

## Supporting Information

# Synthesis of Proposed Structure of Aaptoline B via Transition Metal-Catalyzed Cycloisomerization and Evaluation of Its Neuroprotective Properties in *C. Elegans*

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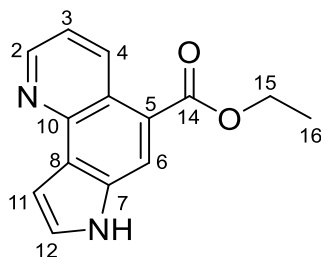
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Table S1. <sup>1</sup>H- and <sup>13</sup>C-NMR assignment of aaptoline B.



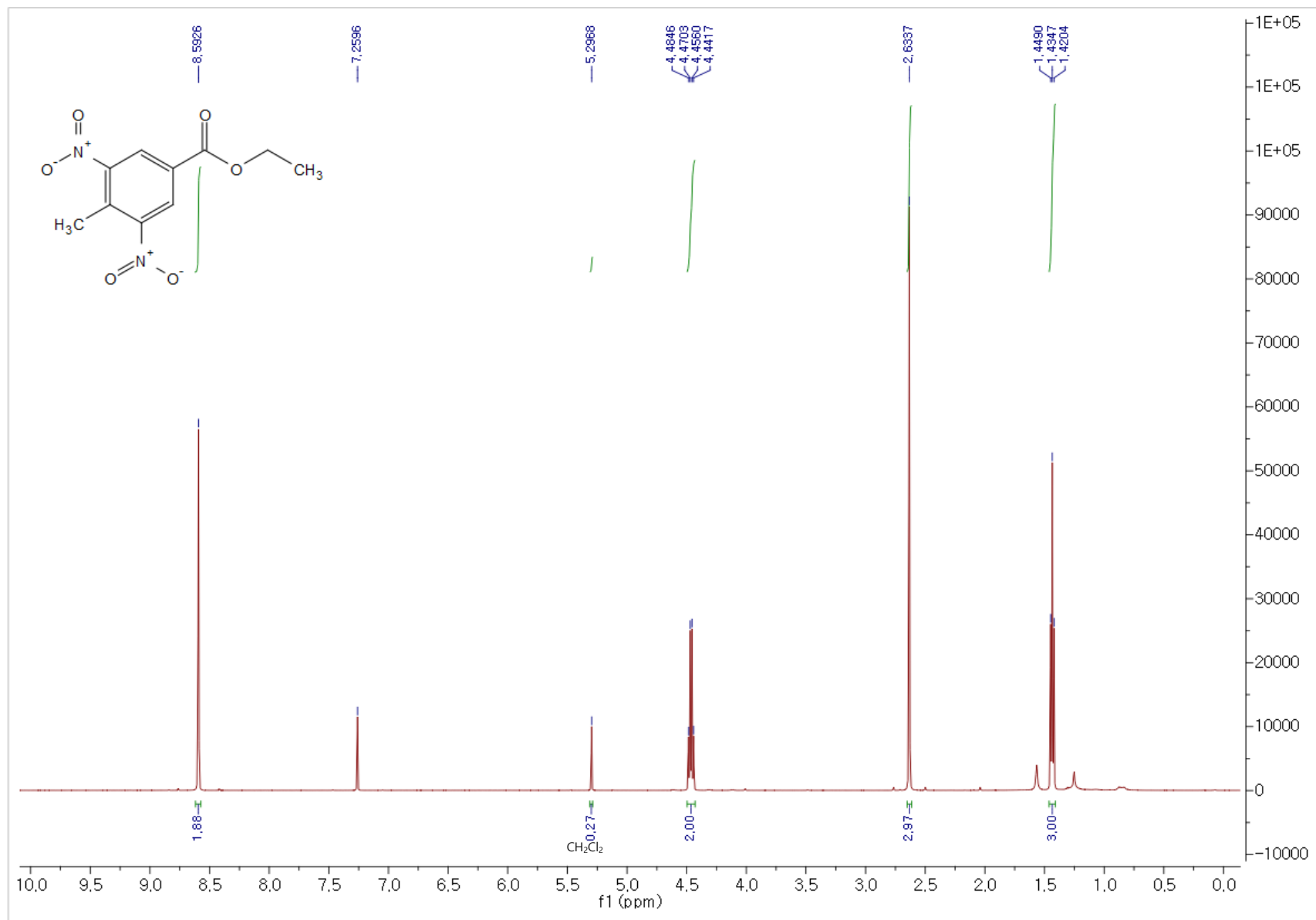
Position	Reported <sup>[a]</sup>		Synthesized <sup>[b]</sup>		Synthesized <sup>[c]</sup>	
	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$	$\delta_H$ (multi, <i>J</i> in Hz)	$\delta_C$
2	9.49 (dd, 10.3, 2.1)	135.3	9.56 (d, 8.4)	136.3	9.52 (dd, 8.4, 1.4)	137.2
3	7.48 (dd, 10.4, 5.0)	120.2	7.52 (m)	120.1	7.51 (dd, 8.8, 4.6)	120.9
4	8.96 (dd, 5.2, 2.0)	149.2	8.96 (d, 3.2)	148.2	8.79 (dd, 4.6, 1.8)	149.2
5		122.9		122.9		124.0
6	8.49 (s)	118.9	8.52 (s)	119.5	8.51 (s)	121.1
7		128.0		127.1		134.7
8		132.8		133.1		128.2
9		-, <sup>[d]</sup>		120.4		120.8
10		120.8		143.1		144.7
11	7.45 (t, 3.0)	104.1	7.52 (m)	104.0	7.34 (t, 1.4)	103.9
12	7.51 (t, 3.0)	126.4	7.52 (m)	126.8	7.59 (d, 2.8)	128.6
13-NH	8.84 (br. s)		9.43 (br.s)			
14		167.4		167.3		168.7
15	4.49 (q, 8.5)	61.1	4.47 (q, 7.1)	61.2	4.45 (q, 7.2)	62.2
16	1.48 (t, 8.5)	14.6	1.46 (t, 7.1)	14.6	1.46 (t, 7.0)	14.9

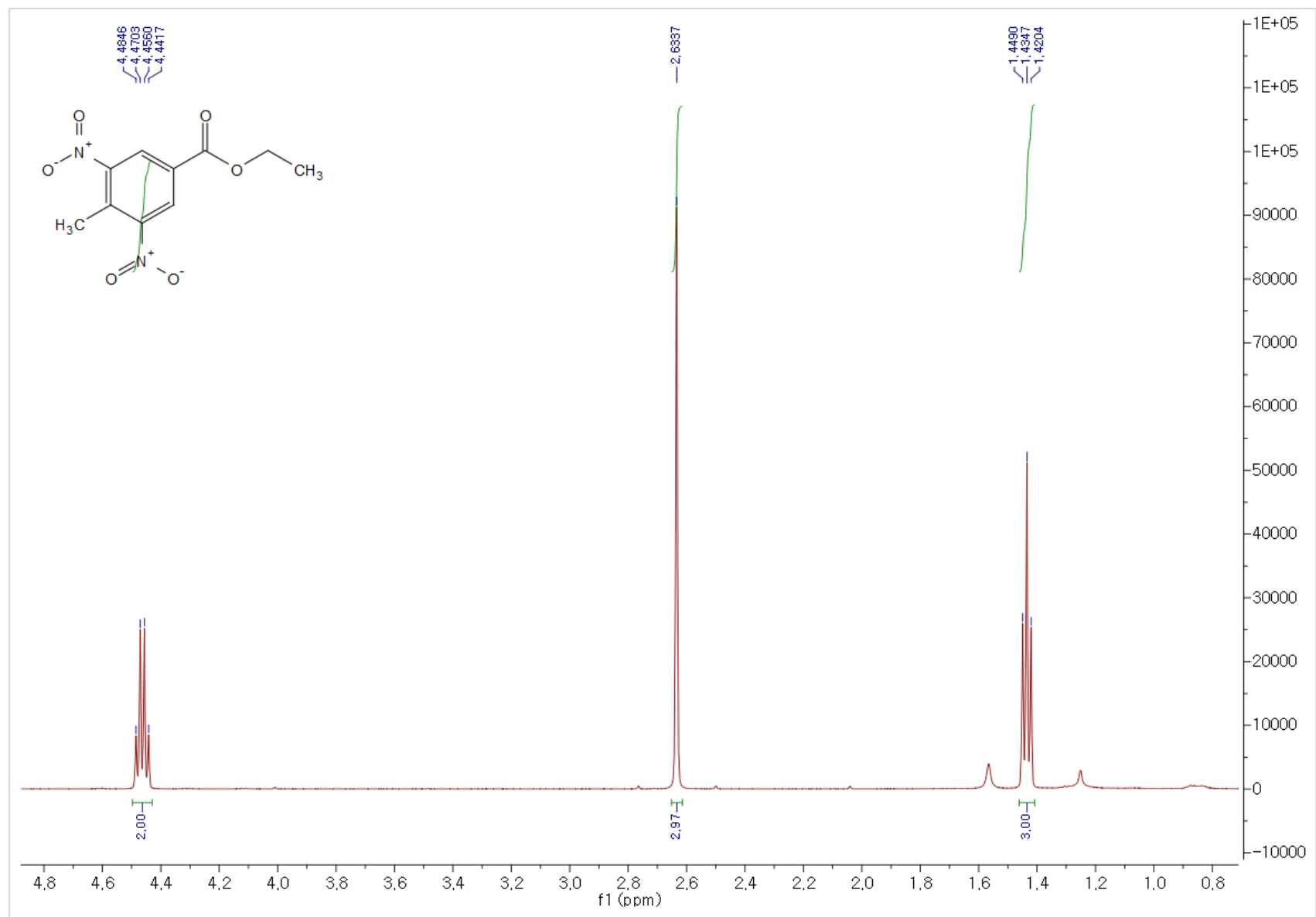
<sup>[a]</sup> <sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded in CDCl<sub>3</sub> at 600 MHz and 150 MHz, respectively.

