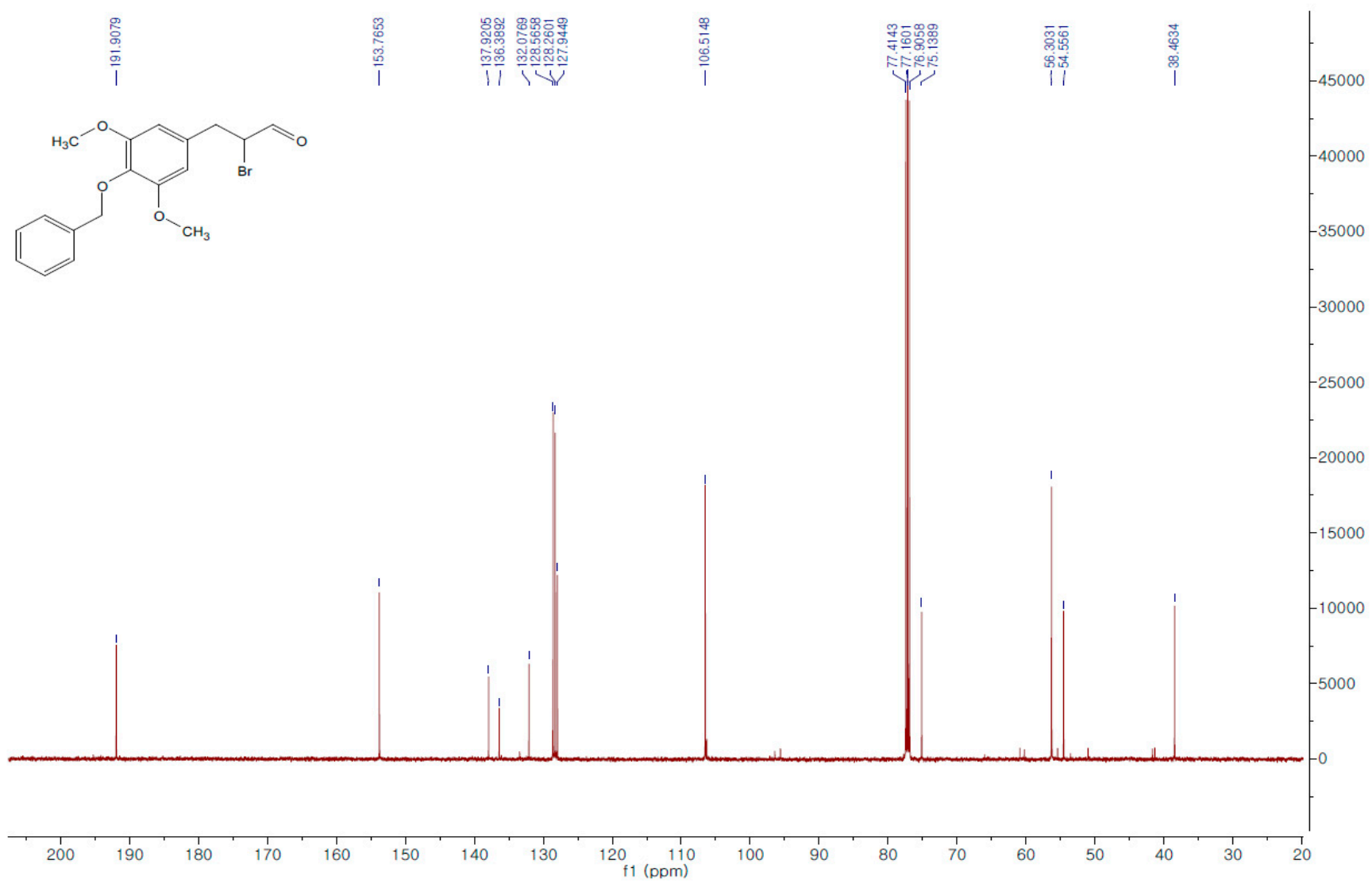
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