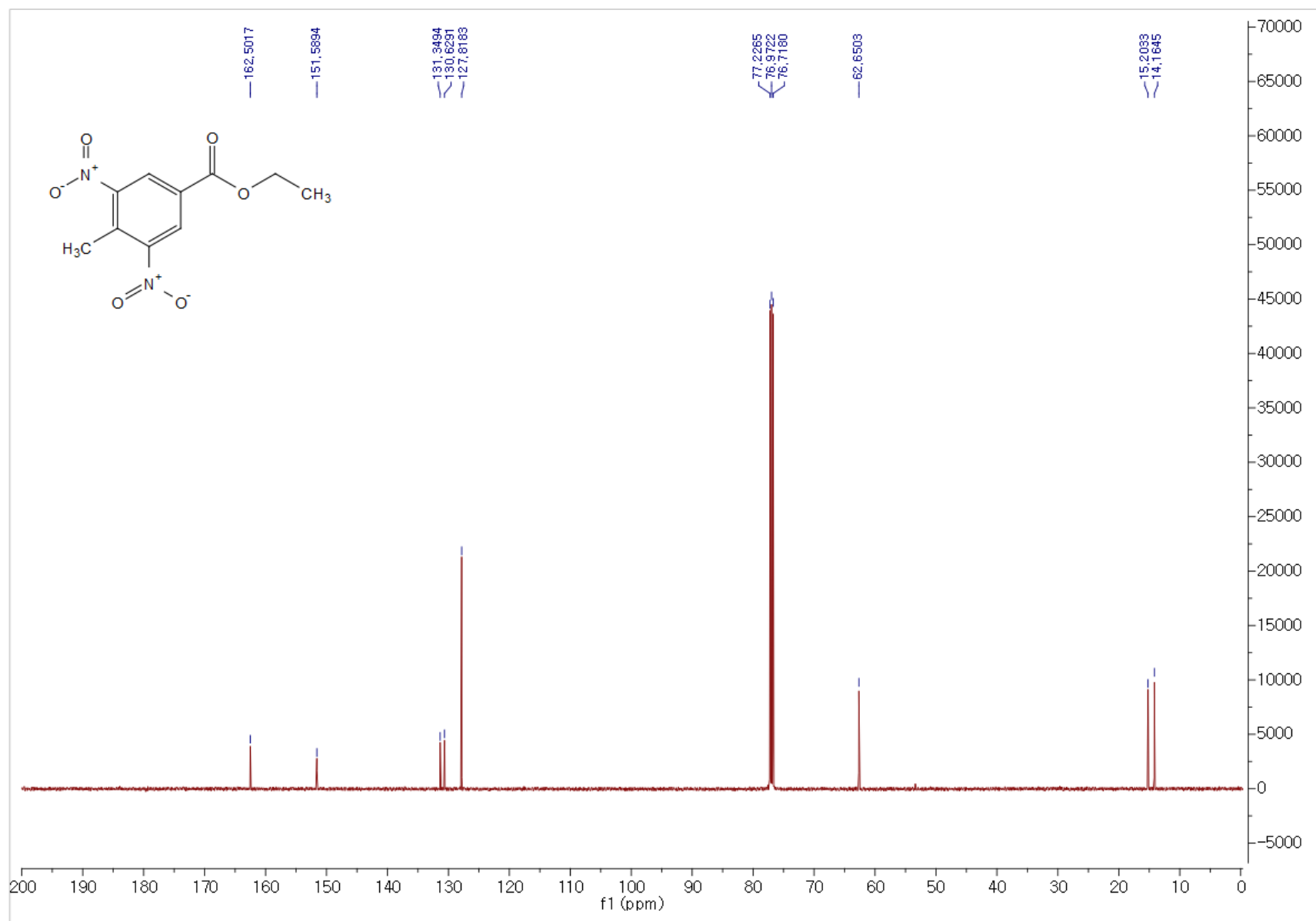
<sup>[b]</sup> <sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded in CDCl<sub>3</sub> at 500 MHz and 125 MHz, respectively.

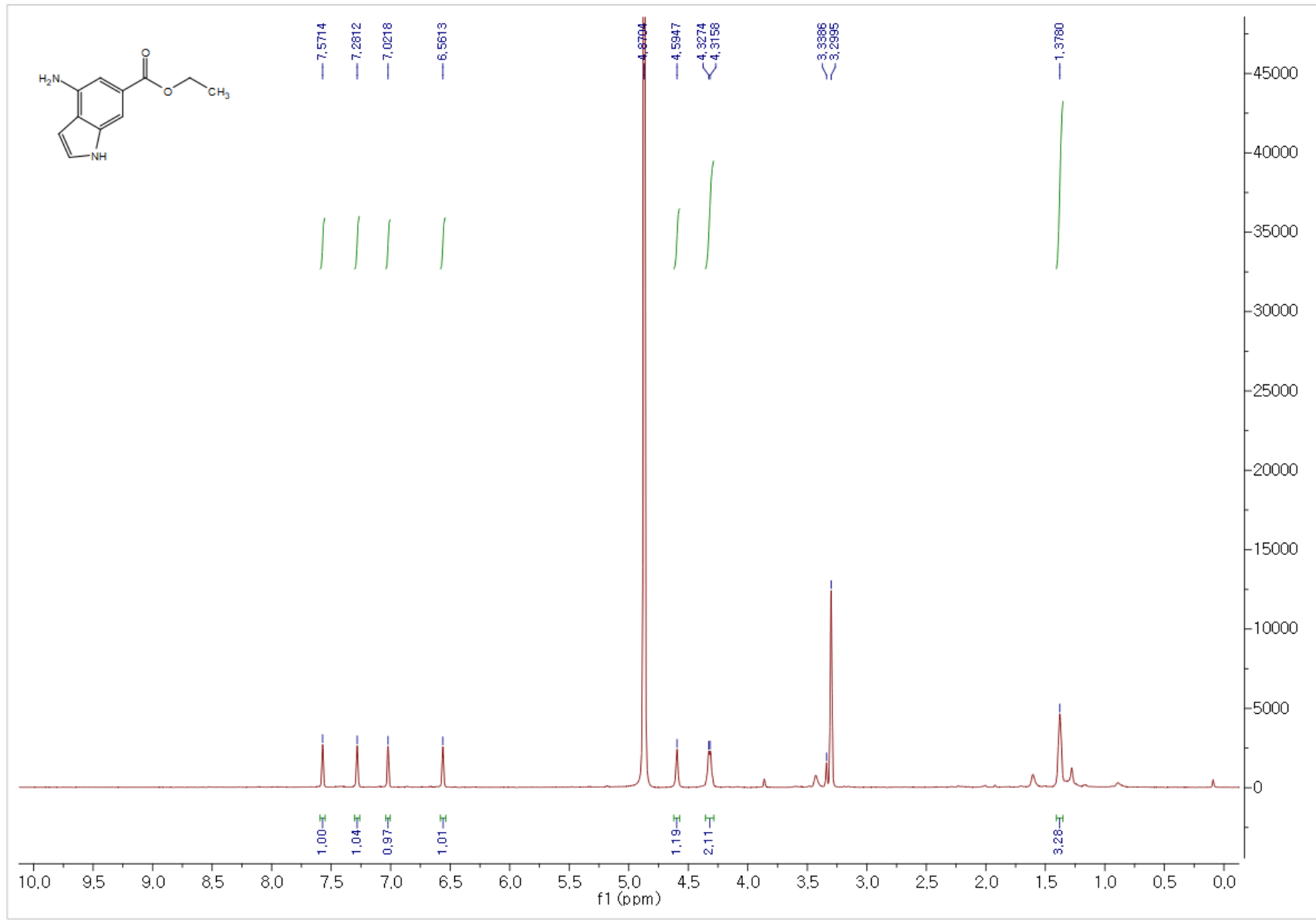
<sup>[c]</sup> <sup>1</sup>H NMR and <sup>13</sup>C spectra were recorded in CD<sub>3</sub>OD at 700 MHz and 175 MHz, respectively.

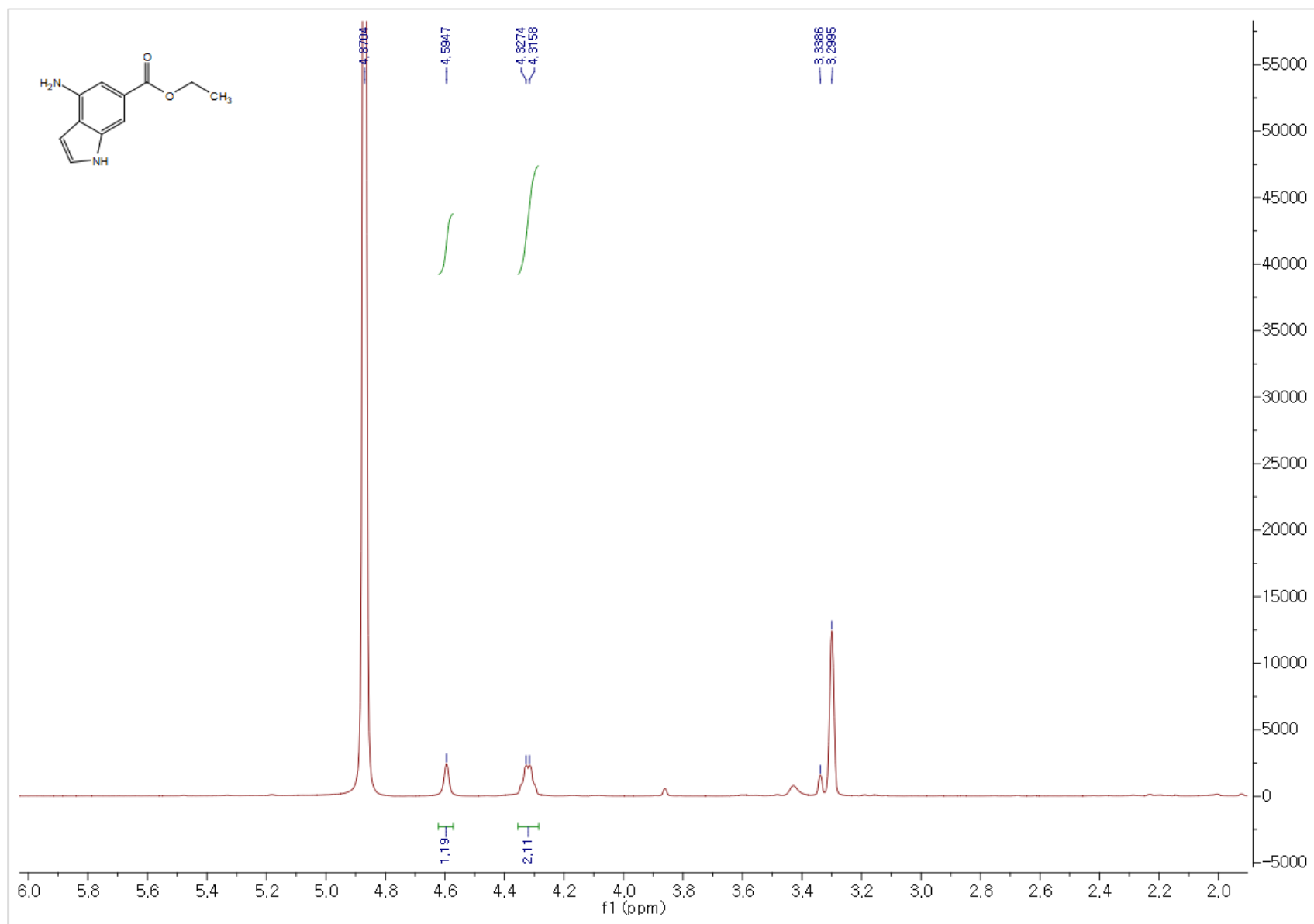
<sup>[d]</sup> Could not be assigned in the previous study.

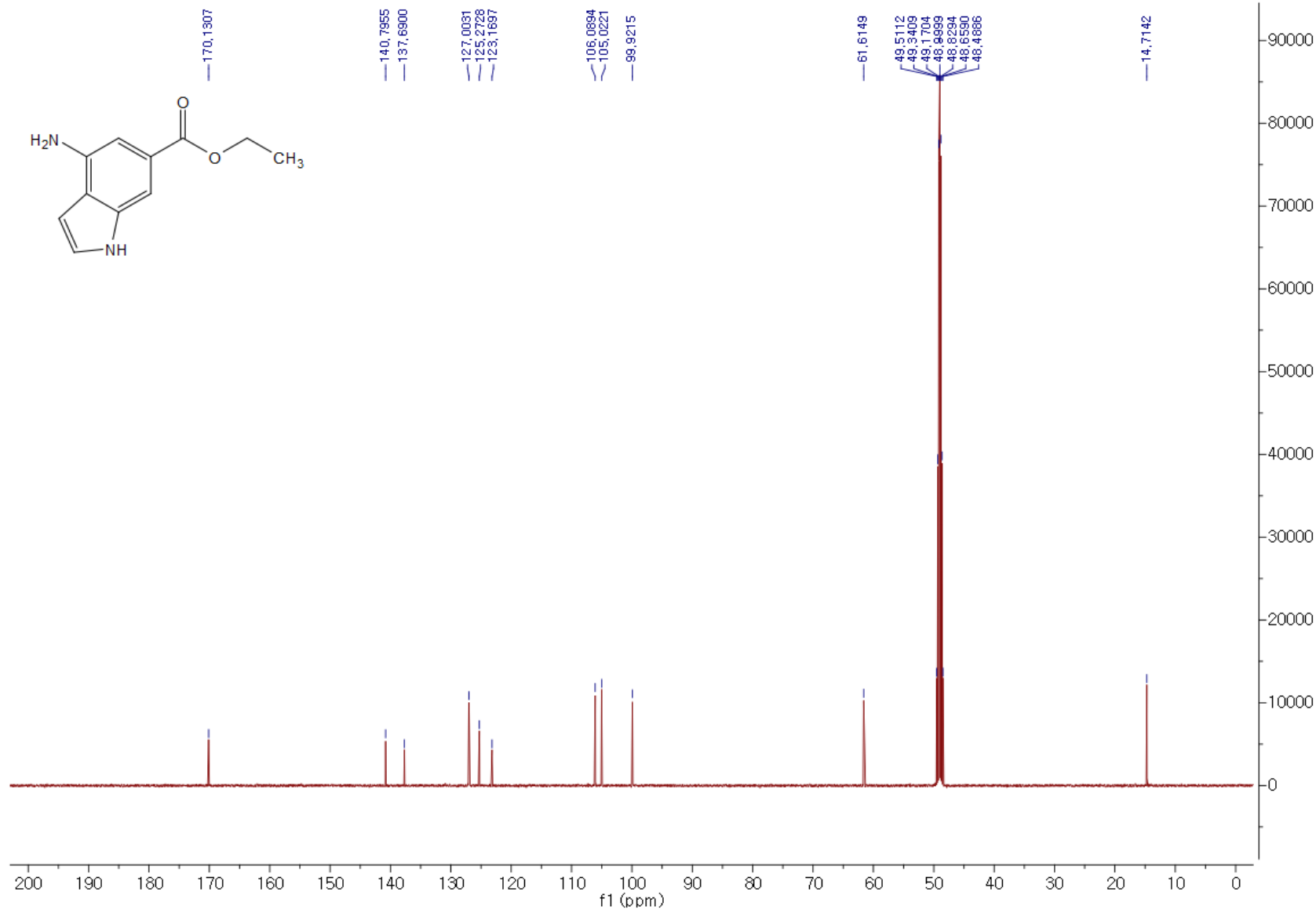
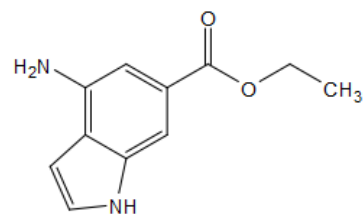