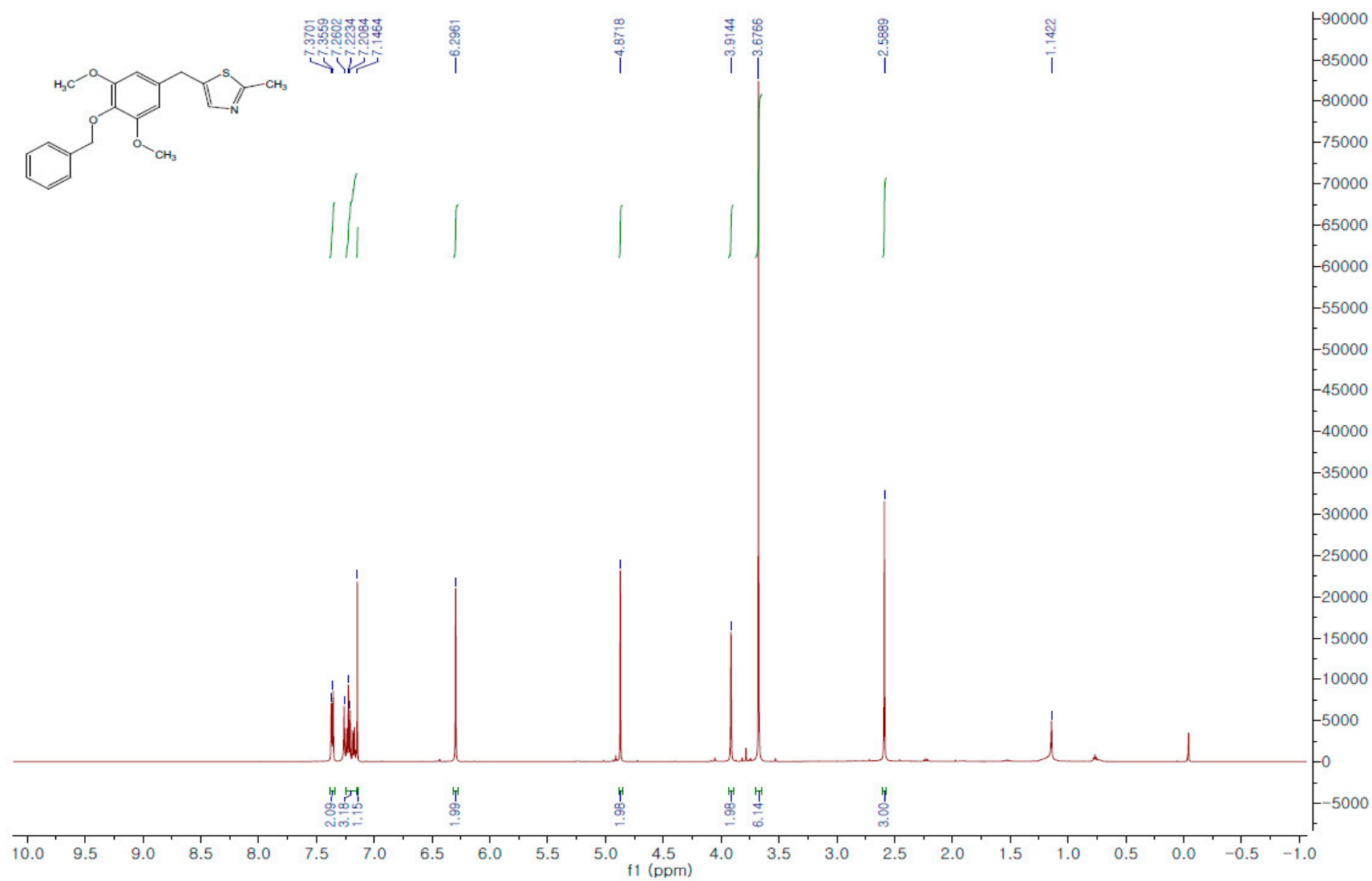
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