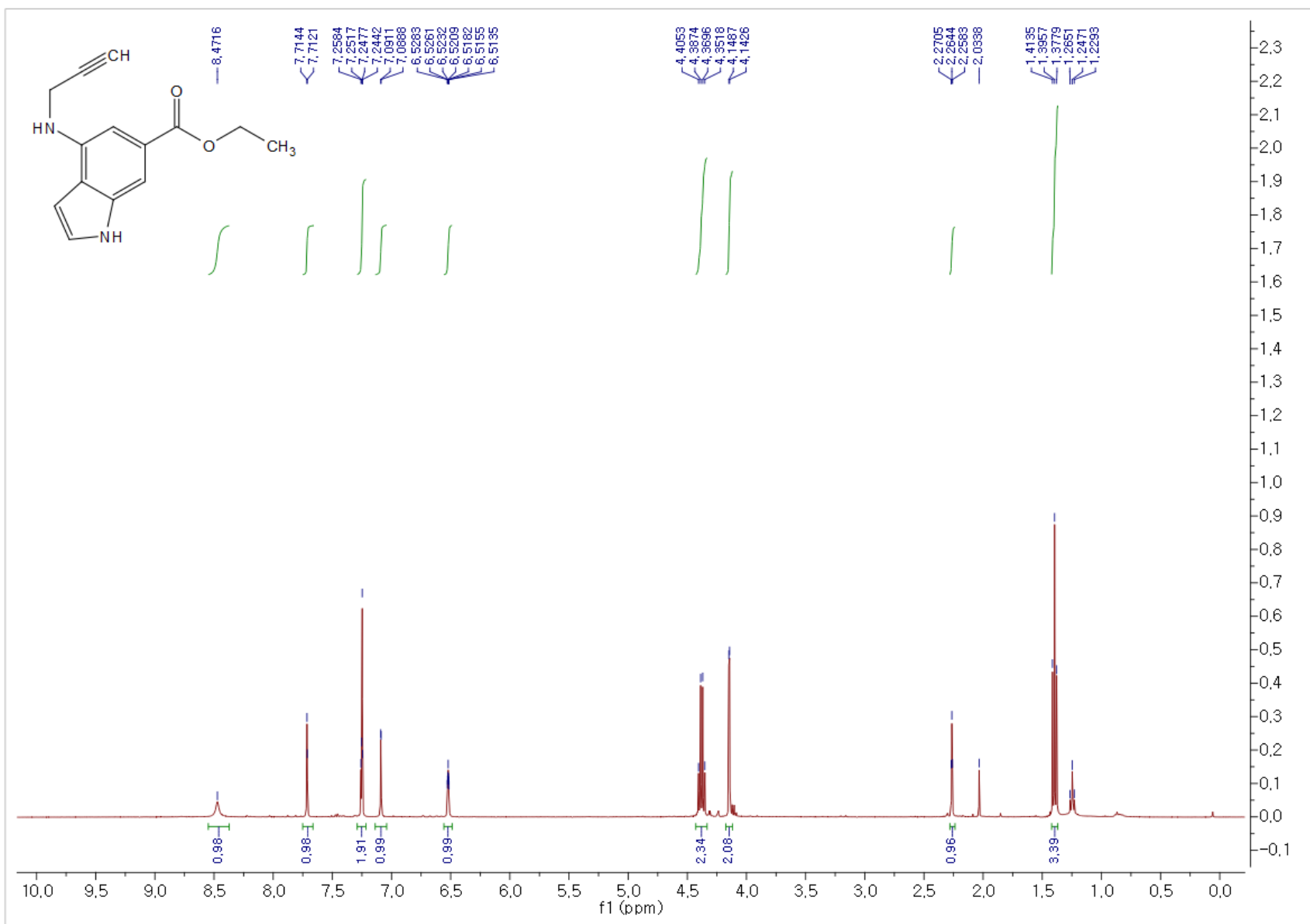


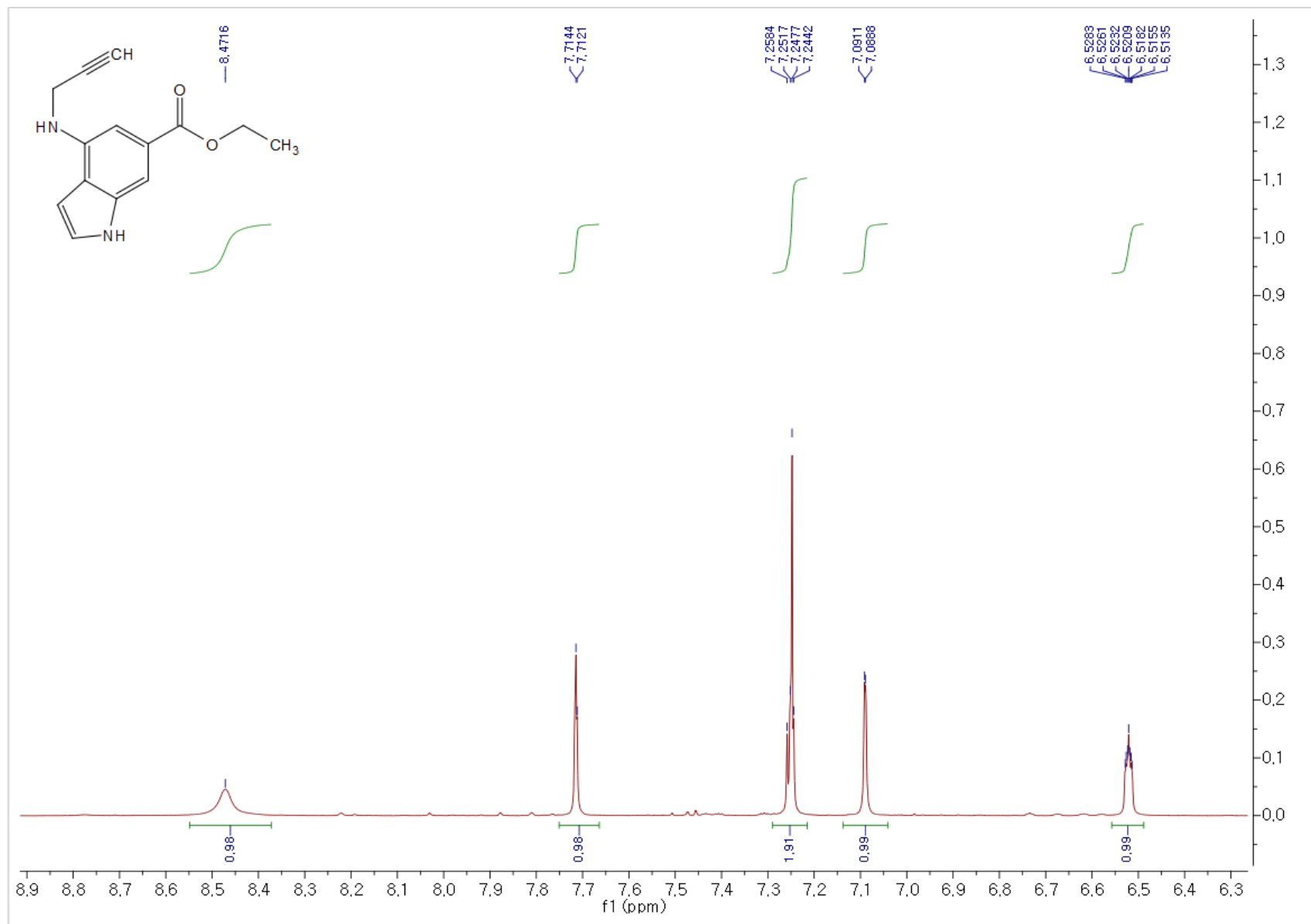


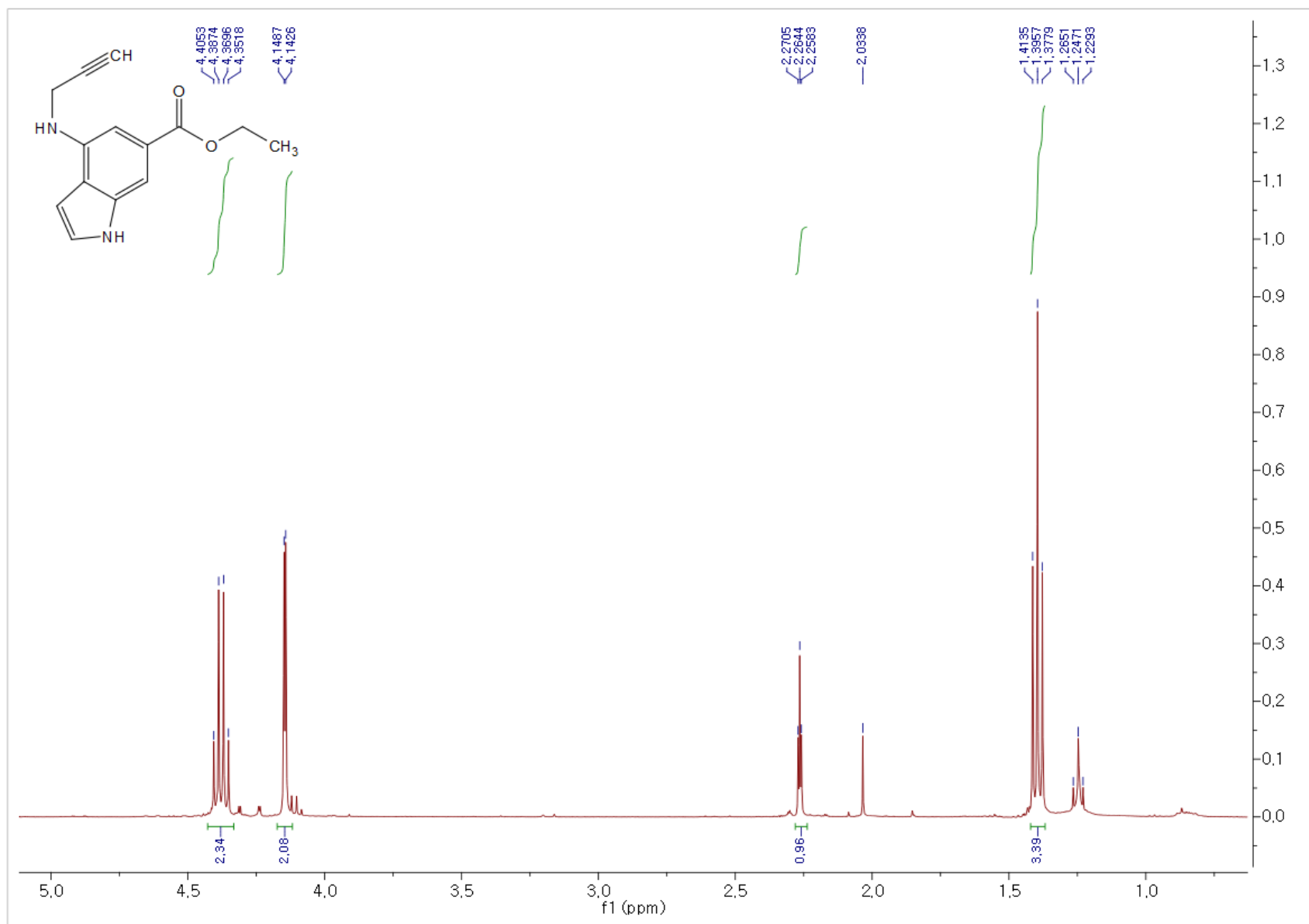


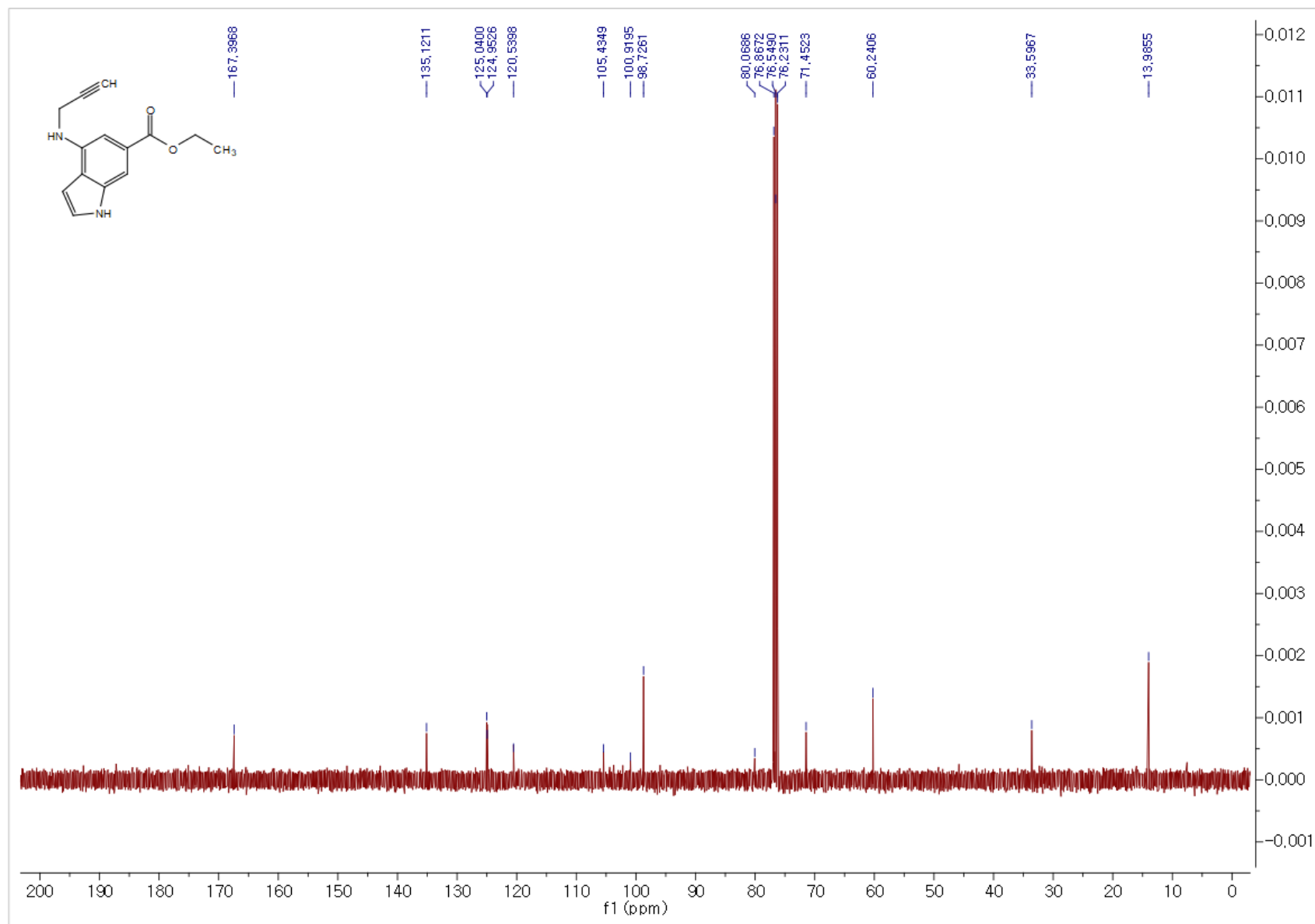


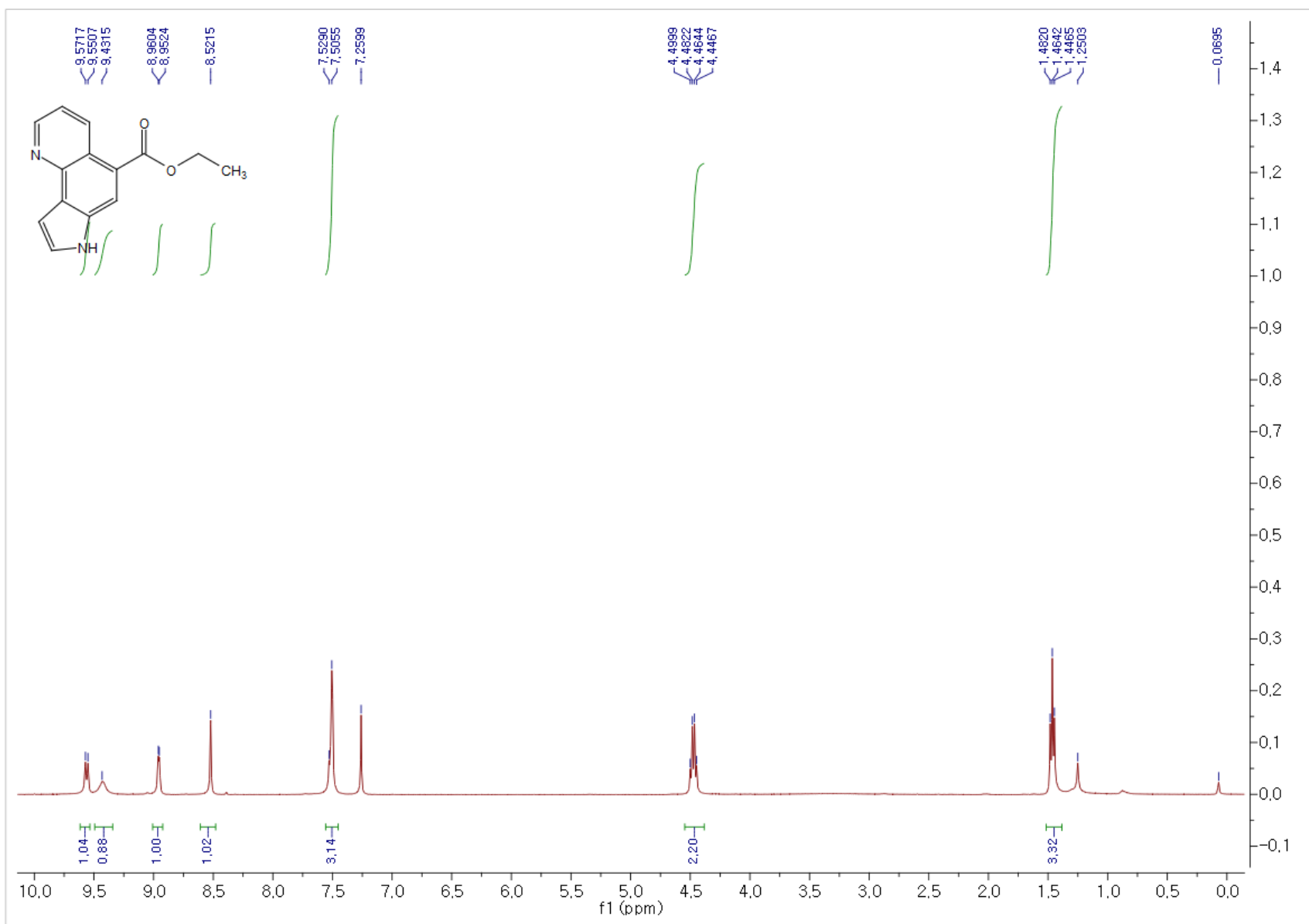


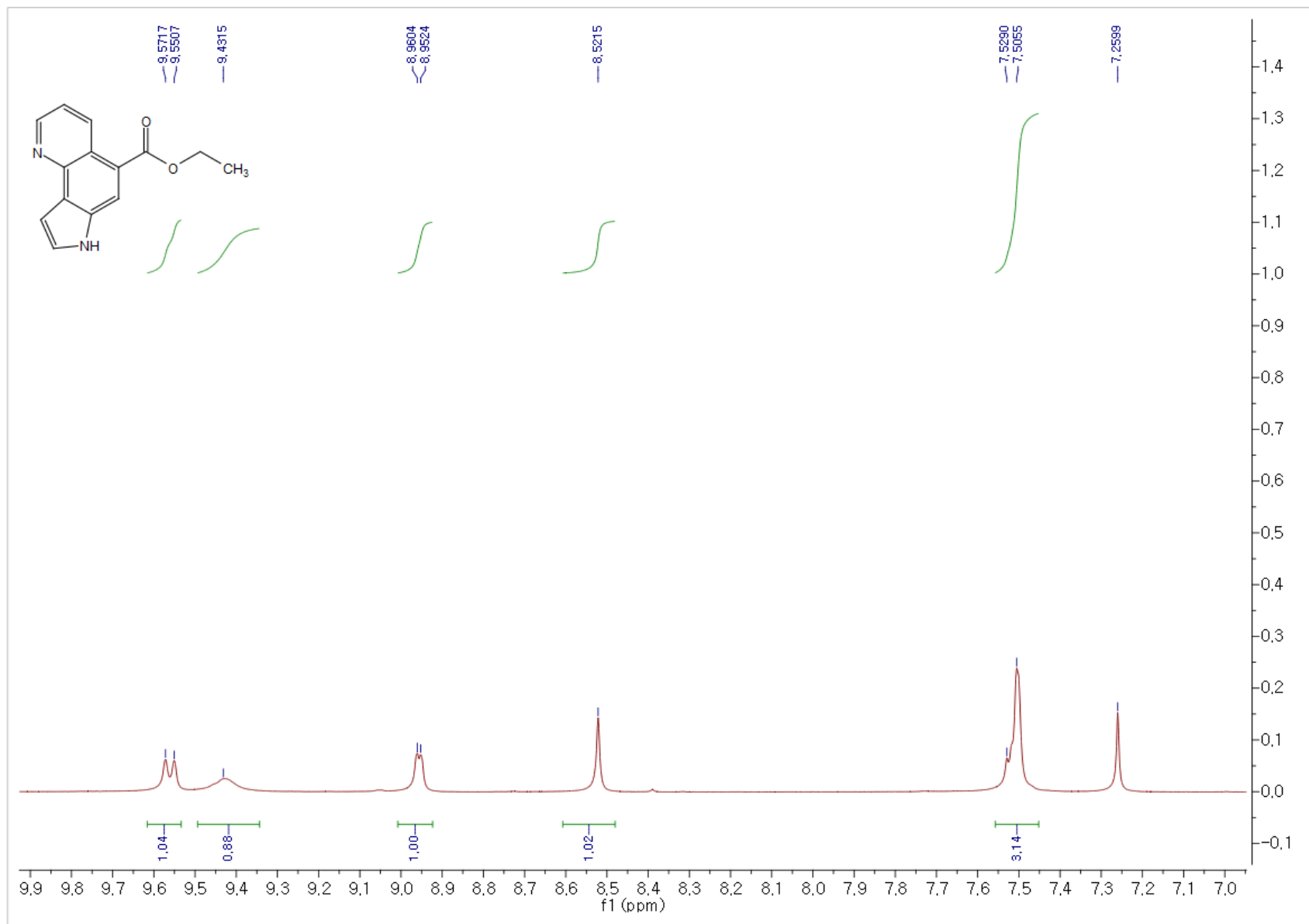


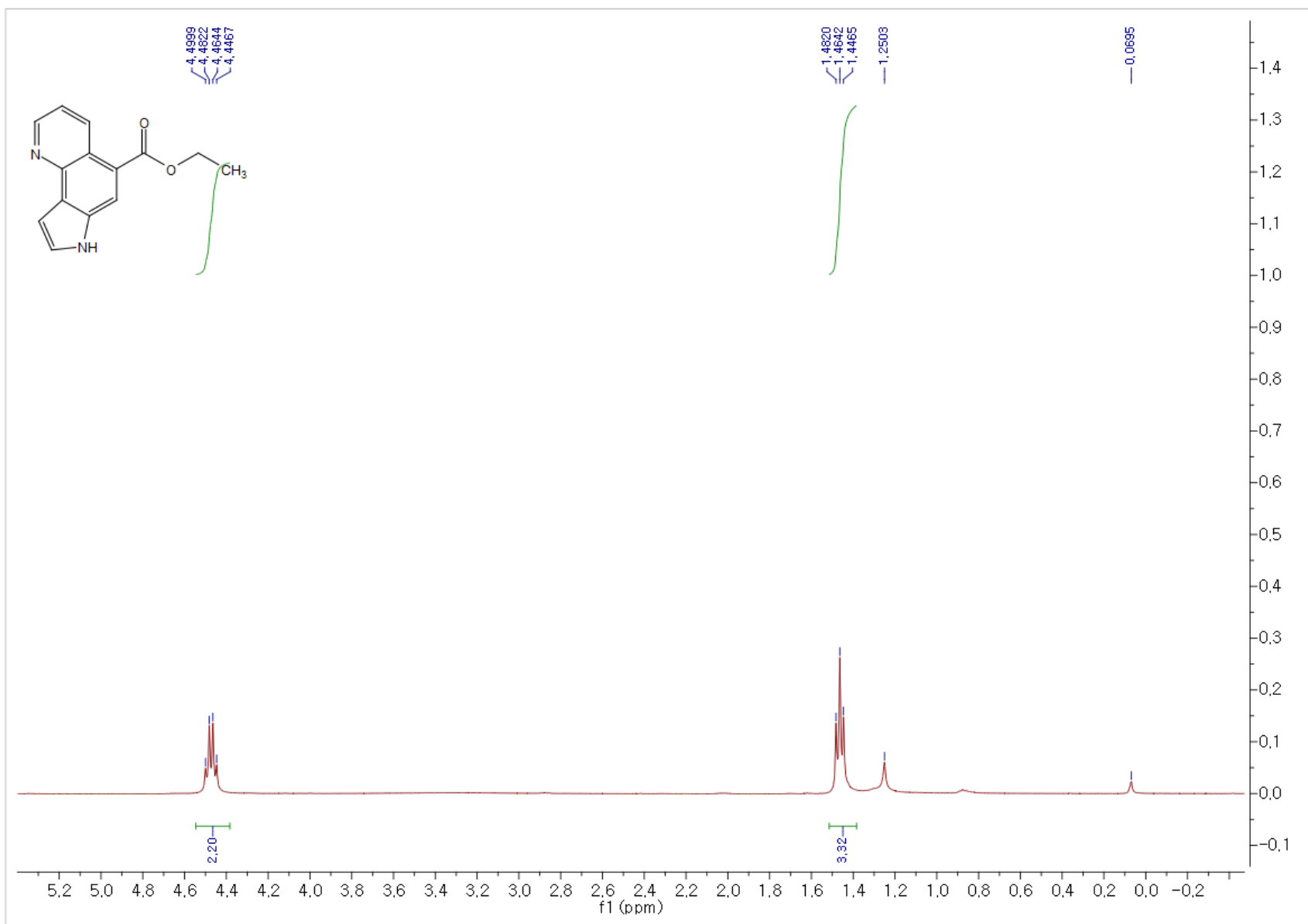