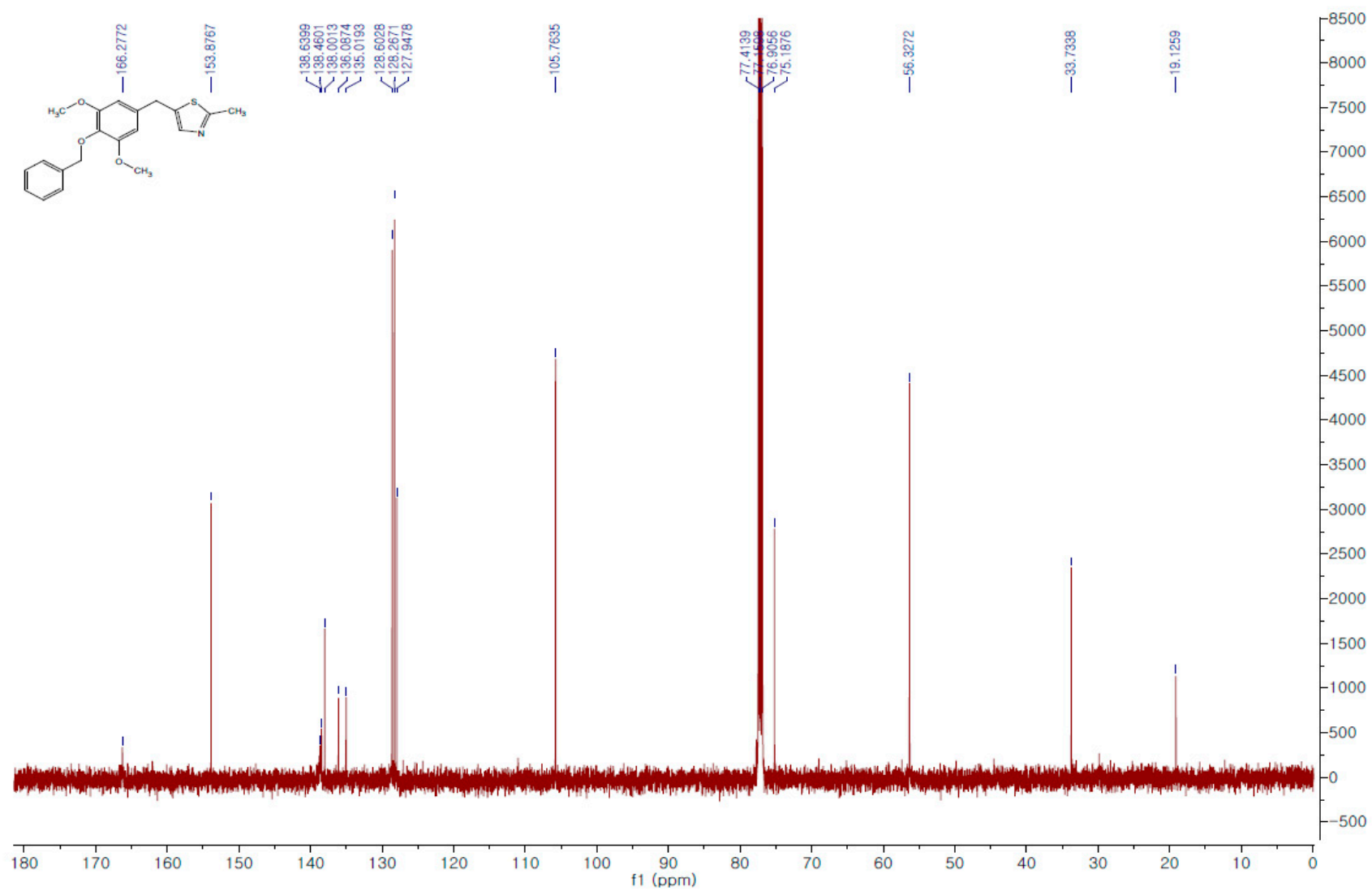


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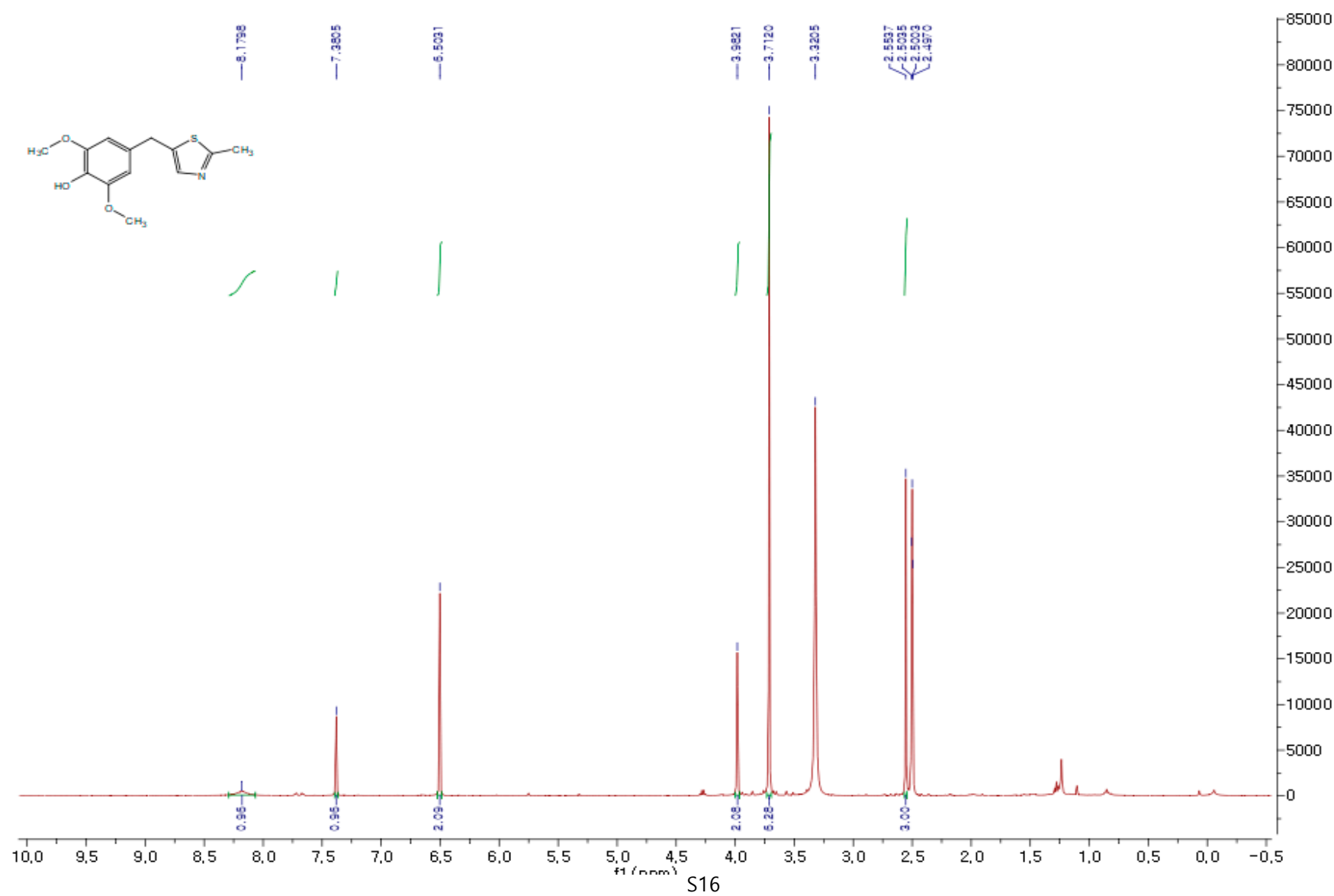