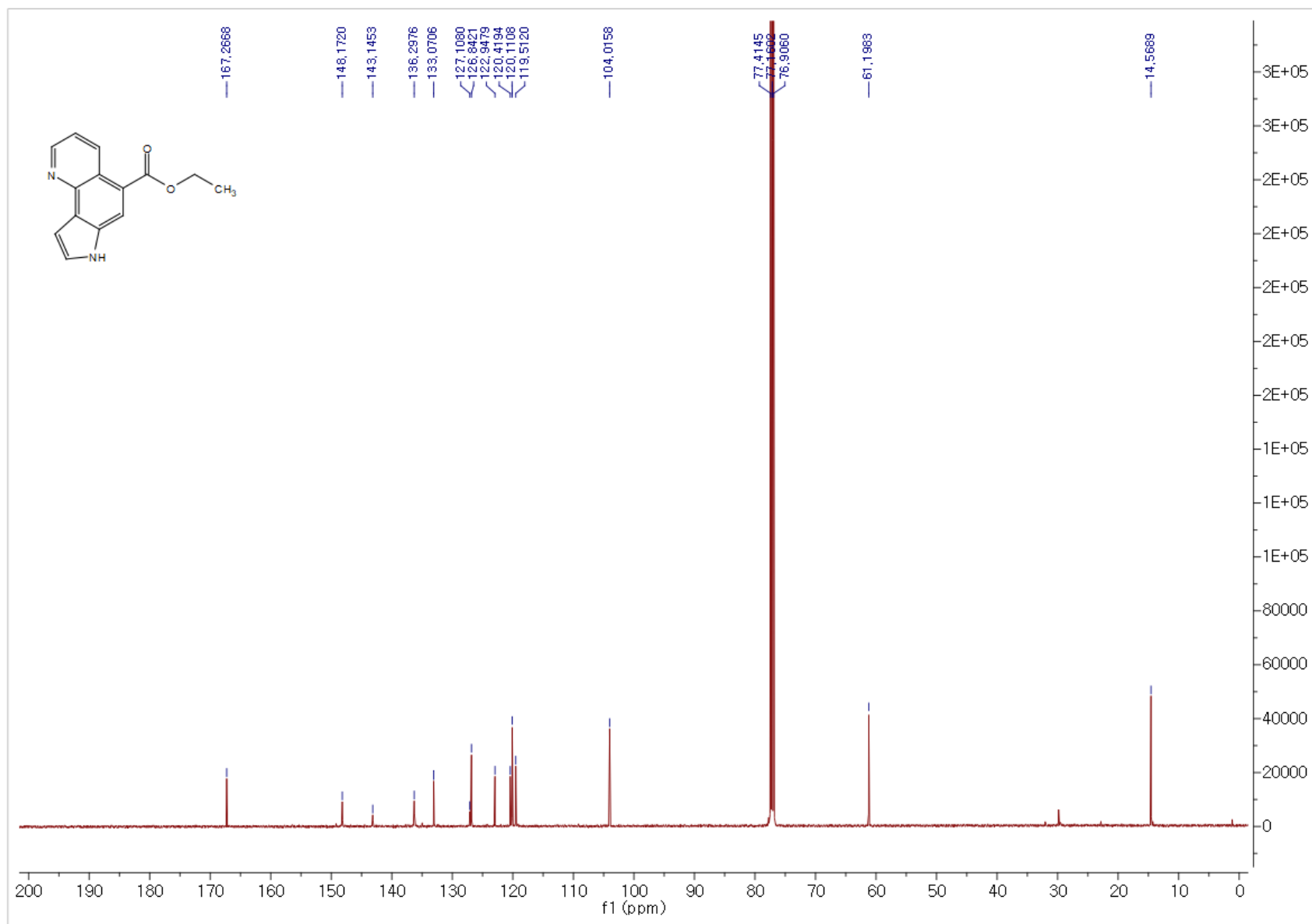






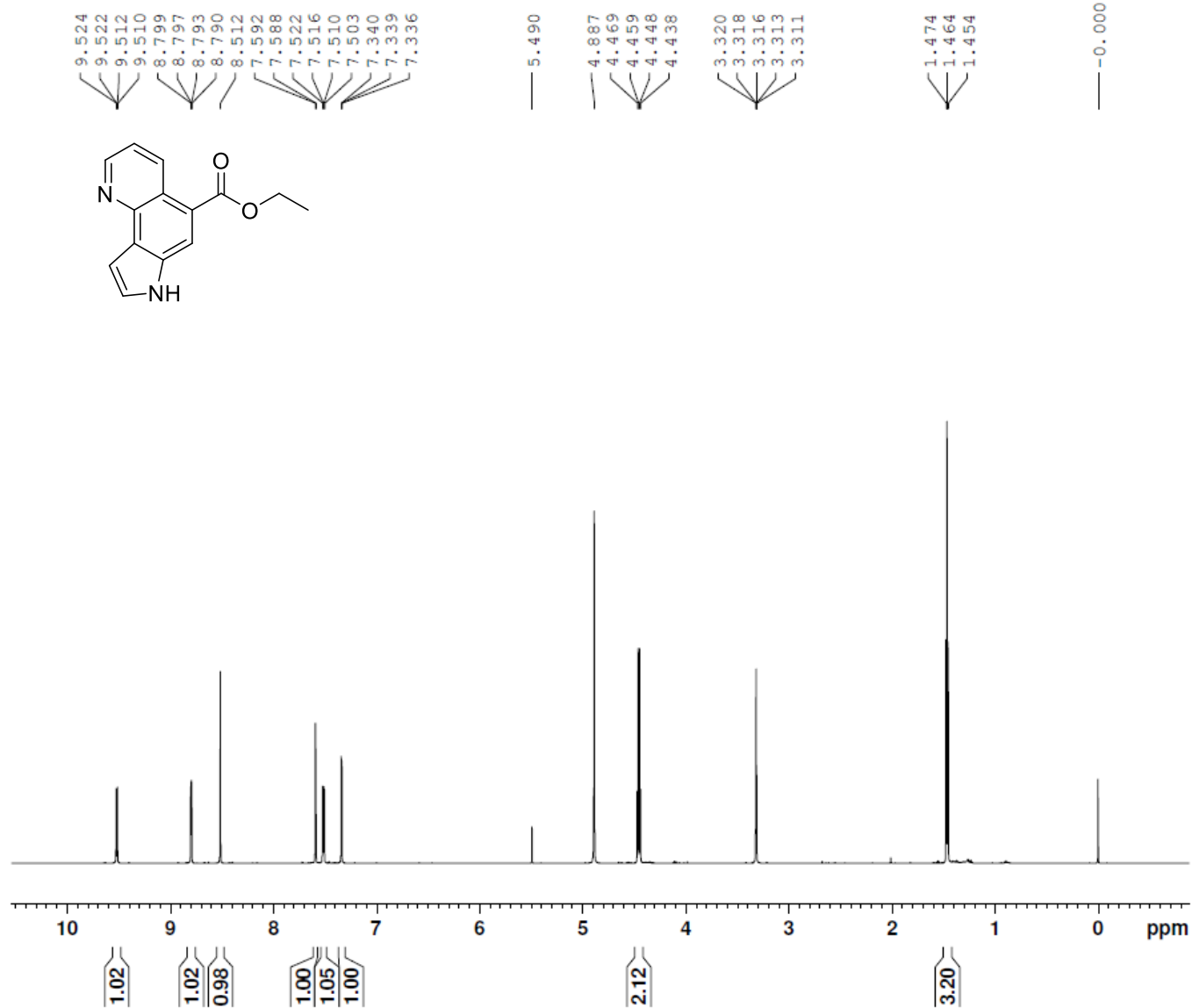








SB-03-08\_1H

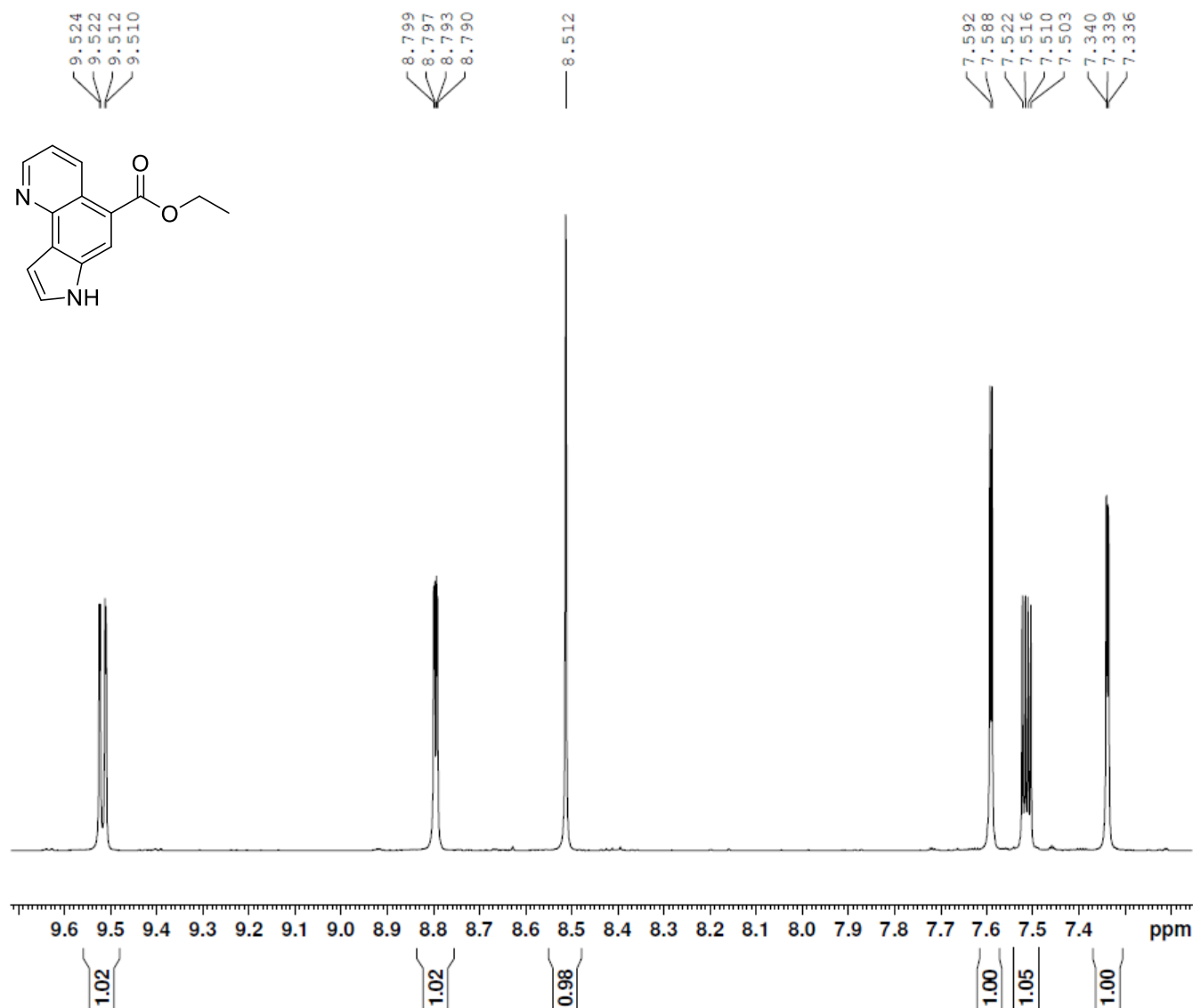


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RG 4.04  
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P1 15.00 usec  