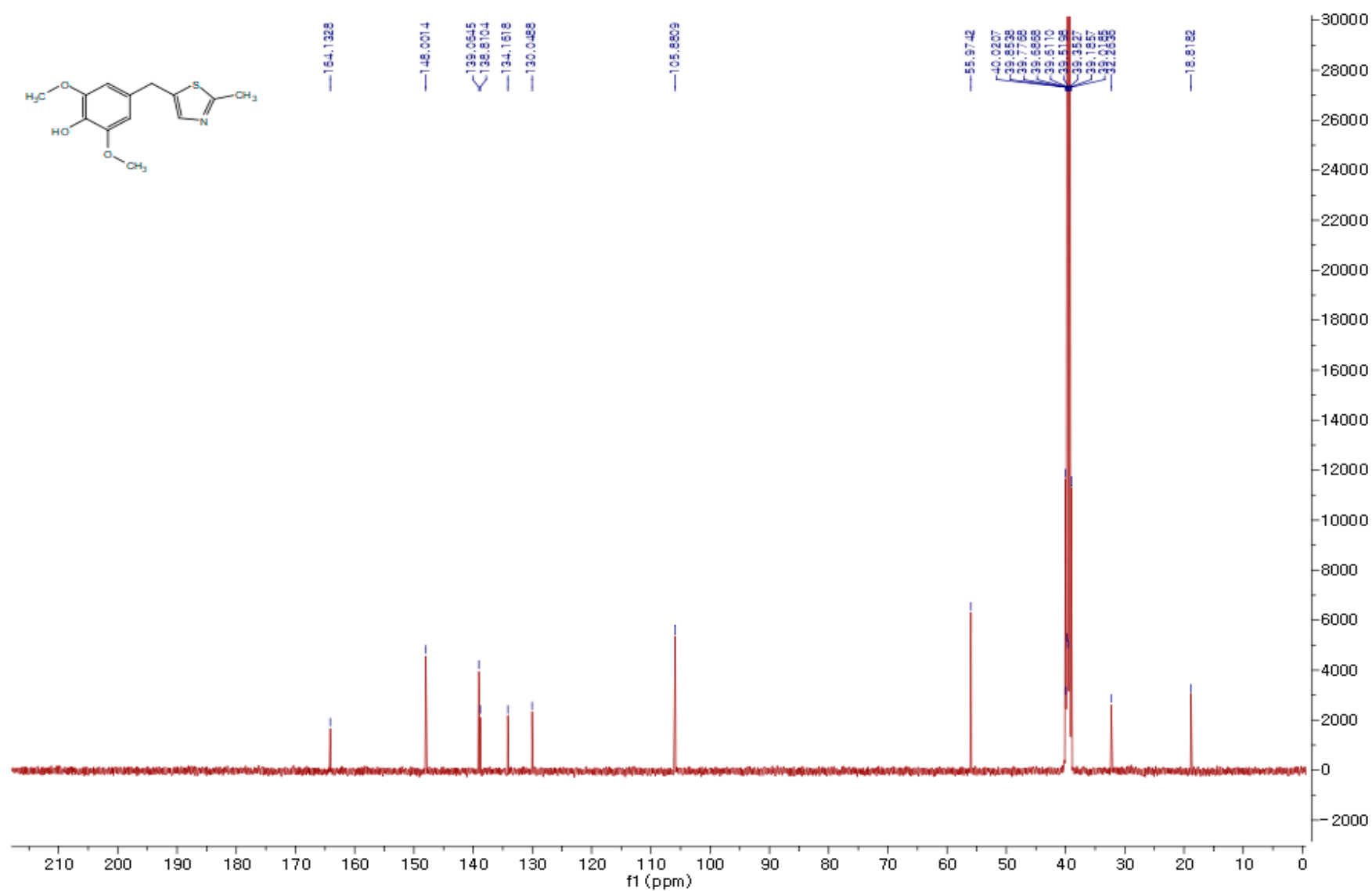
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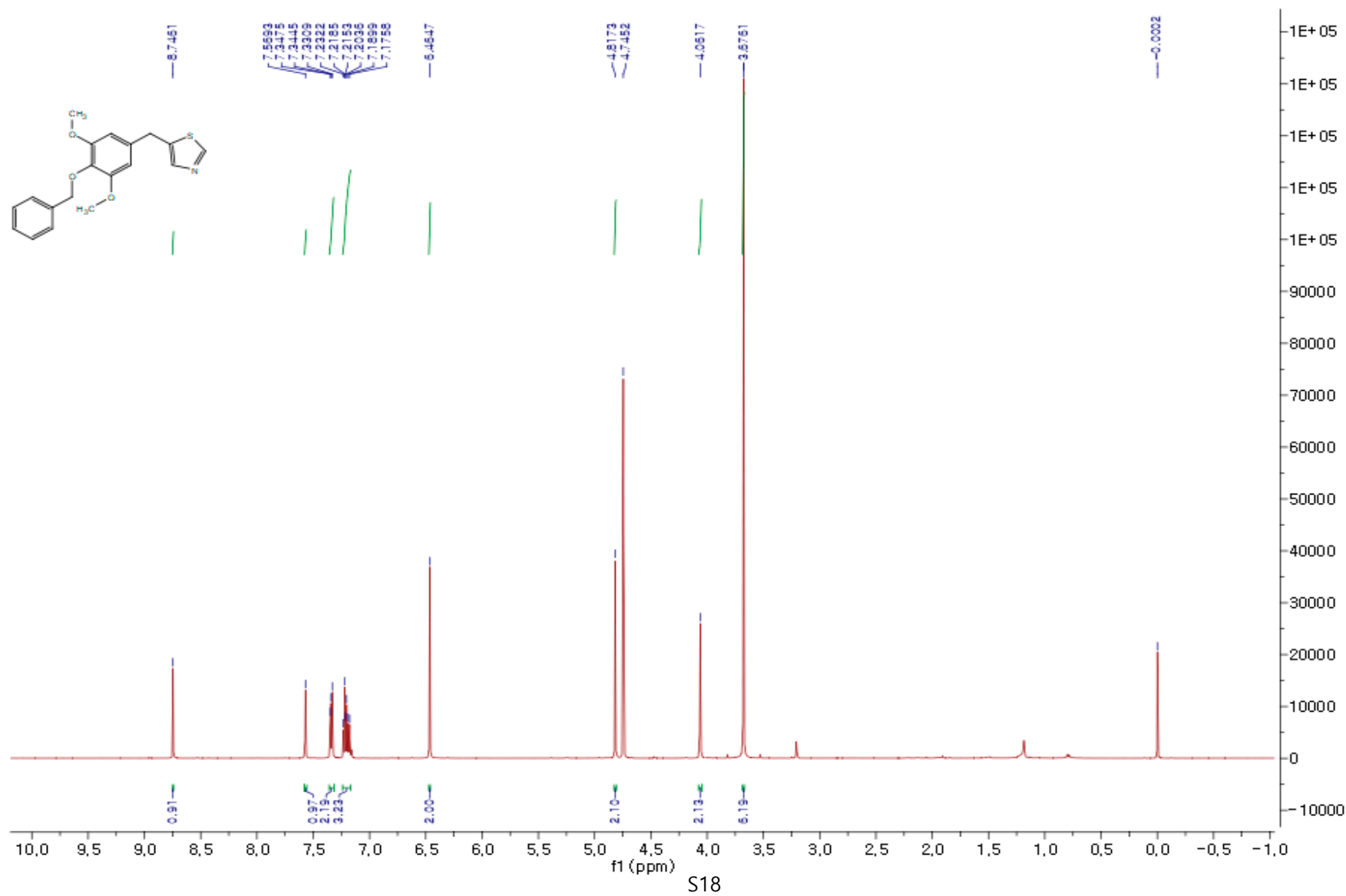


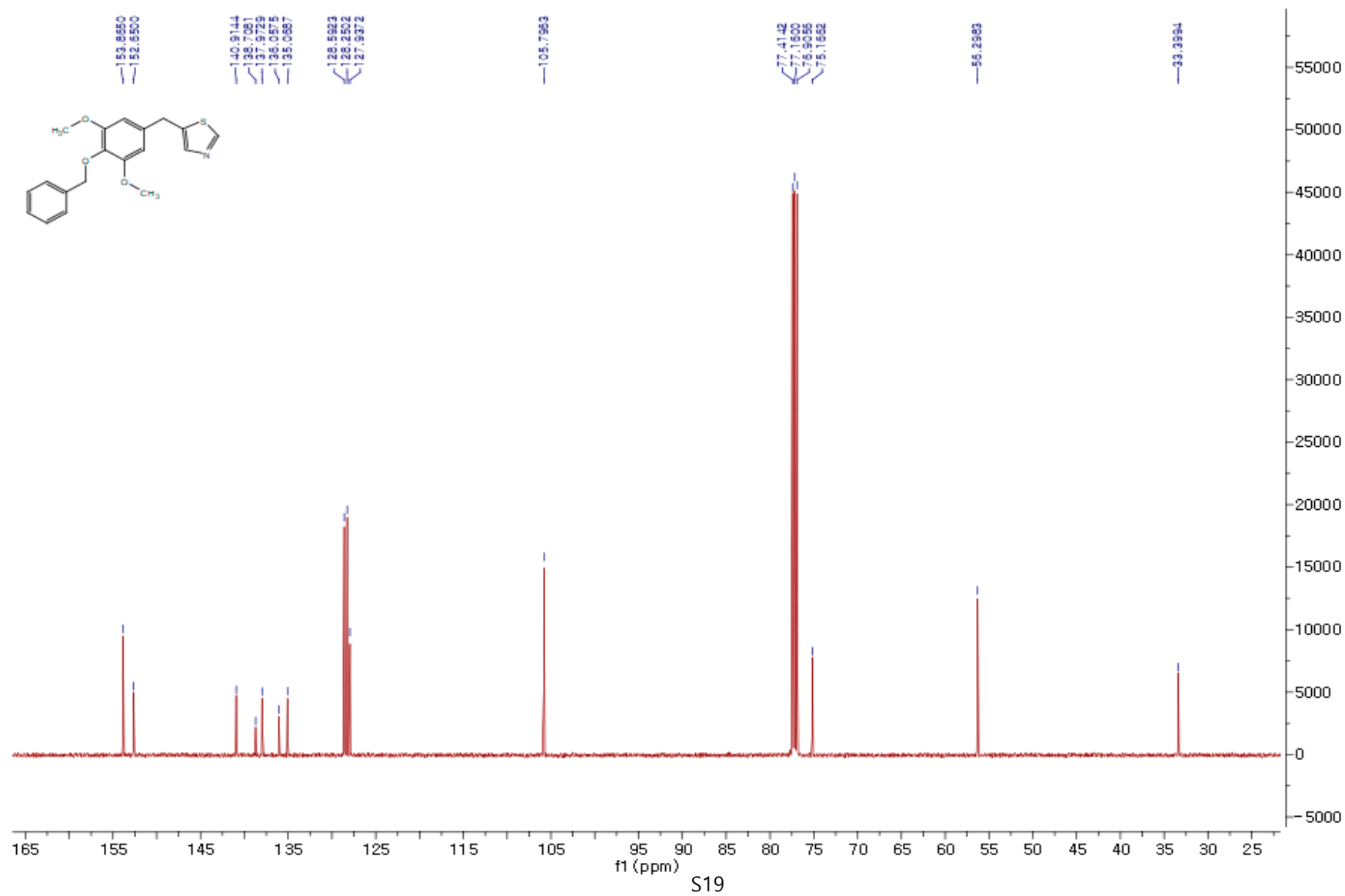