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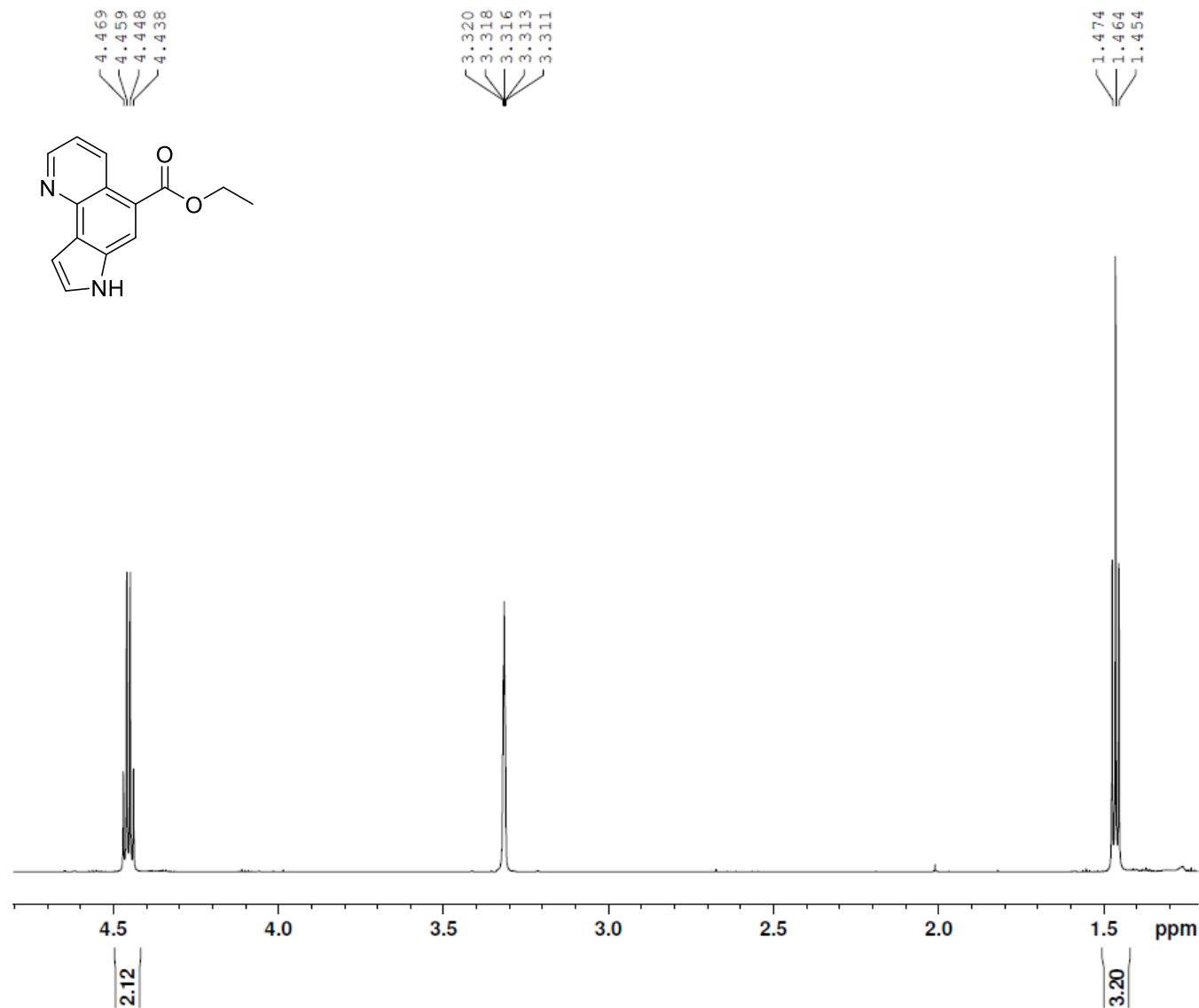
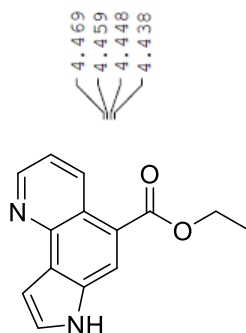


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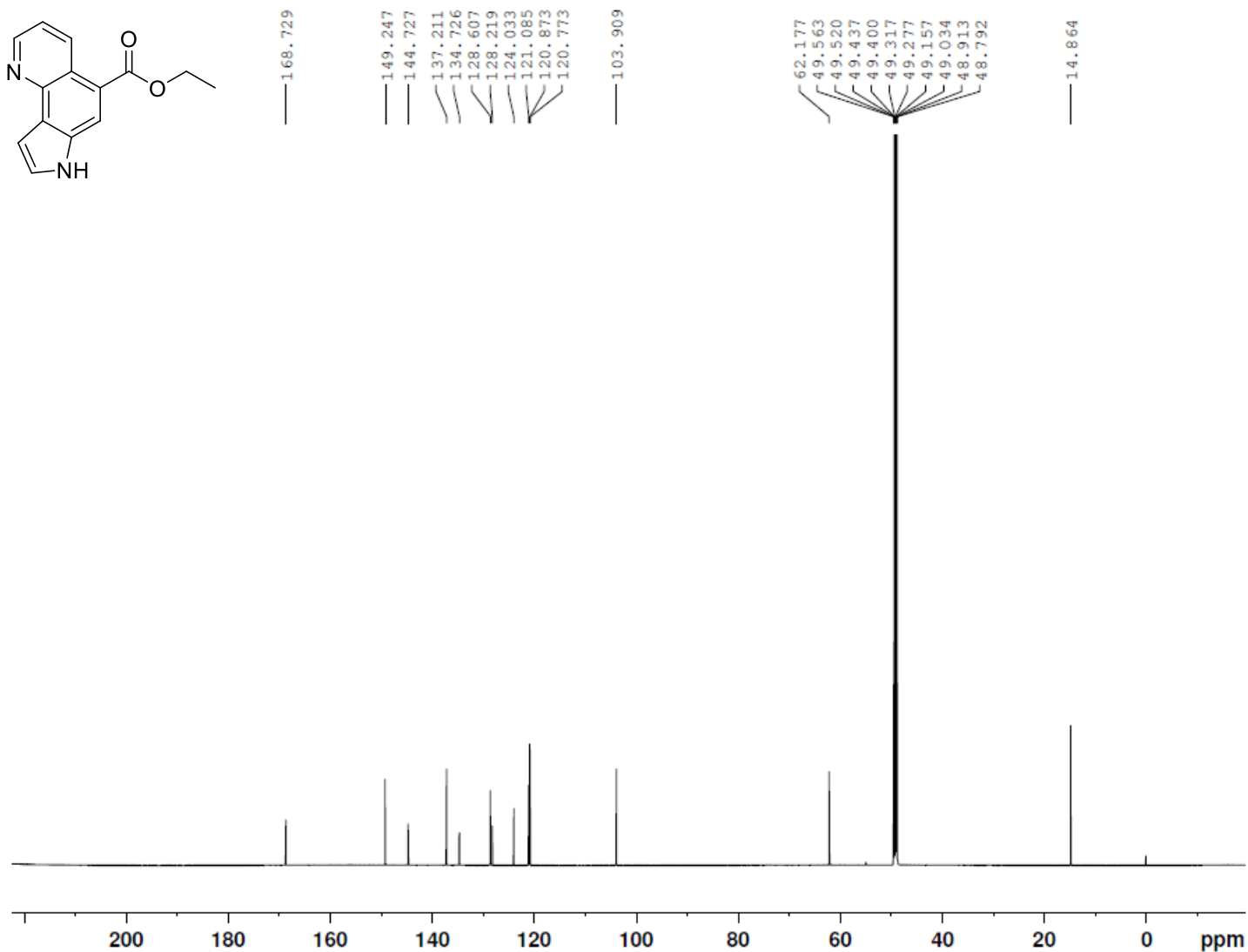
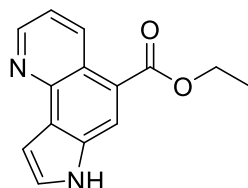