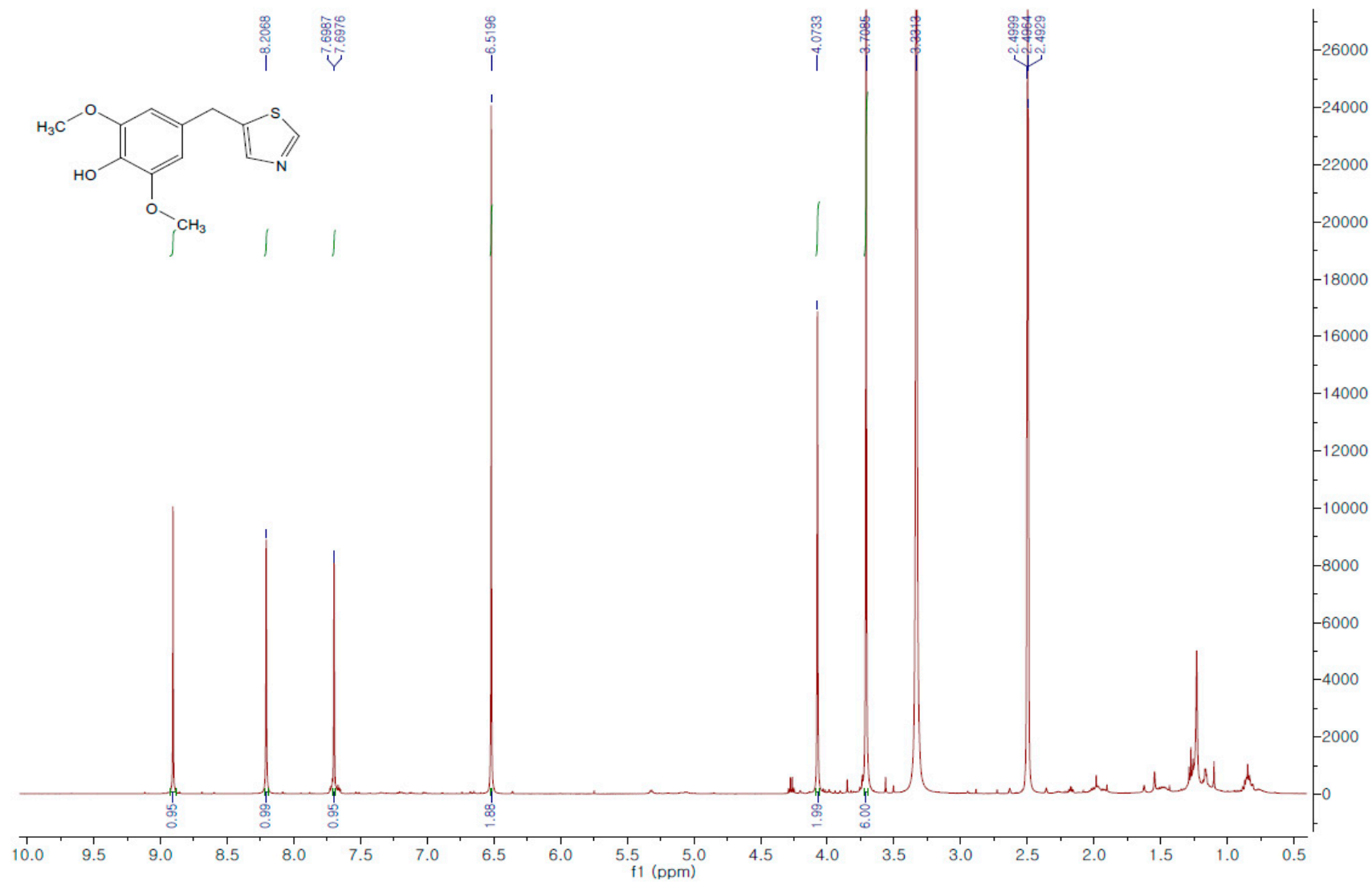
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