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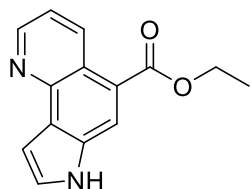


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SB-03-08\_COSY



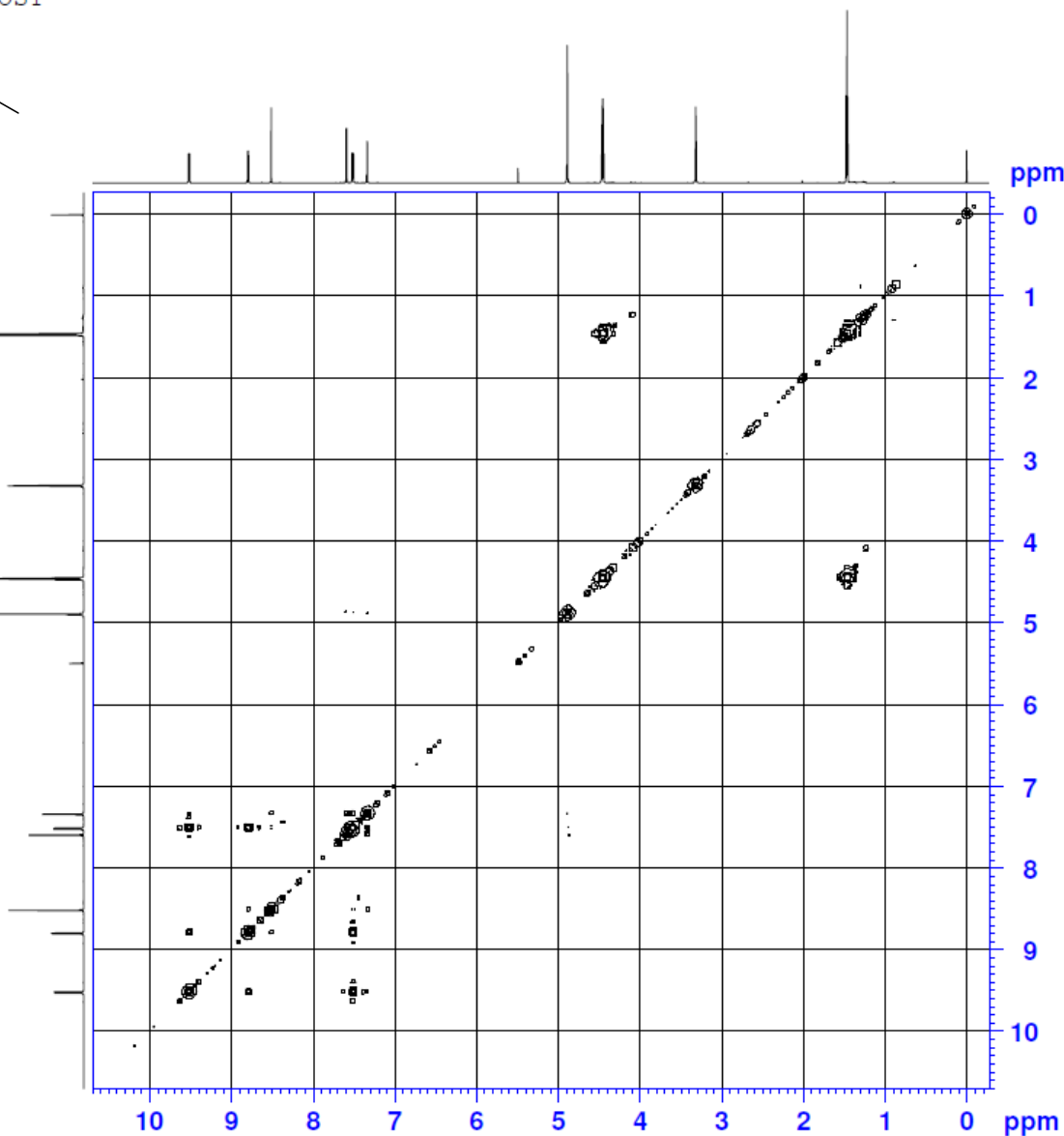
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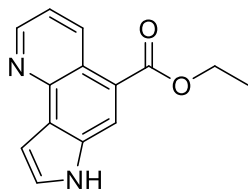
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LB 0 Hz  
GB 0  
PC 1.40

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SB-03-08\_HMBC



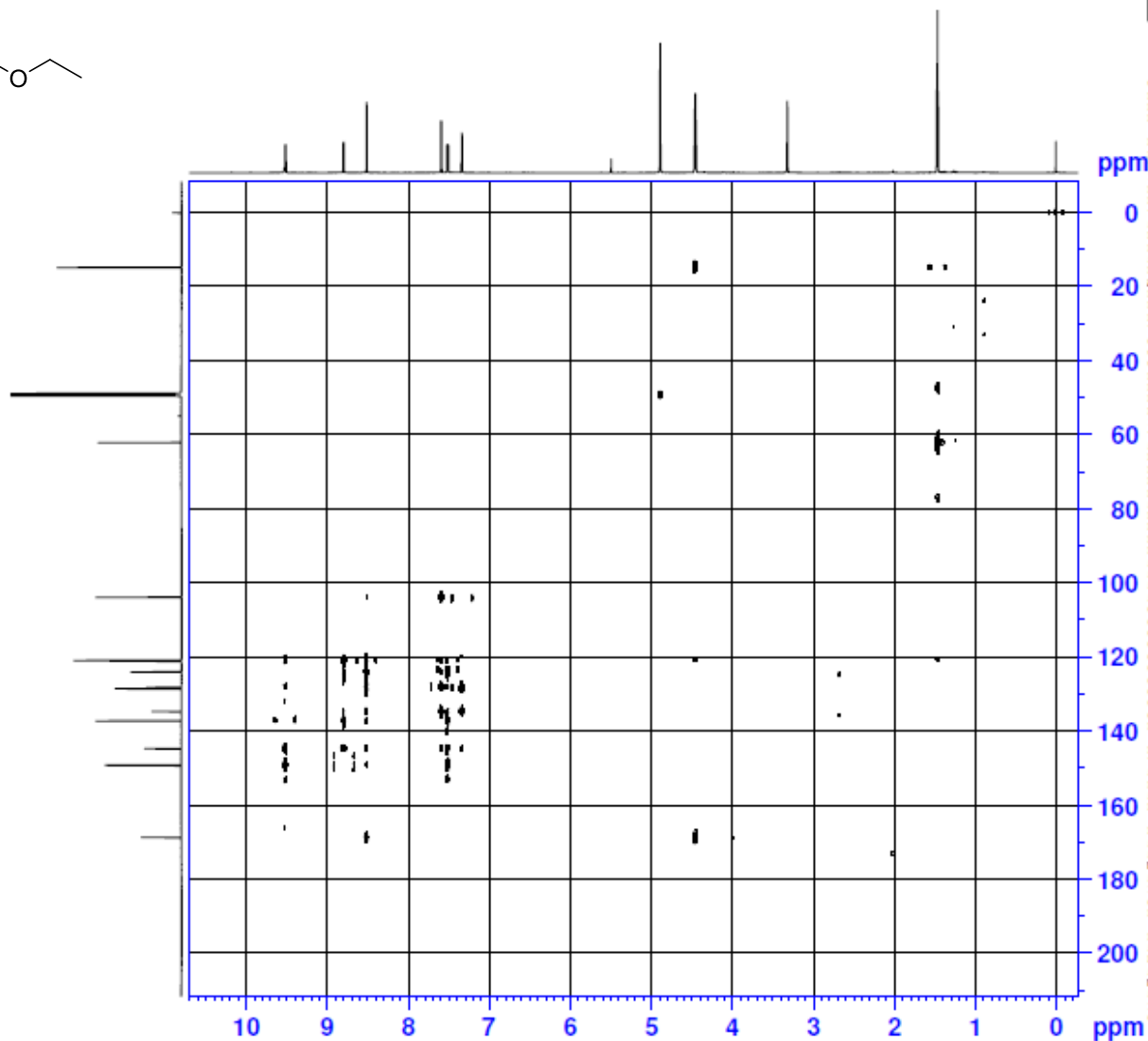
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CMT7 170.0000000  
CMT13 8.0000000  
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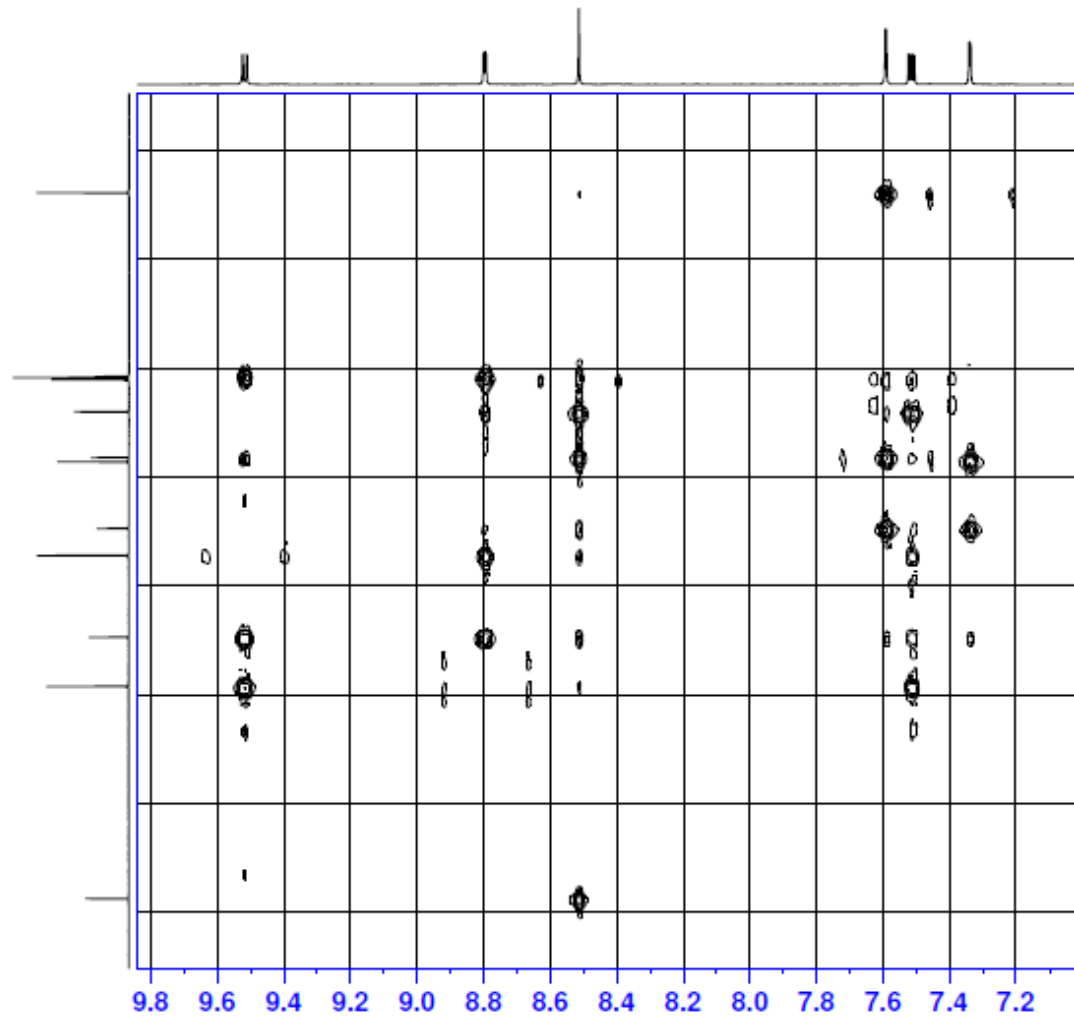
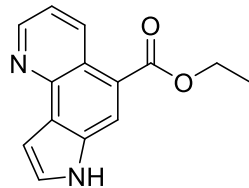
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LB 0  
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SB-03-08\_HMBC