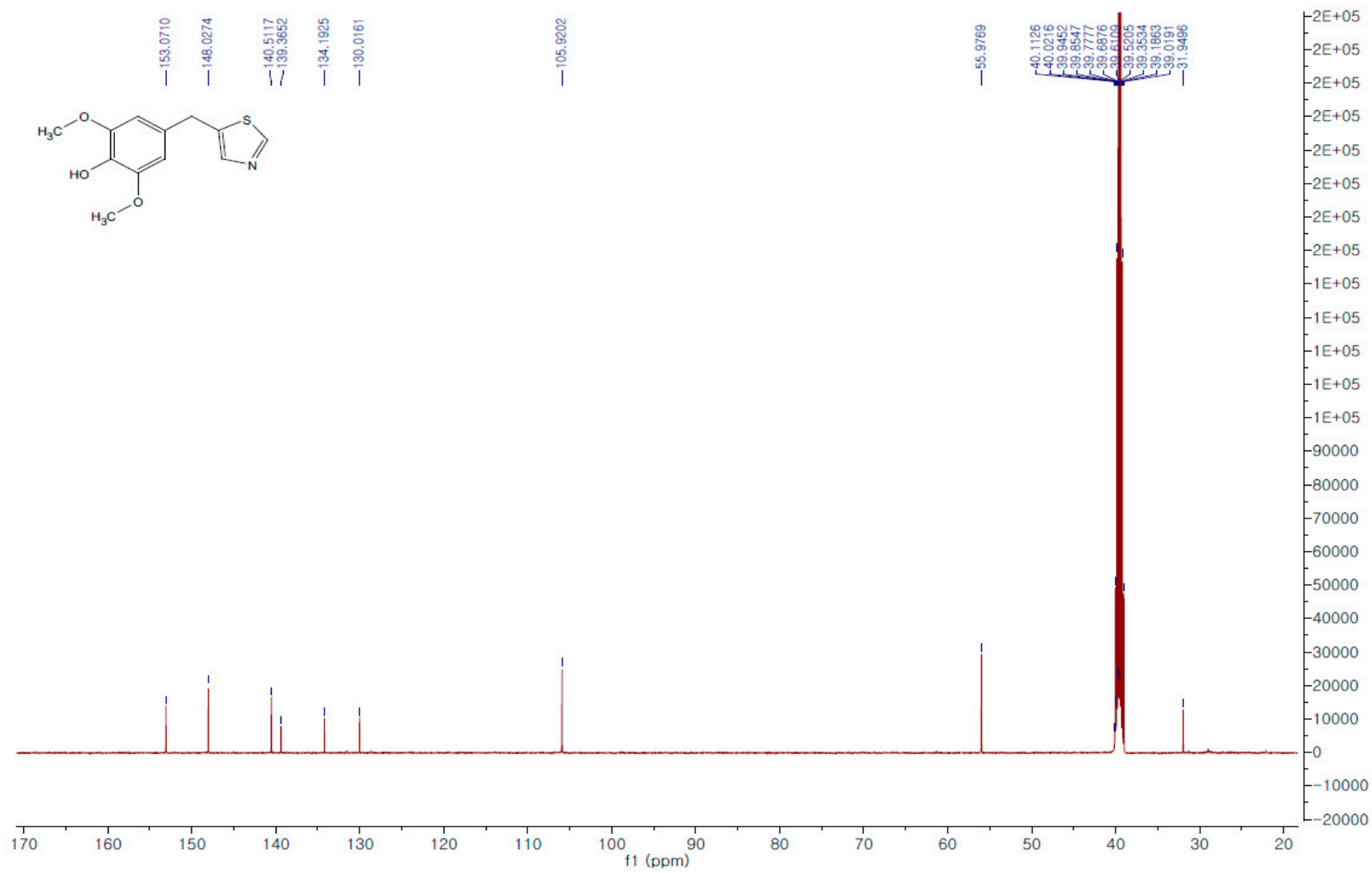








S20



S21