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PROCNO 1

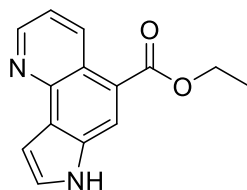
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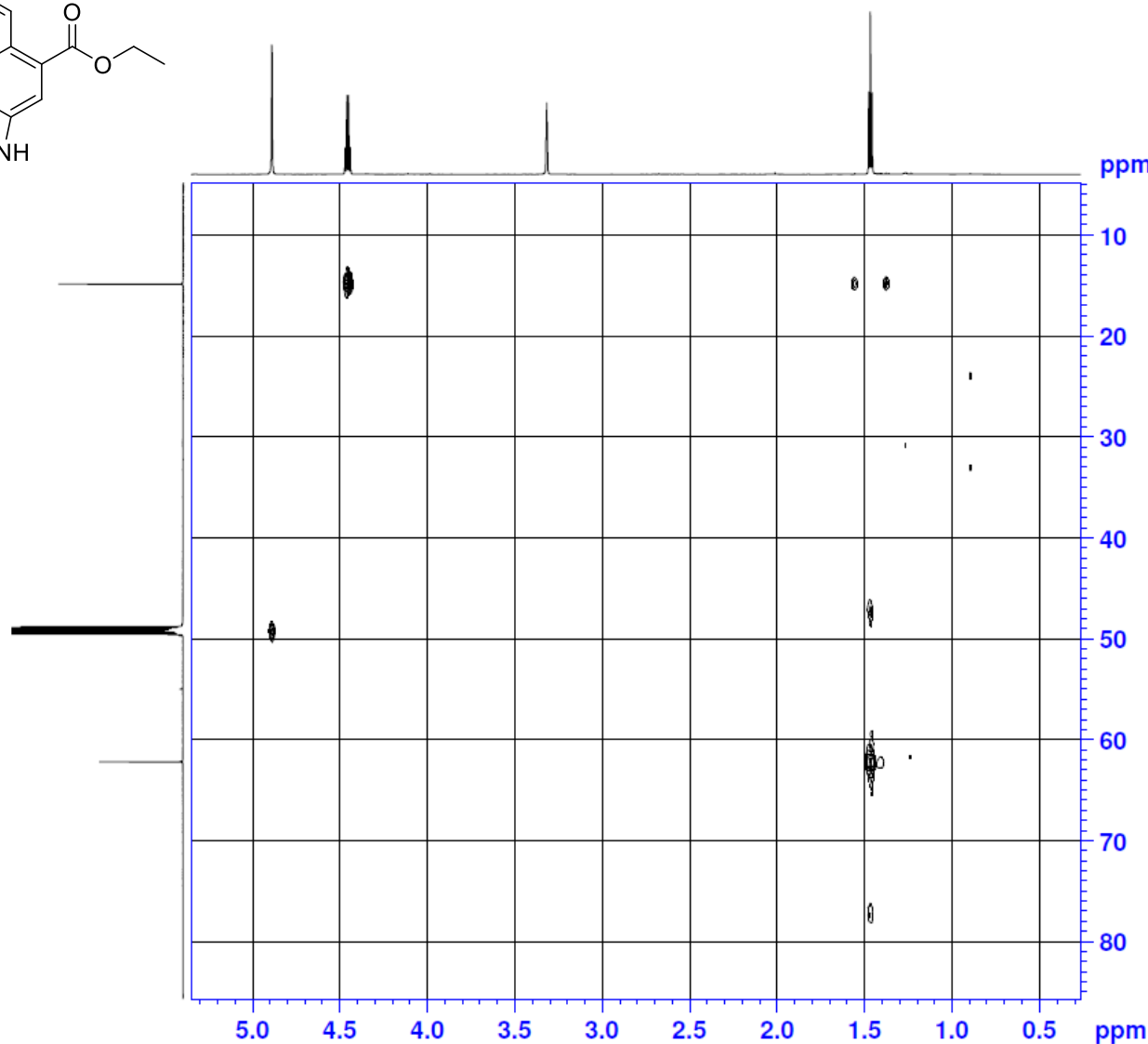
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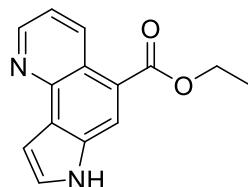
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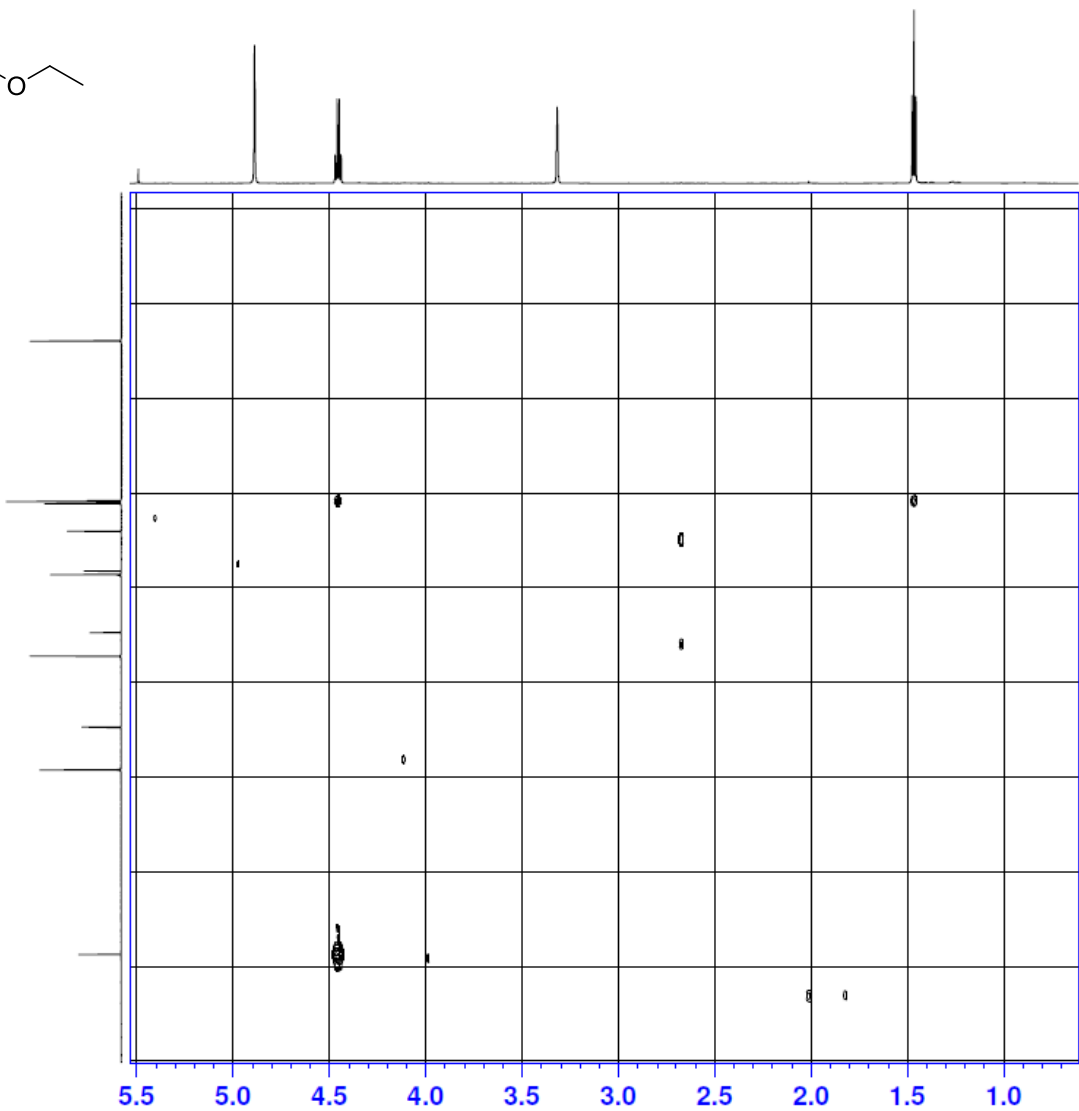


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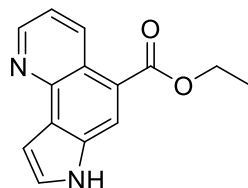
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P2 30.00 usec  
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NUC2 13C  
P3 12.00 usec  
P24 2000.00 usec  
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GPZ4 -8.00 %  
CPNAM[5] SMSQ10.100  
GPZ5 -4.00 %  
CPNAM[6] SMSQ10.100  
GPZ6 -2.00 %  
P16 1000.00 usec  
F1 - Acquisition parameters  
TD 256  
SFO1 176.166 MHz  
FIDRES 302.810089 Hz  
SW 220.018 ppm  
FnMODE Echo-Antiecho  
F2 - Processing parameters  
SI 2048  
SF 700.5300094 MHz  
WDW SINE  
SSB 4  
LB 0 Hz  
GB 0  
PC 1.40  
F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.1481335 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0





SB-03-08\_NOESY



Current Data Parameters  
NAME WS2  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210526  
Time 5.38 h  
INSTRUM spect  
PROBHD z128968\_0001 (   
PULPROG noesygpph  
TD 2048  
SOLVENT MeOD  
NS 32  
DS 32  
SWH 7692.308 Hz  
FIDRES 7.512019 Hz  
AQ 0.1331200 sec  
RG 7.13  
DW 65.000 usec  
DE 10.00 usec  
TE 298.0 K  
D0 0.00004590 sec  
D1 2.01310706 sec  
D8 0.30000001 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
D16 0.00020000 sec  
IN0 0.00013000 sec  
TDav 1  
SF01 700.5336610 MHz  
NUC1 1H  
P1 15.00 usec  
P2 30.00 usec  
P17 2500.00 usec  
PLW1 8.39560032 W  
PLW10 3.02239990 W  
GPNAM[1] SMSQ10.100  
GPZ1 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
ID 256  
SF01 700.5337 MHz  
FIDRES 60.096153 Hz  
SW 10.981 ppm  
FnMODE States-TPPI

F2 - Processing parameters  
SI 1024  
SF 700.5300094 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 States-TPPI  
SF 700.5300094 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

